

# Magnetic Space Groups

Daniel B. Litvin

Department of Physics  
Eberly College of Science  
The Pennsylvania State University

Penn State Berks  
P.O. Box 7009  
Reading PA 19610-6009, USA.

*E-mail: [u3c@psu.edu](mailto:u3c@psu.edu)*

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Dedicated to

**Tikva Sa'eeda**

זכרונה לברכה - may her memory be blessed

to our kids, **Usa Shoshana** and **Steven Yitzchak**,  
who have always done us proud.

and to our granddaughter

**Talia Sa'eeda**



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## Preface

This work discusses the structure, symbols, and properties of magnetic space groups. While the focus is on three-dimensional magnetic space groups, we have included analogous information on the structure, symbols, and properties of one- and two-dimensional magnetic space groups.

Unlike Gaul, this work is divided into two parts. The first is a discussion of the structure of magnetic groups, the Opechowski and Guccione symbols for magnetic space groups and the explicit listing of elements of one representative group from each of the 7, 80, and 1651 types of groups in, respectively, the superfamilies of one- two- and three-dimensional magnetic space groups. The second part of this work is an extension of the classic work on space groups published in the *International Tables for Crystallography, Volume A: Space-Group Symmetry*, my work on non-magnetic subperiodic groups published in the *International Tables for Crystallography, Volume E: Subperiodic Groups*, and my work on international-like tables for magnetic subperiodic groups. A reader familiar with any of these tables should readily recognize most content and format of the magnetic space group tables presented here.

This book was not computer generated. It was hand-calculated, checked, and typed. Consequently, in a massive work as this, the probability of errors and/or typos is then not zero. The author would appreciate being informed of any errors and/or typos found.

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# 1. Magnetic Space Groups: Symbols and Elements

## 1.1 Introduction

Magnetic groups are symmetry groups of arrangements of non-zero magnetic moments (spins). These groups were introduced by Landau and Lifschitz (1951, 1957) by reinterpreting the operation of "change in color" in two-color (black and white) crystallographic groups as "time inversion." Crystallographic two-color groups of rotations had been given by Heesch (1930) and Shubnikov (1951). The 1651 types of two-color three-dimensional space groups were derived by Belov et al (1955, 1957) and by Zamorzaev (1953, 1957) and called *Shubnikov groups*. Koptsik (1966) applied these groups to determine crystallographic and physical properties of magnetic structures.

The three-dimensional magnetic space groups were rederived and a new list of symbols for 1191 types of magnetic space groups was given by Opechowski & Guccione (1965) (see also Opechowski, 1986; Litvin, 2001, and Section 1.3). This number plus 230 space group types gives 1421 types of magnetic groups. The 230 types of groups which are the direct product of a space group and the time inversion group are not magnetic groups as the time inversion element in each such group precludes non-zero magnetic moments. To include these groups, Opechowski (1986) used the concept of *reduced magnetic superfamily* of a space group (see Section 1.2) to give a total of 1651 types of groups commonly referred to as *magnetic space groups*.

The Opechowski & Guccione list consists of a listing of a symbol for one representative magnetic space group from each type. To uniquely specify the meaning of these symbols required a specification of one representative space group chosen

from each of the 230 types of space groups. This specification was made in conjunction with Volume I of the *International Tables for X-ray Crystallography* (1952) (abbreviated here as *ITC52*). In particular, this specification of one space group from each type was based on the specific form of the coordinate triplets of the set of general positions explicitly printed in *ITC52*.

*ITC52* has been replaced by Volume A of the *International Tables for Crystallography* (1983) (abbreviated here as *ITC-A*). One finds that, for some space groups, the set of coordinate triplets of the general positions explicitly printed in *ITC-A* differs from that explicitly printed in *ITC52*. As a consequence, if one attempts to interpret the Opechowski-Guccione symbols using *ITC-A*, one will, in many cases misinterpret the meaning of the symbol (Litvin, 1997, 1998)<sup>1</sup>.

Using the Opechowski-Guccione symbols, a list of symbols of the 1651 superfamilies of magnetic space group types is given in Table 1.1. In distinction from previous listings, where only a set of symbols were given, we specify explicitly the meaning of each symbol (Litvin, 2001). That is, we specify a representative magnetic group of that type. This consists of specifying the coordinate system used, and then relative to that coordinate system, the translational subgroup of the group. We then explicitly give a set of coset representatives of the coset decomposition of the group

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<sup>1</sup> It was suggested in these two papers that the original Opechowski-Guccione set of symbols should be modified so one could correctly interpret them using *ITC-A* instead of *ITC52*. Adopting this ill-advised suggestion would have required in the future a new modification of the Opechowski-Guccione set of symbols whenever changes were made to the coordinate triplets of the general positions in *ITC-A*. Consequently, the meaning of the original Opechowski-Guccione list of symbols was specified by Litvin (2001).

with respect to its translational subgroup.

In Section 1.2, the concept of *reduced magnetic superfamily* of a space group is reviewed. This concept provides for a sub-classification of magnetic space groups. This is followed, in Section 1.3, by a detailed explanation of the contents of Table 1.1., of the magnetic space group type symbols and elements. In Section 1.4 we list the changes in the symbols listed in Opechowski & Guccione (1965) and Opechowski (1986), and those of Table 1.1 . A comparison of the symbols introduced by Opechowski & Guccione (1965) and those of Belov et al (1957) is discussed in Section 1.5 . A side by side comparison is given in Table 1.4.

For one- and two-dimensional black and white space groups, see respectively, Neronova & Belov (1961) and Weber (1929), Heesch (1929), Cochran (1952) and Belov & Tarkhova (1956). The symbols used here for the superfamilies of one- and two-dimensional magnetic space group types are given in Table 1.1 along with a specification of a representative group of each type. A comparison of the symbols for these groups with that of black and white group symbols given by Niggli (1964) and Belov & Tarkhova (1956) are given in Table 1.2 .

## 1.2 Magnetic Superfamily

Let  $\mathbf{F}$  denote a space group type. The *reduced magnetic superfamily* of the space group of type  $\mathbf{F}$  (Opechowski, 1986) consists of <sup>2</sup>

- 1) A group of type  $\mathbf{F}$ .
- 2) The group  $\mathbf{F1}'$ , where  $\mathbf{1}'$  denotes time inversion group consisting of the identity  $1$  and time inversion  $1'$ .
- 3) All non-equivalent groups  $\mathbf{F(D)} = \mathbf{D} + (\mathbf{F} - \mathbf{D})\mathbf{1}'$  where  $\mathbf{D}$  is a subgroup of index two of  $\mathbf{F}$ . Groups of this type will also be denoted by  $\mathbf{M}$ .

The third set of groups is divided into two subdivisions:

- 3a) Groups  $\mathbf{M}_T$ , where  $\mathbf{D}$  is an equi-translational subgroup of  $\mathbf{F}$ .
- 3b) Groups  $\mathbf{M}_R$ , where  $\mathbf{D}$  is an equi-class subgroups of  $\mathbf{F}$ .

A survey of the crystallographic groups of the magnetic superfamily of crystallographic groups of type  $\mathbf{F}$  will consist of a listing of a set of coset representatives called the *standard set of coset representatives*, of the decomposition of the group with respect to its translational subgroup, of one group, called the *representative group*, from the groups of type  $\mathbf{F}$ , one group  $\mathbf{F1}'$ , and each non-equivalent group  $\mathbf{F(D)}$ <sup>3</sup>. The symbol for each listed group is used to denote both the group and the group's type. Reference to *the group*  $\mathbf{F}$ ,  $\mathbf{F1}'$ , or  $\mathbf{F(D)}$  will refer to

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<sup>2</sup> A *magnetic superfamily* as defined by Zamorzaev (1957) does not include groups of type  $\mathbf{F}$ .

<sup>3</sup> Only the relative lengths and mutual orientations of the translation vectors and the standard set of coset representatives with respect to an implied coordinate system are given. The absolute lengths of translation vectors, the position in space of the origin of the coordinate system and the orientation in that space of the basis vectors of the coordinate system are not explicitly given.



the listed group and to *the group type* **F**, **F1'**, or **F(D)** to that group's type.

### 1.3 Tables of Magnetic Space Group Symbols and Elements

The format of Table 1.1 is :

- 1) Serial number of the magnetic space group type.
- 2) Symbol of the magnetic space group type.
- 3) Symbol of the group type of the subgroup **D** of index two of **F** for magnetic space groups **F(D)**, and the position and orientation of the group **D** in the coordinate system of the group **F(D)** [ which is the same as the coordinate system of **F** ].
- 4) The standard set of coset representatives of the decomposition of the magnetic space group with respect to its translational subgroup.

#### 1.3.1 Serial Number

A three part number  $N_1.N_2.N_3$  is used.  $N_1$  is a sequential number for the group type to which **F** belongs. This is the same numbering as given in both *ITC52* and *ITC-A* for the two and three-dimensional space group types.  $N_2$  is a sequential numbering of the magnetic space group types of the superfamily of **F**. Group types **F** always have the assigned number  $N_1.1.N_3$ , and group types **F1'** the assigned number  $N_1.2.N_3$ .  $N_3$  is a global sequential numbering of the 7, 80, and 1651 types of groups in, respectively, the superfamilies of one- two- and three-dimensional magnetic space groups.

#### 1.3.2 Magnetic Space Group Symbol

In Figures 1.1 we give a list of symbols and diagrams for the magnetic group lattices.

The relative lengths and mutual orientations of the translation vectors of the translational subgroups of magnetic space groups are the same as for space groups  $\mathbf{F}$ . These lattice parameters are given in Table 1.2 according to the crystal system of  $\mathbf{F}$ . In Table 1.3.1 we give the symmetry directions of symmetry operations represented by characters in the Hermann-Mauguin symbol of a magnetic space group implied by the characters position in the symbol. In Table 1.3.2 we give the symbols used as subindices on the symmetry operations which represent these symmetry directions.

The symbol for a group  $\mathbf{F}$  is that symbol for the group type  $\mathbf{F}$  given by Opechowski and Guccione (1965). This group  $\mathbf{F}$  is uniquely defined by its translational subgroup and the coset representatives of the coset decomposition of the group with respect to its translational subgroup. These coset representatives, see Section 1.3.4 below, are given in Table 1.1. The symbol for a group  $\mathbf{F1'}$  is that of the group type  $\mathbf{F}$  followed by  $\mathbf{1'}$ .

The symbol for a group  $\mathbf{M}_T = \mathbf{F}(\mathbf{D}) = \mathbf{D} + (\mathbf{F} - \mathbf{D})\mathbf{1'}$  is based on the symbol for the group  $\mathbf{F}$ . As  $\mathbf{D}$  is an equi-translational subgroup of  $\mathbf{F}$ , i.e. the translational subgroup  $\mathbf{T}^{\mathbf{M}_T}$  of the magnetic group  $\mathbf{M}_T$  is  $\mathbf{T}$ , the translational subgroup of  $\mathbf{F}$ . The translational part of the group symbol of a  $\mathbf{M}_T$  group is then the same as that of the corresponding group  $\mathbf{F}$ . A number or letter in the rotational part of the symbol of  $\mathbf{F}$  appears unchanged in the symbol for  $\mathbf{M}_T$  if it is associated with a coset representative of the group  $\mathbf{F}$ , in the coset decomposition of  $\mathbf{F}$  with respect to  $\mathbf{T}$ , which is also an element contained in the subgroup  $\mathbf{D}$ . If not in  $\mathbf{D}$ , i.e. in  $\mathbf{F} - \mathbf{D}$ , the number or letter appears in the symbol for  $\mathbf{M}_T$  with a prime to denote that the element in  $\mathbf{M}_T$  is coupled with  $\mathbf{1'}$ . For example, the

orthorhombic space group  $\mathbf{F} = \mathbf{Pca2}_1$  is listed as the three-dimensional magnetic space group number 29.1.198. This group is defined by a orthorhombic translational subgroup  $\mathbf{T} = \mathbf{P}$ , see Figures 1.1-3D, and the standard set of coset representatives<sup>4</sup>

$$(1|000) \quad (m_x|\frac{1}{2},0,\frac{1}{2}) \quad (m_y|\frac{1}{2},0,0) \quad (2_z|0,0,\frac{1}{2}),$$

the coset decomposition of  $\mathbf{F}$  with respect to  $\mathbf{T}$  can then be written as:

$$\mathbf{F} = \mathbf{T} + (m_x|\frac{1}{2},0,\frac{1}{2})\mathbf{T} + (m_y|\frac{1}{2},0,0)\mathbf{T} + (2_z|0,0,\frac{1}{2})\mathbf{T}.$$

The magnetic space group 29.5.202 is a group  $\mathbf{M}_T$  whose symbol is  $\mathbf{Pc}'\mathbf{a}'\mathbf{2}_1$ . In this case we have

$$\mathbf{Pc}'\mathbf{a}'\mathbf{2}_1 = \mathbf{P2}_1 + (\mathbf{Pca2}_1 - \mathbf{P2}_1)1'$$

i.e.  $\mathbf{F} = \mathbf{Pca2}_1$  and  $\mathbf{D} = \mathbf{P2}_1$ . The symbol "2<sub>1</sub>" in the symbol for  $\mathbf{F} = \mathbf{Pca2}_1$  refers to the coset representative  $(2_z|0,0,\frac{1}{2})$ , an element in  $\mathbf{D} = \mathbf{P2}_1$ . Consequently the symbol appears unprimed in the symbol for  $\mathbf{M}_T$  ( $\mathbf{Pc}'\mathbf{a}'\mathbf{2}_1$ ) and the coset representative  $(2_z|0,0,\frac{1}{2})$  appears as an unprimed coset representative in the standard set of coset representatives of  $\mathbf{M}_T$ . The symbols "c" and "a" in  $\mathbf{F} = \mathbf{Pca2}_1$  refer to the coset representatives  $(m_x|\frac{1}{2},0,\frac{1}{2})$  and  $(m_y|\frac{1}{2},0,0)$ , respectively, neither of which are contained in  $\mathbf{D}$ . Consequently both symbols appear primed in the symbol for  $\mathbf{M}_T$  ( $\mathbf{Pc}'\mathbf{a}'\mathbf{2}_1$ ) and the coset representatives  $(m_x|\frac{1}{2},0,\frac{1}{2})$  and  $(m_y|\frac{1}{2},0,0)$  appear as primed coset representatives in the standard set of coset representatives of  $\mathbf{M}_T$ . The magnetic group  $\mathbf{Pc}'\mathbf{a}'\mathbf{2}_1$  then has the orthorhombic translational subgroup  $\mathbf{T} = \mathbf{P}$  and the standard set of coset representatives

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<sup>4</sup>We use the Seitz notation  $(R|\tau(R) + t)$  for elements of a space group  $\mathbf{F}$ . "R" is a rotation or rotation-inversion, "t" is a translation of the translational subgroup  $\mathbf{T}$  of  $\mathbf{F}$ , and " $\tau(R)$ " is a non-primitive translation associated with "R". The coset representatives are taken to be of the form  $(R|\tau(R))$  which then defines the  $\tau(R)$  associated with the R.

$$(1|000) \quad (m_x|\frac{1}{2},0,\frac{1}{2})' \quad (m_y|\frac{1}{2},0,0)' \quad (2_z|0,0,\frac{1}{2}).$$

The symbol for a group  $\mathbf{M}_R = \mathbf{F}(\mathbf{D}) = \mathbf{D} + (\mathbf{F} - \mathbf{D})1'$  is also based on the symbol for the group  $\mathbf{F}$ . (This is in contradistinction to the “BNS” symbols of  $\mathbf{M}_R$  groups (Belov, Neronova, & Smirnova (1955, 1957)) where the symbol for a  $\mathbf{M}_R$  group is based on the symbol for the group  $\mathbf{D}$ , see below Section 1.5) As this is an equi-class magnetic group, half the translations of  $\mathbf{F}$  are now coupled with  $1'$  in  $\mathbf{M}_R$  and half the translations remain unprimed in  $\mathbf{M}_R$ . The unprimed translations constitute the translational subgroup  $\mathbf{T}^D$  of  $\mathbf{D}$ . We can write the coset decomposition of the translational subgroup  $\mathbf{T}$  of  $\mathbf{F}$  with respect to the translational subgroup  $\mathbf{T}^D$  of  $\mathbf{D}$  as

$$\mathbf{T} = \mathbf{T}^D + \mathbf{t}_\alpha \mathbf{T}^D$$

where  $\mathbf{t}_\alpha$  is a translation of  $\mathbf{F}$  which appears primed (coupled with  $1'$ ) in  $\mathbf{M}_R$ . The translational subgroup of  $\mathbf{M}_R$  can then be written as

$$\mathbf{T}^M_R = \mathbf{T}^D + \mathbf{t}'_\alpha \mathbf{T}^D$$

Symbols for the translational groups  $\mathbf{T}$ , the translational subgroups  $\mathbf{T}^D$  of  $\mathbf{T}$  used in the symbol for  $\mathbf{M}_R$  groups, and the choice of the translations  $\mathbf{t}_\alpha$  for magnetic space groups is given in Figures 1.1 .

The symbol for a magnetic group  $\mathbf{M}_R = \mathbf{F}(\mathbf{D})$  is based on the symbol of the group  $\mathbf{F}$ , and is also a symbol for the subgroup  $\mathbf{D}$  of unprimed elements. The translational part of the symbol of  $\mathbf{F}$  is replaced by the symbol for the translational subgroup  $\mathbf{T}^D$  of  $\mathbf{D}$ . If a coset representative  $(R|\tau(R))$  of  $\mathbf{T}$  in  $\mathbf{F}$  appears as the coset representative  $(R|\tau(R)+\mathbf{t}_\alpha)$  of  $\mathbf{T}^D$  in  $\mathbf{D}$ , then the number or letter corresponding to  $(R|\tau(R))$  in the symbol for  $\mathbf{F}$  is primed. If  $(R|\tau(R))$  appears unchanged as a coset representative of  $\mathbf{T}^D$  in  $\mathbf{D}$ ,

then the number or letter corresponding to  $(R|\tau(R))$  in the symbol for  $\mathbf{F}$  is unchanged.

The resulting symbol is a symbol for  $\mathbf{D}$  based on the symbol for  $\mathbf{F}$  and is also a symbol for the magnetic space group  $\mathbf{M}_R = \mathbf{F}(\mathbf{D})$ . The symbol specifies not only  $\mathbf{D}$  but also  $\mathbf{F}$ : By deleting the subindex on the translational part of the symbol and the primes on the rotational part one obtains the symbol specifying  $\mathbf{F}$ . Having specified  $\mathbf{D}$  and  $\mathbf{F}$  one has specified the group  $\mathbf{M}_R = \mathbf{F}(\mathbf{D})$ . For example: Consider again the three-dimensional space group 29.1.198,  $\mathbf{F} = \mathbf{Pca}2_1$  where

$$\mathbf{F} = \mathbf{T} + (m_x|\frac{1}{2},0,\frac{1}{2})\mathbf{T} + (m_y|\frac{1}{2},0,0)\mathbf{T} + (2_z|0,0,\frac{1}{2})\mathbf{T} .$$

The symbol for the  $\mathbf{M}_R = \mathbf{F}(\mathbf{D})$  group 29.7.204 is  $\mathbf{P}_{2b}\mathbf{c}'\mathbf{a}'2_1$  and is based on the symbol for  $\mathbf{F}$ . The translational subgroup  $\mathbf{T}^D$  of  $\mathbf{D}$  is given by the symbol  $\mathbf{P}_{2b}$  where  $\mathbf{t}_a = \mathbf{b} = (0,1,0)$ . The two primed symbols  $\mathbf{c}'$  and  $\mathbf{a}'$  in  $\mathbf{P}_{2b}\mathbf{c}'\mathbf{a}'2_1$  denote that the two coset representatives  $(m_x|\frac{1}{2},0,\frac{1}{2})$  and  $(m_y|\frac{1}{2},0,0)$  that appear in the set of standard coset representatives of  $\mathbf{T}$  in  $\mathbf{F}$  appear as the coset representatives  $(m_x|\frac{1}{2},1,\frac{1}{2})$  and  $(m_y|\frac{1}{2},1,0)$  in the set of standard coset representatives of  $\mathbf{T}^D$  in  $\mathbf{D}$ . As the symbol  $2_1$  in  $\mathbf{P}_{2b}\mathbf{c}'\mathbf{a}'2_1$  is not primed, the coset representative  $(2_z|0,0,\frac{1}{2})$  of  $\mathbf{T}$  in  $\mathbf{F}$  remains unchanged as a coset representative of  $\mathbf{T}^D$  in  $\mathbf{D}$ . We have then the subgroup:

$$\mathbf{D} = \mathbf{T}^D + (m_x|\frac{1}{2},1,\frac{1}{2})\mathbf{T}^D + (m_y|\frac{1}{2},1,0)\mathbf{T}^D + (2_z|0,0,\frac{1}{2})\mathbf{T}^D$$

We note that these same coset representatives of  $\mathbf{T}^D$  in  $\mathbf{D}$  are also the coset representatives of the standard set of coset representatives of  $\mathbf{T}^M_R$  in  $\mathbf{M}_R$

$$\mathbf{M}_R = \mathbf{T}^M_R + (m_x|\frac{1}{2},1,\frac{1}{2})\mathbf{T}^M_R + (m_y|\frac{1}{2},1,0)\mathbf{T}^M_R + (2_z|0,0,\frac{1}{2})\mathbf{T}^M_R$$

and consequently the standard set of coset representatives of  $\mathbf{P}_{2b}\mathbf{c}'\mathbf{a}'2_1$  listed in the tables is:

$$(1|0,0,0) \quad (m_x|\frac{1}{2},1,\frac{1}{2}) \quad (m_y|\frac{1}{2},1,0) \quad (2_z|0,0,\frac{1}{2})$$

Also, since  $\mathbf{T}_R^M = \mathbf{T}^D + \mathbf{t}_\alpha' \mathbf{T}^D$  it follows that:

$$\mathbf{M}_R = \mathbf{D} + (\mathbf{F}-\mathbf{D})1'$$

$$\begin{aligned} \mathbf{M}_R = & (1|0,0,0) \mathbf{T}^D + (m_x|\frac{1}{2},1,\frac{1}{2}) \mathbf{T}^D + (m_y|\frac{1}{2},1,0) \mathbf{T}^D + (2_z|0,0,\frac{1}{2}) \mathbf{T}^D + \\ & + (1|0,1,0)' \mathbf{T}^D + (m_x|\frac{1}{2},0,\frac{1}{2})' \mathbf{T}^D + (m_y|\frac{1}{2},0,0)' \mathbf{T}^D + (2_z|0,1,\frac{1}{2})' \mathbf{T}^D \end{aligned}$$

Consequently, a primed number or letter in the symbol for  $\mathbf{M}_R$  (which is a symbol for  $\mathbf{D}$ ) denotes that the corresponding coset representative appears in  $\mathbf{D}$  coupled with  $\mathbf{t}_\alpha$  and primed in  $(\mathbf{F}-\mathbf{D})1'$ , e.g.  $\mathbf{a}'$  in  $\mathbf{P}_{2b}\mathbf{c}'\mathbf{a}'\mathbf{2}_1$  denotes that the coset  $(m_x|\frac{1}{2},0,\frac{1}{2})$  appears as  $(m_x|\frac{1}{2},1,\frac{1}{2})$  in  $\mathbf{D}$  and as  $(m_x|\frac{1}{2},0,\frac{1}{2})'$  in  $(\mathbf{F}-\mathbf{D})1'$ . An unprimed number or letter in the symbol for  $\mathbf{M}_R$  (which is a symbol for  $\mathbf{D}$ ) denotes that the corresponding element appears unchanged in  $\mathbf{D}$  and coupled with  $\mathbf{t}_\alpha$  and primed in  $(\mathbf{F}-\mathbf{D})1'$ , e.g. the symbol  $\mathbf{2}_1$  in  $\mathbf{P}_{2b}\mathbf{c}'\mathbf{a}'\mathbf{2}_1$  denotes that  $(2_z|0,0,\frac{1}{2})$  is in  $\mathbf{D}$  and  $(2_z|1,0,\frac{1}{2})'$  in  $(\mathbf{F}-\mathbf{D})1'$ .

### 1.3.3 Symbol of the subgroup $\mathbf{D}$

The third column contains the group type symbol of the subgroup  $\mathbf{D}$  of index two of the magnetic group  $\mathbf{M} = \mathbf{F}(\mathbf{D})$ .

a) For  $\mathbf{M}_T$  groups, the subgroup  $\mathbf{D}$  is defined by the translational subgroup  $\mathbf{T}$  of  $\mathbf{F}$  and the unprimed coset representatives listed in the fourth column.

b) For  $\mathbf{M}_R$  groups,  $\mathbf{D}$  is defined by the translational subgroup  $\mathbf{T}^D$  and the set of all coset representatives listed in the fourth column.

While the group type symbol of  $\mathbf{D}$  is given, the coset representatives of the subgroup  $\mathbf{D}$  of  $\mathbf{M}_T$  or  $\mathbf{M}_R$  defined in a) or b), respectively, may not be identical with the

standard set of coset representatives of the group **D** found in the listing of the magnetic space groups. Consequently, to show the relationship between this group **D** and the group of type **D** listed in the tables, additional information is provided to define a new coordinate system in which the coset representatives of this subgroup of type **D** are identical with the standard set of coset representatives listed for the group **D**.

Let  $(\mathbf{O}; \mathbf{a}, \mathbf{b}, \mathbf{c})$  be the coordinate system in which the three-dimensional space group **F** is defined. “**O**” is the origin of the coordinate system, and **a**, **b**, and **c** are the basis vectors of the coordinate system. **a**, **b**, and **c** represent a set of basis vectors for a primitive cell for primitive lattices and for a conventional cell for centered lattices. A second coordinate system is defined by  $(\mathbf{O}+\mathbf{t}; \mathbf{a}', \mathbf{b}', \mathbf{c}')$ . The origin is first translated from **O** to  $\mathbf{O}+\mathbf{t}$ , and then the basis vectors **a**, **b**, and **c** are changed to **a'**, **b'** and **c'** (for details, see Appendix 1.1).

Immediately following the group type symbol for the subgroup **D** of **F** we give a coordinate system  $(\mathbf{O}+\mathbf{t}; \mathbf{a}', \mathbf{b}', \mathbf{c}')$  [In the tables, for typographical simplicity, the symbols “**O**+” are omitted.] in which the coset representatives of the subgroup **D** of **F** are identical with the standard set of coset representatives of the group **D** found in the listing of the magnetic space groups. **t**, **a'**, **b'**, and **c'** are given in terms of the basis vectors of the coordinate system  $(\mathbf{O}; \mathbf{a}, \mathbf{b}, \mathbf{c})$  of the group **F**.

Example 1: For the  $\mathbf{M}_T$  magnetic group 10.4.52 = P2/m' one finds in the tables:

P2     $(0,0,0; \mathbf{a}, \mathbf{b}, \mathbf{c})$      $(1|0,0,0)$      $(2_y|0,0,0)$      $(\bar{1}|0,0,0)'$      $(m_y|0,0,0)'$

The translational subgroup of **D** is generated by the translations  $(1|1,0,0)$ ,  $(1|0,1,0)$ , and  $(1|0,0,1)$  of **T** since this is a  $\mathbf{M}_T$  magnetic group, and the coset representatives of this group are  $(1|0,0,0)$  and  $(2_y|0,0,0)$ , the unprimed coset representatives on the right. This subgroup **D** is of type P2. In the tables, listed for the group 3.1.8 P2, one finds the identical two coset representatives. Consequently, there is no change the coordinate system, i.e.  $\mathbf{t}=(0,0,0)$  and  $\mathbf{a}'=\mathbf{a}$ ,  $\mathbf{b}'=\mathbf{b}$ , and  $\mathbf{c}'=\mathbf{c}$ . In the coordinate system of the magnetic group P2/m', the coset representatives of its subgroup **D**, of the type P2, are identical with the coset representatives of the group P2 found in the tables.

Example 2: For the  $\mathbf{M}_R$  three-dimensional magnetic space group 16.7.105  $P_{2c}22'2'$  one finds in the tables:

$$P222_1 \quad (0,0,0;\mathbf{a},\mathbf{b},2\mathbf{c}) \quad (1|0,0,0) \quad (2_x|0,0,0) \quad (2_y|0,0,1) \quad (2_z|0,0,1)$$

The translational subgroup of **D** is generated by the translations  $(1|1,0,0)$ ,  $(1|0,1,0)$ , and  $(1|0,0,2)$ , the generators of the unprimed subgroup of  $\mathbf{T}^{\mathbf{M}}_R$ , and the coset representatives of this group are all those coset representatives on the right. This subgroup **D** is of type P222<sub>1</sub>. In the tables, listed for the group 17.1.106 P222<sub>1</sub> one finds a different set of coset representatives:

$$(1|0,0,0) \quad (2_x|0,0,0) \quad (2_y|0,0,\frac{1}{2}) \quad (2_z|0,0,\frac{1}{2})$$

Consequently, to show the relationship between the subgroup **D** of type P222<sub>1</sub> and the



listed group  $P222_1$ , we change the coordinate system in which  $\mathbf{D}$  is defined to  $(0,0,0;\mathbf{a},\mathbf{b},2\mathbf{c})$ . In this new coordinate system the coset representatives of  $\mathbf{D}$  are identical with the coset representatives of the representative group  $P222_1$ .

Example 3: For the  $\mathbf{M}_T$  magnetic group 18.4.116  $P2_12_1'2'$  one finds in the tables:

$$P2_1(0, \frac{1}{4}, 0; \mathbf{c}, \mathbf{a}, \mathbf{b}) \quad (1|000) \quad (2_x|\frac{1}{2}, \frac{1}{2}, 0) \quad (2_y|\frac{1}{2}, \frac{1}{2}, 0)' \quad (2_z|000)'$$

The translational subgroup of  $\mathbf{D}$  is generated by the translations  $(1|0,0,1)$ ,  $(1|1,0,0)$ , and  $(1|0,1,0)$ , and the coset representatives of this group are  $(1|000)$  and  $(2_x|\frac{1}{2}, \frac{1}{2}, 0)$ , the unprimed coset representatives on the right. The group  $\mathbf{D}$  is of type  $P2_1$ . In the tables, for the group 4.1.15  $P2_1$  one finds a different set of coset representatives,  $(1|0,0,0)$  and  $(2_y|0, \frac{1}{2}, 0)$ . Consequently, to show the relationship between the subgroup  $\mathbf{D}$  of type  $P2_1$  and the listed group  $P2_1$ , we change the coordinate system in which the subgroup  $\mathbf{D}$  is defined to  $(0, \frac{1}{4}, 0; \mathbf{c}, \mathbf{a}, \mathbf{b})$ . The origin is first translated from  $\mathbf{O}$  to  $\mathbf{O}+\mathbf{t}$ , where  $\mathbf{t}=(0, \frac{1}{4}, 0)$  and the a new set of basis vectors,  $\mathbf{a}'=\mathbf{c}$ ,  $\mathbf{b}'=\mathbf{a}$ , and  $\mathbf{c}'=\mathbf{b}$  is defined. In this new coordinate system the coset representatives of the subgroup  $\mathbf{D}$  are identical with the standard set of coset representatives of the representative group  $P2_1$ .

### 1.3.4 Coset Representatives

The groups listed are defined by their translational subgroups and a set of coset representatives, the standard set, of the coset decomposition of each group with

respect to its respective translational subgroup. The defining coset representatives are listed on the right hand side of Tables 1.1 .

A two- or three-dimensional space group  $\mathbf{F}$  is defined by its translational subgroup and the set of coset representatives implied by the coordinates of the set of equivalent positions explicitly listed *ITC52*. For example, The three-dimensional space group  $\mathbf{F} = \text{P}222_1$  (17.1.106) has a primitive translational subgroup generated by  $(1|1,0,0)$ ,  $(1|0,1,0)$ , and  $(1|0,0,1)$ . The coordinates of the set of equivalent positions listed in *ITC52* under the group type  $\text{P}222_1$  are:

$$x,y,z; \quad x,\bar{y},\bar{z}; \quad \bar{x}, y, \frac{1}{2}+\bar{z}; \quad \bar{x},\bar{y}, \frac{1}{2}+z$$

The coset representative  $(R|\tau(R))$  corresponding to a specific equivalent position  $\mathbf{r}' = x',y',z'$  is given by the equation  $\mathbf{r}' = (R|\tau(R))\mathbf{r} = R\mathbf{r} + \tau(R)$ . Corresponding to the preceding equivalent positions are the coset representatives

$$(1|0,0,0); \quad (2_x|0,0,0); \quad (2_y|0,0,\frac{1}{2}); \quad (2_z|0,0,\frac{1}{2}),$$

which are listed in Table 1.1.

The coset representatives of groups  $\mathbf{F1}'$  are not explicitly given. These are taken as the coset representatives of  $\mathbf{F}$  plus each of these coset representatives multiplied by  $1'$ . For example, the coset representatives of  $\mathbf{F} = \text{P}222_1$  are given above. The coset representatives of  $\mathbf{F1}' = \text{P}222_11'$  are

$$(1|0,0,0); \quad (2_x|0,0,0); \quad (2_y|0,0,1/2); \quad (2_z|0,0,1/2),$$

$$(1|0,0,0)'; \quad (2_x|0,0,0)'; \quad (2_y|0,0,1/2)'; \quad (2_z|0,0,1/2)'.$$

The coset representatives of groups  $\mathbf{M}_T = \mathbf{F}(\mathbf{D})$  are derived from the coset representatives of  $\mathbf{F}$ . Each coset representative of  $\mathbf{F}$  appears unchanged or primed, see Section 1.3.2 above, as a coset representative of  $\mathbf{M}_T$ . For example, The coset representatives of  $\mathbf{F} = P222_1$  are

$$(1|0,0,0); \quad (2_x|0,0,0); \quad (2_y|0,0,1/2); \quad (2_z|0,0,1/2).$$

The coset representatives of  $\mathbf{M}_T = P2'2'2_1$  are:

$$(1|0,0,0); \quad (2_x|0,0,0)'; \quad (2_y|0,0,1/2)'; \quad (2_z|0,0,1/2).$$

The coset representatives of groups  $\mathbf{M}_R = \mathbf{F}(\mathbf{D})$  are also derived from the coset representatives of  $\mathbf{F}$ . They are also chosen such that they are also coset representatives of  $\mathbf{D}$  with respect to its subgroup  $\mathbf{T}^D$ . Each coset representative of  $\mathbf{F}$  appears either unchanged or multiplied by  $\mathbf{t}_a$ , see Section 1.3.2 above. For example: The coset representatives of  $\mathbf{F} = P222_1$  are

$$(1|0,0,0); \quad (2_x|0,0,0); \quad (2_y|0,0,1/2); \quad (2_z|0,0,1/2).$$

The coset representatives of  $M_R = P_{2a}2'2'2_1$ , where  $t_\alpha = (1,0,0)$ , are:

$$(1|0,0,0); \quad (2_x|1,0,0); \quad (2_y|1,0,\frac{1}{2}); \quad (2_z|0,0,\frac{1}{2}).$$

#### 1.4 Changes in Symbols

Typographical errors in Opechowski & Guccione (1965) corrected in Opechowski (1986) of three-dimensional magnetic space group types are as follows:

Numbering in Table 1.1	Opechowski & Guccione (1965)	Opechowski (1986)
16.4.102	$P_{2s}222$	$P_{2a}222$
43.4.323	$Fd'd'2$	$Fd'd'2$
47.6.352	$P_{2s}mmm$	$P_{2a}mmm$
67.17.593	$C_1m'm'a'$	$C_1m'ma'$
108.8.899	$I4'cm'$	$I_p4'cm'$
108.9.900	$I4c'm'$	$I_p4c'm'$
124.1.1018	$P4/mcr$	$P4/mcc$
132.4.1113	$P4_2/mcm'$	$P4_2'/mcm'$

In both Opechowski & Guccione (1965) and Opechowski (1986) the symbol  $P_{2b}c'ca$  is listed twice, in the numbering of Table 1.1, at entries 54.11.438 and 54.13.440. The second has been changed to  $P_{2b}c'ca'$ , a magnetic group which has a non-magnetic subgroup of the type  $Pnna$ .

Three more changes have been made:

Numbering in Table 1.1	Opechowski & Guccione (1965) Opechowski (1986)	Table 1.1
131.13.1109	$P_p 4_2'/m'mc$	$P_p 4_2'/m'mc'$
177.7.1385	$P_{2c} 6'22$	$P_{2c} 6'22'$
180.7.1402	$P_{2c} 6_2'22$	$P_{2c} 6_2'22'$

The reason for these changes are similar: For the middle case, the group P622 is listed in Table 1.1 as

177.1.1379	P622	$(1 0,0,0)$	$(3_z 0,0,0)$	$(3_z^{-1} 0,0,0)$
		$(2_z 0,0,0)$	$(6_z 0,0,0)$	$(6_z^{-1} 0,0,0)$
		$(2_x 0,0,0)$	$(2_{xy} 0,0,0)$	$(2_y 0,0,0)$
		$(2_1 0,0,0)$	$(2_2 0,0,0)$	$(2_3 0,0,0)$

177.7.1385 is a group with a  $P_{2c}$  lattice. The symbol 6' means that the coset representative  $(6_z|0,0,0)$  in the standard set of coset representatives of the coset decomposition of P622 with respect to P (listed in 177 .1.1379) appears as  $(6_z|0,0,1)$  in the standard set of coset representatives of the coset decomposition of the magnetic group with respect to  $P_{2c}$ . This implies the following coset representatives of 177.7.1385 :

$(1 0,0,0)$	$(3_z 0,0,0)$	$(3_z^{-1} 0,0,0)$
$(2_z 0,0,1)$	$(6_z 0,0,1)$	$(6_z^{-1} 0,0,1)$

The unprimed symbol 2 following the 6' implies that the coset representative  $(2_x|0,0,0)$  remains the same as a coset representative in 177.7.1385. Combining this with the

listed coset representatives implies the complete set of coset representatives found in

Table 1.1:

$(1 0,0,0)$	$(3_z 0,0,0)$	$(3_z^{-1} 0,0,0)$
$(2_z 0,0,1)$	$(6_z 0,0,1)$	$(6_z^{-1} 0,0,1)$
$(2_x 0,0,0)$	$(2_{xy} 0,0,0)$	$(2_y 0,0,0)$
$(2_1 0,0,1)$	$(2_2 0,0,1)$	$(2_3 0,0,1)$

Note that the coset representative  $(2_1|0,0,0)$  of the coset decomposition of P622 with respect to P now appears as the coset representative  $(2_1|0,0,1)$  in the coset decomposition of the magnetic group 177.7.1385 with respect to  $P_{2c}$ . Consequently, the second symbol 2 in P622, appears as 2' in the symbol of 177.7.1385, i.e. the symbol of this magnetic group is  $P_{2c} 6_2' 22'$ .

### 1.5 Relationship to Black and White Space Group Symbols

Opechowski & Guccione symbols (1965) for *all* group types in a three-dimensional magnetic superfamily of type **F** are based on the symbol of the three-dimensional space group **F**. For groups **F**, **F1'**, and **M<sub>T</sub>**, the Belov et al (1955, 1957) symbols do the same. However, for groups of the type **M<sub>R</sub> = F(D) = D + (F - D)1'** Belov et al (1955, 1957) base their symbol on the symbol for the group **D**, the unprimed subgroup of index 2. For example, the Opechowski & Guccione symbol for group 47.11.357 is  $P_C mmm'$ . From this we have that **F** = Pmmm and from Table 1.1 that **D** = Cmma. The Belov et al symbol for this group 47.11.357 is based on the symbol of the subgroup **D**, i.e. the symbol Cmma: A group **M<sub>R</sub>** can be written as **M<sub>R</sub> = F(D) = D + t<sub>α</sub>' D**, where t<sub>α</sub> is a translation of **F** not in **D**. For the group 47.11.357, this translation is chosen as  $a = (1,0,0)$  and is found in the figure for the  $P_C$  lattice in Figures 1.1. The

translational subgroup of this group is symbolically represented by Belov et al as  $C_a$  where C represents the translational subgroup of  $\mathbf{D} = Cmma$  and the subscript "a" denotes the translation  $t_a = a$ . This leads to the Belov et al symbol of  $C_a m'ma$  for the group 47.11.3 57.

A side by side comparison of Opechowski & Guccione symbols for three-dimensional magnetic space groups and Belov et al symbols for three-dimensional black and white space groups is given in Table 1.4-3D. As the Belov et al symbols for groups of type  $\mathbf{F}$ ,  $\mathbf{F1}'$  and  $\mathbf{M}_T$  are the same as Opechowski & Guccione symbols, we list Belov et al symbols explicitly only for groups of type  $\mathbf{M}_R$ . Comparisons of one- and two-dimensional magnetic space groups and black and white space groups are given, respectively, in Tables 1.4-1D and 1.4-2D.

## 2. Guide to the use of the magnetic space groups tables

### 2.1 Introduction

In this section we present a guide to the tabulation of properties of the superfamilies of one-, two-, and three-dimensional magnetic space groups given, respectively, in Table 3 - 1D, Table 3 -2D, and Table 3 - 3D. The format and content of these magnetic group tables are similar to the format and content of the space group tables in *ITC-A: International Tables for Crystallography, Volume A* (1983), the subperiodic group tables in the *ITC-E: International Tables for Crystallography, Volume E* (2002), and the same as that in the magnetic subperiodic group tables (Litvin, 2005).

### 2.2 Contents of the Magnetic Space Group Tables

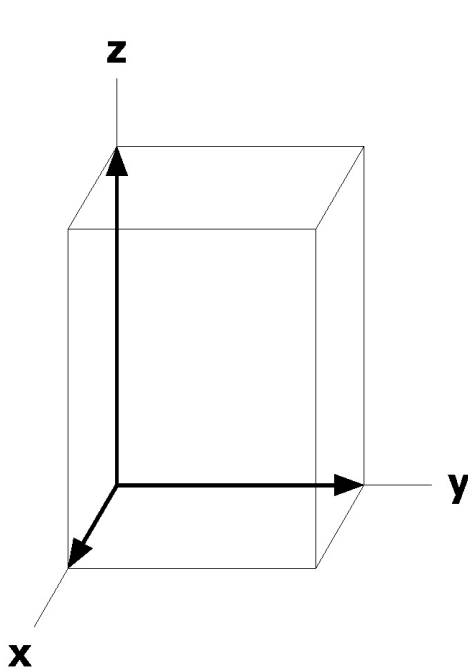
The content of the magnetic group tables consists of the following:

- (1) Lattice Diagram
- (2) Headline
- (3) Diagrams of symmetry elements and of the general positions
- (4) Origin
- (5) Asymmetric unit
- (6) Symmetry operations
- (7) Generators selected
- (8) Positions, with multiplicities, site symmetries, coordinates, and magnetic moments
- (9) Symmetry of special projections

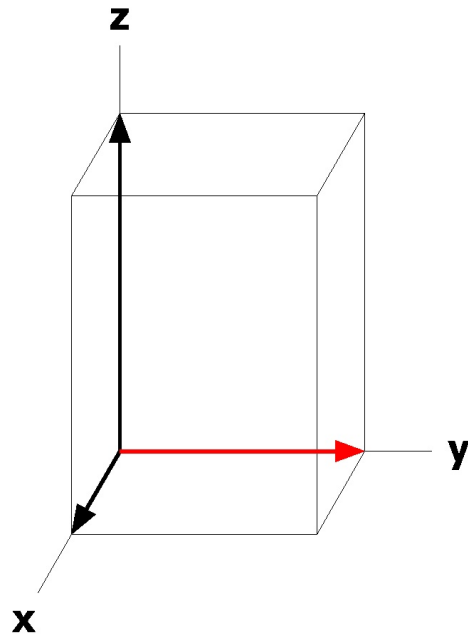


## 2.2.1 Lattice Diagram

In the upper left hand corner of the first page of tables for each magnetic space group is the lattice diagram of the magnetic space group. This lattice diagram depicts the coordinate system used, the conventional unit cell of the space group  $F$ , the magnetic space group's magnetic superfamily type, and the generators of the translational subgroup of the magnetic space group. For example, in Figures 2.2.1.1 and 2.2.1.2 we show the lattice diagrams for the orthorhombic magnetic space groups



**Figure 2.2.1.1:** Lattice Diagram of the group 26.1.168  $F = Pmc2_1$ .



**Figure 2.2.1.2:** Lattice Diagram of the group 26.10.177  $M_R = F(D) = P_{2b} m'c'2_1 = Pmc2_1(Pca2_1)$ .

$Pmc2_1$  and  $P_{2b} m'c'2_1$ , respectively. The generating lattice vectors depicted are color coded. Those colored black are not coupled with time inversion while those colored red are coupled with time inversion. In the former group  $Pmc2_1$ , a magnetic group of the type  $F$ , the lattice is an orthorhombic "P" lattice, see Figures 1.1, and no generating

translation is coupled with time inversion. In the latter group  $P_{2b} m'c'2_1$ , a magnetic group of type  $M_R$ , the lattice is an orthorhombic " $P_{2b}$ " lattice, with the generating lattice vector in the y-direction coupled with time inversion.

### 2.2.2 Headline

To the right of the lattice diagram is a two line heading, an example is given in Figure 2.2.2.1 . On the upper line, starting on the left, are three entries:

P4/m'mm	4/m'mm	Tetragonal
123.3.1001	P4/m'2'/m2'/m	

**Figure 2.2.2.1:** Headline of magnetic space group P4/m'mm.

(1) The *short international* (Hermann-Mauguin) *symbol* of the magnetic space group. Each symbol has two meanings: The first is that of the Hermann-Mauguin symbol of a magnetic space group type. The second is that of a specific magnetic space group which belongs to this magnetic space group type. Given a coordinate system, this group is defined both by the list of symmetry operations (see Section 2.2.6) given on the page with this Hermann-Mauguin symbol in the heading, or by the given list of general positions and magnetic moments (see Section 2.2.8).

(2) The *short international* (Hermann-Mauguin) *point group symbol* for the geometric class to which the magnetic space group belongs.

(3) The crystal system to which the magnetic space group belongs.

The second line has two additional entries:

(1) The three part numerical serial index of the magnetic space group (see

Section 1.3.1 ).

(2) The *long international (Hermann-Mauguin) symbol* of the magnetic space group.

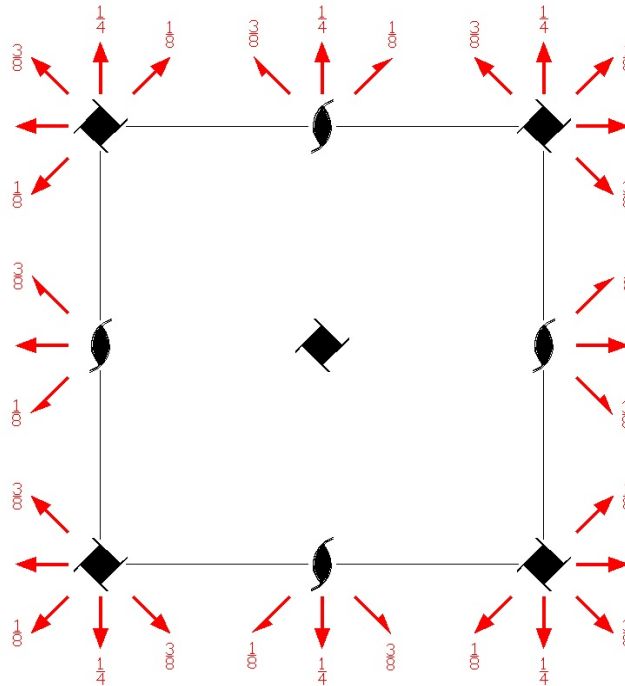
### 2.2.3 Diagrams of symmetry elements and of the general positions

There are two types of diagrams, symmetry diagrams and general position diagrams. The symmetry diagrams show (1) the relative locations and orientations of the symmetry elements and (2) the locations and orientations of the symmetry elements relative to a given coordinate system. The general position diagrams show, in that coordinate system, the arrangement of a set of symmetrically equivalent points and relative orientations of magnetic moments on this set of equivalent points relative to the symmetry elements.





For the three-dimensional magnetic space groups, all diagrams are orthogonal projections and the projection direction is along the **c** basis vector, see Table 1.2 . If the other two basis vectors are not parallel to the plane of the diagram, they are indicated by a subscript "p" , e.g. **a<sub>p</sub>** and **b<sub>p</sub>** . Schematic representations of the diagrams, showing their conventional coordinate system, i.e. the origin "O" and basis vectors, are given in Figures 2.2.3.1 . The general position diagram is shown on the left and indicated by the letter "G". The symmetry diagram is on the right.

The graphical symbols used in the symmetry diagrams are listed in Table 2.2.3 and are an extension of those used in *ITC-A* (1983), *ITC-E* (2002) and Litvin (2005). For three-dimensional magnetic space groups, the symmetry planes and symmetry axes parallel to the plane of diagram, for rotoinversions, and for centers of symmetry, the "heights" *h* along the projection direction above the plane of the diagram are given.

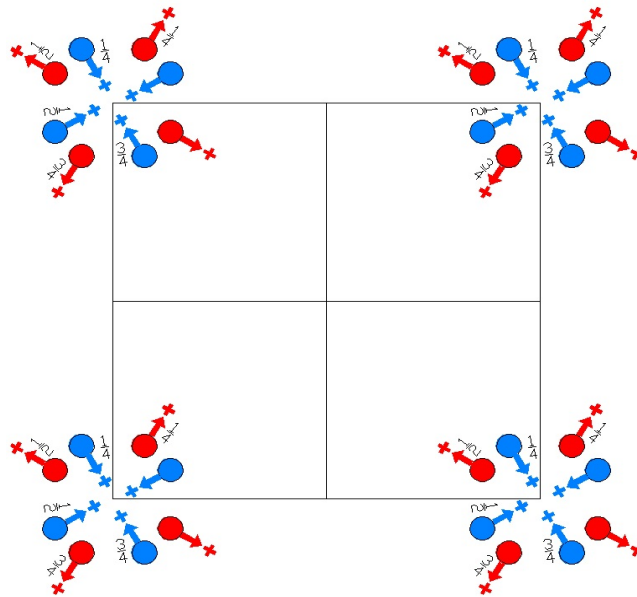
The heights are given as fractions of the shortest translation along the projection direction and if different from zero, are printed next to the graphical symbol, see e.g. Figure 2.2.3.2 .



**Figure 2.2.3.2:** Symmetry diagram of the three-dimensional magnetic space group  $P4_12'2'$

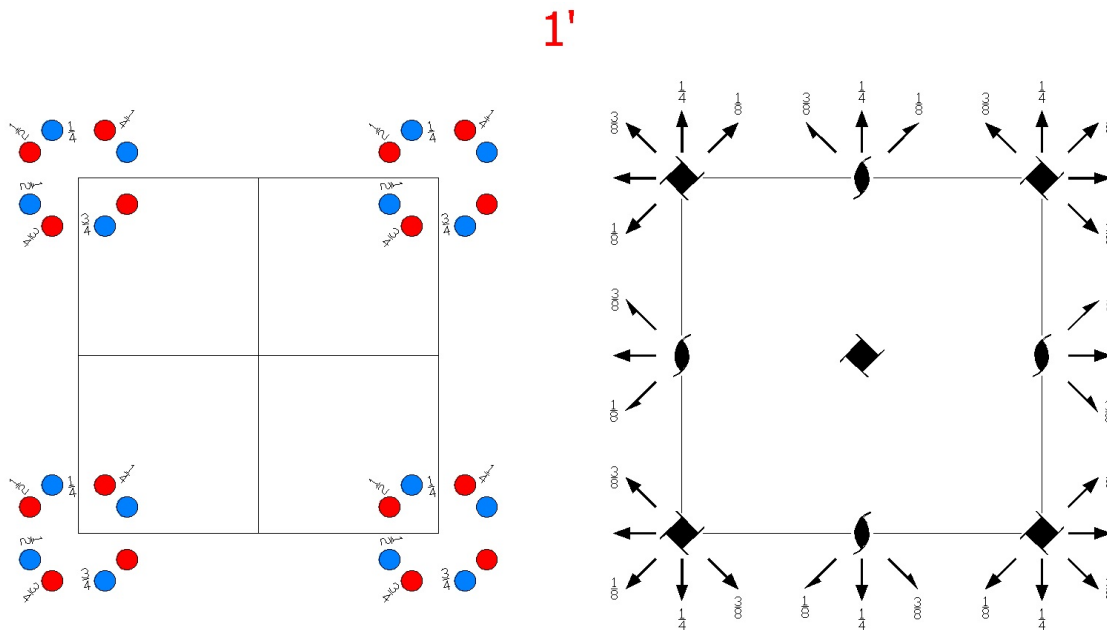
In the general position diagrams, the general positions and corresponding magnetic moments are color coded. Positions with a z-component of "+z" are circles color coded red  and with a z-component of "-z" are circles color coded blue  . If the z-component is either "h+z" or "h-z" with  $h \neq 0$ , then the height "h" is printed next to the general position, e.g.   $\frac{1}{4}$  . If two general positions have the same x-component and y-component, with z-components +z and -z, respectively, the positions are denoted as  . The magnetic moments are color coded to the general position to which they are associated, their direction in the plane of projection is given by an

arrow in the direction of the magnetic moment. A "+" or "-" sign near the tip of the arrow indicates the magnetic moment is inclined, respectively, above or below the plane of projection, as in Figure 2.2.3.3 .



**Figure 2.2.3.3:** General position diagram of the three-dimensional magnetic space group  $P4_12'2'$

For magnetic space groups of the type  $F1'$  , the symmetry diagram is that of the group  $F$ . That each symmetry element also appears coupled with time inversion is represented by a red  $1'$  printed between and above the general position and symmetry diagrams. Because groups of this kind contain the time inversion symmetry, the magnetic moments are all identically zero, and no arrows appear in the general position diagram. An example, the diagrams of three-dimensional magnetic space group  $P4_1221'$  are shown in Figure 2.2.3.4:



**Figure 2.2.3.4:** Diagrams of three-dimensional magnetic space group  $P4_1221'$ .

## 2.2.4 Origin

If the magnetic space group is centrosymmetric then the inversion center or a position of high site symmetry, as on the four-fold axis of tetragonal groups, is chosen as the origin. For noncentrosymmetric groups, the origin is at a point of highest site symmetry. If no symmetry is higher than 1, the origin is placed on a screw axis, a glide plane or at the intersection of several such symmetries.

In the *Origin* line below the diagrams, the site symmetry of the origin is given. An additional symbol indicates all symmetry elements that pass through the origin. For example, for the three-dimensional magnetic space group  $I4/mcm$ , one finds "**Origin** at center (  $4/m$  ) at  $4/mc2_1/c$ ." The site symmetry is  $4/m$  and in addition, two glide planes perpendicular to the  $y$ - and  $z$ -axis, and a screw axis parallel to the  $z$ -axis pass through the origin.

## 2.2.5 Asymmetric Unit

An asymmetric unit of a magnetic space group is a simply connected smallest part of space from which, by application of all symmetry operations of the magnetic space group, exactly fills the whole space. Since the magnetic space groups contain a translational subgroup, the asymmetric unit is a finite part of space. We define the asymmetric unit by setting the limits on the coordinates of points contained in the asymmetric unit. For example, for the three-dimensional magnetic space group  $I4/m'cm$  (140.3.1198) one finds:

$$\text{Asymmetric unit } 0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; y \leq 1/2 - x$$

Drawings showing the boundary planes occurring in the tetragonal, trigonal, and hexagonal systems, together with their algebraic equations are given in Figure 2.8.1 of *ITC-A* (1983). Drawings of asymmetric units for cubic groups have been published by Koch & Fisher (1974). The asymmetric units have complicated shapes in the trigonal, hexagonal, and cubic crystal systems and consequently are also specified by given the vertices of the asymmetric unit. For example, for the three-dimensional magnetic space group  $P6_3/m$  (176.1.1374) one finds:

$$\begin{array}{l} \text{Asymmetric unit } 0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/4; \\ \quad x \leq (1+y)/2; \quad y \leq \min(1-x, (1+x)/2) \\ \text{Vertices } \begin{array}{cccccc} 0,0,0 & 1/2,0,0 & 2/3,1/3,0 & 1/3,2/3,0 & 0,1/2,0 \\ 0,0,1/4 & 1/2,0,1/4 & 2/3,1/3,1/4 & 1/3,2/3,1/4 & 0,1/2,1/4 \end{array} \end{array}$$

Because the asymmetric unit is invariant under time inversion, all magnetic space groups **F**, **F1'**, and **F(D)** of the magnetic superfamily of type **F** have identical asymmetric units.

### 2.2.6 Symmetry operations

Listed under the heading of *Symmetry operations* is the geometric description of the symmetry operations of the magnetic space group. In addition, each symmetry operation is also given in Seitz notation (Burns & Glazer, 1990). The corresponding coordinate triplets of the *General positions* may be interpreted as a second description of the symmetry operations, a description in matrix form. The numbering (1), (2), ... , (p), ... of the entries in the blocks *Symmetry operations* is the same as the numbering of the corresponding coordinate triplets of the *General positions*, the first block below *Positions*. For all magnetic space groups with primitive "P" lattices, the two lists, *Symmetry operations* and *General positions*, have the same number of entries.

For magnetic space groups with centered cells, only one block of several (2,3, or 4) blocks of the *General positions* is explicitly given. A set of (2,3, or 4) centering translations is given below the subheading *Coordinates*. Each of these translations is added to the given block of general positions to obtain the complete set of blocks of general positions. While one of the several blocks of general positions is explicitly given, the corresponding symmetry operations are all explicitly given. Each corresponding block of symmetry operations is listed under a subheading of "centering translation + set" for each centering translation listed below the subheading *Coordinates*.

A symbol denoting the geometric description of each symmetry operation is



given. Details of this symbolism, except for the use of prime to denote time inversion, are given in Section 11.2 of *ITC-A* (1983). For glide planes and screw axes the glide and screw part are always explicitly given in parentheses by fractional coordinates, i.e. by fractions of the basis vectors of the coordinate system of **F** of the superfamily of the magnetic group. A coordinate triplet indicating the location and orientation of the symmetry element is given, and for rotoinversions, the location of the inversion point is also given. These symbols, with the addition of a prime to denote time inversion, follow those used in *ITC-A* (1983), *ITC-E* (2002), and Litvin (2005).

### **2.2.7 Generators selected**

The line *Generators selected* lists the symmetry operations selected to generate the symmetrically equivalent points of the *General position* from a point with coordinates  $x, y, z$ . The first generator is always the identity operation given by (1) followed by generating translations. Additional generators are given as numbers (p) which refer to the coordinate triplets of the *General position* and to corresponding symmetry operations in the first block, if more than one, of *Symmetry operations*.

### **2.2.8 Positions, with multiplicities, site symmetries, coordinates, and magnetic moments**

The entries under *Positions*, referred to as *Wyckoff positions*, consists of the *General positions*, the upper block, followed by blocks of *Special positions*. The upper block of positions, the general positions, is a set of symmetrically equivalent points where each point is left invariant only by the identity operation or, for magnetic groups **F1'**, by the identity operation and time inversion, but by no other

symmetry operations of the magnetic space group. The lower blocks, the special positions, are a set of symmetrically equivalent points where each point is left invariant by at least one additional operation in addition to the identity operation, or , for magnetic space groups  $F1'$  , in addition to the identity operation and time inversion.

For each block of positions information is provided:

**Multiplicity:** The multiplicity is the number of equivalent positions in the conventional unit cell of the non-magnetic group  $F$  associated with the magnetic space group.

**Wyckoff Letter:** This letter is a coding scheme for the blocks of positions, starting with “a” at the bottom block and continuing upwards in alphabetical order.

**Site symmetry:** The site symmetry group is the largest subgroup of the magnetic space group that leaves invariant the first position in each block of positions. This group is isomorphic to a subgroup of the point group of the magnetic space group. An “oriented” symbol is used to show how the symmetry elements at a site are related to the conventional crystallographic basis and the sequence of characters in the symbol correspond to the sequence of symmetry directions as in the magnetic space group symbol, see Table 1.3. Sets of equivalent symmetry directions that do not contribute any element to the site symmetry are represented by dots. Sets of symmetry directions having more than one equivalent direction may require more than one character if the site-symmetry group belongs to a lower crystal system. For example, for the 2c position of the three-dimensional magnetic space group  $P4'm'm$  (99.3.825) the site symmetry group is  $2m'm'$ . where the two characters  $m'm'$  represent the secondary set of tetragonal symmetry directions, whereas the dot represents the tertiary tetragonal symmetry directions.

**Coordinates of Positions and Components of Magnetic Moments :** In each block of positions, the coordinates of each position are given. Immediately following each set of position coordinates are the components of the symmetry allowed magnetic moment at that position. The components of the magnetic moment of the first position is determined from the given site symmetry group. The components of the magnetic moments at the remaining positions are determined by applying the symmetry operations to the components of that magnetic moment at the first position.

### 2.2.9 Symmetry of special projections

Under the heading *Symmetry of special projections* the following information is given for the projections of each magnetic space group:

**Projection direction:** All projections are orthogonal, i.e. the projection, for three-dimensional magnetic space groups, is onto a plane normal to the projection direction.

The projection directions are:

Triclinic, Monoclinic, Orthorhombic	[001] [100] [010]
Tetragonal	[001] [100] [110]
Hexagonal	[001] [100] [210]
Rhombohedral	[111] [1 $\bar{1}$ 0] [2 $\bar{1}$ $\bar{1}$ ]
Cubic	[001] [111] [110]

For two-dimensional magnetic space groups, the projection is onto a line normal to the projection direction. The projection directions are:

Oblique	[10]	[01]
Rectangular	[10]	[01]
Square	[10]	[11]
Hexagonal	[10]	[21]

**Basis vectors:** For three-dimensional magnetic space groups, the relationship between the basis vectors  $\mathbf{a}^*$ ,  $\mathbf{b}^*$  of the two-dimensional magnetic space group symmetry of the projection is given in terms of the basis vectors  $\mathbf{a}, \mathbf{b}, \mathbf{c}$  of the three-dimensional magnetic space group. For triclinic and monoclinic three-dimensional magnetic space groups where basis vectors  $\mathbf{a}, \mathbf{b}$ , or  $\mathbf{c}$  are inclined to the plane of projection, these basis vectors are replaced by  $\mathbf{a}_p$ ,  $\mathbf{b}_p$ , or  $\mathbf{c}_p$ , respectively.

For two-dimensional magnetic space groups, the relationship between the basis vector  $\mathbf{a}^*$  of the one-dimensional magnetic space group symmetry of the projection is given in terms of the basis vectors  $\mathbf{a}$  and  $\mathbf{b}$  of the two-dimensional magnetic space group. For oblique two-dimensional magnetic space groups where basis vectors  $\mathbf{a}$  or  $\mathbf{b}$  are inclined to the plane of projection, these basis vectors are replaced by  $\mathbf{a}_p$  or  $\mathbf{b}_p$ , respectively.

**Location of origin:** For three-dimensional magnetic space groups, the location of the origin of the two-dimensional magnetic space group symmetry of the projection is given with respect to the unit cell of the three-dimensional magnetic space group. For two-dimensional magnetic space groups, the location of the origin of the one-dimensional magnetic space group symmetry of the projection is given with respect to the unit cell of the two-dimensional magnetic space group.

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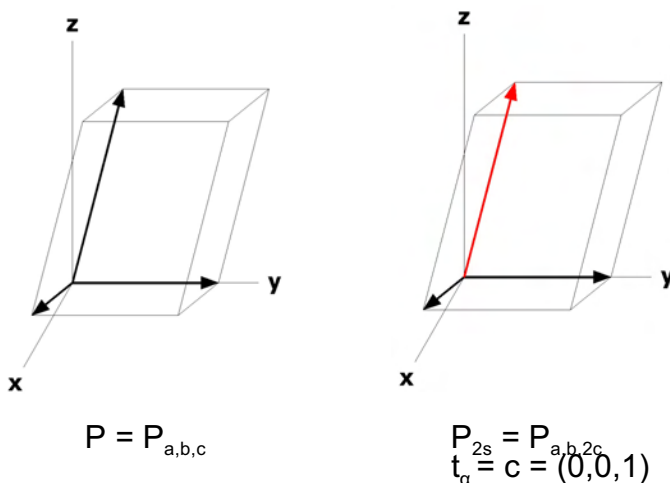
# Figures 1.1: Magnetic Space Group Lattices

Lattices with a first symbol consisting of a single letter with no subscript are lattices of groups  $\mathbf{F}$ ,  $\mathbf{F1}'$  and  $\mathbf{M}_T$ . To the right of an equality sign, a second symbol gives the generators of the lattice in the subscript of the corresponding lattice symbol. These generating translations are also shown as black arrows in the corresponding figure.

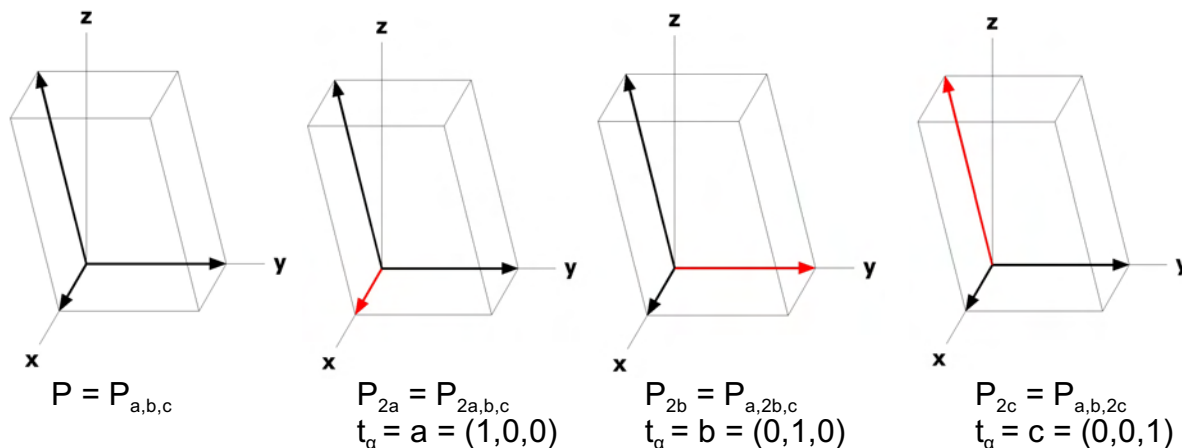
Lattices with a first symbol consisting of a letter with a second letter as a subscript are lattices of magnetic groups  $\mathbf{M}_R$ . The translational subgroup of these groups are of the form  $\mathbf{T}^M = \mathbf{T}^D + \mathbf{t}_\alpha' \mathbf{T}^D$ . To the right of equality signs, additional symbols are given which give the generating translations of  $\mathbf{T}^D$  as a subscript. The translation chosen for  $\mathbf{t}_\alpha$  is also explicitly given. In the corresponding figures, generating translations which are in  $\mathbf{T}^D$  are shown in black and generating translations which are in  $\mathbf{t}_\alpha' \mathbf{T}^D$  are shown in red.

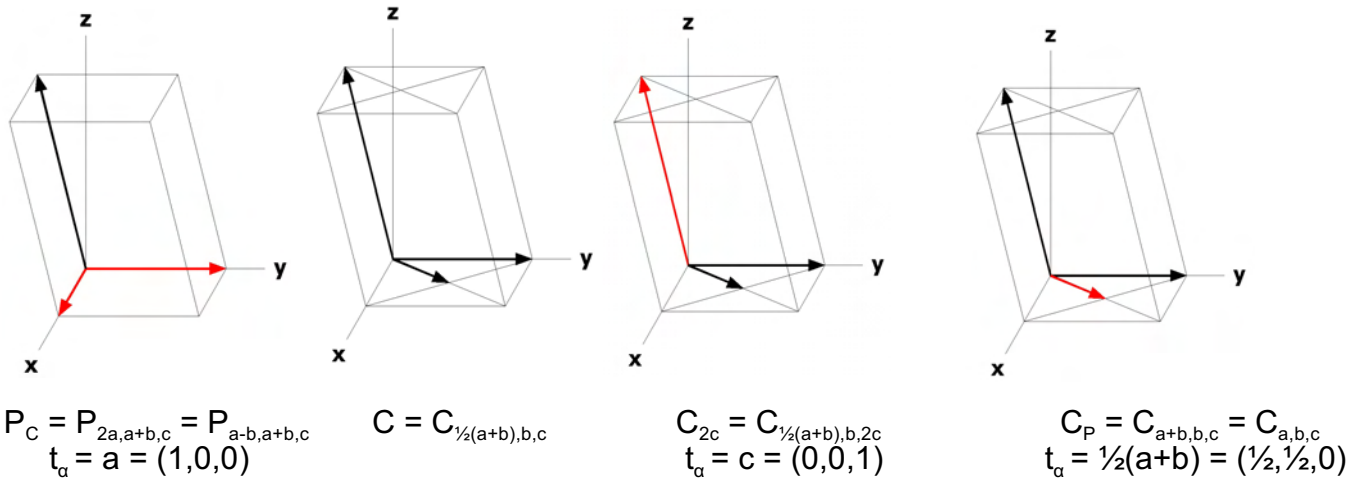
## Three-Dimensional Magnetic Lattices:

Triclinic System

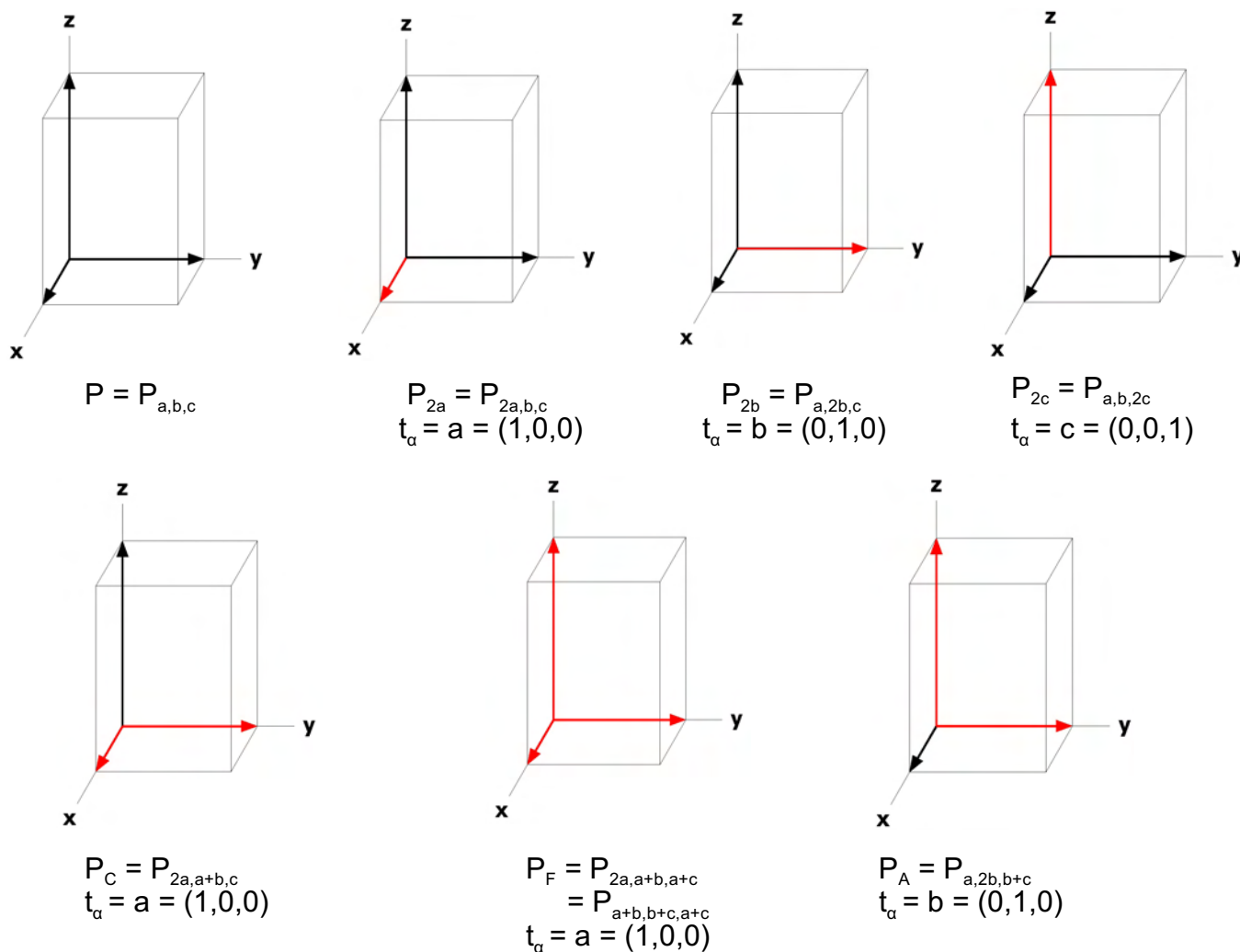


Monoclinic System (2-fold axis along y)



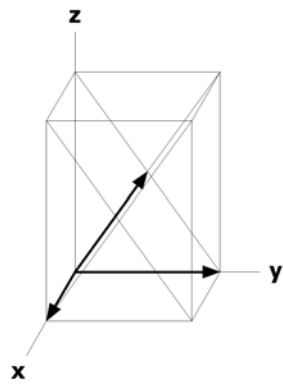


### Orthorhombic System

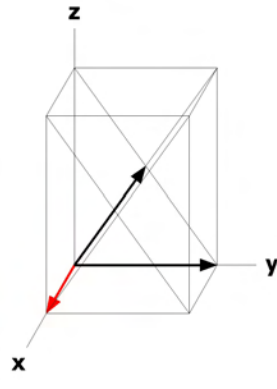


FIGURES 1.1 MAGNETIC SPACE GROUP LATTICES - 2



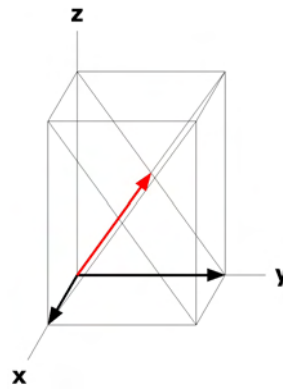


$$A = A_{a,b,\frac{1}{2}(b+c)}$$



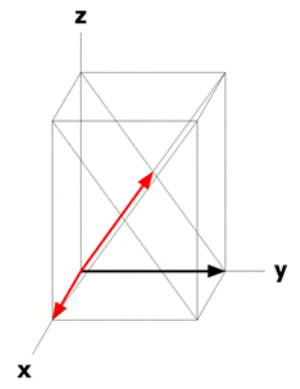
$$A_{2a} = A_{2a,b,b+c}$$

$$t_a = a = (1,0,0)$$



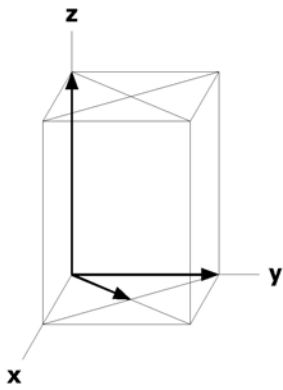
$$A_P = A_{a,b,c}$$

$$t_a = \frac{1}{2}(b+c) = (0,\frac{1}{2},\frac{1}{2})$$

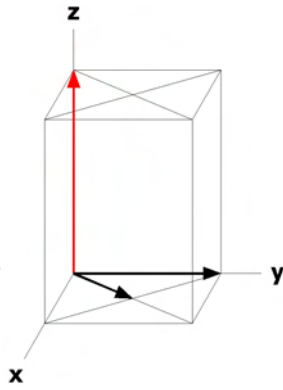


$$A_I = A_{2a,b,\frac{1}{2}(2a+b+c)}$$

$$t_a = a = (1,0,0)$$

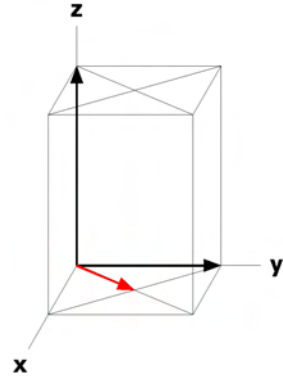


$$C = C_{\frac{1}{2}(a+b),b,c}$$



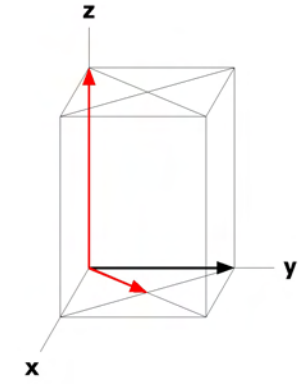
$$C_{2c} = C_{\frac{1}{2}(a+b),b,2c}$$

$$t_a = c = (0,0,1)$$



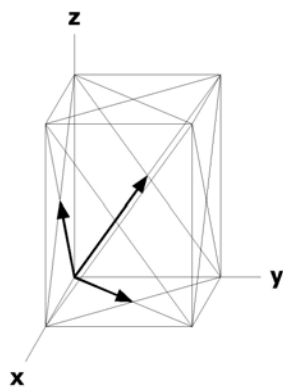
$$C_P = C_{a+b,b,c} = C_{a,b,c}$$

$$t_a = \frac{1}{2}(a+b) = (\frac{1}{2},\frac{1}{2},0)$$

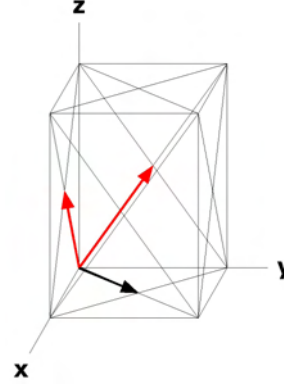


$$C_I = C_{a,b,\frac{1}{2}(a+b+2c)}$$

$$t_a = c = (0,0,1)$$

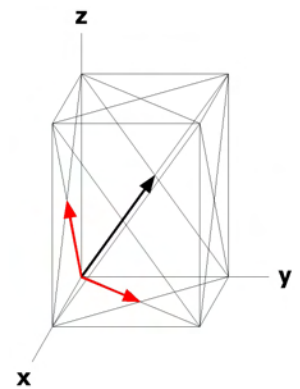


$$F = F_{\frac{1}{2}(a+b),\frac{1}{2}(b+c),\frac{1}{2}(a+c)}$$



$$F_C = F_{\frac{1}{2}(a+b),b,c}$$

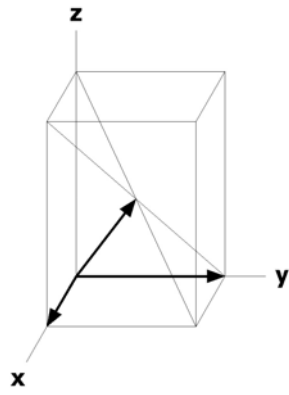
$$t_a = \frac{1}{2}(a+c) = (\frac{1}{2},0,\frac{1}{2})$$



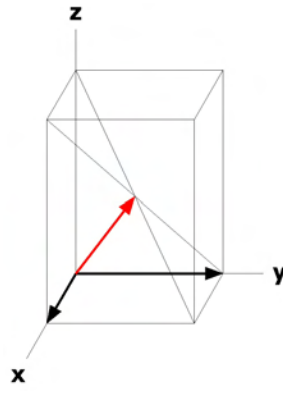
$$F_A = F_{\frac{1}{2}(b+c),c,a}$$

$$t_a = \frac{1}{2}(a+b) = (\frac{1}{2},\frac{1}{2},0)$$

FIGURES 1.1 MAGNETIC SPACE GROUP LATTICES - 3



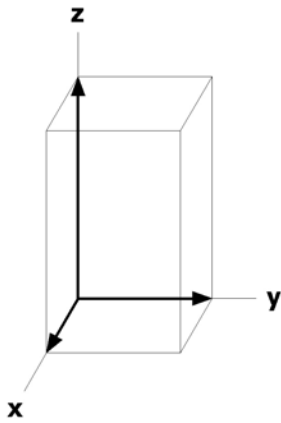
$$l = l_{a,b,\frac{1}{2}(a+b+c)}$$



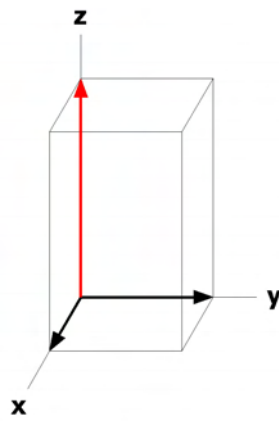
$$l_P = l_{a,b,c}$$

$$t_\alpha = \frac{1}{2}(a+b+c) = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$$

### Tetragonal System

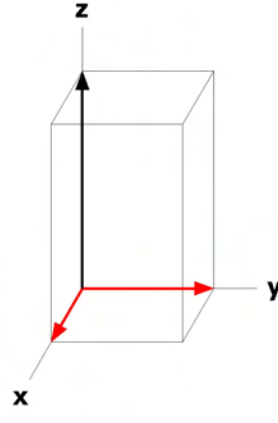


$$P = P_{a,b,c}$$



$$P_{2c} = P_{a,b,2c}$$

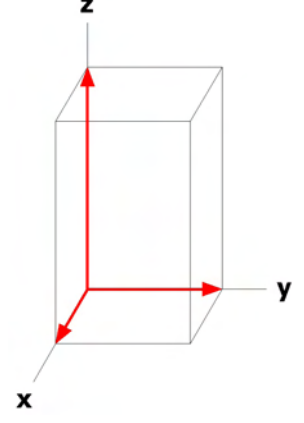
$$t_\alpha = c = (0,0,1)$$



$$P_{a-b,a+b} (P_C) = P_{a-b,a+b,c}$$

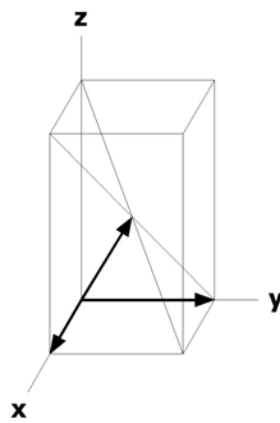
$$= P_P = P_{2a,a+b,c}$$

$$t_\alpha = a = (1,0,0)$$

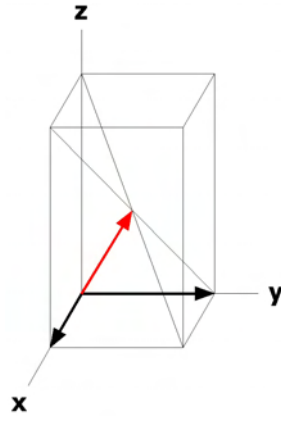


$$P_l = P_{a-b,a+b,a+c}$$

$$t_\alpha = a = (1,0,0)$$



$$l = l_{a,b,\frac{1}{2}(a+b+c)}$$

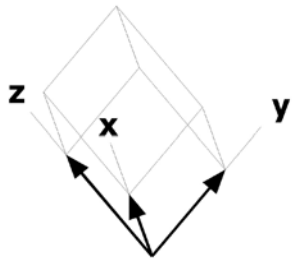


$$l_P = l_{a,b,c}$$

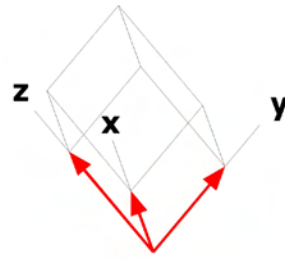
$$t_\alpha = \frac{1}{2}(a+b+c) = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$$

FIGURES 1.1 MAGNETIC SPACE GROUP LATTICES - 4

### Trigonal System (Rhombohedral Axes)



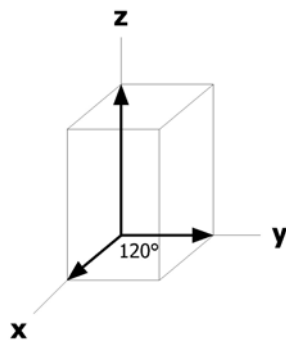
$$R = R_{a,b,c}$$



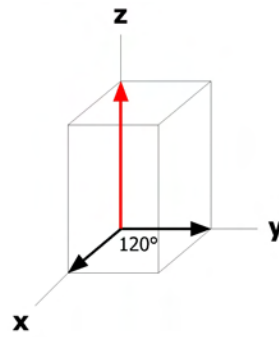
$$R_{2a,a+b,a+c} = R_R = R_{a+b,b+c,a+c}$$

$$t_q = a = (1,0,0)$$

### Trigonal System (Hexagonal Axes) Hexagonal System



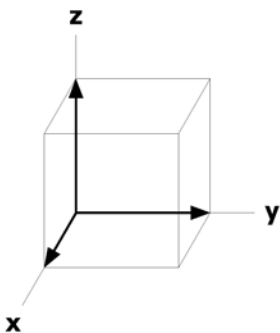
$$P = P_{a,b,c}$$



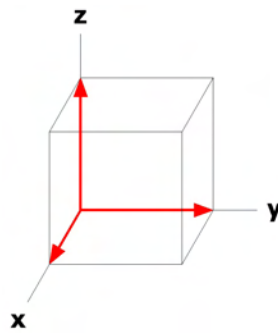
$$P_{2c} = P_{a,b,2c}$$

$$t_q = c = (0,0,1)$$

### Cubic System

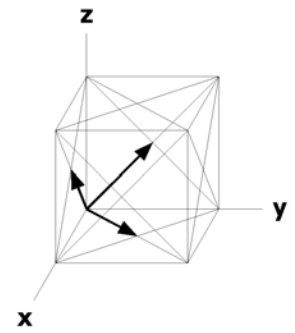


$$P = P_{a,b,c}$$

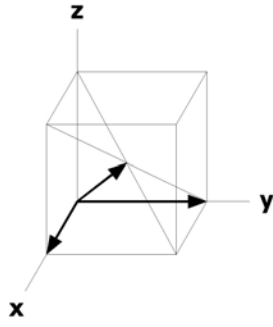


$$P_F = P_{2a,a+b,a+c} = P_{a+b,b+c,a+c}$$

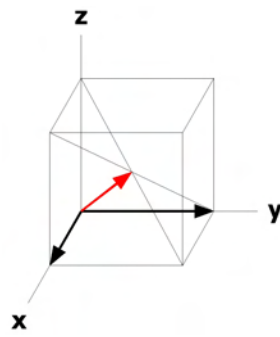
$$t_q = a = (1,0,0)$$



$$F = F_{\frac{1}{2}(a+b), \frac{1}{2}(b+c), \frac{1}{2}(a+c)}$$



$$I = I_{a,b,\frac{1}{2}(a+b+c)}$$

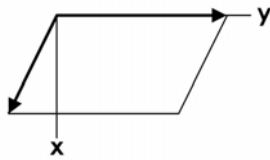


$$I_P = I_{a,b,c}$$

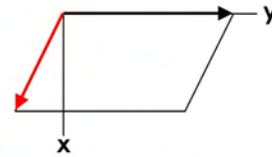
$$t_\alpha = \frac{1}{2}(a+b+c) = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$$

### Two-Dimensional Magnetic Lattices:

#### Oblique System

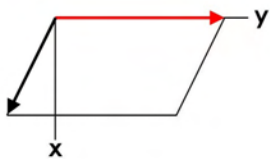


$$p = p_{a,b}$$



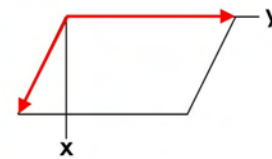
$$p_{2a} = p_{2a,b}$$

$$t_\alpha = a = (1,0)$$



$$p_{2b} = p_{a,2b}$$

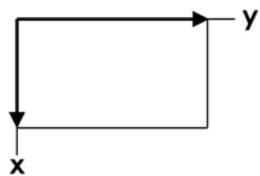
$$t_\alpha = b = (0,1)$$



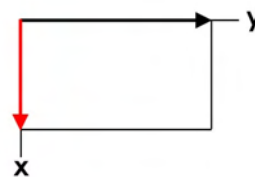
$$p_c = p_{2a,a+b} = p_{a-b,a+b}$$

$$t_\alpha = a = (1,0)$$

# Rectangular System

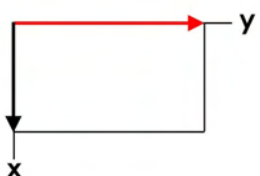


$$p = p_{a,b}$$



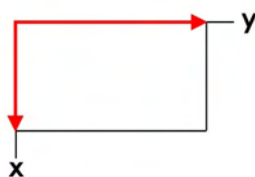
$$p_{2a} = p_{2a,b}$$

$$t_a = a = (1,0)$$



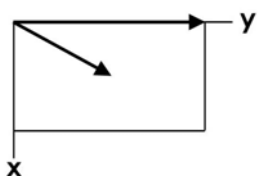
$$p_{2b} = p_{a,2b}$$

$$t_a = b = (0,1)$$

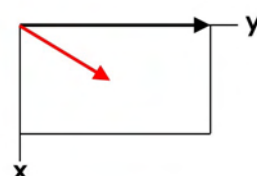


$$p_c = p_{2a,a+b} = p_{a-b,a+b}$$

$$t_a = a = (1,0)$$



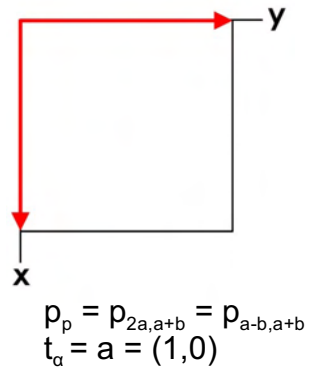
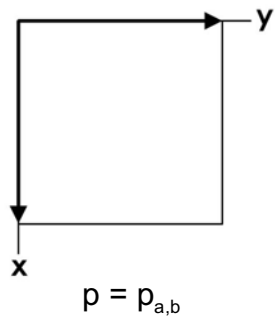
$$c = c_{\frac{1}{2}(a+b),b}$$



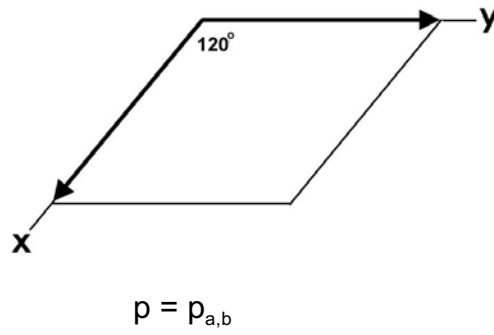
$$c_p = c_{a,b}$$

$$t_a = \frac{1}{2}(a+b)$$

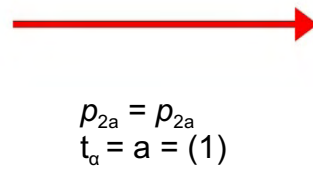
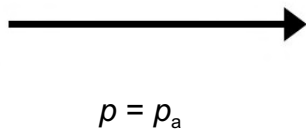
### Square System



### Hexagonal System



### One-Dimensional Magnetic Lattices:



## Figures 2.2.3.1: Projection Diagrams of the Three-Dimensional Magnetic Space Groups

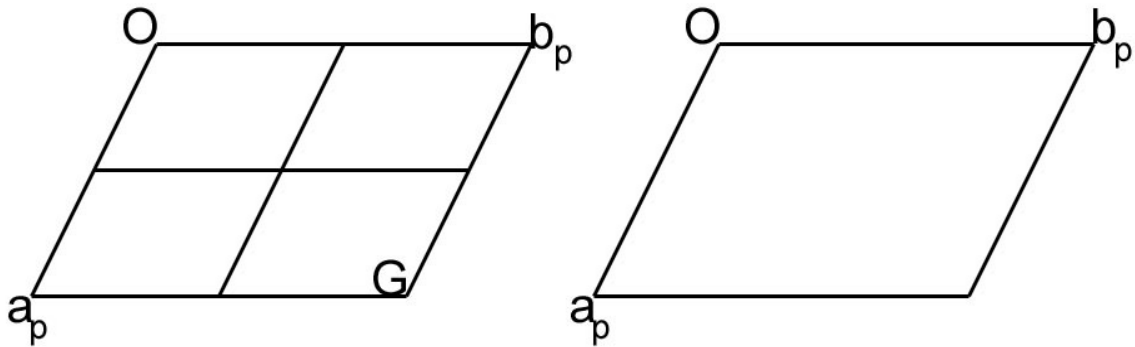


Figure 2.2.3.1a: Diagrams for triclinic 3D-magnetic space groups

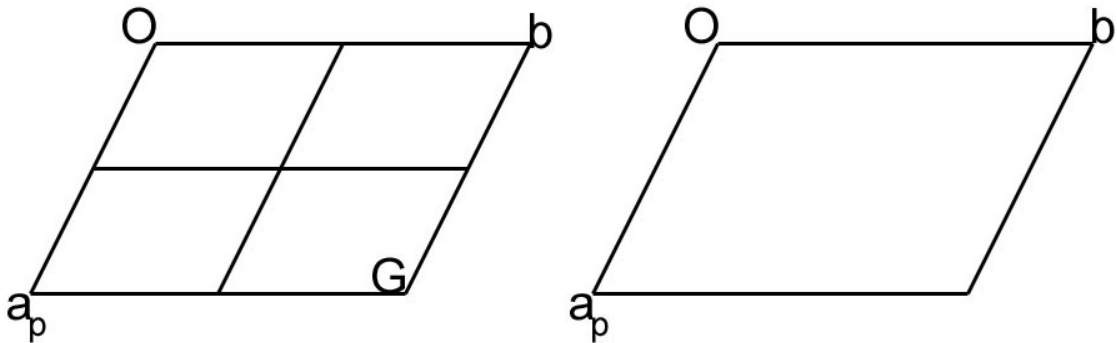
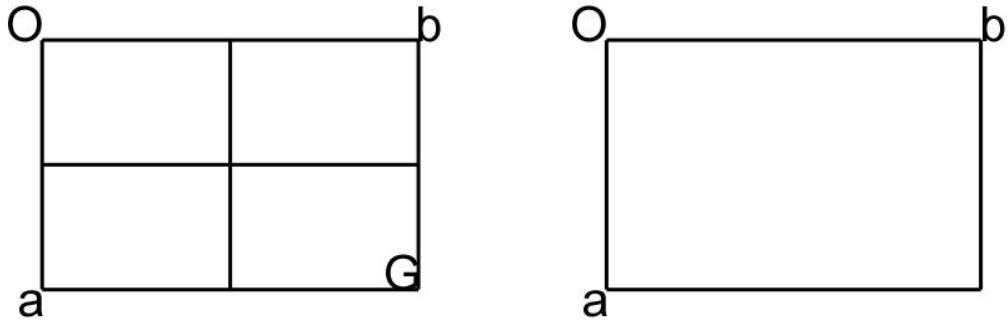
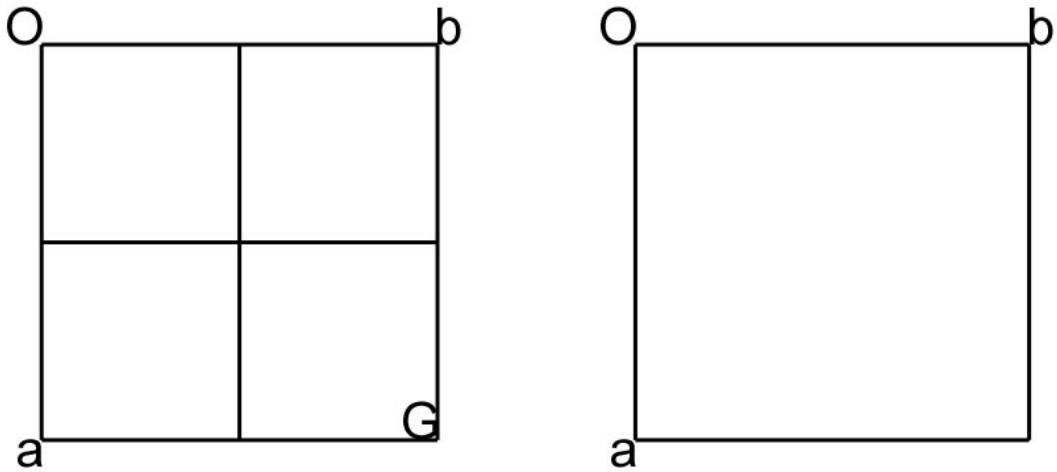


Figure 2.2.3.1b: Diagrams for monoclinic 3D-magnetic space groups

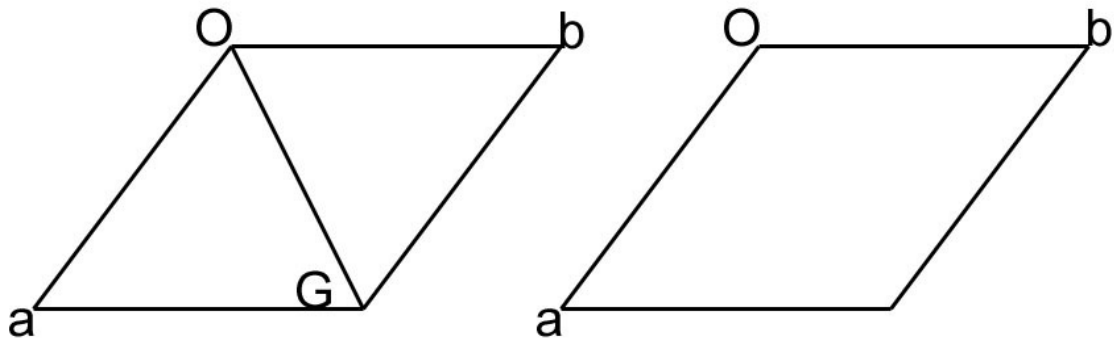


**Figure 2.2.3.1c:** Diagrams for orthorhombic 3D-magnetic space groups.

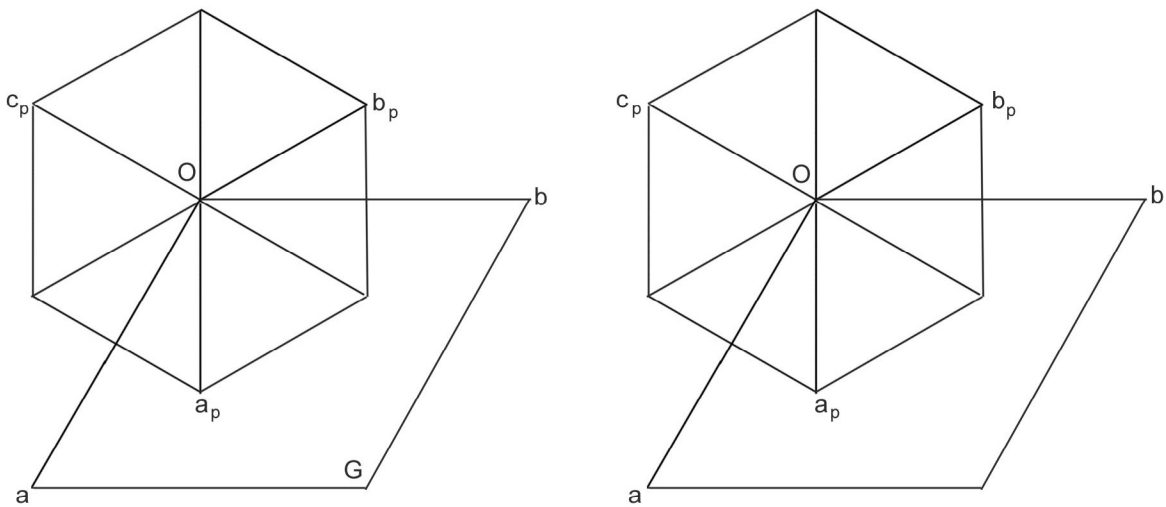


**Figure 2.2.3.1d:** Diagrams for tetragonal and cubic 3D-magnetic space groups.





**Figure 2.2.3.1e:** Diagrams for trigonal P and hexagonal 3D-magnetic space groups.



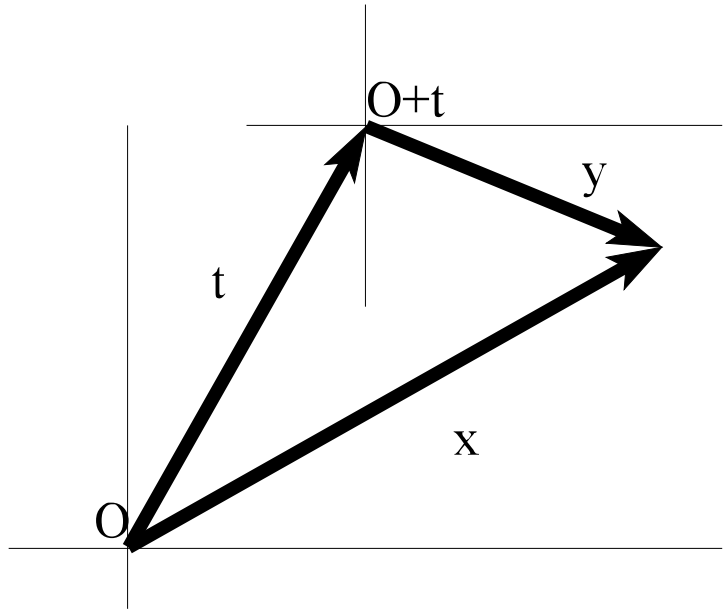
**Figure 2.2.3.1f:** Diagrams for Rhombohedral R 3D-magnetic space groups.

**Appendix 1.1: On characterizing a change in coordinate systems and the non-magnetic subgroup of index two of magnetic groups.**

When given a subgroup  $\mathbf{D}$  of index 2 of a group  $\mathbf{F}$  we want to give enough information to show

- 1) how to change the origin and
- 2) how to change the basis vectors of the coordinate system

$(\mathbf{O}; \mathbf{a}, \mathbf{b}, \mathbf{c})$  in which  $\mathbf{F}$  is defined, such in a second coordinate system  $(\mathbf{O}+\mathbf{t}; \mathbf{a}', \mathbf{b}', \mathbf{c}')$  the



translational subgroup of  $\mathbf{D}$  and the set of coset representatives of

$\mathbf{D}$  with respect to its translational subgroup will be identical with the translational subgroup and standard set of coset representatives of the group of type  $\mathbf{D}$  listed in the tables. Therefore:

- 1) We give, in the coordinate system of  $\mathbf{F}$ , the translation  $\mathbf{t}$  such that the new origin  $\mathbf{O}+\mathbf{t}$  is the origin of the coordinate system in which the subgroup  $\mathbf{D}$  will be of the form of the representative group  $\mathbf{D}$  listed in the tables.
- 2) We give the basis vectors  $\mathbf{a}', \mathbf{b}', \mathbf{c}'$  of a coordinate system  $(\mathbf{O}+\mathbf{t}; \mathbf{a}', \mathbf{b}', \mathbf{c}')$  in terms of the basis vectors of the coordinate system in which  $\mathbf{F}$  is defined, such that the subgroup  $\mathbf{D}$  in  $(\mathbf{O}+\mathbf{t}; \mathbf{a}', \mathbf{b}', \mathbf{c}')$  is identical with the representative group  $\mathbf{D}$ .

The lattices of both **F** and **D** can be either centered or primitive, consequently:

	Primitive	<b>F</b>	Centered
Primitive <b>D</b>	$\mathbf{a}', \mathbf{b}', \mathbf{c}'$ of primitive cell of <b>D</b> given in terms of $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of primitive cell of <b>F</b> .		$\mathbf{a}', \mathbf{b}', \mathbf{c}'$ of primitive cell of <b>D</b> given in terms of $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of the conventional unit cell of <b>F</b> .
Centered	$\mathbf{a}', \mathbf{b}', \mathbf{c}'$ of conventional unit cell of <b>D</b> given in terms of $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of primitive cell of <b>F</b> .		$\mathbf{a}', \mathbf{b}', \mathbf{c}'$ of conventional unit cell of <b>D</b> given in terms of $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of conventional unit cell of <b>F</b> .

To summarize: For the subgroup **D** we will give the following symbol:

$$\mathbf{D} ( \mathbf{t}; \mathbf{a}', \mathbf{b}', \mathbf{c}' )$$

where **D** is the group type symbol for the group **D**, and  $( \mathbf{t}; \mathbf{a}', \mathbf{b}', \mathbf{c}' )$  defines the new coordinate system  $(\mathbf{O}+\mathbf{t}; \mathbf{a}', \mathbf{b}', \mathbf{c}')$  in which the elements of **D** are identical with those of the representative group of the type **D**. Note that in the tables the symbol **t** is given by a trio of numbers  $n_a, n_b, n_c$  and the translation is defined by

$$\mathbf{t} = n_a \mathbf{a} + n_b \mathbf{b} + n_c \mathbf{c} ,$$

i.e. the translation **t** is defined in the coordinate system  $(\mathbf{O}; \mathbf{a}, \mathbf{b}, \mathbf{c})$  of the group **F**. The symbol  $(\mathbf{O}+\mathbf{t}; \mathbf{a}', \mathbf{b}', \mathbf{c}')$  is to be interpreted to define the new coordinate system by *first* moving the origin and *then* inserting the new set of basis vectors at the new origin  $\mathbf{O}+\mathbf{t}$ .

The coset representatives of the group **D** change when changing the origin of

the coordinate system. How they change is as follows:

Given a coordinate system  $(\mathbf{O}; \mathbf{a}, \mathbf{b}, \mathbf{c})$  and two points  $\mathbf{x}$  and  $\mathbf{x}'$  in this coordinate system. Given a second coordinate system  $(\mathbf{O}+\mathbf{t}; \mathbf{a}, \mathbf{b}, \mathbf{c})$  where the two points corresponding to  $\mathbf{x}$  and  $\mathbf{x}'$  are in the second coordinate system denoted respectively by  $\mathbf{y}$  and  $\mathbf{y}'$ .

$$\mathbf{x} = \mathbf{y} + \mathbf{t}$$

$$\mathbf{x}' = \mathbf{y}' + \mathbf{t}$$

If  $\mathbf{x}$  and  $\mathbf{x}'$  are related by  $(R|\tau)$ , in the first coordinate system, how is this relationship represented in the second coordinate system between  $\mathbf{y}$  and  $\mathbf{y}'$  ?

$$\mathbf{x}' = (R|\tau)\mathbf{x}$$

$$\mathbf{x}' = R\mathbf{x} + \tau$$

$$\mathbf{y}' + \mathbf{t} = R(\mathbf{y} + \mathbf{t}) + \tau$$

$$\mathbf{y}' = R\mathbf{y} + \tau + R\mathbf{t} - \mathbf{t}$$

$$\mathbf{y}' = (R|\tau + R\mathbf{t} - \mathbf{t})\mathbf{y}$$

$$\mathbf{y}' = (E|-\mathbf{t})(R|\tau)(E|\mathbf{t})\mathbf{y}$$

Consequently, when the origin is moved from  $\mathbf{O}$  to  $\mathbf{O}+\mathbf{t}$ , the coset  $(R|\tau)$  in the first coordinate system  $(\mathbf{O}; \mathbf{a}, \mathbf{b}, \mathbf{c})$  becomes, in the second coordinate system  $(\mathbf{O}+\mathbf{t}; \mathbf{a}, \mathbf{b}, \mathbf{c})$  the coset  $(E|-\mathbf{t})(R|\tau)(E|\mathbf{t}) = (R|\tau + R\mathbf{t} - \mathbf{t})$ , i.e. the rotational part remains the same, and  $R\mathbf{t}-\mathbf{t}$  is added to the translational part.

## **Table 1.1**

# **MAGNETIC SPACE GROUP SYMBOLS AND ELEMENTS**

**SUPERFAMILIES OF THREE DIMENSIONAL MAGNETIC SPACE GROUPS**

**HIERARCHAL MAGNETIC SPACE GROUP SUPERFAMILY INDEX**

**MAGNETIC SPACE GROUP INDEX**

**SUPERFAMILIES OF TWO-DIMENSIONAL MAGNETIC SPACE GROUPS**

**SUPERFAMILIES OF ONE-DIMENSIONAL MAGNETIC SPACE GROUPS**

**TRICLINIC SYSTEM**

1 P1

2 P $\bar{1}$ **MONOCLINIC SYSTEM**

3 P2

4 P2<sub>1</sub>

5 C2

6 Pm

7 Pc

8 Cm

9 Cc

10 P2/m

11 P2<sub>1</sub>/m

12 C2/m

13 P2/c

14 P2<sub>1</sub>/c

15 C2/c

**ORTHORHOMBIC SYSTEM**

16 P222

17 P222<sub>1</sub>18 P2<sub>1</sub>2<sub>1</sub>219 P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>20 C222<sub>1</sub>

21 C222

22 F222

23 I222

24 I2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>

25 Pmm2

26 Pmc2<sub>1</sub>

27 Pcc2

28 Pma2

29 Pca2<sub>1</sub>

30 Pnc2

31 Pmn2<sub>1</sub>

32 Pba2

33 Pna2<sub>1</sub>

34 Pnn2

35 Cmm2

36 Cmc2<sub>1</sub>

37 Ccc2

38 Amm2

39 Abm2

40 Ama2

41 Aba2

42 Fmm2

43 Fdd2

44 Imm2

45 Iba2

46 Ima2

47 Pmmm

48 Pnnn

49 Pccm

50 Pban

51 Pmma

52 Pnna

53 Pmna

54 Pcca

55 Pbam

56 Pccn

57 Pbcm

58 Pnnm

59 Pmmn

60 Pbcn

61 Pbca

62 Pnma

63 Cmcm

64 Cmca

65 Cmnm

66 Cccm

67 Cmma

68 Ccca

69 Fmmm

70 Fddd

71 Immm

72 Ibam

73 Ibca

74 Imma

**TETRAGONAL SYSTEM**

75 P4

76 P4<sub>1</sub>77 P4<sub>2</sub>78 P4<sub>3</sub>

79 I4

80 I4<sub>1</sub>81 P $\bar{4}$ 82 I $\bar{4}$ 

83 P4/m

84 P4<sub>2</sub>/m

85 P4/n

86 P4<sub>2</sub>/n

87 I4/m

88 I4<sub>1</sub>/a

89 P422

90 P4<sub>2</sub>291 P4<sub>1</sub>2292 P4<sub>1</sub>2<sub>1</sub>293 P4<sub>2</sub>2294 P4<sub>2</sub>2<sub>1</sub>295 P4<sub>3</sub>2296 P4<sub>3</sub>2<sub>1</sub>2

97 I422

98 I4<sub>1</sub>22

99	P4mm	125	P4/nbm	150	P321	175	P6/m
100	P4bm	126	P4/nnc	151	P3 <sub>1</sub> 12	176	P6 <sub>3</sub> /m
101	P4 <sub>2</sub> cm	127	P4/mbm	152	P3 <sub>1</sub> 21	177	P622
102	P4 <sub>2</sub> nm	128	P4/mnc	153	P3 <sub>2</sub> 12	178	P6 <sub>1</sub> 22
103	P4cc	129	P4/nmm	154	P3 <sub>2</sub> 21	179	P6 <sub>5</sub> 22
104	P4nc	130	P4/ncc	155	R32	180	P6 <sub>2</sub> 22
105	P4 <sub>2</sub> mc	131	P4 <sub>2</sub> /mmc	156	P3m1	181	P6 <sub>4</sub> 22
106	P4 <sub>2</sub> bc	132	P4 <sub>2</sub> /mcm	157	P31m	182	p6 <sub>3</sub> 22
107	I4mm	133	P4 <sub>2</sub> /nbc	158	P3c1	183	p6mm
108	I4cm	134	P4 <sub>2</sub> /nnm	159	P31c	184	P6cc
109	I4 <sub>1</sub> md	135	P4 <sub>2</sub> /mbc	160	R3m	185	P6 <sub>3</sub> cm
110	I4 <sub>1</sub> cd	136	P4 <sub>2</sub> /mnm	161	R3c	186	P6 <sub>3</sub> mc
111	P <del>4</del> 2m	137	P4 <sub>2</sub> /nmc	162	P <del>3</del> 1m	187	P <del>6</del> m2
112	P <del>4</del> 2c	138	P4 <sub>2</sub> /ncm	163	P <del>3</del> 1c	188	P <del>6</del> c2
113	P <del>4</del> 2 <sub>1</sub> m	139	I4/mmm	164	P <del>3</del> m1	189	P <del>6</del> 2m
114	P <del>4</del> 2 <sub>1</sub> c	140	I4/mcm	165	P <del>3</del> c1	190	P <del>6</del> 2c
115	P <del>4</del> m2	141	I4 <sub>1</sub> /amd	166	R <del>3</del> m	191	P6/mmm
116	P <del>4</del> c2	142	I4 <sub>1</sub> /acd	167	R <del>3</del> c	192	P6/mcc
117	P <del>4</del> b2		<b>TRIGONAL SYSTEM</b>		<b>HEXAGONAL SYSTEM</b>	193	P6 <sub>3</sub> /mcm
118	P <del>4</del> n2					194	P6 <sub>3</sub> /mmc
119	I <del>4</del> m2	143	P3	168	P6		<b>CUBIC SYSTEM</b>
120	I <del>4</del> c2	144	P3 <sub>1</sub>	169	P6 <sub>1</sub>	195	P23
121	I <del>4</del> 2m	145	P3 <sub>2</sub>	170	P6 <sub>5</sub>	196	F23
122	I <del>4</del> 2d	146	R3	171	P6 <sub>2</sub>	197	I23
123	P4/mmm	147	P <del>3</del>	172	P6 <sub>4</sub>	198	P2 <sub>1</sub> 3
124	P4/mcc	148	R <del>3</del>	173	P6 <sub>3</sub>	199	I2 <sub>1</sub> 3
		149	P312	174	P <del>3</del>		

200	$Pm\bar{2}$	226	$Fm\bar{2}c$
201	$Pn\bar{2}$	227	$Fd\bar{2}m$
202	$Fm\bar{2}$	228	$Fd\bar{2}c$
203	$Fd\bar{2}$	229	$Im\bar{2}m$
204	$Im\bar{2}$	230	$Ia\bar{2}d$
205	$Pa\bar{2}$		
206	$Ia\bar{2}$		
207	$P4_32$		
208	$P4_232$		
209	$F4_32$		
210	$F4_132$		
211	$I4_32$		
212	$P4_332$		
213	$P4_132$		
214	$I4_132$		
215	$P\bar{4}3m$		
216	$F\bar{4}3m$		
217	$I\bar{4}3m$		
218	$P\bar{4}3n$		
219	$F\bar{4}3c$		
220	$I\bar{4}3d$		
221	$Pm\bar{2}m$		
222	$Pn\bar{2}n$		
223	$Pm\bar{2}n$		
224	$Pn\bar{2}m$		
225	$Fm\bar{2}m$		



**TRICLINIC SYSTEM**

		5.5.23	$C_p 2$	9.3.47	$Cc'$
<b>1.1.1</b>	<b>P1</b>	5.6.24	$C_p 2'$	9.4.48	$C_p c$
1.2.2	$P_{11}'$				
1.3.3	$P_{2s} 1$	<b>6.1.25</b>	<b>Pm</b>	<b>10.1.49</b>	<b>P2/m</b>
		6.2.26	$Pm1'$	10.2.50	$P2/m1'$
<b>2.1.4</b>	<b>P&amp;</b>	6.3.27	$Pm'$	10.3.51	$P2'/m$
2.2.5	$P&1'$	6.4.28	$P_{2a} m$	10.4.52	$P2/m'$
2.3.6	$P&'$	6.5.29	$P_{2b} m$	10.5.53	$P2'/m'$
2.4.7	$P_{2s} \&$	6.6.30	$P_C m$	10.6.54	$P_{2a} 2/m$

**MONOCLINIC SYSTEM**

		6.7.31	$P_{2c} m'$	10.7.55	$P_{2b} 2/m$
				10.8.56	$P_C 2/m$
<b>3.1.8</b>	<b>P2</b>	<b>7.1.32</b>	<b>Pc</b>	10.9.57	$P_{2b} 2'/m$
3.2.9	$P21'$	7.2.33	$Pc1'$	10.10.58	$P_{2c} 2/m'$
3.3.10	$P2'$	7.3.34	$Pc'$		
3.4.11	$P_{2a} 2$	7.4.35	$P_{2a} c$	<b>11.1.59</b>	<b>P2<sub>1</sub>/m</b>
3.5.12	$P_{2b} 2$	7.5.36	$P_{2b} c$	11.2.60	$P2_1/m1'$
3.6.13	$P_C 2$	7.6.37	$P_C c$	11.3.61	$P2_1'/m$
3.7.14	$P_{2b} 2'$	<b>8.1.38</b>	<b>Cm</b>	11.4.62	$P2_1/m'$
		8.2.39	$Cm1'$	11.5.63	$P2_1'/m'$
<b>4.1.15</b>	<b>P2<sub>1</sub></b>	8.3.40	$Cm'$	11.6.64	$P_{2a} 2_1/m$
4.2.16	$P2_1 1'$	8.4.41	$C_{2c} m$	11.7.65	$P_{2c} 2_1/m'$
4.3.17	$P2_1'$	8.5.42	$C_p m$	<b>12.1.66</b>	<b>C2/m</b>
4.4.18	$P_{2a} 2_1$	8.6.43	$C_{2c} m'$	12.2.67	$C2/m1'$
<b>5.1.19</b>	<b>C2</b>	8.7.44	$C_p m'$	12.3.68	$C2'/m$
5.2.20	$C21'$			12.4.69	$C2/m'$
5.3.21	$C2'$	<b>9.1.45</b>	<b>Cc</b>	12.5.70	$C2'/m'$
5.4.22	$C_{2c} 2$	9.2.46	$Cc1'$	12.6.71	$C_{2c} 2/m$

12.7.72	$C_P 2/m$	15.5.96	$C2'/c'$	<b>19.1.119</b>	<b><math>P2_1 2_1 2_1</math></b>
12.8.73	$C_{2c} 2/m'$	15.6.97	$C_P 2/c$	19.2.120	$P2_1 2_1 2_1 1'$
12.9.74	$C_P 2'/m$	15.7.98	$C_P 2'/c$	19.3.121	$P2_1' 2_1' 2_1$
12.10.75	$C_P 2/m'$	<b>ORTHORHOMBIC SYSTEM</b>			
12.11.76	$C_P 2'/m'$	<b>16.1.99</b>	<b><math>P222</math></b>	<b>20.1.122</b>	<b><math>C222_1</math></b>
<b>13.1.77</b>	<b><math>P2/c</math></b>	16.2.100	$P2221'$	20.2.123	$C222_1 1'$
13.2.78	$P2/c1'$	16.3.101	$P2'2'2$	20.3.124	$C2'2'2_1$
13.3.79	$P2'/c$	16.4.102	$P_{2a} 222$	20.4.125	$C22'2'_1$
13.4.80	$P2/c'$	16.5.103	$P_C 222$	20.5.126	$C_P 222_1$
13.5.81	$P2'/c'$	16.6.104	$P_F 222$	20.6.127	$C_P 2'2'2_1$
13.6.82	$P_{2a} 2/c$	16.7.105	$P_{2c} 22'2'$	20.7.128	$C_P 22'2'_1$
13.7.83	$P_{2b} 2/c$	<b>17.1.106</b>	<b><math>P222_1</math></b>	<b>21.1.129</b>	<b><math>C222</math></b>
13.8.84	$P_C 2/c$	17.2.107	$P222_1 1'$	21.2.130	$C2221'$
13.9.85	$P_{2b} 2'/c$	17.3.108	$P2'2'2_1$	21.3.131	$C2'2'2$
<b>14.1.86</b>	<b><math>P2_1/c</math></b>	17.4.109	$P22'2'_1$	21.4.132	$C22'2'$
14.2.87	$P2_1/c1'$	17.5.110	$P_{2a} 222_1$	21.5.133	$C_{2c} 222$
14.3.88	$P2_1'/c$	17.6.111	$P_C 222_1$	21.6.134	$C_P 222$
14.4.89	$P2_1/c'$	17.7.112	$P_{2a} 2'2'2_1$	21.7.135	$C_1 222$
14.5.90	$P2_1'/c'$	<b>18.1.113</b>	<b><math>P2_1 2_1 2</math></b>	21.8.136	$C_{2c} 22'2'$
14.6.91	$P_{2a} 2_1/c$	18.2.114	$P2_1 2_1 21'$	21.9.137	$C_P 2'2'2$
<b>15.1.92</b>	<b><math>C2/c</math></b>	18.3.115	$P2_1' 2_1' 2$	21.10.138	$C_P 22'2'$
15.2.93	$C2/c1'$	18.4.116	$P2_1 2_1' 2'$	21.11.139	$C_1 2'22'$
15.3.94	$C2'/c$	18.5.117	$P_{2c} 2_1 2_1 2$	<b>22.1.140</b>	<b><math>F222</math></b>
15.4.95	$C2/c'$	18.6.118	$P_{2c} 2_1 2_1' 2'$	22.2.141	$F2221'$
				22.3.142	$F2'2'2$

22.4.143	$F_C 222$	25.13.167	$P_A m'm'2$	28.7.191	$P_{2c} ma2$
22.5.144	$F_C 22'2'$			28.8.192	$P_A ma2$
<b>23.1.145</b>	<b><math>I222</math></b>	<b>26.1.168</b>	<b><math>Pmc2_1</math></b>	28.9.193	$P_{2b} m'a2'$
23.2.146	$I2221'$	26.2.169	$Pmc2_11'$	28.10.194	$P_{2c} m'a2'$
23.3.147	$I2'2'2$	26.3.170	$Pm'c2_1'$	28.11.195	$P_{2c} ma'2'$
23.4.148	$I_p 222$	26.4.171	$Pmc'2_1'$	28.12.196	$P_{2c} m'a'2$
23.5.149	$I_p 2'2'2$	26.5.172	$Pm'c'2_1$	28.13.197	$P_A m'a'2$
<b>24.1.150</b>	<b><math>I2_12_12_1</math></b>	26.6.173	$P_{2a} mc2_1$		
24.2.151	$I2_12_12_11'$	26.7.174	$P_{2b} mc2_1$	<b>29.1.198</b>	<b><math>Pca2_1</math></b>
24.3.152	$I2_1'2_1'2_1$	26.8.175	$P_C mc2_1$	29.2.199	$Pca2_11'$
24.4.153	$I_p 2_12_12_1$	26.9.176	$P_{2a} mc'2_1'$	29.3.200	$Pc'a2_1'$
24.5.154	$I_p 2_1'2_1'2_1$	26.10.177	$P_{2b} m'c'2_1$	29.4.201	$Pca'2_1'$
<b>25.1.155</b>	<b><math>Pmm2</math></b>	<b>27.1.178</b>	<b><math>Pcc2</math></b>	29.5.202	$Pc'a'2_1$
25.2.156	$Pmm21'$	27.2.179	$Pcc21'$	29.6.203	$P_{2b} ca2_1$
25.3.157	$Pm'm2'$	27.3.180	$Pc'c2'$	29.7.204	$P_{2b} c'a'2_1$
25.4.158	$Pm'm'2$	27.4.181	$Pc'c'2$	<b>30.1.205</b>	<b><math>Pnc2</math></b>
25.5.159	$P_{2c} mm2$	27.5.182	$P_{2a} cc2$	30.2.206	$Pnc21'$
25.6.160	$P_{2a} mm2$	27.6.183	$P_C cc2$	30.3.207	$Pn'c2'$
25.7.161	$P_C mm2$	27.7.184	$P_{2b} c'c2'$	30.4.208	$Pnc'2'$
25.8.162	$P_A mm2$	<b>28.1.185</b>	<b><math>Pma2</math></b>	30.5.209	$Pn'c'2$
25.9.163	$P_F mm2$	28.2.186	$Pma21'$	30.6.210	$P_{2a} nc2$
25.10.164	$P_{2c} mm'2'$	28.3.187	$Pm'a2'$	30.7.211	$P_{2a} nc'2'$
25.11.165	$P_{2c} m'm'2$	28.4.188	$Pma'2'$	<b>31.1.212</b>	<b><math>Pmn2_1</math></b>
25.12.166	$P_{2a} m'm'2$	28.5.189	$Pm'a'2$	31.2.213	$Pmn2_11'$
		28.6.190	$P_{2b} ma2$	31.3.214	$Pm'n2_1'$

31.4.215	Pmn'2 <sub>1</sub> '	35.4.239	Cm'm'2	37.7.264	C <sub>p</sub> c'c'2
31.5.216	Pm'n'2 <sub>1</sub>	35.5.240	C <sub>2c</sub> mm2	<b>38.1.265</b>	<b>Amm2</b>
31.6.217	P <sub>2b</sub> mn2 <sub>1</sub>	35.6.241	C <sub>p</sub> mm2	38.2.266	Amm21'
31.7.218	P <sub>2b</sub> m'n'2 <sub>1</sub> '	35.7.242	C <sub>1</sub> mm2	38.3.267	Am'm'2'
<b>32.1.219</b>	<b>Pba2</b>	35.8.243	C <sub>2c</sub> m'm'2'	38.4.268	Amm'2'
32.2.220	Pba21'	35.9.244	C <sub>2c</sub> m'm'2	38.5.269	Am'm'2
32.3.221	Pb'a2'	35.10.245	C <sub>p</sub> m'm'2'	38.6.270	A <sub>2a</sub> mm2
32.4.222	Pb'a'2	35.11.246	C <sub>p</sub> m'm'2	38.7.271	A <sub>p</sub> mm2
32.5.223	P <sub>2c</sub> ba2	35.12.247	C <sub>1</sub> m'm'2'	38.8.272	A <sub>1</sub> mm2
32.6.224	P <sub>2c</sub> b'a2'	35.13.248	C <sub>1</sub> m'm'2	38.9.273	A <sub>2a</sub> mm'2'
32.7.225	P <sub>2c</sub> b'a'2	<b>36.1.249</b>	<b>Cmc2<sub>1</sub></b>	38.10.274	A <sub>p</sub> m'm'2'
<b>33.1.226</b>	<b>Pna2<sub>1</sub></b>	36.2.250	Cmc2 <sub>1</sub> 1'	38.11.275	A <sub>p</sub> mm'2'
33.2.227	Pna2 <sub>1</sub> 1'	36.3.251	Cm'c'2 <sub>1</sub> '	38.12.276	A <sub>p</sub> m'm'2
33.3.228	Pn'a2 <sub>1</sub> '	36.4.252	Cmc'2 <sub>1</sub> '	38.13.277	A <sub>1</sub> m'm'2
33.4.229	Pna'2 <sub>1</sub> '	36.5.253	Cm'c'2 <sub>1</sub>	<b>39.1.278</b>	<b>Abm2</b>
33.5.230	Pn'a'2 <sub>1</sub>	36.6.254	C <sub>p</sub> mc2 <sub>1</sub>	39.2.279	Abm21'
<b>34.1.231</b>	<b>Pnn2</b>	36.7.255	C <sub>p</sub> m'c'2 <sub>1</sub> '	39.3.280	Ab'm'2'
34.2.232	Pnn21'	36.8.256	C <sub>p</sub> mc'2 <sub>1</sub> '	39.4.281	Abm'2'
34.3.233	Pn'n'2'	36.9.257	C <sub>p</sub> m'c'2 <sub>1</sub>	39.5.282	Ab'm'2
34.4.234	Pn'n'2	<b>37.1.258</b>	<b>Ccc2</b>	39.6.283	A <sub>2a</sub> bm2
34.5.235	P <sub>F</sub> nn2	37.2.259	Ccc21'	39.7.284	A <sub>p</sub> bm2
<b>35.1.236</b>	<b>Cmm2</b>	37.3.260	Cc'c'2'	39.8.285	A <sub>1</sub> bm2
35.2.237	Cmm21'	37.4.261	Cc'c'2	39.9.286	A <sub>2a</sub> b'm'2
35.3.238	Cm'm'2'	37.5.262	C <sub>p</sub> cc2	39.10.287	A <sub>p</sub> b'm'2'
		37.6.263	C <sub>p</sub> c'c'2'	39.11.288	A <sub>p</sub> bm'2'

39.12.289	$A_p b'm^2$	42.5.313	$F_C mm^2$	45.7.337	$I_p b'a^2$
39.13.290	$A_l b'm^2$	42.6.314	$F_A mm^2$	<b>46.1.338</b>	<b>Ima2</b>
<b>40.1.291</b>	<b>Ama2</b>	42.7.315	$F_C mm^2'$	46.2.339	Ima21'
40.2.292	Ama21'	42.8.316	$F_C m'm^2$	46.3.340	Im'a2'
40.3.293	Am'a2'	42.9.317	$F_A m'm^2'$	46.4.341	Ima'2'
40.4.294	Ama'2'	42.10.318	$F_A mm^2'$	46.5.342	Im'a'2
40.5.295	Am'a'2	42.11.319	$F_A m'm^2$	46.6.343	$I_p ma^2$
40.6.296	$A_p ma^2$	<b>43.1.320</b>	<b>Fdd2</b>	46.7.344	$I_p m'a^2'$
40.7.297	$A_p m'a^2'$	43.2.321	Fdd21'	46.8.345	$I_p ma^2'$
40.8.298	$A_p ma^2'$	43.3.322	Fd'd2'	46.9.346	$I_p m'a^2$
40.9.299	$A_p m'a^2$	43.4.323	Fd'd'2	<b>47.1.347</b>	<b>Pmmm</b>
<b>41.1.300</b>	<b>Aba2</b>	<b>44.1.324</b>	<b>Imm2</b>	47.2.348	Pmmm1'
41.2.301	Aba21'	44.2.325	Imm21'	47.3.349	Pm'mm
41.3.302	Ab'a2'	44.3.326	Im'm2'	47.4.350	Pm'm'm
41.4.303	Aba'2'	44.4.327	Im'm'2	47.5.351	Pm'm'm'
41.5.304	Ab'a'2	44.5.328	$I_p mm^2$	47.6.352	$P_{2a} mmm$
41.6.305	$A_p ba^2$	44.6.329	$I_p mm^2'$	47.7.353	$P_C mmm$
41.7.306	$A_p b'a^2'$	44.7.330	$I_p m'm^2$	47.8.354	$P_F mmm$
41.8.307	$A_p ba^2'$	<b>45.1.331</b>	<b>Iba2</b>	47.9.355	$P_{2a} mmm'$
41.9.308	$A_p b'a^2$	45.2.332	Iba21'	47.10.356	$P_{2c} m'm'm$
<b>42.1.309</b>	<b>Fmm2</b>	45.3.333	Ib'a2'	47.11.357	$P_C mmm'$
42.2.310	Fmm21'	45.4.334	Ib'a'2	<b>48.1.358</b>	<b>Pnnn</b>
42.3.311	Fm'm2'	45.5.335	$I_p ba^2$	48.2.359	Pnnn1'
42.4.312	Fm'm'2	45.6.336	$I_p ba^2'$	48.3.360	Pn'nn

48.4.361	Pn'n'n	50.10.386	P <sub>2c</sub> b'a'n	52.6.411	Pn'n'a
48.5.362	Pn'n'n'			52.7.412	Pnn'a'
48.6.363	P <sub>F</sub> nnn	<b>51.1.387</b>	<b>Pmma</b>	52.8.413	Pn'na'
		51.2.388	Pmma1'	52.9.414	Pn'n'a'
<b>49.1.364</b>	<b>Pccm</b>	51.3.389	Pm'ma		
49.2.365	Pccm1'	51.4.390	Pmm'a	<b>53.1.415</b>	<b>Pmna</b>
49.3.366	Pc'cm	51.5.391	Pmma'	53.2.416	Pmna1'
49.4.367	Pccm'	51.6.392	Pm'm'a	53.3.417	Pm'na
49.5.368	Pc'c'm	51.7.393	Pmm'a'	53.4.418	Pmn'a
49.6.369	Pc'cm'	51.8.394	Pm'ma'	53.5.419	Pmna'
49.7.370	Pc'c'm'	51.9.395	Pm'm'a'	53.6.420	Pm'n'a
49.8.371	P <sub>2a</sub> ccm	51.10.396	P <sub>2b</sub> mma	53.7.421	Pmn'a'
49.9.372	P <sub>C</sub> ccm	51.11.397	P <sub>2c</sub> mma	53.8.422	Pm'na'
49.10.373	P <sub>2a</sub> ccm'	51.12.398	P <sub>A</sub> mma	53.9.423	Pm'n'a'
49.11.374	P <sub>2a</sub> c'c'm	51.13.399	P <sub>2b</sub> m'ma	53.10.424	P <sub>2b</sub> mna
49.12.375	P <sub>2a</sub> c'c'm'	51.14.400	P <sub>2b</sub> mma'	53.11.425	P <sub>2b</sub> m'na
49.13.376	P <sub>C</sub> ccm'	51.15.401	P <sub>2b</sub> m'ma'	53.12.426	P <sub>2b</sub> mna'
		51.16.402	P <sub>2c</sub> m'ma	53.13.427	P <sub>2b</sub> m'na'
<b>50.1.377</b>	<b>Pban</b>	51.17.403	P <sub>2c</sub> mm'a		
50.2.378	Pban1'	51.18.404	P <sub>2c</sub> m'm'a	<b>54.1.428</b>	<b>Pcca</b>
50.3.379	Pb'an	51.19.405	P <sub>A</sub> m'ma	54.2.429	Pcca1'
50.4.380	Pban'			54.3.430	Pc'ca
50.5.381	Pb'a'n	<b>52.1.406</b>	<b>Pnna</b>	54.4.431	Pcc'a
50.6.382	Pb'an'	52.2.407	Pnna1'	54.5.432	Pcca'
50.7.383	Pb'a'n'	52.3.408	Pn'na	54.6.433	Pc'c'a
50.8.384	P <sub>2c</sub> ban	52.4.409	Pnn'a	54.7.434	Pcc'a'
50.9.385	P <sub>2c</sub> b'an	52.5.410	Pnna'	54.8.435	Pc'ca'

54.9.436	Pc'c'a'	57.3.460	Pb'cm	59.8.485	P <sub>2c</sub> mmn
54.10.437	P <sub>2b</sub> cca	57.4.461	Pbc'm	59.9.486	P <sub>2c</sub> m'mn
54.11.438	P <sub>2b</sub> c'ca	57.5.462	Pbcm'	59.10.487	P <sub>2c</sub> m'm'n
54.12.439	P <sub>2b</sub> cca'	57.6.463	Pb'c'm	<b>60.1.488</b>	<b>Pbcn</b>
54.13.440	P <sub>2b</sub> c'ca'	57.7.464	Pbc'm'	60.2.489	Pbcn1'
<b>55.1.441</b>	<b>Pbam</b>	57.8.465	Pb'cm'	60.3.490	Pb'cn
55.2.442	Pbam1'	57.9.466	Pb'c'm'	60.4.491	Pbc'n
55.3.443	Pb'am	57.10.467	P <sub>2a</sub> bcm	60.5.492	Pbcn'
55.4.444	Pbam'	57.11.468	P <sub>2a</sub> bc'm	60.6.493	Pb'c'n
55.5.445	Pb'a'm	57.12.469	P <sub>2a</sub> bcm'	60.7.494	Pbc'n'
55.6.446	Pb'am'	57.13.470	P <sub>2a</sub> bc'm'	60.8.495	Pb'cn'
55.7.447	Pb'a'm'	<b>58.1.471</b>	<b>Pnnm</b>	60.9.496	Pb'c'n'
55.8.448	P <sub>2c</sub> bam	58.2.472	Pnnm1'	<b>61.1.497</b>	<b>Pbca</b>
55.9.449	P <sub>2c</sub> b'am	58.3.473	Pn'nm	61.2.498	Pbca1'
55.10.450	P <sub>2c</sub> b'a'm	58.4.474	Pnnm'	61.3.499	Pb'ca
<b>56.1.451</b>	<b>Pccn</b>	58.5.475	Pn'n'm	61.4.500	Pb'c'a
56.2.452	Pccn1'	58.6.476	Pnn'm'	61.5.501	Pb'c'a'
56.3.453	Pc'cn	58.7.477	Pn'n'm'	<b>62.1.502</b>	<b>Pnma</b>
56.4.454	Pccn'	<b>59.1.478</b>	<b>Pmmn</b>	62.2.503	Pnma1'
56.5.455	Pc'c'n	59.2.479	Pmmn1'	62.3.504	Pn'ma
56.6.456	Pc'cn'	59.3.480	Pm'mn	62.4.505	Pnm'a
56.7.457	Pc'c'n'	59.4.481	Pmmn'	62.5.506	Pnma'
<b>57.1.458</b>	<b>Pbcm</b>	59.5.482	Pm'm'n	62.6.507	Pn'm'a
57.2.459	Pbcm1'	59.6.483	Pmm'n'	62.7.508	Pnm'a'
		59.7.484	Pm'm'n'		

62.8.509	Pn'ma'	64.7.534	Cmc'a'	65.15.559	C <sub>p</sub> m'm'm
62.9.510	Pn'm'a'	64.8.535	Cm'ca'	65.16.560	C <sub>p</sub> mm'm'
<b>63.1.511</b>	<b>Cmcm</b>	64.9.536	Cm'c'a'	65.17.561	C <sub>p</sub> m'm'm'
63.2.512	Cmcm1'	64.10.537	C <sub>p</sub> mca	65.18.562	C <sub>1</sub> m'mm
63.3.513	Cm'cm	64.11.538	C <sub>p</sub> m'ca	65.19.563	C <sub>1</sub> m'm'm
63.4.514	Cmc'm	64.12.539	C <sub>p</sub> mc'a	<b>66.1.564</b>	<b>Cccm</b>
63.5.515	Cmcm'	64.13.540	C <sub>p</sub> mca'	66.2.565	Cccm1'
63.6.516	Cm'c'm	64.14.541	C <sub>p</sub> m'c'a	66.3.566	Cc'cm
63.7.517	Cmc'm'	64.15.542	C <sub>p</sub> mc'a'	66.4.567	Cccm'
63.8.518	Cm'cm'	64.16.543	C <sub>p</sub> m'ca'	66.5.568	Cc'c'm
63.9.519	Cm'c'm'	64.17.544	C <sub>p</sub> m'c'a'	66.6.569	Ccc'm'
63.10.520	C <sub>p</sub> mcm	<b>65.1.545</b>	<b>Cmmm</b>	66.7.570	Cc'c'm'
63.11.521	C <sub>p</sub> m'cm	65.2.546	Cmmm1'	66.8.571	C <sub>p</sub> ccm
63.12.522	C <sub>p</sub> mc'm	65.3.547	Cm'mm	66.9.572	C <sub>p</sub> c'cm
63.13.523	C <sub>p</sub> mcm'	65.4.548	Cmmm'	66.10.573	C <sub>p</sub> ccm'
63.14.524	C <sub>p</sub> m'c'm	65.5.549	Cm'm'm	66.11.574	C <sub>p</sub> c'c'm
63.15.525	C <sub>p</sub> mc'm'	65.6.550	Cmm'm'	66.12.575	C <sub>p</sub> cc'm'
63.16.526	C <sub>p</sub> m'cm'	65.7.551	Cm'm'm'	66.13.576	C <sub>p</sub> c'c'm'
63.17.527	C <sub>p</sub> m'c'm'	65.8.552	C <sub>2c</sub> mmm	<b>67.1.577</b>	<b>Cmma</b>
<b>64.1.528</b>	<b>Cmca</b>	65.9.553	C <sub>p</sub> mmm	67.2.578	Cmma1'
64.2.529	Cmca1'	65.10.554	C <sub>1</sub> mmm	67.3.579	Cm'ma
64.3.530	Cm'ca	65.11.555	C <sub>2c</sub> m'm'm	67.4.580	Cmma'
64.4.531	Cmc'a	65.12.556	C <sub>2c</sub> mm'm'	67.5.581	Cm'm'a
64.5.532	Cmca'	65.13.557	C <sub>p</sub> m'mm	67.6.582	Cmm'a'
64.6.533	Cm'c'a	65.14.558	C <sub>p</sub> mmm'	67.7.583	Cm'm'a'



67.8.584	$C_{2c}mma$	69.5.609	$Fm'm'm'$	72.4.633	$lbam'$
67.9.585	$C_p mma$	69.6.610	$F_C mmm$	72.5.634	$lb'a'm$
67.10.586	$C_1 mma$	69.7.611	$F_C m'mm$	72.6.635	$lba'm'$
67.11.587	$C_{2c} m'ma$	69.8.612	$F_C mmm'$	72.7.636	$lb'a'm'$
67.12.588	$C_{2c} m'm'a$	69.9.613	$F_C m'm'm$	72.8.637	$l_p bam$
67.13.589	$C_p m'ma$	69.10.614	$F_C mm'm'$	72.9.638	$l_p b'am$
67.14.590	$C_p mm'a$	69.11.615	$F_C m'm'm'$	72.10.639	$l_p bam'$
67.15.591	$C_p mma'$	<b>70.1.616</b>	<b>Fddd</b>	72.11.640	$l_p b'a'm$
67.16.592	$C_1 mm'a$	70.2.617	$Fddd1'$	72.12.641	$l_p b'am'$
67.17.593	$C_1 m'ma'$	70.3.618	$Fd'dd$	72.13.642	$l_p b'a'm'$
<b>68.1.594</b>	<b>Ccca</b>	70.4.619	$Fd'd'd$	<b>73.1.643</b>	<b>lbca</b>
68.2.595	$Ccca1'$	70.5.620	$Fd'd'd'$	73.2.644	$lbca1'$
68.3.596	$Cc'ca$	<b>71.1.621</b>	<b>Immm</b>	73.3.645	$lb'ca$
68.4.597	$Ccca'$	71.2.622	$Immm1'$	73.4.646	$lb'c'a$
68.5.598	$Cc'c'a$	71.3.623	$Im'mm$	73.5.647	$lb'c'a'$
68.6.599	$Ccc'a'$	71.4.624	$Im'm'm$	73.6.648	$l_p bca$
68.7.600	$Cc'c'a'$	71.5.625	$Im'm'm'$	73.7.649	$l_p b'ca$
68.8.601	$C_p cca$	71.6.626	$l_p mmm$	<b>74.1.650</b>	<b>Imma</b>
68.9.602	$C_p c'ca$	71.7.627	$l_p m'mm$	74.2.651	$Imma1'$
68.10.603	$C_p cca'$	71.8.628	$l_p m'm'm$	74.3.652	$Im'ma$
68.11.604	$C_p cc'a'$	71.9.629	$l_p m'm'm'$	74.4.653	$Imma'$
<b>69.1.605</b>	<b>Fmmm</b>	<b>72.1.630</b>	<b>lbam</b>	74.5.654	$Im'm'a$
69.2.606	$Fmmm1'$	72.2.631	$lbam1'$	74.6.655	$Imm'a'$
69.3.607	$Fm'mm$	72.3.632	$lb'am$	74.7.656	$Im'm'a'$
69.4.608	$Fm'm'm$			74.8.657	$l_p mma$

74.9.658	$I_p m'm'a$	78.2.680	$P4_3 1'$	83.2.704	$P4/m1'$
74.10.659	$I_p mm'a'$	78.3.681	$P4_3'$	83.3.705	$P4'/m$
74.11.660	$I_p m'ma'$	78.4.682	$P_p 4_3$	83.4.706	$P4/m'$
<b>TETRAGONAL SYSTEM</b>		<b>79.1.683</b>	<b><math>I4</math></b>	83.5.707	$P4'/m'$
<b>75.1.661</b>	<b><math>P4</math></b>	79.2.684	$I41'$	83.6.708	$P_{2c} 4/m$
75.2.662	$P41'$	79.3.685	$I4'$	83.7.709	$P_p 4/m$
75.3.663	$P4'$	79.4.686	$I_p 4$	83.8.710	$P_1 4/m$
75.4.664	$P_{2c} 4$	79.5.687	$I_p 4'$	83.9.711	$P_{2c} 4'/m$
75.5.665	$P_p 4$	<b>80.1.688</b>	<b><math>I4_1</math></b>	83.10.712	$P_p 4/m'$
75.6.666	$P_1 4$	80.2.689	$I4_1 1'$	<b>84.1.713</b>	<b><math>P4_2/m</math></b>
75.7.667	$P_{2c} 4'$	80.3.690	$I4_1'$	84.2.714	$P4_2/m1'$
<b>76.1.668</b>	<b><math>P4_1</math></b>	80.4.691	$I_p 4_1$	84.3.715	$P4_2'/m$
76.2.669	$P4_1 1'$	80.5.692	$I_p 4_1'$	84.4.716	$P4_2/m'$
76.3.670	$P4_1'$	<b>81.1.693</b>	<b><math>P\&amp;</math></b>	84.5.717	$P4_2'/m'$
76.4.671	$P_p 4_1$	81.2.694	$P\& 1'$	84.6.718	$P_p 4_2/m$
<b>77.1.672</b>	<b><math>P4_2</math></b>	81.3.695	$P\&'$	84.7.719	$P_p 4_2'/m'$
77.2.673	$P4_2 1'$	81.4.696	$P_{2c} \&$	<b>85.1.720</b>	<b><math>P4/n</math></b>
77.3.674	$P4_2'$	81.5.697	$P_p \&$	85.2.721	$P4/n1'$
77.4.675	$P_{2c} 4_2$	81.6.698	$P_1 \&$	85.3.722	$P4'/n$
77.5.676	$P_p 4_2$	<b>82.1.699</b>	<b><math>I\&amp;</math></b>	85.4.723	$P4/n'$
77.6.677	$P_1 4_2$	82.2.700	$I\& 1'$	85.5.724	$P4'/n'$
77.7.678	$P_{2c} 4_2'$	82.3.701	$I\&'$	85.6.725	$P_{2c} 4/n$
<b>78.1.679</b>	<b><math>P4_3</math></b>	82.4.702	$I_p \&$	85.7.726	$P_{2c} 4'/n$
		<b>83.1.703</b>	<b><math>P4/m</math></b>	<b>86.1.727</b>	<b><math>P4_2/n</math></b>

86.2.728	$P4_2/n1'$	89.6.752	$P_{2c}422$	<b>93.1.776</b>	<b><math>P4_222</math></b>
86.3.729	$P4_2'/n$	89.7.753	$P_P422$	93.2.777	$P4_2221'$
86.4.730	$P4_2/n'$	89.8.754	$P_1422$	93.3.778	$P4_2'22'$
86.5.731	$P4_2'/n'$	89.9.755	$P_{2c}4'22'$	93.4.779	$P4_22'2'$
86.6.732	$P_14_2/n$	89.10.756	$P_P4'22'$	93.5.780	$P4_2'2'2$
<b>87.1.733</b>	<b><math>I4/m</math></b>	<b>90.1.757</b>	<b><math>P42_12</math></b>	93.6.781	$P_{2c}4_222$
87.2.734	$I4/m1'$	90.2.758	$P42_121'$	93.7.782	$P_P4_222$
87.3.735	$I4'/m$	90.3.759	$P4'2_12'$	93.8.783	$P_14_222$
87.4.736	$I4/m'$	90.4.760	$P42_1'2'$	93.9.784	$P_{2c}4_2'22'$
87.5.737	$I4'/m'$	90.5.761	$P4'2_1'2$	93.10.785	$P_P4_2'22'$
87.6.738	$I_P4/m$	90.6.762	$P_{2c}42_12$	<b>94.1.786</b>	<b><math>P4_22_12</math></b>
87.7.739	$I_P4'/m$	90.7.763	$P_{2c}4'2_1'2$	94.2.787	$P4_22_121'$
87.8.740	$I_P4/m'$	<b>91.1.764</b>	<b><math>P4_122</math></b>	94.3.788	$P4_2'2_12'$
87.9.741	$I_P4'/m'$	91.2.765	$P4_1221'$	94.4.789	$P4_22_1'2'$
<b>88.1.742</b>	<b><math>I4_1/a</math></b>	91.3.766	$P4_1'22'$	94.5.790	$P4_2'2_1'2$
88.2.743	$I4_1/a1'$	91.4.767	$P4_12'2'$	94.6.791	$P_{2c}4_22_12$
88.3.744	$I4_1'/a$	91.5.768	$P4_1'2'2$	94.7.792	$P_{2c}4_2'2_1'2$
88.4.745	$I4_1/a'$	91.6.769	$P_P4_122$	<b>95.1.793</b>	<b><math>P4_322</math></b>
88.5.746	$I4_1'/a'$	91.7.770	$P_P4_1'22'$	95.2.794	$P4_3221'$
<b>89.1.747</b>	<b><math>P422</math></b>	<b>92.1.771</b>	<b><math>P4_12_12</math></b>	95.3.795	$P4_3'22'$
89.2.748	$P4221'$	92.2.772	$P4_12_121'$	95.4.796	$P4_32'2'$
89.3.749	$P4'22'$	92.3.773	$P4_1'2_12'$	95.5.797	$P4_3'2'2$
89.4.750	$P42'2'$	92.4.774	$P4_12_1'2'$	95.6.798	$P_P4_322$
89.5.751	$P4'2'2$	92.5.775	$P4_1'2_1'2$	95.7.799	$P_P4_3'22'$

<b>96.1.800</b>	<b>P<sub>4</sub><sub>3</sub>2<sub>1</sub>2</b>	99.2.824	P4mm1'	101.5.849	P4 <sub>2</sub> c'm'
96.2.801	P <sub>4</sub> <sub>3</sub> 2 <sub>1</sub> 21'	99.3.825	P4'm'm	101.6.850	P <sub>p</sub> 4 <sub>2</sub> cm
96.3.802	P <sub>4</sub> <sub>3</sub> '2 <sub>1</sub> 2'	99.4.826	P4'mmm'	101.7.851	P <sub>p</sub> 4 <sub>2</sub> 'cm'
96.4.803	P <sub>4</sub> <sub>3</sub> 2 <sub>1</sub> '2'	99.5.827	P4m'm'm'	<b>102.1.852</b>	<b>P<sub>4</sub><sub>2</sub>nm</b>
96.5.804	P <sub>4</sub> <sub>3</sub> '2 <sub>1</sub> '2	99.6.828	P <sub>2c</sub> 4mm	102.2.853	P4 <sub>2</sub> nm1'
<b>97.1.805</b>	<b>I422</b>	99.7.829	P <sub>p</sub> 4mm	102.3.854	P4 <sub>2</sub> 'n'm
97.2.806	I422	99.8.830	P <sub>1</sub> 4mm	102.4.855	P4 <sub>2</sub> 'nm'
97.3.807	I4'22'	99.9.831	P <sub>2c</sub> 4'm'm	102.5.856	P4 <sub>2</sub> n'm'
97.4.808	I42'2'	99.10.832	P <sub>2c</sub> 4'mm'	102.6.857	P <sub>1</sub> 4 <sub>2</sub> nm
97.5.809	I4'2'2	99.11.833	P <sub>2c</sub> 4m'm'm'	102.7.858	P <sub>1</sub> 4 <sub>2</sub> n'm'
97.6.810	I <sub>p</sub> 422	99.12.834	P <sub>p</sub> 4'mm'	<b>103.1.859</b>	<b>P4cc</b>
97.7.811	I <sub>p</sub> 4'22'	99.13.835	P <sub>1</sub> 4m'm'	103.2.860	P4cc1'
97.8.812	I <sub>p</sub> 42'2'	<b>100.1.836</b>	<b>P4bm</b>	103.3.861	P4'c'c
97.9.813	I <sub>p</sub> 4'2'2	100.2.837	P4bm1'	103.4.862	P4'cc'
<b>98.1.814</b>	<b>I4<sub>1</sub>22</b>	100.3.838	P4'b'm	103.5.863	P4c'c'
98.2.815	I4 <sub>1</sub> 221'	100.4.839	P4'bm'	103.6.864	P <sub>p</sub> 4cc
98.3.816	I4 <sub>1</sub> '22'	100.5.840	P4b'm'	103.7.865	P <sub>p</sub> 4'cc'
98.4.817	I4 <sub>1</sub> 2'2'	100.6.841	P <sub>2c</sub> 4bm	<b>104.1.866</b>	<b>P4nc</b>
98.5.818	I4 <sub>1</sub> '2'2	100.7.842	P <sub>2c</sub> 4'b'm	104.2.867	P4nc1'
98.6.819	I <sub>p</sub> 4 <sub>1</sub> 22	100.8.843	P <sub>2c</sub> 4'bm'	104.3.868	P4'n'c
98.7.820	I <sub>p</sub> 4 <sub>1</sub> '22'	100.9.844	P <sub>2c</sub> 4b'm'	104.4.869	P4'nc'
98.8.821	I <sub>p</sub> 4 <sub>1</sub> 2'2'	<b>101.1.845</b>	<b>P4<sub>2</sub>cm</b>	104.5.870	P4n'c'
98.9.822	I <sub>p</sub> 4 <sub>1</sub> '2'2	101.2.846	P4 <sub>2</sub> cm1'	<b>105.1.871</b>	<b>P4<sub>2</sub>mc</b>
<b>99.1.823</b>	<b>P4mm</b>	101.3.847	P4 <sub>2</sub> 'c'm	105.2.872	P4 <sub>2</sub> mc1'
		101.4.848	P4 <sub>2</sub> 'cm'		

105.3.873	$P4_2'm'c$	108.6.897	$I_p 4cm$	111.11.921	$P_1 \&'2m'$
105.4.874	$P4_2'mc'$	108.7.898	$I_p 4'c'm$	<b>112.1.922</b>	<b><math>P\&amp;2c</math></b>
105.5.875	$P4_2'm'c'$	108.8.899	$I_p 4'cm'$	112.2.923	$P\&2c1'$
105.6.876	$P_p 4_2 mc$	108.9.900	$I_p 4c'm'$	112.3.924	$P\&'2'c$
105.7.877	$P_p 4_2'mc'$	<b>109.1.901</b>	<b><math>I4_1md</math></b>	112.4.925	$P\&'2c'$
<b>106.1.878</b>	<b><math>P4_2 bc</math></b>	109.2.902	$I4_1md1'$	112.5.926	$P\&'2c'$
106.2.879	$P4_2 bc1'$	109.3.903	$I4_1'm'd$	112.6.927	$P_p \&2c$
106.3.880	$P4_2'b'c$	109.4.904	$I4_1'md'$	112.7.928	$P_p \&'2c'$
106.4.881	$P4_2'bc'$	109.5.905	$I4_1m'd'$	<b>113.1.929</b>	<b><math>P\&amp;2_1m</math></b>
106.5.882	$P4_2 b'c'$	<b>110.1.906</b>	<b><math>I4_1cd</math></b>	113.2.930	$P\&2_1m1'$
<b>107.1.883</b>	<b><math>I4mm</math></b>	110.2.907	$I4_1cd1'$	113.3.931	$P\&'2_1'm$
107.2.884	$I4mm1'$	110.3.908	$I4_1'c'd$	113.4.932	$P\&'2_1m'$
107.3.885	$I4'm'm$	110.4.909	$I4_1'cd'$	113.5.933	$P\&2_1'm'$
107.4.886	$I4'mm'$	110.5.910	$I4_1c'd'$	113.6.934	$P_{2c} \&2_1m$
107.5.887	$I4m'm'$	<b>111.1.911</b>	<b><math>P\&amp;2m</math></b>	113.7.935	$P_{2c} \&'2_1m'$
107.6.888	$I_p 4mm$	111.2.912	$P\&2m1'$	<b>114.1.936</b>	<b><math>P\&amp;2_1c</math></b>
107.7.889	$I_p 4'm'm$	111.3.913	$P\&'2'm$	114.2.937	$P\&2_1c1'$
107.8.890	$I_p 4'mm'$	111.4.914	$P\&'2m'$	114.3.938	$P\&'2_1'c$
107.9.891	$I_p 4m'm'$	111.5.915	$P\&'2'm'$	114.4.939	$P\&'2_1c'$
<b>108.1.892</b>	<b><math>I4cm</math></b>	111.6.916	$P_{2c} \&2m$	114.5.940	$P\&2_1'c'$
108.2.893	$I4cm1'$	111.7.917	$P_p \&2m$	<b>115.1.941</b>	<b><math>P\&amp;m2</math></b>
108.3.894	$I4'c'm$	111.8.918	$P_1 \&2m$	115.2.942	$P\&m21'$
108.4.895	$I4'cm'$	111.9.919	$P_{2c} \&'2'm'$	115.3.943	$P\&'m'2$
108.5.896	$I4c'm'$	111.10.920	$P_p \&'2m'$	115.4.944	$P\&'m'2'$

115.5.945	$P\bar{2}m'$	118.5.969	$P\bar{2}n'$	121.9.993	$I\bar{4}2m'$
115.6.946	$P_{2c}\bar{2}m2$	118.6.970	$P_1\bar{2}n2$	<b>122.1.994</b>	<b><math>I\bar{4}2d</math></b>
115.7.947	$P_p\bar{2}m2$	<b>119.1.971</b>	<b><math>I\bar{4}m2</math></b>	122.2.995	$I\bar{4}2d1'$
115.8.948	$P_1\bar{2}m2$	119.2.972	$I\bar{4}m21'$	122.3.996	$I\bar{4}'2'd$
115.9.949	$P_{2c}\bar{2}'m'2$	119.3.973	$I\bar{4}'m'2$	122.4.997	$I\bar{4}'2d'$
115.10.950	$P_p\bar{2}'m'2$	119.4.974	$I\bar{4}'m'2'$	122.5.998	$I\bar{4}'2d'$
<b>116.1.951</b>	<b><math>P\bar{4}c2</math></b>	119.5.975	$I\bar{4}m'2'$	<b>123.1.999</b>	<b><math>P4/mmm</math></b>
116.2.952	$P\bar{4}c21'$	119.6.976	$I_p\bar{4}m2$	123.2.1000	$P4/mmm1'$
116.3.953	$P\bar{4}'c'2$	119.7.977	$I_p\bar{4}'m'2$	123.3.1001	$P4/m'mm$
116.4.954	$P\bar{4}'c'2'$	<b>120.1.978</b>	<b><math>I\bar{4}c2</math></b>	123.4.1002	$P4'/mm'm$
116.5.955	$P\bar{4}c'2'$	120.2.979	$I\bar{4}c21'$	123.5.1003	$P4'/mmm'$
116.6.956	$P_p\bar{4}c2$	120.3.980	$I\bar{4}'c'2$	123.6.1004	$P4'/m'm'm$
116.7.957	$P_p\bar{4}'c'2'$	120.4.981	$I\bar{4}'c'2'$	123.7.1005	$P4/mm'm'$
<b>117.1.958</b>	<b><math>P\bar{4}b2</math></b>	120.5.982	$I\bar{4}c'2'$	123.8.1006	$P4'/m'mm'$
117.2.959	$P\bar{4}b21'$	120.6.983	$I_p\bar{4}c2$	123.9.1007	$P4/m'm'm'$
117.3.960	$P\bar{4}'b'2$	120.7.984	$I_p\bar{4}'c'2'$	123.10.1008	$P_{2c}4/mmm$
117.4.961	$P\bar{4}'b'2'$	<b>121.1.985</b>	<b><math>I\bar{4}2m</math></b>	123.11.1009	$P_p4/mmm$
117.5.962	$P\bar{4}b'2'$	121.2.986	$I\bar{4}2m1'$	123.12.1010	$P_14/mmm$
117.6.963	$P_{2c}\bar{4}b2$	121.3.987	$I\bar{4}'2'm$	123.13.1011	$P_{2c}4'/mm'm$
117.7.964	$P_{2c}\bar{4}'b'2$	121.4.988	$I\bar{4}'2m'$	123.14.1012	$P_{2c}4'/mmm'$
<b>118.1.965</b>	<b><math>P\bar{4}n2</math></b>	121.5.989	$I\bar{4}'2m'$	123.15.1013	$P_{2c}4/mm'm'$
118.2.966	$P\bar{4}n21'$	121.6.990	$I_p\bar{4}2m$	123.16.1014	$P_p4/m'mm$
118.3.967	$P\bar{4}'n'2$	121.7.991	$I_p\bar{4}'2'm$	123.17.1015	$P_p4'/mmm'$
118.4.968	$P\bar{4}'n'2'$	121.8.992	$I_p\bar{4}'2m'$	123.18.1016	$P_p4'/m'mm'$
				123.19.1017	$P_14/mm'm'$

	125.12.1042	$P_{2c}4'/nbm'$	<b>128.1.1066</b>	<b>P4/mnc</b>
<b>124.1.1018</b>		<b>P4/mcc</b>	128.2.1067	P4/mnc1'
124.2.1019		P4/mcc1'	128.3.1068	P4/m'nc
124.3.1020		P4/m'cc	128.4.1069	P4'/mn'c
124.4.1021		P4'/mc'c	128.5.1070	P4'/mnc'
124.5.1022		P4'/mcc'	128.6.1071	P4'/m'n'c
124.6.1023		P4'/m'c'c	128.7.1072	P4/mn'c'
124.7.1024		P4/mc'c'	128.8.1073	P4'/m'nc'
124.8.1025		P4'/m'cc'	128.9.1074	P4/m'n'c'
124.9.1026		P4/m'c'c'	<b>129.1.1075</b>	<b>P4/nmm</b>
124.10.1027		$P_p4/mcc$	129.2.1076	P4/nmm1'
124.11.1028		$P_p4/m'cc$	129.3.1077	P4/n'mm
124.12.1029		$P_p4'/mcc'$	129.4.1078	P4'/nm'm
124.13.1030		$P_p4'/m'cc'$	129.5.1079	P4'/nmm'
<b>125.1.1031</b>		<b>P4/nbm</b>	129.6.1080	P4'/n'm'm
125.2.1032		P4/nbm1'	129.7.1081	P4/nm'm'
125.3.1033		P4/n'bm	129.8.1082	P4'/n'mm'
125.4.1034		P4'/nb'm	129.9.1083	P4/n'm'm'
125.5.1035		P4'/nbm'	129.10.1084	$P_{2c}4/nmm$
125.6.1036		P4'/n'b'm	129.11.1085	$P_{2c}4'/nm'm$
125.7.1037		P4/nb'm'	129.12.1086	$P_{2c}4'/nmm'$
125.8.1038		P4'/n'bm'	129.13.1087	$P_{2c}4/nm'm'$
125.9.1039		P4/n'b'm'	<b>130.1.1088</b>	<b>P4/ncc</b>
125.10.1040		$P_{2c}4/nbm$	130.2.1089	P4/ncc1'
125.11.1041		$P_{2c}4'/nb'm$	130.3.1090	P4/n'cc
	125.13.1043	$P_{2c}4/nb'm'$		
<b>126.1.1044</b>		<b>P4/nnc</b>		
126.2.1045		P4/nnc1'		
126.3.1046		P4/n'nc		
126.4.1047		P4'/nn'c		
126.5.1048		P4'/nnc'		
126.6.1049		P4'/n'n'c		
126.7.1050		P4/nn'c'		
126.8.1051		P4'/n'nc'		
126.9.1052		P4/n'n'c'		
<b>127.1.1053</b>		<b>P4/mbm</b>		
127.2.1054		P4/mbm1'		
127.3.1055		P4/m'bm		
127.4.1056		P4'/mb'm		
127.5.1057		P4'/mbm'		
127.6.1058		P4'/m'b'm		
127.7.1059		P4/mb'm'		
127.8.1060		P4'/m'bm'		
127.9.1061		P4/m'b'm'		
127.10.1062		$P_{2c}4/mbm$		
127.11.1063		$P_{2c}4'/mb'm$		
127.12.1064		$P_{2c}4'/mbm'$		
127.13.1065		$P_{2c}4/mb'm'$		

130.4.1091	$P4'/nc'c$	132.7.1116	$P4_2/mc'm'$	134.10.1141	$P_14_2/nnm$
130.5.1092	$P4'/ncc'$	132.8.1117	$P4_2'/m'cm'$	134.11.1142	$P_14_2/nn'm'$
130.6.1093	$P4'/n'c'c$	132.9.1118	$P4_2/m'c'm'$	<b>135.1.1143</b>	<b><math>P4_2/mbc</math></b>
130.7.1094	$P4/nc'c'$	132.10.1119	$P_P4_2/mcm$	135.2.1144	$P4_2/mbc1'$
130.8.1095	$P4'/n'cc'$	132.11.1120	$P_P4_2/m'cm$	135.3.1145	$P4_2/m'bc$
130.9.1096	$P4/n'c'c'$	132.12.1121	$P_P4_2'/mcm'$	135.4.1146	$P4_2'/mb'c$
<b>131.1.1097</b>	<b><math>P4_2/mmc</math></b>	132.13.1122	$P_P4_2'/m'cm'$	135.5.1147	$P4_2'/mbc'$
131.2.1098	$P4_2/mmc1'$	<b>133.1.1123</b>	<b><math>P4_2/nbc</math></b>	135.6.1148	$P4_2'/m'b'c$
131.3.1099	$P4_2/m'mc$	133.2.1124	$P4_2/nbc1'$	135.7.1149	$P4_2/mb'c'$
131.4.1100	$P4_2'/mm'c$	133.3.1125	$P4_2/n'bc$	135.8.1150	$P4_2'/m'bc'$
131.5.1101	$P4_2'/mmc'$	133.4.1126	$P4_2'/nb'c$	135.9.1151	$P4_2/m'b'c'$
131.6.1102	$P4_2'/m'm'c$	133.5.1127	$P4_2'/nbc'$	<b>136.1.1152</b>	<b><math>P4_2/mnm</math></b>
131.7.1103	$P4_2/mm'c'$	133.6.1128	$P4_2'/n'b'c$	136.2.1153	$P4_2/mnm1'$
131.8.1104	$P4_2'/m'mc'$	133.7.1129	$P4_2/nb'c'$	136.3.1154	$P4_2/m'nm$
131.9.1105	$P4_2/m'm'c'$	133.8.1130	$P4_2'/n'bc'$	136.4.1155	$P4_2'/mn'm$
131.10.1106	$P_P4_2/mmc$	133.9.1131	$P4_2/n'b'c'$	136.5.1156	$P4_2'/mnm'$
131.11.1107	$P_P4_2/m'mc$	<b>134.1.1132</b>	<b><math>P4_2/nnm</math></b>	136.6.1157	$P4_2'/m'n'm$
131.12.1108	$P_P4_2/mm'c'$	134.2.1133	$P4_2/nnm1'$	136.7.1158	$P4_2/mn'm'$
131.13.1109	$P_P4_2'/m'mc'$	134.3.1134	$P4_2/n'nm$	136.8.1159	$P4_2'/m'nm'$
<b>132.1.1110</b>	<b><math>P4_2/mcm</math></b>	134.4.1135	$P4_2'/nn'm$	136.9.1160	$P4_2/m'n'm'$
132.2.1111	$P4_2/mcm1'$	134.5.1136	$P4_2'/nmm'$	<b>137.1.1161</b>	<b><math>P4_2/nmc</math></b>
132.3.1112	$P4_2/m'cm$	134.6.1137	$P4_2'/n'n'm$	137.2.1162	$P4_2/nmc1'$
132.4.1113	$P4_2'/mc'm$	134.7.1138	$P4_2/nn'm'$	137.3.1163	$P4_2/n'mc$
132.5.1114	$P4_2'/mcm'$	134.8.1139	$P4_2'/n'nm'$	137.4.1164	$P4_2'/nm'c$
132.6.1115	$P4_2'/m'c'm$	134.9.1140	$P4_2/n'n'm'$		



137.5.1165	$P4_2/nmc'$	139.12.1190	$I_p 4'/mm'm$	141.3.1215	$I4_1/a'md$
137.6.1166	$P4_2/n'm'c$	139.13.1191	$I_p 4'/mmm'$	141.4.1216	$I4_1'/am'd$
137.7.1167	$P4_2/nm'c'$	139.14.1192	$I_p 4'/m'm'm$	141.5.1217	$I4_1'/amd'$
137.8.1168	$P4_2/n'mc'$	139.15.1193	$I_p 4/mm'm'$	141.6.1218	$I4_1'/a'm'd$
137.9.1169	$P4_2/n'm'c'$	139.16.1194	$I_p 4'/m'mm'$	141.7.1219	$I4_1/am'd'$
<b>138.1.1170</b>	<b><math>P4_2/ncm</math></b>	139.17.1195	$I_p 4/m'm'm'$	141.8.1220	$I4_1'/a'md'$
138.2.1171	$P4_2/ncm1'$	<b>140.1.1196</b>	<b><math>I4/mcm</math></b>	141.9.1221	$I4_1/a'm'd'$
138.3.1172	$P4_2/n'cm$	140.2.1197	$I4/mcm1'$	<b>142.1.1222</b>	<b><math>I4_1/acd</math></b>
138.4.1173	$P4_2/nc'm$	140.3.1198	$I4/m'cm$	142.2.1223	$I4_1/acd1'$
138.5.1174	$P4_2'/ncm'$	140.4.1199	$I4'/mc'm$	142.3.1224	$I4_1/a'cd$
138.6.1175	$P4_2'/n'c'm$	140.5.1200	$I4'/mcm'$	142.4.1225	$I4_1'/ac'd$
138.7.1176	$P4_2/nc'm'$	140.6.1201	$I4'/m'c'm$	142.5.1226	$I4_1'/acd'$
138.8.1177	$P4_2'/n'cm'$	140.7.1202	$I4/mc'm'$	142.6.1227	$I4_1'/a'c'd$
138.9.1178	$P4_2/n'c'm'$	140.8.1203	$I4'/m'cm'$	142.7.1228	$I4_1/ac'd'$
<b>139.1.1179</b>	<b><math>I4/mmm</math></b>	140.9.1204	$I4/m'c'm'$	142.8.1229	$I4_1'/a'cd'$
139.2.1180	$I4/mmm1'$	140.10.1205	$I_p 4/mcm$	142.9.1230	$I4_1/a'c'd'$
139.3.1181	$I4/m'mm$	140.11.1206	$I_p 4/m'cm$		
139.4.1182	$I4'/mm'm$	140.12.1207	$I_p 4'/mc'm$		
139.5.1183	$I4'/mmm'$	140.13.1208	$I_p 4'/mcm'$	<b>143.1.1231</b>	<b><math>P3</math></b>
139.6.1184	$I4'/m'm'm$	140.14.1209	$I_p 4'/m'c'm$	143.2.1232	$P31'$
139.7.1185	$I4/mm'm'$	140.15.1210	$I_p 4/mc'm'$	143.3.1233	$P_{2c} 3$
139.8.1186	$I4'/m'mm'$	140.16.1211	$I_p 4'/m'cm'$	<b>144.1.1234</b>	<b><math>P3_1</math></b>
139.9.1187	$I4/m'm'm'$	140.17.1212	$I_p 4/m'c'm'$	144.2.1235	$P3_11'$
139.10.1188	$I_p 4/mmm$	<b>141.1.1213</b>	<b><math>I4_1/amd</math></b>	144.3.1236	$P_{2c} 3_2$
139.11.1189	$I_p 4/m'mm$	141.2.1214	$I4_1/amd1'$		

## TRIGONAL SYSTEM

<b>145.1.1237</b>	<b>P<sub>3</sub><sub>2</sub></b>				
145.2.1238	P <sub>3</sub> <sub>2</sub> 1'	151.2.1260	P <sub>3</sub> <sub>1</sub> 121'	156.5.1283	P <sub>2c</sub> 3m'1
145.3.1239	P <sub>2c</sub> 3 <sub>1</sub>	151.3.1261	P <sub>3</sub> <sub>1</sub> 12'	<b>157.1.1284</b>	<b>P<sub>31m</sub></b>
<b>146.1.1240</b>	<b>R<sub>3</sub></b>	151.4.1262	P <sub>2c</sub> 3 <sub>2</sub> 12	157.2.1285	P <sub>31m</sub> 1'
146.2.1241	R <sub>3</sub> 1'	<b>152.1.1263</b>	<b>P<sub>3</sub><sub>1</sub>21</b>	157.3.1286	P <sub>31m</sub> '
146.3.1242	R <sub>R</sub> 3	152.2.1264	P <sub>3</sub> <sub>1</sub> 211'	157.4.1287	P <sub>2c</sub> 31m
<b>147.1.1243</b>	<b>P<sub>3</sub><sub>2</sub></b>	152.3.1265	P <sub>3</sub> <sub>1</sub> 2'1	157.5.1288	P <sub>2c</sub> 31m'
147.2.1244	P <sub>3</sub> <sub>2</sub> 1'	152.4.1266	P <sub>2c</sub> 3 <sub>2</sub> 21	<b>158.1.1289</b>	<b>P<sub>3c</sub>1</b>
147.3.1245	P <sub>3</sub> <sub>2</sub> '	<b>153.1.1267</b>	<b>P<sub>3</sub><sub>2</sub>12</b>	158.2.1290	P <sub>3c</sub> 11'
147.4.1246	P <sub>2c</sub> <sub>3</sub>	153.2.1268	P <sub>3</sub> <sub>2</sub> 121'	158.3.1291	P <sub>3c</sub> '1
<b>148.1.1247</b>	<b>R<sub>3</sub><sub>2</sub></b>	153.3.1269	P <sub>3</sub> <sub>2</sub> 12'	<b>159.1.1292</b>	<b>P<sub>31c</sub></b>
148.2.1248	R <sub>3</sub> <sub>2</sub> 1'	153.4.1270	P <sub>2c</sub> 3 <sub>1</sub> 12	159.2.1293	P <sub>31c</sub> 1'
148.3.1249	R <sub>3</sub> <sub>2</sub> '	<b>154.1.1271</b>	<b>P<sub>3</sub><sub>2</sub>21</b>	159.3.1294	P <sub>31c</sub> '
148.4.1250	R <sub>R</sub> <sub>3</sub>	154.2.1272	P <sub>3</sub> <sub>2</sub> 211'	<b>160.1.1295</b>	<b>R<sub>3m</sub></b>
<b>149.1.1251</b>	<b>P<sub>312</sub></b>	154.3.1273	P <sub>3</sub> <sub>2</sub> 2'1	160.2.1296	R <sub>3m</sub> 1'
149.2.1252	P <sub>312</sub> 1'	154.4.1274	P <sub>2c</sub> 3 <sub>1</sub> 21	160.3.1297	R <sub>3m</sub> '
149.3.1253	P <sub>312</sub> '	<b>155.1.1275</b>	<b>R<sub>32</sub></b>	160.4.1298	R <sub>R</sub> 3m
149.4.1254	P <sub>2c</sub> 312	155.2.1276	R <sub>32</sub> 1'	160.5.1299	R <sub>R</sub> 3m'
<b>150.1.1255</b>	<b>P<sub>321</sub></b>	155.3.1277	R <sub>32</sub> '	<b>161.1.1300</b>	<b>R<sub>3c</sub></b>
150.2.1256	P <sub>321</sub> 1'	155.4.1278	R <sub>R</sub> 32	161.2.1301	R <sub>3c</sub> 1'
150.3.1257	P <sub>32</sub> '1	<b>156.1.1279</b>	<b>P<sub>3m</sub>1</b>	161.3.1302	R <sub>3c</sub> '
150.4.1258	P <sub>2c</sub> 321	156.2.1280	P <sub>3m</sub> 11'	<b>162.1.1303</b>	<b>P<sub>3</sub><sub>1</sub>m</b>
<b>151.1.1259</b>	<b>P<sub>3</sub><sub>1</sub>12</b>	156.3.1281	P <sub>3m</sub> '1	162.2.1304	P <sub>3</sub> <sub>1</sub> m1'
		156.4.1282	P <sub>2c</sub> 3m1		

162.3.1305	$P\bar{6}1m$	166.3.1329	$R\bar{6}m$	171.2.1351	$P6_21'$
162.4.1306	$P\bar{6}1m'$	166.4.1330	$R\bar{6}m'$	171.3.1352	$P6_2'$
162.5.1307	$P\bar{6}1m'$	166.5.1331	$R\bar{6}m'$	171.4.1353	$P_{2c}6_2$
162.6.1308	$P_{2c}\bar{6}1m$	166.6.1332	$R_R\bar{6}m$	171.5.1354	$P_{2c}6_2'$
162.7.1309	$P_{2c}\bar{6}1m'$	166.7.1333	$R_R\bar{6}m'$	<b>172.1.1355</b>	<b><math>P6_4</math></b>
<b>163.1.1310</b>	<b><math>P\bar{6}1c</math></b>	<b>167.1.1334</b>	<b><math>R\bar{6}c</math></b>	172.2.1356	$P6_4 1'$
163.2.1311	$P\bar{6}1c1'$	167.2.1335	$R\bar{6}c1'$	172.3.1357	$P6_4'$
163.3.1312	$P\bar{6}1c$	167.3.1336	$R\bar{6}'c$	172.4.1358	$P_{2c}6_4$
163.4.1313	$P\bar{6}'1c'$	167.4.1337	$R\bar{6}'c'$	172.5.1359	$P_{2c}6_4'$
163.5.1314	$P\bar{6}1c'$	167.5.1338	$R\bar{6}c'$	<b>173.1.1360</b>	<b><math>P6_3</math></b>
<b>164.1.1315</b>	<b><math>P\bar{6}m1</math></b>	<b>HEXAGONAL SYSTEM</b>		173.2.1361	$P6_31'$
164.2.1316	$P\bar{6}m11'$	<b>168.1.1339</b>	<b><math>P6</math></b>	173.3.1362	$P6_3'$
164.3.1317	$P\bar{6}'m1$	168.2.1340	$P61'$	<b>174.1.1363</b>	<b><math>P\bar{6}</math></b>
164.4.1318	$P\bar{6}'m'1$	168.3.1341	$P6'$	174.2.1364	$P\bar{6}1'$
164.5.1319	$P\bar{6}m'1$	168.4.1342	$P_{2c}6$	174.3.1365	$P\bar{6}'$
164.6.1320	$P_{2c}\bar{6}m1$	168.5.1343	$P_{2c}6'$	174.4.1366	$P_{2c}\bar{6}$
164.7.1321	$P_{2c}\bar{6}m'1$	<b>169.1.1344</b>	<b><math>P6_1</math></b>	<b>175.1.1367</b>	<b><math>P6/m</math></b>
<b>165.1.1322</b>	<b><math>P\bar{6}c1</math></b>	169.2.1345	$P6_11'$	175.2.1368	$P6/m1'$
165.2.1323	$P\bar{6}c11'$	169.3.1346	$P6_1'$	175.3.1369	$P6'/m$
165.3.1324	$P\bar{6}'c1$	<b>170.1.1347</b>	<b><math>P6_5</math></b>	175.4.1370	$P6/m'$
165.4.1325	$P\bar{6}'c'1$	170.2.1348	$P6_51'$	175.5.1371	$P6'/m'$
165.5.1326	$P\bar{6}c'1$	170.3.1349	$P6_5'$	175.6.1372	$P_{2c}6/m$
<b>166.1.1327</b>	<b><math>R\bar{6}m</math></b>	<b>171.1.1350</b>	<b><math>P6_2</math></b>	175.7.1373	$P_{2c}6'/m$
166.2.1328	$R\bar{6}m1'$				

<b>176.1.1374</b>	<b>P6<sub>3</sub>/m</b>	180.3.1398	P6 <sub>2</sub> '2'2	183.8.1422	P <sub>2c</sub> 6'mm'
176.2.1375	P6 <sub>3</sub> /m1'	180.4.1399	P6 <sub>2</sub> '22'	183.9.1423	P <sub>2c</sub> 6m'm'
176.3.1376	P6 <sub>3</sub> '/m	180.5.1400	P6 <sub>2</sub> '2'2'	<b>184.1.1424</b>	<b>P6cc</b>
176.4.1377	P6 <sub>3</sub> /m'	180.6.1401	P <sub>2c</sub> 6 <sub>2</sub> 22	184.2.1425	P6cc1'
176.5.1378	P6 <sub>3</sub> '/m'	180.7.1402	P <sub>2c</sub> 6 <sub>2</sub> '22'	184.3.1426	P6'c'c
<b>177.1.1379</b>	<b>P622</b>	<b>181.1.1403</b>	<b>P6<sub>4</sub> 22</b>	184.4.1427	P6'cc'
177.2.1380	P6221'	181.2.1404	P6 <sub>4</sub> 221'	184.5.1428	P6c'c'
177.3.1381	P6'2'2	181.3.1405	P6 <sub>4</sub> '2'2	<b>185.1.1429</b>	<b>P6<sub>3</sub> cm</b>
177.4.1382	P6'22'	181.4.1406	P6 <sub>4</sub> '22'	185.2.1430	P6 <sub>3</sub> cm1'
177.5.1383	P6'2'2'	181.5.1407	P6 <sub>4</sub> 2'2'	185.3.1431	P6 <sub>3</sub> 'c'm
177.6.1384	P <sub>2c</sub> 622	181.6.1408	P <sub>2c</sub> 6 <sub>4</sub> 22	185.4.1432	P6 <sub>3</sub> 'cm'
177.7.1385	P <sub>2c</sub> 6'22'	181.7.1409	P <sub>2c</sub> 6 <sub>4</sub> '2'2	185.5.1433	P6 <sub>3</sub> c'm'
<b>178.1.1386</b>	<b>P6<sub>1</sub> 22</b>	<b>182.1.1410</b>	<b>p6<sub>3</sub> 22</b>	<b>186.1.1434</b>	<b>P6<sub>3</sub> mc</b>
178.2.1387	P6 <sub>1</sub> 221'	182.2.1411	p6 <sub>3</sub> 221'	186.2.1435	P6 <sub>3</sub> mc1'
178.3.1388	P6 <sub>1</sub> '2'2	182.3.1412	p6 <sub>3</sub> '2'2	186.3.1436	P6 <sub>3</sub> 'm'c
178.4.1389	P6 <sub>1</sub> '22'	182.4.1413	p6 <sub>3</sub> '22'	186.4.1437	P6 <sub>3</sub> 'mc'
178.5.1390	P6 <sub>1</sub> 2'2'	182.5.1414	p6 <sub>3</sub> 2'2'	186.5.1438	P6 <sub>3</sub> m'c'
<b>179.1.1391</b>	<b>P6<sub>5</sub> 22</b>	<b>183.1.1415</b>	<b>p6mm</b>	<b>187.1.1439</b>	<b>P&amp;m2</b>
179.2.1392	P6 <sub>5</sub> 221'	183.2.1416	P6mm1'	187.2.1440	P&m21'
179.3.1393	P6 <sub>5</sub> '2'2	183.3.1417	P6'm'm	187.3.1441	P&'m'2
179.4.1394	P6 <sub>5</sub> '22'	183.4.1418	P6'mm'	187.4.1442	P&'m'2'
179.5.1395	P6 <sub>5</sub> 2'2'	183.5.1419	P6m'm'	187.5.1443	P&m'2'
<b>180.1.1396</b>	<b>P6<sub>2</sub> 22</b>	183.6.1420	P <sub>2c</sub> 6mm	187.6.1444	P <sub>2c</sub> &m2
180.2.1397	P6 <sub>2</sub> 221'	183.7.1421	P <sub>2c</sub> 6'm'm	187.7.1445	P <sub>2c</sub> &'m'2

**188.1.1446**  **$P\bar{6}c2$**

188.2.1447  $P\bar{6}c21'$

188.3.1448  $P\bar{6}'c'2$

188.4.1449  $P\bar{6}'c'2'$

188.5.1450  $P\bar{6}c'2'$

**189.1.1451**  **$P\bar{6}2m$**

189.2.1452  $P\bar{6}2m1'$

189.3.1453  $P\bar{6}'2'm$

189.4.1454  $P\bar{6}'2m'$

189.5.1455  $P\bar{6}2'm'$

189.6.1456  $P_{2c}\bar{6}2m$

189.7.1457  $P_{2c}\bar{6}'2m'$

**190.1.1458**  **$P\bar{6}2c$**

190.2.1459  $P\bar{6}2c1'$

190.3.1460  $P\bar{6}'2'c$

190.4.1461  $P\bar{6}'2c'$

190.5.1462  $P\bar{6}2'c'$

**191.1.1463**  **$P6/mmm$**

191.2.1464  $P6/mmm1'$

191.3.1465  $P6/m'mm$

191.4.1466  $P6'/mm'm$

191.5.1467  $P6'/mmm'$

191.6.1468  $P6'/m'm'm$

191.7.1469  $P6'/m'mm'$

191.8.1470  $P6/mm'm'$

191.9.1471  $P6/m'm'm'$

191.10.1472  $P_{2c}6/mmm$

191.11.1473  $P_{2c}6'/mm'm$

191.12.1474  $P_{2c}6'/mmm'$

191.13.1475  $P_{2c}6/mm'm'$

**192.1.1476**  **$P6/mcc$**

192.2.1477  $P6/mcc1'$

192.3.1478  $P6/m'cc$

192.4.1479  $P6'/mc'c$

192.5.1480  $P6'/mcc'$

192.6.1481  $P6'/m'c'c$

192.7.1482  $P6'/m'cc'$

192.8.1483  $P6/mc'c'$

192.9.1484  $P6/m'c'c'$

**193.1.1485**  **$P6_3/mcm$**

193.2.1486  $P6_3/mcm1'$

193.3.1487  $P6_3/m'cm$

193.4.1488  $P6_3'/mc'm$

193.5.1489  $P6_3'/mcm'$

193.6.1490  $P6_3'/m'c'm$

193.7.1491  $P6_3'/m'cm'$

193.8.1492  $P6_3/mc'm'$

193.9.1493  $P6_3/m'c'm'$

**194.1.1494**  **$P6_3/mmc$**

194.2.1495  $P6_3/mmc1'$

194.3.1496  $P6_3/m'mc$

194.4.1497  $P6_3'/mm'c$

194.5.1498  $P6_3'/mmc'$

194.6.1499  $P6_3'/m'm'c$

194.7.1500  $P6_3'/m'mc'$

194.8.1501  $P6_3/mm'c'$

194.9.1502  $P6_3/m'm'c'$

## CUBIC SYSTEM

**195.1.1503**  **$P23$**

195.2.1504  $P231'$

195.3.1505  $P_F23$

**196.1.1506**  **$F23$**

196.2.1507  $F231'$

**197.1.1508**  **$I23$**

197.2.1509  $I231'$

197.3.1510  $I_P23$

**198.1.1511**  **$P2_13$**

198.2.1512  $P2_131'$

**199.1.1513**  **$I2_13$**

199.2.1514  $I2_131'$

199.3.1515  $I_P2_13$

		<b>206.1.1538</b>	<b>la</b>		<b>212.1.1561</b>	<b>P<sub>4</sub>32</b>
<b>200.1.1516</b>	<b>Pm</b>	206.2.1539	la <sub>1</sub> '		212.2.1562	P <sub>4</sub> 321'
200.2.1517	Pm <sub>1</sub> '	206.3.1540	la' <sub>1</sub>		212.3.1563	P <sub>4</sub> 3'32'
200.3.1518	Pm' <sub>1</sub>	206.4.1541	I <sub>p</sub> a		<b>213.1.1564</b>	<b>P<sub>4</sub>32</b>
200.4.1519	P <sub>F</sub> m	<b>207.1.1542</b>	<b>P432</b>		213.2.1565	P <sub>4</sub> 321'
<b>201.1.1520</b>	<b>Pn</b>	207.2.1543	P4321'		213.3.1566	P <sub>4</sub> 1'32'
201.2.1521	Pn <sub>1</sub> '	207.3.1544	P4'32'		<b>214.1.1567</b>	<b>I<sub>4</sub>32</b>
201.3.1522	Pn' <sub>1</sub>	207.4.1545	P <sub>F</sub> 432		214.2.1568	I <sub>4</sub> 321'
201.4.1523	P <sub>F</sub> n	<b>208.1.1546</b>	<b>P<sub>4</sub>232</b>		214.3.1569	I <sub>4</sub> 1'32'
<b>202.1.1524</b>	<b>Fm</b>	208.2.1547	P <sub>4</sub> 2321'		214.4.1570	I <sub>p</sub> 4 <sub>1</sub> 32
202.2.1525	Fm <sub>1</sub> '	208.3.1548	P <sub>4</sub> 2'32'		214.5.1571	I <sub>p</sub> 4 <sub>1</sub> '32'
202.3.1526	Fm' <sub>1</sub>	208.4.1549	P <sub>F</sub> 4 <sub>2</sub> 32		<b>215.1.1572</b>	<b>P<sub>4</sub>3m</b>
<b>203.1.1527</b>	<b>Fd</b>	<b>209.1.1550</b>	<b>F432</b>		215.2.1573	P <sub>4</sub> 3m1'
203.2.1528	Fd <sub>1</sub> '	209.2.1551	F4321'		215.3.1574	P <sub>4</sub> 1'3m'
203.3.1529	Fd' <sub>1</sub>	209.3.1552	F4'32'		215.4.1575	P <sub>F</sub> 43m
<b>204.1.1530</b>	<b>Im</b>	<b>210.1.1553</b>	<b>F<sub>4</sub>32</b>		215.5.1576	P <sub>F</sub> 4'3m'
204.2.1531	Im <sub>1</sub> '	210.2.1554	F <sub>4</sub> 321'		<b>216.1.1577</b>	<b>F<sub>4</sub>3m</b>
204.3.1532	Im' <sub>1</sub>	210.3.1555	F <sub>4</sub> 1'32'		216.2.1578	F <sub>4</sub> 3m1'
204.4.1533	I <sub>p</sub> m	<b>211.1.1556</b>	<b>I432</b>		216.3.1579	F <sub>4</sub> 1'3m'
204.5.1534	I <sub>p</sub> m' <sub>1</sub>	211.2.1557	I4321'		<b>217.1.1580</b>	<b>I<sub>4</sub>3m</b>
<b>205.1.1535</b>	<b>Pa</b>	211.3.1558	I4'32'		217.2.1581	I <sub>4</sub> 3m1'
205.2.1536	Pa	211.4.1559	I <sub>p</sub> 432		217.3.1582	I <sub>4</sub> 1'3m'
205.3.1537	Pa' <sub>1</sub>	211.5.1560	I <sub>p</sub> 4'32'		217.4.1583	I <sub>p</sub> 43m

217.5.1584	$I_p \overline{4}3m'$	223.2.1607	$Pm\overline{3}n1'$	227.3.1630	$Fd'\overline{3}'m$
<b>218.1.1585</b>	<b><math>P\overline{4}3n</math></b>	223.3.1608	$Pm'\overline{3}'n$	227.4.1631	$Fd\overline{3}m'$
218.2.1586	$P\overline{4}3n1'$	223.4.1609	$Pm\overline{3}n'$	227.5.1632	$Fd'\overline{3}'m'$
218.3.1587	$P\overline{4}'3n'$	223.5.1610	$Pm'\overline{3}'n'$	<b>228.1633</b>	<b><math>Fd\overline{3}c</math></b>
<b>219.1.1588</b>	<b><math>F\overline{4}3c</math></b>	<b>224.1.1611</b>	<b><math>Pn\overline{3}m</math></b>	228.2.1634	$Fd\overline{3}c1'$
219.2.1589	$F\overline{4}3c1'$	224.2.1612	$Pn\overline{3}m1'$	228.3.1635	$Fd'\overline{3}'c$
219.3.1590	$F\overline{4}'3c'$	224.3.1613	$Pn'\overline{3}'m$	228.4.1636	$Fd\overline{3}c'$
<b>220.1.1591</b>	<b><math>I\overline{4}3d</math></b>	224.4.1614	$Pn\overline{3}m'$	228.5.1637	$Fd'\overline{3}'c'$
220.2.1592	$I\overline{4}3d1'$	224.5.1615	$Pn'\overline{3}'m'$	<b>229.1.1638</b>	<b><math>Im\overline{3}m</math></b>
220.3.1593	$I\overline{4}'3d'$	224.6.1616	$P_F n\overline{3}m$	229.2.1639	$Im\overline{3}m1'$
<b>221.1.1594</b>	<b><math>Pm\overline{3}m</math></b>	224.7.1617	$P_F n\overline{3}m'$	229.3.1640	$Im'\overline{3}'m$
221.2.1595	$Pm\overline{3}m1'$	<b>225.1.1618</b>	<b><math>Fm\overline{3}m</math></b>	229.4.1641	$Im\overline{3}m'$
221.3.1596	$Pm'\overline{3}'m$	225.2.1619	$Fm\overline{3}m1'$	229.5.1642	$Im'\overline{3}'m'$
221.4.1597	$Pm\overline{3}m'$	225.3.1620	$Fm'\overline{3}'m$	229.6.1643	$I_p m\overline{3}m$
221.5.1598	$Pm'\overline{3}'m'$	225.4.1621	$Fm\overline{3}m'$	229.7.1644	$I_p m'\overline{3}'m'$
221.6.1599	$P_F m\overline{3}m$	225.5.1622	$Fm'\overline{3}'m'$	229.8.1645	$I_p m\overline{3}m'$
221.7.1600	$P_F m\overline{3}m'$	<b>226.1.1623</b>	<b><math>Fm\overline{3}c</math></b>	229.9.1646	$I_p m'\overline{3}'m'$
<b>222.1.1601</b>	<b><math>Pn\overline{3}n</math></b>	226.2.1624	$Fm\overline{3}c1'$	<b>230.1.1647</b>	<b><math>la\overline{3}d</math></b>
222.2.1602	$Pn\overline{3}n1'$	226.3.1625	$Fm'\overline{3}'c$	230.2.1648	$la\overline{3}d1'$
222.3.1603	$Pn'\overline{3}'n$	226.4.1626	$Fm\overline{3}c'$	230.3.1649	$la'\overline{3}'d$
222.4.1604	$Pn\overline{3}n'$	226.5.1627	$Fm'\overline{3}'c'$	230.4.1650	$la\overline{3}d'$
222.5.1605	$Pn'\overline{3}'n'$	<b>227.1.1628</b>	<b><math>Fd\overline{3}m</math></b>	230.5.1651	$la'\overline{3}'d'$
<b>223.1.1606</b>	<b><math>Pm\overline{3}n</math></b>	227.2.1629	$Fd\overline{3}m1'$		

## TRICLINIC SYSTEM

1.1.1	<b>P1</b>			<b>(1*0,0,0)</b>	
1.2.2	P11'				
1.3.3	P <sub>2s</sub> 1	P1	(0,0,0;a,b,2c)	(1*0,0,0)	
<b>2.1.4</b>	<b>P&amp;</b>			<b>(1*0,0,0)</b>	<b>(&amp;*0,0,0)</b>
2.2.5	P&1'				
2.3.6	P&'	P1	(0,0,0;a,b,c)	(1*0,0,0)	(&*0,0,0)'
2.4.7	P <sub>2s</sub> &	P&	(0,0,0;a,b,2c)	(1*0,0,0)	(&*0,0,0)

## MONOCLINIC SYSTEM

<b>3.1.8</b>	<b>P2</b>			<b>(1*0,0,0)</b>	<b>(2<sub>y</sub>*0,0,0)</b>
3.2.9	P21'				
3.3.10	P2'	P1	(0,0,0;a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,0)'
3.4.11	P <sub>2a</sub> 2	P2	(0,0,0;2a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,0)
3.5.12	P <sub>2b</sub> 2	P2	(0,0,0;a,2b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,0)
3.6.13	P <sub>C</sub> 2	C2	(0,0,0;2a,2b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,0)
3.7.14	P <sub>2b</sub> 2'	P2 <sub>1</sub>	(0,0,0;a,2b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,1,0)



<b>4.1.15</b>	<b>P2<sub>1</sub></b>			<b>(1*0,0,0)</b>	<b>(2<sub>y</sub>*0,1/2,0)</b>
4.2.16	P2 <sub>1</sub> 1'				
4.3.17	P2 <sub>1</sub> '	P1	(0,0,0;a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,1/2,0)'
4.4.18	P <sub>2a</sub> 2 <sub>1</sub>	P2 <sub>1</sub>	(0,0,0;2a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,1/2,0)
<b>5.1.19</b>	<b>C2</b>			<b>(1*0,0,0)</b>	<b>(2<sub>y</sub>*0,0,0)</b>
5.2.20	C21'				
5.3.21	C2'	P1	(0,0,0;b,{a+b}/2,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,0)'
5.4.22	C <sub>2c</sub> 2	C2	(0,0,0;a,b,2c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,0)
5.5.23	C <sub>p</sub> 2	P2	(0,0,0;a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,0)
5.6.24	C <sub>p</sub> 2'	P2 <sub>1</sub>	(1/4,0,0;a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *1/2,1/2,0)
<b>6.1.25</b>	<b>Pm</b>			<b>(1*0,0,0)</b>	<b>(m<sub>y</sub>*0,0,0)</b>
6.2.26	Pm1'				
6.3.27	Pm'	P1	(0,0,0;a,b,c)	(1*0,0,0)	(m <sub>y</sub> *0,0,0)'
6.4.28	P <sub>2a</sub> m	Pm	(0,0,0;2a,b,c)	(1*0,0,0)	(m <sub>y</sub> *0,0,0)
6.5.29	P <sub>2b</sub> m	Pm	(0,0,0;a,2b,c)	(1*0,0,0)	(m <sub>y</sub> *0,0,0)

6.6.30	$P_C m$	Cm	(0,0,0;2a,2b,c)	(1*0,0,0)	( $m_y$ *0,0,0)
6.7.31	$P_{2c} m'$	Pc	(0,0,0;a,b,2c)	(1*0,0,0)	( $m_y$ *0,0,1)
<b>7.1.32</b>	<b>Pc</b>			<b>(1*0,0,0)</b>	<b>(<math>m_y</math>*0,0,1/2)</b>
7.2.33	$Pc1'$				
7.3.34	$Pc'$	P1	(0,0,0;a,b,c)	(1*0,0,0)	( $m_y$ *0,0,1/2)'
7.4.35	$P_{2a} c$	Pc	(0,0,0;2a,b,c)	(1*0,0,0)	( $m_y$ *0,0,1/2)
7.5.36	$P_{2b} c$	Pc	(0,0,0;a,2b,c)	(1*0,0,0)	( $m_y$ *0,0,1/2)
7.6.37	$P_C c$	Cc	(0,0,0;2a,2b,c)	(1*0,0,0)	( $m_y$ *0,0,1/2)
<b>8.1.38</b>	<b>Cm</b>			<b>(1*0,0,0)</b>	<b>(<math>m_y</math>*0,0,0)</b>
8.2.39	$Cm1'$				
8.3.40	$Cm'$	P1	(0,0,0;b,{a+b}/2,c)	(1*0,0,0)	( $m_y$ *0,0,0)'
8.4.41	$C_{2c} m$	Cm	(0,0,0;a,b,2c)	(1*0,0,0)	( $m_y$ *0,0,0)
8.5.42	$C_P m$	Pm	(0,0,0;a,b,c)	(1*0,0,0)	( $m_y$ *0,0,0)
8.6.43	$C_{2c} m'$	Cc	(0,0,0;a,b,2c)	(1*0,0,0)	( $m_y$ *0,0,1)
8.7.44	$C_P m'$	Pc	(0,1/4,0;c,&a)	(1*0,0,0)	( $m_y$ *1/2,1/2,0)

<b>9.1.45</b>	<b>Cc</b>			<b>(1*0,0,0)</b>	<b>(m<sub>y</sub>*0,0,1/2)</b>		
9.2.46	Cc1'						
9.3.47	Cc'	P1	(0,0,0;b,{a+b}/2,c)	(1*0,0,0)	(m <sub>y</sub> *0,0,1/2)'		
9.4.48	C <sub>p</sub> c	Pc	(0,0,0;a,b,c)	(1*0,0,0)	(m <sub>y</sub> *0,0,1/2)		
<b>10.1.49</b>	<b>P2/m</b>			<b>(1*0,0,0)</b>	<b>(2<sub>y</sub>*0,0,0)</b>	<b>(&amp;*0,0,0)</b>	<b>(m<sub>y</sub>*0,0,0)</b>
10.2.50	P2/m1'						
10.3.51	P2'/m	Pm	(0,0,0;a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,0)'	(&*0,0,0)'	(m <sub>y</sub> *0,0,0)
10.4.52	P2/m'	P2	(0,0,0;a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,0)	(&*0,0,0)'	(m <sub>y</sub> *0,0,0)'
10.5.53	P2'/m'	P&	(0,0,0;a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,0)'	(&*0,0,0)	(m <sub>y</sub> *0,0,0)'
10.6.54	P <sub>2a</sub> 2/m	P2/m	(0,0,0;2a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,0)	(&*0,0,0)	(m <sub>y</sub> *0,0,0)
10.7.55	P <sub>2b</sub> 2/m	P2/m	(0,0,0;a,2b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,0)	(&*0,0,0)	(m <sub>y</sub> *0,0,0)
10.8.56	P <sub>c</sub> 2/m	C2/m	(0,0,0;2a,2b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,0)	(&*0,0,0)	(m <sub>y</sub> *0,0,0)
10.9.57	P <sub>2b</sub> 2'/m	P2 <sub>1</sub> /m	(0,1/2,0;a,2b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,1,0)	(&*0,1,0)	(m <sub>y</sub> *0,0,0)
10.10.58	P <sub>2c</sub> 2/m'	P2/c	(0,0,1/2;a,b,2c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,0)	(&*0,0,1)	(m <sub>y</sub> *0,0,1)
<b>11.1.59</b>	<b>P2<sub>1</sub>/m</b>			<b>(1*0,0,0)</b>	<b>(2<sub>y</sub>*0,1/2,0)</b>	<b>(&amp;*0,0,0)</b>	<b>(m<sub>y</sub>*0,1/2,0)</b>

11.2.60	$P2_1/m1'$						
11.3.61	$P2_1'/m$	$Pm$	$(0,1/4,0;a,b,c)$	$(1^*0,0,0)$	$(2_y^*0,1/2,0)'$	$(\&^*0,0,0)'$	$(m_y^*0,1/2,0)$
11.4.62	$P2_1/m'$	$P2_1$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(2_y^*0,1/2,0)$	$(\&^*0,0,0)'$	$(m_y^*0,1/2,0)'$
11.5.63	$P2_1'/m'$	$P\&$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(2_y^*0,1/2,0)'$	$(\&^*0,0,0)$	$(m_y^*0,1/2,0)'$
11.6.64	$P_{2a}2_1/m$	$P2_1/m$	$(0,0,0;2a,b,c)$	$(1^*0,0,0)$	$(2_y^*0,1/2,0)$	$(\&^*0,0,0)$	$(m_y^*0,1/2,0)$
11.7.65	$P_{2c}2_1/m'$	$P2_1/c$	$(0,0,1/2;a,b,2c)$	$(1^*0,0,0)$	$(2_y^*0,1/2,0)$	$(\&^*0,0,1)$	$(m_y^*0,1/2,1)$
<b>12.1.66</b>	<b><math>C2/m</math></b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(2_y^*0,0,0)</math></b>	<b><math>(\&amp;^*0,0,0)</math></b>	<b><math>(m_y^*0,0,0)</math></b>
12.2.67	$C2/m1'$						
12.3.68	$C2'/m$	$Cm$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(2_y^*0,0,0)'$	$(\&^*0,0,0)'$	$(m_y^*0,0,0)$
12.4.69	$C2/m'$	$C2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(2_y^*0,0,0)$	$(\&^*0,0,0)'$	$(m_y^*0,0,0)'$
12.5.70	$C2'/m'$	$P\&$	$(0,0,0;b,\{a+b\}/2,c)$	$(1^*0,0,0)$	$(2_y^*0,0,0)'$	$(\&^*0,0,0)$	$(m_y^*0,0,0)'$
12.6.71	$C_{2c}2/m$	$C2/m$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$	$(2_y^*0,0,0)$	$(\&^*0,0,0)$	$(m_y^*0,0,0)$
12.7.72	$C_p2/m$	$P2/m$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(2_y^*0,0,0)$	$(\&^*0,0,0)$	$(m_y^*0,0,0)$
12.8.73	$C_{2c}2/m'$	$C2/c$	$(0,0,1/2;a,b,2c)$	$(1^*0,0,0)$	$(2_y^*0,0,0)$	$(\&^*0,0,1)$	$(m_y^*0,0,1)$
12.9.74	$C_p2'/m$	$P2_1/m$	$(1/4,1/4,0;a,b,c)$	$(1^*0,0,0)$	$(2_y^*1/2,1/2,0)$	$(\&^*1/2,1/2,0)$	$(m_y^*0,0,0)$
12.10.75	$C_p2/m'$	$P2/c$	$(1/4,1/4,0;c,\&,a)$	$(1^*0,0,0)$	$(2_y^*0,0,0)$	$(\&^*1/2,1/2,0)$	$(m_y^*1/2,1/2,0)$
12.11.76	$C_p2'/m'$	$P2_1/c$	$(0,0,0;c,\&,a)$	$(1^*0,0,0)$	$(2_y^*1/2,1/2,0)$	$(\&^*0,0,0)$	$(m_y^*1/2,1/2,0)$

<b>13.1.77</b>	<b>P2/c</b>			<b>(1*0,0,0)</b>	<b>(2<sub>y</sub>*0,0,1/2)</b>	<b>(&amp;*0,0,0)</b>	<b>(m<sub>y</sub>*0,0,1/2)</b>
13.2.78	P2/c1'						
13.3.79	P2'/c	Pc	(0,0,0;a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,1/2)'	(&*0,0,0)'	(m <sub>y</sub> *0,0,1/2)
13.4.80	P2/c'	P2	(0,0,1/4;a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,1/2)	(&*0,0,0)'	(m <sub>y</sub> *0,0,1/2)'
13.5.81	P2'/c'	P&	(0,0,0;a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,1/2)'	(&*0,0,0)	(m <sub>y</sub> *0,0,1/2)'
13.6.82	P <sub>2a</sub> 2/c	P2/c	(0,0,0;2a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,1/2)	(&*0,0,0)	(m <sub>y</sub> *0,0,1/2)
13.7.83	P <sub>2b</sub> 2/c	P2/c	(0,0,0;a,2b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,1/2)	(&*0,0,0)	(m <sub>y</sub> *0,0,1/2)
13.8.84	P <sub>c</sub> 2/c	C2/c	(0,0,0;2a,2b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,1/2)	(&*0,0,0)	(m <sub>y</sub> *0,0,1/2)
13.9.85	P <sub>2b</sub> 2'/c	P2 <sub>1</sub> /c	(0,1/2,0;a,2b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,1,1/2)	(&*0,1,0)	(m <sub>y</sub> *0,0,1/2)
<b>14.1.86</b>	<b>P2<sub>1</sub>/c</b>			<b>(1*0,0,0)</b>	<b>(2<sub>y</sub>*0,1/2,1/2)</b>	<b>(&amp;*0,0,0)</b>	<b>(m<sub>y</sub>*0,1/2,1/2)</b>
14.2.87	P2 <sub>1</sub> /c1'						
14.3.88	P2 <sub>1</sub> '/c	Pc	(0,1/4,0;a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,1/2,1/2)'	(&*0,0,0)'	(m <sub>y</sub> *0,1/2,1/2)
14.4.89	P2 <sub>1</sub> /c'	P2 <sub>1</sub>	(0,0,1/4;a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,1/2,1/2)	(&*0,0,0)'	(m <sub>y</sub> *0,1/2,1/2)'
14.5.90	P2 <sub>1</sub> '/c'	P&	(0,0,0;a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,1/2,1/2)'	(&*0,0,0)	(m <sub>y</sub> *0,1/2,1/2)'
14.6.91	P <sub>2a</sub> 2 <sub>1</sub> /c	P2 <sub>1</sub> /c	(0,0,0;2a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,1/2,1/2)	(&*0,0,0)	(m <sub>y</sub> *0,1/2,1/2)

15.1.92	<b>C2/c</b>			<b>(1*0,0,0)</b>	<b>(2<sub>y</sub>*0,0,1/2)</b>	<b>(&amp;*0,0,0)</b>	<b>(m<sub>y</sub>*0,0,1/2)</b>
15.2.93	C2/c1'						
15.3.94	C2'/c	Cc	(0,0,0;a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,1/2)'	(&*0,0,0)'	(m <sub>y</sub> *0,0,1/2)
15.4.95	C2/c'	C2	(0,0,1/4;a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,1/2)	(&*0,0,0)'	(m <sub>y</sub> *0,0,1/2)'
15.5.96	C2'/c'	P&	(0,0,0;b,{a+b}/2,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,1/2)'	(&*0,0,0)	(m <sub>y</sub> *0,0,1/2)'
15.6.97	C <sub>P</sub> 2/c	P2/c	(0,0,0;a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *0,0,1/2)	(&*0,0,0)	(m <sub>y</sub> *0,0,1/2)
15.7.98	C <sub>P</sub> 2'/c	P2 <sub>1</sub> /c	(1/4,1/4,0;a,b,c)	(1*0,0,0)	(2 <sub>y</sub> *1/2,1/2,1/2)	(&*1/2,1/2,0)	(m <sub>y</sub> *0,0,1/2)

## ORTHORHOMBIC SYSTEM

16.1.99	<b>P222</b>			<b>(1*0,0,0)</b>	<b>(2<sub>x</sub>*0,0,0)</b>	<b>(2<sub>y</sub>*0,0,0)</b>	<b>(2<sub>z</sub>*0,0,0)</b>
16.2.100	P2221'						
16.3.101	P2'2'2	P2	(0,0,0;b,c,a)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)'	(2 <sub>y</sub> *0,0,0)'	(2 <sub>z</sub> *0,0,0)
16.4.102	P <sub>2a</sub> 222	P222	(0,0,0;2a,b,c)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)
16.5.103	P <sub>C</sub> 222	C222	(0,0,0;2a,2b,c)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)
16.6.104	P <sub>F</sub> 222	F222	(0,0,0;2a,2b,2c)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)
16.7.105	P <sub>2c</sub> 22'2'	P222 <sub>1</sub>	(0,0,0;a,b,2c)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,1)	(2 <sub>z</sub> *0,0,1)

<b>17.1.106</b>	<b>P222<sub>1</sub></b>			<b>(1*0,0,0)</b>	<b>(2<sub>x</sub>*0,0,0)</b>	<b>(2<sub>y</sub>*0,0,1/2)</b>	<b>(2<sub>z</sub>*0,0,1/2)</b>
17.2.107	P222 <sub>1</sub> 1'						
17.3.108	P2'2'2 <sub>1</sub>	P2 <sub>1</sub>	(0,0,0;b,c,a)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)'	(2 <sub>y</sub> *0,0,1/2)'	(2 <sub>z</sub> *0,0,1/2)
17.4.109	P22'2' <sub>1</sub>	P2	(0,0,0;c,a,b)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,1/2)'	(2 <sub>z</sub> *0,0,1/2)'
17.5.110	P <sub>2a</sub> 222 <sub>1</sub>	P222 <sub>1</sub>	(0,0,0;2a,b,c)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,1/2)	(2 <sub>z</sub> *0,0,1/2)
17.6.111	P <sub>C</sub> 222 <sub>1</sub>	C222 <sub>1</sub>	(0,0,0;2a,2b,c)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,1/2)	(2 <sub>z</sub> *0,0,1/2)
17.7.112	P <sub>2a</sub> 2'2'2 <sub>1</sub>	P2 <sub>1</sub> 2 <sub>1</sub> 2	(1/2,0,1/4;c,2a,b)	(1*0,0,0)	(2 <sub>x</sub> *1,0,0)	(2 <sub>y</sub> *1,0,1/2)	(2 <sub>z</sub> *0,0,1/2)
<b>18.1.113</b>	<b>P2<sub>1</sub>2<sub>1</sub>2</b>			<b>(1*0,0,0)</b>	<b>(2<sub>x</sub>*1/2,1/2,0)</b>	<b>(2<sub>y</sub>*1/2,1/2,0)</b>	<b>(2<sub>z</sub>*0,0,0)</b>
18.2.114	P2 <sub>1</sub> 2 <sub>1</sub> 21'						
18.3.115	P2' <sub>1</sub> 2' <sub>1</sub> 2	P2	(0,0,0;b,c,a)	(1*0,0,0)	(2 <sub>x</sub> *1/2,1/2,0)'	(2 <sub>y</sub> *1/2,1/2,0)'	(2 <sub>z</sub> *0,0,0)
18.4.116	P2 <sub>1</sub> 2' <sub>1</sub> 2'	P2 <sub>1</sub>	(0,1/4,0;c,a,b)	(1*0,0,0)	(2 <sub>x</sub> *1/2,1/2,0)	(2 <sub>y</sub> *1/2,1/2,0)'	(2 <sub>z</sub> *0,0,0)'
18.5.117	P <sub>2c</sub> 2 <sub>1</sub> 2 <sub>1</sub> 2	P2 <sub>1</sub> 2 <sub>1</sub> 2	(0,0,0;a,b,2c)	(1*0,0,0)	(2 <sub>x</sub> *1/2,1/2,0)	(2 <sub>y</sub> *1/2,1/2,0)	(2 <sub>z</sub> *0,0,0)
18.6.118	P <sub>2c</sub> 2 <sub>1</sub> 2' <sub>1</sub> 2'	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	(1/4,0,0;a,b,2c)	(1*0,0,0)	(2 <sub>x</sub> *1/2,1/2,0)	(2 <sub>y</sub> *1/2,1/2,1)	(2 <sub>z</sub> *0,0,1)
<b>19.1.119</b>	<b>P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub></b>			<b>(1*0,0,0)</b>	<b>(2<sub>x</sub>*1/2,1/2,0)</b>	<b>(2<sub>y</sub>*0,1/2,1/2)</b>	<b>(2<sub>z</sub>*1/2,0,1/2)</b>

19.2.120	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> 1'							
19.3.121	P2 <sub>1</sub> '2 <sub>1</sub> '2 <sub>1</sub>	P2 <sub>1</sub>	(1/4,0,0;b,c,a)	(1*0,0,0)	(2 <sub>x</sub> *1/2,1/2,0)'	(2 <sub>y</sub> *0,1/2,1/2)'	(2 <sub>z</sub> *1/2,0,1/2)	
<b>20.1.122</b>	<b>C222<sub>1</sub></b>			<b>(1*0,0,0)</b>	<b>(2<sub>x</sub>*0,0,0)</b>	<b>(2<sub>y</sub>*0,0,1/2)</b>	<b>(2<sub>z</sub>*0,0,1/2)</b>	
20.2.123	C222 <sub>1</sub> 1'							
20.3.124	C2'2'2 <sub>1</sub>	P2 <sub>1</sub>	(0,0,0;b,c,{a+b}/2)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)'	(2 <sub>y</sub> *0,0,1/2)'	(2 <sub>z</sub> *0,0,1/2)	
20.4.125	C22'2 <sub>1</sub> '	P2	(0,0,0;c,a,{a+b}/2)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,1/2)'	(2 <sub>z</sub> *0,0,1/2)'	
20.5.126	C <sub>p</sub> 222 <sub>1</sub>	P222 <sub>1</sub>	(0,0,0;a,b,c)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,1/2)	(2 <sub>z</sub> *0,0,1/2)	
20.6.127	C <sub>p</sub> 2'2'2 <sub>1</sub>	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	(1/4,0,0;a,b,c)	(1*0,0,0)	(2 <sub>x</sub> *1/2,1/2,0)	(2 <sub>y</sub> *1/2,1/2,1/2)	(2 <sub>z</sub> *0,0,1/2)	
20.7.128	C <sub>p</sub> 22'2 <sub>1</sub> '	P2 <sub>1</sub> 2 <sub>1</sub> 2	(1/4,0,0;b,c,a)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *1/2,1/2,1/2)	(2 <sub>z</sub> *1/2,1/2,1/2)	
<b>21.1.129</b>	<b>C222</b>			<b>(1*0,0,0)</b>	<b>(2<sub>x</sub>*0,0,0)</b>	<b>(2<sub>y</sub>*0,0,0)</b>	<b>(2<sub>z</sub>*0,0,0)</b>	
21.2.130	C2221'							
21.3.131	C2'2'2	P2	(0,0,0;b,c,{a+b}/2)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)'	(2 <sub>y</sub> *0,0,0)'	(2 <sub>z</sub> *0,0,0)	
21.4.132	C22'2'	C2	(0,0,0;&a,c)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,0)'	(2 <sub>z</sub> *0,0,0)'	
21.5.133	C <sub>2c</sub> 222	C222	(0,0,0;a,b,2c)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)	
21.6.134	C <sub>p</sub> 222	P222	(0,0,0;a,b,c)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)	
21.7.135	C <sub>i</sub> 222	I222	(0,0,0;a,b,2c)	(1*0,0,0)	(2 <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)	



21.8.136	$C_{2c} 22'2'$	$C222_1$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,1)$	$(2_z^*0,0,1)$
21.9.137	$C_p 2'2'2$	$P2_12_12$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(2_x^*1/2,1/2,0)$	$(2_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$
21.10.138	$C_p 22'2'$	$P222_1$	$(1/4,0,0;a,b,c)$	$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*1/2,1/2,0)$	$(2_z^*1/2,1/2,0)$
21.11.139	$C_1 2'22'$	$I2_12_12_1$	$(1/4,0,0;a,b,2c)$	$(1^*0,0,0)$	$(2_x^*0,0,1)$	$(2_y^*0,0,0)$	$(2_z^*0,0,1)$
<b>22.1.140</b>	<b>F222</b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(2_x^*0,0,0)</math></b>	<b><math>(2_y^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b>
22.2.141	F2221'						
22.3.142	F2'2'2	C2	$(0,0,0;b,c,\{a+b\}/2)$	$(1^*0,0,0)$	$(2_x^*0,0,0)'$	$(2_y^*0,0,0)'$	$(2_z^*0,0,0)$
22.4.143	$F_C 222$	C222	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
22.5.144	$F_C 22'2'$	$C222_1$	$(1/4,0,0;a,b,c)$	$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*1/2,0,1/2)$	$(2_z^*1/2,0,1/2)$
<b>23.1.145</b>	<b>I222</b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(2_x^*0,0,0)</math></b>	<b><math>(2_y^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b>
23.2.146	I2221'						
23.3.147	I2'2'2	C2	$(0,0,0;a+b,c,a)$	$(1^*0,0,0)$	$(2_x^*0,0,0)'$	$(2_y^*0,0,0)'$	$(2_z^*0,0,0)$
23.4.148	$I_p 222$	P222	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
23.5.149	$I_p 2'2'2$	$P2_12_12$	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$	$(2_x^*1/2,1/2,1/2)$	$(2_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$

<b>24.1.150</b>	<b>I<sub>2</sub>2<sub>1</sub>2<sub>1</sub></b>			<b>(1*0,0,0)</b>	<b>(2<sub>x</sub>*1/2,1/2,0)</b>	<b>(2<sub>y</sub>*0,1/2,1/2)</b>	<b>(2<sub>z</sub>*1/2,0,1/2)</b>
24.2.151	I <sub>2</sub> 2 <sub>1</sub> 2 <sub>1</sub> 1'						
24.3.152	I <sub>2</sub> 1'2'12 <sub>1</sub>	C2	(0,1/4,0;a+b,c,a)	(1*0,0,0)	(2 <sub>x</sub> *1/2,1/2,0)'	(2 <sub>y</sub> *0,1/2,1/2)'	(2 <sub>z</sub> *1/2,0,1/2)
24.4.153	I <sub>P</sub> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	(0,0,0;a,b,c)	(1*0,0,0)	(2 <sub>x</sub> *1/2,1/2,0)	(2 <sub>y</sub> *0,1/2,1/2)	(2 <sub>z</sub> *1/2,0,1/2)
24.5.154	I <sub>P</sub> 2 <sub>1</sub> '2 <sub>1</sub> '2 <sub>1</sub>	P222 <sub>1</sub>	(1/4,0,1/4;a,b,c)	(1*0,0,0)	(2 <sub>x</sub> *0,0,1/2)	(2 <sub>y</sub> *1/2,0,0)	(2 <sub>z</sub> *1/2,0,1/2)
<b>25.1.155</b>	<b>Pmm2</b>			<b>(1*0,0,0)</b>	<b>(m<sub>x</sub>*0,0,0)</b>	<b>(m<sub>y</sub>*0,0,0)</b>	<b>(2<sub>z</sub>*0,0,0)</b>
25.2.156	Pmm21'						
25.3.157	Pm'm2'	Pm	(0,0,0;a,b,c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)'	(m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)'
25.4.158	Pm'm'2	P2	(0,0,0;b,c,a)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)'	(m <sub>y</sub> *0,0,0)'	(2 <sub>z</sub> *0,0,0)
25.5.159	P <sub>2c</sub> mm2	Pmm2	(0,0,0;a,b,2c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)
25.6.160	P <sub>2a</sub> mm2	Pmm2	(0,0,0;2a,b,c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)
25.7.161	P <sub>C</sub> mm2	Cmm2	(0,0,0;2a,2b,c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)
25.8.162	P <sub>A</sub> mm2	Amm2	(0,0,0;a,2b,2c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)
25.9.163	P <sub>F</sub> mm2	Fmm2	(0,0,0;2a,2b,2c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)
25.10.164	P <sub>2c</sub> mm'2'	Pmc2 <sub>1</sub>	(0,0,0;a,b,2c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *0,0,1)	(2 <sub>z</sub> *0,0,1)
25.11.165	P <sub>2c</sub> m'm'2	Pcc2	(0,0,0;a,b,2c)	(1*0,0,0)	(m <sub>x</sub> *0,0,1)	(m <sub>y</sub> *0,0,1)	(2 <sub>z</sub> *0,0,0)
25.12.166	P <sub>2a</sub> m'm'2	Pma2	(0,0,0;2a,b,c)	(1*0,0,0)	(m <sub>x</sub> *1,0,0)	(m <sub>y</sub> *1,0,0)	(2 <sub>z</sub> *0,0,0)

25.13.167	$P_A m'm'2$	Abm2	(0,0,0;a,2b,2c)	(1*0,0,0)	( $m_x^*0,1,0$ )	( $m_y^*0,1,0$ )	( $2_z^*0,0,0$ )
<b>26.1.168</b>	<b>Pmc2<sub>1</sub></b>			<b>(1*0,0,0)</b>	<b>(<math>m_x^*0,0,0</math>)</b>	<b>(<math>m_y^*0,0,1/2</math>)</b>	<b>(<math>2_z^*0,0,1/2</math>)</b>
26.2.169	Pmc2 <sub>1</sub> '						
26.3.170	Pm'c2 <sub>1</sub> '	Pc	(0,0,0;a,b,c)	(1*0,0,0)	( $m_x^*0,0,0$ )'	( $m_y^*0,0,1/2$ )	( $2_z^*0,0,1/2$ )'
26.4.171	Pmc'2 <sub>1</sub> '	Pm	(0,0,0;c,a,b)	(1*0,0,0)	( $m_x^*0,0,0$ )	( $m_y^*0,0,1/2$ )'	( $2_z^*0,0,1/2$ )'
26.5.172	Pm'c'2 <sub>1</sub>	P2 <sub>1</sub>	(0,0,0;b,c,a)	(1*0,0,0)	( $m_x^*0,0,0$ )'	( $m_y^*0,0,1/2$ )'	( $2_z^*0,0,1/2$ )
26.6.173	P <sub>2a</sub> mc2 <sub>1</sub>	Pmc2 <sub>1</sub>	(0,0,0;2a,b,c)	(1*0,0,0)	( $m_x^*0,0,0$ )	( $m_y^*0,0,1/2$ )	( $2_z^*0,0,1/2$ )
26.7.174	P <sub>2b</sub> mc2 <sub>1</sub>	Pmc2 <sub>1</sub>	(0,0,0;a,2b,c)	(1*0,0,0)	( $m_x^*0,0,0$ )	( $m_y^*0,0,1/2$ )	( $2_z^*0,0,1/2$ )
26.8.175	P <sub>C</sub> mc2 <sub>1</sub>	Cmc2 <sub>1</sub>	(0,0,0;2a,2b,c)	(1*0,0,0)	( $m_x^*0,0,0$ )	( $m_y^*0,0,1/2$ )	( $2_z^*0,0,1/2$ )
26.9.176	P <sub>2a</sub> mc'2 <sub>1</sub> '	Pmn2 <sub>1</sub>	(0,0,0;2a,b,c)	(1*0,0,0)	( $m_x^*0,0,0$ )	( $m_y^*1,0,1/2$ )	( $2_z^*1,0,1/2$ )
26.10.177	P <sub>2b</sub> m'c'2 <sub>1</sub>	Pca2 <sub>1</sub>	(0,0,0;2b,c,c)	(1*0,0,0)	( $m_x^*0,1,0$ )	( $m_y^*0,1,1/2$ )	( $2_z^*0,0,1/2$ )
<b>27.1.178</b>	<b>Pcc2</b>			<b>(1*0,0,0)</b>	<b>(<math>m_x^*0,0,1/2</math>)</b>	<b>(<math>m_y^*0,0,1/2</math>)</b>	<b>(<math>2_z^*0,0,0</math>)</b>
27.2.179	Pcc21'						
27.3.180	Pc'c2'	Pc	(0,0,0;a,b,c)	(1*0,0,0)	( $m_x^*0,0,1/2$ )'	( $m_y^*0,0,1/2$ )	( $2_z^*0,0,0$ )'
27.4.181	Pc'c'2	P2	(0,0,0;b,c,a)	(1*0,0,0)	( $m_x^*0,0,1/2$ )'	( $m_y^*0,0,1/2$ )'	( $2_z^*0,0,0$ )
27.5.182	P <sub>2a</sub> cc2	Pcc2	(0,0,0;2a,b,c)	(1*0,0,0)	( $m_x^*0,0,1/2$ )	( $m_y^*0,0,1/2$ )	( $2_z^*0,0,0$ )

27.6.183	$P_C cc2$	Ccc2	(0,0,0;2a,2b,c)	$(1^*0,0,0)$	$(m_x^*0,0,1/2)$	$(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$
27.7.184	$P_{2b} c'c2'$	Pnc2	(0,1/2,0;a,2b,c)	$(1^*0,0,0)$	$(m_x^*0,1,1/2)$	$(m_y^*0,0,1/2)$	$(2_z^*0,1,0)$
<b>28.1.185</b>	<b>Pma2</b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(m_x^*1/2,0,0)</math></b>	<b><math>(m_y^*1/2,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b>
28.2.186	Pma21'						
28.3.187	Pm'a2'	Pc	(0,0,0;c,&a)	$(1^*0,0,0)$	$(m_x^*1/2,0,0)'$	$(m_y^*1/2,0,0)$	$(2_z^*0,0,0)'$
28.4.188	Pma'2'	Pm	(1/4,0,0;c,a,b)	$(1^*0,0,0)$	$(m_x^*1/2,0,0)$	$(m_y^*1/2,0,0)'$	$(2_z^*0,0,0)'$
28.5.189	Pm'a'2	P2	(0,0,0;b,c,a)	$(1^*0,0,0)$	$(m_x^*1/2,0,0)'$	$(m_y^*1/2,0,0)'$	$(2_z^*0,0,0)$
28.6.190	$P_{2b} ma2$	Pma2	(0,0,0;a,2b,c)	$(1^*0,0,0)$	$(m_x^*1/2,0,0)$	$(m_y^*1/2,0,0)$	$(2_z^*0,0,0)$
28.7.191	$P_{2c} ma2$	Pma2	(0,0,0;a,b,2c)	$(1^*0,0,0)$	$(m_x^*1/2,0,0)$	$(m_y^*1/2,0,0)$	$(2_z^*0,0,0)$
28.8.192	$P_A ma2$	Ama2	(0,0,0;a,2b,2c)	$(1^*0,0,0)$	$(m_x^*1/2,0,0)$	$(m_y^*1/2,0,0)$	$(2_z^*0,0,0)$
28.9.193	$P_{2b} m'a2'$	Pba2	(0,1/2,0;a,2b,c)	$(1^*0,0,0)$	$(m_x^*1/2,1,0)$	$(m_y^*1/2,0,0)$	$(2_z^*0,1,0)$
28.10.194	$P_{2c} m'a2'$	Pca2 <sub>1</sub>	(0,0,0;a,b,2c)	$(1^*0,0,0)$	$(m_x^*1/2,0,1)$	$(m_y^*1/2,0,0)$	$(2_z^*0,0,1)$
28.11.195	$P_{2c} ma'2'$	Pmn2 <sub>1</sub>	(1/4,0,0;a,b,2c)	$(1^*0,0,0)$	$(m_x^*1/2,0,0)$	$(m_y^*1/2,0,1)$	$(2_z^*0,0,1)$
28.12.196	$P_{2c} m'a'2$	Pnc2	(0,0,0;b,&2c)	$(1^*0,0,0)$	$(m_x^*1/2,0,1)$	$(m_y^*1/2,0,1)$	$(2_z^*0,0,0)$
28.13.197	$P_A m'a'2$	Aba2	(0,0,0;a,2b,2c)	$(1^*0,0,0)$	$(m_x^*1/2,1,0)$	$(m_y^*1/2,1,0)$	$(2_z^*0,0,0)$

<b>29.1.198</b>	<b>Pca2<sub>1</sub></b>			<b>(1*0,0,0)</b>	<b>(m<sub>x</sub>*1/2,0,1/2)</b>	<b>(m<sub>y</sub>*1/2,0,0)</b>	<b>(2<sub>z</sub>*0,0,1/2)</b>
29.2.199	Pca2 <sub>1</sub> 1'						
29.3.200	Pc'a2 <sub>1</sub> '	Pc	(0,0,0;c,&,a)	(1*0,0,0)	(m <sub>x</sub> *1/2,0,1/2)'	(m <sub>y</sub> *1/2,0,0)	(2 <sub>z</sub> *0,0,1/2)'
29.4.201	Pca'2 <sub>1</sub> '	Pc	(1/4,0,0;b,&,c)	(1*0,0,0)	(m <sub>x</sub> *1/2,0,1/2)	(m <sub>y</sub> *1/2,0,0)'	(2 <sub>z</sub> *0,0,1/2)'
29.5.202	Pc'a'2 <sub>1</sub>	P2 <sub>1</sub>	(0,0,0;b,c,a)	(1*0,0,0)	(m <sub>x</sub> *1/2,0,1/2)'	(m <sub>y</sub> *1/2,0,0)'	(2 <sub>z</sub> *0,0,1/2)
29.6.203	P <sub>2b</sub> ca2 <sub>1</sub>	Pca2 <sub>1</sub>	(0,0,0;a,2b,c)	(1*0,0,0)	(m <sub>x</sub> *1/2,0,1/2)	(m <sub>y</sub> *1/2,0,0)	(2 <sub>z</sub> *0,0,1/2)
29.7.204	P <sub>2b</sub> c'a'2 <sub>1</sub>	Pna2 <sub>1</sub>	(0,0,0;a,2b,c)	(1*0,0,0)	(m <sub>x</sub> *1/2,1,1/2)	(m <sub>y</sub> *1/2,1,0)	(2 <sub>z</sub> *0,0,1/2)
<b>30.1.205</b>	<b>Pnc2</b>			<b>(1*0,0,0)</b>	<b>(m<sub>x</sub>*0,1/2,1/2)</b>	<b>(m<sub>y</sub>*0,1/2,1/2)</b>	<b>(2<sub>z</sub>*0,0,0)</b>
30.2.206	Pnc21'						
30.3.207	Pn'c2'	Pc	(0,1/4,0;a,b,c)	(1*0,0,0)	(m <sub>x</sub> *0,1/2,1/2)'	(m <sub>y</sub> *0,1/2,1/2)	(2 <sub>z</sub> *0,0,0)'
30.4.208	Pnc'2'	Pc	(0,0,0;c,a,b+c)	(1*0,0,0)	(m <sub>x</sub> *0,1/2,1/2)	(m <sub>y</sub> *0,1/2,1/2)'	(2 <sub>z</sub> *0,0,0)'
30.5.209	Pn'c'2	P2	(0,0,0;b,c,a)	(1*0,0,0)	(m <sub>x</sub> *0,1/2,1/2)'	(m <sub>y</sub> *0,1/2,1/2)'	(2 <sub>z</sub> *0,0,0)
30.6.210	P <sub>2a</sub> nc2	Pnc2	(0,0,0;2a,b,c)	(1*0,0,0)	(m <sub>x</sub> *0,1/2,1/2)	(m <sub>y</sub> *0,1/2,1/2)	(2 <sub>z</sub> *0,0,0)
30.7.211	P <sub>2a</sub> nc'2'	Pnn2	(1/2,0,0;2a,b,c)	(1*0,0,0)	(m <sub>x</sub> *0,1/2,1/2)	(m <sub>y</sub> *1 1/2 1/2)	(2 <sub>z</sub> *1,0,0)
<b>31.1.212</b>	<b>Pmn2<sub>1</sub></b>			<b>(1*0,0,0)</b>	<b>(m<sub>x</sub>*0,0,0)</b>	<b>(m<sub>y</sub>*1/2,0,1/2)</b>	<b>(2<sub>z</sub>*1/2,0,1/2)</b>

31.2.213	Pmn <sub>2</sub> 1'							
31.3.214	Pm'n <sub>2</sub> 1'	Pc	(0,0,0;a,b,a+c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)'	(m <sub>y</sub> *1/2,0,1/2)	(2 <sub>z</sub> *1/2,0,1/2)'	
31.4.215	Pmn'2 <sub>1</sub> '	Pm	(0,0,0;b,c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *1/2,0,1/2)'	(2 <sub>z</sub> *1/2,0,1/2)'	
31.5.216	Pm'n'2 <sub>1</sub>	P2 <sub>1</sub>	(1/4,0,0;b,c,a)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)'	(m <sub>y</sub> *1/2,0,1/2)'	(2 <sub>z</sub> *1/2,0,1/2)	
31.6.217	P <sub>2b</sub> mn2 <sub>1</sub>	Pmn2 <sub>1</sub>	(0,0,0;a,2b,c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *1/2,0,1/2)	(2 <sub>z</sub> *1/2,0,1/2)	
31.7.218	P <sub>2b</sub> m'n2 <sub>1</sub> '	Pna2 <sub>1</sub>	(1/4,1/2,0;2b,c)	(1*0,0,0)	(m <sub>x</sub> *0,1,0)	(m <sub>y</sub> *1/2,0,1/2)	(2 <sub>z</sub> *1/2,1,1/2)	
<b>32.1.219</b>	<b>Pba2</b>			<b>(1*0,0,0)</b>	<b>(m<sub>x</sub>*1/2,1/2,0)</b>	<b>(m<sub>y</sub>*1/2,1/2,0)</b>	<b>(2<sub>z</sub>*0,0,0)</b>	
32.2.220	Pba21'							
32.3.221	Pb'a2'	Pc	(0,1/4,0;c,a)	(1*0,0,0)	(m <sub>x</sub> *1/2,1/2,0)'	(m <sub>y</sub> *1/2,1/2,0)	(2 <sub>z</sub> *0,0,0)'	
32.4.222	Pb'a'2	P2	(0,0,0;b,c,a)	(1*0,0,0)	(m <sub>x</sub> *1/2,1/2,0)'	(m <sub>y</sub> *1/2,1/2,0)'	(2 <sub>z</sub> *0,0,0)	
32.5.223	P <sub>2c</sub> ba2	Pba2	(0,0,0;a,b,2c)	(1*0,0,0)	(m <sub>x</sub> *1/2,1/2,0)	(m <sub>y</sub> *1/2,1/2,0)	(2 <sub>z</sub> *0,0,0)	
32.6.224	P <sub>2c</sub> b'a2'	Pna2 <sub>1</sub>	(0,0,0;a,b,2c)	(1*0,0,0)	(m <sub>x</sub> *1/2,1/2,1)	(m <sub>y</sub> *1/2,1/2,0)	(2 <sub>z</sub> *0,0,1)	
32.7.225	P <sub>2c</sub> b'a'2	Pnn2	(0,0,0;a,b,2c)	(1*0,0,0)	(m <sub>x</sub> *1/2,1/2,1)	(m <sub>y</sub> *1/2,1/2,1)	(2 <sub>z</sub> *0,0,0)	
<b>33.1.226</b>	<b>Pna2<sub>1</sub></b>			<b>(1*0,0,0)</b>	<b>(m<sub>x</sub>*1/2,1/2,1/2)</b>	<b>(m<sub>y</sub>*1/2,1/2,0)</b>	<b>(2<sub>z</sub>*0,0,1/2)</b>	
33.2.227	Pna2 <sub>1</sub> 1'							
33.3.228	Pn'a2 <sub>1</sub> '	Pc	(0,1/4,0;c,a)	(1*0,0,0)	(m <sub>x</sub> *1/2,1/2,1/2)'	(m <sub>y</sub> *1/2,1/2,0)	(2 <sub>z</sub> *0,0,1/2)'	

33.4.229	Pna'2 <sub>1</sub> '	Pc	(1/4,0,0;c,a,b+c)	(1*0,0,0)	(m <sub>x</sub> *1/2,1/2,1/2)	(m <sub>y</sub> *1/2,1/2,0)'	(2 <sub>z</sub> *0,0,1/2)'
33.5.230	Pn'a'2 <sub>1</sub>	P2 <sub>1</sub>	(0,0,0;b,c,a)	(1*0,0,0)	(m <sub>x</sub> *1/2,1/2,1/2)'	(m <sub>y</sub> *1/2,1/2,0)'	(2 <sub>z</sub> *0,0,1/2)
<b>34.1.231</b>	<b>Pnn2</b>			<b>(1*0,0,0)</b>	<b>(m<sub>x</sub>*1/2,1/2,1/2)</b>	<b>(m<sub>y</sub>*1/2,1/2,1/2)</b>	<b>(2<sub>z</sub>*0,0,0)</b>
34.2.232	Pnn21'						
34.3.233	Pn'n'2'	Pc	(0,1/4,0;a,b,a+c)	(1*0,0,0)	(m <sub>x</sub> *1/2,1/2,1/2)'	(m <sub>y</sub> *1/2,1/2,1/2)	(2 <sub>z</sub> *0,0,0)'
34.4.234	Pn'n'2	P2	(0,0,0;b,c,a)	(1*0,0,0)	(m <sub>x</sub> *1/2,1/2,1/2)'	(m <sub>y</sub> *1/2,1/2,1/2)'	(2 <sub>z</sub> *0,0,0)
34.5.235	P <sub>F</sub> nn2	Fdd2	(0,0,0;2a,2b,2c)	(1*0,0,0)	(m <sub>x</sub> *1/2,1/2,1/2)	(m <sub>y</sub> *1/2,1/2,1/2)	(2 <sub>z</sub> *0,0,0)
<b>35.1.236</b>	<b>Cmm2</b>			<b>(1*0,0,0)</b>	<b>(m<sub>x</sub>*0,0,0)</b>	<b>(m<sub>y</sub>*0,0,0)</b>	<b>(2<sub>z</sub>*0,0,0)</b>
35.2.237	Cmm21'						
35.3.238	Cm'm'2'	Cm	(0,0,0;a,b,c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)'	(m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)'
35.4.239	Cm'm'2	P2	(0,0,0;b,c,{a+b}/2)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)'	(m <sub>y</sub> *0,0,0)'	(2 <sub>z</sub> *0,0,0)
35.5.240	C <sub>2c</sub> mm2	Cmm2	(0,0,0;a,b,2c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)
35.6.241	C <sub>P</sub> mm2	Pmm2	(0,0,0;a,b,c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)
35.7.242	C <sub>1</sub> mm2	Imm2	(0,0,0;a,b,2c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)
35.8.243	C <sub>2c</sub> m'm'2'	Cmc2 <sub>1</sub>	(0,0,0;b,2c)	(1*0,0,0)	(m <sub>x</sub> *0,0,1)	(m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,1)
35.9.244	C <sub>2c</sub> m'm'2	Ccc2	(0,0,0;a,b,2c)	(1*0,0,0)	(m <sub>x</sub> *0,0,1)	(m <sub>y</sub> *0,0,1)	(2 <sub>z</sub> *0,0,0)

35.10.245	$C_p m'm'2'$	Pma2	$(1/4, 1/4, 0; b, \&, c)$	$(1^*0, 0, 0)$	$(m_x^* 1/2, 1/2, 0)$	$(m_y^* 0, 0, 0)$	$(2_z^* 1/2, 1/2, 0)$
35.11.246	$C_p m'm'2$	Pba2	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$	$(m_x^* 1/2, 1/2, 0)$	$(m_y^* 1/2, 1/2, 0)$	$(2_z^* 0, 0, 0)$
35.12.247	$C_1 m'm'2'$	Ima2	$(1/4, 1/4, 0; b, \&, c)$	$(1^*0, 0, 0)$	$(m_x^* 0, 0, 1)$	$(m_y^* 0, 0, 0)$	$(2_z^* 0, 0, 1)$
35.13.248	$C_1 m'm'2$	lba2	$(0, 0, 0; a, b, 2c)$	$(1^*0, 0, 0)$	$(m_x^* 0, 0, 1)$	$(m_y^* 0, 0, 1)$	$(2_z^* 0, 0, 0)$
<b>36.1.249</b>	<b>Cmc2<sub>1</sub></b>			<b><math>(1^*0, 0, 0)</math></b>	<b><math>(m_x^* 0, 0, 0)</math></b>	<b><math>(m_y^* 0, 0, 1/2)</math></b>	<b><math>(2_z^* 0, 0, 1/2)</math></b>
36.2.250	Cmc2 <sub>1</sub> '						
36.3.251	$Cm'c'2_1'$	Cc	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$	$(m_x^* 0, 0, 0)'$	$(m_y^* 0, 0, 1/2)$	$(2_z^* 0, 0, 1/2)'$
36.4.252	$Cmc'2_1'$	Cm	$(0, 0, 0; b, \&, c)$	$(1^*0, 0, 0)$	$(m_x^* 0, 0, 0)$	$(m_y^* 0, 0, 1/2)'$	$(2_z^* 0, 0, 1/2)'$
36.5.253	$Cm'c'2_1$	P2 <sub>1</sub>	$(0, 0, 0; b, c, \{a+b\}/2)$	$(1^*0, 0, 0)$	$(m_x^* 0, 0, 0)'$	$(m_y^* 0, 0, 1/2)'$	$(2_z^* 0, 0, 1/2)$
36.6.254	$C_p mc2_1$	Pmc2 <sub>1</sub>	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$	$(m_x^* 0, 0, 0)$	$(m_y^* 0, 0, 1/2)$	$(2_z^* 0, 0, 1/2)$
36.7.255	$C_p m'c'2_1'$	Pca2 <sub>1</sub>	$(1/4, 1/4, 0; b, \&, c)$	$(1^*0, 0, 0)$	$(m_x^* 1/2, 1/2, 0)$	$(m_y^* 0, 0, 1/2)$	$(2_z^* 1/2, 1/2, 1/2)$
36.8.256	$C_p mc'2_1'$	Pmn2 <sub>1</sub>	$(0, 1/4, 0; a, b, c)$	$(1^*0, 0, 0)$	$(m_x^* 0, 0, 0)$	$(m_y^* 1/2, 1/2, 1/2)$	$(2_z^* 1/2, 1/2, 1/2)$
36.9.257	$C_p m'c'2_1$	Pna2 <sub>1</sub>	$(0, 0, 0; b, \&, c)$	$(1^*0, 0, 0)$	$(m_x^* 1/2, 1/2, 0)$	$(m_y^* 1/2, 1/2, 1/2)$	$(2_z^* 0, 0, 1/2)$
<b>37.1.258</b>	<b>Ccc2</b>			<b><math>(1^*0, 0, 0)</math></b>	<b><math>(m_x^* 0, 0, 1/2)</math></b>	<b><math>(m_y^* 0, 0, 1/2)</math></b>	<b><math>(2_z^* 0, 0, 0)</math></b>
37.2.259	Ccc21'						
37.3.260	$Cc'c'2'$	Cc	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$	$(m_x^* 0, 0, 1/2)'$	$(m_y^* 0, 0, 1/2)$	$(2_z^* 0, 0, 0)'$



37.4.261	Cc'c'2	P2	(0,0,0;b,c,{a+b}/2)	(1*0,0,0)	(m <sub>x</sub> *0,0,1/2)'	(m <sub>y</sub> *0,0,1/2)'	(2 <sub>z</sub> *0,0,0)
37.5.262	C <sub>p</sub> cc2	Pcc2	(0,0,0;a,b,c)	(1*0,0,0)	(m <sub>x</sub> *0,0,1/2)	(m <sub>y</sub> *0,0,1/2)	(2 <sub>z</sub> *0,0,0)
37.6.263	C <sub>p</sub> c'c'2'	Pnc2	(1/4,1/4,0;a,b,c)	(1*0,0,0)	(m <sub>x</sub> *1/2,1/2,1/2)	(m <sub>y</sub> *0,0,1/2)	(2 <sub>z</sub> *1/2,1/2,0)
37.7.264	C <sub>p</sub> c'c'2	Pnn2	(0,0,0;a,b,c)	(1*0,0,0)	(m <sub>x</sub> *1/2,1/2,1/2)	(m <sub>y</sub> *1/2,1/2,1/2)	(2 <sub>z</sub> *0,0,0)
<b>38.1.265</b>	<b>Amm2</b>			<b>(1*0,0,0)</b>	<b>(m<sub>x</sub>*0,0,0)</b>	<b>(m<sub>y</sub>*0,0,0)</b>	<b>(2<sub>z</sub>*0,0,0)</b>
38.2.266	Amm21'						
38.3.267	Am'm2'	Cm	(0,0,0;c,&a)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)'	(m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)'
38.4.268	Amm'2'	Pm	(0,0,0;b,&,{b+c}/2)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *0,0,0)'	(2 <sub>z</sub> *0,0,0)'
38.5.269	Am'm'2	C2	(0,0,0;b,c,a)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)'	(m <sub>y</sub> *0,0,0)'	(2 <sub>z</sub> *0,0,0)
38.6.270	A <sub>2a</sub> mm2	Amm2	(0,0,0;2a,b,c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)
38.7.271	A <sub>p</sub> mm2	Pmm2	(0,0,0;a,b,c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)
38.8.272	A <sub>l</sub> mm2	Imm2	(0,0,0;2a,b,c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)
38.9.273	A <sub>2a</sub> mm'2'	Ama2	(1/2,0,0;2a,b,c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *1,0,0)	(2 <sub>z</sub> *1,0,0)
38.10.274	A <sub>p</sub> m'm2'	Pmn2 <sub>1</sub>	(0,0,0;b,&,c)	(1*0,0,0)	(m <sub>x</sub> *0,1/2,1/2)	(m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,1/2,1/2)
38.11.275	A <sub>p</sub> mm'2'	Pmc2 <sub>1</sub>	(0,1/4,0;a,b,c)	(1*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *0,1/2,1/2)	(2 <sub>z</sub> *0,1/2,1/2)
38.12.276	A <sub>p</sub> m'm'2	Pnc2	(0,0,0;a,b,c)	(1*0,0,0)	(m <sub>x</sub> *0,1/2,1/2)	(m <sub>y</sub> *0,1/2,1/2)	(2 <sub>z</sub> *0,0,0)
38.13.277	A <sub>l</sub> m'm'2	Ima2	(0,0,0;2a,b,c)	(1*0,0,0)	(m <sub>x</sub> *1,0,0)	(m <sub>y</sub> *1,0,0)	(2 <sub>z</sub> *0,0,0)

<b>39.1.278</b>	<b>Abm2</b>			<b>(1*0,0,0)</b>	<b>(m<sub>x</sub>*0,1/2,0)</b>	<b>(m<sub>y</sub>*0,1/2,0)</b>	<b>(2<sub>z</sub>*0,0,0)</b>
39.2.279	Abm21'						
39.3.280	Ab'm2'	Cm	(0,1/4,0;c,&a)	(1*0,0,0)	(m <sub>x</sub> *0,1/2,0)'	(m <sub>y</sub> *0,1/2,0)	(2 <sub>z</sub> *0,0,0)'
39.4.281	Abm'2'	Pc	(0,0,0;{b+c}/2,a,b)	(1*0,0,0)	(m <sub>x</sub> *0,1/2,0)	(m <sub>y</sub> *0,1/2,0)'	(2 <sub>z</sub> *0,0,0)'
39.5.282	Ab'm'2	C2	(0,0,0;b,c,a)	(1*0,0,0)	(m <sub>x</sub> *0,1/2,0)'	(m <sub>y</sub> *0,1/2,0)'	(2 <sub>z</sub> *0,0,0)
39.6.283	A <sub>2a</sub> bm2	Abm2	(0,0,0;2a,b,c)	(1*0,0,0)	(m <sub>x</sub> *0,1/2,0)	(m <sub>y</sub> *0,1/2,0)	(2 <sub>z</sub> *0,0,0)
39.7.284	A <sub>p</sub> bm2	Pma2	(0,0,0;b,&c)	(1*0,0,0)	(m <sub>x</sub> *0,1/2,0)	(m <sub>y</sub> *0,1/2,0)	(2 <sub>z</sub> *0,0,0)
39.8.285	A <sub>l</sub> bm2	Ima2	(0,0,0;b,2&c)	(1*0,0,0)	(m <sub>x</sub> *0,1/2,0)	(m <sub>y</sub> *0,1/2,0)	(2 <sub>z</sub> *0,0,0)
39.9.286	A <sub>2a</sub> b'm'2	Aba2	(0,0,0;2a,b,c)	(1*0,0,0)	(m <sub>x</sub> *1,1/2,0)	(m <sub>y</sub> *1,1/2,0)	(2 <sub>z</sub> *0,0,0)
39.10.287	A <sub>p</sub> b'm'2'	Pmc2 <sub>1</sub>	(0,1/4,0;b,&c)	(1*0,0,0)	(m <sub>x</sub> *0,0,1/2)	(m <sub>y</sub> *0,1/2,0)	(2 <sub>z</sub> *0,1/2,1/2)
39.11.288	A <sub>p</sub> bm'2'	Pca2 <sub>1</sub>	(0,1/4,0;b,&c)	(1*0,0,0)	(m <sub>x</sub> *0,1/2,0)	(m <sub>y</sub> *0,0,1/2)	(2 <sub>z</sub> *0,1/2,1/2)
39.12.289	A <sub>p</sub> b'm'2	Pcc2	(0,0,0;a,b,c)	(1*0,0,0)	(m <sub>x</sub> *0,0,1/2)	(m <sub>y</sub> *0,0,1/2)	(2 <sub>z</sub> *0,0,0)
39.13.290	A <sub>l</sub> b'm'2	lba2	(0,0,0;2a,b,c)	(1*0,0,0)	(m <sub>x</sub> *1,1/2,0)	(m <sub>y</sub> *1,1/2,0)	(2 <sub>z</sub> *0,0,0)
<b>40.1.291</b>	<b>Ama2</b>			<b>(1*0,0,0)</b>	<b>(m<sub>x</sub>*1/2,0,0)</b>	<b>(m<sub>y</sub>*1/2,0,0)</b>	<b>(2<sub>z</sub>*0,0,0)</b>
40.2.292	Ama21'						
40.3.293	Am'a2'	Cc	(0,0,0;c,&a)	(1*0,0,0)	(m <sub>x</sub> *1/2,0,0)'	(m <sub>y</sub> *1/2,0,0)	(2 <sub>z</sub> *0,0,0)'

40.4.294	Ama'2'	Pm	$(1/4, 0, 0; b, \frac{b+c}{2})$	$(1^*0, 0, 0)$	$(m_x^*1/2, 0, 0)$	$(m_y^*1/2, 0, 0)'$	$(2_z^*0, 0, 0)'$
40.5.295	Am'a'2	C2	$(0, 0, 0; b, c, a)$	$(1^*0, 0, 0)$	$(m_x^*1/2, 0, 0)'$	$(m_y^*1/2, 0, 0)'$	$(2_z^*0, 0, 0)$
40.6.296	A <sub>p</sub> ma2	Pma2	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$	$(m_x^*1/2, 0, 0)$	$(m_y^*1/2, 0, 0)$	$(2_z^*0, 0, 0)$
40.7.297	A <sub>p</sub> m'a'2'	Pna2 <sub>1</sub>	$(0, 1/4, 0; a, b, c)$	$(1^*0, 0, 0)$	$(m_x^*1/2, 1/2, 1/2)$	$(m_y^*1/2, 0, 0)$	$(2_z^*0, 1/2, 1/2)$
40.8.298	A <sub>p</sub> ma'2'	Pmn2 <sub>1</sub>	$(1/4, 1/4, 0; a, b, c)$	$(1^*0, 0, 0)$	$(m_x^*1/2, 0, 0)$	$(m_y^*1/2, 1/2, 1/2)$	$(2_z^*0, 1/2, 1/2)$
40.9.299	A <sub>p</sub> m'a'2	Pnn2	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$	$(m_x^*1/2, 1/2, 1/2)$	$(m_y^*1/2, 1/2, 1/2)$	$(2_z^*0, 0, 0)$
<b>41.1.300</b>	<b>Aba2</b>			<b><math>(1^*0, 0, 0)</math></b>	<b><math>(m_x^*1/2, 1/2, 0)</math></b>	<b><math>(m_y^*1/2, 1/2, 0)</math></b>	<b><math>(2_z^*0, 0, 0)</math></b>
41.2.301	Aba21'						
41.3.302	Ab'a'2'	Cc	$(0, 1/4, 0; c, \frac{b+c}{2}, a)$	$(1^*0, 0, 0)$	$(m_x^*1/2, 1/2, 0)'$	$(m_y^*1/2, 1/2, 0)$	$(2_z^*0, 0, 0)'$
41.4.303	Aba'2'	Pc	$(1/4, 0, 0; \frac{b+c}{2}, a, b)$	$(1^*0, 0, 0)$	$(m_x^*1/2, 1/2, 0)$	$(m_y^*1/2, 1/2, 0)'$	$(2_z^*0, 0, 0)'$
41.5.304	Ab'a'2	C2	$(0, 0, 0; b, c, a)$	$(1^*0, 0, 0)$	$(m_x^*1/2, 1/2, 0)'$	$(m_y^*1/2, 1/2, 0)'$	$(2_z^*0, 0, 0)$
41.6.305	A <sub>p</sub> ba2	Pba2	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$	$(m_x^*1/2, 1/2, 0)$	$(m_y^*1/2, 1/2, 0)$	$(2_z^*0, 0, 0)$
41.7.306	A <sub>p</sub> b'a'2'	Pca2 <sub>1</sub>	$(0, 1/4, 0; a, b, c)$	$(1^*0, 0, 0)$	$(m_x^*1/2, 0, 1/2)$	$(m_y^*1/2, 1/2, 0)$	$(2_z^*0, 1/2, 1/2)$
41.8.307	A <sub>p</sub> ba'2'	Pna2 <sub>1</sub>	$(0, 1/4, 0; b, \frac{b+c}{2}, c)$	$(1^*0, 0, 0)$	$(m_x^*1/2, 1/2, 0)$	$(m_y^*1/2, 0, 1/2)$	$(2_z^*0, 1/2, 1/2)$
41.9.308	A <sub>p</sub> b'a'2	Pnc2	$(0, 0, 0; b, \frac{b+c}{2}, c)$	$(1^*0, 0, 0)$	$(m_x^*1/2, 0, 1/2)$	$(m_y^*1/2, 0, 1/2)$	$(2_z^*0, 0, 0)$
<b>42.1.309</b>	<b>Fmm2</b>			<b><math>(1^*0, 0, 0)</math></b>	<b><math>(m_x^*0, 0, 0)</math></b>	<b><math>(m_y^*0, 0, 0)</math></b>	<b><math>(2_z^*0, 0, 0)</math></b>

42.2.310	Fmm21'						
42.3.311	Fm'm2'	Cm	$(0,0,0;a,b,\{a+c\}/2)$	$(1^*0,0,0)$	$(m_x^*0,0,0)'$	$(m_y^*0,0,0)$	$(2_z^*0,0,0)'$
42.4.312	Fm'm'2	C2	$(0,0,0;b,c,\{a+b\}/2)$	$(1^*0,0,0)$	$(m_x^*0,0,0)'$	$(m_y^*0,0,0)'$	$(2_z^*0,0,0)$
42.5.313	F <sub>C</sub> mm2	Cmm2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*0,0,0)$	$(2_z^*0,0,0)$
42.6.314	F <sub>A</sub> mm2	Amm2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*0,0,0)$	$(2_z^*0,0,0)$
42.7.315	F <sub>C</sub> mm'2'	Cmc2 <sub>1</sub>	$(0,1/4,0;a,b,c)$	$(1^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*1/2,0,1/2)$	$(2_z^*1/2,0,1/2)$
42.8.316	F <sub>C</sub> m'm'2	Ccc2	$(1/4,1/4,0;a,b,c)$	$(1^*0,0,0)$	$(m_x^*1/2,0,1/2)$	$(m_y^*1/2,0,1/2)$	$(2_z^*0,0,0)$
42.9.317	F <sub>A</sub> m'm'2'	Abm2	$(1/4,1/4,0;a,b,c)$	$(1^*0,0,0)$	$(m_x^*1/2,1/2,0)$	$(m_y^*0,0,0)$	$(2_z^*1/2,1/2,0)$
42.10.318	F <sub>A</sub> mm'2'	Ama2	$(1/4,1/4,0;a,b,c)$	$(1^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*1/2,1/2,0)$	$(2_z^*1/2,1/2,0)$
42.11.319	F <sub>A</sub> m'm'2	Aba2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(m_x^*1/2,1/2,0)$	$(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$
<b>43.1.320</b>	<b>Fdd2</b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(m_x^*1/4,1/4,1/4)</math></b>	<b><math>(m_y^*1/4,1/4,1/4)</math></b>	<b><math>(2_z^*0,0,0)</math></b>
43.2.321	Fdd21'						
43.3.322	Fd'd2'	Cc	$(0,1/8,0;a,b,\{a+c\}/2)$	$(1^*0,0,0)$	$(m_x^*1/4,1/4,1/4)'$	$(m_y^*1/4,1/4,1/4)$	$(2_z^*0,0,0)'$
43.4.323	Fd'd'2	C2	$(0,0,0;b,c,\{a+b\}/2)$	$(1^*0,0,0)$	$(m_x^*1/4,1/4,1/4)'$	$(m_y^*1/4,1/4,1/4)'$	$(2_z^*0,0,0)$
<b>44.1.324</b>	<b>Imm2</b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(m_x^*0,0,0)</math></b>	<b><math>(m_y^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b>
44.2.325	Imm21'						

44.3.326	$Im'm'2'$	Cm	$(0,0,0;a+c,b,c)$	$(1^*0,0,0)$	$(m_x^*0,0,0)'$	$(m_y^*0,0,0)$	$(2_z^*0,0,0)'$
44.4.327	$Im'm'2$	C2	$(0,0,0;a+b,c,a)$	$(1^*0,0,0)$	$(m_x^*0,0,0)'$	$(m_y^*0,0,0)'$	$(2_z^*0,0,0)$
44.5.328	$I_p mm2$	Pmm2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*0,0,0)$	$(2_z^*0,0,0)$
44.6.329	$I_p mm'2'$	$Pmn2_1$	$(0,1/4,0;a,b,c)$	$(1^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*1/2,1/2,1/2)$	$(2_z^*1/2,1/2,1/2)$
44.7.330	$I_p m'm'2$	Pnn2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(m_x^*1/2,1/2,1/2)$	$(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$
<b>45.1.331</b>	<b><math>Iba2</math></b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(m_x^*0,0,1/2)</math></b>	<b><math>(m_y^*0,0,1/2)</math></b>	<b><math>(2_z^*0,0,0)</math></b>
45.2.332	$Iba21'$						
45.3.333	$Ib'a2'$	Cc	$(0,0,0;a+c,b,c)$	$(1^*0,0,0)$	$(m_x^*0,0,1/2)'$	$(m_y^*0,0,1/2)$	$(2_z^*0,0,0)'$
45.4.334	$Ib'a'2$	C2	$(0,0,0;a+b,c,a)$	$(1^*0,0,0)$	$(m_x^*0,0,1/2)'$	$(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$
45.5.335	$I_p ba2$	Pcc2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(m_x^*0,0,1/2)$	$(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$
45.6.336	$I_p ba'2'$	$Pca2_1$	$(1/4,1/4,0;a,b,c)$	$(1^*0,0,0)$	$(m_x^*0,0,1/2)$	$(m_y^*1/2,1/2,0)$	$(2_z^*1/2,1/2,1/2)$
45.7.337	$I_p b'a'2$	Pba2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(m_x^*1/2,1/2,0)$	$(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$
<b>46.1.338</b>	<b><math>Ima2</math></b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(m_x^*1/2,0,0)</math></b>	<b><math>(m_y^*1/2,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b>
46.2.339	$Ima21'$						
46.3.340	$Im'a2'$	Cc	$(0,0,0;a+c,\&,a)$	$(1^*0,0,0)$	$(m_x^*1/2,0,0)'$	$(m_y^*1/2,0,0)$	$(2_z^*0,0,0)'$
46.4.341	$Ima'2'$	Cm	$(1/4,0,0;\&+\&,a,c)$	$(1^*0,0,0)$	$(m_x^*1/2,0,0)$	$(m_y^*1/2,0,0)'$	$(2_z^*0,0,0)'$

46.5.342	$I_m'a'2$	C2	(0,0,0;a+b,c,a)	(1*0,0,0)	( $m_x^*1/2,0,0$ )'	( $m_y^*1/2,0,0$ )'	( $2_z^*0,0,0$ )
46.6.343	$I_p ma2$	Pma2	(0,0,0;a,b,c)	(1*0,0,0)	( $m_x^*1/2,0,0$ )	( $m_y^*1/2,0,0$ )	( $2_z^*0,0,0$ )
46.7.344	$I_p m'a2'$	Pna2 <sub>1</sub>	(1/4,1/4,0;a,b,c)	(1*0,0,0)	( $m_x^*0,1/2,1/2$ )	( $m_y^*1/2,0,0$ )	( $2_z^*1/2,1/2,1/2$ )
46.8.345	$I_p ma'2'$	Pmc2 <sub>1</sub>	(1/4,1/4,0;a,b,c)	(1*0,0,0)	( $m_x^*1/2,0,0$ )	( $m_y^*0,1/2,1/2$ )	( $2_z^*1/2,1/2,1/2$ )
46.9.346	$I_p m'a'2$	Pnc2	(0,0,0;a,b,c)	(1*0,0,0)	( $m_x^*0,1/2,1/2$ )	( $m_y^*0,1/2,1/2$ )	( $2_z^*0,0,0$ )
<b>47.1.347</b>	<b>Pmmm</b>			<b>(1*0,0,0)</b> <b>(&amp;*0,0,0)</b>	<b>(2<sub>x</sub>*0,0,0)</b> <b>(m<sub>x</sub>*0,0,0)</b>	<b>(2<sub>y</sub>*0,0,0)</b> <b>(m<sub>y</sub>*0,0,0)</b>	<b>(2<sub>z</sub>*0,0,0)</b> <b>(m<sub>z</sub>*0,0,0)</b>
47.2.348	Pmmm1'						
47.3.349	Pm'mm	Pmm2	(0,0,0;b,c,a)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *0,0,0) (m <sub>x</sub> *0,0,0)'	(2 <sub>y</sub> *0,0,0)' (m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)' (m <sub>z</sub> *0,0,0)
47.4.350	Pm'm'm	P2/m	(0,0,0;b,c,a)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *0,0,0)' (m <sub>x</sub> *0,0,0)'	(2 <sub>y</sub> *0,0,0)' (m <sub>y</sub> *0,0,0)'	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *0,0,0)
47.5.351	Pm'm'm'	P222	(0,0,0;a,b,c)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *0,0,0) (m <sub>x</sub> *0,0,0)'	(2 <sub>y</sub> *0,0,0) (m <sub>y</sub> *0,0,0)'	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *0,0,0)'
47.6.352	P <sub>2a</sub> mmm	Pmmm	(0,0,0;2a,b,c)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *0,0,0) (m <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,0) (m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *0,0,0)
47.7.353	P <sub>C</sub> mmm	Cmmm	(0,0,0;2a,2b,c)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *0,0,0) (m <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,0) (m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *0,0,0)
47.8.354	P <sub>F</sub> mmm	Fmmm	(0,0,0;2a,2b,2c)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *0,0,0) (m <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,0) (m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *0,0,0)

47.9.355	$P_{2a}mmm'$	Pmma	$(1/2,0,0;2a,b,c)$	$(1^*0,0,0)$ $(\&^*1,0,0)$	$(2_x^*1,0,0)$ $(m_x^*0,0,0)$	$(2_y^*1,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*1,0,0)$
47.10.356	$P_{2c}m'm'm$	Pccm	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,1)$ $(m_x^*0,0,1)$	$(2_y^*0,0,1)$ $(m_y^*0,0,1)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
47.11.357	$P_Cmmm'$	Cmma	$(1/2,0,0;2b,2\&,c)$	$(1^*0,0,0)$ $(\&^*1,0,0)$	$(2_x^*1,0,0)$ $(m_x^*0,0,0)$	$(2_y^*1,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*1,0,0)$
<b>48.1.358</b>	<b>Pnnn</b>			$(1^*0,0,0)$ $(\&^*1/2,1/2,1/2)$	$(2_x^*0,0,0)$ $(m_x^*1/2,1/2,1/2)$	$(2_y^*0,0,0)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,1/2)$
48.2.359	Pnnn1'						
48.3.360	$Pn'nn$	Pnn2	$(0,0,0;b,c,a)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,1/2)'$	$(2_x^*0,0,0)$ $(m_x^*1/2,1/2,1/2)'$	$(2_y^*0,0,0)'$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)'$ $(m_z^*1/2,1/2,1/2)'$
48.4.361	$Pn'n'n$	P2/c	$(1/4,1/4,1/4;b,c,a+b)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,1/2)$	$(2_x^*0,0,0)'$ $(m_x^*1/2,1/2,1/2)'$	$(2_y^*0,0,0)'$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,1/2)$
48.5.362	$Pn'n'n'$	P222	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,1/2)'$	$(2_x^*0,0,0)$ $(m_x^*1/2,1/2,1/2)'$	$(2_y^*0,0,0)$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,1/2)'$
48.6.363	$P_Fnnn$	Fddd	$(0,0,0;2a,2b,2c)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,1/2)$	$(2_x^*0,0,0)$ $(m_x^*1/2,1/2,1/2)$	$(2_y^*0,0,0)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,1/2)$
<b>49.1.364</b>	<b>Pccm</b>			$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,1/2)$ $(m_x^*0,0,1/2)$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$

49.2.365	Pccm1'						
49.3.366	Pc'cm	Pma2	$(0,0,1/4;c,\&,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,1/2)$ $(m_x^*0,0,1/2)'$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)'$ $(m_z^*0,0,0)$
49.4.367	Pccm'	Pcc2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,1/2)'$ $(m_x^*0,0,1/2)$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)'$
49.5.368	Pc'c'm	P2/m	$(0,0,0;b,c,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,1/2)'$ $(m_x^*0,0,1/2)'$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
49.6.369	Pc'cm'	P2/c	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,1/2)'$ $(m_x^*0,0,1/2)'$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)'$ $(m_z^*0,0,0)'$
49.7.370	Pc'c'm'	P222	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,1/2)$ $(m_x^*0,0,1/2)'$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)'$
49.8.371	P <sub>2a</sub> ccm	Pccm	$(0,0,0;2a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,1/2)$ $(m_x^*0,0,1/2)$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
49.9.372	P <sub>C</sub> ccm	Cccm	$(0,0,0;2a,2b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,1/2)$ $(m_x^*0,0,1/2)$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
49.10.373	P <sub>2a</sub> ccm'	Pcca	$(1/2,0,0;2a,b,c)$	$(1^*0,0,0)$ $(\&^*1,0,0)$	$(2_x^*1,0,1/2)$ $(m_x^*0,0,1/2)$	$(2_y^*1,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_z^*1,0,0)$
49.11.374	P <sub>2a</sub> c'c'm	Pmna	$(0,0,0;c,b,2a)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1,0,1/2)$ $(m_x^*1,0,1/2)$	$(2_y^*1,0,1/2)$ $(m_y^*1,0,1/2)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
49.12.375	P <sub>2a</sub> c'c'm'	Pban	$(0,0,1/4;c,b,2a)$	$(1^*0,0,0)$ $(\&^*1,0,0)$	$(2_x^*0,0,1/2)$ $(m_x^*1,0,1/2)$	$(2_y^*0,0,1/2)$ $(m_y^*1,0,1/2)$	$(2_z^*0,0,0)$ $(m_z^*1,0,0)$
49.13.376	P <sub>C</sub> ccm'	Ccca	$(1/2,1/2,1/4;2a,2b,c)$	$(1^*0,0,0)$ $(\&^*1,0,0)$	$(2_x^*1,0,1/2)$ $(m_x^*0,0,1/2)$	$(2_y^*1,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_z^*1,0,0)$



50.1.377	Pban			$(1^*0,0,0)$ $(\&^*1/2,1/2,0)$	$(2_x^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(2_y^*0,0,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,0)$
50.2.378	Pban1'						
50.3.379	Pb'an	Pnc2	$(0,0,0;c,\&,a)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)'$	$(2_x^*0,0,0)$ $(m_x^*1/2,1/2,0)'$	$(2_y^*0,0,0)'$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)'$ $(m_z^*1/2,1/2,0)$
50.4.380	Pban'	Pba2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)'$	$(2_x^*0,0,0)'$ $(m_x^*1/2,1/2,0)$	$(2_y^*0,0,0)'$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,0)'$
50.5.381	Pb'a'n	P2/c	$(1/4,1/4,0;b,c,a+b)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)$	$(2_x^*0,0,0)'$ $(m_x^*1/2,1/2,0)'$	$(2_y^*0,0,0)'$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,0)$
50.6.382	Pb'an'	P2/c	$(1/4,1/4,0;c,\&,a)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)$	$(2_x^*0,0,0)'$ $(m_x^*1/2,1/2,0)'$	$(2_y^*0,0,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)'$ $(m_z^*1/2,1/2,0)'$
50.7.383	Pb'a'n'	P222	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)'$	$(2_x^*0,0,0)$ $(m_x^*1/2,1/2,0)'$	$(2_y^*0,0,0)$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,0)'$
50.8.384	P <sub>2c</sub> ban	Pban	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)$	$(2_x^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(2_y^*0,0,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,0)$
50.9.385	P <sub>2c</sub> b'an	Pnna	$(1/4,1/4,1/2;a,2\&,b)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,1)$	$(2_x^*0,0,0)$ $(m_x^*1/2,1/2,1)$	$(2_y^*0,0,1)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,1)$ $(m_z^*1/2,1/2,0)$
50.10.386	P <sub>2c</sub> b'a'n	Pnnn	$(0,0,1/2;a,b,2c)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)$	$(2_x^*0,0,1)$ $(m_x^*1/2,1/2,1)$	$(2_y^*0,0,1)$ $(m_y^*1/2,1/2,1)$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,0)$

51.1.387	<b>Pmma</b>			$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,0,0)$ $(m_x^*1/2,0,0)$	$(2_y^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)$
51.2.388	Pmma1'						
51.3.389	Pm'ma	Pmc2 <sub>1</sub>	(0,0,0;b,c,a)	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*1/2,0,0)$ $(m_x^*1/2,0,0)'$	$(2_y^*0,0,0)'$ $(m_y^*0,0,0)$	$(2_z^*1/2,0,0)'$ $(m_z^*1/2,0,0)$
51.4.390	Pmm'a	Pma2	(0,0,0;a,&,b)	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*1/2,0,0)'$ $(m_x^*1/2,0,0)$	$(2_y^*0,0,0)$ $(m_y^*0,0,0)'$	$(2_z^*1/2,0,0)'$ $(m_z^*1/2,0,0)$
51.5.391	Pmma'	Pmm2	(1/4,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*1/2,0,0)'$ $(m_x^*1/2,0,0)$	$(2_y^*0,0,0)'$ $(m_y^*0,0,0)$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)'$
51.6.392	Pm'm'a	P2/c	(0,0,0;b,c,a)	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,0,0)'$ $(m_x^*1/2,0,0)'$	$(2_y^*0,0,0)'$ $(m_y^*0,0,0)'$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)$
51.7.393	Pmm'a'	P2 <sub>1</sub> /m	(0,0,0;c,a,b)	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,0,0)$ $(m_x^*1/2,0,0)$	$(2_y^*0,0,0)'$ $(m_y^*0,0,0)'$	$(2_z^*1/2,0,0)'$ $(m_z^*1/2,0,0)$
51.8.394	Pm'ma'	P2/m	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,0,0)'$ $(m_x^*1/2,0,0)'$	$(2_y^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*1/2,0,0)'$ $(m_z^*1/2,0,0)$
51.9.395	Pm'm'a'	P22 <sub>2</sub> <sub>1</sub>	(0,0,0;b,c,a)	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*1/2,0,0)$ $(m_x^*1/2,0,0)'$	$(2_y^*0,0,0)$ $(m_y^*0,0,0)'$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)$
51.10.396	P <sub>2b</sub> mma	Pmma	(0,0,0;a,2b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,0,0)$ $(m_x^*1/2,0,0)$	$(2_y^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)$
51.11.397	P <sub>2c</sub> mma	Pmma	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,0,0)$ $(m_x^*1/2,0,0)$	$(2_y^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)$
51.12.398	P <sub>A</sub> mma	Cmcm	(0,0,0;2b,2c,a)	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,0,0)$ $(m_x^*1/2,0,0)$	$(2_y^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)$

51.13.399	$P_{2b} m'ma$	Pbcm	$(0, 1/2, 0; c, a, 2b)$	$(1^*0, 0, 0)$ $(\&^*0, 1, 0)$	$(2_x^*1/2, 0, 0)$ $(m_x^*1/2, 1, 0)$	$(2_y^*0, 1, 0)$ $(m_y^*0, 0, 0)$	$(2_z^*1/2, 1, 0)$ $(m_z^*1/2, 0, 0)$
51.14.400	$P_{2b} mma'$	Pmmn	$(1/4, 0, 0; a, 2b, c)$	$(1^*0, 0, 0)$ $(\&^*0, 1, 0)$	$(2_x^*1/2, 1, 0)$ $(m_x^*1/2, 0, 0)$	$(2_y^*0, 1, 0)$ $(m_y^*0, 0, 0)$	$(2_z^*1/2, 0, 0)$ $(m_z^*1/2, 1, 0)$
51.15.401	$P_{2b} m'ma'$	Pmna	$(0, 0, 0; 2b, c, a)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)$	$(2_x^*1/2, 1, 0)$ $(m_x^*1/2, 1, 0)$	$(2_y^*0, 0, 0)$ $(m_y^*0, 0, 0)$	$(2_z^*1/2, 1, 0)$ $(m_z^*1/2, 1, 0)$
51.16.402	$P_{2c} m'ma$	Pbam	$(0, 0, 1/2; 2c, a, b)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 1)$	$(2_x^*1/2, 0, 0)$ $(m_x^*1/2, 0, 1)$	$(2_y^*0, 0, 1)$ $(m_y^*0, 0, 0)$	$(2_z^*1/2, 0, 1)$ $(m_z^*1/2, 0, 0)$
51.17.403	$P_{2c} mm'a$	Pbcm	$(0, 0, 1/2; b, 2c, a)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 1)$	$(2_x^*1/2, 0, 1)$ $(m_x^*1/2, 0, 0)$	$(2_y^*0, 0, 0)$ $(m_y^*0, 0, 1)$	$(2_z^*1/2, 0, 1)$ $(m_z^*1/2, 0, 0)$
51.18.404	$P_{2c} m'm'a$	Pcca	$(0, 0, 0; a, b, 2c)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)$	$(2_x^*1/2, 0, 1)$ $(m_x^*1/2, 0, 1)$	$(2_y^*0, 0, 1)$ $(m_y^*0, 0, 1)$	$(2_z^*1/2, 0, 0)$ $(m_z^*1/2, 0, 0)$
51.19.405	$P_A m'ma$	Cmca	$(0, 0, 1/2; 2b, 2c, a)$	$(1^*0, 0, 0)$ $(\&^*0, 1, 0)$	$(2_x^*1/2, 0, 0)$ $(m_x^*1/2, 1, 0)$	$(2_y^*0, 1, 0)$ $(m_y^*0, 0, 0)$	$(2_z^*1/2, 1, 0)$ $(m_z^*1/2, 0, 0)$
<b>52.1.406</b>	<b>Pnna</b>			$(1^*0, 0, 0)$ $(\&^*0, 0, 0)$	$(2_x^*0, 1/2, 1/2)$ $(m_x^*0, 1/2, 1/2)$	$(2_y^*1/2, 1/2, 1/2)$ $(m_y^*1/2, 1/2, 1/2)$	$(2_z^*1/2, 0, 0)$ $(m_z^*1/2, 0, 0)$
52.2.407	Pnna1'						
52.3.408	Pn'na	Pnc2	$(0, 1/4, 1/4; b, c, a)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)'$	$(2_x^*0, 1/2, 1/2)$ $(m_x^*0, 1/2, 1/2)'$	$(2_y^*1/2, 1/2, 1/2)'$ $(m_y^*1/2, 1/2, 1/2)$	$(2_z^*1/2, 0, 0)'$ $(m_z^*1/2, 0, 0)$
52.4.409	Pnn'a	Pnc2 <sub>1</sub>	$(1/4, 0, 1/4; a, \&, b)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)'$	$(2_x^*0, 1/2, 1/2)'$ $(m_x^*0, 1/2, 1/2)$	$(2_y^*1/2, 1/2, 1/2)$ $(m_y^*1/2, 1/2, 1/2)'$	$(2_z^*1/2, 0, 0)'$ $(m_z^*1/2, 0, 0)$

52.5.410	Pnna'	Pnn2	$(1/4,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,1/2,1/2)'$ $(m_x^*0,1/2,1/2)$	$(2_y^*1/2,1/2,1/2)'$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)'$
52.6.411	Pn'n'a	P2/c	$(0,0,0;b,c,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,1/2,1/2)'$ $(m_x^*0,1/2,1/2)'$	$(2_y^*1/2,1/2,1/2)'$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)$
52.7.412	Pnn'a'	P2/c	$(0,0,0;\&,a,\&+c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,1/2,1/2)$ $(m_x^*0,1/2,1/2)$	$(2_y^*1/2,1/2,1/2)'$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*1/2,0,0)'$ $(m_z^*1/2,0,0)'$
52.8.413	Pn'na'	P2 <sub>1</sub> /c	$(1/4,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,1/2,1/2)'$ $(m_x^*0,1/2,1/2)'$	$(2_y^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*1/2,0,0)'$ $(m_z^*1/2,0,0)'$
52.9.414	Pn'n'a'	P222 <sub>1</sub>	$(1/4,0,1/4;c,a,b)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,1/2,1/2)$ $(m_x^*0,1/2,1/2)'$	$(2_y^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)'$
<b>53.1.415</b>	<b>Pmna</b>			$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*1/2,0,1/2)$ $(m_y^*1/2,0,1/2)$	$(2_z^*1/2,0,1/2)$ $(m_z^*1/2,0,1/2)$
53.2.416	Pmna1'						
53.3.417	Pm'na	Pnc2	$(0,0,0;b,c,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)'$	$(2_y^*1/2,0,1/2)'$ $(m_y^*1/2,0,1/2)$	$(2_z^*1/2,0,1/2)'$ $(m_z^*1/2,0,1/2)$
53.4.418	Pmn'a	Pma2	$(1/4,0,1/4;a,\&,b)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)'$ $(m_x^*0,0,0)$	$(2_y^*1/2,0,1/2)$ $(m_y^*1/2,0,1/2)'$	$(2_z^*1/2,0,1/2)'$ $(m_z^*1/2,0,1/2)$
53.5.419	Pmna'	Pmn2 <sub>1</sub>	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)'$ $(m_x^*0,0,0)$	$(2_y^*1/2,0,1/2)'$ $(m_y^*1/2,0,1/2)$	$(2_z^*1/2,0,1/2)$ $(m_z^*1/2,0,1/2)'$
53.6.420	Pm'n'a	P2 <sub>1</sub> /c	$(0,0,0;b,c,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)'$ $(m_x^*0,0,0)'$	$(2_y^*1/2,0,1/2)'$ $(m_y^*1/2,0,1/2)'$	$(2_z^*1/2,0,1/2)$ $(m_z^*1/2,0,1/2)$
53.7.421	Pmn'a'	P2/m	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*1/2,0,1/2)'$	$(2_z^*1/2,0,1/2)'$

				$(\&^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*1/2,0,1/2)'$	$(m_z^*1/2,0,1/2)'$
53.8.422	Pm'na'	P2/c	$(0,0,0;a,b,a+c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)'$ $(m_x^*0,0,0)'$	$(2_y^*1/2,0,1/2)$ $(m_y^*1/2,0,1/2)$	$(2_z^*1/2,0,1/2)'$ $(m_z^*1/2,0,1/2)'$
53.9.423	Pm'n'a'	P222 <sub>1</sub>	$(1/4,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)'$	$(2_y^*1/2,0,1/2)$ $(m_y^*1/2,0,1/2)'$	$(2_z^*1/2,0,1/2)$ $(m_z^*1/2,0,1/2)'$
53.10.424	P <sub>2b</sub> mna	Pmna	$(0,0,0;a,2b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*1/2,0,1/2)$ $(m_y^*1/2,0,1/2)$	$(2_z^*1/2,0,1/2)$ $(m_z^*1/2,0,1/2)$
53.11.425	P <sub>2b</sub> m'na	Pbcn	$(0,1/2,0;c,a,2b)$	$(1^*0,0,0)$ $(\&^*0,1,0)$	$(2_x^*0,0,0)$ $(m_x^*0,1,0)$	$(2_y^*1/2,1,1/2)$ $(m_y^*1/2,0,1/2)$	$(2_z^*1/2,1,1/2)$ $(m_z^*1/2,0,1/2)$
53.12.426	P <sub>2b</sub> mna'	Pnnm	$(0,1/2,0;2b,c,a)$	$(1^*0,0,0)$ $(\&^*0,1,0)$	$(2_x^*0,1,0)$ $(m_x^*0,0,0)$	$(2_y^*1/2,1,1/2)$ $(m_y^*1/2,0,1/2)$	$(2_z^*1/2,0,1/2)$ $(m_z^*1/2,1,1/2)$
53.13.427	P <sub>2b</sub> m'na'	Pnna	$(0,0,0;2b,c,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,1,0)$ $(m_x^*0,1,0)$	$(2_y^*1/2,0,1/2)$ $(m_y^*1/2,0,1/2)$	$(2_z^*1/2,1,1/2)$ $(m_z^*1/2,1,1/2)$
<b>54.1.428</b>	<b>Pcca</b>			$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,0,1/2)$ $(m_x^*1/2,0,1/2)$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)$
54.2.429	Pcca1'						
54.3.430	Pc'ca	Pca2 <sub>1</sub>	$(0,0,1/4;c,\&,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*1/2,0,1/2)$ $(m_x^*1/2,0,1/2)'$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)$	$(2_z^*1/2,0,0)'$ $(m_z^*1/2,0,0)$
54.4.431	Pcc'a	Pba2	$(0,0,1/4;c,a,b)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*1/2,0,1/2)'$ $(m_x^*1/2,0,1/2)$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)'$	$(2_z^*1/2,0,0)'$ $(m_z^*1/2,0,0)$
54.5.432	Pcca'	Pcc2	$(1/4,0,0;a,b,c)$	$(1^*0,0,0)$	$(2_x^*1/2,0,1/2)'$	$(2_y^*0,0,1/2)'$	$(2_z^*1/2,0,0)$

				$(\&^*0,0,0)'$	$(m_x^*1/2,0,1/2)$	$(m_y^*0,0,1/2)$	$(m_z^*1/2,0,0)'$
54.6.433	Pc'c'a	P2/c	$(0,0,0;b,c,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,0,1/2)'$ $(m_x^*1/2,0,1/2)'$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)'$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)$
54.7.434	Pcc'a'	P2 <sub>1</sub> /c	$(0,0,0;b,\&,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,0,1/2)$ $(m_x^*1/2,0,1/2)$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)'$	$(2_z^*1/2,0,0)'$ $(m_z^*1/2,0,0)'$
54.8.435	Pc'ca'	P2/c	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,0,1/2)'$ $(m_x^*1/2,0,1/2)'$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*1/2,0,0)'$ $(m_z^*1/2,0,0)'$
54.9.436	Pc'c'a'	P222 <sub>1</sub>	$(0,0,1/4;b,c,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*1/2,0,1/2)$ $(m_x^*1/2,0,1/2)'$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)'$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)'$
54.10.437	P <sub>2b</sub> cca	Pcca	$(0,0,0;a,2b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,0,1/2)$ $(m_x^*1/2,0,1/2)$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)$
54.11.438	P <sub>2b</sub> c'ca	Pbcn	$(0,1/2,0;2b,c,a)$	$(1^*0,0,0)$ $(\&^*0,1,0)$	$(2_x^*1/2,0,1/2)$ $(m_x^*1/2,1,1/2)$	$(2_y^*0,1,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*1/2,1,0)$ $(m_z^*1/2,0,0)$
54.12.439	P <sub>2b</sub> cca'	Pccn	$(0,1/2,0;a,2b,c)$	$(1^*0,0,0)$ $(\&^*0,1,0)$	$(2_x^*1/2,1,1/2)$ $(m_x^*1/2,0,1/2)$	$(2_y^*0,1,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,1,0)$
54.13.440	P <sub>2b</sub> c'ca'	Pnna	$(0,0,0;c,a,2b)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,1,1/2)$ $(m_x^*1/2,1,1/2)$	$(2_y^*0,1,1/2)$ $(m_y^*0,1,1/2)$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)$
<b>55.1.441</b>	<b>Pbam</b>			<b><math>(1^*0,0,0)</math></b> <b><math>(\&amp;^*0,0,0)</math></b>	<b><math>(2_x^*1/2,1/2,0)</math></b> <b><math>(m_x^*1/2,1/2,0)</math></b>	<b><math>(2_y^*1/2,1/2,0)</math></b> <b><math>(m_y^*1/2,1/2,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(m_z^*0,0,0)</math></b>
55.2.442	Pbam1'						

55.3.443	Pb'am	Pmc2 <sub>1</sub>	(0,1/4,0;c,&,a)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *1/2,1/2,0) (m <sub>x</sub> *1/2,1/2,0)'	(2 <sub>y</sub> *1/2,1/2,0)' (m <sub>y</sub> *1/2,1/2,0)	(2 <sub>z</sub> *0,0,0)' (m <sub>z</sub> *0,0,0)
55.4.444	Pbam'	Pba2	(0,0,0;a,b,c)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *1/2,1/2,0)' (m <sub>x</sub> *1/2,1/2,0)	(2 <sub>y</sub> *1/2,1/2,0)' (m <sub>y</sub> *1/2,1/2,0)	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *0,0,0)'
55.5.445	Pb'a'm	P2/m	(0,0,0;a,b,c)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *1/2,1/2,0)' (m <sub>x</sub> *1/2,1/2,0)'	(2 <sub>y</sub> *1/2,1/2,0)' (m <sub>y</sub> *1/2,1/2,0)'	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *0,0,0)
55.6.446	Pb'am'	P2 <sub>1</sub> /c	(0,0,0;c,&,a)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *1/2,1/2,0)' (m <sub>x</sub> *1/2,1/2,0)'	(2 <sub>y</sub> *1/2,1/2,0) (m <sub>y</sub> *1/2,1/2,0)	(2 <sub>z</sub> *0,0,0)' (m <sub>z</sub> *0,0,0)'
55.7.447	Pb'a'm'	P2 <sub>1</sub> 2 <sub>1</sub> 2	(0,0,0;a,b,c)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *1/2,1/2,0) (m <sub>x</sub> *1/2,1/2,0)'	(2 <sub>y</sub> *1/2,1/2,0) (m <sub>y</sub> *1/2,1/2,0)'	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *0,0,0)'
55.8.448	P <sub>2c</sub> bam	Pbam	(0,0,0;a,b,2c)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *1/2,1/2,0) (m <sub>x</sub> *1/2,1/2,0)	(2 <sub>y</sub> *1/2,1/2,0) (m <sub>y</sub> *1/2,1/2,0)	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *0,0,0)
55.9.449	P <sub>2c</sub> b'am	Pnma	(0,0,1/2;a,2&,b)	(1*0,0,0) (&*0,0,1)	(2 <sub>x</sub> *1/2,1/2,0) (m <sub>x</sub> *1/2,1/2,1)	(2 <sub>y</sub> *1/2,1/2,1) (m <sub>y</sub> *1/2,1/2,0)	(2 <sub>z</sub> *0,0,1) (m <sub>z</sub> *0,0,0)
55.10.450	P <sub>2c</sub> b'a'm	Pnnm	(0,0,0;a,b,2c)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *1/2,1/2,1) (m <sub>x</sub> *1/2,1/2,1)	(2 <sub>y</sub> *1/2,1/2,1) (m <sub>y</sub> *1/2,1/2,1)	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *0,0,0)
<b>56.1.451</b>	<b>Pccn</b>			<b>(1*0,0,0) (&amp;*0,0,0)</b>	<b>(2<sub>x</sub>*1/2,0,1/2) (m<sub>x</sub>*1/2,0,1/2)</b>	<b>(2<sub>y</sub>*0,1/2,1/2) (m<sub>y</sub>*0,1/2,1/2)</b>	<b>(2<sub>z</sub>*1/2,1/2,0) (m<sub>z</sub>*1/2,1/2,0)</b>
56.2.452	Pccn1'						
56.3.453	Pc'cn	Pna2 <sub>1</sub>	(0,0,1/4;c,&,a)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *1/2,0,1/2) (m <sub>x</sub> *1/2,0,1/2)'	(2 <sub>y</sub> *0,1/2,1/2)' (m <sub>y</sub> *0,1/2,1/2)	(2 <sub>z</sub> *1/2,1/2,0)' (m <sub>z</sub> *1/2,1/2,0)

56.4.454	Pccn'	Pcc2	$(1/4, 1/4, 0; a, b, c)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)'$	$(2_x^*1/2, 0, 1/2)'$ $(m_x^*1/2, 0, 1/2)$	$(2_y^*0, 1/2, 1/2)'$ $(m_y^*0, 1/2, 1/2)$	$(2_z^*1/2, 1/2, 0)$ $(m_z^*1/2, 1/2, 0)'$
56.5.455	Pc'c'n	P2/c	$(0, 0, 0; b, c, a+b)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)$	$(2_x^*1/2, 0, 1/2)'$ $(m_x^*1/2, 0, 1/2)'$	$(2_y^*0, 1/2, 1/2)'$ $(m_y^*0, 1/2, 1/2)'$	$(2_z^*1/2, 1/2, 0)$ $(m_z^*1/2, 1/2, 0)$
56.6.456	Pc'cn'	P2 <sub>1</sub> /c	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)$	$(2_x^*1/2, 0, 1/2)'$ $(m_x^*1/2, 0, 1/2)'$	$(2_y^*0, 1/2, 1/2)$ $(m_y^*0, 1/2, 1/2)$	$(2_z^*1/2, 1/2, 0)'$ $(m_z^*1/2, 1/2, 0)'$
56.7.457	Pc'c'n'	P2 <sub>1</sub> 2 <sub>1</sub> 2	$(1/4, 1/4, 1/4; a, b, c)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)'$	$(2_x^*1/2, 0, 1/2)$ $(m_x^*1/2, 0, 1/2)'$	$(2_y^*0, 1/2, 1/2)$ $(m_y^*0, 1/2, 1/2)'$	$(2_z^*1/2, 1/2, 0)$ $(m_z^*1/2, 1/2, 0)'$
<b>57.1.458</b>	<b>Pbcm</b>			$(1^*0, 0, 0)$ $(\&^*0, 0, 0)$	$(2_x^*0, 1/2, 0)$ $(m_x^*0, 1/2, 0)$	$(2_y^*0, 1/2, 1/2)$ $(m_y^*0, 1/2, 1/2)$	$(2_z^*0, 0, 1/2)$ $(m_z^*0, 0, 1/2)$
57.2.459	Pbcm1'						
57.3.460	Pb'cm	Pma2	$(0, 1/4, 0; c, \&, a)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)'$	$(2_x^*0, 1/2, 0)$ $(m_x^*0, 1/2, 0)'$	$(2_y^*0, 1/2, 1/2)'$ $(m_y^*0, 1/2, 1/2)$	$(2_z^*0, 0, 1/2)'$ $(m_z^*0, 0, 1/2)$
57.4.461	Pbc'm	Pmc2 <sub>1</sub>	$(0, 0, 1/4; c, a, b)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)'$	$(2_x^*0, 1/2, 0)'$ $(m_x^*0, 1/2, 0)$	$(2_y^*0, 1/2, 1/2)$ $(m_y^*0, 1/2, 1/2)'$	$(2_z^*0, 0, 1/2)'$ $(m_z^*0, 0, 1/2)$
57.5.462	Pbcm'	Pca2 <sub>1</sub>	$(0, 0, 0; b, \&, c)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)'$	$(2_x^*0, 1/2, 0)'$ $(m_x^*0, 1/2, 0)$	$(2_y^*0, 1/2, 1/2)'$ $(m_y^*0, 1/2, 1/2)$	$(2_z^*0, 0, 1/2)$ $(m_z^*0, 0, 1/2)'$
57.6.463	Pb'c'm	P2 <sub>1</sub> /m	$(0, 0, 0; b, c, a)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)$	$(2_x^*0, 1/2, 0)'$ $(m_x^*0, 1/2, 0)'$	$(2_y^*0, 1/2, 1/2)'$ $(m_y^*0, 1/2, 1/2)'$	$(2_z^*0, 0, 1/2)$ $(m_z^*0, 0, 1/2)$
57.7.464	Pbc'm'	P2/c	$(0, 0, 0; c, a, b)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)$	$(2_x^*0, 1/2, 0)$ $(m_x^*0, 1/2, 0)$	$(2_y^*0, 1/2, 1/2)'$ $(m_y^*0, 1/2, 1/2)'$	$(2_z^*0, 0, 1/2)'$ $(m_z^*0, 0, 1/2)'$



57.8.465	Pb'cm'	P2 <sub>1</sub> /c	(0,0,0;a,b,c)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *0,1/2,0)' (m <sub>x</sub> *0,1/2,0)'	(2 <sub>y</sub> *0,1/2,1/2) (m <sub>y</sub> *0,1/2,1/2)'	(2 <sub>z</sub> *0,0,1/2)' (m <sub>z</sub> *0,0,1/2)'
57.9.466	Pb'c'm'	P2 <sub>1</sub> 2 <sub>1</sub> 2	(0,1/4,0;c,&,a)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *0,1/2,0) (m <sub>x</sub> *0,1/2,0)'	(2 <sub>y</sub> *0,1/2,1/2) (m <sub>y</sub> *0,1/2,1/2)'	(2 <sub>z</sub> *0,0,1/2) (m <sub>z</sub> *0,0,1/2)'
57.10.467	P <sub>2a</sub> bcm	Pbcm	(0,0,0;2a,b,c)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *0,1/2,0) (m <sub>x</sub> *0,1/2,0)	(2 <sub>y</sub> *0,1/2,1/2) (m <sub>y</sub> *0,1/2,1/2)	(2 <sub>z</sub> *0,0,1/2) (m <sub>z</sub> *0,0,1/2)
57.11.468	P <sub>2a</sub> bc'm	Pnma	(1/2,0,0;b,c,2a)	(1*0,0,0) (&*1,0,0)	(2 <sub>x</sub> *1,1/2,0) (m <sub>x</sub> *0,1/2,0)	(2 <sub>y</sub> *0,1/2,1/2) (m <sub>y</sub> *1,1/2,1/2)	(2 <sub>z</sub> *1,0,1/2) (m <sub>z</sub> *0,0,1/2)
57.12.469	P <sub>2a</sub> bcm'	Pbca	(1/2,0,0;2a,b,c)	(1*0,0,0) (&*1,0,0)	(2 <sub>x</sub> *1,1/2,0) (m <sub>x</sub> *0,1/2,0)	(2 <sub>y</sub> *1,1/2,1/2) (m <sub>y</sub> *0,1/2,1/2)	(2 <sub>z</sub> *0,0,1/2) (m <sub>z</sub> *1,0,1/2)
57.13.470	P <sub>2a</sub> bc'm'	Pbcn	(0,0,0;c,2a,b)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *0,1/2,0) (m <sub>x</sub> *0,1/2,0)	(2 <sub>y</sub> *1,1/2,1/2) (m <sub>y</sub> *1,1/2,1/2)	(2 <sub>z</sub> *1,0,1/2) (m <sub>z</sub> *1,0,1/2)
<b>58.1.471</b>	<b>Pnnm</b>			<b>(1*0,0,0) (&amp;*0,0,0)</b>	<b>(2<sub>x</sub>*1/2,1/2,1/2) (m<sub>x</sub>*1/2,1/2,1/2)</b>	<b>(2<sub>y</sub>*1/2,1/2,1/2) (m<sub>y</sub>*1/2,1/2,1/2)</b>	<b>(2<sub>z</sub>*0,0,0) (m<sub>z</sub>*0,0,0)</b>
58.2.472	Pnnm1'						
58.3.473	Pn'nm	Pmn2 <sub>1</sub>	(0,1/4,0;c,&,a)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *1/2,1/2,1/2) (m <sub>x</sub> *1/2,1/2,1/2)'	(2 <sub>y</sub> *1/2,1/2,1/2)' (m <sub>y</sub> *1/2,1/2,1/2)	(2 <sub>z</sub> *0,0,0)' (m <sub>z</sub> *0,0,0)
58.4.474	Pnnm'	Pnn2	(0,0,0;a,b,c)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *1/2,1/2,1/2)' (m <sub>x</sub> *1/2,1/2,1/2)	(2 <sub>y</sub> *1/2,1/2,1/2)' (m <sub>y</sub> *1/2,1/2,1/2)	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *0,0,0)'
58.5.475	Pn'n'm	P2/m	(0,0,0;a,b,c)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *1/2,1/2,1/2)' (m <sub>x</sub> *1/2,1/2,1/2)'	(2 <sub>y</sub> *1/2,1/2,1/2)' (m <sub>y</sub> *1/2,1/2,1/2)'	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *0,0,0)

58.6.476	Pnn'm'	P2 <sub>1</sub> /c	(0,0,0; & a, & +c)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *1/2,1/2,1/2) (m <sub>x</sub> *1/2,1/2,1/2)	(2 <sub>y</sub> *1/2,1/2,1/2)' (m <sub>y</sub> *1/2,1/2,1/2)'	(2 <sub>z</sub> *0,0,0)' (m <sub>z</sub> *0,0,0)'
58.7.477	Pn'n'm'	P2 <sub>1</sub> 2 <sub>1</sub> 2	(0,0,1/4;a,b,c)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *1/2,1/2,1/2) (m <sub>x</sub> *1/2,1/2,1/2)'	(2 <sub>y</sub> *1/2,1/2,1/2) (m <sub>y</sub> *1/2,1/2,1/2)'	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *0,0,0)'
<b>59.1.478</b>	<b>Pmmn</b>			<b>(1*0,0,0) (&amp;*1/2,1/2,0)</b>	<b>(2<sub>x</sub>*1/2,1/2,0) (m<sub>x</sub>*0,0,0)</b>	<b>(2<sub>y</sub>*1/2,1/2,0) (m<sub>y</sub>*0,0,0)</b>	<b>(2<sub>z</sub>*0,0,0) (m<sub>z</sub>*1/2,1/2,0)</b>
59.2.479	Pmmn1'						
59.3.480	Pm'mn	Pmn2 <sub>1</sub>	(0,0,0;b,c,a)	(1*0,0,0) (&*1/2,1/2,0)'	(2 <sub>x</sub> *1/2,1/2,0) (m <sub>x</sub> *0,0,0)'	(2 <sub>y</sub> *1/2,1/2,0)' (m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)' (m <sub>z</sub> *1/2,1/2,0)
59.4.481	Pmmn'	Pmm2	(0,0,0;a,b,c)	(1*0,0,0) (&*1/2,1/2,0)'	(2 <sub>x</sub> *1/2,1/2,0)' (m <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *1/2,1/2,0)' (m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *1/2,1/2,0)'
59.5.482	Pm'm'n	P2/c	(1/4,1/4,0;b,c,a+b)	(1*0,0,0) (&*1/2,1/2,0)	(2 <sub>x</sub> *1/2,1/2,0)' (m <sub>x</sub> *0,0,0)'	(2 <sub>y</sub> *1/2,1/2,0)' (m <sub>y</sub> *0,0,0)'	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *1/2,1/2,0)
59.6.483	Pmm'n'	P2 <sub>1</sub> /m	(1/4,1/4,0;c,a,b)	(1*0,0,0) (&*1/2,1/2,0)	(2 <sub>x</sub> *1/2,1/2,0) (m <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *1/2,1/2,0)' (m <sub>y</sub> *0,0,0)'	(2 <sub>z</sub> *0,0,0)' (m <sub>z</sub> *1/2,1/2,0)'
59.7.484	Pm'm'n'	P2 <sub>1</sub> 2 <sub>1</sub> 2	(0,0,0;a,b,c)	(1*0,0,0) (&*1/2,1/2,0)'	(2 <sub>x</sub> *1/2,1/2,0) (m <sub>x</sub> *0,0,0)'	(2 <sub>y</sub> *1/2,1/2,0) (m <sub>y</sub> *0,0,0)'	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *1/2,1/2,0)'
59.8.485	P <sub>2c</sub> mmn	Pmmn	(0,0,0;a,b,2c)	(1*0,0,0) (&*1/2,1/2,0)	(2 <sub>x</sub> *1/2,1/2,0) (m <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *1/2,1/2,0) (m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *1/2,1/2,0)
59.9.486	P <sub>2c</sub> m'mn	Pnma	(1/4,1/4,1/2;2c,&,a)	(1*0,0,0) (&*1/2,1/2,1)	(2 <sub>x</sub> *1/2,1/2,0) (m <sub>x</sub> *0,0,1)	(2 <sub>y</sub> *1/2,1/2,1) (m <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,1) (m <sub>z</sub> *1/2,1/2,0)
59.10.487	P <sub>2c</sub> m'm'n	Pccn	(1/4,1/4,0;a,b,2c)	(1*0,0,0)	(2 <sub>x</sub> *1/2,1/2,1)	(2 <sub>y</sub> *1/2,1/2,1)	(2 <sub>z</sub> *0,0,0)

$(\&^*_{1/2,1/2,0})$      $(m_x^*0,0,1)$      $(m_y^*0,0,1)$      $(m_z^*_{1/2,1/2,0})$

<b>60.1.488</b>	<b>Pbcn</b>			$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*_{1/2,1/2,0})$ $(m_x^*_{1/2,1/2,0})$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*_{1/2,1/2,1/2})$ $(m_z^*_{1/2,1/2,1/2})$
60.2.489	Pbcn1'						
60.3.490	Pb'cn	Pna2 <sub>1</sub>	$(0,1/4,0;c,\&,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*_{1/2,1/2,0})$ $(m_x^*_{1/2,1/2,0})'$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)$	$(2_z^*_{1/2,1/2,1/2})'$ $(m_z^*_{1/2,1/2,1/2})$
60.4.491	Pbc'n	Pnc2	$(0,0,1/4;c,a,b)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*_{1/2,1/2,0})'$ $(m_x^*_{1/2,1/2,0})$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)'$	$(2_z^*_{1/2,1/2,1/2})'$ $(m_z^*_{1/2,1/2,1/2})$
60.5.492	Pbcn'	Pca2 <sub>1</sub>	$(1/4,1/4,0;b,\&,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*_{1/2,1/2,0})'$ $(m_x^*_{1/2,1/2,0})$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)$	$(2_z^*_{1/2,1/2,1/2})$ $(m_z^*_{1/2,1/2,1/2})'$
60.6.493	Pb'c'n	P2 <sub>1</sub> /c	$(0,0,0;b,c,a+b)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*_{1/2,1/2,0})'$ $(m_x^*_{1/2,1/2,0})'$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)'$	$(2_z^*_{1/2,1/2,1/2})$ $(m_z^*_{1/2,1/2,1/2})$
60.7.494	Pbc'n'	P2 <sub>1</sub> /c	$(0,0,0;c,a,b)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*_{1/2,1/2,0})$ $(m_x^*_{1/2,1/2,0})$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)'$	$(2_z^*_{1/2,1/2,1/2})'$ $(m_z^*_{1/2,1/2,1/2})'$
60.8.495	Pb'cn'	P2/c	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*_{1/2,1/2,0})'$ $(m_x^*_{1/2,1/2,0})'$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*_{1/2,1/2,1/2})'$ $(m_z^*_{1/2,1/2,1/2})'$
60.9.496	Pb'c'n'	P2 <sub>1</sub> 2 <sub>2</sub>	$(0,1/4,1/4;c,a,b)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*_{1/2,1/2,0})$ $(m_x^*_{1/2,1/2,0})'$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)'$	$(2_z^*_{1/2,1/2,1/2})$ $(m_z^*_{1/2,1/2,1/2})'$
<b>61.1.497</b>	<b>Pbca</b>			$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*_{1/2,1/2,0})$ $(m_x^*_{1/2,1/2,0})$	$(2_y^*0,1/2,1/2)$ $(m_y^*0,1/2,1/2)$	$(2_z^*_{1/2,0,1/2})$ $(m_z^*_{1/2,0,1/2})$

61.2.498	Pbca1'						
61.3.499	Pb'ca	Pca2 <sub>1</sub>	(0,1/4,0;c,&,a)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *1/2,1/2,0) (m <sub>x</sub> *1/2,1/2,0)'	(2 <sub>y</sub> *0,1/2,1/2)' (m <sub>y</sub> *0,1/2,1/2)	(2 <sub>z</sub> *1/2,0,1/2)' (m <sub>z</sub> *1/2,0,1/2)
61.4.500	Pb'c'a	P2 <sub>1</sub> /c	(0,0,0;b,c,a)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *1/2,1/2,0)' (m <sub>x</sub> *1/2,1/2,0)'	(2 <sub>y</sub> *0,1/2,1/2)' (m <sub>y</sub> *0,1/2,1/2)'	(2 <sub>z</sub> *1/2,0,1/2) (m <sub>z</sub> *1/2,0,1/2)
61.5.501	Pb'c'a'	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	(0,0,0;a,b,c)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *1/2,1/2,0) (m <sub>x</sub> *1/2,1/2,0)'	(2 <sub>y</sub> *0,1/2,1/2) (m <sub>y</sub> *0,1/2,1/2)'	(2 <sub>z</sub> *1/2,0,1/2) (m <sub>z</sub> *1/2,0,1/2)'
<b>62.1.502</b>	<b>Pnma</b>			<b>(1*0,0,0) (&amp;*0,0,0)</b>	<b>(2<sub>x</sub>*1/2,1/2,1/2) (m<sub>x</sub>*1/2,1/2,1/2)</b>	<b>(2<sub>y</sub>*0,1/2,0) (m<sub>y</sub>*0,1/2,0)</b>	<b>(2<sub>z</sub>*1/2,0,1/2) (m<sub>z</sub>*1/2,0,1/2)</b>
62.2.503	Pnma1'						
62.3.504	Pn'ma	Pmc2 <sub>1</sub>	(0,1/4,1/4;b,c,a)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *1/2,1/2,1/2) (m <sub>x</sub> *1/2,1/2,1/2)'	(2 <sub>y</sub> *0,1/2,0)' (m <sub>y</sub> *0,1/2,0)	(2 <sub>z</sub> *1/2,0,1/2)' (m <sub>z</sub> *1/2,0,1/2)
62.4.505	Pnm'a	Pna2 <sub>1</sub>	(0,0,0;a,&,b)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *1/2,1/2,1/2)' (m <sub>x</sub> *1/2,1/2,1/2)	(2 <sub>y</sub> *0,1/2,0) (m <sub>y</sub> *0,1/2,0)'	(2 <sub>z</sub> *1/2,0,1/2)' (m <sub>z</sub> *1/2,0,1/2)
62.5.506	Pnma'	Pmn2 <sub>1</sub>	(1/4,1/4,0;b,&,c)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *1/2,1/2,1/2)' (m <sub>x</sub> *1/2,1/2,1/2)	(2 <sub>y</sub> *0,1/2,0)' (m <sub>y</sub> *0,1/2,0)	(2 <sub>z</sub> *1/2,0,1/2) (m <sub>z</sub> *1/2,0,1/2)'
62.6.507	Pn'm'a	P2 <sub>1</sub> /c	(0,0,0;b,c,a)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *1/2,1/2,1/2)' (m <sub>x</sub> *1/2,1/2,1/2)'	(2 <sub>y</sub> *0,1/2,0)' (m <sub>y</sub> *0,1/2,0)'	(2 <sub>z</sub> *1/2,0,1/2) (m <sub>z</sub> *1/2,0,1/2)
62.7.508	Pnm'a'	P2 <sub>1</sub> /c	(0,0,0;&,a,&+c)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *1/2,1/2,1/2) (m <sub>x</sub> *1/2,1/2,1/2)	(2 <sub>y</sub> *0,1/2,0)' (m <sub>y</sub> *0,1/2,0)'	(2 <sub>z</sub> *1/2,0,1/2)' (m <sub>z</sub> *1/2,0,1/2)'
62.8.509	Pn'ma'	P2 <sub>1</sub> /m	(0,0,0;a,b,c)	(1*0,0,0)	(2 <sub>x</sub> *1/2,1/2,1/2)'	(2 <sub>y</sub> *0,1/2,0)	(2 <sub>z</sub> *1/2,0,1/2)'

				$(\&^*0,0,0)$	$(m_x^*1/2,1/2,1/2)'$	$(m_y^*0,1/2,0)$	$(m_z^*1/2,0,1/2)'$
62.9.510	Pn'm'a'	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	(0,0,1/4;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*1/2,1/2,1/2)$ $(m_x^*1/2,1/2,1/2)'$	$(2_y^*0,1/2,0)$ $(m_y^*0,1/2,0)'$	$(2_z^*1/2,0,1/2)$ $(m_z^*1/2,0,1/2)'$
<b>63.1.511</b>	<b>Cmcm</b>			$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,1/2)$ $(m_z^*0,0,1/2)$
63.2.512	Cmcm1'						
63.3.513	Cm'cm	Ama2	(0,0,0;c,&,a)	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)'$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,1/2)'$ $(m_z^*0,0,1/2)$
63.4.514	Cmc'm	Amm2	(0,0,1/4;c,a,b)	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)'$ $(m_x^*0,0,0)$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,1/2)'$ $(m_z^*0,0,1/2)$
63.5.515	Cmcm'	Cmc2 <sub>1</sub>	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)'$ $(m_x^*0,0,0)$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,1/2)$ $(m_z^*0,0,1/2)'$
63.6.516	Cm'c'm	P2 <sub>1</sub> /m	(0,0,0;b,c,{a+b}/2)	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)'$ $(m_x^*0,0,0)'$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,1/2)$ $(m_z^*0,0,1/2)$
63.7.517	Cmc'm'	C2/m	(0,0,0;b,&,c)	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,1/2)'$ $(m_z^*0,0,1/2)'$
63.8.518	Cm'cm'	C2/c	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)'$ $(m_x^*0,0,0)'$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,1/2)'$ $(m_z^*0,0,1/2)'$
63.9.519	Cm'c'm'	C222 <sub>1</sub>	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)'$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,1/2)$ $(m_z^*0,0,1/2)'$
63.10.520	C <sub>p</sub> mcm	Pmma	(0,0,0;c,a,b)	$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,1/2)$	$(2_z^*0,0,1/2)$

				$(\&^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*0,0,1/2)$	$(m_z^*0,0,1/2)$
63.11.521	$C_p m'cm$	Pbcm	$(1/4,1/4,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)$	$(2_x^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(2_y^*1/2,1/2,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*1/2,1/2,1/2)$ $(m_z^*0,0,1/2)$
63.12.522	$C_p mc'm$	Pmmn	$(0,1/4,1/4;a,\&,b)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)$	$(2_x^*1/2,1/2,0)$ $(m_x^*0,0,0)$	$(2_y^*0,0,1/2)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*1/2,1/2,1/2)$ $(m_z^*0,0,1/2)$
63.13.523	$C_p mcm'$	Pnma	$(1/4,1/4,0;c,a,b)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)$	$(2_x^*1/2,1/2,0)$ $(m_x^*0,0,0)$	$(2_y^*1/2,1/2,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,1/2)$ $(m_z^*1/2,1/2,1/2)$
63.14.524	$C_p m'c'm$	Pnma	$(0,0,0;b,c,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,1/2,0)$ $(m_x^*1/2,1/2,0)$	$(2_y^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,1/2)$ $(m_z^*0,0,1/2)$
63.15.525	$C_p mc'm'$	Pnnm	$(0,0,0;b,c,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*1/2,1/2,1/2)$ $(m_z^*1/2,1/2,1/2)$
63.16.526	$C_p m'cm'$	Pbcn	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,1/2,0)$ $(m_x^*1/2,1/2,0)$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*1/2,1/2,1/2)$ $(m_z^*1/2,1/2,1/2)$
63.17.527	$C_p m'c'm'$	Pnna	$(1/4,1/4,0;b,c,a)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)$	$(2_x^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(2_y^*0,0,1/2)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,1/2)$ $(m_z^*1/2,1/2,1/2)$
<b>64.1.528</b>	<b>Cmca</b>			$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*0,1/2,1/2)$ $(m_y^*0,1/2,1/2)$	$(2_z^*0,1/2,1/2)$ $(m_z^*0,1/2,1/2)$
64.2.529	Cmca1'						
64.3.530	Cm'ca	Aba2	$(0,0,0;c,\&,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)'$	$(2_y^*0,1/2,1/2)'$ $(m_y^*0,1/2,1/2)$	$(2_z^*0,1/2,1/2)'$ $(m_z^*0,1/2,1/2)$

64.4.531	Cmc'a	Abm2	$(1/4, 0, 1/4; c, a, b)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)'$	$(2_x^*0, 0, 0)'$ $(m_x^*0, 0, 0)$	$(2_y^*0, 1/2, 1/2)$ $(m_y^*0, 1/2, 1/2)'$	$(2_z^*0, 1/2, 1/2)'$ $(m_z^*0, 1/2, 1/2)$
64.5.532	Cmca'	Cmc2 <sub>1</sub>	$(0, 1/4, 0; a, b, c)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)'$	$(2_x^*0, 0, 0)'$ $(m_x^*0, 0, 0)$	$(2_y^*0, 1/2, 1/2)'$ $(m_y^*0, 1/2, 1/2)$	$(2_z^*0, 1/2, 1/2)$ $(m_z^*0, 1/2, 1/2)'$
64.6.533	Cm'c'a	P2 <sub>1</sub> /c	$(0, 0, 0; \{a+b\}/2, c, b)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)$	$(2_x^*0, 0, 0)'$ $(m_x^*0, 0, 0)'$	$(2_y^*0, 1/2, 1/2)'$ $(m_y^*0, 1/2, 1/2)'$	$(2_z^*0, 1/2, 1/2)$ $(m_z^*0, 1/2, 1/2)$
64.7.534	Cmc'a'	C2/m	$(0, 0, 0; b, \&, c)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)$	$(2_x^*0, 0, 0)$ $(m_x^*0, 0, 0)$	$(2_y^*0, 1/2, 1/2)'$ $(m_y^*0, 1/2, 1/2)'$	$(2_z^*0, 1/2, 1/2)'$ $(m_z^*0, 1/2, 1/2)'$
64.8.535	Cm'ca'	C2/c	$(1/4, 1/4, 0; a, b, c)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)$	$(2_x^*0, 0, 0)'$ $(m_x^*0, 0, 0)'$	$(2_y^*0, 1/2, 1/2)$ $(m_y^*0, 1/2, 1/2)$	$(2_z^*0, 1/2, 1/2)'$ $(m_z^*0, 1/2, 1/2)'$
64.9.536	Cm'c'a'	C222 <sub>1</sub>	$(1/4, 0, 0; a, b, c)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)'$	$(2_x^*0, 0, 0)$ $(m_x^*0, 0, 0)'$	$(2_y^*0, 1/2, 1/2)$ $(m_y^*0, 1/2, 1/2)'$	$(2_z^*0, 1/2, 1/2)$ $(m_z^*0, 1/2, 1/2)'$
64.10.537	C <sub>p</sub> mca	Pbam	$(0, 0, 0; c, \&, a)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)$	$(2_x^*0, 0, 0)$ $(m_x^*0, 0, 0)$	$(2_y^*0, 1/2, 1/2)$ $(m_y^*0, 1/2, 1/2)$	$(2_z^*0, 1/2, 1/2)$ $(m_z^*0, 1/2, 1/2)$
64.11.538	C <sub>p</sub> m'ca	Pcca	$(1/4, 1/4, 0; c, a, b)$	$(1^*0, 0, 0)$ $(\&^*1/2, 1/2, 0)$	$(2_x^*0, 0, 0)$ $(m_x^*1/2, 1/2, 0)$	$(2_y^*1/2, 0, 1/2)$ $(m_y^*0, 1/2, 1/2)$	$(2_z^*1/2, 0, 1/2)$ $(m_z^*0, 1/2, 1/2)$
64.12.539	C <sub>p</sub> mc'a	Pnma	$(1/4, 1/4, 0; b, \&, c)$	$(1^*0, 0, 0)$ $(\&^*1/2, 1/2, 0)$	$(2_x^*1/2, 1/2, 0)$ $(m_x^*0, 0, 0)$	$(2_y^*0, 1/2, 1/2)$ $(m_y^*1/2, 0, 1/2)$	$(2_z^*1/2, 0, 1/2)$ $(m_z^*0, 1/2, 1/2)$
64.13.540	C <sub>p</sub> mca'	Pbcm	$(1/4, 1/4, 0; b, c, a)$	$(1^*0, 0, 0)$ $(\&^*1/2, 1/2, 0)$	$(2_x^*1/2, 1/2, 0)$ $(m_x^*0, 0, 0)$	$(2_y^*1/2, 0, 1/2)$ $(m_y^*0, 1/2, 1/2)$	$(2_z^*0, 1/2, 1/2)$ $(m_z^*1/2, 0, 1/2)$
64.14.541	C <sub>p</sub> m'c'a	Pccn	$(0, 0, 0; c, a, b)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)$	$(2_x^*1/2, 1/2, 0)$ $(m_x^*1/2, 1/2, 0)$	$(2_y^*1/2, 0, 1/2)$ $(m_y^*1/2, 0, 1/2)$	$(2_z^*0, 1/2, 1/2)$ $(m_z^*0, 1/2, 1/2)$
64.15.542	C <sub>p</sub> mc'a'	Pmna	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$	$(2_x^*0, 0, 0)$	$(2_y^*1/2, 0, 1/2)$	$(2_z^*1/2, 0, 1/2)$

				$(\&^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*1/2,0,1/2)$	$(m_z^*1/2,0,1/2)$
64.16.543	$C_p m'ca'$	Pbca	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,1/2,0)$ $(m_x^*1/2,1/2,0)$	$(2_y^*0,1/2,1/2)$ $(m_y^*0,1/2,1/2)$	$(2_z^*1/2,0,1/2)$ $(m_z^*1/2,0,1/2)$
64.17.544	$C_p m'c'a'$	Pbcn	$(1/4,1/4,0;c,a,b)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)$	$(2_x^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(2_y^*0,1/2,1/2)$ $(m_y^*1/2,0,1/2)$	$(2_z^*0,1/2,1/2)$ $(m_z^*1/2,0,1/2)$
<b>65.1.545</b>	<b>Cmmm</b>			$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
65.2.546	Cmmm1'						
65.3.547	$Cm'mm$	Amm2	$(0,0,0;c,\&,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)'$	$(2_y^*0,0,0)'$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)'$ $(m_z^*0,0,0)$
65.4.548	$Cmmm'$	Cmm2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)'$ $(m_x^*0,0,0)$	$(2_y^*0,0,0)'$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)'$
65.5.549	$Cm'm'm$	P2/m	$(0,0,0;b,c,\{a+b\}/2)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)'$ $(m_x^*0,0,0)'$	$(2_y^*0,0,0)'$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
65.6.550	$Cmm'm'$	C2/m	$(0,0,0;b,\&,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*0,0,0)'$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)'$ $(m_z^*0,0,0)'$
65.7.551	$Cm'm'm'$	C222	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)'$	$(2_y^*0,0,0)$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)'$
65.8.552	$C_{2c} mmm$	Cmmm	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
65.9.553	$C_p mmm$	Pmmm	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$



65.10.554	$C_1mmm$	$Immm$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
65.11.555	$C_{2c}m'm'm'$	$Cccm$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,1/2)$ $(m_x^*0,0,1/2)$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
65.12.556	$C_{2c}mm'm'$	$Cmcm$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,1/2)$ $(m_z^*0,0,1/2)$
65.13.557	$C_Pm'mm$	$Pmma$	$(1/4,1/4,0;b,c,a)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)$	$(2_x^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(2_y^*1/2,1/2,0)$ $(m_y^*0,0,0)$	$(2_z^*1/2,1/2,0)$ $(m_z^*0,0,0)$
65.14.558	$C_Pmmm'$	$Pmmn$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)$	$(2_x^*1/2,1/2,0)$ $(m_x^*0,0,0)$	$(2_y^*1/2,1/2,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,0)$
65.15.559	$C_Pm'm'm'$	$Pbam$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,1/2,0)$ $(m_x^*1/2,1/2,0)$	$(2_y^*1/2,1/2,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
65.16.560	$C_Pmm'm'$	$Pmna$	$(0,0,0;a,\&,b)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*1/2,1/2,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*1/2,1/2,0)$ $(m_z^*1/2,1/2,0)$
65.17.561	$C_Pm'm'm'$	$Pban$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)$	$(2_x^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(2_y^*0,0,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,0)$
65.18.562	$C_1m'mm$	$Imma$	$(0,0,1/2;b,2c,a)$	$(1^*0,0,0)$ $(\&^*0,0,1)$	$(2_x^*0,0,0)$ $(m_x^*0,0,1)$	$(2_y^*0,0,1)$ $(m_y^*0,0,0)$	$(2_z^*0,0,1)$ $(m_z^*0,0,0)$
65.19.563	$C_1m'm'm'$	$Ibam$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,1)$ $(m_x^*0,0,1)$	$(2_y^*0,0,1)$ $(m_y^*0,0,1)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
<b>66.1.564</b>	<b><math>Cccm</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(\&amp;^*0,0,0)</math></b>	<b><math>(2_x^*0,0,1/2)</math></b> <b><math>(m_x^*0,0,1/2)</math></b>	<b><math>(2_y^*0,0,1/2)</math></b> <b><math>(m_y^*0,0,1/2)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(m_z^*0,0,0)</math></b>
66.2.565	$Cccm1'$						

66.3.566	Cc'cm	Ama2	$(0,0,1/4;c,\&,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,1/2)$ $(m_x^*0,0,1/2)'$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)'$ $(m_z^*0,0,0)$
66.4.567	Cccm'	Ccc2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,1/2)'$ $(m_x^*0,0,1/2)$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)'$
66.5.568	Cc'c'm	P2/m	$(0,0,0;b,c,\{a+b\}/2)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,1/2)'$ $(m_x^*0,0,1/2)'$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
66.6.569	Ccc'm'	C2/c	$(0,0,0;b,\&,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,1/2)$ $(m_x^*0,0,1/2)$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)'$ $(m_z^*0,0,0)'$
66.7.570	Cc'c'm'	C222	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,1/2)$ $(m_x^*0,0,1/2)'$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)'$
66.8.571	C <sub>p</sub> ccm	Pccm	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,1/2)$ $(m_x^*0,0,1/2)$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
66.9.572	C <sub>p</sub> c'cm	Pmna	$(1/4,1/4,0;c,a,b)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)$	$(2_x^*0,0,1/2)$ $(m_x^*1/2,1/2,1/2)$	$(2_y^*1/2,1/2,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*1/2,1/2,0)$ $(m_z^*0,0,0)$
66.10.573	C <sub>p</sub> ccm'	Pccn	$(1/4,1/4,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)$	$(2_x^*1/2,1/2,1/2)$ $(m_x^*0,0,1/2)$	$(2_y^*1/2,1/2,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,0)$
66.11.574	C <sub>p</sub> c'c'm	Pnnm	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,1/2,1/2)$ $(m_x^*1/2,1/2,1/2)$	$(2_y^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
66.12.575	C <sub>p</sub> cc'm'	Pnna	$(0,0,0;c,\&,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,1/2)$ $(m_x^*0,0,1/2)$	$(2_y^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*1/2,1/2,0)$ $(m_z^*1/2,1/2,0)$
66.13.576	C <sub>p</sub> c'c'm'	Pnnn	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,0)$	$(2_x^*0,0,1/2)$ $(m_x^*1/2,1/2,1/2)$	$(2_y^*0,0,1/2)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,0)$

67.1.577	<b>Cmma</b>			$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*1/2,0,0)$ $(m_y^*1/2,0,0)$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)$
67.2.578	Cmma1'						
67.3.579	Cm'ma	Abm2	$(0,0,0;c,\&,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)'$	$(2_y^*1/2,0,0)'$ $(m_y^*1/2,0,0)$	$(2_z^*1/2,0,0)'$ $(m_z^*1/2,0,0)$
67.4.580	Cmma'	Cmm2	$(0,1/4,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)'$ $(m_x^*0,0,0)$	$(2_y^*1/2,0,0)'$ $(m_y^*1/2,0,0)$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)'$
67.5.581	Cm'm'a	P2/c	$(0,0,0;\{a+b\}/2,c,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)'$ $(m_x^*0,0,0)'$	$(2_y^*1/2,0,0)'$ $(m_y^*1/2,0,0)'$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)$
67.6.582	Cmm'a'	C2/m	$(0,0,0;b,\&,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*1/2,0,0)'$ $(m_y^*1/2,0,0)'$	$(2_z^*1/2,0,0)'$ $(m_z^*1/2,0,0)'$
67.7.583	Cm'm'a'	C222	$(1/4,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)'$	$(2_y^*1/2,0,0)$ $(m_y^*1/2,0,0)'$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)'$
67.8.584	C <sub>2c</sub> mma	Cmma	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*1/2,0,0)$ $(m_y^*1/2,0,0)$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)$
67.9.585	C <sub>p</sub> mma	Pccm	$(0,0,0;b,c,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*1/2,0,0)$ $(m_y^*1/2,0,0)$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)$
67.10.586	C <sub>1</sub> mma	lbam	$(0,0,0;b,2c,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*1/2,0,0)$ $(m_y^*1/2,0,0)$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)$
67.11.587	C <sub>2c</sub> m'ma	Cmca	$(1/4,1/4,1/2;b,2c,a)$	$(1^*0,0,0)$ $(\&^*0,0,1)$	$(2_x^*0,0,0)$ $(m_x^*0,0,1)$	$(2_y^*1/2,0,1)$ $(m_y^*1/2,0,0)$	$(2_z^*1/2,0,1)$ $(m_z^*1/2,0,0)$
67.12.588	C <sub>2c</sub> m'm'a	Ccca	$(1/4,0,1/2;b,\&,2c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,1)$ $(m_x^*0,0,1)$	$(2_y^*1/2,0,1)$ $(m_y^*1/2,0,1)$	$(2_z^*1/2,0,0)$ $(m_z^*1/2,0,0)$

67.13.589	$C_p m' ma$	Pcca	$(1/4, 1/4, 0; b, c, a)$	$(1^*0, 0, 0)$ $(\&^*1/2, 1/2, 0)$	$(2_x^*0, 0, 0)$ $(m_x^*1/2, 1/2, 0)$	$(2_y^*0, 1/2, 0)$ $(m_y^*1/2, 0, 0)$	$(2_z^*0, 1/2, 0)$ $(m_z^*1/2, 0, 0)$
67.14.590	$C_p mm'a$	Pmma	$(1/4, 1/4, 0; a, b, c)$	$(1^*0, 0, 0)$ $(\&^*1/2, 1/2, 0)$	$(2_x^*1/2, 1/2, 0)$ $(m_x^*0, 0, 0)$	$(2_y^*1/2, 0, 0)$ $(m_y^*0, 1/2, 0)$	$(2_z^*0, 1/2, 0)$ $(m_z^*1/2, 0, 0)$
67.15.591	$C_p mma'$	Pbcm	$(1/4, 1/4, 0; c, \&, a)$	$(1^*0, 0, 0)$ $(\&^*1/2, 1/2, 0)$	$(2_x^*1/2, 1/2, 0)$ $(m_x^*0, 0, 0)$	$(2_y^*0, 1/2, 0)$ $(m_y^*1/2, 0, 0)$	$(2_z^*1/2, 0, 0)$ $(m_z^*0, 1/2, 0)$
67.16.592	$C_i mm'a$	Imma	$(0, 0, 1/2; a, b, 2c)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 1)$	$(2_x^*0, 0, 1)$ $(m_x^*0, 0, 0)$	$(2_y^*1/2, 0, 0)$ $(m_y^*1/2, 0, 1)$	$(2_z^*1/2, 0, 1)$ $(m_z^*1/2, 0, 0)$
67.17.593	$C_i m' ma'$	lbca	$(0, 0, 0; a, b, 2c)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)$	$(2_x^*0, 0, 1)$ $(m_x^*0, 0, 1)$	$(2_y^*1/2, 0, 0)$ $(m_y^*1/2, 0, 0)$	$(2_z^*1/2, 0, 1)$ $(m_z^*1/2, 0, 1)$
<b>68.1.594</b>	<b>Ccca</b>			$(1^*0, 0, 0)$ $(\&^*0, 1/2, 1/2)$	$(2_x^*0, 0, 0)$ $(m_x^*0, 1/2, 1/2)$	$(2_y^*0, 0, 0)$ $(m_y^*0, 1/2, 1/2)$	$(2_z^*0, 0, 0)$ $(m_z^*0, 1/2, 1/2)$
68.2.595	Ccca1'						
68.3.596	Cc'ca	Aba2	$(0, 0, 0; c, \&, a)$	$(1^*0, 0, 0)$ $(\&^*0, 1/2, 1/2)'$	$(2_x^*0, 0, 0)$ $(m_x^*0, 1/2, 1/2)'$	$(2_y^*0, 0, 0)'$ $(m_y^*0, 1/2, 1/2)$	$(2_z^*0, 0, 0)'$ $(m_z^*0, 1/2, 1/2)$
68.4.597	Ccca'	Ccc2	$(1/4, 1/4, 0; a, b, c)$	$(1^*0, 0, 0)$ $(\&^*0, 1/2, 1/2)'$	$(2_x^*0, 0, 0)'$ $(m_x^*0, 1/2, 1/2)$	$(2_y^*0, 0, 0)'$ $(m_y^*0, 1/2, 1/2)$	$(2_z^*0, 0, 0)$ $(m_z^*0, 1/2, 1/2)'$
68.5.598	Cc'c'a	P2/c	$(0, 1/4, 1/4; \{a+b\}/2, c, \&)$	$(1^*0, 0, 0)$ $(\&^*0, 1/2, 1/2)$	$(2_x^*0, 0, 0)'$ $(m_x^*0, 1/2, 1/2)'$	$(2_y^*0, 0, 0)'$ $(m_y^*0, 1/2, 1/2)'$	$(2_z^*0, 0, 0)$ $(m_z^*0, 1/2, 1/2)$
68.6.599	Ccc'a'	C2/c	$(1/4, 0, 1/4; b, \&, c)$	$(1^*0, 0, 0)$ $(\&^*0, 1/2, 1/2)$	$(2_x^*0, 0, 0)$ $(m_x^*0, 1/2, 1/2)$	$(2_y^*0, 0, 0)'$ $(m_y^*0, 1/2, 1/2)'$	$(2_z^*0, 0, 0)'$ $(m_z^*0, 1/2, 1/2)'$
68.7.600	Cc'c'a'	C222	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$	$(2_x^*0, 0, 0)$	$(2_y^*0, 0, 0)$	$(2_z^*0, 0, 0)$

				$(\&^*0,1/2,1/2)'$	$(m_x^*0,1/2,1/2)'$	$(m_y^*0,1/2,1/2)'$	$(m_z^*0,1/2,1/2)'$
68.8.601	$C_p cca$	Pban	$(0,0,0;c,\&,a)$	$(1^*0,0,0)$ $(\&^*0,1/2,1/2)$	$(2_x^*0,0,0)$ $(m_x^*0,1/2,1/2)$	$(2_y^*0,0,0)$ $(m_y^*0,1/2,1/2)$	$(2_z^*0,0,0)$ $(m_z^*0,1/2,1/2)$
68.9.602	$C_p c'ca$	Pcca	$(1/4,0,1/4;b,\&,c)$	$(1^*0,0,0)$ $(\&^*1/2,0,1/2)$	$(2_x^*0,0,0)$ $(m_x^*1/2,0,1/2)$	$(2_y^*1/2,1/2,0)$ $(m_y^*0,1/2,1/2)$	$(2_z^*1/2,1/2,0)$ $(m_z^*0,1/2,1/2)$
68.10.603	$C_p cca'$	Pbcn	$(1/4,0,1/4;b,c,a)$	$(1^*0,0,0)$ $(\&^*1/2,0,1/2)$	$(2_x^*1/2,1/2,0)$ $(m_x^*0,1/2,1/2)$	$(2_y^*1/2,1/2,0)$ $(m_y^*0,1/2,1/2)$	$(2_z^*0,0,0)$ $(m_z^*1/2,0,1/2)$
68.11.604	$C_p cc'a'$	Pnna	$(0,1/4,1/4;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,1/2,1/2)$	$(2_x^*0,0,0)$ $(m_x^*0,1/2,1/2)$	$(2_y^*1/2,1/2,0)$ $(m_y^*1/2,0,1/2)$	$(2_z^*1/2,1/2,0)$ $(m_z^*1/2,0,1/2)$
<b>69.1.605</b>	<b>Fmmm</b>			$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
69.2.606	Fmmm1'						
69.3.607	Fm'mm	Fmm2	$(0,0,0;b,c,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)'$	$(2_y^*0,0,0)'$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)'$ $(m_z^*0,0,0)$
69.4.608	Fm'm'm	C2/m	$(0,0,0;b,c,\{a+b\}/2)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)'$ $(m_x^*0,0,0)'$	$(2_y^*0,0,0)'$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
69.5.609	Fm'm'm'	F222	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)'$	$(2_y^*0,0,0)$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)'$
69.6.610	$F_C mmm$	Cmmm	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
69.7.611	$F_C m'mm$	Cmcm	$(1/4,0,1/4;b,c,a)$	$(1^*0,0,0)$ $(\&^*1/2,0,1/2)$	$(2_x^*0,0,0)$ $(m_x^*1/2,0,1/2)$	$(2_y^*1/2,0,1/2)$ $(m_y^*0,0,0)$	$(2_z^*1/2,0,1/2)$ $(m_z^*0,0,0)$

69.8.612	$F_C mmm'$	Cmma	$(1/4, 0, 1/4; b, \&, c)$	$(1^*0, 0, 0)$ $(\&^*1/2, 0, 1/2)$	$(2_x^*1/2, 0, 1/2)$ $(m_x^*0, 0, 0)$	$(2_y^*1/2, 0, 1/2)$ $(m_y^*0, 0, 0)$	$(2_z^*0, 0, 0)$ $(m_z^*1/2, 0, 1/2)$
69.9.613	$F_C m'm'm$	Cccm	$(1/4, 1/4, 0; a, b, c)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)$	$(2_x^*1/2, 0, 1/2)$ $(m_x^*1/2, 0, 1/2)$	$(2_y^*1/2, 0, 1/2)$ $(m_y^*1/2, 0, 1/2)$	$(2_z^*0, 0, 0)$ $(m_z^*0, 0, 0)$
69.10.614	$F_C mm'm'$	Cmca	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$ $(\&^*0, 0, 0)$	$(2_x^*0, 0, 0)$ $(m_x^*0, 0, 0)$	$(2_y^*1/2, 0, 1/2)$ $(m_y^*1/2, 0, 1/2)$	$(2_z^*1/2, 0, 1/2)$ $(m_z^*1/2, 0, 1/2)$
69.11.615	$F_C m'm'm'$	Ccca	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$ $(\&^*1/2, 0, 1/2)$	$(2_x^*0, 0, 0)$ $(m_x^*1/2, 0, 1/2)$	$(2_y^*0, 0, 0)$ $(m_y^*1/2, 0, 1/2)$	$(2_z^*0, 0, 0)$ $(m_z^*1/2, 0, 1/2)$
<b>70.1.616</b>	<b>Fddd</b>			<b><math>(1^*0, 0, 0)</math></b> <b><math>(\&amp;^*1/4, 1/4, 1/4)</math></b>	<b><math>(2_x^*0, 0, 0)</math></b> <b><math>(m_x^*1/4, 1/4, 1/4)</math></b>	<b><math>(2_y^*0, 0, 0)</math></b> <b><math>(m_y^*1/4, 1/4, 1/4)</math></b>	<b><math>(2_z^*0, 0, 0)</math></b> <b><math>(m_z^*1/4, 1/4, 1/4)</math></b>
70.2.617	Fddd1'						
70.3.618	Fd'dd	Fdd2	$(0, 0, 0; b, c, a)$	$(1^*0, 0, 0)$ $(\&^*1/4, 1/4, 1/4)'$	$(2_x^*0, 0, 0)$ $(m_x^*1/4, 1/4, 1/4)'$	$(2_y^*0, 0, 0)'$ $(m_y^*1/4, 1/4, 1/4)$	$(2_z^*0, 0, 0)'$ $(m_z^*1/4, 1/4, 1/4)$
70.4.619	Fd'd'd	C2/c	$(1/8, 1/8, 1/8; b, c, \{a+b\}/2)$	$(1^*0, 0, 0)$ $(\&^*1/4, 1/4, 1/4)$	$(2_x^*0, 0, 0)'$ $(m_x^*1/4, 1/4, 1/4)'$	$(2_y^*0, 0, 0)'$ $(m_y^*1/4, 1/4, 1/4)'$	$(2_z^*0, 0, 0)$ $(m_z^*1/4, 1/4, 1/4)$
70.5.620	Fd'd'd'	F222	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$ $(\&^*1/4, 1/4, 1/4)'$	$(2_x^*0, 0, 0)$ $(m_x^*1/4, 1/4, 1/4)'$	$(2_y^*0, 0, 0)$ $(m_y^*1/4, 1/4, 1/4)'$	$(2_z^*0, 0, 0)$ $(m_z^*1/4, 1/4, 1/4)'$
<b>71.1.621</b>	<b>Immm</b>			<b><math>(1^*0, 0, 0)</math></b> <b><math>(\&amp;^*0, 0, 0)</math></b>	<b><math>(2_x^*0, 0, 0)</math></b> <b><math>(m_x^*0, 0, 0)</math></b>	<b><math>(2_y^*0, 0, 0)</math></b> <b><math>(m_y^*0, 0, 0)</math></b>	<b><math>(2_z^*0, 0, 0)</math></b> <b><math>(m_z^*0, 0, 0)</math></b>
71.2.622	Immm1'						

71.3.623	Im'mm	Imm2	(0,0,0;b,c,a)	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)'$	$(2_y^*0,0,0)'$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)'$ $(m_z^*0,0,0)$
71.4.624	Im'm'm	C2/m	(0,0,0;a+b,c,a)	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)'$ $(m_x^*0,0,0)'$	$(2_y^*0,0,0)'$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
71.5.625	Im'm'm'	Imm2	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)'$	$(2_y^*0,0,0)$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)'$
71.6.626	I <sub>p</sub> mmm	Pmmm	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
71.7.627	I <sub>p</sub> m'mm	Pmmn	(1/4,0,0;b,c,a)	$(1^*0,0,0)$ $(\&^*1/2,1/2,1/2)$	$(2_x^*0,0,0)$ $(m_x^*1/2,1/2,1/2)$	$(2_y^*1/2,1/2,1/2)$ $(m_y^*0,0,0)$	$(2_z^*1/2,1/2,1/2)$ $(m_z^*0,0,0)$
71.8.628	I <sub>p</sub> m'm'm	Pnnm	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,1/2,1/2)$ $(m_x^*1/2,1/2,1/2)$	$(2_y^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
71.9.629	I <sub>p</sub> m'm'm'	Pnnn	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*1/2,1/2,1/2)$	$(2_x^*0,0,0)$ $(m_x^*1/2,1/2,1/2)$	$(2_y^*0,0,0)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,1/2)$
<b>72.1.630</b>	<b>lbam</b>			$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,1/2)$ $(m_x^*0,0,1/2)$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
72.2.631	lbam1'						
72.3.632	lb'am	Ima2	(0,0,1/4;c,&,a)	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,1/2)$ $(m_x^*0,0,1/2)'$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)'$ $(m_z^*0,0,0)$
72.4.633	lbam'	lba2	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,1/2)'$ $(m_x^*0,0,1/2)$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)'$
72.5.634	lb'a'm	C2/m	(0,0,0;a+b,c,a)	$(1^*0,0,0)$	$(2_x^*0,0,1/2)'$	$(2_y^*0,0,1/2)'$	$(2_z^*0,0,0)$

				$(\&^*0,0,0)$	$(m_x^*0,0,1/2)'$	$(m_y^*0,0,1/2)'$	$(m_z^*0,0,0)$
72.6.635	lba'm'	C2/c	$(0,0,0;b+c,\&,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,1/2)$ $(m_x^*0,0,1/2)$	$(2_y^*0,0,1/2)'$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)'$ $(m_z^*0,0,0)'$
72.7.636	lb'a'm'	I222	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*0,0,1/2)$ $(m_x^*0,0,1/2)'$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)'$
72.8.637	I <sub>p</sub> bam	Pccm	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*0,0,1/2)$ $(m_x^*0,0,1/2)$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
72.9.638	I <sub>p</sub> b'am	Pbcm	$(1/4,1/4,1/4;a,b,c)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,1/2)$	$(2_x^*0,0,1/2)$ $(m_x^*1/2,1/2,0)$	$(2_y^*1/2,1/2,0)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,1/2)$
72.10.639	I <sub>p</sub> bam'	Pccn	$(1/4,1/4,1/4;a,b,c)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,1/2)$	$(2_x^*1/2,1/2,0)$ $(m_x^*0,0,1/2)$	$(2_y^*1/2,1/2,0)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,1/2)$
72.11.640	I <sub>p</sub> b'a'm	Pbam	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,1/2,0)$ $(m_x^*1/2,1/2,0)$	$(2_y^*1/2,1/2,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$
72.12.641	I <sub>p</sub> b'am'	Pbcn	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(2_x^*1/2,1/2,0)$ $(m_x^*1/2,1/2,0)$	$(2_y^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*1/2,1/2,1/2)$ $(m_z^*1/2,1/2,1/2)$
72.13.642	I <sub>p</sub> b'a'm'	Pban	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(\&^*1/2,1/2,1/2)$	$(2_x^*0,0,1/2)$ $(m_x^*1/2,1/2,0)$	$(2_y^*0,0,1/2)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,1/2)$
<b>73.1.643</b>	<b>lbca</b>			<b><math>(1^*0,0,0)</math></b> <b><math>(\&amp;^*0,0,0)</math></b>	<b><math>(2_x^*1/2,1/2,0)</math></b> <b><math>(m_x^*1/2,1/2,0)</math></b>	<b><math>(2_y^*0,1/2,1/2)</math></b> <b><math>(m_y^*0,1/2,1/2)</math></b>	<b><math>(2_z^*1/2,0,1/2)</math></b> <b><math>(m_z^*1/2,0,1/2)</math></b>
73.2.644	lbca1'						
73.3.645	lb'ca	lba2	$(0,0,1/4;b,c,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(2_x^*1/2,1/2,0)$ $(m_x^*1/2,1/2,0)'$	$(2_y^*0,1/2,1/2)'$ $(m_y^*0,1/2,1/2)$	$(2_z^*1/2,0,1/2)'$ $(m_z^*1/2,0,1/2)$



73.4.646	Ib'c'a	C2/c	(0,0,0;a+b,c,&)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *1/2,1/2,0)' (m <sub>x</sub> *1/2,1/2,0)'	(2 <sub>y</sub> *0,1/2,1/2)' (m <sub>y</sub> *0,1/2,1/2)'	(2 <sub>z</sub> *1/2,0,1/2) (m <sub>z</sub> *1/2,0,1/2)
73.5.647	Ib'c'a'	I2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	(0,0,0;a,b,c)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *1/2,1/2,0) (m <sub>x</sub> *1/2,1/2,0)'	(2 <sub>y</sub> *0,1/2,1/2) (m <sub>y</sub> *0,1/2,1/2)'	(2 <sub>z</sub> *1/2,0,1/2) (m <sub>z</sub> *1/2,0,1/2)'
73.6.648	I <sub>p</sub> bca	Pbca	(0,0,0;a,b,c)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *1/2,1/2,0) (m <sub>x</sub> *1/2,1/2,0)	(2 <sub>y</sub> *0,1/2,1/2) (m <sub>y</sub> *0,1/2,1/2)	(2 <sub>z</sub> *1/2,0,1/2) (m <sub>z</sub> *1/2,0,1/2)
73.7.649	I <sub>p</sub> b'ca	Pcca	(1/4,1/4,1/4;a,b,c)	(1*0,0,0) (&*1/2,1/2,1/2)	(2 <sub>x</sub> *1/2,1/2,0) (m <sub>x</sub> *0,0,1/2)	(2 <sub>y</sub> *1/2,0,0) (m <sub>y</sub> *0,1/2,1/2)	(2 <sub>z</sub> *0,1/2,0) (m <sub>z</sub> *1/2,0,1/2)
<b>74.1.650</b>	<b>Imma</b>			<b>(1*0,0,0) (&amp;*0,0,0)</b>	<b>(2<sub>x</sub>*0,0,0) (m<sub>x</sub>*0,0,0)</b>	<b>(2<sub>y</sub>*0,1/2,0) (m<sub>y</sub>*0,1/2,0)</b>	<b>(2<sub>z</sub>*0,1/2,0) (m<sub>z</sub>*0,1/2,0)</b>
74.2.651	Imma1'						
74.3.652	Im'ma	Ima2	(0,0,0;b,c,a)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *0,0,0) (m <sub>x</sub> *0,0,0)'	(2 <sub>y</sub> *0,1/2,0)' (m <sub>y</sub> *0,1/2,0)	(2 <sub>z</sub> *0,1/2,0)' (m <sub>z</sub> *0,1/2,0)
74.4.653	Imma'	Imm2	(0,1/4,0;a,b,c)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *0,0,0)' (m <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,1/2,0)' (m <sub>y</sub> *0,1/2,0)	(2 <sub>z</sub> *0,1/2,0) (m <sub>z</sub> *0,1/2,0)'
74.5.654	Im'm'a	C2/c	(0,0,0;a+b,c,&)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *0,0,0)' (m <sub>x</sub> *0,0,0)'	(2 <sub>y</sub> *0,1/2,0)' (m <sub>y</sub> *0,1/2,0)'	(2 <sub>z</sub> *0,1/2,0) (m <sub>z</sub> *0,1/2,0)
74.6.655	Imm'a'	C2/m	(0,0,0;a+b,&,c)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *0,0,0) (m <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,1/2,0)' (m <sub>y</sub> *0,1/2,0)'	(2 <sub>z</sub> *0,1/2,0)' (m <sub>z</sub> *0,1/2,0)'
74.7.656	Im'm'a'	I2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	(0,0,1/4;a,b,c)	(1*0,0,0) (&*0,0,0)'	(2 <sub>x</sub> *0,0,0) (m <sub>x</sub> *0,0,0)'	(2 <sub>y</sub> *0,1/2,0) (m <sub>y</sub> *0,1/2,0)'	(2 <sub>z</sub> *0,1/2,0) (m <sub>z</sub> *0,1/2,0)'
74.8.657	I <sub>p</sub> mma	Pmma	(0,0,0;b,&,c)	(1*0,0,0) (&*0,0,0)	(2 <sub>x</sub> *0,0,0) (m <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,1/2,0) (m <sub>y</sub> *0,1/2,0)	(2 <sub>z</sub> *0,1/2,0) (m <sub>z</sub> *0,1/2,0)

74.9.658	$I_p m'm'a$	Pnna	$(0,0,0;b,\frac{1}{2},c)$	$(1^*0,0,0)$ $(\frac{1}{2}^*0,0,0)$	$(2_x^*1/2,1/2,1/2)$ $(m_x^*1/2,1/2,1/2)$	$(2_y^*1/2,0,1/2)$ $(m_y^*1/2,0,1/2)$	$(2_z^*0,1/2,0)$ $(m_z^*0,1/2,0)$
74.10.659	$I_p mm'a'$	Pmna	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\frac{1}{2}^*0,0,0)$	$(2_x^*0,0,0)$ $(m_x^*0,0,0)$	$(2_y^*1/2,0,1/2)$ $(m_y^*1/2,0,1/2)$	$(2_z^*1/2,0,1/2)$ $(m_z^*1/2,0,1/2)$
74.11.660	$I_p m'ma'$	Pnma	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\frac{1}{2}^*0,0,0)$	$(2_x^*1/2,1/2,1/2)$ $(m_x^*1/2,1/2,1/2)$	$(2_y^*0,1/2,0)$ $(m_y^*0,1/2,0)$	$(2_z^*1/2,0,1/2)$ $(m_z^*1/2,0,1/2)$

## TETRAGONAL SYSTEM

<b>75.1.661</b>	<b>P4</b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(4_z^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b>	<b><math>(4_z^{-1*}0,0,0)</math></b>
75.2.662	P41'						
75.3.663	P4'	P2	$(0,0,0;b,c,a)$	$(1^*0,0,0)$	$(4_z^*0,0,0)'$	$(2_z^*0,0,0)$	$(4_z^{-1*}0,0,0)'$
75.4.664	$P_{2c}4$	P4	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$	$(4_z^*0,0,0)$	$(2_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$
75.5.665	$P_p4$	P4	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$	$(4_z^*0,0,0)$	$(2_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$
75.6.666	$P_14$	I4	$(0,0,0;a-b,a+b,2c)$	$(1^*0,0,0)$	$(4_z^*0,0,0)$	$(2_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$
75.7.667	$P_{2c}4'$	$P4_2$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$	$(4_z^*0,0,1)$	$(2_z^*0,0,0)$	$(4_z^{-1*}0,0,1)$
<b>76.1.668</b>	<b><math>P4_1</math></b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(4_z^*0,0,1/4)</math></b>	<b><math>(2_z^*0,0,1/2)</math></b>	<b><math>(4_z^{-1*}0,0,3/4)</math></b>
76.2.669	$P4_11'$						
76.3.670	$P4_1'$	$P2_1$	$(0,0,0;b,c,a)$	$(1^*0,0,0)$	$(4_z^*0,0,1/4)'$	$(2_z^*0,0,1/2)$	$(4_z^{-1*}0,0,3/4)'$
76.4.671	$P_p4_1$	$P4_1$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$	$(4_z^*0,0,1/4)$	$(2_z^*0,0,1/2)$	$(4_z^{-1*}0,0,3/4)$

<b>77.1.672</b>	<b>P4<sub>2</sub></b>			<b>(1*0,0,0)</b>	<b>(4<sub>z</sub>*0,0,1/2)</b>	<b>(2<sub>z</sub>*0,0,0)</b>	<b>(4<sub>z</sub><sup>-1</sup>*0,0,1/2)</b>
77.2.673	P4 <sub>2</sub> 1'						
77.3.674	P4 <sub>2</sub> '	P2	(0,0,0;b,c,a)	(1*0,0,0)	(4 <sub>z</sub> *0,0,1/2)'	(2 <sub>z</sub> *0,0,0)	(4 <sub>z</sub> <sup>-1</sup> *0,0,1/2)'
77.4.675	P <sub>2c</sub> 4 <sub>2</sub>	P4 <sub>1</sub>	(0,0,0;a,b,2c)	(1*0,0,0)	(4 <sub>z</sub> *0,0,1/2)	(2 <sub>z</sub> *0,0,1)	(4 <sub>z</sub> <sup>-1</sup> *0,0,3/2)
77.5.676	P <sub>P</sub> 4 <sub>2</sub>	P4 <sub>2</sub>	(0,0,0;a-b,a+b,c)	(1*0,0,0)	(4 <sub>z</sub> *0,0,1/2)	(2 <sub>z</sub> *0,0,0)	(4 <sub>z</sub> <sup>-1</sup> *0,0,1/2)
77.6.677	P <sub>1</sub> 4 <sub>2</sub>	I4 <sub>1</sub>	(0,0,0;a-b,a+b,2c)	(1*0,0,0)	(4 <sub>z</sub> *0,0,1/2)	(2 <sub>z</sub> *0,0,1)	(4 <sub>z</sub> <sup>-1</sup> *0,0,3/2)
77.7.678	P <sub>2c</sub> 4 <sub>2</sub> '	P4 <sub>3</sub>	(0,0,0;a,b,2c)	(1*0,0,0)	(4 <sub>z</sub> *0,0,3/2)	(2 <sub>z</sub> *0,0,1)	(4 <sub>z</sub> <sup>-1</sup> *0,0,1/2)
<b>78.1.679</b>	<b>P4<sub>3</sub></b>			<b>(1*0,0,0)</b>	<b>(4<sub>z</sub>*0,0,3/4)</b>	<b>(2<sub>z</sub>*0,0,1/2)</b>	<b>(4<sub>z</sub><sup>-1</sup>*0,0,1/4)</b>
78.2.680	P4 <sub>3</sub> 1'						
78.3.681	P4 <sub>3</sub> '	P2 <sub>1</sub>	(0,0,0;b,c,a)	(1*0,0,0)	(4 <sub>z</sub> *0,0,3/4)'	(2 <sub>z</sub> *0,0,1/2)	(4 <sub>z</sub> <sup>-1</sup> *0,0,1/4)'
78.4.682	P <sub>P</sub> 4 <sub>3</sub>	P4 <sub>3</sub>	(0,0,0;a-b,a+b,c)	(1*0,0,0)	(4 <sub>z</sub> *0,0,3/4)	(2 <sub>z</sub> *0,0,1/2)	(4 <sub>z</sub> <sup>-1</sup> *0,0,1/4)
<b>79.1.683</b>	<b>I4</b>			<b>(1*0,0,0)</b>	<b>(4<sub>z</sub>*0,0,0)</b>	<b>(2<sub>z</sub>*0,0,0)</b>	<b>(4<sub>z</sub><sup>-1</sup>*0,0,0)</b>
79.2.684	I41'						
79.3.685	I4'	C2	(0,0,0;a+b,c,a)	(1*0,0,0)	(4 <sub>z</sub> *0,0,0)'	(2 <sub>z</sub> *0,0,0)	(4 <sub>z</sub> <sup>-1</sup> *0,0,0)'

79.4.686	$I_p 4$	$P4$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(4_z^*0,0,0)$	$(2_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$
79.5.687	$I_p 4'$	$P4_2$	$(0,1/2,0;a,b,c)$	$(1^*0,0,0)$	$(4_z^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)$
<b>80.1.688</b>	<b><math>I4_1</math></b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(4_z^*0,1/2,1/4)</math></b>	<b><math>(2_z^*0,0,0)</math></b>	<b><math>(4_z^{-1*}0,1/2,1/4)</math></b>
80.2.689	$I4_1 1'$						
80.3.690	$I4_1'$	$C2$	$(0,0,0;a+b,c,a)$	$(1^*0,0,0)$	$(4_z^*0,1/2,1/4)'$	$(2_z^*0,0,0)$	$(4_z^{-1*}0,1/2,1/4)'$
80.4.691	$I_p 4_1$	$P4_1$	$(1/4,-1/4,0;a,b,c)$	$(1^*0,0,0)$	$(4_z^*0,1/2,1/4)$	$(2_z^*1/2,1/2,1/2)$	$(4_z^{-1*}1/2,0,3/4)$
80.5.692	$I_p 4_1'$	$P4_3$	$(1/4,1/4,0;a,b,c)$	$(1^*0,0,0)$	$(4_z^*1/2,0,3/4)$	$(2_z^*1/2,1/2,1/2)$	$(4_z^{-1*}0,1/2,1/4)$
<b>81.1.693</b>	<b><math>P\&amp;</math></b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(\&amp;_z^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b>	<b><math>(\&amp;_z^{-1*}0,0,0)</math></b>
81.2.694	$P\& 1'$						
81.3.695	$P\&'$	$P2$	$(0,0,0;b,c,a)$	$(1^*0,0,0)$	$(\&_z^*0,0,0)'$	$(2_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)'$
81.4.696	$P_{2c} \&$	$P\&$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$	$(\&_z^*0,0,0)$	$(2_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
81.5.697	$P_p \&$	$P\&$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$	$(\&_z^*0,0,0)$	$(2_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
81.6.698	$P_1 \&$	$I\&$	$(0,0,0;a-b,a+b,2c)$	$(1^*0,0,0)$	$(\&_z^*0,0,0)$	$(2_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
<b>82.1.699</b>	<b><math>I\&amp;</math></b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(\&amp;_z^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b>	<b><math>(\&amp;_z^{-1*}0,0,0)</math></b>
82.2.700	$I\& 1'$						

82.3.701	$I\&'$	C2	$(0,0,0;a+b,c,a)$	$(1^*0,0,0)$	$(\&_z^*0,0,0)'$	$(2_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)'$
82.4.702	$I_p \&$	$P\&$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(\&_z^*0,0,0)$	$(2_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
<b>83.1.703</b>	<b><math>P4/m</math></b>			<b><math>(1^*0,0,0)</math> <math>(\&amp;^*0,0,0)</math></b>	<b><math>(4_z^*0,0,0)</math> <math>(\&amp;_z^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math> <math>(m_z^*0,0,0)</math></b>	<b><math>(4_z^{-1*}0,0,0)</math> <math>(\&amp;_z^{-1*}0,0,0)</math></b>
83.2.704	$P4/m1'$						
83.3.705	$P4'/m$	$P2/m$	$(0,0,0;b,c,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(4_z^*0,0,0)'$ $(\&_z^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$	$(4_z^{-1*}0,0,0)'$ $(\&_z^{-1*}0,0,0)'$
83.4.706	$P4/m'$	$P4$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(4_z^*0,0,0)$ $(\&_z^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)'$	$(4_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)'$
83.5.707	$P4'/m'$	$P\&$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(4_z^*0,0,0)'$ $(\&_z^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)'$	$(4_z^{-1*}0,0,0)'$ $(\&_z^{-1*}0,0,0)$
83.6.708	$P_{2c}4/m$	$P4/m$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(4_z^*0,0,0)$ $(\&_z^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$
83.7.709	$P_p4/m$	$P4/m$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(4_z^*0,0,0)$ $(\&_z^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$
83.8.710	$P_14/m$	$P4/m$	$(0,0,0;a-b,a+b,2c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(4_z^*0,0,0)$ $(\&_z^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$
83.9.711	$P_{2c}4'/m$	$P4_2/m$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(4_z^*0,0,1)$ $(\&_z^*0,0,1)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$	$(4_z^{-1*}0,0,1)$ $(\&_z^{-1*}0,0,1)$
83.10.712	$P_p4/m'$	$P4/n$	$(1/2,1/2,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(\&^*1,0,0)$	$(4_z^*0,0,0)$ $(\&_z^*1,0,0)$	$(2_z^*0,0,0)$ $(m_z^*1,0,0)$	$(4_z^{-1*}0,0,0)$ $(\&_z^{-1*}1,0,0)$

<b>84.1.713</b>	<b>P4<sub>2</sub>/m</b>			<b>(1*0,0,0)</b> <b>(&amp;*0,0,0)</b>	<b>(4<sub>z</sub>*0,0,1/2)</b> <b>(&amp;<sub>z</sub>*0,0,1/2)</b>	<b>(2<sub>z</sub>*0,0,0)</b> <b>(m<sub>z</sub>*0,0,0)</b>	<b>(4<sub>z</sub><sup>-1</sup>*0,0,1/2)</b> <b>(&amp;<sub>z</sub><sup>-1</sup>*0,0,1/2)</b>
84.2.714	P4 <sub>2</sub> /m1'						
84.3.715	P4 <sub>2</sub> '/m	P2/m	(0,0,0;b,c,a)	(1*0,0,0) (&*0,0,0)	(4 <sub>z</sub> *0,0,1/2)' (& <sub>z</sub> *0,0,1/2)'	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *0,0,0)	(4 <sub>z</sub> <sup>-1</sup> *0,0,1/2)' (& <sub>z</sub> <sup>-1</sup> *0,0,1/2)'
84.4.716	P4 <sub>2</sub> /m'	P4 <sub>2</sub>	(0,0,0;a,b,c)	(1*0,0,0) (&*0,0,0)'	(4 <sub>z</sub> *0,0,1/2) (& <sub>z</sub> *0,0,1/2)'	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *0,0,0)'	(4 <sub>z</sub> <sup>-1</sup> *0,0,1/2) (& <sub>z</sub> <sup>-1</sup> *0,0,1/2)'
84.5.717	P4 <sub>2</sub> '/m'	P&	(0,0,1/4;a,b,c)	(1*0,0,0) (&*0,0,0)'	(4 <sub>z</sub> *0,0,1/2)' (& <sub>z</sub> *0,0,1/2)'	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *0,0,0)'	(4 <sub>z</sub> <sup>-1</sup> *0,0,1/2)' (& <sub>z</sub> <sup>-1</sup> *0,0,1/2)'
84.6.718	P <sub>P</sub> 4 <sub>2</sub> /m	P4 <sub>2</sub> /m	(0,0,0;a-b,a+b,c)	(1*0,0,0) (&*0,0,0)	(4 <sub>z</sub> *0,0,1/2) (& <sub>z</sub> *0,0,1/2)	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *0,0,0)	(4 <sub>z</sub> <sup>-1</sup> *0,0,1/2) (& <sub>z</sub> <sup>-1</sup> *0,0,1/2)
84.7.719	P <sub>P</sub> 4 <sub>2</sub> /m'	P4 <sub>2</sub> /n	(1/2,1/2,1/4;a-b,a+b,c)	(1*0,0,0) (&*1,0,0)	(4 <sub>z</sub> *0,0,1/2) (& <sub>z</sub> *1,0,1/2)	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *1,0,0)	(4 <sub>z</sub> <sup>-1</sup> *0,0,1/2) (& <sub>z</sub> <sup>-1</sup> *1,0,1/2)
<b>85.1.720</b>	<b>P4/n</b>			<b>(1*0,0,0)</b> <b>(&amp;*1/2,1/2,0)</b>	<b>(4<sub>z</sub>*1/2,1/2,0)</b> <b>(&amp;<sub>z</sub>*0,0,0)</b>	<b>(2<sub>z</sub>*0,0,0)</b> <b>(m<sub>z</sub>*1/2,1/2,0)</b>	<b>(4<sub>z</sub><sup>-1</sup>*1/2,1/2,0)</b> <b>(&amp;<sub>z</sub><sup>-1</sup>*0,0,0)</b>
85.2.721	P4/n1'						
85.3.722	P4'/n	P2/c	(1/4,1/4,0;a,c,a+b)	(1*0,0,0) (&*1/2,1/2,0)	(4 <sub>z</sub> *1/2,1/2,0)' (& <sub>z</sub> *0,0,0)'	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *1/2,1/2,0)	(4 <sub>z</sub> <sup>-1</sup> *1/2,1/2,0)' (& <sub>z</sub> <sup>-1</sup> *0,0,0)'
85.4.723	P4'/n'	P4	(1/2,0,0;a,b,c)	(1*0,0,0) (&*1/2,1/2,0)'	(4 <sub>z</sub> *1/2,1/2,0) (& <sub>z</sub> *0,0,0)'	(2 <sub>z</sub> *0,0,0) (m <sub>z</sub> *1/2,1/2,0)'	(4 <sub>z</sub> <sup>-1</sup> *1/2,1/2,0) (& <sub>z</sub> <sup>-1</sup> *0,0,0)'
85.5.724	P4'/n'	P&	(0,0,0;a,b,c)	(1*0,0,0)	(4 <sub>z</sub> *1/2,1/2,0)'	(2 <sub>z</sub> *0,0,0)	(4 <sub>z</sub> <sup>-1</sup> *1/2,1/2,0)'

				$(\&^*_{1/2,1/2,0})'$	$(\&_z^*0,0,0)$	$(m_z^*_{1/2,1/2,0})'$	$(\&_z^{-1*}0,0,0)$
85.6.725	$P_{2c}4/n$	$P4/n$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(\&^*_{1/2,1/2,0})'$	$(4_z^*_{1/2,1/2,0})'$ $(\&_z^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*_{1/2,1/2,0})'$	$(4_z^{-1*}_{1/2,1/2,0})'$ $(\&_z^{-1*}0,0,0)$
85.7.726	$P_{2c}4'/n$	$P4_2/n$	$(1/2,0,0;a,b,2c)$	$(1^*0,0,0)$ $(\&^*_{1/2,1/2,0})'$	$(4_z^*_{1/2,1/2,1})'$ $(\&_z^*0,0,1)$	$(2_z^*0,0,0)$ $(m_z^*_{1/2,1/2,0})'$	$(4_z^{-1*}_{1/2,1/2,1})'$ $(\&_z^{-1*}0,0,1)$
<b>86.1.727</b>	<b><math>P4_2/n</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(\&amp;^*_{1/2,1/2,1/2})'</math></b>	<b><math>(4_z^*_{1/2,1/2,1/2})'</math></b> <b><math>(\&amp;_z^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(m_z^*_{1/2,1/2,1/2})'</math></b>	<b><math>(4_z^{-1*}_{1/2,1/2,1/2})'</math></b> <b><math>(\&amp;_z^{-1*}0,0,0)</math></b>
86.2.728	$P4_2/n1'$						
86.3.729	$P4_2'/n$	$P2/c$	$(1/4,1/4,1/4;a,c,a+b)$	$(1^*0,0,0)$ $(\&^*_{1/2,1/2,1/2})'$	$(4_z^*_{1/2,1/2,1/2})'$ $(\&_z^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_z^*_{1/2,1/2,1/2})'$	$(4_z^{-1*}_{1/2,1/2,1/2})'$ $(\&_z^{-1*}0,0,0)'$
86.4.730	$P4_2/n'$	$P4_2$	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*_{1/2,1/2,1/2})'$	$(4_z^*_{1/2,1/2,1/2})'$ $(\&_z^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_z^*_{1/2,1/2,1/2})'$	$(4_z^{-1*}_{1/2,1/2,1/2})'$ $(\&_z^{-1*}0,0,0)'$
86.5.731	$P4_2'/n'$	$P\&$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*_{1/2,1/2,1/2})'$	$(4_z^*_{1/2,1/2,1/2})'$ $(\&_z^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*_{1/2,1/2,1/2})'$	$(4_z^{-1*}_{1/2,1/2,1/2})'$ $(\&_z^{-1*}0,0,0)$
86.6.732	$P_14_2/n$	$I4_1/a$	$(0,0,0;a-b,a+b,2c)$	$(1^*0,0,0)$ $(\&^*_{1/2,1/2,1/2})'$	$(4_z^*_{1/2,1/2,1/2})'$ $(\&_z^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*_{1/2,1/2,1/2})'$	$(4_z^{-1*}_{1/2,1/2,1/2})'$ $(\&_z^{-1*}0,0,0)$
<b>87.1.733</b>	<b><math>I4/m</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(\&amp;^*0,0,0)</math></b>	<b><math>(4_z^*0,0,0)</math></b> <b><math>(\&amp;_z^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(m_z^*0,0,0)</math></b>	<b><math>(4_z^{-1*}0,0,0)</math></b> <b><math>(\&amp;_z^{-1*}0,0,0)</math></b>
87.2.734	$I4/m1'$						
87.3.735	$I4'/m$	$C2/m$	$(0,0,0;a+b,c,a)$	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(4_z^*0,0,0)'$ $(\&_z^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$	$(4_z^{-1*}0,0,0)'$ $(\&_z^{-1*}0,0,0)'$

87.4.736	I4/m'	I4	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(4_z^*0,0,0)$ $(\&_z^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)'$	$(4_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)'$
87.5.737	I4'/m'	I&	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)'$	$(4_z^*0,0,0)'$ $(\&_z^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)'$	$(4_z^{-1*}0,0,0)'$ $(\&_z^{-1*}0,0,0)$
87.6.738	I <sub>p</sub> 4/m	P4/m	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(4_z^*0,0,0)$ $(\&_z^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$
87.7.739	I <sub>p</sub> 4'/m	P4 <sub>2</sub> /m	(1/2,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(4_z^*1/2,1/2,1/2)$ $(\&_z^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(m_z^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(\&_z^{-1*}1/2,1/2,1/2)$
87.8.740	I <sub>p</sub> 4/m'	P4/n	(1/2,0,1/4;a,b,c)	$(1^*0,0,0)$ $(\&^*1/2,1/2,1/2)$	$(4_z^*0,0,0)$ $(\&_z^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,1/2)$	$(4_z^{-1*}0,0,0)$ $(\&_z^{-1*}1/2,1/2,1/2)$
87.9.741	I <sub>p</sub> 4'/m'	P4 <sub>2</sub> /n	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*1/2,1/2,1/2)$	$(4_z^*1/2,1/2,1/2)$ $(\&_z^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*1/2,1/2,1/2)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(\&_z^{-1*}0,0,0)$
<b>88.1.742</b>	<b>I4<sub>1</sub>/a</b>			<b><math>(1^*0,0,0)</math></b> <b><math>(\&amp;^*0,1/2,1/4)</math></b>	<b><math>(4_z^*0,1/2,1/4)</math></b> <b><math>(\&amp;_z^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(m_z^*0,1/2,1/4)</math></b>	<b><math>(4_z^{-1*}0,1/2,1/4)</math></b> <b><math>(\&amp;_z^{-1*}0,0,0)</math></b>
88.2.743	I4 <sub>1</sub> /a1'						
88.3.744	I4 <sub>1</sub> '/a	C2/c	(0,1/4,3/8;a,&,b)	$(1^*0,0,0)$ $(\&^*0,1/2,1/4)$	$(4_z^*0,1/2,1/4)'$ $(\&_z^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_z^*0,1/2,1/4)$	$(4_z^{-1*}0,1/2,1/4)'$ $(\&_z^{-1*}0,0,0)'$
88.4.745	I4 <sub>1</sub> /a'	I4 <sub>1</sub>	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,1/2,1/4)'$	$(4_z^*0,1/2,1/4)$ $(\&_z^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_z^*0,1/2,1/4)'$	$(4_z^{-1*}0,1/2,1/4)$ $(\&_z^{-1*}0,0,0)'$
88.5.746	I4 <sub>1</sub> '/a'	I&	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,1/2,1/4)'$	$(4_z^*0,1/2,1/4)'$ $(\&_z^*0,0,0)$	$(2_z^*0,0,0)$ $(m_z^*0,1/2,1/4)'$	$(4_z^{-1*}0,1/2,1/4)'$ $(\&_z^{-1*}0,0,0)$



<b>89.1.747</b>	<b>P422</b>			$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)$ $(2_{&y}^*0,0,0)$
89.2.748	P4221'						
89.3.749	P4'22'	P222	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(4_z^*0,0,0)'$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,0)'$ $(2_{&y}^*0,0,0)'$
89.4.750	P42'2'	P4	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)'$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,0)$ $(2_{&y}^*0,0,0)'$
89.5.751	P4'2'2	C222	(0,0,0;a-b,a+b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)'$	$(4_z^*0,0,0)'$ $(2_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)'$ $(2_{&y}^*0,0,0)$
89.6.752	P <sub>2c</sub> 422	P422	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)$ $(2_{&y}^*0,0,0)$
89.7.753	P <sub>p</sub> 422	P422	(0,0,0;a-b,a+b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)$ $(2_{&y}^*0,0,0)$
89.8.754	P <sub>l</sub> 422	I422	(0,0,0;a-b,a+b,2c)	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)$ $(2_{&y}^*0,0,0)$
89.9.755	P <sub>2c</sub> 4'22'	P4 <sub>2</sub> 22	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(4_z^*0,0,1)$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1)$	$(4_z^{-1*}0,0,1)$ $(2_{&y}^*0,0,1)$
89.10.756	P <sub>p</sub> 4'22'	P42 <sub>1</sub> 2	(0,0,0;a-b,a+b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(4_z^*1,0,0)$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1,0,0)$	$(4_z^{-1*}1,0,0)$ $(2_{&y}^*1,0,0)$
<b>90.1.757</b>	<b>P42<sub>1</sub>2</b>			$(1^*0,0,0)$	$(4_z^*1/2,1/2,0)$	$(2_z^*0,0,0)$	$(4_z^{-1*}1/2,1/2,0)$

				$(2_x^* 1/2, 1/2, 0)$	$(2_y^* 1/2, 1/2, 0)$	$(2_{xy}^* 0, 0, 0)$	$(2_{\&y}^* 0, 0, 0)$
90.2.758	P4 <sub>2</sub> 21'						
90.3.759	P4'2 <sub>1</sub> 2'	P2 <sub>1</sub> 2 <sub>1</sub> 2	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^* 1/2, 1/2, 0)$	$(4_z^* 1/2, 1/2, 0)'$ $(2_y^* 1/2, 1/2, 0)$	$(2_z^* 0, 0, 0)$ $(2_{xy}^* 0, 0, 0)'$	$(4_z^{-1*} 1/2, 1/2, 0)'$ $(2_{\&y}^* 0, 0, 0)'$
90.4.760	P4 <sub>2</sub> 1'2'	P4	(1/2,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^* 1/2, 1/2, 0)'$	$(4_z^* 1/2, 1/2, 0)$ $(2_y^* 1/2, 1/2, 0)'$	$(2_z^* 0, 0, 0)$ $(2_{xy}^* 0, 0, 0)'$	$(4_z^{-1*} 1/2, 1/2, 0)$ $(2_{\&y}^* 0, 0, 0)'$
90.5.761	P4'2 <sub>1</sub> '2	C222	(0,0,0;a-b,a+b,c)	$(1^*0,0,0)$ $(2_x^* 1/2, 1/2, 0)'$	$(4_z^* 1/2, 1/2, 0)'$ $(2_y^* 1/2, 1/2, 0)'$	$(2_z^* 0, 0, 0)$ $(2_{xy}^* 0, 0, 0)$	$(4_z^{-1*} 1/2, 1/2, 0)'$ $(2_{\&y}^* 0, 0, 0)$
90.6.762	P <sub>2c</sub> 4 <sub>2</sub> 1'2	P4 <sub>2</sub> 1'2	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^* 1/2, 1/2, 0)$	$(4_z^* 1/2, 1/2, 0)$ $(2_y^* 1/2, 1/2, 0)$	$(2_z^* 0, 0, 0)$ $(2_{xy}^* 0, 0, 0)$	$(4_z^{-1*} 1/2, 1/2, 0)$ $(2_{\&y}^* 0, 0, 0)$
90.7.763	P <sub>2c</sub> 4'2 <sub>1</sub> '2	P4 <sub>2</sub> 2 <sub>1</sub> 2	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(2_x^* 1/2, 1/2, 1)$	$(4_z^* 1/2, 1/2, 1)$ $(2_y^* 1/2, 1/2, 1)$	$(2_z^* 0, 0, 0)$ $(2_{xy}^* 0, 0, 0)$	$(4_z^{-1*} 1/2, 1/2, 1)$ $(2_{\&y}^* 0, 0, 0)$
<b>91.1.764</b>	<b>P4<sub>1</sub>22</b>			$(1^*0,0,0)$ $(2_x^* 0, 0, 1/2)$	$(4_z^* 0, 0, 1/4)$ $(2_y^* 0, 0, 0)$	$(2_z^* 0, 0, 1/2)$ $(2_{xy}^* 0, 0, 3/4)$	$(4_z^{-1*} 0, 0, 3/4)$ $(2_{\&y}^* 0, 0, 1/4)$
91.2.765	P4 <sub>1</sub> 221'						
91.3.766	P4 <sub>1</sub> '22'	P222 <sub>1</sub>	(0,0,0;b,&,c)	$(1^*0,0,0)$ $(2_x^* 0, 0, 1/2)$	$(4_z^* 0, 0, 1/4)'$ $(2_y^* 0, 0, 0)$	$(2_z^* 0, 0, 1/2)$ $(2_{xy}^* 0, 0, 3/4)'$	$(4_z^{-1*} 0, 0, 3/4)'$ $(2_{\&y}^* 0, 0, 1/4)'$
91.4.767	P4 <sub>1</sub> 2'2'	P4 <sub>1</sub>	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^* 0, 0, 1/2)'$	$(4_z^* 0, 0, 1/4)$ $(2_y^* 0, 0, 0)'$	$(2_z^* 0, 0, 1/2)$ $(2_{xy}^* 0, 0, 3/4)'$	$(4_z^{-1*} 0, 0, 3/4)$ $(2_{\&y}^* 0, 0, 1/4)'$
91.5.768	P4 <sub>1</sub> '2'2	C222 <sub>1</sub>	(0,0,0;a-b,a+b,c)	$(1^*0,0,0)$ $(2_x^* 0, 0, 1/2)'$	$(4_z^* 0, 0, 1/4)'$ $(2_y^* 0, 0, 0)'$	$(2_z^* 0, 0, 1/2)$ $(2_{xy}^* 0, 0, 3/4)$	$(4_z^{-1*} 0, 0, 3/4)'$ $(2_{\&y}^* 0, 0, 1/4)$
91.6.769	P <sub>p</sub> 4 <sub>1</sub> 22	P4 <sub>1</sub> 22	(0,0,1/8;a-b,a+b,c)	$(1^*0,0,0)$	$(4_z^* 0, 0, 1/4)$	$(2_z^* 0, 0, 1/2)$	$(4_z^{-1*} 0, 0, 3/4)$

				$(2_x^*0,0,1/2)$	$(2_y^*0,0,0)$	$(2_{xy}^*0,0,3/4)$	$(2_{&y}^*0,0,1/4)$
91.7.770	$P_p4_1'22'$	$P4_12_12$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)$	$(4_z^*1,0,1/4)$ $(2_y^*0,0,0)$	$(2_z^*0,0,1/2)$ $(2_{xy}^*1,0,3/4)$	$(4_z^{-1*}1,0,3/4)$ $(2_{&y}^*1,0,1/4)$
<b>92.1.771</b>	<b><math>P4_12_12</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(2_x^*1/2,1/2,3/4)</math></b>	<b><math>(4_z^*1/2,1/2,1/4)</math></b> <b><math>(2_y^*1/2,1/2,1/4)</math></b>	<b><math>(2_z^*0,0,1/2)</math></b> <b><math>(2_{xy}^*0,0,0)</math></b>	<b><math>(4_z^{-1*}1/2,1/2,3/4)</math></b> <b><math>(2_{&amp;y}^*0,0,1/2)</math></b>
92.2.772	$P4_12_121'$						
92.3.773	$P4_1'2_12'$	$P2_12_12_1$	$(1/4,0,1/8;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,3/4)'$	$(4_z^*1/2,1/2,1/4)'$ $(2_y^*1/2,1/2,1/4)'$	$(2_z^*0,0,1/2)$ $(2_{xy}^*0,0,0)'$	$(4_z^{-1*}1/2,1/2,3/4)'$ $(2_{&y}^*0,0,1/2)'$
92.4.774	$P4_12_1'2'$	$P4_1$	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,3/4)'$	$(4_z^*1/2,1/2,1/4)'$ $(2_y^*1/2,1/2,1/4)'$	$(2_z^*0,0,1/2)$ $(2_{xy}^*0,0,0)'$	$(4_z^{-1*}1/2,1/2,3/4)'$ $(2_{&y}^*0,0,1/2)'$
92.5.775	$P4_1'2_1'2$	$C222_1$	$(0,0,0;a+b,-a-b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,3/4)'$	$(4_z^*1/2,1/2,1/4)'$ $(2_y^*1/2,1/2,1/4)'$	$(2_z^*0,0,1/2)$ $(2_{xy}^*0,0,0)$	$(4_z^{-1*}1/2,1/2,3/4)'$ $(2_{&y}^*0,0,1/2)$
<b>93.1.776</b>	<b><math>P4_222</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(2_x^*0,0,0)</math></b>	<b><math>(4_z^*0,0,1/2)</math></b> <b><math>(2_y^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(2_{xy}^*0,0,1/2)</math></b>	<b><math>(4_z^{-1*}0,0,1/2)</math></b> <b><math>(2_{&amp;y}^*0,0,1/2)</math></b>
93.2.777	$P4_2221'$						
93.3.778	$P4_2'22'$	$P222$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(4_z^*0,0,1/2)'$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)'$	$(4_z^{-1*}0,0,1/2)'$ $(2_{&y}^*0,0,1/2)'$
93.4.779	$P4_2'2'2'$	$P4_2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)'$	$(4_z^*0,0,1/2)$ $(2_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)'$	$(4_z^{-1*}0,0,1/2)$ $(2_{&y}^*0,0,1/2)'$

93.5.780	$P4_2'2'2$	C222	$(0,0,1/4;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)'$	$(4_z^*0,0,1/2)'$ $(2_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$	$(4_z^{-1*}0,0,1/2)'$ $(2_{&y}^*0,0,1/2)$
93.6.781	$P_{2c}4_222$	$P4_122$	$(0,0,0;b,\&,2c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(4_z^*0,0,1/2)$ $(2_y^*0,0,1)$	$(2_z^*0,0,1)$ $(2_{xy}^*0,0,1/2)$	$(4_z^{-1*}0,0,3/2)$ $(2_{&y}^*0,0,3/2)$
93.7.782	$P_P4_222$	$P4_222$	$(0,0,1/4;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(4_z^*0,0,1/2)$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$	$(4_z^{-1*}0,0,1/2)$ $(2_{&y}^*0,0,1/2)$
93.8.783	$P_I4_222$	$I4_122$	$(-1/2,0,0;-a-b,a-b,2c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(4_z^*0,0,1/2)$ $(2_y^*0,0,1)$	$(2_z^*0,0,1)$ $(2_{xy}^*0,0,1/2)$	$(4_z^{-1*}0,0,3/2)$ $(2_{&y}^*0,0,3/2)$
93.9.784	$P_{2c}4_2'22'$	$P4_322$	$(0,0,0;b,\&,2c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(4_z^*0,0,3/2)$ $(2_y^*0,0,1)$	$(2_z^*0,0,1)$ $(2_{xy}^*0,0,3/2)$	$(4_z^{-1*}0,0,1/2)$ $(2_{&y}^*0,0,1/2)$
93.10.785	$P_P4_2'22'$	$P4_22_12$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(4_z^*1,0,1/2)$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1,0,1/2)$	$(4_z^{-1*}1,0,1/2)$ $(2_{&y}^*1,0,1/2)$
<b>94.1.786</b>	<b><math>P4_22_12</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(2_x^*1/2,1/2,1/2)</math></b>	<b><math>(4_z^*1/2,1/2,1/2)</math></b> <b><math>(2_y^*1/2,1/2,1/2)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(2_{xy}^*0,0,0)</math></b>	<b><math>(4_z^{-1*}1/2,1/2,1/2)</math></b> <b><math>(2_{&amp;y}^*0,0,0)</math></b>
94.2.787	$P4_22_121'$						
94.3.788	$P4_2'2_12'$	$P2_12_12$	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)$	$(4_z^*1/2,1/2,1/2)'$ $(2_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$	$(4_z^{-1*}1/2,1/2,1/2)'$ $(2_{&y}^*0,0,0)'$
94.4.789	$P4_22_1'2'$	$P4_2$	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)'$	$(4_z^*1/2,1/2,1/2)$ $(2_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$	$(4_z^{-1*}1/2,1/2,1/2)$ $(2_{&y}^*0,0,0)'$
94.5.790	$P4_2'2_1'2$	C222	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)'$	$(4_z^*1/2,1/2,1/2)'$ $(2_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)'$ $(2_{&y}^*0,0,0)$
94.6.791	$P_{2c}4_22_12$	$P4_12_12$	$(0,0,0;b,\&,c)$	$(1^*0,0,0)$	$(4_z^*1/2,1/2,1/2)$	$(2_z^*0,0,1)$	$(4_z^{-1*}1/2,1/2,3/2)$

				$(2_x^*1/2, 1/2, 1/2)$	$(2_y^*1/2, 1/2, 3/2)$	$(2_{xy}^*0, 0, 1)$	$(2_{\&y}^*0, 0, 0)$
94.7.792	$P_{2c}4_2'2_1'2$	$P4_32_12$	$(0, 0, 0; b, \&, c)$	$(1^*0, 0, 0)$ $(2_x^*1/2, 1/2, 3/2)$	$(4_z^*1/2, 1/2, 3/2)$ $(2_y^*1/2, 1/2, 1/2)$	$(2_z^*0, 0, 1)$ $(2_{xy}^*0, 0, 1)$	$(4_z^{-1*}1/2, 1/2, 1/2)$ $(2_{\&y}^*0, 0, 0)$
<b>95.1.793</b>	<b><math>P4_322</math></b>			<b><math>(1^*0, 0, 0)</math></b> <b><math>(2_x^*0, 0, 1/2)</math></b>	<b><math>(4_z^*0, 0, 3/4)</math></b> <b><math>(2_y^*0, 0, 0)</math></b>	<b><math>(2_z^*0, 0, 1/2)</math></b> <b><math>(2_{xy}^*0, 0, 1/4)</math></b>	<b><math>(4_z^{-1*}0, 0, 1/4)</math></b> <b><math>(2_{\&amp;y}^*0, 0, 3/4)</math></b>
95.2.794	$P4_3221'$						
95.3.795	$P4_3'22'$	$P222_1$	$(0, 0, 0; b, \&, c)$	$(1^*0, 0, 0)$ $(2_x^*0, 0, 1/2)$	$(4_z^*0, 0, 3/4)'$ $(2_y^*0, 0, 0)$	$(2_z^*0, 0, 1/2)$ $(2_{xy}^*0, 0, 1/4)'$	$(4_z^{-1*}0, 0, 1/4)'$ $(2_{\&y}^*0, 0, 3/4)'$
95.4.796	$P4_32'2'$	$P4_3$	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$ $(2_x^*0, 0, 1/2)'$	$(4_z^*0, 0, 3/4)$ $(2_y^*0, 0, 0)'$	$(2_z^*0, 0, 1/2)$ $(2_{xy}^*0, 0, 1/4)'$	$(4_z^{-1*}0, 0, 1/4)$ $(2_{\&y}^*0, 0, 3/4)'$
95.5.797	$P4_3'2'2$	$C222_1$	$(0, 0, 1/8; a-b, a+b, c)$	$(1^*0, 0, 0)$ $(2_x^*0, 0, 1/2)'$	$(4_z^*0, 0, 3/4)'$ $(2_y^*0, 0, 0)'$	$(2_z^*0, 0, 1/2)$ $(2_{xy}^*0, 0, 1/4)$	$(4_z^{-1*}0, 0, 1/4)'$ $(2_{\&y}^*0, 0, 3/4)$
95.6.798	$P_P4_322$	$P4_322$	$(0, 0, 1/8; a+b, -a+b, c)$	$(1^*0, 0, 0)$ $(2_x^*0, 0, 1/2)$	$(4_z^*0, 0, 3/4)$ $(2_y^*0, 0, 0)$	$(2_z^*0, 0, 1/2)$ $(2_{xy}^*0, 0, 1/4)$	$(4_z^{-1*}0, 0, 1/4)$ $(2_{\&y}^*0, 0, 3/4)$
95.7.799	$P_P4_3'22'$	$P4_32_12$	$(0, 0, 0; a+b, -a+b, c)$	$(1^*0, 0, 0)$ $(2_x^*0, 0, 1/2)$	$(4_z^*1, 0, 3/4)$ $(2_y^*0, 0, 0)$	$(2_z^*0, 0, 1/2)$ $(2_{xy}^*1, 0, 1/4)$	$(4_z^{-1*}1, 0, 1/4)$ $(2_{\&y}^*1, 0, 3/4)$
<b>96.1.800</b>	<b><math>P4_32_12</math></b>			<b><math>(1^*0, 0, 0)</math></b> <b><math>(2_x^*1/2, 1/2, 1/4)</math></b>	<b><math>(4_z^*1/2, 1/2, 3/4)</math></b> <b><math>(2_y^*1/2, 1/2, 3/4)</math></b>	<b><math>(2_z^*0, 0, 1/2)</math></b> <b><math>(2_{xy}^*0, 0, 0)</math></b>	<b><math>(4_z^{-1*}1/2, 1/2, 1/4)</math></b> <b><math>(2_{\&amp;y}^*0, 0, 1/2)</math></b>
96.2.801	$P4_32_121'$						

96.3.802	$P4_3'2_1'2'$	$P2_12_12_1$	$(1/4,0,-1/8;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/4)'$	$(4_z^*1/2,1/2,3/4)'$ $(2_y^*1/2,1/2,3/4)'$	$(2_z^*0,0,1/2)$ $(2_{xy}^*0,0,0)'$	$(4_z^{-1*}1/2,1/2,1/4)'$ $(2_{&y}^*0,0,1/2)'$
96.4.803	$P4_3'2_1'2'$	$P4_3$	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/4)'$	$(4_z^*1/2,1/2,3/4)'$ $(2_y^*1/2,1/2,3/4)'$	$(2_z^*0,0,1/2)$ $(2_{xy}^*0,0,0)'$	$(4_z^{-1*}1/2,1/2,1/4)'$ $(2_{&y}^*0,0,1/2)'$
96.5.804	$P4_3'2_1'2'$	$C222_1$	$(0,0,0;a+b,-a+b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/4)'$	$(4_z^*1/2,1/2,3/4)'$ $(2_y^*1/2,1/2,3/4)'$	$(2_z^*0,0,1/2)$ $(2_{xy}^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/4)'$ $(2_{&y}^*0,0,1/2)$
<b>97.1.805</b>	<b>I422</b>			<b><math>(1^*0,0,0)</math></b> <b><math>(2_x^*0,0,0)</math></b>	<b><math>(4_z^*0,0,0)</math></b> <b><math>(2_y^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(2_{xy}^*0,0,0)</math></b>	<b><math>(4_z^{-1*}0,0,0)</math></b> <b><math>(2_{&amp;y}^*0,0,0)</math></b>
97.2.806	I4221'						
97.3.807	I4'22'	I222	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(4_z^*0,0,0)'$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,0)'$ $(2_{&y}^*0,0,0)'$
97.4.808	I42'2'	I4	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)'$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,0)$ $(2_{&y}^*0,0,0)'$
97.5.809	I4'2'2	F222	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)'$	$(4_z^*0,0,0)'$ $(2_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)'$ $(2_{&y}^*0,0,0)$
97.6.810	I <sub>p</sub> 422	P422	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)$ $(2_{&y}^*0,0,0)$
97.7.811	I <sub>p</sub> 4'22'	P4 <sub>2</sub> 22	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(4_z^*1/2,1/2,1/2)$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(2_{&y}^*1/2,1/2,1/2)$
97.8.812	I <sub>p</sub> 42'2'	P4 <sub>2</sub> 2	$(1/2,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)$	$(4_z^*0,0,0)$ $(2_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}0,0,0)$ $(2_{&y}^*1/2,1/2,1/2)$

97.9.813	$I_p 4'2'2$	$P4_2 2_1 2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^* 1/2, 1/2, 1/2)$	$(4_z^* 1/2, 1/2, 1/2)$ $(2_y^* 1/2, 1/2, 1/2)$	$(2_z^* 0,0,0)$ $(2_{xy}^* 0,0,0)$	$(4_z^{-1*} 1/2, 1/2, 1/2)$ $(2_{&y}^* 0,0,0)$
<b>98.1.814</b>	<b><math>I4_1 22</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(2_x^* 0, 1/2, 1/4)</math></b>	<b><math>(4_z^* 0, 1/2, 1/4)</math></b> <b><math>(2_y^* 0, 1/2, 1/4)</math></b>	<b><math>(2_z^* 0,0,0)</math></b> <b><math>(2_{xy}^* 0,0,0)</math></b>	<b><math>(4_z^{-1*} 0, 1/2, 1/4)</math></b> <b><math>(2_{&amp;y}^* 0,0,0)</math></b>
98.2.815	$I4_1 221'$						
98.3.816	$I4_1' 22'$	$I2_1 2_1 2_1$	$(0, 1/4, 1/4; a, b, c)$	$(1^*0,0,0)$ $(2_x^* 0, 1/2, 1/4)$	$(4_z^* 0, 1/2, 1/4)'$ $(2_y^* 0, 1/2, 1/4)$	$(2_z^* 0,0,0)$ $(2_{xy}^* 0,0,0)'$	$(4_z^{-1*} 0, 1/2, 1/4)'$ $(2_{&y}^* 0,0,0)'$
98.4.817	$I4_1 2'2'$	$I4_1$	$(1/4, -1/4, 0; a, b, c)$	$(1^*0,0,0)$ $(2_x^* 0, 1/2, 1/4)'$	$(4_z^* 0, 1/2, 1/4)$ $(2_y^* 0, 1/2, 1/4)'$	$(2_z^* 0,0,0)$ $(2_{xy}^* 0,0,0)'$	$(4_z^{-1*} 0, 1/2, 1/4)$ $(2_{&y}^* 0,0,0)'$
98.5.818	$I4_1' 2'2'$	$F222$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^* 0, 1/2, 1/4)'$	$(4_z^* 0, 1/2, 1/4)'$ $(2_y^* 0, 1/2, 1/4)'$	$(2_z^* 0,0,0)$ $(2_{xy}^* 0,0,0)$	$(4_z^{-1*} 0, 1/2, 1/4)'$ $(2_{&y}^* 0,0,0)$
98.6.819	$I_p 4_1 22$	$P4_1 22$	$(1/4, -1/4, 1/8; a, b, c)$	$(1^*0,0,0)$ $(2_x^* 0, 1/2, 1/4)$	$(4_z^* 0, 1/2, 1/4)$ $(2_y^* 1/2, 0, 3/4)$	$(2_z^* 1/2, 1/2, 1/2)$ $(2_{xy}^* 1/2, 1/2, 1/2)$	$(4_z^{-1*} 1/2, 0, 3/4)$ $(2_{&y}^* 0,0,0)$
98.7.820	$I_p 4_1' 22'$	$P4_3 22$	$(1/4, 1/4, 1/8; a, b, c)$	$(1^*0,0,0)$ $(2_x^* 0, 1/2, 1/4)$	$(4_z^* 1/2, 0, 3/4)$ $(2_y^* 1/2, 0, 3/4)$	$(2_z^* 1/2, 1/2, 1/2)$ $(2_{xy}^* 0,0,0)$	$(4_z^{-1*} 0, 1/2, 1/4)$ $(2_{&y}^* 1/2, 1/2, 1/2)$
98.8.821	$I_p 4_1 2'2'$	$P4_1 2_1 2$	$(1/4, 1/4, 0; a, b, c)$	$(1^*0,0,0)$ $(2_x^* 1/2, 0, 3/4)$	$(4_z^* 0, 1/2, 1/4)$ $(2_y^* 0, 1/2, 1/4)$	$(2_z^* 1/2, 1/2, 1/2)$ $(2_{xy}^* 0,0,0)$	$(4_z^{-1*} 1/2, 0, 3/4)$ $(2_{&y}^* 1/2, 1/2, 1/2)$
98.9.822	$I_p 4_1' 2'2'$	$P4_3 2_1 2$	$(1/4, -1/4, 1/4; a, b, c)$	$(1^*0,0,0)$ $(2_x^* 1/2, 0, 3/4)$	$(4_z^* 1/2, 0, 3/4)$ $(2_y^* 0, 1/2, 1/4)$	$(2_z^* 1/2, 1/2, 1/2)$ $(2_{xy}^* 1/2, 1/2, 1/2)$	$(4_z^{-1*} 0, 1/2, 1/4)$ $(2_{&y}^* 0,0,0)$
<b>99.1.823</b>	<b><math>P4mm</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(m_x^* 0,0,0)</math></b>	<b><math>(4_z^* 0,0,0)</math></b> <b><math>(m_y^* 0,0,0)</math></b>	<b><math>(2_z^* 0,0,0)</math></b> <b><math>(m_{xy}^* 0,0,0)</math></b>	<b><math>(4_z^{-1*} 0,0,0)</math></b> <b><math>(m_{&amp;y}^* 0,0,0)</math></b>

99.2.824	P4mm1'						
99.3.825	P4'm'm	Cmm2	(0,0,0;a-b,a+b,c)	$(1^*0,0,0)$ $(m_x^*0,0,0)'$	$(4_z^*0,0,0)'$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)'$ $(m_{&y}^*0,0,0)$
99.4.826	P4'mm'	Pmm2	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,0)'$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,0)'$ $(m_{&y}^*0,0,0)'$
99.5.827	P4m'm'	P4	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(m_x^*0,0,0)'$	$(4_z^*0,0,0)$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,0)$ $(m_{&y}^*0,0,0)'$
99.6.828	P <sub>2c</sub> 4mm	P4mm	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)$ $(m_{&y}^*0,0,0)$
99.7.829	P <sub>p</sub> 4mm	P4mm	(0,0,0;a-b,a+b,c)	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)$ $(m_{&y}^*0,0,0)$
99.8.830	P <sub>l</sub> 4mm	I4mm	(0,0,0;a-b,a+b,2c)	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)$ $(m_{&y}^*0,0,0)$
99.9.831	P <sub>2c</sub> 4'm'm	P4 <sub>2</sub> cm	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(m_x^*0,0,1)$	$(4_z^*0,0,1)$ $(m_y^*0,0,1)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,1)$ $(m_{&y}^*0,0,0)$
99.10.832	P <sub>2c</sub> 4'mm'	P4 <sub>2</sub> mc	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,1)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,1)$	$(4_z^{-1*}0,0,1)$ $(m_{&y}^*0,0,1)$
99.11.833	P <sub>2c</sub> 4m'm'	P4cc	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(m_x^*0,0,1)$	$(4_z^*0,0,0)$ $(m_y^*0,0,1)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,1)$	$(4_z^{-1*}0,0,0)$ $(m_{&y}^*0,0,1)$
99.12.834	P <sub>p</sub> 4'mm'	P4bm	(1/2,1/2,0;a-b,a+b,c)	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*1,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*1,0,0)$	$(4_z^{-1*}1,0,0)$ $(m_{&y}^*1,0,0)$
99.13.835	P <sub>l</sub> 4m'm'	I4cm	(0,0,0;a-b,a+b,2c)	$(1^*0,0,0)$ $(m_x^*1,0,0)$	$(4_z^*0,0,0)$ $(m_y^*1,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*1,0,0)$	$(4_z^{-1*}0,0,0)$ $(m_{&y}^*1,0,0)$



<b>100.1.836</b>	<b>P4bm</b>			$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(4_z^*0,0,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}0,0,0)$ $(m_{&y}^*1/2,1/2,0)$
100.2.837	P4bm1'						
100.3.838	P4'b'm	Cmm2	$(1/2,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)'$	$(4_z^*0,0,0)'$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}0,0,0)'$ $(m_{&y}^*1/2,1/2,0)$
100.4.839	P4'bm'	Pba2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(4_z^*0,0,0)'$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)'$	$(4_z^{-1*}0,0,0)'$ $(m_{&y}^*1/2,1/2,0)'$
100.5.840	P4b'm'	P4	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)'$	$(4_z^*0,0,0)$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)'$	$(4_z^{-1*}0,0,0)$ $(m_{&y}^*1/2,1/2,0)$
100.6.841	P <sub>2c</sub> 4bm	P4bm	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(4_z^*0,0,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}0,0,0)$ $(m_{&y}^*1/2,1/2,0)$
100.7.842	P <sub>2c</sub> 4'b'm	P4 <sub>2</sub> nm	$(0,1/2,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,1)$	$(4_z^*0,0,1)$ $(m_y^*1/2,1/2,1)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}0,0,1)$ $(m_{&y}^*1/2,1/2,0)$
100.8.843	P <sub>2c</sub> 4'bm'	P4 <sub>2</sub> bc	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(4_z^*0,0,1)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1)$	$(4_z^{-1*}0,0,1)$ $(m_{&y}^*1/2,1/2,1)$
100.9.844	P <sub>2c</sub> 4b'm'	P4nc	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,1)$	$(4_z^*0,0,0)$ $(m_y^*1/2,1/2,1)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1)$	$(4_z^{-1*}0,0,0)$ $(m_{&y}^*1/2,1/2,1)$
<b>101.1.845</b>	<b>P4<sub>2</sub>cm</b>			$(1^*0,0,0)$ $(m_x^*0,0,1/2)$	$(4_z^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,1/2)$ $(m_{&y}^*0,0,0)$
101.2.846	P4 <sub>2</sub> cm1'						

101.3.847	$P4_2'c'm$	Cmm2	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,1/2)'$	$(4_z^*0,0,1/2)'$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,1/2)'$ $(m_{&y}^*0,0,0)$
101.4.848	$P4_2'cm'$	Pcc2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,1/2)$	$(4_z^*0,0,1/2)'$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,1/2)'$ $(m_{&y}^*0,0,0)'$
101.5.849	$P4_2c'm'$	$P4_2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,1/2)'$	$(4_z^*0,0,1/2)$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,1/2)$ $(m_{&y}^*0,0,0)'$
101.6.850	$P_P4_2cm$	$P4_2mc$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,1/2)$	$(4_z^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,1/2)$ $(m_{&y}^*0,0,0)$
101.7.851	$P_P4_2'cm'$	$P4_2bc$	$(1/2,1/2,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,1/2)$	$(4_z^*1,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_{xy}^*1,0,0)$	$(4_z^{-1*}1,0,1/2)$ $(m_{&y}^*1,0,0)$
<b>102.1.852</b>	<b><math>P4_2nm</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(m_x^*1/2,1/2,1/2)</math></b>	<b><math>(4_z^*1/2,1/2,1/2)</math></b> <b><math>(m_y^*1/2,1/2,1/2)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(m_{xy}^*0,0,0)</math></b>	<b><math>(4_z^{-1*}1/2,1/2,1/2)</math></b> <b><math>(m_{&amp;y}^*0,0,0)</math></b>
102.2.853	$P4_2nm1'$						
102.3.854	$P4_2'n'm$	Cmm2	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,1/2)'$	$(4_z^*1/2,1/2,1/2)'$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)'$ $(m_{&y}^*0,0,0)$
102.4.855	$P4_2'nm'$	Pnn2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,1/2)$	$(4_z^*1/2,1/2,1/2)'$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}1/2,1/2,1/2)'$ $(m_{&y}^*0,0,0)'$
102.5.856	$P4_2n'm'$	$P4_2$	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,1/2)'$	$(4_z^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}1/2,1/2,1/2)$ $(m_{&y}^*0,0,0)'$
102.6.857	$P_I4_2nm$	$I4_1md$	$(0,0,0;a-b,a+b,2c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,1/2)$	$(4_z^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(m_{&y}^*0,0,0)$

102.7.858	$P_1 4_2 n' m'$	$I 4_1 cd$	$(0,0,0;a-b,a+b,2c)$	$(1^*0,0,0)$ $(m_x^* 3/2, 1/2, 1/2)$	$(4_z^* 1/2, 1/2, 1/2)$ $(m_y^* 3/2, 1/2, 1/2)$	$(2_z^* 0,0,0)$ $(m_{xy}^* 1,0,0)$	$(4_z^{-1*} 1/2, 1/2, 1/2)$ $(m_{\&y}^* 1,0,0)$
<b>103.1.859</b>	<b><math>P 4cc</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(m_x^* 0,0,1/2)</math></b>	<b><math>(4_z^* 0,0,0)</math></b> <b><math>(m_y^* 0,0,1/2)</math></b>	<b><math>(2_z^* 0,0,0)</math></b> <b><math>(m_{xy}^* 0,0,1/2)</math></b>	<b><math>(4_z^{-1*} 0,0,0)</math></b> <b><math>(m_{\&amp;y}^* 0,0,1/2)</math></b>
103.2.860	$P 4cc 1'$						
103.3.861	$P 4'c'c$	$Ccc 2$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^* 0,0,1/2)'$	$(4_z^* 0,0,0)'$ $(m_y^* 0,0,1/2)'$	$(2_z^* 0,0,0)$ $(m_{xy}^* 0,0,1/2)$	$(4_z^{-1*} 0,0,0)'$ $(m_{\&y}^* 0,0,1/2)$
103.4.862	$P 4'cc'$	$Pcc 2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^* 0,0,1/2)$	$(4_z^* 0,0,0)'$ $(m_y^* 0,0,1/2)$	$(2_z^* 0,0,0)$ $(m_{xy}^* 0,0,1/2)'$	$(4_z^{-1*} 0,0,0)'$ $(m_{\&y}^* 0,0,1/2)'$
103.5.863	$P 4c'c'$	$P 4$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^* 0,0,1/2)'$	$(4_z^* 0,0,0)$ $(m_y^* 0,0,1/2)'$	$(2_z^* 0,0,0)$ $(m_{xy}^* 0,0,1/2)'$	$(4_z^{-1*} 0,0,0)$ $(m_{\&y}^* 0,0,1/2)'$
103.6.864	$P_p 4cc$	$P 4cc$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^* 0,0,1/2)$	$(4_z^* 0,0,0)$ $(m_y^* 0,0,1/2)$	$(2_z^* 0,0,0)$ $(m_{xy}^* 0,0,1/2)$	$(4_z^{-1*} 0,0,0)$ $(m_{\&y}^* 0,0,1/2)$
103.7.865	$P_p 4'cc'$	$P 4nc$	$(1/2,1/2,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^* 0,0,1/2)$	$(4_z^* 1,0,0)$ $(m_y^* 0,0,1/2)$	$(2_z^* 0,0,0)$ $(m_{xy}^* 1,0,1/2)$	$(4_z^{-1*} 1,0,0)$ $(m_{\&y}^* 1,0,1/2)$
<b>104.1.866</b>	<b><math>P 4nc</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(m_x^* 1/2, 1/2, 1/2)</math></b>	<b><math>(4_z^* 0,0,0)</math></b> <b><math>(m_y^* 1/2, 1/2, 1/2)</math></b>	<b><math>(2_z^* 0,0,0)</math></b> <b><math>(m_{xy}^* 1/2, 1/2, 1/2)</math></b>	<b><math>(4_z^{-1*} 0,0,0)</math></b> <b><math>(m_{\&amp;y}^* 1/2, 1/2, 1/2)</math></b>
104.2.867	$P 4nc 1'$						
104.3.868	$P 4'n'c$	$Ccc 2$	$(1/2,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^* 1/2, 1/2, 1/2)'$	$(4_z^* 0,0,0)'$ $(m_y^* 1/2, 1/2, 1/2)'$	$(2_z^* 0,0,0)$ $(m_{xy}^* 1/2, 1/2, 1/2)$	$(4_z^{-1*} 0,0,0)'$ $(m_{\&y}^* 1/2, 1/2, 1/2)$
104.4.869	$P 4'nc'$	$Pnn 2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^* 1/2, 1/2, 1/2)$	$(4_z^* 0,0,0)'$ $(m_y^* 1/2, 1/2, 1/2)$	$(2_z^* 0,0,0)$ $(m_{xy}^* 1/2, 1/2, 1/2)'$	$(4_z^{-1*} 0,0,0)'$ $(m_{\&y}^* 1/2, 1/2, 1/2)'$

104.5.870	P4n'c'	P4	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(m_x^*1/2,1/2,1/2)'$	$(4_z^*0,0,0)$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)'$	$(4_z^{-1*}0,0,0)$ $(m_{&y}^*1/2,1/2,1/2)'$
<b>105.1.871</b>	<b>P4<sub>2</sub>mc</b>			<b><math>(1^*0,0,0)</math></b> <b><math>(m_x^*0,0,0)</math></b>	<b><math>(4_z^*0,0,1/2)</math></b> <b><math>(m_y^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(m_{xy}^*0,0,1/2)</math></b>	<b><math>(4_z^{-1*}0,0,1/2)</math></b> <b><math>(m_{&amp;y}^*0,0,1/2)</math></b>
105.2.872	P4 <sub>2</sub> mc1'						
105.3.873	P4 <sub>2</sub> 'm'c	Ccc2	(0,0,0;a-b,a+b,c)	$(1^*0,0,0)$ $(m_x^*0,0,0)'$	$(4_z^*0,0,1/2)'$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)$	$(4_z^{-1*}0,0,1/2)'$ $(m_{&y}^*0,0,1/2)$
105.4.874	P4 <sub>2</sub> 'mc'	Pmm2	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,1/2)'$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)'$	$(4_z^{-1*}0,0,1/2)'$ $(m_{&y}^*0,0,1/2)'$
105.5.875	P4 <sub>2</sub> m'c'	P4 <sub>2</sub>	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(m_x^*0,0,0)'$	$(4_z^*0,0,1/2)$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)'$	$(4_z^{-1*}0,0,1/2)$ $(m_{&y}^*0,0,1/2)'$
105.6.876	P <sub>P</sub> 4 <sub>2</sub> mc	P4 <sub>2</sub> cm	(0,0,0;a-b,a+b,c)	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,1/2)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)$	$(4_z^{-1*}0,0,1/2)$ $(m_{&y}^*0,0,1/2)$
105.7.877	P <sub>P</sub> 4 <sub>2</sub> 'mc'	P4 <sub>2</sub> nm	(0,0,0;a-b,a+b,c)	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*1,0,1/2)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*1,0,1/2)$	$(4_z^{-1*}1,0,1/2)$ $(m_{&y}^*1,0,1/2)$
<b>106.1.878</b>	<b>P4<sub>2</sub>bc</b>			<b><math>(1^*0,0,0)</math></b> <b><math>(m_x^*1/2,1/2,0)</math></b>	<b><math>(4_z^*0,0,1/2)</math></b> <b><math>(m_y^*1/2,1/2,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(m_{xy}^*1/2,1/2,1/2)</math></b>	<b><math>(4_z^{-1*}0,0,1/2)</math></b> <b><math>(m_{&amp;y}^*1/2,1/2,1/2)</math></b>
106.2.879	P4 <sub>2</sub> bc1'						
106.3.880	P4 <sub>2</sub> 'b'c	Ccc2	(1/2,0,0;a-b,a+b,c)	$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)'$	$(4_z^*0,0,1/2)'$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}0,0,1/2)'$ $(m_{&y}^*1/2,1/2,1/2)$
106.4.881	P4 <sub>2</sub> 'bc'	Pba2	(0,0,0;a,b,c)	$(1^*0,0,0)$	$(4_z^*0,0,1/2)'$	$(2_z^*0,0,0)$	$(4_z^{-1*}0,0,1/2)'$

				$(m_x^*1/2,1/2,0)$	$(m_y^*1/2,1/2,0)$	$(m_{xy}^*1/2,1/2,1/2)'$	$(m_{\&y}^*1/2,1/2,1/2)'$
106.5.882	$P4_2b'c'$	$P4_2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)'$	$(4_z^*0,0,1/2)$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)'$	$(4_z^{-1*}0,0,1/2)$ $(m_{\&y}^*1/2,1/2,1/2)'$
<b>107.1.883</b>	<b><math>I4mm</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(m_x^*0,0,0)</math></b>	<b><math>(4_z^*0,0,0)</math></b> <b><math>(m_y^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(m_{xy}^*0,0,0)</math></b>	<b><math>(4_z^{-1*}0,0,0)</math></b> <b><math>(m_{\&amp;y}^*0,0,0)</math></b>
107.2.884	$I4mm1'$						
107.3.885	$I4'm'm$	$Fmm2$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,0)'$	$(4_z^*0,0,0)'$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)'$ $(m_{\&y}^*0,0,0)$
107.4.886	$I4'mm'$	$Imm2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,0)'$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,0)'$ $(m_{\&y}^*0,0,0)$
107.5.887	$I4m'm'$	$I4$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,0)'$	$(4_z^*0,0,0)$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,0)$ $(m_{\&y}^*0,0,0)$
107.6.888	$I_p4mm$	$P4mm$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)$ $(m_{\&y}^*0,0,0)$
107.7.889	$I_p4'm'm$	$P4_2nm$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,1/2)$	$(4_z^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(m_{\&y}^*0,0,0)$
107.8.890	$I_p4'mm'$	$P4_2mc$	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*1/2,1/2,1/2)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(m_{\&y}^*1/2,1/2,1/2)$
107.9.891	$I_p4m'm'$	$P4nc$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,1/2)$	$(4_z^*0,0,0)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,1/2)$

<b>108.1.892</b>	<b>I4cm</b>			$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(4_z^*0,0,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}0,0,0)$ $(m_{&y}^*1/2,1/2,0)$
108.2.893	I4cm1'						
108.3.894	I4'c'm	Fmm2	$(1/2,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)'$	$(4_z^*0,0,0)'$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}0,0,0)'$ $(m_{&y}^*1/2,1/2,0)$
108.4.895	I4'cm'	Iba2	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(4_z^*0,0,0)'$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)'$	$(4_z^{-1*}0,0,0)'$ $(m_{&y}^*1/2,1/2,0)'$
108.5.896	I4c'm'	I4	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)'$	$(4_z^*0,0,0)$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)'$	$(4_z^{-1*}0,0,0)$ $(m_{&y}^*1/2,1/2,0)'$
108.6.897	I <sub>p</sub> 4cm	P4bm	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(4_z^*0,0,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}0,0,0)$ $(m_{&y}^*1/2,1/2,0)$
108.7.898	I <sub>p</sub> 4'c'm	P4 <sub>2</sub> cm	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,1/2)$	$(4_z^*1/2,1/2,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(m_{&y}^*1/2,1/2,0)$
108.8.899	I <sub>p</sub> 4'cm'	P4 <sub>2</sub> bc	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(4_z^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(m_{&y}^*0,0,1/2)$
108.9.900	I <sub>p</sub> 4c'm'	P4cc	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,1/2)$	$(4_z^*0,0,0)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)$	$(4_z^{-1*}0,0,0)$ $(m_{&y}^*0,0,1/2)$
<b>109.1.901</b>	<b>I4<sub>1</sub>md</b>			$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,1/2,1/4)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,1/2,1/4)$	$(4_z^{-1*}0,1/2,1/4)$ $(m_{&y}^*0,1/2,1/4)$
109.2.902	I4 <sub>1</sub> md1'						
109.3.903	I4 <sub>1</sub> 'm'd	Fdd2	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,0)'$	$(4_z^*0,1/2,1/4)'$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,1/2,1/4)$	$(4_z^{-1*}0,1/2,1/4)'$ $(m_{&y}^*0,1/2,1/4)$

109.4.904	$I4_1'$ md'	Imm2	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,1/2,1/4)'$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,1/2,1/4)'$	$(4_z^{-1*}0,1/2,1/4)'$ $(m_{&y}^*0,1/2,1/4)'$
109.5.905	$I4_1$ m'd'	$I4_1$	(1/4,-1/4,0;a,b,c)	$(1^*0,0,0)$ $(m_x^*0,0,0)'$	$(4_z^*0,1/2,1/4)$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,1/2,1/4)'$	$(4_z^{-1*}0,1/2,1/4)$ $(m_{&y}^*0,1/2,1/4)'$
<b>110.1.906</b>	<b><math>I4_1</math>cd</b>			<b><math>(1^*0,0,0)</math></b> <b><math>(m_x^*0,0,1/2)</math></b>	<b><math>(4_z^*0,1/2,1/4)</math></b> <b><math>(m_y^*0,0,1/2)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(m_{xy}^*0,1/2,3/4)</math></b>	<b><math>(4_z^{-1*}0,1/2,1/4)</math></b> <b><math>(m_{&amp;y}^*0,1/2,3/4)</math></b>
110.2.907	$I4_1$ cd1'						
110.3.908	$I4_1'$ c'd	Fdd2	(0,0,0;a-b,a+b,c)	$(1^*0,0,0)$ $(m_x^*0,0,1/2)'$	$(4_z^*0,1/2,1/4)'$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,1/2,3/4)$	$(4_z^{-1*}0,1/2,1/4)'$ $(m_{&y}^*0,1/2,3/4)$
110.4.909	$I4_1'$ cd'	Iba2	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(m_x^*0,0,1/2)$	$(4_z^*0,1/2,1/4)'$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,1/2,3/4)'$	$(4_z^{-1*}0,1/2,1/4)'$ $(m_{&y}^*0,1/2,3/4)'$
110.5.910	$I4_1$ c'd'	$I4_1$	(1/4,-1/4,0;a,b,c)	$(1^*0,0,0)$ $(m_x^*0,0,1/2)'$	$(4_z^*0,1/2,1/4)$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,1/2,3/4)'$	$(4_z^{-1*}0,1/2,1/4)$ $(m_{&y}^*0,1/2,3/4)'$
<b>111.1.911</b>	<b><math>P&amp;2m</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(2_x^*0,0,0)</math></b>	<b><math>(&amp;_z^*0,0,0)</math></b> <b><math>(2_y^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(m_{xy}^*0,0,0)</math></b>	<b><math>(&amp;_z^{-1*}0,0,0)</math></b> <b><math>(m_{&amp;y}^*0,0,0)</math></b>
111.2.912	$P&2m1'$						
111.3.913	$P&2'm$	Cmm2	(0,0,0;a-b,a+b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)'$	$(&_z^*0,0,0)'$ $(2_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(&_z^{-1*}0,0,0)'$ $(m_{&y}^*0,0,0)$
111.4.914	$P&2m'$	P222	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(&_z^*0,0,0)'$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(&_z^{-1*}0,0,0)'$ $(m_{&y}^*0,0,0)'$

111.5.915	$P\bar{2}'m'$	$P\bar{2}$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)'$	$(\bar{2}_z^*0,0,0)$ $(2_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(\bar{2}_z^{-1*}0,0,0)$ $(m_{\bar{y}}^*0,0,0)'$
111.6.916	$P_{2c}\bar{2}m$	$P\bar{2}m$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(\bar{2}_z^*0,0,0)$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(\bar{2}_z^{-1*}0,0,0)$ $(m_{\bar{y}}^*0,0,0)$
111.7.917	$P_p\bar{2}m$	$P\bar{2}m2$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(\bar{2}_z^*0,0,0)$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(\bar{2}_z^{-1*}0,0,0)$ $(m_{\bar{y}}^*0,0,0)$
111.8.918	$P_1\bar{2}m$	$I\bar{2}m$	$(0,0,0;a-b,a+b,2c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(\bar{2}_z^*0,0,0)$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(\bar{2}_z^{-1*}0,0,0)$ $(m_{\bar{y}}^*0,0,0)$
111.9.919	$P_{2c}\bar{2}'m'$	$P\bar{2}2c$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1)$	$(\bar{2}_z^*0,0,0)$ $(2_y^*0,0,1)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,1)$	$(\bar{2}_z^{-1*}0,0,0)$ $(m_{\bar{y}}^*0,0,1)$
111.10.920	$P_p\bar{2}'2m'$	$P\bar{2}b2$	$(1/2,1/2,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(\bar{2}_z^*1,0,0)$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*1,0,0)$	$(\bar{2}_z^{-1*}1,0,0)$ $(m_{\bar{y}}^*1,0,0)$
111.11.921	$P_1\bar{2}'2m'$	$I\bar{2}c2$	$(1/2,-1/2,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(\bar{2}_z^*1,0,0)$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*1,0,0)$	$(\bar{2}_z^{-1*}1,0,0)$ $(m_{\bar{y}}^*1,0,0)$
<b>112.1.922</b>	<b><math>P\bar{2}2c</math></b>			<b><math>(1^*0,0,0)</math> <math>(2_x^*0,0,1/2)</math></b>	<b><math>(\bar{2}_z^*0,0,0)</math> <math>(2_y^*0,0,1/2)</math></b>	<b><math>(2_z^*0,0,0)</math> <math>(m_{xy}^*0,0,1/2)</math></b>	<b><math>(\bar{2}_z^{-1*}0,0,0)</math> <math>(m_{\bar{y}}^*0,0,1/2)</math></b>
112.2.923	$P\bar{2}c1'$						
112.3.924	$P\bar{2}'2c$	$Ccc2$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)'$	$(\bar{2}_z^*0,0,0)'$ $(2_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)$	$(\bar{2}_z^{-1*}0,0,0)'$ $(m_{\bar{y}}^*0,0,1/2)$
112.4.925	$P\bar{2}'2c'$	$P222$	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)$	$(\bar{2}_z^*0,0,0)'$ $(2_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)'$	$(\bar{2}_z^{-1*}0,0,0)'$ $(m_{\bar{y}}^*0,0,1/2)$
112.5.926	$P\bar{2}'2c'$	$P\bar{2}$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(\bar{2}_z^*0,0,0)$	$(2_z^*0,0,0)$	$(\bar{2}_z^{-1*}0,0,0)$



				$(2_x^*0,0,1/2)'$	$(2_y^*0,0,1/2)'$	$(m_{xy}^*0,0,1/2)'$	$(m_{&y}^*0,0,1/2)'$
112.6.927	$P_p \&2c$	$P\&c2$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)$	$(\&z^*0,0,0)$ $(2_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)$	$(\&z^{-1*}0,0,0)$ $(m_{&y}^*0,0,1/2)$
112.7.928	$P_p \&'2c'$	$P\&n2$	$(1/2,-1/2,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)$	$(\&z^*1,0,0)$ $(2_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(m_{xy}^*1,0,1/2)$	$(\&z^{-1*}1,0,0)$ $(m_{&y}^*1,0,1/2)$
<b>113.1.929</b>	<b><math>P\&amp;2,m</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(2_x^*1/2,1/2,0)</math></b>	<b><math>(\&amp;z^*0,0,0)</math></b> <b><math>(2_y^*1/2,1/2,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(m_{xy}^*1/2,1/2,0)</math></b>	<b><math>(\&amp;z^{-1*}0,0,0)</math></b> <b><math>(m_{&amp;y}^*1/2,1/2,0)</math></b>
113.2.930	$P\&2,m1'$						
113.3.931	$P\&'2_1,m$	$Cmm2$	$(1/2,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)'$	$(\&z^*0,0,0)'$ $(2_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)$	$(\&z^{-1*}0,0,0)'$ $(m_{&y}^*1/2,1/2,0)$
113.4.932	$P\&'2_1,m'$	$P2_12_2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$	$(\&z^*0,0,0)'$ $(2_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)'$	$(\&z^{-1*}0,0,0)'$ $(m_{&y}^*1/2,1/2,0)'$
113.5.933	$P\&2_1,m'$	$P\&$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)'$	$(\&z^*0,0,0)$ $(2_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)'$	$(\&z^{-1*}0,0,0)$ $(m_{&y}^*1/2,1/2,0)'$
113.6.934	$P_{2c} \&2_1,m$	$P\&2_1,m$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$	$(\&z^*0,0,0)$ $(2_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)$	$(\&z^{-1*}0,0,0)$ $(m_{&y}^*1/2,1/2,0)$
113.7.935	$P_{2c} \&'2_1,m'$	$P\&2_1,c$	$(0,0,1/2;a,b,2c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$	$(\&z^*0,0,1)$ $(2_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1)$	$(\&z^{-1*}0,0,1)$ $(m_{&y}^*1/2,1/2,1)$
<b>114.1.936</b>	<b><math>P\&amp;2_1,c</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(2_x^*1/2,1/2,1/2)</math></b>	<b><math>(\&amp;z^*0,0,0)</math></b> <b><math>(2_y^*1/2,1/2,1/2)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(m_{xy}^*1/2,1/2,1/2)</math></b>	<b><math>(\&amp;z^{-1*}0,0,0)</math></b> <b><math>(m_{&amp;y}^*1/2,1/2,1/2)</math></b>

114.2.937	$P\bar{2}_1c1'$						
114.3.938	$P\bar{2}_1'c$	Ccc2	$(1/2,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)'$	$(\bar{2}_z^*0,0,0)'$ $(2_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)$	$(\bar{2}_z^{-1*}0,0,0)'$ $(m_{\bar{y}}^*1/2,1/2,1/2)'$
114.4.939	$P\bar{2}_1'c$	P2 <sub>1</sub> 2 <sub>2</sub>	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)$	$(\bar{2}_z^*0,0,0)'$ $(2_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)'$	$(\bar{2}_z^{-1*}0,0,0)'$ $(m_{\bar{y}}^*1/2,1/2,1/2)'$
114.5.940	$P\bar{2}_1'c$	$P\bar{2}$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)'$	$(\bar{2}_z^*0,0,0)$ $(2_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)'$	$(\bar{2}_z^{-1*}0,0,0)$ $(m_{\bar{y}}^*1/2,1/2,1/2)'$
<b>115.1.941</b>	<b><math>P\bar{2}m2</math></b>			<b><math>(1^*0,0,0)</math> <math>(m_x^*0,0,0)</math></b>	<b><math>(\bar{2}_z^*0,0,0)</math> <math>(m_y^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math> <math>(2_{xy}^*0,0,0)</math></b>	<b><math>(\bar{2}_z^{-1*}0,0,0)</math> <math>(2_{\bar{y}}^*0,0,0)</math></b>
115.2.942	$P\bar{2}m21'$						
115.3.943	$P\bar{2}'m'2$	C222	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,0)'$	$(\bar{2}_z^*0,0,0)'$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(\bar{2}_z^{-1*}0,0,0)'$ $(2_{\bar{y}}^*0,0,0)$
115.4.944	$P\bar{2}'m'2'$	Pmm2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(\bar{2}_z^*0,0,0)'$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$	$(\bar{2}_z^{-1*}0,0,0)'$ $(2_{\bar{y}}^*0,0,0)'$
115.5.945	$P\bar{2}'m'2'$	$P\bar{2}$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,0)'$	$(\bar{2}_z^*0,0,0)$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$	$(\bar{2}_z^{-1*}0,0,0)$ $(2_{\bar{y}}^*0,0,0)'$
115.6.946	$P_{2c}\bar{2}m2$	$P\bar{2}m2$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(\bar{2}_z^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(\bar{2}_z^{-1*}0,0,0)$ $(2_{\bar{y}}^*0,0,0)$
115.7.947	$P_p\bar{2}m2$	$P\bar{2}2m$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(\bar{2}_z^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(\bar{2}_z^{-1*}0,0,0)$ $(2_{\bar{y}}^*0,0,0)$

115.8.948	$P_1 \& m_2$	$I \& 2m$	$(0,0,0;a-b,a+b,2c)$	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(\&_z^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(\&_z^{-1*}0,0,0)$ $(2_{\&y}^*0,0,0)$
115.9.949	$P_{2c} \& 'm'2$	$P \& c2$	$(0,0,1/2;a,b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,1)$	$(\&_z^*0,0,1)$ $(m_y^*0,0,1)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(\&_z^{-1*}0,0,1)$ $(2_{\&y}^*0,0,0)$
115.10.950	$P_p \& 'm'2'$	$P \& 2_1m$	$(1/2,-1/2,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(\&_z^*1,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1,0,0)$	$(\&_z^{-1*}1,0,0)$ $(2_{\&y}^*1,0,0)$
<b>116.1.951</b>	<b><math>P \&amp; c2</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(m_x^*0,0,1/2)</math></b>	<b><math>(\&amp;_z^*0,0,0)</math></b> <b><math>(m_y^*0,0,1/2)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(2_{xy}^*0,0,1/2)</math></b>	<b><math>(\&amp;_z^{-1*}0,0,0)</math></b> <b><math>(2_{\&amp;y}^*0,0,1/2)</math></b>
116.2.952	$P \& c21'$						
116.3.953	$P \& 'c'2$	$C222$	$(0,0,1/4;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,1/2)'$	$(\&_z^*0,0,0)'$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$	$(\&_z^{-1*}0,0,0)'$ $(2_{\&y}^*0,0,1/2)$
116.4.954	$P \& 'c'2'$	$Pcc2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,1/2)$	$(\&_z^*0,0,0)'$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)'$	$(\&_z^{-1*}0,0,0)'$ $(2_{\&y}^*0,0,1/2)'$
116.5.955	$P \& 'c'2'$	$P \&$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,1/2)'$	$(\&_z^*0,0,0)$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)'$	$(\&_z^{-1*}0,0,0)$ $(2_{\&y}^*0,0,1/2)'$
116.6.956	$P_p \& c2$	$P \& 2c$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,1/2)$	$(\&_z^*0,0,0)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$	$(\&_z^{-1*}0,0,0)$ $(2_{\&y}^*0,0,1/2)$
116.7.957	$P_p \& 'c'2'$	$P \& 2_1c$	$(1/2,-1/2,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,1/2)$	$(\&_z^*1,0,0)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*1,0,1/2)$	$(\&_z^{-1*}1,0,0)$ $(2_{\&y}^*1,0,1/2)$

<b>117.1.958</b>	<b>P&amp;b2</b>			$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(\&z^*0,0,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,0)$	$(\&z^{-1*}0,0,0)$ $(2_{\&y}^*1/2,1/2,0)$
117.2.959	P&b21'						
117.3.960	P&'b'2	C222	$(1/2,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)'$	$(\&z^*0,0,0)'$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,0)$	$(\&z^{-1*}0,0,0)'$ $(2_{\&y}^*1/2,1/2,0)$
117.4.961	P&'b'2'	Pba2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(\&z^*0,0,0)'$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,0)'$	$(\&z^{-1*}0,0,0)'$ $(2_{\&y}^*1/2,1/2,0)'$
117.5.962	P&'b'2'	P&	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)'$	$(\&z^*0,0,0)$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,0)'$	$(\&z^{-1*}0,0,0)$ $(2_{\&y}^*1/2,1/2,0)'$
117.6.963	P <sub>2c</sub> &b2	P&b2	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(\&z^*0,0,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,0)$	$(\&z^{-1*}0,0,0)$ $(2_{\&y}^*1/2,1/2,0)$
117.7.964	P <sub>2c</sub> &'b'2	P&n2	$(0,0,1/2;a,b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,1)$	$(\&z^*0,0,1)$ $(m_y^*1/2,1/2,1)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,0)$	$(\&z^{-1*}0,0,1)$ $(2_{\&y}^*1/2,1/2,0)$
<b>118.1.965</b>	<b>P&amp;n2</b>			$(1^*0,0,0)$ $(m_x^*1/2,1/2,1/2)$	$(\&z^*0,0,0)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)$	$(\&z^{-1*}0,0,0)$ $(2_{\&y}^*1/2,1/2,1/2)$
118.2.966	P&n21'						
118.3.967	P&'n'2	C222	$(1/2,0,1/4;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,1/2)'$	$(\&z^*0,0,0)'$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)$	$(\&z^{-1*}0,0,0)'$ $(2_{\&y}^*1/2,1/2,1/2)$
118.4.968	P&'n'2'	Pnn2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,1/2)$	$(\&z^*0,0,0)'$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)'$	$(\&z^{-1*}0,0,0)'$ $(2_{\&y}^*1/2,1/2,1/2)'$
118.5.969	P&'n'2'	P&	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(\&z^*0,0,0)$	$(2_z^*0,0,0)$	$(\&z^{-1*}0,0,0)$

118.6.970	$P_1 \&n2$	$I\&2d$	$(0,0,0;a-b,a+b,2c)$	$(m_x^{*1/2,1/2,1/2})'$ $(1^*0,0,0)$	$(m_y^{*1/2,1/2,1/2})'$ $(\&z^{*0,0,0})$	$(2_{xy}^{*1/2,1/2,1/2})'$ $(2_z^{*0,0,0})$	$(2_{\&y}^{*1/2,1/2,1/2})'$ $(\&z^{-1*0,0,0})$ $(2_{\&y}^{*1/2,1/2,1/2})$
<b>119.1.971</b>	<b><math>I\&amp;m2</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(m_x^{*0,0,0})</math></b>	<b><math>(\&amp;z^{*0,0,0})</math></b> <b><math>(m_y^{*0,0,0})</math></b>	<b><math>(2_z^{*0,0,0})</math></b> <b><math>(2_{xy}^{*0,0,0})</math></b>	<b><math>(\&amp;z^{-1*0,0,0})</math></b> <b><math>(2_{\&amp;y}^{*0,0,0})</math></b>
119.2.972	$I\&m21'$						
119.3.973	$I\&'m'2$	$F222$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^{*0,0,0})'$	$(\&z^{*0,0,0})'$ $(m_y^{*0,0,0})'$	$(2_z^{*0,0,0})$ $(2_{xy}^{*0,0,0})$	$(\&z^{-1*0,0,0})'$ $(2_{\&y}^{*0,0,0})$
119.4.974	$I\&'m'2'$	$Imm2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^{*0,0,0})$	$(\&z^{*0,0,0})'$ $(m_y^{*0,0,0})$	$(2_z^{*0,0,0})$ $(2_{xy}^{*0,0,0})'$	$(\&z^{-1*0,0,0})'$ $(2_{\&y}^{*0,0,0})'$
119.5.975	$I\&'m'2'$	$I\&$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^{*0,0,0})'$	$(\&z^{*0,0,0})'$ $(m_y^{*0,0,0})'$	$(2_z^{*0,0,0})$ $(2_{xy}^{*0,0,0})'$	$(\&z^{-1*0,0,0})'$ $(2_{\&y}^{*0,0,0})'$
119.6.976	$I_p \&m2$	$P\&m2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^{*0,0,0})$	$(\&z^{*0,0,0})'$ $(m_y^{*0,0,0})$	$(2_z^{*0,0,0})$ $(2_{xy}^{*0,0,0})$	$(\&z^{-1*0,0,0})'$ $(2_{\&y}^{*0,0,0})$
119.7.977	$I_p \&'m'2$	$P\&n2$	$(1/2,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(m_x^{*1/2,1/2,1/2})$	$(\&z^{*1/2,1/2,1/2})'$ $(m_y^{*1/2,1/2,1/2})$	$(2_z^{*0,0,0})$ $(2_{xy}^{*0,0,0})$	$(\&z^{-1*1/2,1/2,1/2})'$ $(2_{\&y}^{*0,0,0})$
<b>120.1.978</b>	<b><math>I\&amp;c2</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(m_x^{*0,0,1/2})</math></b>	<b><math>(\&amp;z^{*0,0,0})'</math></b> <b><math>(m_y^{*0,0,1/2})</math></b>	<b><math>(2_z^{*0,0,0})</math></b> <b><math>(2_{xy}^{*0,0,1/2})</math></b>	<b><math>(\&amp;z^{-1*0,0,0})'</math></b> <b><math>(2_{\&amp;y}^{*0,0,1/2})</math></b>
120.2.979	$I\&c21'$						
120.3.980	$I\&'c'2$	$F222$	$(0,0,1/4;a-b,a+b,c)$	$(1^*0,0,0)$	$(\&z^{*0,0,0})'$	$(2_z^{*0,0,0})$	$(\&z^{-1*0,0,0})'$

				$(m_x^*0,0,1/2)'$	$(m_y^*0,0,1/2)'$	$(2_{xy}^*0,0,1/2)$	$(2_{&y}^*0,0,1/2)$
120.4.981	$I&'c2'$	$Iba2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,1/2)$	$(&_z^*0,0,0)'$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)'$	$(&_z^{-1*}0,0,0)'$ $(2_{&y}^*0,0,1/2)'$
120.5.982	$I&'c2'$	$I&$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,1/2)'$	$(&_z^*0,0,0)$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)'$	$(&_z^{-1*}0,0,0)$ $(2_{&y}^*0,0,1/2)'$
120.6.983	$I_p \&c2$	$P&c2$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,1/2)$	$(&_z^*0,0,0)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$	$(&_z^{-1*}0,0,0)$ $(2_{&y}^*0,0,1/2)$
120.7.984	$I_p \&'c2'$	$P&b2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(&_z^*0,0,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,0)$	$(&_z^{-1*}0,0,0)$ $(2_{&y}^*1/2,1/2,0)$
<b>121.1.985</b>	<b><math>I&amp;2m</math></b>			<b><math>(1^*0,0,0)</math> <math>(2_x^*0,0,0)</math></b>	<b><math>(&amp;_z^*0,0,0)</math> <math>(2_y^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math> <math>(m_{xy}^*0,0,0)</math></b>	<b><math>(&amp;_z^{-1*}0,0,0)</math> <math>(m_{&amp;y}^*0,0,0)</math></b>
121.2.986	$I&2m1'$						
121.3.987	$I&'2'm$	$Fmm2$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)'$	$(&_z^*0,0,0)'$ $(2_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(&_z^{-1*}0,0,0)'$ $(m_{&y}^*0,0,0)$
121.4.988	$I&'2m'$	$I222$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(&_z^*0,0,0)'$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(&_z^{-1*}0,0,0)'$ $(m_{&y}^*0,0,0)'$
121.5.989	$I&'2'm'$	$I&$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)'$	$(&_z^*0,0,0)$ $(2_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(&_z^{-1*}0,0,0)$ $(m_{&y}^*0,0,0)'$
121.6.990	$I_p \&2m$	$P&2m$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(&_z^*0,0,0)$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(&_z^{-1*}0,0,0)$ $(m_{&y}^*0,0,0)$

121.7.991	$I_p \&2'm$	$P\&2_1m$	$(1/2,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)$	$(\&z^*1/2,1/2,1/2)$ $(2_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(\&z^{-1*}1/2,1/2,1/2)$ $(m_{\&y}^*0,0,0)$
121.8.992	$I_p \&2m'$	$P\&2c$	$(1/2,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(\&z^*1/2,1/2,1/2)$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)$	$(\&z^{-1*}1/2,1/2,1/2)$ $(m_{\&y}^*1/2,1/2,1/2)$
121.9.993	$I_p \&2'm'$	$P\&2_1c$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)$	$(\&z^*0,0,0)$ $(2_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)$	$(\&z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,1/2)$
<b>122.1.994</b>	<b><math>I\&amp;2d</math></b>			<b><math>(1^*0,0,0)</math> <math>(2_x^*0,1/2,1/4)</math></b>	<b><math>(\&amp;z^*0,0,0)</math> <math>(2_y^*0,1/2,1/4)</math></b>	<b><math>(2_z^*0,0,0)</math> <math>(m_{xy}^*0,1/2,1/4)</math></b>	<b><math>(\&amp;z^{-1*}0,0,0)</math> <math>(m_{\&amp;y}^*0,1/2,1/4)</math></b>
122.2.995	$I\&2d1'$						
122.3.996	$I\&2'd$	$Fdd2$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,1/2,1/4)'$	$(\&z^*0,0,0)'$ $(2_y^*0,1/2,1/4)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,1/2,1/4)$	$(\&z^{-1*}0,0,0)'$ $(m_{\&y}^*0,1/2,1/4)$
122.4.997	$I\&2'd'$	$I2_12_12_1$	$(0,1/4,1/8;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,1/2,1/4)$	$(\&z^*0,0,0)'$ $(2_y^*0,1/2,1/4)$	$(2_z^*0,0,0)$ $(m_{xy}^*0,1/2,1/4)'$	$(\&z^{-1*}0,0,0)'$ $(m_{\&y}^*0,1/2,1/4)'$
122.5.998	$I\&2'd'$	$I\&$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,1/2,1/4)'$	$(\&z^*0,0,0)$ $(2_y^*0,1/2,1/4)'$	$(2_z^*0,0,0)$ $(m_{xy}^*0,1/2,1/4)'$	$(\&z^{-1*}0,0,0)$ $(m_{\&y}^*0,1/2,1/4)'$
<b>123.1.999</b>	<b><math>P4/mmm</math></b>			<b><math>(1^*0,0,0)</math> <math>(2_x^*0,0,0)</math> <math>(\&amp;^*0,0,0)</math> <math>(m_x^*0,0,0)</math></b>	<b><math>(4_z^*0,0,0)</math> <math>(2_y^*0,0,0)</math> <math>(\&amp;z^*0,0,0)</math> <math>(m_y^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math> <math>(2_{xy}^*0,0,0)</math> <math>(m_z^*0,0,0)</math> <math>(m_{xy}^*0,0,0)</math></b>	<b><math>(4_z^{-1*}0,0,0)</math> <math>(2_{\&amp;y}^*0,0,0)</math> <math>(\&amp;z^{-1*}0,0,0)</math> <math>(m_{\&amp;y}^*0,0,0)</math></b>
123.2.1000	$P4/mmm1'$						

123.3.1001	P4/m'mm	P4mm	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)'$ $(\&^*0,0,0)'$ $(m_x^*0,0,0)$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)'$ $(\&_z^*0,0,0)'$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*0,0,0)'$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*0,0,0)$
123.4.1002	P4'/mm'm	Cmmm	(0,0,0;a-b,a+b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)'$ $(\&^*0,0,0)$ $(m_x^*0,0,0)'$	$(4_z^*0,0,0)'$ $(2_y^*0,0,0)'$ $(\&_z^*0,0,0)'$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)'$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*0,0,0)$
123.5.1003	P4'/mmm'	Pmmm	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,0)'$ $(2_y^*0,0,0)$ $(\&_z^*0,0,0)'$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,0)'$ $(2_{\&y}^*0,0,0)'$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*0,0,0)$
123.6.1004	P4'/m'm'm	P&2m	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&^*0,0,0)'$ $(m_x^*0,0,0)'$	$(4_z^*0,0,0)'$ $(2_y^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*0,0,0)'$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)'$ $(2_{\&y}^*0,0,0)'$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*0,0,0)$
123.7.1005	P4/mm'm'	P4/m	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)'$ $(\&^*0,0,0)$ $(m_x^*0,0,0)'$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)'$ $(\&_z^*0,0,0)$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*0,0,0)'$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*0,0,0)'$
123.8.1006	P4'/m'mm'	P&m2	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)'$ $(\&^*0,0,0)'$ $(m_x^*0,0,0)$	$(4_z^*0,0,0)'$ $(2_y^*0,0,0)'$ $(\&_z^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*0,0,0)'$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,0)'$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*0,0,0)'$
123.9.1007	P4/m'm'm'	P422	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&^*0,0,0)'$ $(m_x^*0,0,0)'$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)$ $(\&_z^*0,0,0)'$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*0,0,0)'$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*0,0,0)'$



123.10.1008	$P_{2c}4/mmm$	$P4/mmm$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1}^*0,0,0)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1}^*0,0,0)$ $(m_{\&y}^*0,0,0)$
123.11.1009	$P_p4/mmm$	$P4/mmm$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1}^*0,0,0)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1}^*0,0,0)$ $(m_{\&y}^*0,0,0)$
123.12.1010	$P_l4/mmm$	$I4/mmm$	$(0,0,0;a-b,a+b,2c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1}^*0,0,0)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1}^*0,0,0)$ $(m_{\&y}^*0,0,0)$
123.13.1011	$P_{2c}4'/mm'm$	$P4_2/mcm$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(2_x^*0,0,1)$ $(\&^*0,0,0)$ $(m_x^*0,0,1)$	$(4_z^*0,0,1)$ $(2_y^*0,0,1)$ $(\&_z^*0,0,1)$ $(m_y^*0,0,1)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1}^*0,0,1)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1}^*0,0,1)$ $(m_{\&y}^*0,0,0)$
123.14.1012	$P_{2c}4'/mmm'$	$P4_2/mmc$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,1)$ $(2_y^*0,0,0)$ $(\&_z^*0,0,1)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1)$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,1)$	$(4_z^{-1}^*0,0,1)$ $(2_{\&y}^*0,0,1)$ $(\&_z^{-1}^*0,0,1)$ $(m_{\&y}^*0,0,1)$
123.15.1013	$P_{2c}4'/mm'm'$	$P4/mcc$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(2_x^*0,0,1)$ $(\&^*0,0,0)$ $(m_x^*0,0,1)$	$(4_z^*0,0,0)$ $(2_y^*0,0,1)$ $(\&_z^*0,0,0)$ $(m_y^*0,0,1)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1)$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,1)$	$(4_z^{-1}^*0,0,0)$ $(2_{\&y}^*0,0,1)$ $(\&_z^{-1}^*0,0,0)$ $(m_{\&y}^*0,0,1)$
123.16.1014	$P_p4/m'mm$	$P4/nmm$	$(1/2,1/2,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*1,0,0)$ $(\&^*1,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,0)$ $(2_y^*1,0,0)$ $(\&_z^*1,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1,0,0)$ $(m_z^*1,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1}^*0,0,0)$ $(2_{\&y}^*1,0,0)$ $(\&_z^{-1}^*1,0,0)$ $(m_{\&y}^*0,0,0)$

123.17.1015	$P_4/mmm'$	$P4/mbm$	$(1/2, 1/2, 0; a-b, a+b, c)$	$(1^*0, 0, 0)$ $(2_x^*0, 0, 0)$ $(\&^*0, 0, 0)$ $(m_x^*0, 0, 0)$	$(4_z^*1, 0, 0)$ $(2_y^*0, 0, 0)$ $(\&_z^*1, 0, 0)$ $(m_y^*0, 0, 0)$	$(2_z^*0, 0, 0)$ $(2_{xy}^*1, 0, 0)$ $(m_z^*0, 0, 0)$ $(m_{xy}^*1, 0, 0)$	$(4_z^{-1*}1, 0, 0)$ $(2_{\&y}^*1, 0, 0)$ $(\&_z^{-1*}1, 0, 0)$ $(m_{\&y}^*1, 0, 0)$
123.18.1016	$P_4/m'mm'$	$P4/nbm$	$(1/2, 1/2, 0; a-b, a+b, c)$	$(1^*0, 0, 0)$ $(2_x^*1, 0, 0)$ $(\&^*1, 0, 0)$ $(m_x^*0, 0, 0)$	$(4_z^*1, 0, 0)$ $(2_y^*1, 0, 0)$ $(\&_z^*0, 0, 0)$ $(m_y^*0, 0, 0)$	$(2_z^*0, 0, 0)$ $(2_{xy}^*0, 0, 0)$ $(m_z^*1, 0, 0)$ $(m_{xy}^*1, 0, 0)$	$(4_z^{-1*}1, 0, 0)$ $(2_{\&y}^*0, 0, 0)$ $(\&_z^{-1*}0, 0, 0)$ $(m_{\&y}^*1, 0, 0)$
123.19.1017	$P_14/mm'm'$	$I4/mcm$	$(1/2, 1/2, 0; a-b, a+b, 2c)$	$(1^*0, 0, 0)$ $(2_x^*1, 0, 0)$ $(\&^*0, 0, 0)$ $(m_x^*1, 0, 0)$	$(4_z^*0, 0, 0)$ $(2_y^*1, 0, 0)$ $(\&_z^*0, 0, 0)$ $(m_y^*1, 0, 0)$	$(2_z^*0, 0, 0)$ $(2_{xy}^*1, 0, 0)$ $(m_z^*0, 0, 0)$ $(m_{xy}^*1, 0, 0)$	$(4_z^{-1*}0, 0, 0)$ $(2_{\&y}^*1, 0, 0)$ $(\&_z^{-1*}0, 0, 0)$ $(m_{\&y}^*1, 0, 0)$
<b>124.1.1018</b>	<b><math>P4/mcc</math></b>			$(1^*0, 0, 0)$ $(2_x^*0, 0, 1/2)$ $(\&^*0, 0, 0)$ $(m_x^*0, 0, 1/2)$	$(4_z^*0, 0, 0)$ $(2_y^*0, 0, 1/2)$ $(\&_z^*0, 0, 0)$ $(m_y^*0, 0, 1/2)$	$(2_z^*0, 0, 0)$ $(2_{xy}^*0, 0, 1/2)$ $(m_z^*0, 0, 0)$ $(m_{xy}^*0, 0, 1/2)$	$(4_z^{-1*}0, 0, 0)$ $(2_{\&y}^*0, 0, 1/2)$ $(\&_z^{-1*}0, 0, 0)$ $(m_{\&y}^*0, 0, 1/2)$
124.2.1019	$P4/mcc1'$						
124.3.1020	$P4/m'cc$	$P4cc$	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$ $(2_x^*0, 0, 1/2)'$ $(\&^*0, 0, 0)'$ $(m_x^*0, 0, 1/2)$	$(4_z^*0, 0, 0)$ $(2_y^*0, 0, 1/2)'$ $(\&_z^*0, 0, 0)'$ $(m_y^*0, 0, 1/2)$	$(2_z^*0, 0, 0)$ $(2_{xy}^*0, 0, 1/2)'$ $(m_z^*0, 0, 0)'$ $(m_{xy}^*0, 0, 1/2)$	$(4_z^{-1*}0, 0, 0)$ $(2_{\&y}^*0, 0, 1/2)'$ $(\&_z^{-1*}0, 0, 0)'$ $(m_{\&y}^*0, 0, 1/2)$
124.4.1021	$P4'/mc'c$	$Cccm$	$(0, 0, 0; a-b, a+b, c)$	$(1^*0, 0, 0)$ $(2_x^*0, 0, 1/2)'$ $(\&^*0, 0, 0)$ $(m_x^*0, 0, 1/2)'$	$(4_z^*0, 0, 0)'$ $(2_y^*0, 0, 1/2)'$ $(\&_z^*0, 0, 0)'$ $(m_y^*0, 0, 1/2)'$	$(2_z^*0, 0, 0)$ $(2_{xy}^*0, 0, 1/2)$ $(m_z^*0, 0, 0)$ $(m_{xy}^*0, 0, 1/2)$	$(4_z^{-1*}0, 0, 0)'$ $(2_{\&y}^*0, 0, 1/2)$ $(\&_z^{-1*}0, 0, 0)'$ $(m_{\&y}^*0, 0, 1/2)$

124.5.1022	P4'/mcc'	Pccm	(0,0,0;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *0,0,1/2) (&_z*0,0,0) (m <sub>x</sub> *0,0,1/2)	(4 <sub>z</sub> *0,0,0)' (2 <sub>xy</sub> *0,0,1/2) (&_z*0,0,0)' (m <sub>y</sub> *0,0,1/2)	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *0,0,1/2)' (m <sub>z</sub> *0,0,0) (m <sub>xy</sub> *0,0,1/2)'	(4 <sub>z</sub> <sup>-1</sup> *0,0,0)' (2 <sub>&amp;y</sub> *0,0,1/2)' (&_z <sup>-1</sup> *0,0,0)' (m <sub>&amp;y</sub> *0,0,1/2)'
124.6.1023	P4'/m'c'c	P&2c	(0,0,0;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *0,0,1/2) (&_z*0,0,0)' (m <sub>x</sub> *0,0,1/2)'	(4 <sub>z</sub> *0,0,0)' (2 <sub>y</sub> *0,0,1/2) (&_z*0,0,0) (m <sub>y</sub> *0,0,1/2)'	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *0,0,1/2)' (m <sub>z</sub> *0,0,0)' (m <sub>xy</sub> *0,0,1/2)'	(4 <sub>z</sub> <sup>-1</sup> *0,0,0)' (2 <sub>&amp;y</sub> *0,0,1/2)' (&_z <sup>-1</sup> *0,0,0) (m <sub>&amp;y</sub> *0,0,1/2)'
124.7.1024	P4/mc'c'	P4/m	(0,0,0;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *0,0,1/2)' (&_z*0,0,0) (m <sub>x</sub> *0,0,1/2)'	(4 <sub>z</sub> *0,0,0) (2 <sub>y</sub> *0,0,1/2)' (&_z*0,0,0) (m <sub>y</sub> *0,0,1/2)'	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *0,0,1/2)' (m <sub>z</sub> *0,0,0) (m <sub>xy</sub> *0,0,1/2)'	(4 <sub>z</sub> <sup>-1</sup> *0,0,0) (2 <sub>&amp;y</sub> *0,0,1/2)' (&_z <sup>-1</sup> *0,0,0) (m <sub>&amp;y</sub> *0,0,1/2)'
124.8.1025	P4'/m'cc'	P&c2	(0,0,0;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *0,0,1/2)' (&_z*0,0,0)' (m <sub>x</sub> *0,0,1/2)	(4 <sub>z</sub> *0,0,0)' (2 <sub>y</sub> *0,0,1/2)' (&_z*0,0,0) (m <sub>y</sub> *0,0,1/2)	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *0,0,1/2) (m <sub>z</sub> *0,0,0)' (m <sub>xy</sub> *0,0,1/2)'	(4 <sub>z</sub> <sup>-1</sup> *0,0,0)' (2 <sub>&amp;y</sub> *0,0,1/2) (&_z <sup>-1</sup> *0,0,0) (m <sub>&amp;y</sub> *0,0,1/2)'
124.9.1026	P4/m'c'c'	P422	(0,0,1/4;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *0,0,1/2) (&_z*0,0,0)' (m <sub>x</sub> *0,0,1/2)'	(4 <sub>z</sub> *0,0,0) (2 <sub>y</sub> *0,0,1/2) (&_z*0,0,0)' (m <sub>y</sub> *0,0,1/2)'	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *0,0,1/2) (m <sub>z</sub> *0,0,0)' (m <sub>xy</sub> *0,0,1/2)'	(4 <sub>z</sub> <sup>-1</sup> *0,0,0) (2 <sub>&amp;y</sub> *0,0,1/2) (&_z <sup>-1</sup> *0,0,0)' (m <sub>&amp;y</sub> *0,0,1/2)'
124.10.1027	P <sub>p</sub> 4/mcc	P4/mcc	(0,0,0;a-b,a+b,c)	(1*0,0,0) (2 <sub>x</sub> *0,0,1/2) (&_z*0,0,0) (m <sub>x</sub> *0,0,1/2)	(4 <sub>z</sub> *0,0,0) (2 <sub>y</sub> *0,0,1/2) (&_z*0,0,0) (m <sub>y</sub> *0,0,1/2)	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *0,0,1/2) (m <sub>z</sub> *0,0,0) (m <sub>xy</sub> *0,0,1/2)	(4 <sub>z</sub> <sup>-1</sup> *0,0,0) (2 <sub>&amp;y</sub> *0,0,1/2) (&_z <sup>-1</sup> *0,0,0) (m <sub>&amp;y</sub> *0,0,1/2)
124.11.1028	P <sub>p</sub> 4/m'cc	P4/ncc	(1/2,1/2,0;a-b,a+b,c)	(1*0,0,0) (2 <sub>x</sub> *1,0,1/2) (&_z*1,0,0)	(4 <sub>z</sub> *0,0,0) (2 <sub>y</sub> *1,0,1/2) (&_z*1,0,0)	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *1,0,1/2) (m <sub>z</sub> *1,0,0)	(4 <sub>z</sub> <sup>-1</sup> *0,0,0) (2 <sub>&amp;y</sub> *1,0,1/2) (&_z <sup>-1</sup> *1,0,0)

				$(m_x^*0,0,1/2)$	$(m_y^*0,0,1/2)$	$(m_{xy}^*0,0,1/2)$	$(m_{\&y}^*0,0,1/2)$
124.12.1029	$P_4/mcc'$	P4/mnc	$(1/2,1/2,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)$ $(\&^*0,0,0)$ $(m_x^*0,0,1/2)$	$(4_z^*1,0,0)$ $(2_y^*0,0,1/2)$ $(\&_z^*1,0,0)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*1,0,1/2)$ $(m_z^*0,0,0)$ $(m_{xy}^*1,0,1/2)$	$(4_z^{-1*}1,0,0)$ $(2_{\&y}^*1,0,1/2)$ $(\&_z^{-1*}1,0,0)$ $(m_{\&y}^*1,0,1/2)$
124.13.1030	$P_4/m'cc'$	P4/nnc	$(1/2,1/2,1/4;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*1,0,1/2)$ $(\&^*1,0,0)$ $(m_x^*0,0,1/2)$	$(4_z^*1,0,0)$ $(2_y^*1,0,1/2)$ $(\&_z^*0,0,0)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$ $(m_z^*1,0,0)$ $(m_{xy}^*1,0,1/2)$	$(4_z^{-1*}1,0,0)$ $(2_{\&y}^*0,0,1/2)$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*1,0,1/2)$
<b>125.1.1031</b>	<b>P4/nbm</b>			$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&^*1/2,1/2,0)$ $(m_x^*1/2,1/2,0)$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)$ $(\&_z^*1/2,1/2,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*1/2,1/2,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}1/2,1/2,0)$ $(m_{\&y}^*1/2,1/2,0)$
125.2.1032	P4/nbm1'						
125.3.1033	$P4/n'bm$	P4bm	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)'$ $(\&^*1/2,1/2,0)'$ $(m_x^*1/2,1/2,0)$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)'$ $(\&_z^*1/2,1/2,0)'$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*1/2,1/2,0)'$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*0,0,0)'$ $(\&_z^{-1*}1/2,1/2,0)'$ $(m_{\&y}^*1/2,1/2,0)$
125.4.1034	$P4'/nb'm$	Cmma	$(1/4,1/4,0;a+b,-a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)'$ $(\&^*1/2,1/2,0)$ $(m_x^*1/2,1/2,0)'$	$(4_z^*0,0,0)'$ $(2_y^*0,0,0)'$ $(\&_z^*1/2,1/2,0)'$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*1/2,1/2,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}0,0,0)'$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}1/2,1/2,0)'$ $(m_{\&y}^*1/2,1/2,0)$
125.5.1035	$P4'/nbm'$	Pban	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(4_z^*0,0,0)'$ $(2_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,0)'$ $(2_{\&y}^*0,0,0)'$

				$(\&_z^*1/2,1/2,0)$ $(m_x^*1/2,1/2,0)$	$(\&_z^*1/2,1/2,0)'$ $(m_y^*1/2,1/2,0)$	$(m_z^*1/2,1/2,0)$ $(m_{xy}^*1/2,1/2,0)'$	$(\&_z^{-1*}1/2,1/2,0)'$ $(m_{\&y}^*1/2,1/2,0)'$
125.6.1036	P4'/n'b'm	P&2m	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&_z^*1/2,1/2,0)'$ $(m_x^*1/2,1/2,0)'$	$(4_z^*0,0,0)'$ $(2_y^*0,0,0)$ $(\&_z^*1/2,1/2,0)$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*1/2,1/2,0)'$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}0,0,0)'$ $(2_{\&y}^*0,0,0)'$ $(\&_z^{-1*}1/2,1/2,0)$ $(m_{\&y}^*1/2,1/2,0)$
125.7.1037	P4/nb'm'	P4/n	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)'$ $(\&_z^*1/2,1/2,0)$ $(m_x^*1/2,1/2,0)'$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)'$ $(\&_z^*1/2,1/2,0)$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*1/2,1/2,0)$ $(m_{xy}^*1/2,1/2,0)'$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*0,0,0)'$ $(\&_z^{-1*}1/2,1/2,0)$ $(m_{\&y}^*1/2,1/2,0)'$
125.8.1038	P4'/n'bm'	P&b2	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)'$ $(\&_z^*1/2,1/2,0)'$ $(m_x^*1/2,1/2,0)$	$(4_z^*0,0,0)'$ $(2_y^*0,0,0)'$ $(\&_z^*1/2,1/2,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*1/2,1/2,0)'$ $(m_{xy}^*1/2,1/2,0)'$	$(4_z^{-1*}0,0,0)'$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}1/2,1/2,0)$ $(m_{\&y}^*1/2,1/2,0)'$
125.9.1039	P4/n'b'm'	P422	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&_z^*1/2,1/2,0)'$ $(m_x^*1/2,1/2,0)'$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)$ $(\&_z^*1/2,1/2,0)'$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*1/2,1/2,0)'$ $(m_{xy}^*1/2,1/2,0)'$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}1/2,1/2,0)'$ $(m_{\&y}^*1/2,1/2,0)'$
125.10.1040	P <sub>2c</sub> 4'/nbm	P4/nbm	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&_z^*1/2,1/2,0)$ $(m_x^*1/2,1/2,0)$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)$ $(\&_z^*1/2,1/2,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*1/2,1/2,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}1/2,1/2,0)$ $(m_{\&y}^*1/2,1/2,0)$
125.11.1041	P <sub>2c</sub> 4'/nb'm	P4 <sub>2</sub> /nmm	$(1/2,0,1/2;a,b,2c)$	$(1^*0,0,0)$ $(2_x^*0,0,1)$ $(\&_z^*1/2,1/2,0)$ $(m_x^*1/2,1/2,1)$	$(4_z^*0,0,1)$ $(2_y^*0,0,1)$ $(\&_z^*1/2,1/2,1)$ $(m_y^*1/2,1/2,1)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*1/2,1/2,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}0,0,1)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}1/2,1/2,1)$ $(m_{\&y}^*1/2,1/2,0)$
125.12.1042	P <sub>2c</sub> 4'/nbm'	P4 <sub>2</sub> /nbc	$(1/2,0,1/2;a,b,2c)$	$(1^*0,0,0)$	$(4_z^*0,0,1)$	$(2_z^*0,0,0)$	$(4_z^{-1*}0,0,1)$

				$(2_x^*0,0,0)$ $(\&_x^*1/2,1/2,0)$ $(m_x^*1/2,1/2,0)$	$(2_y^*0,0,0)$ $(\&_z^*1/2,1/2,1)$ $(m_y^*1/2,1/2,0)$	$(2_{xy}^*0,0,1)$ $(m_z^*1/2,1/2,0)$ $(m_{xy}^*1/2,1/2,1)$	$(2_{\&y}^*0,0,1)$ $(\&_z^{-1*}1/2,1/2,1)$ $(m_{\&y}^*1/2,1/2,1)$
125.13.1043	$P_{2c}4/nb'm'$	P4nnc	$(0,0,1/2;a,b,2c)$	$(1^*0,0,0)$ $(2_x^*0,0,1)$ $(\&_x^*1/2,1/2,0)$ $(m_x^*1/2,1/2,1)$	$(4_z^*0,0,0)$ $(2_y^*0,0,1)$ $(\&_z^*1/2,1/2,0)$ $(m_y^*1/2,1/2,1)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1)$ $(m_z^*1/2,1/2,0)$ $(m_{xy}^*1/2,1/2,1)$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*0,0,1)$ $(\&_z^{-1*}1/2,1/2,0)$ $(m_{\&y}^*1/2,1/2,1)$
<b>126.1.1044</b>	<b>P4/nnc</b>			$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&_x^*1/2,1/2,1/2)$ $(m_x^*1/2,1/2,1/2)$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)$ $(\&_z^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*1/2,1/2,1/2)$ $(m_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}1/2,1/2,1/2)$ $(m_{\&y}^*1/2,1/2,1/2)$
126.2.1045	P4/nnc1'						
126.3.1046	P4/n'nc	P4nc	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)'$ $(\&_x^*1/2,1/2,1/2)'$ $(m_x^*1/2,1/2,1/2)$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)'$ $(\&_z^*1/2,1/2,1/2)'$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*1/2,1/2,1/2)'$ $(m_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*0,0,0)'$ $(\&_z^{-1*}1/2,1/2,1/2)'$ $(m_{\&y}^*1/2,1/2,1/2)$
126.4.1047	P4'/nn'c	Ccca	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)'$ $(\&_x^*1/2,1/2,1/2)$ $(m_x^*1/2,1/2,1/2)'$	$(4_z^*0,0,0)'$ $(2_y^*0,0,0)'$ $(\&_z^*1/2,1/2,1/2)'$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*1/2,1/2,1/2)$ $(m_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}0,0,0)'$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}1/2,1/2,1/2)'$ $(m_{\&y}^*1/2,1/2,1/2)$
126.5.1048	P4'/nnc'	Pnnn	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&_x^*1/2,1/2,1/2)$ $(m_x^*1/2,1/2,1/2)$	$(4_z^*0,0,0)'$ $(2_y^*0,0,0)$ $(\&_z^*1/2,1/2,1/2)'$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*1/2,1/2,1/2)$ $(m_{xy}^*1/2,1/2,1/2)'$	$(4_z^{-1*}0,0,0)'$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}1/2,1/2,1/2)'$ $(m_{\&y}^*1/2,1/2,1/2)$
126.6.1049	P4'/n'n'c	P&2c	$(1/2,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&_x^*1/2,1/2,1/2)'$	$(4_z^*0,0,0)'$ $(2_y^*0,0,0)$ $(\&_z^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*1/2,1/2,1/2)'$	$(4_z^{-1*}0,0,0)'$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}1/2,1/2,1/2)$

				$(m_x^* 1/2, 1/2, 1/2)'$	$(m_y^* 1/2, 1/2, 1/2)'$	$(m_{xy}^* 1/2, 1/2, 1/2)$	$(m_{\&y}^* 1/2, 1/2, 1/2)$
126.7.1050	P4/nn'c'	P4/n	$(1/2, 0, 1/4; a, b, c)$	$(1^* 0, 0, 0)$ $(2_x^* 0, 0, 0)'$ $(\&^* 1/2, 1/2, 1/2)$ $(m_x^* 1/2, 1/2, 1/2)'$	$(4_z^* 0, 0, 0)$ $(2_y^* 0, 0, 0)'$ $(\&_z^* 1/2, 1/2, 1/2)$ $(m_y^* 1/2, 1/2, 1/2)'$	$(2_z^* 0, 0, 0)$ $(2_{xy}^* 0, 0, 0)'$ $(m_z^* 1/2, 1/2, 1/2)$ $(m_{xy}^* 1/2, 1/2, 1/2)'$	$(4_z^{-1} 0, 0, 0)$ $(2_{\&y}^* 0, 0, 0)'$ $(\&_z^{-1} 1/2, 1/2, 1/2)$ $(m_{\&y}^* 1/2, 1/2, 1/2)'$
126.8.1051	P4'/n'nc'	P&n2	$(1/2, 0, 1/4; a, b, c)$	$(1^* 0, 0, 0)$ $(2_x^* 0, 0, 0)'$ $(\&^* 1/2, 1/2, 1/2)'$ $(m_x^* 1/2, 1/2, 1/2)$	$(4_z^* 0, 0, 0)'$ $(2_y^* 0, 0, 0)'$ $(\&_z^* 1/2, 1/2, 1/2)$ $(m_y^* 1/2, 1/2, 1/2)$	$(2_z^* 0, 0, 0)$ $(2_{xy}^* 0, 0, 0)$ $(m_z^* 1/2, 1/2, 1/2)'$ $(m_{xy}^* 1/2, 1/2, 1/2)'$	$(4_z^{-1} 0, 0, 0)'$ $(2_{\&y}^* 0, 0, 0)$ $(\&_z^{-1} 1/2, 1/2, 1/2)$ $(m_{\&y}^* 1/2, 1/2, 1/2)'$
126.9.1052	P4/n'n'c'	P422	$(0, 0, 0; a, b, c)$	$(1^* 0, 0, 0)$ $(2_x^* 0, 0, 0)$ $(\&^* 1/2, 1/2, 1/2)'$ $(m_x^* 1/2, 1/2, 1/2)'$	$(4_z^* 0, 0, 0)$ $(2_y^* 0, 0, 0)$ $(\&_z^* 1/2, 1/2, 1/2)'$ $(m_y^* 1/2, 1/2, 1/2)'$	$(2_z^* 0, 0, 0)$ $(2_{xy}^* 0, 0, 0)$ $(m_z^* 1/2, 1/2, 1/2)'$ $(m_{xy}^* 1/2, 1/2, 1/2)'$	$(4_z^{-1} 0, 0, 0)$ $(2_{\&y}^* 0, 0, 0)$ $(\&_z^{-1} 1/2, 1/2, 1/2)'$ $(m_{\&y}^* 1/2, 1/2, 1/2)'$
<b>127.1.1053</b>	<b>P4/mbm</b>			$(1^* 0, 0, 0)$ $(2_x^* 1/2, 1/2, 0)$ $(\&^* 0, 0, 0)$ $(m_x^* 1/2, 1/2, 0)$	$(4_z^* 0, 0, 0)$ $(2_y^* 1/2, 1/2, 0)$ $(\&_z^* 0, 0, 0)$ $(m_y^* 1/2, 1/2, 0)$	$(2_z^* 0, 0, 0)$ $(2_{xy}^* 1/2, 1/2, 0)$ $(m_z^* 0, 0, 0)$ $(m_{xy}^* 1/2, 1/2, 0)$	$(4_z^{-1} 0, 0, 0)$ $(2_{\&y}^* 1/2, 1/2, 0)$ $(\&_z^{-1} 0, 0, 0)$ $(m_{\&y}^* 1/2, 1/2, 0)$
127.2.1054	P4/mbm1'						
127.3.1055	P4/m'bm	P4bm	$(0, 0, 0; a, b, c)$	$(1^* 0, 0, 0)$ $(2_x^* 1/2, 1/2, 0)'$ $(\&^* 0, 0, 0)'$ $(m_x^* 1/2, 1/2, 0)$	$(4_z^* 0, 0, 0)$ $(2_y^* 1/2, 1/2, 0)'$ $(\&_z^* 0, 0, 0)'$ $(m_y^* 1/2, 1/2, 0)$	$(2_z^* 0, 0, 0)$ $(2_{xy}^* 1/2, 1/2, 0)'$ $(m_z^* 0, 0, 0)'$ $(m_{xy}^* 1/2, 1/2, 0)$	$(4_z^{-1} 0, 0, 0)$ $(2_{\&y}^* 1/2, 1/2, 0)'$ $(\&_z^{-1} 0, 0, 0)'$ $(m_{\&y}^* 1/2, 1/2, 0)$
127.4.1056	P4'/mb'm	Cmmm	$(1/2, 0, 0; a-b, a+b, c)$	$(1^* 0, 0, 0)$ $(2_x^* 1/2, 1/2, 0)'$ $(\&^* 0, 0, 0)$ $(m_x^* 1/2, 1/2, 0)'$	$(4_z^* 0, 0, 0)'$ $(2_y^* 1/2, 1/2, 0)'$ $(\&_z^* 0, 0, 0)'$ $(m_y^* 1/2, 1/2, 0)'$	$(2_z^* 0, 0, 0)$ $(2_{xy}^* 1/2, 1/2, 0)$ $(m_z^* 0, 0, 0)$ $(m_{xy}^* 1/2, 1/2, 0)$	$(4_z^{-1} 0, 0, 0)'$ $(2_{\&y}^* 1/2, 1/2, 0)$ $(\&_z^{-1} 0, 0, 0)'$ $(m_{\&y}^* 1/2, 1/2, 0)$

127.5.1057	P4'/mbm'	Pbam	(0,0,0;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *1/2,1/2,0) (&*0,0,0) (m <sub>x</sub> *1/2,1/2,0)	(4 <sub>z</sub> *0,0,0)' (2 <sub>xy</sub> *1/2,1/2,0) (& <sub>z</sub> *0,0,0)' (m <sub>y</sub> *1/2,1/2,0)	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *1/2,1/2,0)' (m <sub>z</sub> *0,0,0) (m <sub>xy</sub> *1/2,1/2,0)'	(4 <sub>z</sub> <sup>-1</sup> *0,0,0)' (2 <sub>&amp;y</sub> *1/2,1/2,0)' (& <sub>z</sub> <sup>-1</sup> *0,0,0)' (m <sub>&amp;y</sub> *1/2,1/2,0)'
127.6.1058	P4'/m'b'm	P&2 <sub>1</sub> m	(0,0,0;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *1/2,1/2,0) (&*0,0,0)' (m <sub>x</sub> *1/2,1/2,0)'	(4 <sub>z</sub> *0,0,0)' (2 <sub>y</sub> *1/2,1/2,0) (& <sub>z</sub> *0,0,0) (m <sub>y</sub> *1/2,1/2,0)'	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *1/2,1/2,0)' (m <sub>z</sub> *0,0,0)' (m <sub>xy</sub> *1/2,1/2,0)	(4 <sub>z</sub> <sup>-1</sup> *0,0,0)' (2 <sub>&amp;y</sub> *1/2,1/2,0)' (& <sub>z</sub> <sup>-1</sup> *0,0,0) (m <sub>&amp;y</sub> *1/2,1/2,0)
127.7.1059	P4/mb'm'	P4/m	(0,0,0;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *1/2,1/2,0)' (&*0,0,0) (m <sub>x</sub> *1/2,1/2,0)'	(4 <sub>z</sub> *0,0,0) (2 <sub>y</sub> *1/2,1/2,0)' (& <sub>z</sub> *0,0,0) (m <sub>y</sub> *1/2,1/2,0)'	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *1/2,1/2,0)' (m <sub>z</sub> *0,0,0) (m <sub>xy</sub> *1/2,1/2,0)'	(4 <sub>z</sub> <sup>-1</sup> *0,0,0) (2 <sub>&amp;y</sub> *1/2,1/2,0)' (& <sub>z</sub> <sup>-1</sup> *0,0,0) (m <sub>&amp;y</sub> *1/2,1/2,0)'
127.8.1060	P4'/m'bm'	P&b2	(0,0,0;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *1/2,1/2,0)' (&*0,0,0)' (m <sub>x</sub> *1/2,1/2,0)	(4 <sub>z</sub> *0,0,0)' (2 <sub>y</sub> *1/2,1/2,0)' (& <sub>z</sub> *0,0,0) (m <sub>y</sub> *1/2,1/2,0)	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *1/2,1/2,0) (m <sub>z</sub> *0,0,0)' (m <sub>xy</sub> *1/2,1/2,0)'	(4 <sub>z</sub> <sup>-1</sup> *0,0,0)' (2 <sub>&amp;y</sub> *1/2,1/2,0) (& <sub>z</sub> <sup>-1</sup> *0,0,0) (m <sub>&amp;y</sub> *1/2,1/2,0)'
127.9.1061	P4/m'b'm'	P4 <sub>2</sub> ,2	(1/2,0,0;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *1/2,1/2,0) (&*0,0,0)' (m <sub>x</sub> *1/2,1/2,0)'	(4 <sub>z</sub> *0,0,0) (2 <sub>y</sub> *1/2,1/2,0) (& <sub>z</sub> *0,0,0)' (m <sub>y</sub> *1/2,1/2,0)'	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *1/2,1/2,0) (m <sub>z</sub> *0,0,0)' (m <sub>xy</sub> *1/2,1/2,0)'	(4 <sub>z</sub> <sup>-1</sup> *0,0,0) (2 <sub>&amp;y</sub> *1/2,1/2,0) (& <sub>z</sub> <sup>-1</sup> *0,0,0)' (m <sub>&amp;y</sub> *1/2,1/2,0)'
127.10.1062	P <sub>2c</sub> 4'/mbm	P4'/mbm	(0,0,0;a,b,2c)	(1*0,0,0) (2 <sub>x</sub> *1/2,1/2,0) (&*0,0,0) (m <sub>x</sub> *1/2,1/2,0)	(4 <sub>z</sub> *0,0,0) (2 <sub>y</sub> *1/2,1/2,0) (& <sub>z</sub> *0,0,0) (m <sub>y</sub> *1/2,1/2,0)	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *1/2,1/2,0) (m <sub>z</sub> *0,0,0) (m <sub>xy</sub> *1/2,1/2,0)	(4 <sub>z</sub> <sup>-1</sup> *0,0,0) (2 <sub>&amp;y</sub> *1/2,1/2,0) (& <sub>z</sub> <sup>-1</sup> *0,0,0) (m <sub>&amp;y</sub> *1/2,1/2,0)
127.11.1063	P <sub>2c</sub> 4'/mb'm	P4 <sub>2</sub> /mnm	(1/2,0,0;a,b,2c)	(1*0,0,0) (2 <sub>x</sub> *1/2,1/2,1) (&*0,0,0)	(4 <sub>z</sub> *0,0,1) (2 <sub>y</sub> *1/2,1/2,1) (& <sub>z</sub> *0,0,1)	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *1/2,1/2,0) (m <sub>z</sub> *0,0,0)	(4 <sub>z</sub> <sup>-1</sup> *0,0,1) (2 <sub>&amp;y</sub> *1/2,1/2,0) (& <sub>z</sub> <sup>-1</sup> *0,0,1)



				$(m_x^*1/2,1/2,1)$	$(m_y^*1/2,1/2,1)$	$(m_{xy}^*1/2,1/2,0)$	$(m_{\&y}^*1/2,1/2,0)$
127.12.1064	$P_{2c}4'/mbm'$	$P4_2/mbc$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$ $(\&^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(4_z^*0,0,1)$ $(2_y^*1/2,1/2,0)$ $(\&_z^*0,0,1)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1)$ $(m_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1)$	$(4_z^{-1*}0,0,1)$ $(2_{\&y}^*1/2,1/2,1)$ $(\&_z^{-1*}0,0,1)$ $(m_{\&y}^*1/2,1/2,1)$
127.13.1065	$P_{2c}4'/mb'm'$	$P4/mnc$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1)$ $(\&^*0,0,0)$ $(m_x^*1/2,1/2,1)$	$(4_z^*0,0,0)$ $(2_y^*1/2,1/2,1)$ $(\&_z^*0,0,0)$ $(m_y^*1/2,1/2,1)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1)$ $(m_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1)$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*1/2,1/2,1)$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,1)$
<b>128.1.1066</b>	<b><math>P4/mnc</math></b>			$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)$ $(\&^*0,0,0)$ $(m_x^*1/2,1/2,1/2)$	$(4_z^*0,0,0)$ $(2_y^*1/2,1/2,1/2)$ $(\&_z^*0,0,0)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)$ $(m_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*1/2,1/2,1/2)$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,1/2)$
128.2.1067	$P4/mnc1'$						
128.3.1068	$P4/m'nc$	$P4nc$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)'$ $(\&^*0,0,0)'$ $(m_x^*1/2,1/2,1/2)$	$(4_z^*0,0,0)$ $(2_y^*1/2,1/2,1/2)'$ $(\&_z^*0,0,0)'$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)'$ $(m_z^*0,0,0)'$ $(m_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*1/2,1/2,1/2)'$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*1/2,1/2,1/2)$
128.4.1069	$P4'/mn'c$	$Cccm$	$(1/2,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)'$ $(\&^*0,0,0)$ $(m_x^*1/2,1/2,1/2)'$	$(4_z^*0,0,0)'$ $(2_y^*1/2,1/2,1/2)'$ $(\&_z^*0,0,0)'$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)$ $(m_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}0,0,0)'$ $(2_{\&y}^*1/2,1/2,1/2)$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*1/2,1/2,1/2)$
128.5.1070	$P4'/mnc'$	$Pnnm$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)$	$(4_z^*0,0,0)'$ $(2_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)'$	$(4_z^{-1*}0,0,0)'$ $(2_{\&y}^*1/2,1/2,1/2)'$

				$(\&^*0,0,0)$ $(m_x^*1/2,1/2,1/2)$	$(\&_z^*0,0,0)'$ $(m_y^*1/2,1/2,1/2)$	$(m_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)'$	$(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*1/2,1/2,1/2)'$
128.6.1071	P4'/m'n'c	P&2 <sub>1</sub> c	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)$ $(\&^*0,0,0)'$ $(m_x^*1/2,1/2,1/2)'$	$(4_z^*0,0,0)'$ $(2_y^*1/2,1/2,1/2)$ $(\&_z^*0,0,0)$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)'$ $(m_z^*0,0,0)'$ $(m_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}0,0,0)'$ $(2_{\&y}^*1/2,1/2,1/2)'$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,1/2)$
128.7.1072	P4/mn'c'	P4/m	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)'$ $(\&^*0,0,0)$ $(m_x^*1/2,1/2,1/2)'$	$(4_z^*0,0,0)$ $(2_y^*1/2,1/2,1/2)'$ $(\&_z^*0,0,0)$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)'$ $(m_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)'$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*1/2,1/2,1/2)'$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,1/2)'$
128.8.1073	P4'/m'nc'	P&n <sub>2</sub>	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)'$ $(\&^*0,0,0)'$ $(m_x^*1/2,1/2,1/2)$	$(4_z^*0,0,0)'$ $(2_y^*1/2,1/2,1/2)'$ $(\&_z^*0,0,0)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)$ $(m_z^*0,0,0)'$ $(m_{xy}^*1/2,1/2,1/2)'$	$(4_z^{-1*}0,0,0)'$ $(2_{\&y}^*1/2,1/2,1/2)$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,1/2)'$
128.9.1074	P4/m'n'c'	P4 <sub>2</sub> , <sub>2</sub>	(1/2,0,1/4;a,b,c)	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)$ $(\&^*0,0,0)'$ $(m_x^*1/2,1/2,1/2)'$	$(4_z^*0,0,0)$ $(2_y^*1/2,1/2,1/2)$ $(\&_z^*0,0,0)'$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)$ $(m_z^*0,0,0)'$ $(m_{xy}^*1/2,1/2,1/2)'$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*1/2,1/2,1/2)$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*1/2,1/2,1/2)'$
<b>129.1.1075</b>	<b>P4/nmm</b>			$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$ $(\&^*1/2,1/2,0)$ $(m_x^*0,0,0)$	$(4_z^*1/2,1/2,0)$ $(2_y^*1/2,1/2,0)$ $(\&_z^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*1/2,1/2,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}1/2,1/2,0)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,0)$
129.2.1076	P4/nmm1'						

129.3.1077	P4/n'mm	P4mm	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)'$ $(\&^*1/2,1/2,0)'$ $(m_x^*0,0,0)$	$(4_z^*1/2,1/2,0)$ $(2_y^*1/2,1/2,0)'$ $(\&_z^*0,0,0)'$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*1/2,1/2,0)'$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}1/2,1/2,0)$ $(2_{\&y}^*0,0,0)'$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*1/2,1/2,0)$
129.4.1078	P4'/nm'm	Cmma	$(1/4,1/4,0;a+b,-a+b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)'$ $(\&^*1/2,1/2,0)$ $(m_x^*0,0,0)'$	$(4_z^*1/2,1/2,0)'$ $(2_y^*1/2,1/2,0)'$ $(\&_z^*0,0,0)'$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*1/2,1/2,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}1/2,1/2,0)'$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*1/2,1/2,0)$
129.5.1079	P4'/nmm'	Pmmn	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$ $(\&^*1/2,1/2,0)$ $(m_x^*0,0,0)$	$(4_z^*1/2,1/2,0)'$ $(2_y^*1/2,1/2,0)$ $(\&_z^*0,0,0)'$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*1/2,1/2,0)$ $(m_{xy}^*1/2,1/2,0)'$	$(4_z^{-1*}1/2,1/2,0)'$ $(2_{\&y}^*0,0,0)'$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*1/2,1/2,0)'$
129.6.1080	P4'/n'm'm	P&2 <sub>1</sub> m	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$ $(\&^*1/2,1/2,0)'$ $(m_x^*0,0,0)'$	$(4_z^*1/2,1/2,0)'$ $(2_y^*1/2,1/2,0)$ $(\&_z^*0,0,0)$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*1/2,1/2,0)'$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}1/2,1/2,0)'$ $(2_{\&y}^*0,0,0)'$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,0)$
129.7.1081	P4/nm'm'	P4/n	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)'$ $(\&^*1/2,1/2,0)$ $(m_x^*0,0,0)'$	$(4_z^*1/2,1/2,0)$ $(2_y^*1/2,1/2,0)'$ $(\&_z^*0,0,0)$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*1/2,1/2,0)$ $(m_{xy}^*1/2,1/2,0)'$	$(4_z^{-1*}1/2,1/2,0)$ $(2_{\&y}^*0,0,0)'$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,0)'$
129.8.1082	P4'/n'mm'	P&m2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)'$ $(\&^*1/2,1/2,0)'$ $(m_x^*0,0,0)$	$(4_z^*1/2,1/2,0)'$ $(2_y^*1/2,1/2,0)'$ $(\&_z^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*1/2,1/2,0)'$ $(m_{xy}^*1/2,1/2,0)'$	$(4_z^{-1*}1/2,1/2,0)'$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,0)'$
129.9.1083	P4/n'm'm'	P4 <sub>2</sub> ,2	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$ $(\&^*1/2,1/2,0)'$ $(m_x^*0,0,0)'$	$(4_z^*1/2,1/2,0)$ $(2_y^*1/2,1/2,0)$ $(\&_z^*0,0,0)'$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*1/2,1/2,0)'$ $(m_{xy}^*1/2,1/2,0)'$	$(4_z^{-1*}1/2,1/2,0)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*1/2,1/2,0)'$

129.10.1084	$P_{2c}4/nmm$	$P4/nmm$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$ $(\&^*1/2,1/2,0)$ $(m_x^*0,0,0)$	$(4_z^*1/2,1/2,0)$ $(2_y^*1/2,1/2,0)$ $(\&_z^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*1/2,1/2,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}1/2,1/2,0)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,0)$
129.11.1085	$P_{2c}4'/nm'm$	$P4_2/ncm$	$(0,0,1/2;a,b,2c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1)$ $(\&^*1/2,1/2,0)$ $(m_x^*0,0,1)$	$(4_z^*1/2,1/2,1)$ $(2_y^*1/2,1/2,1)$ $(\&_z^*0,0,1)$ $(m_y^*0,0,1)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*1/2,1/2,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}1/2,1/2,1)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,1)$ $(m_{\&y}^*1/2,1/2,0)$
129.12.1086	$P_{2c}4'/nmm'$	$P4_2/nmc$	$(0,0,1/2;a,b,2c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$ $(\&^*1/2,1/2,0)$ $(m_x^*0,0,0)$	$(4_z^*1/2,1/2,1)$ $(2_y^*1/2,1/2,0)$ $(\&_z^*0,0,1)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1)$ $(m_z^*1/2,1/2,0)$ $(m_{xy}^*1/2,1/2,1)$	$(4_z^{-1*}1/2,1/2,1)$ $(2_{\&y}^*0,0,1)$ $(\&_z^{-1*}0,0,1)$ $(m_{\&y}^*1/2,1/2,1)$
129.13.1087	$P_{2c}4/nm'm'$	$P4/ncc$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1)$ $(\&^*1/2,1/2,0)$ $(m_x^*0,0,1)$	$(4_z^*1/2,1/2,0)$ $(2_y^*1/2,1/2,1)$ $(\&_z^*0,0,0)$ $(m_y^*0,0,1)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1)$ $(m_z^*1/2,1/2,0)$ $(m_{xy}^*1/2,1/2,1)$	$(4_z^{-1*}1/2,1/2,0)$ $(2_{\&y}^*0,0,1)$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,1)$
<b>130.1.1088</b>	<b><math>P4/ncc</math></b>			<b><math>(1^*0,0,0)</math> <math>(2_x^*1/2,1/2,1/2)</math> <math>(\&amp;^*1/2,1/2,0)</math> <math>(m_x^*0,0,1/2)</math></b>	<b><math>(4_z^*1/2,1/2,0)</math> <math>(2_y^*1/2,1/2,1/2)</math> <math>(\&amp;_z^*0,0,0)</math> <math>(m_y^*0,0,1/2)</math></b>	<b><math>(2_z^*0,0,0)</math> <math>(2_{xy}^*0,0,1/2)</math> <math>(m_z^*1/2,1/2,0)</math> <math>(m_{xy}^*1/2,1/2,1/2)</math></b>	<b><math>(4_z^{-1*}1/2,1/2,0)</math> <math>(2_{\&amp;y}^*0,0,1/2)</math> <math>(\&amp;_z^{-1*}0,0,0)</math> <math>(m_{\&amp;y}^*1/2,1/2,1/2)</math></b>
130.2.1089	$P4/ncc1'$						
130.3.1090	$P4/n'cc$	$P4cc$	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)'$	$(4_z^*1/2,1/2,0)$ $(2_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)'$	$(4_z^{-1*}1/2,1/2,0)$ $(2_{\&y}^*0,0,1/2)'$

				$(\&_z^{*1/2,1/2,0})'$ $(m_x^{*0,0,1/2})'$	$(\&_z^{*0,0,0})'$ $(m_y^{*0,0,1/2})'$	$(m_z^{*1/2,1/2,0})'$ $(m_{xy}^{*1/2,1/2,1/2})'$	$(\&_z^{-1*0,0,0})'$ $(m_{\&y}^{*1/2,1/2,1/2})'$
130.4.1091	P4'/nc'c	Ccca	(0,0,1/4;a-b,a+b,c)	$(1^{*0,0,0})$ $(2_x^{*1/2,1/2,1/2})'$ $(\&_z^{*1/2,1/2,0})'$ $(m_x^{*0,0,1/2})'$	$(4_z^{*1/2,1/2,0})'$ $(2_y^{*1/2,1/2,1/2})'$ $(\&_z^{*0,0,0})'$ $(m_y^{*0,0,1/2})'$	$(2_z^{*0,0,0})$ $(2_{xy}^{*0,0,1/2})'$ $(m_z^{*1/2,1/2,0})'$ $(m_{xy}^{*1/2,1/2,1/2})'$	$(4_z^{-1*1/2,1/2,0})'$ $(2_{\&y}^{*0,0,1/2})'$ $(\&_z^{-1*0,0,0})'$ $(m_{\&y}^{*1/2,1/2,1/2})'$
130.5.1092	P4'/ncc'	Pccn	(1/4,1/4,0;a,b,c)	$(1^{*0,0,0})$ $(2_x^{*1/2,1/2,1/2})'$ $(\&_z^{*1/2,1/2,0})'$ $(m_x^{*0,0,1/2})'$	$(4_z^{*1/2,1/2,0})'$ $(2_y^{*1/2,1/2,1/2})'$ $(\&_z^{*0,0,0})'$ $(m_y^{*0,0,1/2})'$	$(2_z^{*0,0,0})$ $(2_{xy}^{*0,0,1/2})'$ $(m_z^{*1/2,1/2,0})'$ $(m_{xy}^{*1/2,1/2,1/2})'$	$(4_z^{-1*1/2,1/2,0})'$ $(2_{\&y}^{*0,0,1/2})'$ $(\&_z^{-1*0,0,0})'$ $(m_{\&y}^{*1/2,1/2,1/2})'$
130.6.1093	P4'/n'c'c	P&2 <sub>1</sub> c	(0,0,0;a,b,c)	$(1^{*0,0,0})$ $(2_x^{*1/2,1/2,1/2})'$ $(\&_z^{*1/2,1/2,0})'$ $(m_x^{*0,0,1/2})'$	$(4_z^{*1/2,1/2,0})'$ $(2_y^{*1/2,1/2,1/2})'$ $(\&_z^{*0,0,0})'$ $(m_y^{*0,0,1/2})'$	$(2_z^{*0,0,0})$ $(2_{xy}^{*0,0,1/2})'$ $(m_z^{*1/2,1/2,0})'$ $(m_{xy}^{*1/2,1/2,1/2})'$	$(4_z^{-1*1/2,1/2,0})'$ $(2_{\&y}^{*0,0,1/2})'$ $(\&_z^{-1*0,0,0})'$ $(m_{\&y}^{*1/2,1/2,1/2})'$
130.7.1094	P4'/nc'c'	P4/n	(0,0,0;a,b,c)	$(1^{*0,0,0})$ $(2_x^{*1/2,1/2,1/2})'$ $(\&_z^{*1/2,1/2,0})'$ $(m_x^{*0,0,1/2})'$	$(4_z^{*1/2,1/2,0})'$ $(2_y^{*1/2,1/2,1/2})'$ $(\&_z^{*0,0,0})'$ $(m_y^{*0,0,1/2})'$	$(2_z^{*0,0,0})$ $(2_{xy}^{*0,0,1/2})'$ $(m_z^{*1/2,1/2,0})'$ $(m_{xy}^{*1/2,1/2,1/2})'$	$(4_z^{-1*1/2,1/2,0})'$ $(2_{\&y}^{*0,0,1/2})'$ $(\&_z^{-1*0,0,0})'$ $(m_{\&y}^{*1/2,1/2,1/2})'$
130.8.1095	P4'/n'cc'	P&c2	(0,0,0;a,b,c)	$(1^{*0,0,0})$ $(2_x^{*1/2,1/2,1/2})'$ $(\&_z^{*1/2,1/2,0})'$ $(m_x^{*0,0,1/2})'$	$(4_z^{*1/2,1/2,0})'$ $(2_y^{*1/2,1/2,1/2})'$ $(\&_z^{*0,0,0})'$ $(m_y^{*0,0,1/2})'$	$(2_z^{*0,0,0})$ $(2_{xy}^{*0,0,1/2})'$ $(m_z^{*1/2,1/2,0})'$ $(m_{xy}^{*1/2,1/2,1/2})'$	$(4_z^{-1*1/2,1/2,0})'$ $(2_{\&y}^{*0,0,1/2})'$ $(\&_z^{-1*0,0,0})'$ $(m_{\&y}^{*1/2,1/2,1/2})'$
130.9.1096	P4'/n'c'c'	P4 <sub>2</sub> ,2	(0,0,1/4;a,b,c)	$(1^{*0,0,0})$ $(2_x^{*1/2,1/2,1/2})'$	$(4_z^{*1/2,1/2,0})'$ $(2_y^{*1/2,1/2,1/2})'$	$(2_z^{*0,0,0})$ $(2_{xy}^{*0,0,1/2})'$	$(4_z^{-1*1/2,1/2,0})'$ $(2_{\&y}^{*0,0,1/2})'$

$$\begin{matrix} (\&_z^{*1/2,1/2,0})' & (\&_z^{*0,0,0})' & (m_z^{*1/2,1/2,0})' & (\&_z^{-1*0,0,0})' \\ (m_x^{*0,0,1/2})' & (m_y^{*0,0,1/2})' & (m_{xy}^{*1/2,1/2,1/2})' & (m_{\&y}^{*1/2,1/2,1/2})' \end{matrix}$$

131.1.1097  $P4_2/mmc$

$$\begin{matrix} (1^{*0,0,0}) & (4_z^{*0,0,1/2}) & (2_z^{*0,0,0}) & (4_z^{-1*0,0,1/2}) \\ (2_x^{*0,0,0}) & (2_y^{*0,0,0}) & (2_{xy}^{*0,0,1/2}) & (2_{\&y}^{*0,0,1/2}) \\ (\&_z^{*0,0,0}) & (\&_z^{*0,0,1/2}) & (m_z^{*0,0,0}) & (\&_z^{-1*0,0,1/2}) \\ (m_x^{*0,0,0}) & (m_y^{*0,0,0}) & (m_{xy}^{*0,0,1/2}) & (m_{\&y}^{*0,0,1/2}) \end{matrix}$$

131.2.1098  $P4_2/mmc1'$

131.3.1099  $P4_2/m'mc$   $P4_2mc$  (0,0,0;a,b,c)

$$\begin{matrix} (1^{*0,0,0}) & (4_z^{*0,0,1/2}) & (2_z^{*0,0,0}) & (4_z^{-1*0,0,1/2}) \\ (2_x^{*0,0,0})' & (2_y^{*0,0,0})' & (2_{xy}^{*0,0,1/2})' & (2_{\&y}^{*0,0,1/2})' \\ (\&_z^{*0,0,0})' & (\&_z^{*0,0,1/2})' & (m_z^{*0,0,0})' & (\&_z^{-1*0,0,1/2})' \\ (m_x^{*0,0,0}) & (m_y^{*0,0,0}) & (m_{xy}^{*0,0,1/2}) & (m_{\&y}^{*0,0,1/2}) \end{matrix}$$

131.4.1100  $P4_2'/mm'c$   $Cccm$  (0,0,0;a-b,a+b,c)

$$\begin{matrix} (1^{*0,0,0}) & (4_z^{*0,0,1/2})' & (2_z^{*0,0,0}) & (4_z^{-1*0,0,1/2})' \\ (2_x^{*0,0,0})' & (2_y^{*0,0,0})' & (2_{xy}^{*0,0,1/2}) & (2_{\&y}^{*0,0,1/2}) \\ (\&_z^{*0,0,0}) & (\&_z^{*0,0,1/2})' & (m_z^{*0,0,0}) & (\&_z^{-1*0,0,1/2})' \\ (m_x^{*0,0,0})' & (m_y^{*0,0,0})' & (m_{xy}^{*0,0,1/2}) & (m_{\&y}^{*0,0,1/2}) \end{matrix}$$

131.5.1101  $P4_2'/mmc'$   $Pmmm$  (0,0,0;a,b,c)

$$\begin{matrix} (1^{*0,0,0}) & (4_z^{*0,0,1/2})' & (2_z^{*0,0,0}) & (4_z^{-1*0,0,1/2})' \\ (2_x^{*0,0,0}) & (2_y^{*0,0,0}) & (2_{xy}^{*0,0,1/2})' & (2_{\&y}^{*0,0,1/2})' \\ (\&_z^{*0,0,0}) & (\&_z^{*0,0,1/2})' & (m_z^{*0,0,0}) & (\&_z^{-1*0,0,1/2})' \\ (m_x^{*0,0,0}) & (m_y^{*0,0,0}) & (m_{xy}^{*0,0,1/2})' & (m_{\&y}^{*0,0,1/2})' \end{matrix}$$

131.6.1102  $P4_2'/m'm'c$   $P\&2c$  (0,0,1/4;a,b,c)

$$\begin{matrix} (1^{*0,0,0}) & (4_z^{*0,0,1/2})' & (2_z^{*0,0,0}) & (4_z^{-1*0,0,1/2})' \\ (2_x^{*0,0,0}) & (2_y^{*0,0,0}) & (2_{xy}^{*0,0,1/2})' & (2_{\&y}^{*0,0,1/2})' \\ (\&_z^{*0,0,0})' & (\&_z^{*0,0,1/2})' & (m_z^{*0,0,0})' & (\&_z^{-1*0,0,1/2})' \\ (m_x^{*0,0,0})' & (m_y^{*0,0,0})' & (m_{xy}^{*0,0,1/2}) & (m_{\&y}^{*0,0,1/2}) \end{matrix}$$

131.7.1103  $P4_2'/mm'c'$   $P4_2/m$  (0,0,0;a,b,c)

$$\begin{matrix} (1^{*0,0,0}) & (4_z^{*0,0,1/2}) & (2_z^{*0,0,0}) & (4_z^{-1*0,0,1/2}) \\ (2_x^{*0,0,0})' & (2_y^{*0,0,0})' & (2_{xy}^{*0,0,1/2})' & (2_{\&y}^{*0,0,1/2})' \end{matrix}$$

				$(\&_z^*0,0,0)$ $(m_x^*0,0,0)'$	$(\&_z^*0,0,1/2)$ $(m_y^*0,0,0)'$	$(m_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)'$	$(\&_z^{-1*}0,0,1/2)$ $(m_{\&y}^*0,0,1/2)'$
131.8.1104	$P4_2/m'mc'$	$P\&m2$	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)'$ $(\&^*0,0,0)'$ $(m_x^*0,0,0)$	$(4_z^*0,0,1/2)'$ $(2_y^*0,0,0)'$ $(\&_z^*0,0,1/2)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$ $(m_z^*0,0,0)'$ $(m_{xy}^*0,0,1/2)'$	$(4_z^{-1*}0,0,1/2)'$ $(2_{\&y}^*0,0,1/2)$ $(\&_z^{-1*}0,0,1/2)$ $(m_{\&y}^*0,0,1/2)'$
131.9.1105	$P4_2/m'm'c'$	$P4_22$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&^*0,0,0)'$ $(m_x^*0,0,0)'$	$(4_z^*0,0,1/2)$ $(2_y^*0,0,0)$ $(\&_z^*0,0,1/2)'$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$ $(m_z^*0,0,0)'$ $(m_{xy}^*0,0,1/2)'$	$(4_z^{-1*}0,0,1/2)$ $(2_{\&y}^*0,0,1/2)$ $(\&_z^{-1*}0,0,1/2)'$ $(m_{\&y}^*0,0,1/2)'$
131.10.1106	$P_P4_2/mmc$	$P4_2/mcm$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,1/2)$ $(2_y^*0,0,0)$ $(\&_z^*0,0,1/2)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)$	$(4_z^{-1*}0,0,1/2)$ $(2_{\&y}^*0,0,1/2)$ $(\&_z^{-1*}0,0,1/2)$ $(m_{\&y}^*0,0,1/2)$
131.11.1107	$P_P4_2/m'mc$	$P4_2/ncm$	$(1/2,1/2,1/4;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*1,0,0)$ $(\&^*1,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,1/2)$ $(2_y^*1,0,0)$ $(\&_z^*1,0,1/2)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1,0,1/2)$ $(m_z^*1,0,0)$ $(m_{xy}^*0,0,1/2)$	$(4_z^{-1*}0,0,1/2)$ $(2_{\&y}^*1,0,1/2)$ $(\&_z^{-1*}1,0,1/2)$ $(m_{\&y}^*0,0,1/2)$
131.12.1108	$P_P4_2/mm'c'$	$P4_2/mnm$	$(1/2,1/2,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*1,0,0)$ $(\&^*0,0,0)$ $(m_x^*1,0,0)$	$(4_z^*0,0,1/2)$ $(2_y^*1,0,0)$ $(\&_z^*0,0,1/2)$ $(m_y^*1,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1,0,1/2)$ $(m_z^*0,0,0)$ $(m_{xy}^*1,0,1/2)$	$(4_z^{-1*}0,0,1/2)$ $(2_{\&y}^*1,0,1/2)$ $(\&_z^{-1*}0,0,1/2)$ $(m_{\&y}^*1,0,1/2)$
131.13.1109	$P_P4_2'/m'mc'$	$P4_2/nm$	$(0,0,1/4;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*1,0,0)$ $(\&^*1,0,0)$ $(m_x^*0,0,0)$	$(4_z^*1,0,1/2)$ $(2_y^*1,0,0)$ $(\&_z^*0,0,1/2)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$ $(m_z^*1,0,0)$ $(m_{xy}^*1,0,1/2)$	$(4_z^{-1*}1,0,1/2)$ $(2_{\&y}^*0,0,1/2)$ $(\&_z^{-1*}0,0,1/2)$ $(m_{\&y}^*1,0,1/2)$

132.1.1110	$P4_2/mcm$			$(1^*0,0,0)$ $(2_x^*0,0,1/2)$ $(\&^*0,0,0)$ $(m_x^*0,0,1/2)$	$(4_z^*0,0,1/2)$ $(2_y^*0,0,1/2)$ $(\&_z^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,1/2)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,1/2)$ $(m_{\&y}^*0,0,0)$
132.2.1111	$P4_2/mcm1'$						
132.3.1112	$P4_2/m'cm$	$P4_2 cm$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)'$ $(\&^*0,0,0)'$ $(m_x^*0,0,1/2)$	$(4_z^*0,0,1/2)$ $(2_y^*0,0,1/2)'$ $(\&_z^*0,0,1/2)'$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*0,0,0)'$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,1/2)$ $(2_{\&y}^*0,0,0)'$ $(\&_z^{-1*}0,0,1/2)'$ $(m_{\&y}^*0,0,0)$
132.4.1113	$P4_2'/mc'm$	$Cmmm$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)'$ $(\&^*0,0,0)$ $(m_x^*0,0,1/2)'$	$(4_z^*0,0,1/2)'$ $(2_y^*0,0,1/2)'$ $(\&_z^*0,0,1/2)'$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,1/2)'$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,1/2)'$ $(m_{\&y}^*0,0,0)$
132.5.1114	$P4_2'/mcm'$	$Pccm$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)$ $(\&^*0,0,0)$ $(m_x^*0,0,1/2)$	$(4_z^*0,0,1/2)'$ $(2_y^*0,0,1/2)$ $(\&_z^*0,0,1/2)'$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,1/2)'$ $(2_{\&y}^*0,0,0)'$ $(\&_z^{-1*}0,0,1/2)'$ $(m_{\&y}^*0,0,0)'$
132.6.1115	$P4_2'/m'c'm$	$P\&2m$	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)$ $(\&^*0,0,0)'$ $(m_x^*0,0,1/2)'$	$(4_z^*0,0,1/2)'$ $(2_y^*0,0,1/2)$ $(\&_z^*0,0,1/2)$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*0,0,0)'$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,1/2)'$ $(2_{\&y}^*0,0,0)'$ $(\&_z^{-1*}0,0,1/2)'$ $(m_{\&y}^*0,0,0)$
132.7.1116	$P4_2/mc'm'$	$P4_2/m$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)'$ $(\&^*0,0,0)$ $(m_x^*0,0,1/2)'$	$(4_z^*0,0,1/2)$ $(2_y^*0,0,1/2)'$ $(\&_z^*0,0,1/2)$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,1/2)$ $(2_{\&y}^*0,0,0)'$ $(\&_z^{-1*}0,0,1/2)$ $(m_{\&y}^*0,0,0)'$
132.8.1117	$P4_2'/m'cm'$	$P\&c2$	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$	$(4_z^*0,0,1/2)'$	$(2_z^*0,0,0)$	$(4_z^{-1*}0,0,1/2)'$



				$(2_x^*0,0,1/2)'$ $(\&^*0,0,0)'$ $(m_x^*0,0,1/2)$	$(2_y^*0,0,1/2)'$ $(\&_z^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_{xy}^*0,0,0)$ $(m_z^*0,0,0)'$ $(m_{xy}^*0,0,0)'$	$(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,1/2)$ $(m_{\&y}^*0,0,0)'$
132.9.1118	$P4_2/m'c'm'$	$P4_222$	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)$ $(\&^*0,0,0)'$ $(m_x^*0,0,1/2)'$	$(4_z^*0,0,1/2)$ $(2_y^*0,0,1/2)$ $(\&_z^*0,0,1/2)'$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*0,0,0)'$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,1/2)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,1/2)'$ $(m_{\&y}^*0,0,0)'$
132.10.1119	$P_p4_2/mcm$	$P4_2/mmc$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)$ $(\&^*0,0,0)$ $(m_x^*0,0,1/2)$	$(4_z^*0,0,1/2)$ $(2_y^*0,0,1/2)$ $(\&_z^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,1/2)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,1/2)$ $(m_{\&y}^*0,0,0)$
132.11.1120	$P_p4_2/m'cm$	$P4_2/nmc$	$(1/2,1/2,1/4;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*1,0,1/2)$ $(\&^*1,0,0)$ $(m_x^*0,0,1/2)$	$(4_z^*0,0,1/2)$ $(2_y^*1,0,1/2)$ $(\&_z^*1,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*1,0,0)$ $(m_z^*1,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,1/2)$ $(2_{\&y}^*1,0,0)$ $(\&_z^{-1*}1,0,1/2)$ $(m_{\&y}^*0,0,0)$
132.12.1121	$P_p4_2'/mcm'$	$P4_2/mbc$	$(1/2,1/2,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)$ $(\&^*0,0,0)$ $(m_x^*0,0,1/2)$	$(4_z^*1,0,1/2)$ $(2_y^*0,0,1/2)$ $(\&_z^*1,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*1,0,0)$ $(m_z^*0,0,0)$ $(m_{xy}^*1,0,0)$	$(4_z^{-1*}1,0,1/2)$ $(2_{\&y}^*1,0,0)$ $(\&_z^{-1*}1,0,1/2)$ $(m_{\&y}^*1,0,0)$
132.13.1122	$P_p4_2'/m'cm'$	$P4_2/nbc$	$(0,0,1/4;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*1,0,1/2)$ $(\&^*1,0,0)$ $(m_x^*0,0,1/2)$	$(4_z^*1,0,1/2)$ $(2_y^*1,0,1/2)$ $(\&_z^*0,0,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*1,0,0)$ $(m_{xy}^*1,0,0)$	$(4_z^{-1*}1,0,1/2)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,1/2)$ $(m_{\&y}^*1,0,0)$
133.1.1123	$P4_2/nbc$			$(1^*0,0,0)$ $(2_x^*0,0,1/2)$ $(\&^*1/2,1/2,1/2)$	$(4_z^*1/2,1/2,1/2)$ $(2_y^*0,0,1/2)$ $(\&_z^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,0)$ $(m_z^*1/2,1/2,1/2)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(2_{\&y}^*1/2,1/2,0)$ $(\&_z^{-1*}0,0,0)$

				$(m_x^* 1/2, 1/2, 0)$	$(m_y^* 1/2, 1/2, 0)$	$(m_{xy}^* 0, 0, 1/2)$	$(m_{&y}^* 0, 0, 1/2)$
133.2.1124	$P4_2/nbc1'$						
133.3.1125	$P4_2/n'bc$	$P4_2 bc$	$(1/2, 0, 0; a, b, c)$	$(1^* 0, 0, 0)$ $(2_x^* 0, 0, 1/2)'$ $(\&^* 1/2, 1/2, 1/2)'$ $(m_x^* 1/2, 1/2, 0)$	$(4_z^* 1/2, 1/2, 1/2)$ $(2_y^* 0, 0, 1/2)'$ $(\&_z^* 0, 0, 0)'$ $(m_y^* 1/2, 1/2, 0)$	$(2_z^* 0, 0, 0)$ $(2_{xy}^* 1/2, 1/2, 0)'$ $(m_z^* 1/2, 1/2, 1/2)'$ $(m_{xy}^* 0, 0, 1/2)$	$(4_z^{-1*} 1/2, 1/2, 1/2)$ $(2_{&y}^* 1/2, 1/2, 0)'$ $(\&_z^{-1*} 0, 0, 0)'$ $(m_{&y}^* 0, 0, 1/2)$
133.4.1126	$P4_2/nb'c$	$Ccca$	$(1/2, 0, 0; a-b, a+b, c)$	$(1^* 0, 0, 0)$ $(2_x^* 0, 0, 1/2)'$ $(\&^* 1/2, 1/2, 1/2)$ $(m_x^* 1/2, 1/2, 0)'$	$(4_z^* 1/2, 1/2, 1/2)'$ $(2_y^* 0, 0, 1/2)'$ $(\&_z^* 0, 0, 0)'$ $(m_y^* 1/2, 1/2, 0)'$	$(2_z^* 0, 0, 0)$ $(2_{xy}^* 1/2, 1/2, 0)$ $(m_z^* 1/2, 1/2, 1/2)$ $(m_{xy}^* 0, 0, 1/2)$	$(4_z^{-1*} 1/2, 1/2, 1/2)'$ $(2_{&y}^* 1/2, 1/2, 0)$ $(\&_z^{-1*} 0, 0, 0)'$ $(m_{&y}^* 0, 0, 1/2)$
133.5.1127	$P4_2/nbc'$	$Pban$	$(0, 0, 1/4; a, b, c)$	$(1^* 0, 0, 0)$ $(2_x^* 0, 0, 1/2)$ $(\&^* 1/2, 1/2, 1/2)$ $(m_x^* 1/2, 1/2, 0)$	$(4_z^* 1/2, 1/2, 1/2)'$ $(2_y^* 0, 0, 1/2)$ $(\&_z^* 0, 0, 0)'$ $(m_y^* 1/2, 1/2, 0)$	$(2_z^* 0, 0, 0)$ $(2_{xy}^* 1/2, 1/2, 0)'$ $(m_z^* 1/2, 1/2, 1/2)$ $(m_{xy}^* 0, 0, 1/2)'$	$(4_z^{-1*} 1/2, 1/2, 1/2)'$ $(2_{&y}^* 1/2, 1/2, 0)'$ $(\&_z^{-1*} 0, 0, 0)'$ $(m_{&y}^* 0, 0, 1/2)'$
133.6.1128	$P4_2/n'b'c$	$P\&2c$	$(0, 0, 0; a, b, c)$	$(1^* 0, 0, 0)$ $(2_x^* 0, 0, 1/2)$ $(\&^* 1/2, 1/2, 1/2)'$ $(m_x^* 1/2, 1/2, 0)'$	$(4_z^* 1/2, 1/2, 1/2)'$ $(2_y^* 0, 0, 1/2)$ $(\&_z^* 0, 0, 0)$ $(m_y^* 1/2, 1/2, 0)'$	$(2_z^* 0, 0, 0)$ $(2_{xy}^* 1/2, 1/2, 0)'$ $(m_z^* 1/2, 1/2, 1/2)'$ $(m_{xy}^* 0, 0, 1/2)$	$(4_z^{-1*} 1/2, 1/2, 1/2)'$ $(2_{&y}^* 1/2, 1/2, 0)'$ $(\&_z^{-1*} 0, 0, 0)$ $(m_{&y}^* 0, 0, 1/2)$
133.7.1129	$P4_2/nb'c'$	$P4_2/n$	$(0, 0, 0; a, b, c)$	$(1^* 0, 0, 0)$ $(2_x^* 0, 0, 1/2)'$ $(\&^* 1/2, 1/2, 1/2)$ $(m_x^* 1/2, 1/2, 0)'$	$(4_z^* 1/2, 1/2, 1/2)$ $(2_y^* 0, 0, 1/2)'$ $(\&_z^* 0, 0, 0)$ $(m_y^* 1/2, 1/2, 0)'$	$(2_z^* 0, 0, 0)$ $(2_{xy}^* 1/2, 1/2, 0)'$ $(m_z^* 1/2, 1/2, 1/2)$ $(m_{xy}^* 0, 0, 1/2)'$	$(4_z^{-1*} 1/2, 1/2, 1/2)$ $(2_{&y}^* 1/2, 1/2, 0)'$ $(\&_z^{-1*} 0, 0, 0)$ $(m_{&y}^* 0, 0, 1/2)'$
133.8.1130	$P4_2/n'bc'$	$P\&b2$	$(0, 0, 0; a, b, c)$	$(1^* 0, 0, 0)$ $(2_x^* 0, 0, 1/2)'$ $(\&^* 1/2, 1/2, 1/2)'$ $(m_x^* 1/2, 1/2, 0)$	$(4_z^* 1/2, 1/2, 1/2)'$ $(2_y^* 0, 0, 1/2)'$ $(\&_z^* 0, 0, 0)$ $(m_y^* 1/2, 1/2, 0)$	$(2_z^* 0, 0, 0)$ $(2_{xy}^* 1/2, 1/2, 0)$ $(m_z^* 1/2, 1/2, 1/2)'$ $(m_{xy}^* 0, 0, 1/2)'$	$(4_z^{-1*} 1/2, 1/2, 1/2)'$ $(2_{&y}^* 1/2, 1/2, 0)$ $(\&_z^{-1*} 0, 0, 0)$ $(m_{&y}^* 0, 0, 1/2)'$

133.9.1131	$P4_2/n'b'c'$	$P4_22$	$(1/2,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)$ $(\&^*1/2,1/2,1/2)'$ $(m_x^*1/2,1/2,0)'$	$(4_z^*1/2,1/2,1/2)$ $(2_y^*0,0,1/2)$ $(\&_z^*0,0,0)'$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,0)$ $(m_z^*1/2,1/2,1/2)'$ $(m_{xy}^*0,0,1/2)'$	$(4_z^{-1*}1/2,1/2,1/2)$ $(2_{\&y}^*1/2,1/2,0)$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*0,0,1/2)'$
134.1.1132	$P4_2/nnm$			$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&^*1/2,1/2,1/2)$ $(m_x^*1/2,1/2,1/2)$	$(4_z^*1/2,1/2,1/2)$ $(2_y^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)$ $(m_z^*1/2,1/2,1/2)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(2_{\&y}^*1/2,1/2,1/2)$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*0,0,0)$
134.2.1133	$P4_2/nm1'$						
134.3.1134	$P4_2/n'nm$	$P4_2nm$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)'$ $(\&^*1/2,1/2,1/2)'$ $(m_x^*1/2,1/2,1/2)$	$(4_z^*1/2,1/2,1/2)$ $(2_y^*0,0,0)'$ $(\&_z^*0,0,0)'$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)'$ $(m_z^*1/2,1/2,1/2)'$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(2_{\&y}^*1/2,1/2,1/2)'$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*0,0,0)$
134.4.1135	$P4_2'/nn'm$	$Cmma$	$(1/4,1/4,1/4;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)'$ $(\&^*1/2,1/2,1/2)$ $(m_x^*1/2,1/2,1/2)'$	$(4_z^*1/2,1/2,1/2)'$ $(2_y^*0,0,0)'$ $(\&_z^*0,0,0)'$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)$ $(m_z^*1/2,1/2,1/2)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)'$ $(2_{\&y}^*1/2,1/2,1/2)$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*0,0,0)$
134.5.1136	$P4_2'/nm'$	$Pnnn$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&^*1/2,1/2,1/2)$ $(m_x^*1/2,1/2,1/2)$	$(4_z^*1/2,1/2,1/2)'$ $(2_y^*0,0,0)$ $(\&_z^*0,0,0)'$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)'$ $(m_z^*1/2,1/2,1/2)$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}1/2,1/2,1/2)'$ $(2_{\&y}^*1/2,1/2,1/2)'$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*0,0,0)$
134.6.1137	$P4_2'/n'n'm$	$P\&2m$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&^*1/2,1/2,1/2)'$ $(m_x^*1/2,1/2,1/2)'$	$(4_z^*1/2,1/2,1/2)'$ $(2_y^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)'$ $(m_z^*1/2,1/2,1/2)'$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)'$ $(2_{\&y}^*1/2,1/2,1/2)'$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*0,0,0)$

134.7.1138	$P4_2/nm'$	$P4_2/n$	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)'$ $(\&^*_{1/2,1/2,1/2})$ $(m_x^*_{1/2,1/2,1/2})'$	$(4_z^*_{1/2,1/2,1/2})$ $(2_y^*0,0,0)'$ $(\&^*_{z^*0,0,0})$ $(m_y^*_{1/2,1/2,1/2})'$	$(2_z^*0,0,0)$ $(2_{xy}^*_{1/2,1/2,1/2})'$ $(m_z^*_{1/2,1/2,1/2})$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}_{1/2,1/2,1/2})$ $(2_{\&y}^*_{1/2,1/2,1/2})'$ $(\&^*_{z^{-1*}0,0,0})$ $(m_{\&y}^*0,0,0)'$
134.8.1139	$P4_2/n'm'$	$P\&n2$	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)'$ $(\&^*_{1/2,1/2,1/2})'$ $(m_x^*_{1/2,1/2,1/2})$	$(4_z^*_{1/2,1/2,1/2})'$ $(2_y^*0,0,0)'$ $(\&^*_{z^*0,0,0})$ $(m_y^*_{1/2,1/2,1/2})$	$(2_z^*0,0,0)$ $(2_{xy}^*_{1/2,1/2,1/2})$ $(m_z^*_{1/2,1/2,1/2})'$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}_{1/2,1/2,1/2})'$ $(2_{\&y}^*_{1/2,1/2,1/2})$ $(\&^*_{z^{-1*}0,0,0})$ $(m_{\&y}^*0,0,0)'$
134.9.1140	$P4_2/n'n'm'$	$P4_22$	(1/2,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&^*_{1/2,1/2,1/2})'$ $(m_x^*_{1/2,1/2,1/2})'$	$(4_z^*_{1/2,1/2,1/2})$ $(2_y^*0,0,0)$ $(\&^*_{z^*0,0,0})'$ $(m_y^*_{1/2,1/2,1/2})'$	$(2_z^*0,0,0)$ $(2_{xy}^*_{1/2,1/2,1/2})$ $(m_z^*_{1/2,1/2,1/2})'$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}_{1/2,1/2,1/2})$ $(2_{\&y}^*_{1/2,1/2,1/2})$ $(\&^*_{z^{-1*}0,0,0})'$ $(m_{\&y}^*0,0,0)'$
134.10.1141	$P_14_2/nm$	$I4_1/amd$	(0,0,0 ;a-b,a+b,2c)	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&^*_{1/2,1/2,1/2})$ $(m_x^*_{1/2,1/2,1/2})$	$(4_z^*_{1/2,1/2,1/2})$ $(2_y^*0,0,0)$ $(\&^*_{z^*0,0,0})$ $(m_y^*_{1/2,1/2,1/2})$	$(2_z^*0,0,0)$ $(2_{xy}^*_{1/2,1/2,1/2})$ $(m_z^*_{1/2,1/2,1/2})$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}_{1/2,1/2,1/2})$ $(2_{\&y}^*_{1/2,1/2,1/2})$ $(\&^*_{z^{-1*}0,0,0})$ $(m_{\&y}^*0,0,0)$
134.11.1142	$P_14_2/nn'm'$	$I4_1/acd$	(0,0,0 ;a-b,a+b,2c)	$(1^*0,0,0)$ $(2_x^*1,0,0)$ $(\&^*_{1/2,1/2,1/2})$ $(m_x^*_{3/2,1/2,1/2})$	$(4_z^*_{1/2,1/2,1/2})$ $(2_y^*1,0,0)$ $(\&^*_{z^*0,0,0})$ $(m_y^*_{3/2,1/2,1/2})$	$(2_z^*0,0,0)$ $(2_{xy}^*_{3/2,1/2,1/2})$ $(m_z^*_{1/2,1/2,1/2})$ $(m_{xy}^*1,0,0)$	$(4_z^{-1*}_{1/2,1/2,1/2})$ $(2_{\&y}^*_{3/2,1/2,1/2})$ $(\&^*_{z^{-1*}0,0,0})$ $(m_{\&y}^*1,0,0)$
135.1.1143	$P4_2/mbc$			$(1^*0,0,0)$ $(2_x^*_{1/2,1/2,0})$ $(\&^*0,0,0)$ $(m_x^*_{1/2,1/2,0})$	$(4_z^*0,0,1/2)$ $(2_y^*_{1/2,1/2,0})$ $(\&^*_{z^*0,0,1/2})$ $(m_y^*_{1/2,1/2,0})$	$(2_z^*0,0,0)$ $(2_{xy}^*_{1/2,1/2,1/2})$ $(m_z^*0,0,0)$ $(m_{xy}^*_{1/2,1/2,1/2})$	$(4_z^{-1*}0,0,1/2)$ $(2_{\&y}^*_{1/2,1/2,1/2})$ $(\&^*_{z^{-1*}0,0,1/2})$ $(m_{\&y}^*_{1/2,1/2,1/2})$
135.2.1144	$P4_2/mbc1'$						

135.3.1145	$P4_2/m'bc$	$P4_2bc$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)'$ $(\&^*0,0,0)'$ $(m_x^*1/2,1/2,0)$	$(4_z^*0,0,1/2)$ $(2_y^*1/2,1/2,0)'$ $(\&_z^*0,0,1/2)'$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)'$ $(m_z^*0,0,0)'$ $(m_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}0,0,1/2)$ $(2_{\&y}^*1/2,1/2,1/2)'$ $(\&_z^{-1*}0,0,1/2)'$ $(m_{\&y}^*1/2,1/2,1/2)$
135.4.1146	$P4_2'/mb'c$	Cccm	$(1/2,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)'$ $(\&^*0,0,0)$ $(m_x^*1/2,1/2,0)'$	$(4_z^*0,0,1/2)'$ $(2_y^*1/2,1/2,0)'$ $(\&_z^*0,0,1/2)'$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)$ $(m_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}0,0,1/2)'$ $(2_{\&y}^*1/2,1/2,1/2)$ $(\&_z^{-1*}0,0,1/2)'$ $(m_{\&y}^*1/2,1/2,1/2)$
135.5.1147	$P4_2'/mbc'$	Pbam	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$ $(\&^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(4_z^*0,0,1/2)'$ $(2_y^*1/2,1/2,0)$ $(\&_z^*0,0,1/2)'$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)'$ $(m_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)'$	$(4_z^{-1*}0,0,1/2)'$ $(2_{\&y}^*1/2,1/2,1/2)'$ $(\&_z^{-1*}0,0,1/2)'$ $(m_{\&y}^*1/2,1/2,1/2)'$
135.6.1148	$P4_2'/m'b'c$	$P\&2_1c$	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$ $(\&^*0,0,0)'$ $(m_x^*1/2,1/2,0)'$	$(4_z^*0,0,1/2)'$ $(2_y^*1/2,1/2,0)$ $(\&_z^*0,0,1/2)$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)'$ $(m_z^*0,0,0)'$ $(m_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}0,0,1/2)'$ $(2_{\&y}^*1/2,1/2,1/2)'$ $(\&_z^{-1*}0,0,1/2)$ $(m_{\&y}^*1/2,1/2,1/2)$
135.7.1149	$P4_2'/mb'c'$	$P4_2/m$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)'$ $(\&^*0,0,0)$ $(m_x^*1/2,1/2,0)'$	$(4_z^*0,0,1/2)$ $(2_y^*1/2,1/2,0)'$ $(\&_z^*0,0,1/2)$ $(m_y^*1/2,1/2,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)'$ $(m_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)'$	$(4_z^{-1*}0,0,1/2)$ $(2_{\&y}^*1/2,1/2,1/2)'$ $(\&_z^{-1*}0,0,1/2)$ $(m_{\&y}^*1/2,1/2,1/2)'$
135.8.1150	$P4_2'/m'bc'$	$P\&b2$	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)'$ $(\&^*0,0,0)'$ $(m_x^*1/2,1/2,0)$	$(4_z^*0,0,1/2)'$ $(2_y^*1/2,1/2,0)'$ $(\&_z^*0,0,1/2)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)$ $(m_z^*0,0,0)'$ $(m_{xy}^*1/2,1/2,1/2)'$	$(4_z^{-1*}0,0,1/2)'$ $(2_{\&y}^*1/2,1/2,1/2)$ $(\&_z^{-1*}0,0,1/2)$ $(m_{\&y}^*1/2,1/2,1/2)'$
135.9.1151	$P4_2'/m'b'c'$	$P4_22_12$	$(1/2,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$ $(\&^*0,0,0)'$	$(4_z^*0,0,1/2)$ $(2_y^*1/2,1/2,0)$ $(\&_z^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)$ $(m_z^*0,0,0)'$	$(4_z^{-1*}0,0,1/2)$ $(2_{\&y}^*1/2,1/2,1/2)$ $(\&_z^{-1*}0,0,1/2)'$

$$(m_x^*1/2,1/2,0)' \quad (m_y^*1/2,1/2,0)' \quad (m_{xy}^*1/2,1/2,1/2)' \quad (m_{\&y}^*1/2,1/2,1/2)'$$

136.1.1152  $P4_2/mnm$

$$\begin{matrix} (1^*0,0,0) & (4_z^*1/2,1/2,1/2) & (2_z^*0,0,0) & (4_z^{-1*}1/2,1/2,1/2) \\ (2_x^*1/2,1/2,1/2) & (2_y^*1/2,1/2,1/2) & (2_{xy}^*0,0,0) & (2_{\&y}^*0,0,0) \\ (\&^*0,0,0) & (\&z^*1/2,1/2,1/2) & (m_z^*0,0,0) & (\&z^{-1*}1/2,1/2,1/2) \\ (m_x^*1/2,1/2,1/2) & (m_y^*1/2,1/2,1/2) & (m_{xy}^*0,0,0) & (m_{\&y}^*0,0,0) \end{matrix}$$

136.2.1153  $P4_2/mnm1'$

136.3.1154  $P4_2/m'nm$   $P4_2nm$  (0,0,0;a,b,c)

$$\begin{matrix} (1^*0,0,0) & (4_z^*1/2,1/2,1/2) & (2_z^*0,0,0) & (4_z^{-1*}1/2,1/2,1/2) \\ (2_x^*1/2,1/2,1/2)' & (2_y^*1/2,1/2,1/2)' & (2_{xy}^*0,0,0)' & (2_{\&y}^*0,0,0)' \\ (\&^*0,0,0)' & (\&z^*1/2,1/2,1/2)' & (m_z^*0,0,0)' & (\&z^{-1*}1/2,1/2,1/2)' \\ (m_x^*1/2,1/2,1/2) & (m_y^*1/2,1/2,1/2) & (m_{xy}^*0,0,0) & (m_{\&y}^*0,0,0) \end{matrix}$$

136.4.1155  $P4_2'/mn'm$   $Cmmm$  (0,0,0;a-b,a+b,c)

$$\begin{matrix} (1^*0,0,0) & (4_z^*1/2,1/2,1/2)' & (2_z^*0,0,0) & (4_z^{-1*}1/2,1/2,1/2)' \\ (2_x^*1/2,1/2,1/2)' & (2_y^*1/2,1/2,1/2)' & (2_{xy}^*0,0,0) & (2_{\&y}^*0,0,0) \\ (\&^*0,0,0) & (\&z^*1/2,1/2,1/2)' & (m_z^*0,0,0) & (\&z^{-1*}1/2,1/2,1/2)' \\ (m_x^*1/2,1/2,1/2)' & (m_y^*1/2,1/2,1/2)' & (m_{xy}^*0,0,0) & (m_{\&y}^*0,0,0) \end{matrix}$$

136.5.1156  $P4_2'/mnm'$   $Pnm$  (0,0,0;a,b,c)

$$\begin{matrix} (1^*0,0,0) & (4_z^*1/2,1/2,1/2)' & (2_z^*0,0,0) & (4_z^{-1*}1/2,1/2,1/2)' \\ (2_x^*1/2,1/2,1/2) & (2_y^*1/2,1/2,1/2) & (2_{xy}^*0,0,0)' & (2_{\&y}^*0,0,0)' \\ (\&^*0,0,0) & (\&z^*1/2,1/2,1/2)' & (m_z^*0,0,0) & (\&z^{-1*}1/2,1/2,1/2)' \\ (m_x^*1/2,1/2,1/2) & (m_y^*1/2,1/2,1/2) & (m_{xy}^*0,0,0)' & (m_{\&y}^*0,0,0)' \end{matrix}$$

136.6.1157  $P4_2'/m'n'm$   $P\&2_1m$  (1/2,0,1/4;a,b,c)

$$\begin{matrix} (1^*0,0,0) & (4_z^*1/2,1/2,1/2)' & (2_z^*0,0,0) & (4_z^{-1*}1/2,1/2,1/2)' \\ (2_x^*1/2,1/2,1/2) & (2_y^*1/2,1/2,1/2) & (2_{xy}^*0,0,0)' & (2_{\&y}^*0,0,0)' \\ (\&^*0,0,0)' & (\&z^*1/2,1/2,1/2) & (m_z^*0,0,0)' & (\&z^{-1*}1/2,1/2,1/2) \\ (m_x^*1/2,1/2,1/2)' & (m_y^*1/2,1/2,1/2)' & (m_{xy}^*0,0,0) & (m_{\&y}^*0,0,0) \end{matrix}$$

136.7.1158  $P4_2'/mn'm'$   $P4_2/m$  (1/2,0,0;a,b,c)

$$\begin{matrix} (1^*0,0,0) & (4_z^*1/2,1/2,1/2) & (2_z^*0,0,0) & (4_z^{-1*}1/2,1/2,1/2) \\ (2_x^*1/2,1/2,1/2)' & (2_y^*1/2,1/2,1/2)' & (2_{xy}^*0,0,0)' & (2_{\&y}^*0,0,0)' \end{matrix}$$

				$(\&^*0,0,0)$ $(m_x^*1/2,1/2,1/2)'$	$(\&_z^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,1/2)'$	$(m_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(\&_z^{-1*}1/2,1/2,1/2)$ $(m_{\&y}^*0,0,0)'$
136.8.1159	$P4_2/m'nm'$	$P\&n2$	$(1/2,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)'$ $(\&^*0,0,0)'$ $(m_x^*1/2,1/2,1/2)$	$(4_z^*1/2,1/2,1/2)'$ $(2_y^*1/2,1/2,1/2)'$ $(\&_z^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*0,0,0)'$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}1/2,1/2,1/2)'$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}1/2,1/2,1/2)$ $(m_{\&y}^*0,0,0)'$
136.9.1160	$P4_2/m'n'm'$	$P4_22_12$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)$ $(\&^*0,0,0)'$ $(m_x^*1/2,1/2,1/2)'$	$(4_z^*1/2,1/2,1/2)$ $(2_y^*1/2,1/2,1/2)$ $(\&_z^*1/2,1/2,1/2)'$ $(m_y^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*0,0,0)'$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}1/2,1/2,1/2)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}1/2,1/2,1/2)'$ $(m_{\&y}^*0,0,0)'$
<b>137.1.1161</b>	<b><math>P4_2/nmc</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(2_x^*1/2,1/2,1/2)</math></b> <b><math>(\&amp;^*1/2,1/2,1/2)</math></b> <b><math>(m_x^*0,0,0)</math></b>	<b><math>(4_z^*1/2,1/2,1/2)</math></b> <b><math>(2_y^*1/2,1/2,1/2)</math></b> <b><math>(\&amp;_z^*0,0,0)</math></b> <b><math>(m_y^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b> <b><math>(2_{xy}^*0,0,0)</math></b> <b><math>(m_z^*1/2,1/2,1/2)</math></b> <b><math>(m_{xy}^*1/2,1/2,1/2)</math></b>	<b><math>(4_z^{-1*}1/2,1/2,1/2)</math></b> <b><math>(2_{\&amp;y}^*0,0,0)</math></b> <b><math>(\&amp;_z^{-1*}0,0,0)</math></b> <b><math>(m_{\&amp;y}^*1/2,1/2,1/2)</math></b>
137.2.1162	$P4_2/nmc1'$						
137.3.1163	$P4_2/n'mc$	$P4_2mc$	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)'$ $(\&^*1/2,1/2,1/2)'$ $(m_x^*0,0,0)$	$(4_z^*1/2,1/2,1/2)$ $(2_y^*1/2,1/2,1/2)'$ $(\&_z^*0,0,0)'$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_z^*1/2,1/2,1/2)'$ $(m_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(2_{\&y}^*0,0,0)'$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*1/2,1/2,1/2)$
137.4.1164	$P4_2/nm'c$	$Ccca$	$(0,0,0;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)'$ $(\&^*1/2,1/2,1/2)$ $(m_x^*0,0,0)'$	$(4_z^*1/2,1/2,1/2)'$ $(2_y^*1/2,1/2,1/2)'$ $(\&_z^*0,0,0)'$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*1/2,1/2,1/2)$ $(m_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}1/2,1/2,1/2)'$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*1/2,1/2,1/2)$
137.5.1165	$P4_2/nmc'$	$Pmmn$	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$	$(4_z^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)'$

				$(2_x^*1/2,1/2,1/2)$	$(2_y^*1/2,1/2,1/2)$	$(2_{xy}^*0,0,0)'$	$(2_{&y}^*0,0,0)'$
				$(\&^*1/2,1/2,1/2)$	$(\&_z^*0,0,0)'$	$(m_z^*1/2,1/2,1/2)$	$(\&_z^{-1*}0,0,0)'$
				$(m_x^*0,0,0)$	$(m_y^*0,0,0)$	$(m_{xy}^*1/2,1/2,1/2)'$	$(m_{&y}^*1/2,1/2,1/2)'$
137.6.1166	$P4_2/n'm'c$	$P\&2_1c$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(4_z^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)'$
				$(2_x^*1/2,1/2,1/2)$	$(2_y^*1/2,1/2,1/2)$	$(2_{xy}^*0,0,0)'$	$(2_{&y}^*0,0,0)'$
				$(\&^*1/2,1/2,1/2)'$	$(\&_z^*0,0,0)$	$(m_z^*1/2,1/2,1/2)'$	$(\&_z^{-1*}0,0,0)$
				$(m_x^*0,0,0)'$	$(m_y^*0,0,0)'$	$(m_{xy}^*1/2,1/2,1/2)$	$(m_{&y}^*1/2,1/2,1/2)$
137.7.1167	$P4_2/nm'c'$	$P4_2/n$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(4_z^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)$
				$(2_x^*1/2,1/2,1/2)'$	$(2_y^*1/2,1/2,1/2)'$	$(2_{xy}^*0,0,0)'$	$(2_{&y}^*0,0,0)'$
				$(\&^*1/2,1/2,1/2)$	$(\&_z^*0,0,0)$	$(m_z^*1/2,1/2,1/2)$	$(\&_z^{-1*}0,0,0)$
				$(m_x^*0,0,0)'$	$(m_y^*0,0,0)'$	$(m_{xy}^*1/2,1/2,1/2)'$	$(m_{&y}^*1/2,1/2,1/2)'$
137.8.1168	$P4_2/n'mc'$	$P\&m2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(4_z^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)'$
				$(2_x^*1/2,1/2,1/2)'$	$(2_y^*1/2,1/2,1/2)'$	$(2_{xy}^*0,0,0)$	$(2_{&y}^*0,0,0)$
				$(\&^*1/2,1/2,1/2)'$	$(\&_z^*0,0,0)$	$(m_z^*1/2,1/2,1/2)'$	$(\&_z^{-1*}0,0,0)$
				$(m_x^*0,0,0)$	$(m_y^*0,0,0)$	$(m_{xy}^*1/2,1/2,1/2)'$	$(m_{&y}^*1/2,1/2,1/2)'$
137.9.1169	$P4_2/n'm'c'$	$P4_22_12$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(4_z^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)$
				$(2_x^*1/2,1/2,1/2)$	$(2_y^*1/2,1/2,1/2)$	$(2_{xy}^*0,0,0)$	$(2_{&y}^*0,0,0)$
				$(\&^*1/2,1/2,1/2)'$	$(\&_z^*0,0,0)'$	$(m_z^*1/2,1/2,1/2)'$	$(\&_z^{-1*}0,0,0)'$
				$(m_x^*0,0,0)'$	$(m_y^*0,0,0)'$	$(m_{xy}^*1/2,1/2,1/2)'$	$(m_{&y}^*1/2,1/2,1/2)'$
<b>138.1.1170</b>	<b><math>P4_2/ncm</math></b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(4_z^*1/2,1/2,1/2)</math></b>	<b><math>(2_z^*0,0,0)</math></b>	<b><math>(4_z^{-1*}1/2,1/2,1/2)</math></b>
				<b><math>(2_x^*1/2,1/2,0)</math></b>	<b><math>(2_y^*1/2,1/2,0)</math></b>	<b><math>(2_{xy}^*0,0,1/2)</math></b>	<b><math>(2_{&amp;y}^*0,0,1/2)</math></b>
				<b><math>(\&amp;^*1/2,1/2,1/2)</math></b>	<b><math>(\&amp;_z^*0,0,0)</math></b>	<b><math>(m_z^*1/2,1/2,1/2)</math></b>	<b><math>(\&amp;_z^{-1*}0,0,0)</math></b>
				<b><math>(m_x^*0,0,1/2)</math></b>	<b><math>(m_y^*0,0,1/2)</math></b>	<b><math>(m_{xy}^*1/2,1/2,0)</math></b>	<b><math>(m_{&amp;y}^*1/2,1/2,0)</math></b>
138.2.1171	$P4_2/ncm1'$						
138.3.1172	$P4_2/n'cm$	$P4_2cm$	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$	$(4_z^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)$
				$(2_x^*1/2,1/2,0)'$	$(2_y^*1/2,1/2,0)'$	$(2_{xy}^*0,0,1/2)'$	$(2_{&y}^*0,0,1/2)'$
				$(\&^*1/2,1/2,1/2)'$	$(\&_z^*0,0,0)'$	$(m_z^*1/2,1/2,1/2)'$	$(\&_z^{-1*}0,0,0)'$



				$(m_x^*0,0,1/2)$	$(m_y^*0,0,1/2)$	$(m_{xy}^*1/2,1/2,0)$	$(m_{\&y}^*1/2,1/2,0)$
138.4.1173	$P4_2/n'c'm$	Cmma	$(1/4,1/4,1/4;a+b,-a+b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)'$ $(\&z^*1/2,1/2,1/2)$ $(m_x^*0,0,1/2)'$	$(4_z^*1/2,1/2,1/2)'$ $(2_y^*1/2,1/2,0)'$ $(\&z^*0,0,0)'$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$ $(m_z^*1/2,1/2,1/2)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}1/2,1/2,1/2)'$ $(2_{\&y}^*0,0,1/2)$ $(\&z^{-1*}0,0,0)'$ $(m_{\&y}^*1/2,1/2,0)$
138.5.1174	$P4_2/n'cm'$	Pccn	$(1/4,1/4,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$ $(\&z^*1/2,1/2,1/2)$ $(m_x^*0,0,1/2)$	$(4_z^*1/2,1/2,1/2)'$ $(2_y^*1/2,1/2,0)$ $(\&z^*0,0,0)'$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)'$ $(m_z^*1/2,1/2,1/2)$ $(m_{xy}^*1/2,1/2,0)'$	$(4_z^{-1*}1/2,1/2,1/2)'$ $(2_{\&y}^*0,0,1/2)$ $(\&z^{-1*}0,0,0)'$ $(m_{\&y}^*1/2,1/2,0)$
138.6.1175	$P4_2/n'c'm$	$P\&2_1m$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$ $(\&z^*1/2,1/2,1/2)'$ $(m_x^*0,0,1/2)'$	$(4_z^*1/2,1/2,1/2)'$ $(2_y^*1/2,1/2,0)$ $(\&z^*0,0,0)$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)'$ $(m_z^*1/2,1/2,1/2)'$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}1/2,1/2,1/2)'$ $(2_{\&y}^*0,0,1/2)'$ $(\&z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,0)$
138.7.1176	$P4_2/n'c'm'$	$P4_2/n$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)'$ $(\&z^*1/2,1/2,1/2)$ $(m_x^*0,0,1/2)'$	$(4_z^*1/2,1/2,1/2)$ $(2_y^*1/2,1/2,0)'$ $(\&z^*0,0,0)$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)'$ $(m_z^*1/2,1/2,1/2)$ $(m_{xy}^*1/2,1/2,0)'$	$(4_z^{-1*}1/2,1/2,1/2)$ $(2_{\&y}^*0,0,1/2)'$ $(\&z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,0)$
138.8.1177	$P4_2/n'cm'$	$P\&c2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)'$ $(\&z^*1/2,1/2,1/2)'$ $(m_x^*0,0,1/2)$	$(4_z^*1/2,1/2,1/2)'$ $(2_y^*1/2,1/2,0)'$ $(\&z^*0,0,0)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$ $(m_z^*1/2,1/2,1/2)'$ $(m_{xy}^*1/2,1/2,0)'$	$(4_z^{-1*}1/2,1/2,1/2)'$ $(2_{\&y}^*0,0,1/2)$ $(\&z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,0)$
138.9.1178	$P4_2/n'c'm'$	$P4_22_12$	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$ $(\&z^*1/2,1/2,1/2)'$ $(m_x^*0,0,1/2)'$	$(4_z^*1/2,1/2,1/2)$ $(2_y^*1/2,1/2,0)$ $(\&z^*0,0,0)'$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$ $(m_z^*1/2,1/2,1/2)'$ $(m_{xy}^*1/2,1/2,0)'$	$(4_z^{-1*}1/2,1/2,1/2)$ $(2_{\&y}^*0,0,1/2)$ $(\&z^{-1*}0,0,0)'$ $(m_{\&y}^*1/2,1/2,0)$
<b>139.1.1179</b>	<b>I4/mmm</b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(4_z^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b>	<b><math>(4_z^{-1*}0,0,0)</math></b>

$$\begin{array}{cccc}
 (2_x^*0,0,0) & (2_y^*0,0,0) & (2_{xy}^*0,0,0) & (2_{\&y}^*0,0,0) \\
 (\&^*0,0,0) & (\&z^*0,0,0) & (m_z^*0,0,0) & (\&z^{-1*}0,0,0) \\
 (m_x^*0,0,0) & (m_y^*0,0,0) & (m_{xy}^*0,0,0) & (m_{\&y}^*0,0,0)
 \end{array}$$

139.2.1180 I4/mmm1'

139.3.1181 I4/m'mm I4mm (0,0,0;a,b,c)  $(1^*0,0,0)$   $(4_z^*0,0,0)$   $(2_z^*0,0,0)$   $(4_z^{-1*}0,0,0)$   
 $(2_x^*0,0,0)'$   $(2_y^*0,0,0)'$   $(2_{xy}^*0,0,0)'$   $(2_{\&y}^*0,0,0)'$   
 $(\&^*0,0,0)'$   $(\&z^*0,0,0)'$   $(m_z^*0,0,0)'$   $(\&z^{-1*}0,0,0)'$   
 $(m_x^*0,0,0)$   $(m_y^*0,0,0)$   $(m_{xy}^*0,0,0)$   $(m_{\&y}^*0,0,0)$

139.4.1182 I4'/mm'm Fmmm (0,0,0 ;a-b,a+b,c)  $(1^*0,0,0)$   $(4_z^*0,0,0)'$   $(2_z^*0,0,0)$   $(4_z^{-1*}0,0,0)'$   
 $(2_x^*0,0,0)'$   $(2_y^*0,0,0)'$   $(2_{xy}^*0,0,0)$   $(2_{\&y}^*0,0,0)$   
 $(\&^*0,0,0)$   $(\&z^*0,0,0)'$   $(m_z^*0,0,0)$   $(\&z^{-1*}0,0,0)'$   
 $(m_x^*0,0,0)'$   $(m_y^*0,0,0)'$   $(m_{xy}^*0,0,0)$   $(m_{\&y}^*0,0,0)$

139.5.1183 I4'/mmm' Immm (0,0,0;a,b,c)  $(1^*0,0,0)$   $(4_z^*0,0,0)'$   $(2_z^*0,0,0)$   $(4_z^{-1*}0,0,0)'$   
 $(2_x^*0,0,0)$   $(2_y^*0,0,0)$   $(2_{xy}^*0,0,0)'$   $(2_{\&y}^*0,0,0)'$   
 $(\&^*0,0,0)$   $(\&z^*0,0,0)'$   $(m_z^*0,0,0)$   $(\&z^{-1*}0,0,0)'$   
 $(m_x^*0,0,0)$   $(m_y^*0,0,0)$   $(m_{xy}^*0,0,0)'$   $(m_{\&y}^*0,0,0)'$

139.6.1184 I4'/m'm'm I&2m (0,0,0;a,b,c)  $(1^*0,0,0)$   $(4_z^*0,0,0)'$   $(2_z^*0,0,0)$   $(4_z^{-1*}0,0,0)'$   
 $(2_x^*0,0,0)$   $(2_y^*0,0,0)$   $(2_{xy}^*0,0,0)'$   $(2_{\&y}^*0,0,0)'$   
 $(\&^*0,0,0)'$   $(\&z^*0,0,0)$   $(m_z^*0,0,0)'$   $(\&z^{-1*}0,0,0)'$   
 $(m_x^*0,0,0)'$   $(m_y^*0,0,0)'$   $(m_{xy}^*0,0,0)$   $(m_{\&y}^*0,0,0)$

139.7.1185 I4/mm'm' I4/m (0,0,0;a,b,c)  $(1^*0,0,0)$   $(4_z^*0,0,0)$   $(2_z^*0,0,0)$   $(4_z^{-1*}0,0,0)$   
 $(2_x^*0,0,0)'$   $(2_y^*0,0,0)'$   $(2_{xy}^*0,0,0)'$   $(2_{\&y}^*0,0,0)'$   
 $(\&^*0,0,0)$   $(\&z^*0,0,0)$   $(m_z^*0,0,0)$   $(\&z^{-1*}0,0,0)$   
 $(m_x^*0,0,0)'$   $(m_y^*0,0,0)'$   $(m_{xy}^*0,0,0)'$   $(m_{\&y}^*0,0,0)'$

139.8.1186 I4'/m'mm' I&m2 (0,0,0;a,b,c)  $(1^*0,0,0)$   $(4_z^*0,0,0)'$   $(2_z^*0,0,0)$   $(4_z^{-1*}0,0,0)'$   
 $(2_x^*0,0,0)'$   $(2_y^*0,0,0)'$   $(2_{xy}^*0,0,0)$   $(2_{\&y}^*0,0,0)$

				$(\&_z^*0,0,0)'$ $(m_x^*0,0,0)$	$(\&_z^*0,0,0)$ $(m_y^*0,0,0)$	$(m_z^*0,0,0)'$ $(m_{xy}^*0,0,0)'$	$(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*0,0,0)'$
139.9.1187	I4/m'm'm'	I422	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&_z^*0,0,0)'$ $(m_x^*0,0,0)'$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)$ $(\&_z^*0,0,0)'$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*0,0,0)'$ $(m_{xy}^*0,0,0)'$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*0,0,0)'$
139.10.1188	I <sub>p</sub> 4/mmm	P4/mmm	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*0,0,0)$ $(2_y^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*0,0,0)$
139.11.1189	I <sub>p</sub> 4/m'mm	P4/nmm	(1/2,0,1/4;a,b,c)	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)$ $(\&_z^*1/2,1/2,1/2)$ $(m_x^*0,0,0)$	$(4_z^*0,0,0)$ $(2_y^*1/2,1/2,1/2)$ $(\&_z^*1/2,1/2,1/2)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)$ $(m_z^*1/2,1/2,1/2)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*1/2,1/2,1/2)$ $(\&_z^{-1*}1/2,1/2,1/2)$ $(m_{\&y}^*0,0,0)$
139.12.1190	I <sub>p</sub> 4'/mm'm	P4 <sub>2</sub> /mnm	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*1/2,1/2,1/2)$ $(\&_z^*0,0,0)$ $(m_x^*1/2,1/2,1/2)$	$(4_z^*1/2,1/2,1/2)$ $(2_y^*1/2,1/2,1/2)$ $(\&_z^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}1/2,1/2,1/2)$ $(m_{\&y}^*0,0,0)$
139.13.1191	I <sub>p</sub> 4'/mmm'	P4 <sub>2</sub> /mmc	(1/2,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_x^*0,0,0)$	$(4_z^*1/2,1/2,1/2)$ $(2_y^*0,0,0)$ $(\&_z^*1/2,1/2,1/2)$ $(m_y^*0,0,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)$ $(m_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(2_{\&y}^*1/2,1/2,1/2)$ $(\&_z^{-1*}1/2,1/2,1/2)$ $(m_{\&y}^*1/2,1/2,1/2)$
139.14.1192	I <sub>p</sub> 4'/m'm'm	P4 <sub>2</sub> /nm	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)$ $(\&_z^*1/2,1/2,1/2)$ $(m_x^*1/2,1/2,1/2)$	$(4_z^*1/2,1/2,1/2)$ $(2_y^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_y^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)$ $(m_z^*1/2,1/2,1/2)$ $(m_{xy}^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(2_{\&y}^*1/2,1/2,1/2)$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*0,0,0)$
139.15.1193	I <sub>p</sub> 4/mm'm'	P4/mnc	(0,0,0;a,b,c)	$(1^*0,0,0)$	$(4_z^*0,0,0)$	$(2_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$

				$(2_x^*1/2,1/2,1/2)$	$(2_y^*1/2,1/2,1/2)$	$(2_{xy}^*1/2,1/2,1/2)$	$(2_{&y}^*1/2,1/2,1/2)$
				$(\&^*0,0,0)$	$(\&_z^*0,0,0)$	$(m_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
				$(m_x^*1/2,1/2,1/2)$	$(m_y^*1/2,1/2,1/2)$	$(m_{xy}^*1/2,1/2,1/2)$	$(m_{&y}^*1/2,1/2,1/2)$
139.16.1194	$I_p 4'/m'mm'$	$P4_2/nmc$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(4_z^*1/2,1/2,1/2)$	$(2_z^*0,0,0)$	$(4_z^{-1*}1/2,1/2,1/2)$
				$(2_x^*1/2,1/2,1/2)$	$(2_y^*1/2,1/2,1/2)$	$(2_{xy}^*0,0,0)$	$(2_{&y}^*0,0,0)$
				$(\&^*1/2,1/2,1/2)$	$(\&_z^*0,0,0)$	$(m_z^*1/2,1/2,1/2)$	$(\&_z^{-1*}0,0,0)$
				$(m_x^*0,0,0)$	$(m_y^*0,0,0)$	$(m_{xy}^*1/2,1/2,1/2)$	$(m_{&y}^*1/2,1/2,1/2)$
139.17.1195	$I_p 4/m'm'm'$	$P4/nnc$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(4_z^*0,0,0)$	$(2_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$
				$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_{&y}^*0,0,0)$
				$(\&^*1/2,1/2,1/2)$	$(\&_z^*1/2,1/2,1/2)$	$(m_z^*1/2,1/2,1/2)$	$(\&_z^{-1*}1/2,1/2,1/2)$
				$(m_x^*1/2,1/2,1/2^*)$	$(m_y^*1/2,1/2,1/2)$	$(m_{xy}^*1/2,1/2,1/2)$	$(m_{&y}^*1/2,1/2,1/2)$
<b>140.1.1196</b>	<b><math>I4/mcm</math></b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(4_z^*0,0,0)</math></b>	<b><math>(2_z^*0,0,0)</math></b>	<b><math>(4_z^{-1*}0,0,0)</math></b>
				<b><math>(2_x^*0,0,1/2)</math></b>	<b><math>(2_y^*0,0,1/2)</math></b>	<b><math>(2_{xy}^*0,0,1/2)</math></b>	<b><math>(2_{&amp;y}^*0,0,1/2)</math></b>
				<b><math>(\&amp;^*0,0,0)</math></b>	<b><math>(\&amp;_z^*0,0,0)</math></b>	<b><math>(m_z^*0,0,0)</math></b>	<b><math>(\&amp;_z^{-1*}0,0,0)</math></b>
				<b><math>(m_x^*0,0,1/2)</math></b>	<b><math>(m_y^*0,0,1/2)</math></b>	<b><math>(m_{xy}^*0,0,1/2)</math></b>	<b><math>(m_{&amp;y}^*0,0,1/2)</math></b>
140.2.1197	$I4/mcm1'$						
140.3.1198	$I4/m'cm$	$I4cm$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(4_z^*0,0,0)$	$(2_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$
				$(2_x^*0,0,1/2)'$	$(2_y^*0,0,1/2)'$	$(2_{xy}^*0,0,1/2)'$	$(2_{&y}^*0,0,1/2)'$
				$(\&^*0,0,0)'$	$(\&_z^*0,0,0)'$	$(m_z^*0,0,0)'$	$(\&_z^{-1*}0,0,0)'$
				$(m_x^*0,0,1/2)$	$(m_y^*0,0,1/2)$	$(m_{xy}^*0,0,1/2)$	$(m_{&y}^*0,0,1/2)$
140.4.1199	$I4'/mc'm$	$Fmmm$	$(1/2,0,0;a-b,a+b,c)$	$(1^*0,0,0)$	$(4_z^*0,0,0)'$	$(2_z^*0,0,0)$	$(4_z^{-1*}0,0,0)'$
				$(2_x^*0,0,1/2)'$	$(2_y^*0,0,1/2)'$	$(2_{xy}^*0,0,1/2)$	$(2_{&y}^*0,0,1/2)$
				$(\&^*0,0,0)$	$(\&_z^*0,0,0)'$	$(m_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)'$
				$(m_x^*0,0,1/2)'$	$(m_y^*0,0,1/2)'$	$(m_{xy}^*0,0,1/2)$	$(m_{&y}^*0,0,1/2)$

140.5.1200	I4'/mcm'	Ibam	(1/2,0,0;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *0,0,1/2) (&*0,0,0) (m <sub>x</sub> *0,0,1/2)	(4 <sub>z</sub> *0,0,0)' (2 <sub>y</sub> *0,0,1/2) (& <sub>z</sub> *0,0,0)' (m <sub>y</sub> *0,0,1/2)'	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *0,0,1/2)' (m <sub>z</sub> *0,0,0) (m <sub>xy</sub> *0,0,1/2)'	(4 <sub>z</sub> <sup>-1</sup> *0,0,0)' (2 <sub>&amp;y</sub> *0,0,1/2)' (& <sub>z</sub> <sup>-1</sup> *0,0,0)' (m <sub>&amp;y</sub> *0,0,1/2)'
140.6.1201	I4'/m'c'm	I&2m	(1/2,0,1/4;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *0,0,1/2) (&*0,0,0)' (m <sub>x</sub> *0,0,1/2)'	(4 <sub>z</sub> *0,0,0)' (2 <sub>y</sub> *0,0,1/2) (& <sub>z</sub> *0,0,0) (m <sub>y</sub> *0,0,1/2)'	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *0,0,1/2)' (m <sub>z</sub> *0,0,0) (m <sub>xy</sub> *0,0,1/2)'	(4 <sub>z</sub> <sup>-1</sup> *0,0,0)' (2 <sub>&amp;y</sub> *0,0,1/2)' (& <sub>z</sub> <sup>-1</sup> *0,0,0) (m <sub>&amp;y</sub> *0,0,1/2)'
140.7.1202	I4/mc'm'	I4/m	(0,0,0;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *0,0,1/2)' (&*0,0,0) (m <sub>x</sub> *0,0,1/2)'	(4 <sub>z</sub> *0,0,0) (2 <sub>y</sub> *0,0,1/2)' (& <sub>z</sub> *0,0,0) (m <sub>y</sub> *0,0,1/2)'	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *0,0,1/2)' (m <sub>z</sub> *0,0,0) (m <sub>xy</sub> *0,0,1/2)'	(4 <sub>z</sub> <sup>-1</sup> *0,0,0) (2 <sub>&amp;y</sub> *0,0,1/2)' (& <sub>z</sub> <sup>-1</sup> *0,0,0) (m <sub>&amp;y</sub> *0,0,1/2)'
140.8.1203	I4'/m'cm'	I&c2	(0,0,0;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *0,0,1/2)' (&*0,0,0)' (m <sub>x</sub> *0,0,1/2)	(4 <sub>z</sub> *0,0,0)' (2 <sub>y</sub> *0,0,1/2)' (& <sub>z</sub> *0,0,0) (m <sub>y</sub> *0,0,1/2)	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *0,0,1/2) (m <sub>z</sub> *0,0,0)' (m <sub>xy</sub> *0,0,1/2)'	(4 <sub>z</sub> <sup>-1</sup> *0,0,0)' (2 <sub>&amp;y</sub> *0,0,1/2) (& <sub>z</sub> <sup>-1</sup> *0,0,0) (m <sub>&amp;y</sub> *0,0,1/2)'
140.9.1204	I4/m'c'm'	I422	(0,0,1/4;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *0,0,1/2) (&*0,0,0)' (m <sub>x</sub> *0,0,1/2)'	(4 <sub>z</sub> *0,0,0) (2 <sub>y</sub> *0,0,1/2) (& <sub>z</sub> *0,0,0)' (m <sub>y</sub> *0,0,1/2)'	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *0,0,1/2) (m <sub>z</sub> *0,0,0)' (m <sub>xy</sub> *0,0,1/2)'	(4 <sub>z</sub> <sup>-1</sup> *0,0,0) (2 <sub>&amp;y</sub> *0,0,1/2) (& <sub>z</sub> <sup>-1</sup> *0,0,0)' (m <sub>&amp;y</sub> *0,0,1/2)'
140.10.1205	I <sub>p</sub> 4/mcm	P4/mcc	(0,0,0;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *0,0,1/2) (&*0,0,0) (m <sub>x</sub> *0,0,1/2)	(4 <sub>z</sub> *0,0,0) (2 <sub>y</sub> *0,0,1/2) (& <sub>z</sub> *0,0,0) (m <sub>y</sub> *0,0,1/2)	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *0,0,1/2) (m <sub>z</sub> *0,0,0) (m <sub>xy</sub> *0,0,1/2)	(4 <sub>z</sub> <sup>-1</sup> *0,0,0) (2 <sub>&amp;y</sub> *0,0,1/2) (& <sub>z</sub> <sup>-1</sup> *0,0,0) (m <sub>&amp;y</sub> *0,0,1/2)
140.11.1206	I <sub>p</sub> 4/m'cm	P4/ncc	(1/2,0,1/4;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *1/2,1/2,0) (&*1/2,1/2,1/2)	(4 <sub>z</sub> *0,0,0) (2 <sub>y</sub> *1/2,1/2,0) (& <sub>z</sub> *1/2,1/2,1/2)	(2 <sub>z</sub> *0,0,0) (2 <sub>xy</sub> *1/2,1/2,0) (m <sub>z</sub> *1/2,1/2,1/2)	(4 <sub>z</sub> <sup>-1</sup> *0,0,0) (2 <sub>&amp;y</sub> *1/2,1/2,0) (& <sub>z</sub> <sup>-1</sup> *1/2,1/2,1/2)

			$(m_x^*0,0,1/2)$	$(m_y^*0,0,1/2)$	$(m_{xy}^*0,0,1/2)$	$(m_{\&y}^*0,0,1/2)$	
140.12.1207	$I_p 4'/mc'm$	$P4_2/mbc$	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$ $(\&^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(4_z^*1/2,1/2,1/2)$ $(2_y^*1/2,1/2,0)$ $(\&_z^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$ $(m_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(2_{\&y}^*0,0,1/2)$ $(\&_z^{-1*}1/2,1/2,1/2)$ $(m_{\&y}^*0,0,1/2)$
140.13.1208	$I_p 4'/mcm'$	$P4_2/mcm$	$(1/2,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)$ $(\&^*0,0,0)$ $(m_x^*0,0,1/2)$	$(4_z^*1/2,1/2,1/2)$ $(2_y^*0,0,1/2)$ $(\&_z^*1/2,1/2,1/2)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,0)$ $(m_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(2_{\&y}^*1/2,1/2,0)$ $(\&_z^{-1*}1/2,1/2,1/2)$ $(m_{\&y}^*1/2,1/2,0)$
140.14.1209	$I_p 4'/m'c'm$	$P4_2/nbc$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)$ $(\&^*1/2,1/2,1/2)$ $(m_x^*1/2,1/2,0)$	$(4_z^*1/2,1/2,1/2)$ $(2_y^*0,0,1/2)$ $(\&_z^*0,0,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,0)$ $(m_z^*1/2,1/2,1/2)$ $(m_{xy}^*0,0,1/2)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(2_{\&y}^*1/2,1/2,0)$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*0,0,1/2)$
140.15.1210	$I_p 4'/mc'm'$	$P4/mbm$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$ $(\&^*0,0,0)$ $(m_x^*1/2,1/2,0)$	$(4_z^*0,0,0)$ $(2_y^*1/2,1/2,0)$ $(\&_z^*0,0,0)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*1/2,1/2,0)$ $(m_z^*0,0,0)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*1/2,1/2,0)$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,0)$
140.16.1211	$I_p 4'/m'cm'$	$P4_2/ncm$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*1/2,1/2,0)$ $(\&^*1/2,1/2,1/2)$ $(m_x^*0,0,1/2)$	$(4_z^*1/2,1/2,1/2)$ $(2_y^*1/2,1/2,0)$ $(\&_z^*0,0,0)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$ $(m_z^*1/2,1/2,1/2)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}1/2,1/2,1/2)$ $(2_{\&y}^*0,0,1/2)$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*1/2,1/2,0)$
140.17.1212	$I_p 4'/m'c'm'$	$P4/nbm$	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,1/2)$ $(\&^*1/2,1/2,1/2)$ $(m_x^*1/2,1/2,0)$	$(4_z^*0,0,0)$ $(2_y^*0,0,1/2)$ $(\&_z^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,0)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$ $(m_z^*1/2,1/2,1/2)$ $(m_{xy}^*1/2,1/2,0)$	$(4_z^{-1*}0,0,0)$ $(2_{\&y}^*0,0,1/2)$ $(\&_z^{-1*}1/2,1/2,1/2)$ $(m_{\&y}^*1/2,1/2,0)$
<b>141.1.1213</b>	<b><math>I_4'/amd</math></b>			$(1^*0,0,0)$ $(2_x^*0,1/2,1/4)$	$(4_z^*0,1/2,1/4)$ $(2_y^*0,1/2,1/4)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(4_z^{-1*}0,1/2,1/4)$ $(2_{\&y}^*0,0,0)$

				$(\&_z^*0, 1/2, 1/4)$ $(m_x^*0, 0, 0)$	$(\&_z^*0, 0, 0)$ $(m_y^*0, 0, 0)$	$(m_z^*0, 1/2, 1/4)$ $(m_{xy}^*0, 1/2, 1/4)$	$(\&_z^{-1*}0, 0, 0)$ $(m_{\&y}^*0, 1/2, 1/4)$
141.2.1214	$I4_1/a$	$I4_1/a$					
141.3.1215	$I4_1/a$	$I4_1/m$	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$ $(2_x^*0, 1/2, 1/4)'$ $(\&^*0, 1/2, 1/4)'$ $(m_x^*0, 0, 0)$	$(4_z^*0, 1/2, 1/4)$ $(2_y^*0, 1/2, 1/4)'$ $(\&_z^*0, 0, 0)'$ $(m_y^*0, 0, 0)$	$(2_z^*0, 0, 0)$ $(2_{xy}^*0, 0, 0)'$ $(m_z^*0, 1/2, 1/4)'$ $(m_{xy}^*0, 1/2, 1/4)$	$(4_z^{-1*}0, 1/2, 1/4)$ $(2_{\&y}^*0, 0, 0)'$ $(\&_z^{-1*}0, 0, 0)'$ $(m_{\&y}^*0, 1/2, 1/4)$
141.4.1216	$I4_1/a$	$Fddd$	$(0, 0, 0; a+b, -a+b, c)$	$(1^*0, 0, 0)$ $(2_x^*0, 1/2, 1/4)'$ $(\&^*0, 1/2, 1/4)$ $(m_x^*0, 0, 0)'$	$(4_z^*0, 1/2, 1/4)'$ $(2_y^*0, 1/2, 1/4)'$ $(\&_z^*0, 0, 0)'$ $(m_y^*0, 0, 0)'$	$(2_z^*0, 0, 0)$ $(2_{xy}^*0, 0, 0)$ $(m_z^*0, 1/2, 1/4)$ $(m_{xy}^*0, 1/2, 1/4)$	$(4_z^{-1*}0, 1/2, 1/4)'$ $(2_{\&y}^*0, 0, 0)$ $(\&_z^{-1*}0, 0, 0)'$ $(m_{\&y}^*0, 1/2, 1/4)$
141.5.1217	$I4_1/a$	$I4_1/m$	$(0, 1/4, 1/8; c, \&, a)$	$(1^*0, 0, 0)$ $(2_x^*0, 1/2, 1/4)$ $(\&^*0, 1/2, 1/4)$ $(m_x^*0, 0, 0)$	$(4_z^*0, 1/2, 1/4)'$ $(2_y^*0, 1/2, 1/4)$ $(\&_z^*0, 0, 0)'$ $(m_y^*0, 0, 0)$	$(2_z^*0, 0, 0)$ $(2_{xy}^*0, 0, 0)'$ $(m_z^*0, 1/2, 1/4)$ $(m_{xy}^*0, 1/2, 1/4)'$	$(4_z^{-1*}0, 1/2, 1/4)'$ $(2_{\&y}^*0, 0, 0)'$ $(\&_z^{-1*}0, 0, 0)'$ $(m_{\&y}^*0, 1/2, 1/4)'$
141.6.1218	$I4_1/a$	$I4_1/m$	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$ $(2_x^*0, 1/2, 1/4)$ $(\&^*0, 1/2, 1/4)'$ $(m_x^*0, 0, 0)'$	$(4_z^*0, 1/2, 1/4)'$ $(2_y^*0, 1/2, 1/4)$ $(\&_z^*0, 0, 0)$ $(m_y^*0, 0, 0)'$	$(2_z^*0, 0, 0)$ $(2_{xy}^*0, 0, 0)'$ $(m_z^*0, 1/2, 1/4)'$ $(m_{xy}^*0, 1/2, 1/4)$	$(4_z^{-1*}0, 1/2, 1/4)'$ $(2_{\&y}^*0, 0, 0)'$ $(\&_z^{-1*}0, 0, 0)$ $(m_{\&y}^*0, 1/2, 1/4)$
141.7.1219	$I4_1/a$	$I4_1/a$	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$ $(2_x^*0, 1/2, 1/4)'$ $(\&^*0, 1/2, 1/4)$ $(m_x^*0, 0, 0)'$	$(4_z^*0, 1/2, 1/4)$ $(2_y^*0, 1/2, 1/4)'$ $(\&_z^*0, 0, 0)$ $(m_y^*0, 0, 0)'$	$(2_z^*0, 0, 0)$ $(2_{xy}^*0, 0, 0)'$ $(m_z^*0, 1/2, 1/4)$ $(m_{xy}^*0, 1/2, 1/4)'$	$(4_z^{-1*}0, 1/2, 1/4)$ $(2_{\&y}^*0, 0, 0)'$ $(\&_z^{-1*}0, 0, 0)$ $(m_{\&y}^*0, 1/2, 1/4)'$
141.8.1220	$I4_1/a$	$I4_1/m$	$(0, 0, 0; a, b, c)$	$(1^*0, 0, 0)$ $(2_x^*0, 1/2, 1/4)'$ $(\&^*0, 1/2, 1/4)'$ $(m_x^*0, 0, 0)$	$(4_z^*0, 1/2, 1/4)'$ $(2_y^*0, 1/2, 1/4)'$ $(\&_z^*0, 0, 0)$ $(m_y^*0, 0, 0)$	$(2_z^*0, 0, 0)$ $(2_{xy}^*0, 0, 0)$ $(m_z^*0, 1/2, 1/4)'$ $(m_{xy}^*0, 1/2, 1/4)'$	$(4_z^{-1*}0, 1/2, 1/4)'$ $(2_{\&y}^*0, 0, 0)$ $(\&_z^{-1*}0, 0, 0)$ $(m_{\&y}^*0, 1/2, 1/4)'$

141.9.1221	$I4_1/a'm'd'$	$I4_122$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,1/2,1/4)$ $(\&^*0,1/2,1/4)'$ $(m_x^*0,0,0)'$	$(4_z^*0,1/2,1/4)$ $(2_y^*0,1/2,1/4)$ $(\&_z^*0,0,0)'$ $(m_y^*0,0,0)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_z^*0,1/2,1/4)'$ $(m_{xy}^*0,1/2,1/4)'$	$(4_z^{-1*}0,1/2,1/4)$ $(2_{\&y}^*0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*0,1/2,1/4)'$
<b>142.1.1222</b>	<b><math>I4_1/acd</math></b>			$(1^*0,0,0)$ $(2_x^*0,1/2,3/4)$ $(\&^*0,1/2,1/4)$ $(m_x^*0,0,1/2)$	$(4_z^*0,1/2,1/4)$ $(2_y^*0,1/2,3/4)$ $(\&_z^*0,0,0)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$ $(m_z^*0,1/2,1/4)$ $(m_{xy}^*0,1/2,3/4)$	$(4_z^{-1*}0,1/2,1/4)$ $(2_{\&y}^*0,0,1/2)$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*0,1/2,3/4)$
142.2.1223	$I4_1/acd1'$						
142.3.1224	$I4_1/a'cd$	$I4_1cd$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,1/2,3/4)'$ $(\&^*0,1/2,1/4)'$ $(m_x^*0,0,1/2)$	$(4_z^*0,1/2,1/4)$ $(2_y^*0,1/2,3/4)'$ $(\&_z^*0,0,0)'$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)'$ $(m_z^*0,1/2,1/4)'$ $(m_{xy}^*0,1/2,3/4)$	$(4_z^{-1*}0,1/2,1/4)$ $(2_{\&y}^*0,0,1/2)'$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*0,1/2,3/4)$
142.4.1225	$I4_1'/ac'd$	$Fddd$	$(0,0,1/4;a-b,a+b,c)$	$(1^*0,0,0)$ $(2_x^*0,1/2,3/4)'$ $(\&^*0,1/2,1/4)$ $(m_x^*0,0,1/2)'$	$(4_z^*0,1/2,1/4)'$ $(2_y^*0,1/2,3/4)'$ $(\&_z^*0,0,0)'$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$ $(m_z^*0,1/2,1/4)$ $(m_{xy}^*0,1/2,3/4)$	$(4_z^{-1*}0,1/2,1/4)'$ $(2_{\&y}^*0,0,1/2)$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*0,1/2,3/4)$
142.5.1226	$I4_1'/acd'$	$Ibca$	$(1/4,0,1/8;b,\&,c)$	$(1^*0,0,0)$ $(2_x^*0,1/2,3/4)$ $(\&^*0,1/2,1/4)$ $(m_x^*0,0,1/2)$	$(4_z^*0,1/2,1/4)'$ $(2_y^*0,1/2,3/4)$ $(\&_z^*0,0,0)'$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)'$ $(m_z^*0,1/2,1/4)$ $(m_{xy}^*0,1/2,3/4)'$	$(4_z^{-1*}0,1/2,1/4)'$ $(2_{\&y}^*0,0,1/2)'$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*0,1/2,3/4)'$
142.6.1227	$I4_1'/a'c'd$	$I\&2d$	$(0,0,0;b,\&,c)$	$(1^*0,0,0)$ $(2_x^*0,1/2,3/4)$ $(\&^*0,1/2,1/4)'$ $(m_x^*0,0,1/2)'$	$(4_z^*0,1/2,1/4)'$ $(2_y^*0,1/2,3/4)$ $(\&_z^*0,0,0)$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)'$ $(m_z^*0,1/2,1/4)'$ $(m_{xy}^*0,1/2,3/4)$	$(4_z^{-1*}0,1/2,1/4)'$ $(2_{\&y}^*0,0,1/2)'$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*0,1/2,3/4)'$



142.7.1228	$I4_1/ac'd'$	$I4_1/a$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,1/2,3/4)'$ $(\&^*0,1/2,1/4)$ $(m_x^*0,0,1/2)'$	$(4_z^*0,1/2,1/4)$ $(2_y^*0,1/2,3/4)'$ $(\&_z^*0,0,0)$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)'$ $(m_z^*0,1/2,1/4)$ $(m_{xy}^*0,1/2,3/4)'$	$(4_z^{-1*}0,1/2,1/4)$ $(2_{\&y}^*0,0,1/2)'$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*0,1/2,3/4)'$
142.8.1229	$I4_1/a'cd'$	$I\&c2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,1/2,3/4)'$ $(\&^*0,1/2,1/4)$ $(m_x^*0,0,1/2)$	$(4_z^*0,1/2,1/4)'$ $(2_y^*0,1/2,3/4)'$ $(\&_z^*0,0,0)$ $(m_y^*0,0,1/2)$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$ $(m_z^*0,1/2,1/4)'$ $(m_{xy}^*0,1/2,3/4)'$	$(4_z^{-1*}0,1/2,1/4)'$ $(2_{\&y}^*0,0,1/2)$ $(\&_z^{-1*}0,0,0)$ $(m_{\&y}^*0,1/2,3/4)'$
142.9.1230	$I4_1/a'c'd'$	$I4_1,22$	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,1/2,3/4)$ $(\&^*0,1/2,1/4)'$ $(m_x^*0,0,1/2)'$	$(4_z^*0,1/2,1/4)$ $(2_y^*0,1/2,3/4)$ $(\&_z^*0,0,0)'$ $(m_y^*0,0,1/2)'$	$(2_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$ $(m_z^*0,1/2,1/4)'$ $(m_{xy}^*0,1/2,3/4)'$	$(4_z^{-1*}0,1/2,1/4)$ $(2_{\&y}^*0,0,1/2)$ $(\&_z^{-1*}0,0,0)'$ $(m_{\&y}^*0,1/2,3/4)'$

## TRIGONAL SYSTEM

<b>143.1.1231</b>	<b>P3</b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(3_z^*0,0,0)</math></b>	<b><math>(3_z^{-1*}0,0,0)</math></b>
143.2.1232	P31'					
143.3.1233	$P_{2c}3$	P3	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
<b>144.1.1234</b>	<b>P3<sub>1</sub></b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(3_z^*0,0,1/3)</math></b>	<b><math>(3_z^{-1*}0,0,2/3)</math></b>
144.2.1235	P3 <sub>1</sub> '					
144.3.1236	$P_{2c}3_2$	P3 <sub>2</sub>	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$	$(3_z^*0,0,4/3)$	$(3_z^{-1*}0,0,2/3)$

<b>145.1.1237</b>	<b>P3<sub>2</sub></b>			<b>(1*0,0,0)</b>	<b>(3<sub>z</sub>*0,0,2/3)</b>	<b>(3<sub>z</sub><sup>-1</sup>*0,0,1/3)</b>
145.2.1238	P3 <sub>2</sub> 1'					
145.3.1239	P <sub>2c</sub> 3 <sub>1</sub>	P3 <sub>1</sub>	(0,0,0;a,b,2c)	(1*0,0,0)	(3 <sub>z</sub> *0,0,2/3)	(3 <sub>z</sub> <sup>-1</sup> *0,0,4/3)
<b>146.1.1240</b>	<b>R3</b>			<b>(1*0,0,0)</b>	<b>(3<sub>z</sub>*0,0,0)</b>	<b>(3<sub>z</sub><sup>-1</sup>*0,0,0)</b>
146.2.1241	R31'					
146.3.1242	R <sub>R</sub> 3	R3	(0,0,0;a+b,b+c,a+c)	(1*0,0,0)	(3 <sub>z</sub> *0,0,0)	(3 <sub>z</sub> <sup>-1</sup> *0,0,0)
<b>147.1.1243</b>	<b>P&amp;</b>			<b>(1*0,0,0)</b> <b>(&amp;*0,0,0)</b>	<b>(3<sub>z</sub>*0,0,0)</b> <b>(&amp;<sub>z</sub>*0,0,0)</b>	<b>(3<sub>z</sub><sup>-1</sup>*0,0,0)</b> <b>(&amp;<sub>z</sub><sup>-1</sup>*0,0,0)</b>
147.2.1244	P&1'					
147.3.1245	P&'	P3	(0,0,0;a,b,c)	(1*0,0,0) (&*0,0,0)'	(3 <sub>z</sub> *0,0,0) (& <sub>z</sub> *0,0,0)'	(3 <sub>z</sub> <sup>-1</sup> *0,0,0) (& <sub>z</sub> <sup>-1</sup> *0,0,0)'
147.4.1246	P <sub>2c</sub> &	P&	(0,0,0;a,b,2c)	(1*0,0,0) (&*0,0,0)	(3 <sub>z</sub> *0,0,0) (& <sub>z</sub> *0,0,0)	(3 <sub>z</sub> <sup>-1</sup> *0,0,0) (& <sub>z</sub> <sup>-1</sup> *0,0,0)
<b>148.1.1247</b>	<b>R&amp;</b>			<b>(1*0,0,0)</b> <b>(&amp;*0,0,0)</b>	<b>(3<sub>z</sub>*0,0,0)</b> <b>(&amp;<sub>z</sub>*0,0,0)</b>	<b>(3<sub>z</sub><sup>-1</sup>*0,0,0)</b> <b>(&amp;<sub>z</sub><sup>-1</sup>*0,0,0)</b>
148.2.1248	R&1'					
148.3.1249	R&'	R3	(0,0,0;a,b,c)	(1*0,0,0)	(3 <sub>z</sub> *0,0,0)	(3 <sub>z</sub> <sup>-1</sup> *0,0,0)

148.4.1250	$R_R \&$	$R \&$	$(0,0,0;a+b,b+c,a+c)$	$(\&^*0,0,0)'$ $(1^*0,0,0)$ $(\&^*0,0,0)$	$(\&_z^*0,0,0)'$ $(3_z^*0,0,0)$ $(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)'$ $(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$
<b>149.1.1251</b>	<b>P312</b>			<b><math>(1^*0,0,0)</math></b> <b><math>(2_1^*0,0,0)</math></b>	<b><math>(3_z^*0,0,0)</math></b> <b><math>(2_2^*0,0,0)</math></b>	<b><math>(3_z^{-1*}0,0,0)</math></b> <b><math>(2_3^*0,0,0)</math></b>
149.2.1252	P3121'					
149.3.1253	P312'	P3	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_1^*0,0,0)'$	$(3_z^*0,0,0)$ $(2_2^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(2_3^*0,0,0)'$
149.4.1254	$P_{2c} 312$	P312	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(2_1^*0,0,0)$	$(3_z^*0,0,0)$ $(2_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(2_3^*0,0,0)$
<b>150.1.1255</b>	<b>P321</b>			<b><math>(1^*0,0,0)</math></b> <b><math>(2_x^*0,0,0)</math></b>	<b><math>(3_z^*0,0,0)</math></b> <b><math>(2_{xy}^*0,0,0)</math></b>	<b><math>(3_z^{-1*}0,0,0)</math></b> <b><math>(2_y^*0,0,0)</math></b>
150.2.1256	P3211'					
150.3.1257	P32'1	P3	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)'$	$(3_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(2_y^*0,0,0)'$
150.4.1258	$P_{2c} 321$	P321	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(3_z^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(2_y^*0,0,0)$
<b>151.1.1259</b>	<b>P3<sub>12</sub></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(2_1^*0,0,0)</math></b>	<b><math>(3_z^*0,0,1/3)</math></b> <b><math>(2_2^*0,0,1/3)</math></b>	<b><math>(3_z^{-1*}0,0,2/3)</math></b> <b><math>(2_3^*0,0,2/3)</math></b>

151.2.1260	P <sub>3</sub> ,121'					
151.3.1261	P <sub>3</sub> ,12'	P <sub>3</sub> <sub>1</sub>	(0,0,0;a,b,c)	(1*0,0,0) (2 <sub>1</sub> *0,0,0)'	(3 <sub>z</sub> *0,0,1/3) (2 <sub>2</sub> *0,0,1/3)'	(3 <sub>z</sub> <sup>-1</sup> *0,0,2/3) (2 <sub>3</sub> *0,0,2/3)'
151.4.1262	P <sub>2c</sub> 3 <sub>2</sub> 12	P <sub>3</sub> <sub>2</sub> 12	(0,0,0;a,b,2c)	(1*0,0,0) (2 <sub>1</sub> *0,0,0)	(3 <sub>z</sub> *0,0,4/3) (2 <sub>2</sub> *0,0,4/3)	(3 <sub>z</sub> <sup>-1</sup> *0,0,2/3) (2 <sub>3</sub> *0,0,2/3)
<b>152.1.1263</b>	<b>P<sub>3</sub>,21</b>			<b>(1*0,0,0) (2<sub>x</sub>*0,0,2/3)</b>	<b>(3<sub>z</sub>*0,0,1/3) (2<sub>xy</sub>*0,0,0)</b>	<b>(3<sub>z</sub><sup>-1</sup>*0,0,2/3) (2<sub>y</sub>*0,0,1/3)</b>
152.2.1264	P <sub>3</sub> ,211'					
152.3.1265	P <sub>3</sub> ,2'1	P <sub>3</sub> <sub>1</sub>	(0,0,0;a,b,c)	(1*0,0,0) (2 <sub>x</sub> *0,0,2/3)'	(3 <sub>z</sub> *0,0,1/3) (2 <sub>xy</sub> *0,0,0)'	(3 <sub>z</sub> <sup>-1</sup> *0,0,2/3) (2 <sub>y</sub> *0,0,1/3)'
152.4.1266	P <sub>2c</sub> 3 <sub>2</sub> 21	P <sub>3</sub> <sub>2</sub> 21	(0,0,0;a,b,2c)	(1*0,0,0) (2 <sub>x</sub> *0,0,2/3)	(3 <sub>z</sub> *0,0,4/3) (2 <sub>xy</sub> *0,0,0)	(3 <sub>z</sub> <sup>-1</sup> *0,0,2/3) (2 <sub>y</sub> *0,0,4/3)
<b>153.1.1267</b>	<b>P<sub>3</sub>,12</b>			<b>(1*0,0,0) (2<sub>1</sub>*0,0,0)</b>	<b>(3<sub>z</sub>*0,0,2/3) (2<sub>2</sub>*0,0,2/3)</b>	<b>(3<sub>z</sub><sup>-1</sup>*0,0,1/3) (2<sub>3</sub>*0,0,1/3)</b>
153.2.1268	P <sub>3</sub> <sub>2</sub> 121'					
153.3.1269	P <sub>3</sub> <sub>2</sub> 12'	P <sub>3</sub> <sub>2</sub>	(0,0,0;a,b,c)	(1*0,0,0) (2 <sub>1</sub> *0,0,0)'	(3 <sub>z</sub> *0,0,2/3) (2 <sub>2</sub> *0,0,2/3)'	(3 <sub>z</sub> <sup>-1</sup> *0,0,1/3) (2 <sub>3</sub> *0,0,1/3)'
153.4.1270	P <sub>2c</sub> 3 <sub>1</sub> 12	P <sub>3</sub> <sub>1</sub> 12	(0,0,0;a,b,2c)	(1*0,0,0) (2 <sub>1</sub> *0,0,0)	(3 <sub>z</sub> *0,0,2/3) (2 <sub>2</sub> *0,0,2/3)	(3 <sub>z</sub> <sup>-1</sup> *0,0,4/3) (2 <sub>3</sub> *0,0,4/3)

<b>154.1.1271</b>	<b>P3<sub>2</sub>21</b>			$(1^*0,0,0)$ $(2_x^*0,0,1/3)$	$(3_z^*0,0,2/3)$ $(2_{xy}^*0,0,0)$	$(3_z^{-1*}0,0,1/3)$ $(2_y^*0,0,2/3)$
154.2.1272	P3 <sub>2</sub> 211'					
154.3.1273	P3 <sub>2</sub> 2'1	P3 <sub>2</sub>	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,1/3)'$	$(3_z^*0,0,2/3)$ $(2_{xy}^*0,0,0)'$	$(3_z^{-1*}0,0,1/3)$ $(2_y^*0,0,2/3)'$
154.4.1274	P <sub>2c</sub> 3 <sub>1</sub> 21	P3 <sub>1</sub> 21	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(2_x^*0,0,4/3)$	$(3_z^*0,0,2/3)$ $(2_{xy}^*0,0,0)$	$(3_z^{-1*}0,0,4/3)$ $(2_y^*0,0,2/3)$
<b>155.1.1275</b>	<b>R32</b>			$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(3_z^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(2_y^*0,0,0)$
155.2.1276	R321'					
155.3.1277	R32'	R3	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_x^*0,0,0)'$	$(3_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(2_y^*0,0,0)'$
155.4.1278	R <sub>R</sub> 32	R32	(0,0,0;a+b,b+c,a+c)	$(1^*0,0,0)$ $(2_x^*0,0,0)$	$(3_z^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(2_y^*0,0,0)$
<b>156.1.1279</b>	<b>P3m1</b>			$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(3_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(m_y^*0,0,0)$
156.2.1280	P3m11'					
156.3.1281	P3m'1	P3	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(m_x^*0,0,0)'$	$(3_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(m_y^*0,0,0)'$

156.4.1282	$P_{2c} 3m1$	P3m1	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(3_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(3_z^{-1}0,0,0)$ $(m_y^*0,0,0)$
156.5.1283	$P_{2c} 3m'1$	P3c1	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(m_x^*0,0,1)$	$(3_z^*0,0,0)$ $(m_{xy}^*0,0,1)$	$(3_z^{-1}0,0,0)$ $(m_y^*0,0,1)$
<b>157.1.1284</b>	<b>P31m</b>			<b><math>(1^*0,0,0)</math></b> <b><math>(m_1^*0,0,0)</math></b>	<b><math>(3_z^*0,0,0)</math></b> <b><math>(m_2^*0,0,0)</math></b>	<b><math>(3_z^{-1}0,0,0)</math></b> <b><math>(m_3^*0,0,0)</math></b>
157.2.1285	P31m1'					
157.3.1286	P31m'	P3	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(m_1^*0,0,0)'$	$(3_z^*0,0,0)$ $(m_2^*0,0,0)'$	$(3_z^{-1}0,0,0)$ $(m_3^*0,0,0)'$
157.4.1287	$P_{2c} 31m$	P31m	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(m_1^*0,0,0)$	$(3_z^*0,0,0)$ $(m_2^*0,0,0)$	$(3_z^{-1}0,0,0)$ $(m_3^*0,0,0)$
157.5.1288	$P_{2c} 31m'$	P31c	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(m_1^*0,0,1)$	$(3_z^*0,0,0)$ $(m_2^*0,0,1)$	$(3_z^{-1}0,0,0)$ $(m_3^*0,0,1)$
<b>158.1.1289</b>	<b>P3c1</b>			<b><math>(1^*0,0,0)</math></b> <b><math>(m_x^*0,0,1/2)</math></b>	<b><math>(3_z^*0,0,0)</math></b> <b><math>(m_{xy}^*0,0,1/2)</math></b>	<b><math>(3_z^{-1}0,0,0)</math></b> <b><math>(m_y^*0,0,1/2)</math></b>
158.2.1290	P3c11'					
158.3.1291	P3c'1	P3	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(m_x^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)'$	$(3_z^{-1}0,0,0)$ $(m_y^*0,0,1/2)'$
<b>159.1.1292</b>	<b>P31c</b>			<b><math>(1^*0,0,0)</math></b>	<b><math>(3_z^*0,0,0)</math></b>	<b><math>(3_z^{-1}0,0,0)</math></b>

				$(m_1^*0,0,1/2)$	$(m_2^*0,0,1/2)$	$(m_3^*0,0,1/2)$
159.2.1293	P31c1'					
159.3.1294	P31c'	P3	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_1^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(m_2^*0,0,1/2)'$	$(3_z^{-1*}0,0,0)$ $(m_3^*0,0,1/2)'$
<b>160.1.1295</b>	<b>R3m</b>			$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(3_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(m_y^*0,0,0)$
160.2.1296	R3m1'					
160.3.1297	R3m'	R3	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,0)'$	$(3_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(m_y^*0,0,0)'$
160.4.1298	R <sub>R</sub> 3m	R3m	$(0,0,0;a+b,b+c,a+c)$	$(1^*0,0,0)$ $(m_x^*0,0,0)$	$(3_z^*0,0,0)$ $(m_{xy}^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(m_y^*0,0,0)$
160.5.1299	R <sub>R</sub> 3m'	R3c	$(0,0,0;a+b,b+c,2a)$	$(1^*0,0,0)$ $(m_x^*1,0,0)$	$(3_z^*0,0,0)$ $(m_{xy}^*1,0,0)$	$(3_z^{-1*}0,0,0)$ $(m_y^*1,0,0)$
<b>161.1.1300</b>	<b>R3c</b>			$(1^*0,0,0)$ $(m_x^*0,0,1/2)$	$(3_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)$	$(3_z^{-1*}0,0,0)$ $(m_y^*0,0,1/2)$
161.2.1301	R3c1'					
161.3.1302	R3c'	R3	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_x^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)'$	$(3_z^{-1*}0,0,0)$ $(m_y^*0,0,1/2)'$

<b>162.1.1303</b>	<b>P&amp;1m</b>			$(1^*0,0,0)$ $(\&^*0,0,0)$ $(m_1^*0,0,0)$ $(2_1^*0,0,0)$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_2^*0,0,0)$ $(2_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$ $(m_3^*0,0,0)$ $(2_3^*0,0,0)$
162.2.1304	P&1m1'					
162.3.1305	P&'1m	P31m	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)'$ $(m_1^*0,0,0)$ $(2_1^*0,0,0)'$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)'$ $(m_2^*0,0,0)$ $(2_2^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(m_3^*0,0,0)$ $(2_3^*0,0,0)'$
162.4.1306	P&'1m'	P312	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)'$ $(m_1^*0,0,0)$ $(2_1^*0,0,0)$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)'$ $(m_2^*0,0,0)$ $(2_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(m_3^*0,0,0)'$ $(2_3^*0,0,0)$
162.5.1307	P&1m'	P&	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)$ $(m_1^*0,0,0)'$ $(2_1^*0,0,0)'$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_2^*0,0,0)'$ $(2_2^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$ $(m_3^*0,0,0)'$ $(2_3^*0,0,0)'$
162.6.1308	P <sub>2c</sub> &1m	P&1m	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(\&^*0,0,0)$ $(m_1^*0,0,0)$ $(2_1^*0,0,0)$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_2^*0,0,0)$ $(2_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$ $(m_3^*0,0,0)$ $(2_3^*0,0,0)$
162.7.1309	P <sub>2c</sub> &1m'	P&1c	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(\&^*0,0,0)$ $(m_1^*0,0,1)$ $(2_1^*0,0,1)$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_2^*0,0,1)$ $(2_2^*0,0,1)$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$ $(m_3^*0,0,1)$ $(2_3^*0,0,1)$
<b>163.1.1310</b>	<b>P&amp;1c</b>			$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$



$$\begin{matrix} (\& *0,0,0) \\ (m_1 *0,0,1/2) \\ (2_1 *0,0,1/2) \end{matrix} \quad \begin{matrix} (\&_z *0,0,0) \\ (m_2 *0,0,1/2) \\ (2_2 *0,0,1/2) \end{matrix} \quad \begin{matrix} (\&_z^{-1} *0,0,0) \\ (m_3 *0,0,1/2) \\ (2_3 *0,0,1/2) \end{matrix}$$

163.2.1311 P&1c1'

163.3.1312 P&'1c P31c (0,0,0;a,b,c)  $\begin{matrix} (1^*0,0,0) \\ (\& *0,0,0)' \\ (m_1^*0,0,1/2) \\ (2_1^*0,0,1/2)' \end{matrix}$   $\begin{matrix} (3_z^*0,0,0) \\ (\&_z *0,0,0)' \\ (m_2^*0,0,1/2) \\ (2_2^*0,0,1/2)' \end{matrix}$   $\begin{matrix} (3_z^{-1} *0,0,0) \\ (\&_z^{-1} *0,0,0)' \\ (m_3^*0,0,1/2) \\ (2_3^*0,0,1/2)' \end{matrix}$

163.4.1313 P&'1c' P312 (0,0,1/4;a,b,c)  $\begin{matrix} (1^*0,0,0) \\ (\& *0,0,0)' \\ (m_1^*0,0,1/2)' \\ (2_1^*0,0,1/2) \end{matrix}$   $\begin{matrix} (3_z^*0,0,0) \\ (\&_z *0,0,0)' \\ (m_2^*0,0,1/2)' \\ (2_2^*0,0,1/2) \end{matrix}$   $\begin{matrix} (3_z^{-1} *0,0,0) \\ (\&_z^{-1} *0,0,0)' \\ (m_3^*0,0,1/2)' \\ (2_3^*0,0,1/2) \end{matrix}$

163.5.1314 P&1c' P& (0,0,0;a,b,c)  $\begin{matrix} (1^*0,0,0) \\ (\& *0,0,0) \\ (m_1^*0,0,1/2)' \\ (2_1^*0,0,1/2)' \end{matrix}$   $\begin{matrix} (3_z^*0,0,0) \\ (\&_z *0,0,0) \\ (m_2^*0,0,1/2)' \\ (2_2^*0,0,1/2)' \end{matrix}$   $\begin{matrix} (3_z^{-1} *0,0,0) \\ (\&_z^{-1} *0,0,0) \\ (m_3^*0,0,1/2)' \\ (2_3^*0,0,1/2)' \end{matrix}$

**164.1.1315 P&m1**  $\begin{matrix} (1^*0,0,0) \\ (\& *0,0,0) \\ (m_x^*0,0,0) \\ (2_x^*0,0,0) \end{matrix}$   $\begin{matrix} (3_z^*0,0,0) \\ (\&_z *0,0,0) \\ (m_{xy}^*0,0,0) \\ (2_{xy}^*0,0,0) \end{matrix}$   $\begin{matrix} (3_z^{-1} *0,0,0) \\ (\&_z^{-1} *0,0,0) \\ (m_y^*0,0,0) \\ (2_y^*0,0,0) \end{matrix}$

164.2.1316 P&m11'

164.3.1317 P&'m1 P3m1 (0,0,0;a,b,c)  $\begin{matrix} (1^*0,0,0) \\ (\& *0,0,0)' \\ (m_x^*0,0,0) \\ (2_x^*0,0,0)' \end{matrix}$   $\begin{matrix} (3_z^*0,0,0) \\ (\&_z *0,0,0)' \\ (m_{xy}^*0,0,0) \\ (2_{xy}^*0,0,0)' \end{matrix}$   $\begin{matrix} (3_z^{-1} *0,0,0) \\ (\&_z^{-1} *0,0,0)' \\ (m_y^*0,0,0) \\ (2_y^*0,0,0)' \end{matrix}$

164.4.1318	$P\bar{4}m'1$	P321	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\bar{4}^*0,0,0)'$ $(m_x^*0,0,0)'$ $(2_x^*0,0,0)$	$(3_z^*0,0,0)$ $(\bar{4}_z^*0,0,0)'$ $(m_{xy}^*0,0,0)'$ $(2_{xy}^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\bar{4}_z^{-1*}0,0,0)'$ $(m_y^*0,0,0)'$ $(2_y^*0,0,0)$
164.5.1319	$P\bar{4}m'1$	$P\bar{4}$	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\bar{4}^*0,0,0)$ $(m_x^*0,0,0)'$ $(2_x^*0,0,0)'$	$(3_z^*0,0,0)$ $(\bar{4}_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$ $(2_{xy}^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(\bar{4}_z^{-1*}0,0,0)$ $(m_y^*0,0,0)'$ $(2_y^*0,0,0)'$
164.6.1320	$P_{2c}\bar{4}m1$	$P\bar{4}m1$	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(\bar{4}^*0,0,0)$ $(m_x^*0,0,0)$ $(2_x^*0,0,0)$	$(3_z^*0,0,0)$ $(\bar{4}_z^*0,0,0)$ $(m_{xy}^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\bar{4}_z^{-1*}0,0,0)$ $(m_y^*0,0,0)$ $(2_y^*0,0,0)$
164.7.1321	$P_{2c}\bar{4}m'1$	$P\bar{4}c1$	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(\bar{4}^*0,0,0)$ $(m_x^*0,0,1)$ $(2_x^*0,0,1)$	$(3_z^*0,0,0)$ $(\bar{4}_z^*0,0,0)$ $(m_{xy}^*0,0,1)$ $(2_{xy}^*0,0,1)$	$(3_z^{-1*}0,0,0)$ $(\bar{4}_z^{-1*}0,0,0)$ $(m_y^*0,0,1)$ $(2_y^*0,0,1)$
<b>165.1.1322</b>	<b><math>P\bar{4}c1</math></b>			<b><math>(1^*0,0,0)</math> <math>(\bar{4}^*0,0,0)</math> <math>(m_x^*0,0,1/2)</math> <math>(2_x^*0,0,1/2)</math></b>	<b><math>(3_z^*0,0,0)</math> <math>(\bar{4}_z^*0,0,0)</math> <math>(m_{xy}^*0,0,1/2)</math> <math>(2_{xy}^*0,0,1/2)</math></b>	<b><math>(3_z^{-1*}0,0,0)</math> <math>(\bar{4}_z^{-1*}0,0,0)</math> <math>(m_y^*0,0,1/2)</math> <math>(2_y^*0,0,1/2)</math></b>
165.2.1323	$P\bar{4}c11'$					
165.3.1324	$P\bar{4}c1$	P3c1	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\bar{4}^*0,0,0)'$ $(m_x^*0,0,1/2)$	$(3_z^*0,0,0)$ $(\bar{4}_z^*0,0,0)'$ $(m_{xy}^*0,0,1/2)$	$(3_z^{-1*}0,0,0)$ $(\bar{4}_z^{-1*}0,0,0)'$ $(m_y^*0,0,1/2)$

165.4.1325	P&'c'1	P321	(0,0,1/4;a,b,c)	$(2_x^*0,0,1/2)'$ $(1^*0,0,0)$ $(\&^*0,0,0)'$ $(m_x^*0,0,1/2)'$ $(2_x^*0,0,1/2)$	$(2_{xy}^*0,0,1/2)'$ $(3_z^*0,0,0)$ $(\&_z^*0,0,0)'$ $(m_{xy}^*0,0,1/2)'$ $(2_{xy}^*0,0,1/2)$	$(2_y^*0,0,1/2)'$ $(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(m_y^*0,0,1/2)'$ $(2_y^*0,0,1/2)$
165.5.1326	P&'c'1	P&	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)$ $(m_x^*0,0,1/2)'$ $(2_x^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)'$ $(2_{xy}^*0,0,1/2)'$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$ $(m_y^*0,0,1/2)'$ $(2_y^*0,0,1/2)'$
<b>166.1.1327</b>	<b>R&amp;m</b>			$(1^*0,0,0)$ $(\&^*0,0,0)$ $(m_x^*0,0,0)$ $(2_x^*0,0,0)$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_{xy}^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$ $(m_y^*0,0,0)$ $(2_y^*0,0,0)$
166.2.1328	R&m1'					
166.3.1329	R&'m	R3m	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)'$ $(m_x^*0,0,0)$ $(2_x^*0,0,0)'$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)'$ $(m_{xy}^*0,0,0)$ $(2_{xy}^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(m_y^*0,0,0)$ $(2_y^*0,0,0)'$
166.4.1330	R&'m'	R32	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)'$ $(m_x^*0,0,0)$ $(2_x^*0,0,0)$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)'$ $(m_{xy}^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(m_y^*0,0,0)$ $(2_y^*0,0,0)$
166.5.1331	R&'m'	R&	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$

				$(m_x^*0,0,0)'$ $(2_x^*0,0,0)'$	$(m_{xy}^*0,0,0)'$ $(2_{xy}^*0,0,0)'$	$(m_y^*0,0,0)'$ $(2_y^*0,0,0)'$
166.6.1332	$R_R\&m$	$R\&m$	$(0,0,0;a+b,b+c,a+c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$ $(m_x^*0,0,0)$ $(2_x^*0,0,0)$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_{xy}^*0,0,0)$ $(2_{xy}^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$ $(m_y^*0,0,0)$ $(2_y^*0,0,0)$
166.7.1333	$R_R\&m'$	$R\&c$	$(0,0,0;a+b,b+c,a+c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$ $(m_x^*0,0,1)$ $(2_x^*0,0,1)$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_{xy}^*0,0,1)$ $(2_{xy}^*0,0,1)$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$ $(m_y^*0,0,1)$ $(2_y^*0,0,1)$
<b>167.1.1334</b>	<b><math>R\&amp;c</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(\&amp;^*0,0,0)</math></b> <b><math>(m_x^*0,0,1/2)</math></b> <b><math>(2_x^*0,0,1/2)</math></b>	<b><math>(3_z^*0,0,0)</math></b> <b><math>(\&amp;_z^*0,0,0)</math></b> <b><math>(m_{xy}^*0,0,1/2)</math></b> <b><math>(2_{xy}^*0,0,1/2)</math></b>	<b><math>(3_z^{-1*}0,0,0)</math></b> <b><math>(\&amp;_z^{-1*}0,0,0)</math></b> <b><math>(m_y^*0,0,1/2)</math></b> <b><math>(2_y^*0,0,1/2)</math></b>
167.2.1335	$R\&c1'$					
167.3.1336	$R\&'c$	$R3c$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$ $(m_x^*0,0,1/2)$ $(2_x^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)'$ $(m_{xy}^*0,0,1/2)$ $(2_{xy}^*0,0,1/2)'$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(m_y^*0,0,1/2)$ $(2_y^*0,0,1/2)'$
167.4.1337	$R\&'c'$	$R32$	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$ $(m_x^*0,0,1/2)'$ $(2_x^*0,0,1/2)$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)'$ $(m_{xy}^*0,0,1/2)'$ $(2_{xy}^*0,0,1/2)$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(m_y^*0,0,1/2)'$ $(2_y^*0,0,1/2)$
167.5.1338	$R\&c'$	$R\&$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$

$$\begin{array}{ccc}
 (\mathbb{1}^*0,0,0) & (\mathbb{3}_z^*0,0,0) & (\mathbb{3}_z^{-1*}0,0,0) \\
 (m_x^*0,0,1/2)' & (m_{xy}^*0,0,1/2)' & (m_y^*0,0,1/2)' \\
 (2_x^*0,0,1/2)' & (2_{xy}^*0,0,1/2)' & (2_y^*0,0,1/2)'
 \end{array}$$

## HEXAGONAL SYSTEM

<b>168.1.1339</b>	<b>P6</b>			<b>(1*0,0,0)</b>	<b>(3<sub>z</sub>*0,0,0)</b>	<b>(3<sub>z</sub><sup>-1</sup>*0,0,0)</b>
				<b>(2<sub>z</sub>*0,0,0)</b>	<b>(6<sub>z</sub>*0,0,0)</b>	<b>(6<sub>z</sub><sup>-1</sup>*0,0,0)</b>
168.2.1340	P61'					
168.3.1341	P6'	P3	(0,0,0;a,b,c)	(1*0,0,0)	(3 <sub>z</sub> *0,0,0)	(3 <sub>z</sub> <sup>-1</sup> *0,0,0)
				(2 <sub>z</sub> *0,0,0)'	(6 <sub>z</sub> *0,0,0)'	(6 <sub>z</sub> <sup>-1</sup> *0,0,0)'
168.4.1342	P <sub>2c</sub> 6	P6	(0,0,0;a,b,2c)	(1*0,0,0)	(3 <sub>z</sub> *0,0,0)	(3 <sub>z</sub> <sup>-1</sup> *0,0,0)
				(2 <sub>z</sub> *0,0,0)	(6 <sub>z</sub> *0,0,0)	(6 <sub>z</sub> <sup>-1</sup> *0,0,0)
168.5.1343	P <sub>2c</sub> 6'	P6 <sub>3</sub>	(0,0,0;a,b,2c)	(1*0,0,0)	(3 <sub>z</sub> *0,0,0)	(3 <sub>z</sub> <sup>-1</sup> *0,0,0)
				(2 <sub>z</sub> *0,0,1)	(6 <sub>z</sub> *0,0,1)	(6 <sub>z</sub> <sup>-1</sup> *0,0,1)
<b>169.1.1344</b>	<b>P6<sub>1</sub></b>			<b>(1*0,0,0)</b>	<b>(3<sub>z</sub>*0,0,1/3)</b>	<b>(3<sub>z</sub><sup>-1</sup>*0,0,2/3)</b>
				<b>(2<sub>z</sub>*0,0,1/2)</b>	<b>(6<sub>z</sub>*0,0,1/6)</b>	<b>(6<sub>z</sub><sup>-1</sup>*0,0,5/6)</b>
169.2.1345	P6 <sub>1</sub> 1'					
169.3.1346	P6 <sub>1</sub> '	P3 <sub>1</sub>	(0,0,0;a,b,c)	(1*0,0,0)	(3 <sub>z</sub> *0,0,1/3)	(3 <sub>z</sub> <sup>-1</sup> *0,0,2/3)

$$(2_z^*0,0,1/2)' \quad (6_z^*0,0,1/6)' \quad (6_z^{-1*}0,0,5/6)'$$

**170.1.1347**  $P6_5$

$$\begin{matrix} (1^*0,0,0) \\ (2_z^*0,0,1/2) \end{matrix} \quad \begin{matrix} (3_z^*0,0,2/3) \\ (6_z^*0,0,5/6) \end{matrix} \quad \begin{matrix} (3_z^{-1*}0,0,1/3) \\ (6_z^{-1*}0,0,1/6) \end{matrix}$$

170.2.1348  $P6_51'$

170.3.1349  $P6_5'$

$P3_2$

(0,0,0;a,b,c)

$$\begin{matrix} (1^*0,0,0) \\ (2_z^*0,0,1/2)' \end{matrix} \quad \begin{matrix} (3_z^*0,0,2/3) \\ (6_z^*0,0,5/6)' \end{matrix} \quad \begin{matrix} (3_z^{-1*}0,0,1/3) \\ (6_z^{-1*}0,0,1/6)' \end{matrix}$$

**171.1.1350**  $P6_2$

$$\begin{matrix} (1^*0,0,0) \\ (2_z^*0,0,0) \end{matrix} \quad \begin{matrix} (3_z^*0,0,2/3) \\ (6_z^*0,0,1/3) \end{matrix} \quad \begin{matrix} (3_z^{-1*}0,0,1/3) \\ (6_z^{-1*}0,0,2/3) \end{matrix}$$

171.2.1351  $P6_21'$

171.3.1352  $P6_2'$

$P3_2$

(0,0,0;a,b,c)

$$\begin{matrix} (1^*0,0,0) \\ (2_z^*0,0,0)' \end{matrix} \quad \begin{matrix} (3_z^*0,0,2/3) \\ (6_z^*0,0,1/3)' \end{matrix} \quad \begin{matrix} (3_z^{-1*}0,0,1/3) \\ (6_z^{-1*}0,0,2/3)' \end{matrix}$$

171.4.1353  $P_{2c}6_2$

$P6_1$

(0,0,0;a,b,2c)

$$\begin{matrix} (1^*0,0,0) \\ (2_z^*0,0,1) \end{matrix} \quad \begin{matrix} (3_z^*0,0,2/3) \\ (6_z^*0,0,1/3) \end{matrix} \quad \begin{matrix} (3_z^{-1*}0,0,4/3) \\ (6_z^{-1*}0,0,5/3) \end{matrix}$$

171.5.1354  $P_{2c}6_2'$

$P6_4$

(0,0,0;a,b,2c)

$$\begin{matrix} (1^*0,0,0) \\ (2_z^*0,0,0) \end{matrix} \quad \begin{matrix} (3_z^*0,0,2/3) \\ (6_z^*0,0,4/3) \end{matrix} \quad \begin{matrix} (3_z^{-1*}0,0,4/3) \\ (6_z^{-1*}0,0,2/3) \end{matrix}$$

**172.1.1355**  $P6_4$

$$\begin{matrix} (1^*0,0,0) \\ (2_z^*0,0,0) \end{matrix} \quad \begin{matrix} (3_z^*0,0,1/3) \\ (6_z^*0,0,2/3) \end{matrix} \quad \begin{matrix} (3_z^{-1*}0,0,2/3) \\ (6_z^{-1*}0,0,1/3) \end{matrix}$$

172.2.1356  $P6_4 1'$

172.3.1357  $P6_4'$

$P3_1$

(0,0,0;a,b,c)

$$(1^*0,0,0) \quad (3_z^*0,0,1/3) \quad (3_z^{-1*}0,0,2/3)$$

				$(2_z^*0,0,0)'$	$(6_z^*0,0,2/3)'$	$(6_z^{-1*}0,0,1/3)'$
172.4.1358	$P_{2c}6_4$	$P6_2$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(2_z^*0,0,0)$	$(3_z^*0,0,4/3)$ $(6_z^*0,0,2/3)$	$(3_z^{-1*}0,0,2/3)$ $(6_z^{-1*}0,0,4/3)$
172.5.1359	$P_{2c}6_4'$	$P6_5$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(2_z^*0,0,1)$	$(3_z^*0,0,4/3)$ $(6_z^*0,0,5/3)$	$(3_z^{-1*}0,0,2/3)$ $(6_z^{-1*}0,0,1/3)$
<b>173.1.1360</b>	<b><math>P6_3</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(2_z^*0,0,1/2)</math></b>	<b><math>(3_z^*0,0,0)</math></b> <b><math>(6_z^*0,0,1/2)</math></b>	<b><math>(3_z^{-1*}0,0,0)</math></b> <b><math>(6_z^{-1*}0,0,1/2)</math></b>
173.2.1361	$P6_31'$					
173.3.1362	$P6_3'$	$P3$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,1/2)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)'$
<b>174.1.1363</b>	<b><math>P\&amp;</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(m_z^*0,0,0)</math></b>	<b><math>(3_z^*0,0,0)</math></b> <b><math>(\&amp;_z^*0,0,0)</math></b>	<b><math>(3_z^{-1*}0,0,0)</math></b> <b><math>(\&amp;_z^{-1*}0,0,0)</math></b>
174.2.1364	$P\&1'$					
174.3.1365	$P\&'$	$P3$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_z^*0,0,0)'$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)'$
174.4.1366	$P_{2c}\&$	$P\&$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(m_z^*0,0,0)$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$
<b>175.1.1367</b>	<b><math>P6/m</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(\&amp;^*0,0,0)</math></b>	<b><math>(3_z^*0,0,0)</math></b> <b><math>(\&amp;_z^*0,0,0)</math></b>	<b><math>(3_z^{-1*}0,0,0)</math></b> <b><math>(\&amp;_z^{-1*}0,0,0)</math></b>

				$(2_z^*0,0,0)$ $(m_z^*0,0,0)$	$(6_z^*0,0,0)$ $(\&_z^*0,0,0)$	$(6_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$
175.2.1368	P6/m1'					
175.3.1369	P6'/m	P&	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)'$ $(2_z^*0,0,0)'$ $(m_z^*0,0,0)$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)'$ $(6_z^*0,0,0)'$ $(\&_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(6_z^{-1*}0,0,0)'$ $(\&_z^{-1*}0,0,0)$
175.4.1370	P6/m'	P6	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)'$ $(2_z^*0,0,0)$ $(m_z^*0,0,0)'$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)'$ $(6_z^*0,0,0)$ $(\&_z^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(6_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)'$
175.5.1371	P6'/m'	P&	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(\&^*0,0,0)$ $(2_z^*0,0,0)'$ $(m_z^*0,0,0)'$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)$ $(6_z^*0,0,0)'$ $(\&_z^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)'$ $(\&_z^{-1*}0,0,0)'$
175.6.1372	P <sub>2c</sub> 6/m	P6/m	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(\&^*0,0,0)$ $(2_z^*0,0,0)$ $(m_z^*0,0,0)$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)$ $(6_z^*0,0,0)$ $(\&_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$
175.7.1373	P <sub>2c</sub> 6'/m	P6 <sub>3</sub> /m	(0,0,1/2;a,b,2c)	$(1^*0,0,0)$ $(\&^*0,0,1)$ $(2_z^*0,0,1)$ $(m_z^*0,0,0)$	$(3_z^*0,0,0)$ $(\&_z^*0,0,1)$ $(6_z^*0,0,1)$ $(\&_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,1)$ $(6_z^{-1*}0,0,1)$ $(\&_z^{-1*}0,0,0)$
176.1.1374	P6 <sub>3</sub> /m			$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$



				$(\&^*0,0,0)$ $(2_z^*0,0,1/2)$ $(m_z^*0,0,1/2)$	$(\&_z^*0,0,0)$ $(6_z^*0,0,1/2)$ $(\&_z^*0,0,1/2)$	$(\&_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)$ $(\&_z^{-1*}0,0,1/2)$
176.2.1375	$P6_3/m1'$					
176.3.1376	$P6_3'/m$	$P\&$	$(0,0,1/4;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$ $(2_z^*0,0,1/2)'$ $(m_z^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)'$ $(6_z^*0,0,1/2)'$ $(\&_z^*0,0,1/2)'$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(6_z^{-1*}0,0,1/2)'$ $(\&_z^{-1*}0,0,1/2)'$
176.4.1377	$P6_3/m'$	$P6_3$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)'$ $(2_z^*0,0,1/2)$ $(m_z^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)'$ $(6_z^*0,0,1/2)$ $(\&_z^*0,0,1/2)'$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)'$ $(6_z^{-1*}0,0,1/2)$ $(\&_z^{-1*}0,0,1/2)'$
176.5.1378	$P6_3'/m'$	$P\&$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(\&^*0,0,0)$ $(2_z^*0,0,1/2)'$ $(m_z^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(\&_z^*0,0,0)$ $(6_z^*0,0,1/2)'$ $(\&_z^*0,0,1/2)'$	$(3_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)'$ $(\&_z^{-1*}0,0,1/2)'$
<b>177.1.1379</b>	<b><math>P622</math></b>			$(1^*0,0,0)$ $(2_z^*0,0,0)$ $(2_x^*0,0,0)$ $(2_1^*0,0,0)$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(2_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)$ $(2_y^*0,0,0)$ $(2_3^*0,0,0)$
177.2.1380	$P6221'$					
177.3.1381	$P6'2'2$	$P312$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,0)'$ $(2_x^*0,0,0)'$ $(2_1^*0,0,0)$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)'$ $(2_{xy}^*0,0,0)'$ $(2_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)'$ $(2_y^*0,0,0)'$ $(2_3^*0,0,0)$

177.4.1382	P6'22'	P321	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,0)'$ $(2_x^*0,0,0)$ $(2_1^*0,0,0)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)'$ $(2_{xy}^*0,0,0)$ $(2_2^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)'$ $(2_y^*0,0,0)$ $(2_3^*0,0,0)'$
177.5.1383	P62'2'	P6	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,0)$ $(2_x^*0,0,0)'$ $(2_1^*0,0,0)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(2_2^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)$ $(2_y^*0,0,0)'$ $(2_3^*0,0,0)'$
177.6.1384	P <sub>2c</sub> 622	P622	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(2_z^*0,0,0)$ $(2_x^*0,0,0)$ $(2_1^*0,0,0)$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(2_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)$ $(2_y^*0,0,0)$ $(2_3^*0,0,0)$
177.7.1385	P <sub>2c</sub> 6'22'	P6 <sub>3</sub> 22	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(2_z^*0,0,1)$ $(2_x^*0,0,0)$ $(2_1^*0,0,1)$	$(3_z^*0,0,0)$ $(6_z^*0,0,1)$ $(2_{xy}^*0,0,0)$ $(2_2^*0,0,1)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1)$ $(2_y^*0,0,0)$ $(2_3^*0,0,1)$
<b>178.1.1386</b>	<b>P6<sub>1</sub>22</b>			$(1^*0,0,0)$ $(2_z^*0,0,1/2)$ $(2_x^*0,0,0)$ $(2_1^*0,0,1/6)$	$(3_z^*0,0,1/3)$ $(6_z^*0,0,1/6)$ $(2_{xy}^*0,0,1/3)$ $(2_2^*0,0,1/2)$	$(3_z^{-1*}0,0,2/3)$ $(6_z^{-1*}0,0,5/6)$ $(2_y^*0,0,2/3)$ $(2_3^*0,0,5/6)$
178.2.1387	P6 <sub>1</sub> 221'					
178.3.1388	P6 <sub>1</sub> '2'2	P3 <sub>1</sub> 12	(0,0,1/12;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,1/2)'$ $(2_x^*0,0,0)'$ $(2_1^*0,0,1/6)$	$(3_z^*0,0,1/3)$ $(6_z^*0,0,1/6)'$ $(2_{xy}^*0,0,1/3)'$ $(2_2^*0,0,1/2)$	$(3_z^{-1*}0,0,2/3)$ $(6_z^{-1*}0,0,5/6)'$ $(2_y^*0,0,2/3)'$ $(2_3^*0,0,5/6)$

178.4.1389	P6 <sub>1</sub> '22'	P3 <sub>1</sub> 21	(0,0,1/6;a,b,c)	(1*0,0,0) (2 <sub>z</sub> *0,0,1/2)' (2 <sub>x</sub> *0,0,0) (2 <sub>1</sub> *0,0,1/6)'	(3 <sub>z</sub> *0,0,1/3) (6 <sub>z</sub> *0,0,1/6)' (2 <sub>xy</sub> *0,0,1/3) (2 <sub>2</sub> *0,0,1/2)'	(3 <sub>z</sub> <sup>-1</sup> *0,0,2/3) (6 <sub>z</sub> <sup>-1</sup> *0,0,5/6)' (2 <sub>y</sub> *0,0,2/3) (2 <sub>3</sub> *0,0,5/6)'
178.5.1390	P6 <sub>1</sub> 2'2'	P6 <sub>1</sub>	(0,0,0;a,b,c)	(1*0,0,0) (2 <sub>z</sub> *0,0,1/2) (2 <sub>x</sub> *0,0,0)' (2 <sub>1</sub> *0,0,1/6)'	(3 <sub>z</sub> *0,0,1/3) (6 <sub>z</sub> *0,0,1/6) (2 <sub>xy</sub> *0,0,1/3)' (2 <sub>2</sub> *0,0,1/2)'	(3 <sub>z</sub> <sup>-1</sup> *0,0,2/3) (6 <sub>z</sub> <sup>-1</sup> *0,0,5/6) (2 <sub>y</sub> *0,0,2/3)' (2 <sub>3</sub> *0,0,5/6)'
<b>179.1.1391</b>	<b>P6<sub>5</sub>22</b>			<b>(1*0,0,0) (2<sub>z</sub>*0,0,1/2) (2<sub>x</sub>*0,0,0) (2<sub>1</sub>*0,0,5/6)</b>	<b>(3<sub>z</sub>*0,0,2/3) (6<sub>z</sub>*0,0,5/6) (2<sub>xy</sub>*0,0,2/3) (2<sub>2</sub>*0,0,1/2)</b>	<b>(3<sub>z</sub><sup>-1</sup>*0,0,1/3) (6<sub>z</sub><sup>-1</sup>*0,0,1/6) (2<sub>y</sub>*0,0,1/3) (2<sub>3</sub>*0,0,1/6)</b>
179.2.1392	P6 <sub>5</sub> 221'					
179.3.1393	P6 <sub>5</sub> '2'2	P3 <sub>2</sub> 12	(0,0,-1/12;a,b,c)	(1*0,0,0) (2 <sub>z</sub> *0,0,1/2)' (2 <sub>x</sub> *0,0,0)' (2 <sub>1</sub> *0,0,5/6)	(3 <sub>z</sub> *0,0,2/3) (6 <sub>z</sub> *0,0,5/6)' (2 <sub>xy</sub> *0,0,2/3)' (2 <sub>2</sub> *0,0,1/2)	(3 <sub>z</sub> <sup>-1</sup> *0,0,1/3) (6 <sub>z</sub> <sup>-1</sup> *0,0,1/6)' (2 <sub>y</sub> *0,0,1/3)' (2 <sub>3</sub> *0,0,1/6)
179.4.1394	P6 <sub>5</sub> '22'	P3 <sub>2</sub> 21	(0,0,-1/6;a,b,c)	(1*0,0,0) (2 <sub>z</sub> *0,0,1/2)' (2 <sub>x</sub> *0,0,0) (2 <sub>1</sub> *0,0,5/6)'	(3 <sub>z</sub> *0,0,2/3) (6 <sub>z</sub> *0,0,5/6)' (2 <sub>xy</sub> *0,0,2/3) (2 <sub>2</sub> *0,0,1/2)'	(3 <sub>z</sub> <sup>-1</sup> *0,0,1/3) (6 <sub>z</sub> <sup>-1</sup> *0,0,1/6)' (2 <sub>y</sub> *0,0,1/3) (2 <sub>3</sub> *0,0,1/6)'
179.5.1395	P6 <sub>5</sub> 2'2'	P6 <sub>5</sub>	(0,0,0;a,b,c)	(1*0,0,0) (2 <sub>z</sub> *0,0,1/2) (2 <sub>x</sub> *0,0,0)' (2 <sub>1</sub> *0,0,5/6)'	(3 <sub>z</sub> *0,0,2/3) (6 <sub>z</sub> *0,0,5/6) (2 <sub>xy</sub> *0,0,2/3)' (2 <sub>2</sub> *0,0,1/2)'	(3 <sub>z</sub> <sup>-1</sup> *0,0,1/3) (6 <sub>z</sub> <sup>-1</sup> *0,0,1/6) (2 <sub>y</sub> *0,0,1/3)' (2 <sub>3</sub> *0,0,1/6)'

180.1.1396	$P6_2 22$			$(1^*0,0,0)$ $(2_z^*0,0,0)$ $(2_x^*0,0,0)$ $(2_1^*0,0,1/3)$	$(3_z^*0,0,2/3)$ $(6_z^*0,0,1/3)$ $(2_{xy}^*0,0,2/3)$ $(2_2^*0,0,0)$	$(3_z^{-1*}0,0,1/3)$ $(6_z^{-1*}0,0,2/3)$ $(2_y^*0,0,1/3)$ $(2_3^*0,0,2/3)$
180.2.1397	$P6_2 221'$					
180.3.1398	$P6_2'2'2$	$P3_2 12$	$(0,0,1/6;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,0)'$ $(2_x^*0,0,0)'$ $(2_1^*0,0,1/3)$	$(3_z^*0,0,2/3)$ $(6_z^*0,0,1/3)'$ $(2_{xy}^*0,0,2/3)'$ $(2_2^*0,0,0)$	$(3_z^{-1*}0,0,1/3)$ $(6_z^{-1*}0,0,2/3)'$ $(2_y^*0,0,1/3)'$ $(2_3^*0,0,2/3)$
180.4.1399	$P6_2'2'2'$	$P3_2 21$	$(0,0,-1/6;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,0)'$ $(2_x^*0,0,0)$ $(2_1^*0,0,1/3)'$	$(3_z^*0,0,2/3)$ $(6_z^*0,0,1/3)'$ $(2_{xy}^*0,0,2/3)$ $(2_2^*0,0,0)'$	$(3_z^{-1*}0,0,1/3)$ $(6_z^{-1*}0,0,2/3)'$ $(2_y^*0,0,1/3)$ $(2_3^*0,0,2/3)'$
180.5.1400	$P6_2 2'2'$	$P6_2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,0)$ $(2_x^*0,0,0)'$ $(2_1^*0,0,1/3)'$	$(3_z^*0,0,2/3)$ $(6_z^*0,0,1/3)$ $(2_{xy}^*0,0,2/3)'$ $(2_2^*0,0,0)'$	$(3_z^{-1*}0,0,1/3)$ $(6_z^{-1*}0,0,2/3)$ $(2_y^*0,0,1/3)'$ $(2_3^*0,0,2/3)'$
180.6.1401	$P_{2c} 6_2 22$	$P6_1 22$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(2_z^*0,0,1)$ $(2_x^*0,0,0)$ $(2_1^*0,0,1/3)$	$(3_z^*0,0,2/3)$ $(6_z^*0,0,1/3)$ $(2_{xy}^*0,0,2/3)$ $(2_2^*0,0,1)$	$(3_z^{-1*}0,0,4/3)$ $(6_z^{-1*}0,0,5/3)$ $(2_y^*0,0,4/3)$ $(2_3^*0,0,5/3)$
180.7.1402	$P_{2c} 6_2'2'2'$	$P6_4 22$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(2_z^*0,0,0)$ $(2_x^*0,0,0)$ $(2_1^*0,0,4/3)$	$(3_z^*0,0,2/3)$ $(6_z^*0,0,4/3)$ $(2_{xy}^*0,0,2/3)$ $(2_2^*0,0,0)$	$(3_z^{-1*}0,0,4/3)$ $(6_z^{-1*}0,0,2/3)$ $(2_y^*0,0,4/3)$ $(2_3^*0,0,2/3)$

181.1.1403	$P6_4 22$			$(1^*0,0,0)$ $(2_z^*0,0,0)$ $(2_x^*0,0,0)$ $(2_1^*0,0,2/3)$	$(3_z^*0,0,1/3)$ $(6_z^*0,0,2/3)$ $(2_{xy}^*0,0,1/3)$ $(2_2^*0,0,0)$	$(3_z^{-1*}0,0,2/3)$ $(6_z^{-1*}0,0,1/3)$ $(2_y^*0,0,2/3)$ $(2_3^*0,0,1/3)$
181.2.1404	$P6_4 221'$					
181.3.1405	$P6_4'2'2$	$P3_1 12$	$(0,0,1/3;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,0)'$ $(2_x^*0,0,0)'$ $(2_1^*0,0,2/3)$	$(3_z^*0,0,1/3)$ $(6_z^*0,0,2/3)'$ $(2_{xy}^*0,0,1/3)'$ $(2_2^*0,0,0)$	$(3_z^{-1*}0,0,2/3)$ $(6_z^{-1*}0,0,1/3)'$ $(2_y^*0,0,2/3)'$ $(2_3^*0,0,1/3)$
181.4.1406	$P6_4'2'2'$	$P3_1 21$	$(0,0,1/6;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,0)'$ $(2_x^*0,0,0)$ $(2_1^*0,0,2/3)'$	$(3_z^*0,0,1/3)$ $(6_z^*0,0,2/3)'$ $(2_{xy}^*0,0,1/3)$ $(2_2^*0,0,0)'$	$(3_z^{-1*}0,0,2/3)$ $(6_z^{-1*}0,0,1/3)'$ $(2_y^*0,0,2/3)$ $(2_3^*0,0,1/3)'$
181.5.1407	$P6_4 2'2'$	$P6_4$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,0)$ $(2_x^*0,0,0)'$ $(2_1^*0,0,2/3)'$	$(3_z^*0,0,1/3)$ $(6_z^*0,0,2/3)$ $(2_{xy}^*0,0,1/3)'$ $(2_2^*0,0,0)'$	$(3_z^{-1*}0,0,2/3)$ $(6_z^{-1*}0,0,1/3)$ $(2_y^*0,0,2/3)'$ $(2_3^*0,0,1/3)'$
181.6.1408	$P_{2c} 6_4 22$	$P6_2 22$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,0)$ $(2_x^*0,0,0)$ $(2_1^*0,0,2/3)$	$(3_z^*0,0,4/3)$ $(6_z^*0,0,2/3)$ $(2_{xy}^*0,0,4/3)$ $(2_2^*0,0,0)$	$(3_z^{-1*}0,0,2/3)$ $(6_z^{-1*}0,0,4/3)$ $(2_y^*0,0,2/3)$ $(2_3^*0,0,4/3)$
181.7.1409	$P_{2c} 6_4'2'2$	$P6_5 22$	$(0,0,1/2;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,1)$ $(2_x^*0,0,1)$ $(2_1^*0,0,2/3)$	$(3_z^*0,0,4/3)$ $(6_z^*0,0,5/3)$ $(2_{xy}^*0,0,1/3)$ $(2_2^*0,0,0)$	$(3_z^{-1*}0,0,2/3)$ $(6_z^{-1*}0,0,1/3)$ $(2_y^*0,0,5/3)$ $(2_3^*0,0,4/3)$

<b>182.1.1410</b>	<b>p6<sub>3</sub>22</b>			$(1^*0,0,0)$ $(2_z^*0,0,1/2)$ $(2_x^*0,0,0)$ $(2_1^*0,0,1/2)$	$(3_z^*0,0,0)$ $(6_z^*0,0,1/2)$ $(2_{xy}^*0,0,0)$ $(2_2^*0,0,1/2)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)$ $(2_y^*0,0,0)$ $(2_3^*0,0,1/2)$
182.2.1411	p6 <sub>3</sub> 221'					
182.3.1412	p6 <sub>3</sub> '2'2	P312	(0,0,1/4;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,1/2)'$ $(2_x^*0,0,0)'$ $(2_1^*0,0,1/2)$	$(3_z^*0,0,0)$ $(6_z^*0,0,1/2)'$ $(2_{xy}^*0,0,0)'$ $(2_2^*0,0,1/2)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)'$ $(2_y^*0,0,0)'$ $(2_3^*0,0,1/2)$
182.4.1413	p6 <sub>3</sub> '2'2'	P321	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,1/2)'$ $(2_x^*0,0,0)$ $(2_1^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,1/2)'$ $(2_{xy}^*0,0,0)$ $(2_2^*0,0,1/2)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)'$ $(2_y^*0,0,0)$ $(2_3^*0,0,1/2)'$
182.5.1414	p6 <sub>3</sub> 2'2'	P6 <sub>3</sub>	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,1/2)$ $(2_x^*0,0,0)'$ $(2_1^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,1/2)$ $(2_{xy}^*0,0,0)'$ $(2_2^*0,0,1/2)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)$ $(2_y^*0,0,0)'$ $(2_3^*0,0,1/2)'$
<b>183.1.1415</b>	<b>p6mm</b>			$(1^*0,0,0)$ $(2_z^*0,0,0)$ $(m_x^*0,0,0)$ $(m_1^*0,0,0)$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)$ $(m_{xy}^*0,0,0)$ $(m_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)$ $(m_y^*0,0,0)$ $(m_3^*0,0,0)$
183.2.1416	P6mm1'					
183.3.1417	P6'm'm	P31m	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,0)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)'$

				$(m_x^*0,0,0)'$ $(m_1^*0,0,0)$	$(m_{xy}^*0,0,0)'$ $(m_2^*0,0,0)$	$(m_y^*0,0,0)'$ $(m_3^*0,0,0)$
183.4.1418	P6'mm'	P3m1	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,0)'$ $(m_x^*0,0,0)$ $(m_1^*0,0,0)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)'$ $(m_{xy}^*0,0,0)$ $(m_2^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)'$ $(m_y^*0,0,0)$ $(m_3^*0,0,0)'$
183.5.1419	P6m'm'	P6	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,0)$ $(m_x^*0,0,0)'$ $(m_1^*0,0,0)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)$ $(m_{xy}^*0,0,0)'$ $(m_2^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)$ $(m_y^*0,0,0)'$ $(m_3^*0,0,0)'$
183.6.1420	P <sub>2c</sub> 6mm	P6mm	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,0)$ $(m_x^*0,0,0)$ $(m_1^*0,0,0)$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)$ $(m_{xy}^*0,0,0)$ $(m_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)$ $(m_y^*0,0,0)$ $(m_3^*0,0,0)$
183.7.1421	P <sub>2c</sub> 6'm'm	P6 <sub>3</sub> cm	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(2_z^*0,0,1)$ $(m_x^*0,0,1)$ $(m_1^*0,0,0)$	$(3_z^*0,0,0)$ $(6_z^*0,0,1)$ $(m_{xy}^*0,0,1)$ $(m_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1)$ $(m_y^*0,0,1)$ $(m_3^*0,0,0)$
183.8.1422	P <sub>2c</sub> 6'mm'	P6 <sub>3</sub> mc	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(2_z^*0,0,1)$ $(m_x^*0,0,0)$ $(m_1^*0,0,1)$	$(3_z^*0,0,0)$ $(6_z^*0,0,1)$ $(m_{xy}^*0,0,0)$ $(m_2^*0,0,1)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1)$ $(m_y^*0,0,0)$ $(m_3^*0,0,1)$
183.9.1423	P <sub>2c</sub> 6m'm'	P6cc	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(2_z^*0,0,0)$ $(m_x^*0,0,1)$ $(m_1^*0,0,1)$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)$ $(m_{xy}^*0,0,1)$ $(m_2^*0,0,1)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)$ $(m_y^*0,0,1)$ $(m_3^*0,0,1)$

184.1.1424	P6cc			$(1^*0,0,0)$ $(2_z^*0,0,0)$ $(m_x^*0,0,1/2)$ $(m_1^*0,0,1/2)$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)$ $(m_2^*0,0,1/2)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)$ $(m_y^*0,0,1/2)$ $(m_3^*0,0,1/2)$
184.2.1425	P6cc1'					
184.3.1426	P6'c'c	P31c	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,0)'$ $(m_x^*0,0,1/2)'$ $(m_1^*0,0,1/2)$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)'$ $(m_{xy}^*0,0,1/2)'$ $(m_2^*0,0,1/2)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)'$ $(m_y^*0,0,1/2)'$ $(m_3^*0,0,1/2)$
184.4.1427	P6'cc'	P3c1	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,0)'$ $(m_x^*0,0,1/2)$ $(m_1^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)'$ $(m_{xy}^*0,0,1/2)$ $(m_2^*0,0,1/2)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)'$ $(m_y^*0,0,1/2)$ $(m_3^*0,0,1/2)'$
184.5.1428	P6c'c'	P6	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,0)$ $(m_x^*0,0,1/2)'$ $(m_1^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)'$ $(m_2^*0,0,1/2)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)$ $(m_y^*0,0,1/2)'$ $(m_3^*0,0,1/2)'$
185.1.1429	P6 <sub>3</sub> cm			$(1^*0,0,0)$ $(2_z^*0,0,1/2)$ $(m_x^*0,0,1/2)$ $(m_1^*0,0,0)$	$(3_z^*0,0,0)$ $(6_z^*0,0,1/2)$ $(m_{xy}^*0,0,1/2)$ $(m_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)$ $(m_y^*0,0,1/2)$ $(m_3^*0,0,0)$
185.2.1430	P6 <sub>3</sub> cm1'					
185.3.1431	P6 <sub>3</sub> 'c'm	P312	(0,0,0;a,b,c)	$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$



				$(2_z^*0,0,1/2)'$ $(m_x^*0,0,1/2)'$ $(m_1^*0,0,0)$	$(6_z^*0,0,1/2)'$ $(m_{xy}^*0,0,1/2)'$ $(m_2^*0,0,0)$	$(6_z^{-1*}0,0,1/2)'$ $(m_y^*0,0,1/2)'$ $(m_3^*0,0,0)$
185.4.1432	$P6_3'cm'$	$P3c1$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,1/2)'$ $(m_x^*0,0,1/2)$ $(m_1^*0,0,0)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,1/2)'$ $(m_{xy}^*0,0,1/2)$ $(m_2^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)'$ $(m_y^*0,0,1/2)$ $(m_3^*0,0,0)'$
185.5.1433	$P6_3c'm'$	$P6_3$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,1/2)$ $(m_x^*0,0,1/2)'$ $(m_1^*0,0,0)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,1/2)$ $(m_{xy}^*0,0,1/2)'$ $(m_2^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)$ $(m_y^*0,0,1/2)'$ $(m_3^*0,0,0)'$
<b>186.1.1434</b>	<b><math>P6_3mc</math></b>			<b><math>(1^*0,0,0)</math></b> <b><math>(2_z^*0,0,1/2)</math></b> <b><math>(m_x^*0,0,0)</math></b> <b><math>(m_1^*0,0,1/2)</math></b>	<b><math>(3_z^*0,0,0)</math></b> <b><math>(6_z^*0,0,1/2)</math></b> <b><math>(m_{xy}^*0,0,0)</math></b> <b><math>(m_2^*0,0,1/2)</math></b>	<b><math>(3_z^{-1*}0,0,0)</math></b> <b><math>(6_z^{-1*}0,0,1/2)</math></b> <b><math>(m_y^*0,0,0)</math></b> <b><math>(m_3^*0,0,1/2)</math></b>
186.2.1435	$P6_3mc1'$					
186.3.1436	$P6_3'm'c$	$P31c$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,1/2)'$ $(m_x^*0,0,0)'$ $(m_1^*0,0,1/2)$	$(3_z^*0,0,0)$ $(6_z^*0,0,1/2)'$ $(m_{xy}^*0,0,0)'$ $(m_2^*0,0,1/2)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)'$ $(m_y^*0,0,0)'$ $(m_3^*0,0,1/2)$
186.4.1437	$P6_3'mc'$	$P3m1$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,1/2)'$ $(m_x^*0,0,0)$ $(m_1^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,1/2)'$ $(m_{xy}^*0,0,0)$ $(m_2^*0,0,1/2)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)'$ $(m_y^*0,0,0)$ $(m_3^*0,0,1/2)'$
186.5.1438	$P6_3m'c'$	$P6_3$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$

$$\begin{array}{ccc} (2_z^*0,0,1/2) & (6_z^*0,0,1/2) & (6_z^{-1*}0,0,1/2) \\ (m_x^*0,0,0)' & (m_{xy}^*0,0,0)' & (m_y^*0,0,0)' \\ (m_1^*0,0,1/2)' & (m_2^*0,0,1/2)' & (m_3^*0,0,1/2)' \end{array}$$

187.1.1439  $P\bar{6}m2$

$$\begin{array}{ccc} (1^*0,0,0) & (3_z^*0,0,0) & (3_z^{-1*}0,0,0) \\ (m_z^*0,0,0) & (\bar{6}_z^*0,0,0) & (\bar{6}_z^{-1*}0,0,0) \\ (m_x^*0,0,0) & (m_{xy}^*0,0,0) & (m_y^*0,0,0) \\ (2_1^*0,0,0) & (2_2^*0,0,0) & (2_3^*0,0,0) \end{array}$$

187.2.1440  $P\bar{6}m21'$

187.3.1441  $P\bar{6}m'2$  P312 (0,0,0;a,b,c)

$$\begin{array}{ccc} (1^*0,0,0) & (3_z^*0,0,0) & (3_z^{-1*}0,0,0) \\ (m_z^*0,0,0)' & (\bar{6}_z^*0,0,0)' & (\bar{6}_z^{-1*}0,0,0)' \\ (m_x^*0,0,0)' & (m_{xy}^*0,0,0)' & (m_y^*0,0,0)' \\ (2_1^*0,0,0) & (2_2^*0,0,0) & (2_3^*0,0,0) \end{array}$$

187.4.1442  $P\bar{6}m'2$  P3m1 (0,0,0;a,b,c)

$$\begin{array}{ccc} (1^*0,0,0) & (3_z^*0,0,0) & (3_z^{-1*}0,0,0) \\ (m_z^*0,0,0)' & (\bar{6}_z^*0,0,0)' & (\bar{6}_z^{-1*}0,0,0)' \\ (m_x^*0,0,0) & (m_{xy}^*0,0,0) & (m_y^*0,0,0) \\ (2_1^*0,0,0)' & (2_2^*0,0,0)' & (2_3^*0,0,0)' \end{array}$$

187.5.1443  $P\bar{6}m'2$   $P\bar{6}$  (0,0,0;a,b,c)

$$\begin{array}{ccc} (1^*0,0,0) & (3_z^*0,0,0) & (3_z^{-1*}0,0,0) \\ (m_z^*0,0,0) & (\bar{6}_z^*0,0,0) & (\bar{6}_z^{-1*}0,0,0) \\ (m_x^*0,0,0)' & (m_{xy}^*0,0,0)' & (m_y^*0,0,0)' \\ (2_1^*0,0,0)' & (2_2^*0,0,0)' & (2_3^*0,0,0)' \end{array}$$

187.6.1444  $P_{2c}\bar{6}m2$   $P\bar{6}m2$  (0,0,0;a,b,2c)

$$\begin{array}{ccc} (1^*0,0,0) & (3_z^*0,0,0) & (3_z^{-1*}0,0,0) \\ (m_z^*0,0,0) & (\bar{6}_z^*0,0,0) & (\bar{6}_z^{-1*}0,0,0) \\ (m_x^*0,0,0) & (m_{xy}^*0,0,0) & (m_y^*0,0,0) \\ (2_1^*0,0,0) & (2_2^*0,0,0) & (2_3^*0,0,0) \end{array}$$

187.7.1445	$P_{2c}\bar{6}m'2$	$P\bar{6}c2$	(0,0,0;a,b,2c)	$(1^*0,0,0)$ $(m_z^*0,0,1)$ $(m_x^*0,0,1)$ $(2_1^*0,0,0)$	$(3_z^*0,0,0)$ $(\bar{6}_z^*0,0,1)$ $(m_{xy}^*0,0,1)$ $(2_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\bar{6}_z^{-1*}0,0,1)$ $(m_y^*0,0,1)$ $(2_3^*0,0,0)$
188.1.1446	$P\bar{6}c2$			$(1^*0,0,0)$ $(m_z^*0,0,1/2)$ $(m_x^*0,0,1/2)$ $(2_1^*0,0,0)$	$(3_z^*0,0,0)$ $(\bar{6}_z^*0,0,1/2)$ $(m_{xy}^*0,0,1/2)$ $(2_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\bar{6}_z^{-1*}0,0,1/2)$ $(m_y^*0,0,1/2)$ $(2_3^*0,0,0)$
188.2.1447	$P\bar{6}c21'$					
188.3.1448	$P\bar{6}'c'2$	P312	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(m_z^*0,0,1/2)'$ $(m_x^*0,0,1/2)'$ $(2_1^*0,0,0)$	$(3_z^*0,0,0)$ $(\bar{6}_z^*0,0,1/2)'$ $(m_{xy}^*0,0,1/2)'$ $(2_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\bar{6}_z^{-1*}0,0,1/2)'$ $(m_y^*0,0,1/2)'$ $(2_3^*0,0,0)$
188.4.1449	$P\bar{6}'c'2'$	P3c1	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(m_z^*0,0,1/2)'$ $(m_x^*0,0,1/2)$ $(2_1^*0,0,0)'$	$(3_z^*0,0,0)$ $(\bar{6}_z^*0,0,1/2)'$ $(m_{xy}^*0,0,1/2)$ $(2_2^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(\bar{6}_z^{-1*}0,0,1/2)'$ $(m_y^*0,0,1/2)$ $(2_3^*0,0,0)'$
188.5.1450	$P\bar{6}'c'2'$	$P\bar{6}$	(0,0,1/4;a,b,c)	$(1^*0,0,0)$ $(m_z^*0,0,1/2)$ $(m_x^*0,0,1/2)'$ $(2_1^*0,0,0)'$	$(3_z^*0,0,0)$ $(\bar{6}_z^*0,0,1/2)$ $(m_{xy}^*0,0,1/2)'$ $(2_2^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(\bar{6}_z^{-1*}0,0,1/2)$ $(m_y^*0,0,1/2)'$ $(2_3^*0,0,0)'$
189.1.1451	$P\bar{6}2m$			$(1^*0,0,0)$ $(m_z^*0,0,0)$ $(2_x^*0,0,0)$ $(m_1^*0,0,0)$	$(3_z^*0,0,0)$ $(\bar{6}_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\bar{6}_z^{-1*}0,0,0)$ $(2_y^*0,0,0)$ $(m_3^*0,0,0)$

189.2.1452	$P\bar{2}m1'$					
189.3.1453	$P\bar{2}'m$	P31m	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_z^*0,0,0)'$ $(2_x^*0,0,0)'$ $(m_1^*0,0,0)$	$(3_z^*0,0,0)$ $(\bar{2}_z^*0,0,0)'$ $(2_{xy}^*0,0,0)'$ $(m_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\bar{2}_z^{-1*}0,0,0)'$ $(2_y^*0,0,0)'$ $(m_3^*0,0,0)$
189.4.1454	$P\bar{2}'m'$	P321	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_z^*0,0,0)'$ $(2_x^*0,0,0)$ $(m_1^*0,0,0)'$	$(3_z^*0,0,0)$ $(\bar{2}_z^*0,0,0)'$ $(2_{xy}^*0,0,0)$ $(m_2^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(\bar{2}_z^{-1*}0,0,0)'$ $(2_y^*0,0,0)$ $(m_3^*0,0,0)'$
189.5.1455	$P\bar{2}'m'$	$P\bar{2}$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(m_z^*0,0,0)$ $(2_x^*0,0,0)'$ $(m_1^*0,0,0)'$	$(3_z^*0,0,0)$ $(\bar{2}_z^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(m_2^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(\bar{2}_z^{-1*}0,0,0)$ $(2_y^*0,0,0)'$ $(m_3^*0,0,0)'$
189.6.1456	$P_{2c}\bar{2}m$	$P\bar{2}m$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(m_z^*0,0,0)$ $(2_x^*0,0,0)$ $(m_1^*0,0,0)$	$(3_z^*0,0,0)$ $(\bar{2}_z^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(m_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\bar{2}_z^{-1*}0,0,0)$ $(2_y^*0,0,0)$ $(m_3^*0,0,0)$
189.7.1457	$P_{2c}\bar{2}'m'$	$P\bar{2}c$	$(0,0,0;a,b,2c)$	$(1^*0,0,0)$ $(m_z^*0,0,1)$ $(2_x^*0,0,0)$ $(m_1^*0,0,1)$	$(3_z^*0,0,0)$ $(\bar{2}_z^*0,0,1)$ $(2_{xy}^*0,0,0)$ $(m_2^*0,0,1)$	$(3_z^{-1*}0,0,0)$ $(\bar{2}_z^{-1*}0,0,1)$ $(2_y^*0,0,0)$ $(m_3^*0,0,1)$
190.1.1458	$P\bar{2}c$			$(1^*0,0,0)$ $(m_z^*0,0,1/2)$ $(2_x^*0,0,0)$	$(3_z^*0,0,0)$ $(\bar{2}_z^*0,0,1/2)$ $(2_{xy}^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(\bar{2}_z^{-1*}0,0,1/2)$ $(2_y^*0,0,0)$

$(m_1^*0,0,1/2)$        $(m_2^*0,0,1/2)$        $(m_3^*0,0,1/2)$

190.2.1459 P $\bar{6}$ 2c1'

190.3.1460	P $\bar{6}$ '2'c	P31c	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(m_z^*0,0,1/2)'$ $(2_x^*0,0,0)'$ $(m_1^*0,0,1/2)$	$(3_z^*0,0,0)$ $(\bar{6}_z^*0,0,1/2)'$ $(2_{xy}^*0,0,0)'$ $(m_2^*0,0,1/2)$	$(3_z^{-1*}0,0,0)$ $(\bar{6}_z^{-1*}0,0,1/2)'$ $(2_y^*0,0,0)'$ $(m_3^*0,0,1/2)$
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190.4.1461	P $\bar{6}$ '2'c'	P321	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(m_z^*0,0,1/2)'$ $(2_x^*0,0,0)$ $(m_1^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(\bar{6}_z^*0,0,1/2)'$ $(2_{xy}^*0,0,0)$ $(m_2^*0,0,1/2)'$	$(3_z^{-1*}0,0,0)$ $(\bar{6}_z^{-1*}0,0,1/2)'$ $(2_y^*0,0,0)$ $(m_3^*0,0,1/2)'$
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190.5.1462	P $\bar{6}$ '2'c'	P $\bar{6}$	(0,0,1/4;a,b,c)	$(1^*0,0,0)$ $(m_z^*0,0,1/2)$ $(2_x^*0,0,0)'$ $(m_1^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(\bar{6}_z^*0,0,1/2)$ $(2_{xy}^*0,0,0)'$ $(m_2^*0,0,1/2)'$	$(3_z^{-1*}0,0,0)$ $(\bar{6}_z^{-1*}0,0,1/2)$ $(2_y^*0,0,0)'$ $(m_3^*0,0,1/2)'$
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191.1.1463 P6/mmm

$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
$(2_z^*0,0,0)$	$(6_z^*0,0,0)$	$(6_z^{-1*}0,0,0)$
$(2_x^*0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_y^*0,0,0)$
$(2_1^*0,0,0)$	$(2_2^*0,0,0)$	$(2_3^*0,0,0)$
$(\bar{6}^*0,0,0)$	$(\bar{6}_z^*0,0,0)$	$(\bar{6}_z^{-1*}0,0,0)$
$(m_z^*0,0,0)$	$(\bar{6}_z^*0,0,0)$	$(\bar{6}_z^{-1*}0,0,0)$
$(m_x^*0,0,0)$	$(m_{xy}^*0,0,0)$	$(m_y^*0,0,0)$
$(m_1^*0,0,0)$	$(m_2^*0,0,0)$	$(m_3^*0,0,0)$

191.2.1464 P6/mmm1'

191.3.1465	P6/m'mm	P6mm	(0,0,0;a,b,c)	(1*0,0,0)	(3 <sub>z</sub> *0,0,0)	(3 <sub>z</sub> <sup>-1</sup> *0,0,0)
				(2 <sub>z</sub> *0,0,0)	(6 <sub>z</sub> *0,0,0)	(6 <sub>z</sub> <sup>-1</sup> *0,0,0)
				(2 <sub>x</sub> *0,0,0)'	(2 <sub>xy</sub> *0,0,0)'	(2 <sub>y</sub> *0,0,0)'
				(2 <sub>1</sub> *0,0,0)'	(2 <sub>2</sub> *0,0,0)'	(2 <sub>3</sub> *0,0,0)'
				( $\mathcal{E}$ *0,0,0)'	( $\mathcal{E}_z$ *0,0,0)'	( $\mathcal{E}_z$ <sup>-1</sup> *0,0,0)'
				(m <sub>z</sub> *0,0,0)'	( $\mathcal{E}_z$ *0,0,0)'	( $\mathcal{E}_z$ <sup>-1</sup> *0,0,0)'
				(m <sub>x</sub> *0,0,0)	(m <sub>xy</sub> *0,0,0)	(m <sub>y</sub> *0,0,0)
				(m <sub>1</sub> *0,0,0)	(m <sub>2</sub> *0,0,0)	(m <sub>3</sub> *0,0,0)

191.4.1466	P6'/mm'm	P $\mathcal{E}$ 2m	(0,0,0;a,b,c)	(1*0,0,0)	(3 <sub>z</sub> *0,0,0)	(3 <sub>z</sub> <sup>-1</sup> *0,0,0)
				(2 <sub>z</sub> *0,0,0)'	(6 <sub>z</sub> *0,0,0)'	(6 <sub>z</sub> <sup>-1</sup> *0,0,0)'
				(2 <sub>x</sub> *0,0,0)	(2 <sub>xy</sub> *0,0,0)	(2 <sub>y</sub> *0,0,0)
				(2 <sub>1</sub> *0,0,0)'	(2 <sub>2</sub> *0,0,0)'	(2 <sub>3</sub> *0,0,0)'
				( $\mathcal{E}$ *0,0,0)'	( $\mathcal{E}_z$ *0,0,0)'	( $\mathcal{E}_z$ <sup>-1</sup> *0,0,0)'
				(m <sub>z</sub> *0,0,0)	( $\mathcal{E}_z$ *0,0,0)	( $\mathcal{E}_z$ <sup>-1</sup> *0,0,0)
				(m <sub>x</sub> *0,0,0)'	(m <sub>xy</sub> *0,0,0)'	(m <sub>y</sub> *0,0,0)'
				(m <sub>1</sub> *0,0,0)	(m <sub>2</sub> *0,0,0)	(m <sub>3</sub> *0,0,0)

191.5.1467	P6'/mmm'	P $\mathcal{E}$ m2	(0,0,0;a,b,c)	(1*0,0,0)	(3 <sub>z</sub> *0,0,0)	(3 <sub>z</sub> <sup>-1</sup> *0,0,0)
				(2 <sub>z</sub> *0,0,0)'	(6 <sub>z</sub> *0,0,0)'	(6 <sub>z</sub> <sup>-1</sup> *0,0,0)'
				(2 <sub>x</sub> *0,0,0)'	(2 <sub>xy</sub> *0,0,0)'	(2 <sub>y</sub> *0,0,0)'
				(2 <sub>1</sub> *0,0,0)	(2 <sub>2</sub> *0,0,0)	(2 <sub>3</sub> *0,0,0)
				( $\mathcal{E}$ *0,0,0)'	( $\mathcal{E}_z$ *0,0,0)'	( $\mathcal{E}_z$ <sup>-1</sup> *0,0,0)'
				(m <sub>z</sub> *0,0,0)	( $\mathcal{E}_z$ *0,0,0)	( $\mathcal{E}_z$ <sup>-1</sup> *0,0,0)
				(m <sub>x</sub> *0,0,0)	(m <sub>xy</sub> *0,0,0)	(m <sub>y</sub> *0,0,0)
				(m <sub>1</sub> *0,0,0)'	(m <sub>2</sub> *0,0,0)'	(m <sub>3</sub> *0,0,0)'

191.6.1468	P6'/m'm'm	P $\mathcal{E}$ 1m	(0,0,0;a,b,c)	(1*0,0,0)	(3 <sub>z</sub> *0,0,0)	(3 <sub>z</sub> <sup>-1</sup> *0,0,0)
				(2 <sub>z</sub> *0,0,0)'	(6 <sub>z</sub> *0,0,0)'	(6 <sub>z</sub> <sup>-1</sup> *0,0,0)'

				$(2_x^*0,0,0)'$	$(2_{xy}^*0,0,0)'$	$(2_y^*0,0,0)'$
				$(2_1^*0,0,0)$	$(2_2^*0,0,0)$	$(2_3^*0,0,0)$
				$(\&^*0,0,0)$	$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
				$(m_z^*0,0,0)'$	$(\&_z^*0,0,0)'$	$(\&_z^{-1*}0,0,0)'$
				$(m_x^*0,0,0)'$	$(m_{xy}^*0,0,0)'$	$(m_y^*0,0,0)'$
				$(m_1^*0,0,0)$	$(m_2^*0,0,0)$	$(m_3^*0,0,0)$
191.7.1469	P6'/m'mm'	P&m1	(0,0,0;a,b,c)	$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
				$(2_z^*0,0,0)'$	$(6_z^*0,0,0)'$	$(6_z^{-1*}0,0,0)'$
				$(2_x^*0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_y^*0,0,0)$
				$(2_1^*0,0,0)'$	$(2_2^*0,0,0)'$	$(2_3^*0,0,0)'$
				$(\&^*0,0,0)$	$(\&^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
				$(m_z^*0,0,0)'$	$(\&_z^*0,0,0)'$	$(\&_z^{-1*}0,0,0)'$
				$(m_x^*0,0,0)$	$(m_{xy}^*0,0,0)$	$(m_y^*0,0,0)$
				$(m_1^*0,0,0)'$	$(m_2^*0,0,0)'$	$(m_3^*0,0,0)'$
191.8.1470	P6/mm'm'	P6/m	(0,0,0;a,b,c)	$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
				$(2_z^*0,0,0)$	$(6_z^*0,0,0)$	$(6_z^{-1*}0,0,0)$
				$(2_x^*0,0,0)'$	$(2_{xy}^*0,0,0)'$	$(2_y^*0,0,0)'$
				$(2_1^*0,0,0)'$	$(2_2^*0,0,0)'$	$(2_3^*0,0,0)'$
				$(\&^*0,0,0)$	$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
				$(m_z^*0,0,0)$	$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
				$(m_x^*0,0,0)'$	$(m_{xy}^*0,0,0)'$	$(m_y^*0,0,0)'$
				$(m_1^*0,0,0)'$	$(m_2^*0,0,0)'$	$(m_3^*0,0,0)'$
191.9.1471	P6/m'm'm'	P622	(0,0,0;a,b,c)	$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
				$(2_z^*0,0,0)$	$(6_z^*0,0,0)$	$(6_z^{-1*}0,0,0)$
				$(2_x^*0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_y^*0,0,0)$
				$(2_1^*0,0,0)$	$(2_2^*0,0,0)$	$(2_3^*0,0,0)$
				$(\&^*0,0,0)'$	$(\&_z^*0,0,0)'$	$(\&_z^{-1*}0,0,0)'$
				$(m_z^*0,0,0)'$	$(\&_z^*0,0,0)'$	$(\&_z^{-1*}0,0,0)'$
				$(m_x^*0,0,0)'$	$(m_{xy}^*0,0,0)'$	$(m_y^*0,0,0)'$
				$(m_1^*0,0,0)'$	$(m_2^*0,0,0)'$	$(m_3^*0,0,0)'$
191.10.1472	P <sub>2c</sub> 6/mmm	P6/mmm	(0,0,0;a,b,2c)	$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$

$(2_z^*0,0,0)$	$(6_z^*0,0,0)$	$(6_z^{-1*}0,0,0)$
$(2_x^*0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_y^*0,0,0)$
$(2_1^*0,0,0)$	$(2_2^*0,0,0)$	$(2_3^*0,0,0)$
$(\&^*0,0,0)$	$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
$(m_z^*0,0,0)$	$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
$(m_x^*0,0,0)$	$(m_{xy}^*0,0,0)$	$(m_y^*0,0,0)$
$(m_1^*0,0,0)$	$(m_2^*0,0,0)$	$(m_3^*0,0,0)$

191.11.1473  $P_{2c}6'/mm'm$   $P6_3/mcm$   $(0,0,1/2;a,b,2c)$

$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
$(2_z^*0,0,1)$	$(6_z^*0,0,1)$	$(6_z^{-1*}0,0,1)$
$(2_x^*0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_y^*0,0,0)$
$(2_1^*0,0,1)$	$(2_2^*0,0,1)$	$(2_3^*0,0,1)$
$(\&^*0,0,1)$	$(\&_z^*0,0,1)$	$(\&_z^{-1*}0,0,1)$
$(m_z^*0,0,0)$	$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
$(m_x^*0,0,1)$	$(m_{xy}^*0,0,1)$	$(m_y^*0,0,1)$
$(m_1^*0,0,0)$	$(m_2^*0,0,0)$	$(m_3^*0,0,0)$

191.12.1474  $P_{2c}6'/mmm'$   $P6_3/mmc$   $(0,0,1/2;a,b,2c)$

$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
$(2_z^*0,0,1)$	$(6_z^*0,0,1)$	$(6_z^{-1*}0,0,1)$
$(2_x^*0,0,1)$	$(2_{xy}^*0,0,1)$	$(2_y^*0,0,1)$
$(2_1^*0,0,0)$	$(2_2^*0,0,0)$	$(2_3^*0,0,0)$
$(\&^*0,0,1)$	$(\&_z^*0,0,1)$	$(\&_z^{-1*}0,0,1)$
$(m_z^*0,0,0)$	$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
$(m_x^*0,0,0)$	$(m_{xy}^*0,0,0)$	$(m_y^*0,0,0)$
$(m_1^*0,0,1)$	$(m_2^*0,0,1)$	$(m_3^*0,0,1)$

191.13.1475  $P_{2c}6'/mm'm'$   $P6/mcc$   $(0,0,0;a,b,2c)$

$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
$(2_z^*0,0,0)$	$(6_z^*0,0,0)$	$(6_z^{-1*}0,0,0)$
$(2_x^*0,0,1)$	$(2_{xy}^*0,0,1)$	$(2_y^*0,0,1)$
$(2_1^*0,0,1)$	$(2_2^*0,0,1)$	$(2_3^*0,0,1)$
$(\&^*0,0,0)$	$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
$(m_z^*0,0,0)$	$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
$(m_x^*0,0,1)$	$(m_{xy}^*0,0,1)$	$(m_y^*0,0,1)$
$(m_1^*0,0,1)$	$(m_2^*0,0,1)$	$(m_3^*0,0,1)$



192.1.1476	P6/mcc			$(1^*0,0,0)$ $(2_z^*0,0,0)$ $(2_x^*0,0,1/2)$ $(2_1^*0,0,1/2)$ $(\&^*0,0,0)$ $(m_z^*0,0,0)$ $(m_x^*0,0,1/2)$ $(m_1^*0,0,1/2)$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)$ $(2_2^*0,0,1/2)$ $(\&_z^*0,0,0)$ $(\&_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)$ $(m_2^*0,0,1/2)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)$ $(2_y^*0,0,1/2)$ $(2_3^*0,0,1/2)$ $(\&_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,0)$ $(m_y^*0,0,1/2)$ $(m_3^*0,0,1/2)$
192.2.1477	P6/mcc1'					
192.3.1478	P6/m'cc	P6cc	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,0)$ $(2_x^*0,0,1/2)'$ $(2_1^*0,0,1/2)'$ $(\&^*0,0,0)'$ $(m_z^*0,0,0)'$ $(m_x^*0,0,1/2)$ $(m_1^*0,0,1/2)$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)$ $(2_{xy}^*0,0,1/2)'$ $(2_2^*0,0,1/2)'$ $(\&_z^*0,0,0)'$ $(\&_z^*0,0,0)'$ $(m_{xy}^*0,0,1/2)$ $(m_2^*0,0,1/2)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)$ $(2_y^*0,0,1/2)'$ $(2_3^*0,0,1/2)'$ $(\&_z^{-1*}0,0,0)'$ $(\&_z^{-1*}0,0,0)'$ $(m_y^*0,0,1/2)$ $(m_3^*0,0,1/2)$
192.4.1479	P6'/mc'c	P&2c	(0,0,1/4;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,0)'$ $(2_x^*0,0,1/2)$ $(2_1^*0,0,1/2)'$ $(\&^*0,0,0)'$ $(m_z^*0,0,0)$ $(m_x^*0,0,1/2)'$ $(m_1^*0,0,1/2)$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)'$ $(2_{xy}^*0,0,1/2)$ $(2_2^*0,0,1/2)'$ $(\&_z^*0,0,0)'$ $(\&_z^*0,0,0)$ $(m_{xy}^*0,0,1/2)'$ $(m_2^*0,0,1/2)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)'$ $(2_y^*0,0,1/2)$ $(2_3^*0,0,1/2)'$ $(\&_z^{-1*}0,0,0)'$ $(\&_z^{-1*}0,0,0)$ $(m_y^*0,0,1/2)'$ $(m_3^*0,0,1/2)$
192.5.1480	P6'/mcc'	P&c2	(0,0,1/4;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,0)'$ $(2_x^*0,0,1/2)'$ $(2_1^*0,0,1/2)$ $(\&^*0,0,0)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,0)'$ $(2_{xy}^*0,0,1/2)'$ $(2_2^*0,0,1/2)$ $(\&_z^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,0)'$ $(2_y^*0,0,1/2)'$ $(2_3^*0,0,1/2)$ $(\&_z^{-1*}0,0,0)'$

				$(m_z^*0,0,0)$	$(\mathcal{E}_z^*0,0,0)$	$(\mathcal{E}_z^{-1*}0,0,0)$
				$(m_x^*0,0,1/2)$	$(m_{xy}^*0,0,1/2)$	$(m_y^*0,0,1/2)$
				$(m_1^*0,0,1/2)'$	$(m_2^*0,0,1/2)'$	$(m_3^*0,0,1/2)'$
192.6.1481	P6'/m'c'c	P&1c	(0,0,0;a,b,c)	$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
				$(2_z^*0,0,0)'$	$(6_z^*0,0,0)'$	$(6_z^{-1*}0,0,0)'$
				$(2_x^*0,0,1/2)'$	$(2_{xy}^*0,0,1/2)'$	$(2_y^*0,0,1/2)'$
				$(2_1^*0,0,1/2)$	$(2_2^*0,0,1/2)$	$(2_3^*0,0,1/2)$
				$(\mathcal{E}^*0,0,0)$	$(\mathcal{E}_z^*0,0,0)$	$(\mathcal{E}_z^{-1*}0,0,0)$
				$(m_z^*0,0,0)'$	$(\mathcal{E}_z^*0,0,0)'$	$(\mathcal{E}_z^{-1*}0,0,0)'$
				$(m_x^*0,0,1/2)'$	$(m_{xy}^*0,0,1/2)'$	$(m_y^*0,0,1/2)'$
				$(m_1^*0,0,1/2)$	$(m_2^*0,0,1/2)$	$(m_3^*0,0,1/2)$
192.7.1482	P6'/m'cc'	P&c1	(0,0,0;a,b,c)	$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
				$(2_z^*0,0,0)'$	$(6_z^*0,0,0)'$	$(6_z^{-1*}0,0,0)'$
				$(2_x^*0,0,1/2)$	$(2_{xy}^*0,0,1/2)$	$(2_y^*0,0,1/2)$
				$(2_1^*0,0,1/2)'$	$(2_2^*0,0,1/2)'$	$(2_3^*0,0,1/2)'$
				$(\mathcal{E}^*0,0,0)$	$(\mathcal{E}_z^*0,0,0)$	$(\mathcal{E}_z^{-1*}0,0,0)$
				$(m_z^*0,0,0)'$	$(\mathcal{E}_z^*0,0,0)'$	$(\mathcal{E}_z^{-1*}0,0,0)'$
				$(m_x^*0,0,1/2)$	$(m_{xy}^*0,0,1/2)$	$(m_y^*0,0,1/2)$
				$(m_1^*0,0,1/2)'$	$(m_2^*0,0,1/2)'$	$(m_3^*0,0,1/2)'$
192.8.1483	P6/mc'c'	P6/m	(0,0,0;a,b,c)	$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
				$(2_z^*0,0,0)$	$(6_z^*0,0,0)$	$(6_z^{-1*}0,0,0)$
				$(2_x^*0,0,1/2)'$	$(2_{xy}^*0,0,1/2)'$	$(2_y^*0,0,1/2)'$
				$(2_1^*0,0,1/2)'$	$(2_2^*0,0,1/2)'$	$(2_3^*0,0,1/2)'$
				$(\mathcal{E}^*0,0,0)$	$(\mathcal{E}_z^*0,0,0)$	$(\mathcal{E}_z^{-1*}0,0,0)$
				$(m_z^*0,0,0)$	$(\mathcal{E}_z^*0,0,0)$	$(\mathcal{E}_z^{-1*}0,0,0)$
				$(m_x^*0,0,1/2)'$	$(m_{xy}^*0,0,1/2)'$	$(m_y^*0,0,1/2)'$
				$(m_1^*0,0,1/2)'$	$(m_2^*0,0,1/2)'$	$(m_3^*0,0,1/2)'$
192.9.1484	P6/m'c'c'	P622	(0,0,1/4;a,b,c)	$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
				$(2_z^*0,0,0)$	$(6_z^*0,0,0)$	$(6_z^{-1*}0,0,0)$
				$(2_x^*0,0,1/2)$	$(2_{xy}^*0,0,1/2)$	$(2_y^*0,0,1/2)$
				$(2_1^*0,0,1/2)$	$(2_2^*0,0,1/2)$	$(2_3^*0,0,1/2)$

$(\&^*0,0,0)'$	$(\&_z^*0,0,0)'$	$(\&_z^{-1*}0,0,0)'$
$(m_z^*0,0,0)'$	$(\&_z^*0,0,0)'$	$(\&_z^{-1*}0,0,0)'$
$(m_x^*0,0,1/2)'$	$(m_{xy}^*0,0,1/2)'$	$(m_y^*0,0,1/2)'$
$(m_1^*0,0,1/2)'$	$(m_2^*0,0,1/2)'$	$(m_3^*0,0,1/2)'$

193.1.1485  $P6_3/mcm$

$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
$(2_z^*0,0,1/2)$	$(6_z^*0,0,1/2)$	$(6_z^{-1*}0,0,1/2)$
$(2_x^*0,0,1/2)$	$(2_{xy}^*0,0,1/2)$	$(2_y^*0,0,1/2)$
$(2_1^*0,0,0)$	$(2_2^*0,0,0)$	$(2_3^*0,0,0)$
$(\&^*0,0,0)$	$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
$(m_z^*0,0,1/2)$	$(\&_z^*0,0,1/2)$	$(\&_z^{-1*}0,0,1/2)$
$(m_x^*0,0,1/2)$	$(m_{xy}^*0,0,1/2)$	$(m_y^*0,0,1/2)$
$(m_1^*0,0,0)$	$(m_2^*0,0,0)$	$(m_3^*0,0,0)$

193.2.1486  $P6_3/mcm1'$

193.3.1487  $P6_3/m'cm$   $P6_3cm$   $(0,0,0;a,b,c)$

$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
$(2_z^*0,0,1/2)$	$(6_z^*0,0,1/2)$	$(6_z^{-1*}0,0,1/2)$
$(2_x^*0,0,1/2)'$	$(2_{xy}^*0,0,1/2)'$	$(2_y^*0,0,1/2)'$
$(2_1^*0,0,0)'$	$(2_2^*0,0,0)'$	$(2_3^*0,0,0)'$
$(\&^*0,0,0)'$	$(\&_z^*0,0,0)'$	$(\&_z^{-1*}0,0,0)'$
$(m_z^*0,0,1/2)'$	$(\&_z^*0,0,1/2)'$	$(\&_z^{-1*}0,0,1/2)'$
$(m_x^*0,0,1/2)$	$(m_{xy}^*0,0,1/2)$	$(m_y^*0,0,1/2)$
$(m_1^*0,0,0)$	$(m_2^*0,0,0)$	$(m_3^*0,0,0)$

193.4.1488  $P6_3'/mc'm$   $P\&2m$   $(0,0,1/4;a,b,c)$

$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
$(2_z^*0,0,1/2)'$	$(6_z^*0,0,1/2)'$	$(6_z^{-1*}0,0,1/2)'$
$(2_x^*0,0,1/2)$	$(2_{xy}^*0,0,1/2)$	$(2_y^*0,0,1/2)$
$(2_1^*0,0,0)'$	$(2_2^*0,0,0)'$	$(2_3^*0,0,0)'$
$(\&^*0,0,0)'$	$(\&_z^*0,0,0)'$	$(\&_z^{-1*}0,0,0)'$
$(m_z^*0,0,1/2)$	$(\&_z^*0,0,1/2)$	$(\&_z^{-1*}0,0,1/2)$
$(m_x^*0,0,1/2)'$	$(m_{xy}^*0,0,1/2)'$	$(m_y^*0,0,1/2)'$

				$(m_1^*0,0,0)$	$(m_2^*0,0,0)$	$(m_3^*0,0,0)$
193.5.1489	$P6_3/mcm'$	$P\bar{6}c2$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,1/2)'$ $(2_x^*0,0,1/2)'$ $(2_1^*0,0,0)$ $(\bar{6}_z^*0,0,0)'$ $(m_z^*0,0,1/2)$ $(m_x^*0,0,1/2)$ $(m_1^*0,0,0)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,1/2)'$ $(2_{xy}^*0,0,1/2)'$ $(2_2^*0,0,0)$ $(\bar{6}_z^*0,0,0)'$ $(\bar{6}_z^*0,0,1/2)$ $(m_{xy}^*0,0,1/2)$ $(m_2^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)'$ $(2_y^*0,0,1/2)'$ $(2_3^*0,0,0)$ $(\bar{6}_z^{-1*}0,0,0)'$ $(\bar{6}_z^{-1*}0,0,1/2)$ $(m_y^*0,0,1/2)$ $(m_3^*0,0,0)'$
193.6.1490	$P6_3/m'c'm$	$P\bar{6}1m$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,1/2)'$ $(2_x^*0,0,1/2)'$ $(2_1^*0,0,0)$ $(\bar{6}_z^*0,0,0)$ $(m_z^*0,0,1/2)'$ $(m_x^*0,0,1/2)'$ $(m_1^*0,0,0)$	$(3_z^*0,0,0)$ $(6_z^*0,0,1/2)'$ $(2_{xy}^*0,0,1/2)'$ $(2_2^*0,0,0)$ $(\bar{6}_z^*0,0,0)$ $(\bar{6}_z^*0,0,1/2)'$ $(m_{xy}^*0,0,1/2)'$ $(m_2^*0,0,0)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)'$ $(2_y^*0,0,1/2)'$ $(2_3^*0,0,0)$ $(\bar{6}_z^{-1*}0,0,0)$ $(\bar{6}_z^{-1*}0,0,1/2)'$ $(m_y^*0,0,1/2)'$ $(m_3^*0,0,0)$
193.7.1491	$P6_3/m'cm'$	$P\bar{6}c1$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,1/2)'$ $(2_x^*0,0,1/2)$ $(2_1^*0,0,0)'$ $(\bar{6}_z^*0,0,0)$ $(m_z^*0,0,1/2)'$ $(m_x^*0,0,1/2)$ $(m_1^*0,0,0)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,1/2)'$ $(2_{xy}^*0,0,1/2)$ $(2_2^*0,0,0)'$ $(\bar{6}_z^*0,0,0)$ $(\bar{6}_z^*0,0,1/2)'$ $(m_{xy}^*0,0,1/2)$ $(m_2^*0,0,0)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)'$ $(2_y^*0,0,1/2)$ $(2_3^*0,0,0)'$ $(\bar{6}_z^{-1*}0,0,0)$ $(\bar{6}_z^{-1*}0,0,1/2)'$ $(m_y^*0,0,1/2)$ $(m_3^*0,0,0)'$
193.8.1492	$P6_3/mc'm'$	$P6_3/m$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(2_z^*0,0,1/2)$ $(2_x^*0,0,1/2)'$ $(2_1^*0,0,0)'$ $(\bar{6}_z^*0,0,0)$ $(m_z^*0,0,1/2)$	$(3_z^*0,0,0)$ $(6_z^*0,0,1/2)$ $(2_{xy}^*0,0,1/2)'$ $(2_2^*0,0,0)'$ $(\bar{6}_z^*0,0,0)$ $(\bar{6}_z^*0,0,1/2)$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)$ $(2_y^*0,0,1/2)'$ $(2_3^*0,0,0)'$ $(\bar{6}_z^{-1*}0,0,0)$ $(\bar{6}_z^{-1*}0,0,1/2)$

$(m_x^*0,0,1/2)'$	$(m_{xy}^*0,0,1/2)'$	$(m_y^*0,0,1/2)'$
$(m_1^*0,0,0)'$	$(m_2^*0,0,0)'$	$(m_3^*0,0,0)'$

193.9.1493  $P6_3/m'c'm'$   $P6_322$  (0,0,1/4;a,b,c)

$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
$(2_z^*0,0,1/2)$	$(6_z^*0,0,1/2)$	$(6_z^{-1*}0,0,1/2)$
$(2_x^*0,0,1/2)$	$(2_{xy}^*0,0,1/2)$	$(2_y^*0,0,1/2)$
$(2_1^*0,0,0)$	$(2_2^*0,0,0)$	$(2_3^*0,0,0)$
$(\&^*0,0,0)'$	$(\&_z^*0,0,0)'$	$(\&_z^{-1*}0,0,0)'$
$(m_z^*0,0,1/2)'$	$(\&_z^*0,0,1/2)'$	$(\&_z^{-1*}0,0,1/2)'$
$(m_x^*0,0,1/2)'$	$(m_{xy}^*0,0,1/2)'$	$(m_y^*0,0,1/2)'$
$(m_1^*0,0,0)'$	$(m_2^*0,0,0)'$	$(m_3^*0,0,0)'$

194.1.1494  $P6_3/mmc$

$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
$(2_z^*0,0,1/2)$	$(6_z^*0,0,1/2)$	$(6_z^{-1*}0,0,1/2)$
$(2_x^*0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_y^*0,0,0)$
$(2_1^*0,0,1/2)$	$(2_2^*0,0,1/2)$	$(2_3^*0,0,1/2)$
$(\&^*0,0,0)$	$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
$(m_z^*0,0,1/2)$	$(\&_z^*0,0,1/2)$	$(\&_z^{-1*}0,0,1/2)$
$(m_x^*0,0,0)$	$(m_{xy}^*0,0,0)$	$(m_y^*0,0,0)$
$(m_1^*0,0,1/2)$	$(m_2^*0,0,1/2)$	$(m_3^*0,0,1/2)$

194.2.1495  $P6_3/mmc1'$

194.3.1496  $P6_3/m'mc$   $P6_3mc$  (0,0,0;a,b,c)

$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
$(2_z^*0,0,1/2)$	$(6_z^*0,0,1/2)$	$(6_z^{-1*}0,0,1/2)$
$(2_x^*0,0,0)'$	$(2_{xy}^*0,0,0)'$	$(2_y^*0,0,0)'$
$(2_1^*0,0,1/2)'$	$(2_2^*0,0,1/2)'$	$(2_3^*0,0,1/2)'$
$(\&^*0,0,0)'$	$(\&_z^*0,0,0)'$	$(\&_z^{-1*}0,0,0)'$
$(m_z^*0,0,1/2)'$	$(\&_z^*0,0,1/2)'$	$(\&_z^{-1*}0,0,1/2)'$
$(m_x^*0,0,0)$	$(m_{xy}^*0,0,0)$	$(m_y^*0,0,0)$
$(m_1^*0,0,1/2)$	$(m_2^*0,0,1/2)$	$(m_3^*0,0,1/2)$

194.4.1497  $P6_3'/mm'c$   $P\&2c$  (0,0,0;a,b,c)

$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
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$(2_z^*0,0,1/2)'$	$(6_z^*0,0,1/2)'$	$(6_z^{-1*}0,0,1/2)'$
$(2_x^*0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_y^*0,0,0)$
$(2_1^*0,0,1/2)'$	$(2_2^*0,0,1/2)'$	$(2_3^*0,0,1/2)'$
$(\&^*0,0,0)'$	$(\&_z^*0,0,0)'$	$(\&_z^{-1*}0,0,0)'$
$(m_z^*0,0,1/2)$	$(\&_z^*0,0,1/2)$	$(\&_z^{-1*}0,0,1/2)$
$(m_x^*0,0,0)'$	$(m_{xy}^*0,0,0)'$	$(m_y^*0,0,0)'$
$(m_1^*0,0,1/2)$	$(m_2^*0,0,1/2)$	$(m_3^*0,0,1/2)$

194.5.1498  $P6_3'/mmc'$   $P\&m2$   $(0,0,1/4;a,b,c)$

$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
$(2_z^*0,0,1/2)'$	$(6_z^*0,0,1/2)'$	$(6_z^{-1*}0,0,1/2)'$
$(2_x^*0,0,0)'$	$(2_{xy}^*0,0,0)'$	$(2_y^*0,0,0)'$
$(2_1^*0,0,1/2)$	$(2_2^*0,0,1/2)$	$(2_3^*0,0,1/2)$
$(\&^*0,0,0)'$	$(\&_z^*0,0,0)'$	$(\&_z^{-1*}0,0,0)'$
$(m_z^*0,0,1/2)$	$(\&_z^*0,0,1/2)$	$(\&_z^{-1*}0,0,1/2)$
$(m_x^*0,0,0)'$	$(m_{xy}^*0,0,0)'$	$(m_y^*0,0,0)'$
$(m_1^*0,0,1/2)'$	$(m_2^*0,0,1/2)'$	$(m_3^*0,0,1/2)'$

194.6.1499  $P6_3'/m'm'c$   $P\&1c$   $(0,0,0;a,b,c)$

$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
$(2_z^*0,0,1/2)'$	$(6_z^*0,0,1/2)'$	$(6_z^{-1*}0,0,1/2)'$
$(2_x^*0,0,0)'$	$(2_{xy}^*0,0,0)'$	$(2_y^*0,0,0)'$
$(2_1^*0,0,1/2)$	$(2_2^*0,0,1/2)$	$(2_3^*0,0,1/2)$
$(\&^*0,0,0)$	$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
$(m_z^*0,0,1/2)'$	$(\&_z^*0,0,1/2)'$	$(\&_z^{-1*}0,0,1/2)'$
$(m_x^*0,0,0)'$	$(m_{xy}^*0,0,0)'$	$(m_y^*0,0,0)'$
$(m_1^*0,0,1/2)$	$(m_2^*0,0,1/2)$	$(m_3^*0,0,1/2)$

194.7.1500  $P6_3'/m'm'c'$   $P\&m1$   $(0,0,0;a,b,c)$

$(1^*0,0,0)$	$(3_z^*0,0,0)$	$(3_z^{-1*}0,0,0)$
$(2_z^*0,0,1/2)'$	$(6_z^*0,0,1/2)'$	$(6_z^{-1*}0,0,1/2)'$
$(2_x^*0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_y^*0,0,0)$
$(2_1^*0,0,1/2)'$	$(2_2^*0,0,1/2)'$	$(2_3^*0,0,1/2)'$
$(\&^*0,0,0)$	$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$
$(m_z^*0,0,1/2)'$	$(\&_z^*0,0,1/2)'$	$(\&_z^{-1*}0,0,1/2)'$
$(m_x^*0,0,0)$	$(m_{xy}^*0,0,0)$	$(m_y^*0,0,0)$
$(m_1^*0,0,1/2)'$	$(m_2^*0,0,1/2)'$	$(m_3^*0,0,1/2)'$

194.8.1501	$P6_3/mm'c'$	$P6_3/m$	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,1/2)$ $(2_x^*0,0,0)'$ $(2_1^*0,0,1/2)'$ $(\&^*0,0,0)$ $(m_z^*0,0,1/2)$ $(m_x^*0,0,0)'$ $(m_1^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,1/2)$ $(2_{xy}^*0,0,0)'$ $(2_2^*0,0,1/2)'$ $(\&_z^*0,0,0)$ $(\&_z^*0,0,1/2)$ $(m_{xy}^*0,0,0)'$ $(m_2^*0,0,1/2)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)$ $(2_y^*0,0,0)'$ $(2_3^*0,0,1/2)'$ $(\&_z^{-1*}0,0,0)$ $(\&_z^{-1*}0,0,1/2)$ $(m_y^*0,0,0)'$ $(m_3^*0,0,1/2)'$
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194.9.1502	$P6_3/m'm'c'$	$P6_3/22$	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(2_z^*0,0,1/2)$ $(2_x^*0,0,0)$ $(2_1^*0,0,1/2)$ $(\&^*0,0,0)'$ $(m_z^*0,0,1/2)'$ $(m_x^*0,0,0)'$ $(m_1^*0,0,1/2)'$	$(3_z^*0,0,0)$ $(6_z^*0,0,1/2)$ $(2_{xy}^*0,0,0)$ $(2_2^*0,0,1/2)$ $(\&_z^*0,0,0)'$ $(\&_z^*0,0,1/2)'$ $(m_{xy}^*0,0,0)'$ $(m_2^*0,0,1/2)'$	$(3_z^{-1*}0,0,0)$ $(6_z^{-1*}0,0,1/2)$ $(2_y^*0,0,0)$ $(2_3^*0,0,1/2)$ $(\&_z^{-1*}0,0,0)'$ $(\&_z^{-1*}0,0,1/2)'$ $(m_y^*0,0,0)'$ $(m_3^*0,0,1/2)'$
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**CUBIC SYSTEM**

195.1.1503	$P23$			$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\&z}^*0,0,0)$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\&z}^{-1*}0,0,0)$	$(2_y^*0,0,0)$ $(3_{\&yz}^*0,0,0)$ $(3_{xy\&}^*0,0,0)$	$(2_z^*0,0,0)$ $(3_{\&yz}^{-1*}0,0,0)$ $(3_{xy\&}^{-1*}0,0,0)$
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195.2.1504  $P231'$

195.3.1505	$P_F23$	$F23$	(0,0,0;2a,2b,2c)	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\&z}^*0,0,0)$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\&z}^{-1*}0,0,0)$	$(2_y^*0,0,0)$ $(3_{\&yz}^*0,0,0)$ $(3_{xy\&}^*0,0,0)$	$(2_z^*0,0,0)$ $(3_{\&yz}^{-1*}0,0,0)$ $(3_{xy\&}^{-1*}0,0,0)$
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196.1.1506	F23				$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\&z}^*0,0,0)$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\&z}^{-1*}0,0,0)$	$(2_y^*0,0,0)$ $(3_{\&yz}^*0,0,0)$ $(3_{xy\&}^*0,0,0)$	$(2_z^*0,0,0)$ $(3_{\&yz}^{-1*}0,0,0)$ $(3_{xy\&}^{-1*}0,0,0)$
196.2.1507	F231'							
197.1.1508	I23				$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\&z}^*0,0,0)$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\&z}^{-1*}0,0,0)$	$(2_y^*0,0,0)$ $(3_{\&yz}^*0,0,0)$ $(3_{xy\&}^*0,0,0)$	$(2_z^*0,0,0)$ $(3_{\&yz}^{-1*}0,0,0)$ $(3_{xy\&}^{-1*}0,0,0)$
197.2.1509	I231'							
197.3.1510	I <sub>p</sub> 23	P23	(0,0,0;a,b,c)		$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\&z}^*0,0,0)$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\&z}^{-1*}0,0,0)$	$(2_y^*0,0,0)$ $(3_{\&yz}^*0,0,0)$ $(3_{xy\&}^*0,0,0)$	$(2_z^*0,0,0)$ $(3_{\&yz}^{-1*}0,0,0)$ $(3_{xy\&}^{-1*}0,0,0)$
198.1.1511	P2 <sub>1</sub> 3				$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\&z}^*1/2,0,1/2)$	$(2_x^*1/2,1/2,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\&z}^{-1*}1/2,1/2,0)$	$(2_y^*0,1/2,1/2)$ $(3_{\&yz}^*0,1/2,1/2)$ $(3_{xy\&}^*1/2,1/2,0)$	$(2_z^*1/2,0,1/2)$ $(3_{\&yz}^{-1*}1/2,0,1/2)$ $(3_{xy\&}^{-1*}0,1/2,1/2)$
198.2.1512	P2 <sub>1</sub> 31'							
199.1.1513	I2 <sub>1</sub> 3				$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\&z}^*1/2,0,1/2)$	$(2_x^*1/2,1/2,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\&z}^{-1*}1/2,1/2,0)$	$(2_y^*0,1/2,1/2)$ $(3_{\&yz}^*0,1/2,1/2)$ $(3_{xy\&}^*1/2,1/2,0)$	$(2_z^*1/2,0,1/2)$ $(3_{\&yz}^{-1*}1/2,0,1/2)$ $(3_{xy\&}^{-1*}0,1/2,1/2)$
199.2.1514	I2 <sub>1</sub> 31'							



199.3.1515	$I_{p2,3}$	$P2_13$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\&z}^*1/2,0,1/2)$	$(2_x^*1/2,1/2,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\&z}^{-1*}1/2,1/2,0)$	$(2_y^*0,1/2,1/2)$ $(3_{\&yz}^*0,1/2,1/2)$ $(3_{xy\&}^*1/2,1/2,0)$	$(2_z^*1/2,0,1/2)$ $(3_{\&yz}^{-1*}1/2,0,1/2)$ $(3_{xy\&}^{-1*}0,1/2,1/2)$
200.1.1516	$Pm\&$			$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\&z}^*0,0,0)$ $(\&^*0,0,0)$ $(\&_{xyz}^*0,0,0)$ $(\&_{x\&z}^*0,0,0)$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\&z}^{-1*}0,0,0)$ $(m_x^*0,0,0)$ $(\&_{xyz}^{-1*}0,0,0)$ $(\&_{x\&z}^{-1*}0,0,0)$	$(2_y^*0,0,0)$ $(3_{\&yz}^*0,0,0)$ $(3_{xy\&}^*0,0,0)$ $(m_y^*0,0,0)$ $(\&_{\&yz}^*0,0,0)$ $(\&_{xy\&}^*0,0,0)$	$(2_z^*0,0,0)$ $(3_{\&yz}^{-1*}0,0,0)$ $(3_{xy\&}^{-1*}0,0,0)$ $(m_z^*0,0,0)$ $(\&_{\&yz}^{-1*}0,0,0)$ $(\&_{xy\&}^{-1*}0,0,0)$
200.2.1517	$Pm\&1'$						
200.3.1518	$Pm'\&'$	$P23$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\&z}^*0,0,0)$ $(\&^*0,0,0)'$ $(\&_{xyz}^*0,0,0)'$ $(\&_{x\&z}^*0,0,0)'$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\&z}^{-1*}0,0,0)$ $(m_x^*0,0,0)'$ $(\&_{xyz}^{-1*}0,0,0)'$ $(\&_{x\&z}^{-1*}0,0,0)'$	$(2_y^*0,0,0)$ $(3_{\&yz}^*0,0,0)$ $(3_{xy\&}^*0,0,0)$ $(m_y^*0,0,0)'$ $(\&_{\&yz}^*0,0,0)'$ $(\&_{xy\&}^*0,0,0)'$	$(2_z^*0,0,0)$ $(3_{\&yz}^{-1*}0,0,0)$ $(3_{xy\&}^{-1*}0,0,0)$ $(m_z^*0,0,0)'$ $(\&_{\&yz}^{-1*}0,0,0)'$ $(\&_{xy\&}^{-1*}0,0,0)'$
200.4.1519	$P_F m\&$	$Fm\&$	$(0,0,0;2a,2b,2c)$	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\&z}^*0,0,0)$ $(\&^*0,0,0)$ $(\&_{xyz}^*0,0,0)$ $(\&_{x\&z}^*0,0,0)$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\&z}^{-1*}0,0,0)$ $(m_x^*0,0,0)$ $(\&_{xyz}^{-1*}0,0,0)$ $(\&_{x\&z}^{-1*}0,0,0)$	$(2_y^*0,0,0)$ $(3_{\&yz}^*0,0,0)$ $(3_{xy\&}^*0,0,0)$ $(m_y^*0,0,0)$ $(\&_{\&yz}^*0,0,0)$ $(\&_{xy\&}^*0,0,0)$	$(2_z^*0,0,0)$ $(3_{\&yz}^{-1*}0,0,0)$ $(3_{xy\&}^{-1*}0,0,0)$ $(m_z^*0,0,0)$ $(\&_{\&yz}^{-1*}0,0,0)$ $(\&_{xy\&}^{-1*}0,0,0)$

201.1.1520 Pn&

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{&yz}^*0,0,0)$	$(3_{&yz}^{-1*}0,0,0)$
$(3_{x&z}^*0,0,0)$	$(3_{x&z}^{-1*}0,0,0)$	$(3_{xy&}^*0,0,0)$	$(3_{xy&}^{-1*}0,0,0)$
$(\&_x^*1/2,1/2,1/2)$	$(m_x^*1/2,1/2,1/2)$	$(m_y^*1/2,1/2,1/2)$	$(m_z^*1/2,1/2,1/2)$
$(\&_{xyz}^*1/2,1/2,1/2)$	$(\&_{xyz}^{-1*}1/2,1/2,1/2)$	$(\&_{&yz}^*1/2,1/2,1/2)$	$(\&_{&yz}^{-1*}1/2,1/2,1/2)$
$(\&_{x&z}^*1/2,1/2,1/2)$	$(\&_{x&z}^{-1*}1/2,1/2,1/2)$	$(\&_{xy&}^*1/2,1/2,1/2)$	$(\&_{xy&}^{-1*}1/2,1/2,1/2)$

201.2.1521 Pn&1'

201.3.1522 Pn'&'

P23

(0,0,0;a,b,c)

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{&yz}^*0,0,0)$	$(3_{&yz}^{-1*}0,0,0)$
$(3_{x&z}^*0,0,0)$	$(3_{x&z}^{-1*}0,0,0)$	$(3_{xy&}^*0,0,0)$	$(3_{xy&}^{-1*}0,0,0)$
$(\&_x^*1/2,1/2,1/2)'$	$(m_x^*1/2,1/2,1/2)'$	$(m_y^*1/2,1/2,1/2)$	$(m_z^*1/2,1/2,1/2)$
$(\&_{xyz}^*1/2,1/2,1/2)'$	$(\&_{xyz}^{-1*}1/2,1/2,1/2)'$	$(\&_{&yz}^*1/2,1/2,1/2)'$	$(\&_{&yz}^{-1*}1/2,1/2,1/2)'$
$(\&_{x&z}^*1/2,1/2,1/2)'$	$(\&_{x&z}^{-1*}1/2,1/2,1/2)'$	$(\&_{xy&}^*1/2,1/2,1/2)'$	$(\&_{xy&}^{-1*}1/2,1/2,1/2)'$

201.4.1523 P<sub>F</sub>n&

Fd&

(0,0,0;2a,2b,2c)

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{&yz}^*0,0,0)$	$(3_{&yz}^{-1*}0,0,0)$
$(3_{x&z}^*0,0,0)$	$(3_{x&z}^{-1*}0,0,0)$	$(3_{xy&}^*0,0,0)$	$(3_{xy&}^{-1*}0,0,0)$
$(\&_x^*1/2,1/2,1/2)$	$(m_x^*1/2,1/2,1/2)$	$(m_y^*1/2,1/2,1/2)$	$(m_z^*1/2,1/2,1/2)$
$(\&_{xyz}^*1/2,1/2,1/2)$	$(\&_{xyz}^{-1*}1/2,1/2,1/2)$	$(\&_{&yz}^*1/2,1/2,1/2)$	$(\&_{&yz}^{-1*}1/2,1/2,1/2)$
$(\&_{x&z}^*1/2,1/2,1/2)$	$(\&_{x&z}^{-1*}1/2,1/2,1/2)$	$(\&_{xy&}^*1/2,1/2,1/2)$	$(\&_{xy&}^{-1*}1/2,1/2,1/2)$

202.1.1524 Fm&

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{&yz}^*0,0,0)$	$(3_{&yz}^{-1*}0,0,0)$
$(3_{x&z}^*0,0,0)$	$(3_{x&z}^{-1*}0,0,0)$	$(3_{xy&}^*0,0,0)$	$(3_{xy&}^{-1*}0,0,0)$
$(\&_x^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*0,0,0)$	$(m_z^*0,0,0)$
$(\&_{xyz}^*0,0,0)$	$(\&_{xyz}^{-1*}0,0,0)$	$(\&_{&yz}^*0,0,0)$	$(\&_{&yz}^{-1*}0,0,0)$

$(\&_{x\&z}^*0,0,0)$    
  $(\&_{x\&z}^{-1*}0,0,0)$    
  $(\&_{xy\&}^*0,0,0)$    
  $(\&_{xy\&}^{-1*}0,0,0)$

202.2.1525 Fm $\&1'$

202.3.1526 Fm' $\&'$     F23    (0,0,0;a,b,c)

$(1^*0,0,0)$      $(2_x^*0,0,0)$      $(2_y^*0,0,0)$      $(2_z^*0,0,0)$   
 $(3_{xyz}^*0,0,0)$      $(3_{xyz}^{-1*}0,0,0)$      $(3_{\&yz}^*0,0,0)$      $(3_{\&yz}^{-1*}0,0,0)$   
 $(3_{x\&z}^*0,0,0)$      $(3_{x\&z}^{-1*}0,0,0)$      $(3_{xy\&}^*0,0,0)$      $(3_{xy\&}^{-1*}0,0,0)$   
 $(\&^*0,0,0)'$      $(m_x^*0,0,0)'$      $(m_y^*0,0,0)'$      $(m_z^*0,0,0)'$   
 $(\&_{xyz}^*0,0,0)'$      $(\&_{xyz}^{-1*}0,0,0)'$      $(\&_{\&yz}^*0,0,0)'$      $(\&_{\&yz}^{-1*}0,0,0)'$   
 $(\&_{x\&z}^*0,0,0)'$      $(\&_{x\&z}^{-1*}0,0,0)'$      $(\&_{xy\&}^*0,0,0)'$      $(\&_{xy\&}^{-1*}0,0,0)'$

203.1.1527 Fd $\&$

$(1^*0,0,0)$      $(2_x^*0,0,0)$      $(2_y^*0,0,0)$      $(2_z^*0,0,0)$   
 $(3_{xyz}^*0,0,0)$      $(3_{xyz}^{-1*}0,0,0)$      $(3_{\&yz}^*0,0,0)$      $(3_{\&yz}^{-1*}0,0,0)$   
 $(3_{x\&z}^*0,0,0)$      $(3_{x\&z}^{-1*}0,0,0)$      $(3_{xy\&}^*0,0,0)$      $(3_{xy\&}^{-1*}0,0,0)$   
 $(\&^*1/4,1/4,1/4)$      $(m_x^*1/4,1/4,1/4)$      $(m_y^*1/4,1/4,1/4)$      $(m_z^*1/4,1/4,1/4)$   
 $(\&_{xyz}^*1/4,1/4,1/4)$      $(\&_{xyz}^{-1*}1/4,1/4,1/4)$      $(\&_{\&yz}^*1/4,1/4,1/4)$      $(\&_{\&yz}^{-1*}1/4,1/4,1/4)$   
 $(\&_{x\&z}^*1/4,1/4,1/4)$      $(\&_{x\&z}^{-1*}1/4,1/4,1/4)$      $(\&_{xy\&}^*1/4,1/4,1/4)$      $(\&_{xy\&}^{-1*}1/4,1/4,1/4)$

203.2.1528 Fd $\&1'$

203.3.1529 Fd' $\&'$     F23    (0,0,0;a,b,c)

$(1^*0,0,0)$      $(2_x^*0,0,0)$      $(2_y^*0,0,0)$      $(2_z^*0,0,0)$   
 $(3_{xyz}^*0,0,0)$      $(3_{xyz}^{-1*}0,0,0)$      $(3_{\&yz}^*0,0,0)$      $(3_{\&yz}^{-1*}0,0,0)$   
 $(3_{x\&z}^*0,0,0)$      $(3_{x\&z}^{-1*}0,0,0)$      $(3_{xy\&}^*0,0,0)$      $(3_{xy\&}^{-1*}0,0,0)$   
 $(\&^*1/4,1/4,1/4)'$      $(m_x^*1/4,1/4,1/4)'$      $(m_y^*1/4,1/4,1/4)'$      $(m_z^*1/4,1/4,1/4)'$   
 $(\&_{xyz}^*1/4,1/4,1/4)'$      $(\&_{xyz}^{-1*}1/4,1/4,1/4)'$      $(\&_{\&yz}^*1/4,1/4,1/4)'$      $(\&_{\&yz}^{-1*}1/4,1/4,1/4)'$   
 $(\&_{x\&z}^*1/4,1/4,1/4)'$      $(\&_{x\&z}^{-1*}1/4,1/4,1/4)'$      $(\&_{xy\&}^*1/4,1/4,1/4)'$      $(\&_{xy\&}^{-1*}1/4,1/4,1/4)'$

204.1.1530 Im $\&$

$(1^*0,0,0)$      $(2_x^*0,0,0)$      $(2_y^*0,0,0)$      $(2_z^*0,0,0)$   
 $(3_{xyz}^*0,0,0)$      $(3_{xyz}^{-1*}0,0,0)$      $(3_{\&yz}^*0,0,0)$      $(3_{\&yz}^{-1*}0,0,0)$   
 $(3_{x\&z}^*0,0,0)$      $(3_{x\&z}^{-1*}0,0,0)$      $(3_{xy\&}^*0,0,0)$      $(3_{xy\&}^{-1*}0,0,0)$

$$\begin{array}{cccc}
 (\&^*0,0,0) & (m_x^*0,0,0) & (m_y^*0,0,0) & (m_z^*0,0,0) \\
 (\&_{xyz}^*0,0,0) & (\&_{xyz}^{-1*}0,0,0) & (\&_{\&yz}^*0,0,0) & (\&_{\&yz}^{-1*}0,0,0) \\
 (\&_{x\&z}^*0,0,0) & (\&_{x\&z}^{-1*}0,0,0) & (\&_{xy\&}^*0,0,0) & (\&_{xy\&}^{-1*}0,0,0)
 \end{array}$$

204.2.1531 Im $\&$ '

204.3.1532	Im' $\&$ '	I23	(0,0,0;a,b,c)	$  \begin{array}{l}  (1^*0,0,0) \\  (3_{xyz}^*0,0,0) \\  (3_{x\&z}^*0,0,0) \\  (\&^*0,0,0)' \\  (\&_{xyz}^*0,0,0)' \\  (\&_{x\&z}^*0,0,0)'  \end{array}  $	$  \begin{array}{l}  (2_x^*0,0,0) \\  (3_{xyz}^{-1*}0,0,0) \\  (3_{x\&z}^{-1*}0,0,0) \\  (m_x^*0,0,0)' \\  (\&_{xyz}^{-1*}0,0,0)' \\  (\&_{x\&z}^{-1*}0,0,0)'  \end{array}  $	$  \begin{array}{l}  (2_y^*0,0,0) \\  (3_{\&yz}^*0,0,0) \\  (3_{xy\&}^*0,0,0) \\  (m_y^*0,0,0)' \\  (\&_{\&yz}^*0,0,0)' \\  (\&_{xy\&}^*0,0,0)'  \end{array}  $	$  \begin{array}{l}  (2_z^*0,0,0) \\  (3_{\&yz}^{-1*}0,0,0) \\  (3_{xy\&}^{-1*}0,0,0) \\  (m_z^*0,0,0)' \\  (\&_{\&yz}^{-1*}0,0,0)' \\  (\&_{xy\&}^{-1*}0,0,0)'  \end{array}  $
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204.4.1533	I <sub>p</sub> m $\&$	Pm $\&$	(0,0,0;a,b,c)	$  \begin{array}{l}  (1^*0,0,0) \\  (3_{xyz}^*0,0,0) \\  (3_{x\&z}^*0,0,0) \\  (\&^*0,0,0) \\  (\&_{xyz}^*0,0,0) \\  (\&_{x\&z}^*0,0,0)  \end{array}  $	$  \begin{array}{l}  (2_x^*0,0,0) \\  (3_{xyz}^{-1*}0,0,0) \\  (3_{x\&z}^{-1*}0,0,0) \\  (m_x^*0,0,0) \\  (\&_{xyz}^{-1*}0,0,0) \\  (\&_{x\&z}^{-1*}0,0,0)  \end{array}  $	$  \begin{array}{l}  (2_y^*0,0,0) \\  (3_{\&yz}^*0,0,0) \\  (3_{xy\&}^*0,0,0) \\  (m_y^*0,0,0) \\  (\&_{\&yz}^*0,0,0) \\  (\&_{xy\&}^*0,0,0)  \end{array}  $	$  \begin{array}{l}  (2_z^*0,0,0) \\  (3_{\&yz}^{-1*}0,0,0) \\  (3_{xy\&}^{-1*}0,0,0) \\  (m_z^*0,0,0) \\  (\&_{\&yz}^{-1*}0,0,0) \\  (\&_{xy\&}^{-1*}0,0,0)  \end{array}  $
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204.5.1534	I <sub>p</sub> m' $\&$ '	Pn $\&$	(0,0,0;a,b,c)	$  \begin{array}{l}  (1^*0,0,0) \\  (3_{xyz}^*0,0,0) \\  (3_{x\&z}^*0,0,0) \\  (\&^*1/2,1/2,1/2) \\  (\&_{xyz}^*1/2,1/2,1/2) \\  (\&_{x\&z}^*1/2,1/2,1/2)  \end{array}  $	$  \begin{array}{l}  (2_x^*0,0,0) \\  (3_{xyz}^{-1*}0,0,0) \\  (3_{x\&z}^{-1*}0,0,0) \\  (m_x^*1/2,1/2,1/2) \\  (\&_{xyz}^{-1*}1/2,1/2,1/2) \\  (\&_{x\&z}^{-1*}1/2,1/2,1/2)  \end{array}  $	$  \begin{array}{l}  (2_y^*0,0,0) \\  (3_{\&yz}^*0,0,0) \\  (3_{xy\&}^*0,0,0) \\  (m_y^*1/2,1/2,1/2) \\  (\&_{\&yz}^*1/2,1/2,1/2) \\  (\&_{xy\&}^*1/2,1/2,1/2)  \end{array}  $	$  \begin{array}{l}  (2_z^*0,0,0) \\  (3_{\&yz}^{-1*}0,0,0) \\  (3_{xy\&}^{-1*}0,0,0) \\  (m_z^*1/2,1/2,1/2) \\  (\&_{\&yz}^{-1*}1/2,1/2,1/2) \\  (\&_{xy\&}^{-1*}1/2,1/2,1/2)  \end{array}  $
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205.1.1535	Pa $\&$			$  \begin{array}{l}  (1^*0,0,0) \\  (3_{xyz}^*0,0,0) \\  (3_{x\&z}^*1/2,0,1/2) \\  (\&^*0,0,0) \\  (\&_{xyz}^*0,0,0) \\  (\&_{x\&z}^*1/2,0,1/2)  \end{array}  $	$  \begin{array}{l}  (2_x^*1/2,1/2,0) \\  (3_{xyz}^{-1*}0,0,0) \\  (3_{x\&z}^{-1*}1/2,1/2,0) \\  (m_x^*1/2,1/2,0) \\  (\&_{xyz}^{-1*}0,0,0) \\  (\&_{x\&z}^{-1*}1/2,1/2,0)  \end{array}  $	$  \begin{array}{l}  (2_y^*0,1/2,1/2) \\  (3_{\&yz}^*0,1/2,1/2) \\  (3_{xy\&}^*1/2,1/2,0) \\  (m_y^*0,1/2,1/2) \\  (\&_{\&yz}^*0,1/2,1/2) \\  (\&_{xy\&}^*1/2,1/2,0)  \end{array}  $	$  \begin{array}{l}  (2_z^*1/2,0,1/2) \\  (3_{\&yz}^{-1*}1/2,0,1/2) \\  (3_{xy\&}^{-1*}0,1/2,1/2) \\  (m_z^*1/2,0,1/2) \\  (\&_{\&yz}^{-1*}1/2,0,1/2) \\  (\&_{xy\&}^{-1*}0,1/2,1/2)  \end{array}  $
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205.2.1536 Pa $\bar{1}$ '

205.3.1537 Pa' $\bar{1}$ '

P2<sub>1</sub>3

(0,0,0;a,b,c)

$(1^*0,0,0)$	$(2_x^*1/2,1/2,0)$	$(2_y^*0,1/2,1/2)$	$(2_z^*1/2,0,1/2)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\bar{y}z}^*0,1/2,1/2)$	$(3_{\bar{y}z}^{-1*}1/2,0,1/2)$
$(3_{x\bar{z}}^*1/2,0,1/2)$	$(3_{x\bar{z}}^{-1*}1/2,1/2,0)$	$(3_{xy\bar{z}}^*1/2,1/2,0)$	$(3_{xy\bar{z}}^{-1*}0,1/2,1/2)$
$(\bar{1}^*0,0,0)'$	$(m_x^*1/2,1/2,0)'$	$(m_y^*0,1/2,1/2)'$	$(m_z^*1/2,0,1/2)'$
$(\bar{1}_{xyz}^*0,0,0)'$	$(\bar{1}_{xyz}^{-1*}0,0,0)'$	$(\bar{1}_{\bar{y}z}^*0,1/2,1/2)'$	$(\bar{1}_{\bar{y}z}^{-1*}1/2,0,1/2)'$
$(\bar{1}_{x\bar{z}}^*1/2,0,1/2)'$	$(\bar{1}_{x\bar{z}}^{-1*}1/2,1/2,0)'$	$(\bar{1}_{xy\bar{z}}^*1/2,1/2,0)'$	$(\bar{1}_{xy\bar{z}}^{-1*}0,1/2,1/2)'$

206.1.1538 Ia $\bar{1}$

$(1^*0,0,0)$	$(2_x^*1/2,1/2,0)$	$(2_y^*0,1/2,1/2)$	$(2_z^*1/2,0,1/2)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\bar{y}z}^*0,1/2,1/2)$	$(3_{\bar{y}z}^{-1*}1/2,0,1/2)$
$(3_{x\bar{z}}^*1/2,0,1/2)$	$(3_{x\bar{z}}^{-1*}1/2,1/2,0)$	$(3_{xy\bar{z}}^*1/2,1/2,0)$	$(3_{xy\bar{z}}^{-1*}0,1/2,1/2)$
$(\bar{1}^*0,0,0)$	$(m_x^*1/2,1/2,0)$	$(m_y^*0,1/2,1/2)$	$(m_z^*1/2,0,1/2)$
$(\bar{1}_{xyz}^*0,0,0)$	$(\bar{1}_{xyz}^{-1*}0,0,0)$	$(\bar{1}_{\bar{y}z}^*0,1/2,1/2)$	$(\bar{1}_{\bar{y}z}^{-1*}1/2,0,1/2)$
$(\bar{1}_{x\bar{z}}^*1/2,0,1/2)$	$(\bar{1}_{x\bar{z}}^{-1*}1/2,1/2,0)$	$(\bar{1}_{xy\bar{z}}^*1/2,1/2,0)$	$(\bar{1}_{xy\bar{z}}^{-1*}0,1/2,1/2)$

206.2.1539 Ia $\bar{1}$ '

206.3.1540 Ia' $\bar{1}$ '

I2<sub>1</sub>3

(0,0,0;a,b,c)

$(1^*0,0,0)$	$(2_x^*1/2,1/2,0)$	$(2_y^*0,1/2,1/2)$	$(2_z^*1/2,0,1/2)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\bar{y}z}^*0,1/2,1/2)$	$(3_{\bar{y}z}^{-1*}1/2,0,1/2)$
$(3_{x\bar{z}}^*1/2,0,1/2)$	$(3_{x\bar{z}}^{-1*}1/2,1/2,0)$	$(3_{xy\bar{z}}^*1/2,1/2,0)$	$(3_{xy\bar{z}}^{-1*}0,1/2,1/2)$
$(\bar{1}^*0,0,0)'$	$(m_x^*1/2,1/2,0)'$	$(m_y^*0,1/2,1/2)'$	$(m_z^*1/2,0,1/2)'$
$(\bar{1}_{xyz}^*0,0,0)'$	$(\bar{1}_{xyz}^{-1*}0,0,0)'$	$(\bar{1}_{\bar{y}z}^*0,1/2,1/2)'$	$(\bar{1}_{\bar{y}z}^{-1*}1/2,0,1/2)'$
$(\bar{1}_{x\bar{z}}^*1/2,0,1/2)'$	$(\bar{1}_{x\bar{z}}^{-1*}1/2,1/2,0)'$	$(\bar{1}_{xy\bar{z}}^*1/2,1/2,0)'$	$(\bar{1}_{xy\bar{z}}^{-1*}0,1/2,1/2)'$

206.4.1541 I<sub>p</sub>a $\bar{1}$

Pa $\bar{1}$

(0,0,0;a,b,c)

$(1^*0,0,0)$	$(2_x^*1/2,1/2,0)$	$(2_y^*0,1/2,1/2)$	$(2_z^*1/2,0,1/2)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\bar{y}z}^*0,1/2,1/2)$	$(3_{\bar{y}z}^{-1*}1/2,0,1/2)$
$(3_{x\bar{z}}^*1/2,0,1/2)$	$(3_{x\bar{z}}^{-1*}1/2,1/2,0)$	$(3_{xy\bar{z}}^*1/2,1/2,0)$	$(3_{xy\bar{z}}^{-1*}0,1/2,1/2)$

$$\begin{array}{cccc}
 (\mathbb{1}^*0,0,0) & (m_x^*1/2,1/2,0) & (m_y^*0,1/2,1/2) & (m_z^*1/2,0,1/2) \\
 (\mathbb{3}_{xyz}^*0,0,0) & (\mathbb{3}_{xyz}^{-1*}0,0,0) & (\mathbb{3}_{\&yz}^*0,1/2,1/2) & (\mathbb{3}_{\&yz}^{-1*}1/2,0,1/2) \\
 (\mathbb{3}_{x\&z}^*1/2,0,1/2) & (\mathbb{3}_{x\&z}^{-1*}1/2,1/2,0) & (\mathbb{3}_{xy\&}^*1/2,1/2,0) & (\mathbb{3}_{xy\&}^{-1*}0,1/2,1/2)
 \end{array}$$

207.1.1542 P432

$$\begin{array}{cccc}
 (1^*0,0,0) & (2_x^*0,0,0) & (2_y^*0,0,0) & (2_z^*0,0,0) \\
 (3_{xyz}^*0,0,0) & (3_{xyz}^{-1*}0,0,0) & (3_{\&yz}^*0,0,0) & (3_{\&yz}^{-1*}0,0,0) \\
 (3_{x\&z}^*0,0,0) & (3_{x\&z}^{-1*}0,0,0) & (3_{xy\&}^*0,0,0) & (3_{xy\&}^{-1*}0,0,0) \\
 (4_x^*0,0,0) & (4_x^{-1*}0,0,0) & (2_{xy}^*0,0,0) & (2_{\&y}^*0,0,0) \\
 (4_y^*0,0,0) & (4_y^{-1*}0,0,0) & (2_{xz}^*0,0,0) & (2_{\&z}^*0,0,0) \\
 (4_z^*0,0,0) & (4_z^{-1*}0,0,0) & (2_{yz}^*0,0,0) & (2_{\&z}^*0,0,0)
 \end{array}$$

207.2.1543 P4321'

207.3.1544 P4'32' P23

(0,0,0;a,b,c)

$$\begin{array}{cccc}
 (1^*0,0,0) & (2_x^*0,0,0) & (2_y^*0,0,0) & (2_z^*0,0,0) \\
 (3_{xyz}^*0,0,0) & (3_{xyz}^{-1*}0,0,0) & (3_{\&yz}^*0,0,0) & (3_{\&yz}^{-1*}0,0,0) \\
 (3_{x\&z}^*0,0,0) & (3_{x\&z}^{-1*}0,0,0) & (3_{xy\&}^*0,0,0) & (3_{xy\&}^{-1*}0,0,0) \\
 (4_x^*0,0,0)' & (4_x^{-1*}0,0,0) & (2_{xy}^*0,0,0)' & (2_{\&y}^*0,0,0)' \\
 (4_y^*0,0,0)' & (4_y^{-1*}0,0,0)' & (2_{xz}^*0,0,0)' & (2_{\&z}^*0,0,0)' \\
 (4_z^*0,0,0)' & (4_z^{-1*}0,0,0)' & (2_{yz}^*0,0,0)' & (2_{\&z}^*0,0,0)'
 \end{array}$$

207.4.1545 P<sub>F</sub>432

F432

(0,0,0;2a,2b,2c)

$$\begin{array}{cccc}
 (1^*0,0,0) & (2_x^*0,0,0) & (2_y^*0,0,0) & (2_z^*0,0,0) \\
 (3_{xyz}^*0,0,0) & (3_{xyz}^{-1*}0,0,0) & (3_{\&yz}^*0,0,0) & (3_{\&yz}^{-1*}0,0,0) \\
 (3_{x\&z}^*0,0,0) & (3_{x\&z}^{-1*}0,0,0) & (3_{xy\&}^*0,0,0) & (3_{xy\&}^{-1*}0,0,0) \\
 (4_x^*0,0,0) & (4_x^{-1*}0,0,0) & (2_{xy}^*0,0,0) & (2_{\&y}^*0,0,0) \\
 (4_y^*0,0,0) & (4_y^{-1*}0,0,0) & (2_{xz}^*0,0,0) & (2_{\&z}^*0,0,0) \\
 (4_z^*0,0,0) & (4_z^{-1*}0,0,0) & (2_{yz}^*0,0,0) & (2_{\&z}^*0,0,0)
 \end{array}$$

208.1.1546 P<sub>4</sub><sub>2</sub>32

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(4_x^*1/2,1/2,1/2)$	$(4_x^{-1*}1/2,1/2,1/2)$	$(2_{xy}^*1/2,1/2,1/2)$	$(2_{\&y}^*1/2,1/2,1/2)$
$(4_y^*1/2,1/2,1/2)$	$(4_y^{-1*}1/2,1/2,1/2)$	$(2_{xz}^*1/2,1/2,1/2)$	$(2_{\&z}^*1/2,1/2,1/2)$
$(4_z^*1/2,1/2,1/2)$	$(4_z^{-1*}1/2,1/2,1/2)$	$(2_{yz}^*1/2,1/2,1/2)$	$(2_{\&z}^*1/2,1/2,1/2)$

208.2.1547 P<sub>4</sub><sub>2</sub>321'

208.3.1548 P<sub>4</sub><sub>2</sub>'32'

P23

(0,0,0;a,b,c)

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(4_x^*1/2,1/2,1/2)'$	$(4_x^{-1*}1/2,1/2,1/2)'$	$(2_{xy}^*1/2,1/2,1/2)'$	$(2_{\&y}^*1/2,1/2,1/2)'$
$(4_y^*1/2,1/2,1/2)'$	$(4_y^{-1*}1/2,1/2,1/2)'$	$(2_{xz}^*1/2,1/2,1/2)'$	$(2_{\&z}^*1/2,1/2,1/2)'$
$(4_z^*1/2,1/2,1/2)'$	$(4_z^{-1*}1/2,1/2,1/2)'$	$(2_{yz}^*1/2,1/2,1/2)'$	$(2_{\&z}^*1/2,1/2,1/2)'$

208.4.1549 P<sub>F</sub>4<sub>2</sub>32

F4<sub>1</sub>32

(0,0,0;2a,2b,2c)

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(4_x^*1/2,1/2,1/2)$	$(4_x^{-1*}1/2,1/2,1/2)$	$(2_{xy}^*1/2,1/2,1/2)$	$(2_{\&y}^*1/2,1/2,1/2)$
$(4_y^*1/2,1/2,1/2)$	$(4_y^{-1*}1/2,1/2,1/2)$	$(2_{xz}^*1/2,1/2,1/2)$	$(2_{\&z}^*1/2,1/2,1/2)$
$(4_z^*1/2,1/2,1/2)$	$(4_z^{-1*}1/2,1/2,1/2)$	$(2_{yz}^*1/2,1/2,1/2)$	$(2_{\&z}^*1/2,1/2,1/2)$

209.1.1550 F432

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(4_x^*0,0,0)$	$(4_x^{-1*}0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_{\&y}^*0,0,0)$
$(4_y^*0,0,0)$	$(4_y^{-1*}0,0,0)$	$(2_{xz}^*0,0,0)$	$(2_{\&z}^*0,0,0)$
$(4_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$	$(2_{yz}^*0,0,0)$	$(2_{\&z}^*0,0,0)$

209.2.1551 F4321'

209.3.1552	F4'32'	F23	(0,0,0;a,b,c)	$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
				$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
				$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
				$(4_x^*0,0,0)'$	$(4_x^{-1*}0,0,0)'$	$(2_{xy}^*0,0,0)'$	$(2_{\&y}^*0,0,0)'$
				$(4_y^*0,0,0)'$	$(4_y^{-1*}0,0,0)'$	$(2_{xz}^*0,0,0)'$	$(2_{\&z}^*0,0,0)'$
				$(4_z^*0,0,0)'$	$(4_z^{-1*}0,0,0)'$	$(2_{yz}^*0,0,0)'$	$(2_{\&z}^*0,0,0)'$

210.1.1553	F4 <sub>1</sub> 32			$(1^*0,0,0)$	$(2_x^*1/2,0,1/2)$	$(2_y^*1/2,1/2,0)$	$(2_z^*0,1/2,1/2)$
				$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*1/2,1/2,0)$	$(3_{\&yz}^{-1*}0,1/2,1/2)$
				$(3_{x\&z}^*0,1/2,1/2)$	$(3_{x\&z}^{-1*}1/2,0,1/2)$	$(3_{xy\&}^*1/2,0,1/2)$	$(3_{xy\&}^{-1*}1/2,1/2,0)$
				$(4_x^*1/4,3/4,3/4)$	$(4_x^{-1*}3/4,1/4,3/4)$	$(2_{xy}^*3/4,1/4,3/4)$	$(2_{\&y}^*1/4,1/4,1/4)$
				$(4_y^*3/4,1/4,3/4)$	$(4_y^{-1*}3/4,3/4,1/4)$	$(2_{xz}^*1/4,3/4,3/4)$	$(2_{\&z}^*1/4,1/4,1/4)$
				$(4_z^*3/4,3/4,1/4)$	$(4_z^{-1*}1/4,3/4,3/4)$	$(2_{yz}^*3/4,3/4,1/4)$	$(2_{\&z}^*1/4,1/4,1/4)$

210.2.1554 F4<sub>1</sub>321'

210.3.1555	F4 <sub>1</sub> '32'	F23	(0,0,0;a,b,c)	$(1^*0,0,0)$	$(2_x^*1/2,0,1/2)$	$(2_y^*1/2,1/2,0)$	$(2_z^*0,1/2,1/2)$
				$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*1/2,1/2,0)$	$(3_{\&yz}^{-1*}0,1/2,1/2)$
				$(3_{x\&z}^*0,1/2,1/2)$	$(3_{x\&z}^{-1*}1/2,0,1/2)$	$(3_{xy\&}^*1/2,0,1/2)$	$(3_{xy\&}^{-1*}1/2,1/2,0)$
				$(4_x^*1/4,3/4,3/4)'$	$(4_x^{-1*}3/4,1/4,3/4)'$	$(2_{xy}^*3/4,1/4,3/4)'$	$(2_{\&y}^*1/4,1/4,1/4)'$
				$(4_y^*3/4,1/4,3/4)'$	$(4_y^{-1*}3/4,3/4,1/4)'$	$(2_{xz}^*1/4,3/4,3/4)'$	$(2_{\&z}^*1/4,1/4,1/4)'$
				$(4_z^*3/4,3/4,1/4)'$	$(4_z^{-1*}1/4,3/4,3/4)'$	$(2_{yz}^*3/4,3/4,1/4)'$	$(2_{\&z}^*1/4,1/4,1/4)'$

211.1.1556 I432

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(4_x^*0,0,0)$	$(4_x^{-1*}0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_{\&y}^*0,0,0)$
$(4_y^*0,0,0)$	$(4_y^{-1*}0,0,0)$	$(2_{xz}^*0,0,0)$	$(2_{\&z}^*0,0,0)$



$(4_z^*0,0,0)$        $(4_z^{-1*}0,0,0)$        $(2_{yz}^*0,0,0)$        $(2_{yz}^*0,0,0)$

211.2.1557 I4321'

211.3.1558 I4'32' I23 (0,0,0;a,b,c)

$(1^*0,0,0)$        $(2_x^*0,0,0)$        $(2_y^*0,0,0)$        $(2_z^*0,0,0)$   
 $(3_{xyz}^*0,0,0)$        $(3_{xyz}^{-1*}0,0,0)$        $(3_{yz}^*0,0,0)$        $(3_{yz}^{-1*}0,0,0)$   
 $(3_{xz}^*0,0,0)$        $(3_{xz}^{-1*}0,0,0)$        $(3_{xy}^*0,0,0)$        $(3_{xy}^{-1*}0,0,0)$   
 $(4_x^*0,0,0)'$        $(4_x^{-1*}0,0,0)'$        $(2_{xy}^*0,0,0)'$        $(2_{xy}^*0,0,0)'$   
 $(4_y^*0,0,0)'$        $(4_y^{-1*}0,0,0)'$        $(2_{xz}^*0,0,0)'$        $(2_{xz}^*0,0,0)'$   
 $(4_z^*0,0,0)'$        $(4_z^{-1*}0,0,0)'$        $(2_{yz}^*0,0,0)'$        $(2_{yz}^*0,0,0)'$

211.4.1559 I<sub>p</sub>432 P432 (0,0,0;a,b,c)

$(1^*0,0,0)$        $(2_x^*0,0,0)$        $(2_y^*0,0,0)$        $(2_z^*0,0,0)$   
 $(3_{xyz}^*0,0,0)$        $(3_{xyz}^{-1*}0,0,0)$        $(3_{yz}^*0,0,0)$        $(3_{yz}^{-1*}0,0,0)$   
 $(3_{xz}^*0,0,0)$        $(3_{xz}^{-1*}0,0,0)$        $(3_{xy}^*0,0,0)$        $(3_{xy}^{-1*}0,0,0)$   
 $(4_x^*0,0,0)$        $(4_x^{-1*}0,0,0)$        $(2_{xy}^*0,0,0)$        $(2_{xy}^*0,0,0)$   
 $(4_y^*0,0,0)$        $(4_y^{-1*}0,0,0)$        $(2_{xz}^*0,0,0)$        $(2_{xz}^*0,0,0)$   
 $(4_z^*0,0,0)$        $(4_z^{-1*}0,0,0)$        $(2_{yz}^*0,0,0)$        $(2_{yz}^*0,0,0)$

211.5.1560 I<sub>p</sub>4'32' P4<sub>2</sub>32 (0,0,0;a,b,c)

$(1^*0,0,0)$        $(2_x^*0,0,0)$        $(2_y^*0,0,0)$        $(2_z^*0,0,0)$   
 $(3_{xyz}^*0,0,0)$        $(3_{xyz}^{-1*}0,0,0)$        $(3_{yz}^*0,0,0)$        $(3_{yz}^{-1*}0,0,0)$   
 $(3_{xz}^*0,0,0)$        $(3_{xz}^{-1*}0,0,0)$        $(3_{xy}^*0,0,0)$        $(3_{xy}^{-1*}0,0,0)$   
 $(4_x^*1/2,1/2,1/2)$        $(4_x^{-1*}1/2,1/2,1/2)$        $(2_{xy}^*1/2,1/2,1/2)$        $(2_{xy}^*1/2,1/2,1/2)$   
 $(4_y^*1/2,1/2,1/2)$        $(4_y^{-1*}1/2,1/2,1/2)$        $(2_{xz}^*1/2,1/2,1/2)$        $(2_{xz}^*1/2,1/2,1/2)$   
 $(4_z^*1/2,1/2,1/2)$        $(4_z^{-1*}1/2,1/2,1/2)$        $(2_{yz}^*1/2,1/2,1/2)$        $(2_{yz}^*1/2,1/2,1/2)$

212.1.1561 P4<sub>3</sub>32

$(1^*0,0,0)$        $(2_x^*1/2,1/2,0)$        $(2_y^*0,1/2,1/2)$        $(2_z^*1/2,0,1/2)$   
 $(3_{xyz}^*0,0,0)$        $(3_{xyz}^{-1*}0,0,0)$        $(3_{yz}^*0,1/2,1/2)$        $(3_{yz}^{-1*}1/2,0,1/2)$   
 $(3_{xz}^*1/2,0,1/2)$        $(3_{xz}^{-1*}1/2,1/2,0)$        $(3_{xy}^*1/2,1/2,0)$        $(3_{xy}^{-1*}0,1/2,1/2)$   
 $(4_x^*3/4,3/4,1/4)$        $(4_x^{-1*}1/4,3/4,3/4)$        $(2_{xy}^*1/4,3/4,3/4)$        $(2_{xy}^*1/4,1/4,1/4)$   
 $(4_y^*1/4,3/4,3/4)$        $(4_y^{-1*}3/4,1/4,3/4)$        $(2_{xz}^*3/4,3/4,1/4)$        $(2_{xz}^*1/4,1/4,1/4)$   
 $(4_z^*3/4,1/4,3/4)$        $(4_z^{-1*}3/4,3/4,1/4)$        $(2_{yz}^*3/4,1/4,3/4)$        $(2_{yz}^*1/4,1/4,1/4)$

212.2.1562 P4<sub>3</sub>321'

212.3.1563 P4<sub>3</sub>'32' P2,3 (0,0,0;a,b,c)

$(1^*0,0,0)$	$(2_x^*1/2,1/2,0)$	$(2_y^*0,1/2,1/2)$	$(2_z^*1/2,0,1/2)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,1/2,1/2)$	$(3_{\&yz}^{-1*}1/2,0,1/2)$
$(3_{x\&z}^*1/2,0,1/2)$	$(3_{x\&z}^{-1*}1/2,1/2,0)$	$(3_{xy\&}^*1/2,1/2,0)$	$(3_{xy\&}^{-1*}0,1/2,1/2)$
$(4_x^*3/4,3/4,1/4)'$	$(4_x^{-1*}1/4,3/4,3/4)'$	$(2_{xy}^*1/4,3/4,3/4)'$	$(2_{\&y}^*1/4,1/4,1/4)'$
$(4_y^*1/4,3/4,3/4)'$	$(4_y^{-1*}3/4,1/4,3/4)'$	$(2_{xz}^*3/4,3/4,1/4)'$	$(2_{\&z}^*1/4,1/4,1/4)'$
$(4_z^*3/4,1/4,3/4)'$	$(4_z^{-1*}3/4,3/4,1/4)'$	$(2_{yz}^*3/4,1/4,3/4)'$	$(2_{\&z}^*1/4,1/4,1/4)'$

213.1.1564 P4<sub>1</sub>32

$(1^*0,0,0)$	$(2_x^*1/2,1/2,0)$	$(2_y^*0,1/2,1/2)$	$(2_z^*1/2,0,1/2)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,1/2,1/2)$	$(3_{\&yz}^{-1*}1/2,0,1/2)$
$(3_{x\&z}^*1/2,0,1/2)$	$(3_{x\&z}^{-1*}1/2,1/2,0)$	$(3_{xy\&}^*1/2,1/2,0)$	$(3_{xy\&}^{-1*}0,1/2,1/2)$
$(4_x^*1/4,1/4,3/4)$	$(4_x^{-1*}3/4,1/4,1/4)$	$(2_{xy}^*3/4,1/4,1/4)$	$(2_{\&y}^*3/4,3/4,3/4)$
$(4_y^*3/4,1/4,1/4)$	$(4_y^{-1*}1/4,3/4,1/4)$	$(2_{xz}^*1/4,1/4,3/4)$	$(2_{\&z}^*3/4,3/4,3/4)$
$(4_z^*1/4,3/4,1/4)$	$(4_z^{-1*}1/4,1/4,3/4)$	$(2_{yz}^*1/4,3/4,1/4)$	$(2_{\&z}^*3/4,3/4,3/4)$

213.2.1565 P4<sub>1</sub>321'

213.3.1566 P4<sub>1</sub>'32' P2,3 (0,0,0;a,b,c)

$(1^*0,0,0)$	$(2_x^*1/2,1/2,0)$	$(2_y^*0,1/2,1/2)$	$(2_z^*1/2,0,1/2)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,1/2,1/2)$	$(3_{\&yz}^{-1*}1/2,0,1/2)$
$(3_{x\&z}^*1/2,0,1/2)$	$(3_{x\&z}^{-1*}1/2,1/2,0)$	$(3_{xy\&}^*1/2,1/2,0)$	$(3_{xy\&}^{-1*}0,1/2,1/2)$
$(4_x^*1/4,1/4,3/4)'$	$(4_x^{-1*}3/4,1/4,1/4)'$	$(2_{xy}^*3/4,1/4,1/4)'$	$(2_{\&y}^*3/4,3/4,3/4)'$
$(4_y^*3/4,1/4,1/4)'$	$(4_y^{-1*}1/4,3/4,1/4)'$	$(2_{xz}^*1/4,1/4,3/4)'$	$(2_{\&z}^*3/4,3/4,3/4)'$
$(4_z^*1/4,3/4,1/4)'$	$(4_z^{-1*}1/4,1/4,3/4)'$	$(2_{yz}^*1/4,3/4,1/4)'$	$(2_{\&z}^*3/4,3/4,3/4)'$

214.1.1567 I4<sub>1</sub>32

$(1^*0,0,0)$	$(2_x^*1/2,1/2,0)$	$(2_y^*0,1/2,1/2)$	$(2_z^*1/2,0,1/2)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,1/2,1/2)$	$(3_{\&yz}^{-1*}1/2,0,1/2)$
$(3_{x\&z}^*1/2,0,1/2)$	$(3_{x\&z}^{-1*}1/2,1/2,0)$	$(3_{xy\&}^*1/2,1/2,0)$	$(3_{xy\&}^{-1*}0,1/2,1/2)$
$(4_x^*1/4,1/4,3/4)$	$(4_x^{-1*}3/4,1/4,1/4)$	$(2_{xy}^*3/4,1/4,1/4)$	$(2_{\&y}^*3/4,3/4,3/4)$

214.2.1568	$I_4 321'$			$(4_y^* 3/4, 1/4, 1/4)$ $(4_z^* 1/4, 3/4, 1/4)$	$(4_y^{-1*} 1/4, 3/4, 1/4)$ $(4_z^{-1*} 1/4, 1/4, 3/4)$	$(2_{xz}^* 1/4, 1/4, 3/4)$ $(2_{yz}^* 1/4, 3/4, 1/4)$	$(2_{\&z}^* 3/4, 3/4, 3/4)$ $(2_{\&z}^* 3/4, 3/4, 3/4)$
214.3.1569	$I_4 32'$	$I_2 3$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\&z}^*1/2,0,1/2)$ $(4_x^*1/4,1/4,3/4)'$ $(4_y^*3/4,1/4,1/4)'$ $(4_z^*1/4,3/4,1/4)'$	$(2_x^*1/2,1/2,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\&z}^{-1*}1/2,1/2,0)$ $(4_x^{-1*}3/4,1/4,1/4)'$ $(4_y^{-1*}1/4,3/4,1/4)'$ $(4_z^{-1*}1/4,1/4,3/4)'$	$(2_y^*0,1/2,1/2)$ $(3_{\&yz}^*0,1/2,1/2)$ $(3_{xy\&}^*1/2,1/2,0)$ $(2_{xy}^*3/4,1/4,1/4)'$ $(2_{xz}^*1/4,1/4,3/4)'$ $(2_{yz}^*1/4,3/4,1/4)'$	$(2_z^*1/2,0,1/2)$ $(3_{\&yz}^{-1*}1/2,0,1/2)$ $(3_{xy\&}^{-1*}0,1/2,1/2)$ $(2_{\&y}^*3/4,3/4,3/4)'$ $(2_{\&z}^*3/4,3/4,3/4)'$ $(2_{\&z}^*3/4,3/4,3/4)'$
214.4.1570	$I_p 4_1 32$	$P4_1 32$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\&z}^*1/2,0,1/2)$ $(4_x^*1/4,1/4,3/4)$ $(4_y^*3/4,1/4,1/4)$ $(4_z^*1/4,3/4,1/4)$	$(2_x^*1/2,1/2,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\&z}^{-1*}1/2,1/2,0)$ $(4_x^{-1*}3/4,1/4,1/4)$ $(4_y^{-1*}1/4,3/4,1/4)$ $(4_z^{-1*}1/4,1/4,3/4)$	$(2_y^*0,1/2,1/2)$ $(3_{\&yz}^*0,1/2,1/2)$ $(3_{xy\&}^*1/2,1/2,0)$ $(2_{xy}^*3/4,1/4,1/4)$ $(2_{xz}^*1/4,1/4,3/4)$ $(2_{yz}^*1/4,3/4,1/4)$	$(2_z^*1/2,0,1/2)$ $(3_{\&yz}^{-1*}1/2,0,1/2)$ $(3_{xy\&}^{-1*}0,1/2,1/2)$ $(2_{\&y}^*3/4,3/4,3/4)$ $(2_{\&z}^*3/4,3/4,3/4)$ $(2_{\&z}^*3/4,3/4,3/4)$
214.5.1571	$I_p 4_1 32'$	$P4_3 32$	$(0,0,0;a,b,c)$	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\&z}^*1/2,0,1/2)$ $(4_x^*3/4,3/4,1/4)$ $(4_y^*1/4,3/4,3/4)$ $(4_z^*3/4,1/4,3/4)$	$(2_x^*1/2,1/2,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\&z}^{-1*}1/2,1/2,0)$ $(4_x^{-1*}1/4,3/4,3/4)$ $(4_y^{-1*}3/4,1/4,3/4)$ $(4_z^{-1*}3/4,3/4,1/4)$	$(2_y^*0,1/2,1/2)$ $(3_{\&yz}^*0,1/2,1/2)$ $(3_{xy\&}^*1/2,1/2,0)$ $(2_{xy}^*1/4,3/4,3/4)$ $(2_{xz}^*3/4,3/4,1/4)$ $(2_{yz}^*3/4,1/4,3/4)$	$(2_z^*1/2,0,1/2)$ $(3_{\&yz}^{-1*}1/2,0,1/2)$ $(3_{xy\&}^{-1*}0,1/2,1/2)$ $(2_{\&y}^*1/4,1/4,1/4)$ $(2_{\&z}^*1/4,1/4,1/4)$ $(2_{\&z}^*1/4,1/4,1/4)$
215.1.1572	$P\&3m$			$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\&z}^*0,0,0)$ $(\&x^*0,0,0)$ $(\&y^*0,0,0)$ $(\&z^*0,0,0)$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\&z}^{-1*}0,0,0)$ $(\&x^{-1*}0,0,0)$ $(\&y^{-1*}0,0,0)$ $(\&z^{-1*}0,0,0)$	$(2_y^*0,0,0)$ $(3_{\&yz}^*0,0,0)$ $(3_{xy\&}^*0,0,0)$ $(m_{xy}^*0,0,0)$ $(m_{xz}^*0,0,0)$ $(m_{yz}^*0,0,0)$	$(2_z^*0,0,0)$ $(3_{\&yz}^{-1*}0,0,0)$ $(3_{xy\&}^{-1*}0,0,0)$ $(m_{\&y}^*0,0,0)$ $(m_{\&z}^*0,0,0)$ $(m_{\&z}^*0,0,0)$
215.2.1573	$P\&3m1'$						

215.3.1574	P $\bar{3}m'$	P23	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\bar{y}z}^*0,0,0)$ $(\bar{2}_x^*0,0,0)'$ $(\bar{2}_y^*0,0,0)'$ $(\bar{2}_z^*0,0,0)'$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\bar{y}z}^{-1*}0,0,0)$ $(\bar{2}_x^{-1*}0,0,0)'$ $(\bar{2}_y^{-1*}0,0,0)'$ $(\bar{2}_z^{-1*}0,0,0)'$	$(2_y^*0,0,0)$ $(3_{\bar{x}yz}^*0,0,0)$ $(3_{xy\bar{z}}^*0,0,0)$ $(m_{xy}^*0,0,0)'$ $(m_{xz}^*0,0,0)'$ $(m_{yz}^*0,0,0)'$	$(2_z^*0,0,0)$ $(3_{\bar{x}yz}^{-1*}0,0,0)$ $(3_{xy\bar{z}}^{-1*}0,0,0)$ $(m_{\bar{x}y}^*0,0,0)'$ $(m_{\bar{x}z}^*0,0,0)'$ $(m_{\bar{x}z}^*0,0,0)'$
215.4.1575	P $\bar{F}\bar{3}m$	F $\bar{3}m$	(0,0,0;2a,2b,2c)	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\bar{y}z}^*0,0,0)$ $(\bar{2}_x^*0,0,0)$ $(\bar{2}_y^*0,0,0)$ $(\bar{2}_z^*0,0,0)$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\bar{y}z}^{-1*}0,0,0)$ $(\bar{2}_x^{-1*}0,0,0)$ $(\bar{2}_y^{-1*}0,0,0)$ $(\bar{2}_z^{-1*}0,0,0)$	$(2_y^*0,0,0)$ $(3_{\bar{x}yz}^*0,0,0)$ $(3_{xy\bar{z}}^*0,0,0)$ $(m_{xy}^*0,0,0)$ $(m_{xz}^*0,0,0)$ $(m_{yz}^*0,0,0)$	$(2_z^*0,0,0)$ $(3_{\bar{x}yz}^{-1*}0,0,0)$ $(3_{xy\bar{z}}^{-1*}0,0,0)$ $(m_{\bar{x}y}^*0,0,0)$ $(m_{\bar{x}z}^*0,0,0)$ $(m_{\bar{x}z}^*0,0,0)$
215.5.1576	P $\bar{F}\bar{3}m'$	F $\bar{3}c$	(0,0,0;2a,2b,2c)	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\bar{y}z}^*0,0,0)$ $(\bar{2}_x^*1,0,0)$ $(\bar{2}_y^*1,0,0)$ $(\bar{2}_z^*1,0,0)$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\bar{y}z}^{-1*}0,0,0)$ $(\bar{2}_x^{-1*}1,0,0)$ $(\bar{2}_y^{-1*}1,0,0)$ $(\bar{2}_z^{-1*}1,0,0)$	$(2_y^*0,0,0)$ $(3_{\bar{x}yz}^*0,0,0)$ $(3_{xy\bar{z}}^*0,0,0)$ $(m_{xy}^*1,0,0)$ $(m_{xz}^*1,0,0)$ $(m_{yz}^*1,0,0)$	$(2_z^*0,0,0)$ $(3_{\bar{x}yz}^{-1*}0,0,0)$ $(3_{xy\bar{z}}^{-1*}0,0,0)$ $(m_{\bar{x}y}^*1,0,0)$ $(m_{\bar{x}z}^*1,0,0)$ $(m_{\bar{x}z}^*1,0,0)$
216.1.1577	F $\bar{3}m$			$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\bar{y}z}^*0,0,0)$ $(\bar{2}_x^*0,0,0)$ $(\bar{2}_y^*0,0,0)$ $(\bar{2}_z^*0,0,0)$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\bar{y}z}^{-1*}0,0,0)$ $(\bar{2}_x^{-1*}0,0,0)$ $(\bar{2}_y^{-1*}0,0,0)$ $(\bar{2}_z^{-1*}0,0,0)$	$(2_y^*0,0,0)$ $(3_{\bar{x}yz}^*0,0,0)$ $(3_{xy\bar{z}}^*0,0,0)$ $(m_{xy}^*0,0,0)$ $(m_{xz}^*0,0,0)$ $(m_{yz}^*0,0,0)$	$(2_z^*0,0,0)$ $(3_{\bar{x}yz}^{-1*}0,0,0)$ $(3_{xy\bar{z}}^{-1*}0,0,0)$ $(m_{\bar{x}y}^*0,0,0)$ $(m_{\bar{x}z}^*0,0,0)$ $(m_{\bar{x}z}^*0,0,0)$
216.2.1578	F $\bar{3}m1'$						
216.3.1579	F $\bar{3}m'$	F23	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$	$(2_y^*0,0,0)$ $(3_{\bar{x}yz}^*0,0,0)$	$(2_z^*0,0,0)$ $(3_{\bar{x}yz}^{-1*}0,0,0)$

$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(\&x^*0,0,0)'$	$(\&x^{-1*}0,0,0)'$	$(m_{xy}^*0,0,0)'$	$(m_{\&y}^*0,0,0)'$
$(\&y^*0,0,0)'$	$(\&y^{-1*}0,0,0)'$	$(m_{xz}^*0,0,0)'$	$(m_{\&z}^*0,0,0)'$
$(\&z^*0,0,0)'$	$(\&z^{-1*}0,0,0)'$	$(m_{yz}^*0,0,0)'$	$(m_{\&z}^*0,0,0)'$

217.1.1580  $I\&3m$

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(\&x^*0,0,0)$	$(\&x^{-1*}0,0,0)$	$(m_{xy}^*0,0,0)$	$(m_{\&y}^*0,0,0)$
$(\&y^*0,0,0)$	$(\&y^{-1*}0,0,0)$	$(m_{xz}^*0,0,0)$	$(m_{\&z}^*0,0,0)$
$(\&z^*0,0,0)$	$(\&z^{-1*}0,0,0)$	$(m_{yz}^*0,0,0)$	$(m_{\&z}^*0,0,0)$

217.2.1581  $I\&3m1'$

217.3.1582  $I\&'3m'$   $I23$   $(0,0,0;a,b,c)$

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(\&x^*0,0,0)'$	$(\&x^{-1*}0,0,0)'$	$(m_{xy}^*0,0,0)'$	$(m_{\&y}^*0,0,0)'$
$(\&y^*0,0,0)'$	$(\&y^{-1*}0,0,0)'$	$(m_{xz}^*0,0,0)'$	$(m_{\&z}^*0,0,0)'$
$(\&z^*0,0,0)'$	$(\&z^{-1*}0,0,0)'$	$(m_{yz}^*0,0,0)'$	$(m_{\&z}^*0,0,0)'$

217.4.1583  $I_p\&3m$   $P\&3m$   $(0,0,0;a,b,c)$

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(\&x^*0,0,0)$	$(\&x^{-1*}0,0,0)$	$(m_{xy}^*0,0,0)$	$(m_{\&y}^*0,0,0)$
$(\&y^*0,0,0)$	$(\&y^{-1*}0,0,0)$	$(m_{xz}^*0,0,0)$	$(m_{\&z}^*0,0,0)$
$(\&z^*0,0,0)$	$(\&z^{-1*}0,0,0)$	$(m_{yz}^*0,0,0)$	$(m_{\&z}^*0,0,0)$

217.5.1584  $I_p\&'3m'$   $P\&3n$   $(0,0,0;a,b,c)$

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(\&x^*1/2,1/2,1/2)$	$(\&x^{-1*}1/2,1/2,1/2)$	$(m_{xy}^*1/2,1/2,1/2)$	$(m_{\&y}^*1/2,1/2,1/2)$

$$\begin{pmatrix} g_y^* & 1/2, 1/2, 1/2 \\ g_z^* & 1/2, 1/2, 1/2 \end{pmatrix} \quad \begin{pmatrix} g_y^{-1*} & 1/2, 1/2, 1/2 \\ g_z^{-1*} & 1/2, 1/2, 1/2 \end{pmatrix} \quad \begin{pmatrix} m_{xz}^* & 1/2, 1/2, 1/2 \\ m_{yz}^* & 1/2, 1/2, 1/2 \end{pmatrix} \quad \begin{pmatrix} m_{\&z}^* & 1/2, 1/2, 1/2 \\ m_{\&z}^* & 1/2, 1/2, 1/2 \end{pmatrix}$$

218.1.1585 P&3n

$$\begin{pmatrix} 1^* & 0, 0, 0 \\ 3_{xyz}^* & 0, 0, 0 \\ 3_{x\&z}^* & 0, 0, 0 \\ g_x^* & 1/2, 1/2, 1/2 \\ g_y^* & 1/2, 1/2, 1/2 \\ g_z^* & 1/2, 1/2, 1/2 \end{pmatrix} \quad \begin{pmatrix} 2_x^* & 0, 0, 0 \\ 3_{xyz}^{-1*} & 0, 0, 0 \\ 3_{x\&z}^{-1*} & 0, 0, 0 \\ g_x^{-1*} & 1/2, 1/2, 1/2 \\ g_y^{-1*} & 1/2, 1/2, 1/2 \\ g_z^{-1*} & 1/2, 1/2, 1/2 \end{pmatrix} \quad \begin{pmatrix} 2_y^* & 0, 0, 0 \\ 3_{\&yz}^* & 0, 0, 0 \\ 3_{xy\&}^* & 0, 0, 0 \\ m_{xy}^* & 1/2, 1/2, 1/2 \\ m_{xz}^* & 1/2, 1/2, 1/2 \\ m_{yz}^* & 1/2, 1/2, 1/2 \end{pmatrix} \quad \begin{pmatrix} 2_z^* & 0, 0, 0 \\ 3_{\&yz}^{-1*} & 0, 0, 0 \\ 3_{xy\&}^{-1*} & 0, 0, 0 \\ m_{\&y}^* & 1/2, 1/2, 1/2 \\ m_{\&z}^* & 1/2, 1/2, 1/2 \\ m_{\&z}^* & 1/2, 1/2, 1/2 \end{pmatrix}$$

218.2.1586 P&3n1'

218.3.1587 P&'3n'

P23

(0,0,0;a,b,c)

$$\begin{pmatrix} 1^* & 0, 0, 0 \\ 3_{xyz}^* & 0, 0, 0 \\ 3_{x\&z}^* & 0, 0, 0 \\ g_x^* & 1/2, 1/2, 1/2 \\ g_y^* & 1/2, 1/2, 1/2 \\ g_z^* & 1/2, 1/2, 1/2 \end{pmatrix}' \quad \begin{pmatrix} 2_x^* & 0, 0, 0 \\ 3_{xyz}^{-1*} & 0, 0, 0 \\ 3_{x\&z}^{-1*} & 0, 0, 0 \\ g_x^{-1*} & 1/2, 1/2, 1/2 \\ g_y^{-1*} & 1/2, 1/2, 1/2 \\ g_z^{-1*} & 1/2, 1/2, 1/2 \end{pmatrix}' \quad \begin{pmatrix} 2_y^* & 0, 0, 0 \\ 3_{\&yz}^* & 0, 0, 0 \\ 3_{xy\&}^* & 0, 0, 0 \\ m_{xy}^* & 1/2, 1/2, 1/2 \\ m_{xz}^* & 1/2, 1/2, 1/2 \\ m_{yz}^* & 1/2, 1/2, 1/2 \end{pmatrix}' \quad \begin{pmatrix} 2_z^* & 0, 0, 0 \\ 3_{\&yz}^{-1*} & 0, 0, 0 \\ 3_{xy\&}^{-1*} & 0, 0, 0 \\ m_{\&y}^* & 1/2, 1/2, 1/2 \\ m_{\&z}^* & 1/2, 1/2, 1/2 \\ m_{\&z}^* & 1/2, 1/2, 1/2 \end{pmatrix}'$$

219.1.1588 F&3c

$$\begin{pmatrix} 1^* & 0, 0, 0 \\ 3_{xyz}^* & 0, 0, 0 \\ 3_{x\&z}^* & 0, 0, 0 \\ g_x^* & 1/2, 1/2, 1/2 \\ g_y^* & 1/2, 1/2, 1/2 \\ g_z^* & 1/2, 1/2, 1/2 \end{pmatrix} \quad \begin{pmatrix} 2_x^* & 0, 0, 0 \\ 3_{xyz}^{-1*} & 0, 0, 0 \\ 3_{x\&z}^{-1*} & 0, 0, 0 \\ g_x^{-1*} & 1/2, 1/2, 1/2 \\ g_y^{-1*} & 1/2, 1/2, 1/2 \\ g_z^{-1*} & 1/2, 1/2, 1/2 \end{pmatrix} \quad \begin{pmatrix} 2_y^* & 0, 0, 0 \\ 3_{\&yz}^* & 0, 0, 0 \\ 3_{xy\&}^* & 0, 0, 0 \\ m_{xy}^* & 1/2, 1/2, 1/2 \\ m_{xz}^* & 1/2, 1/2, 1/2 \\ m_{yz}^* & 1/2, 1/2, 1/2 \end{pmatrix} \quad \begin{pmatrix} 2_z^* & 0, 0, 0 \\ 3_{\&yz}^{-1*} & 0, 0, 0 \\ 3_{xy\&}^{-1*} & 0, 0, 0 \\ m_{\&y}^* & 1/2, 1/2, 1/2 \\ m_{\&z}^* & 1/2, 1/2, 1/2 \\ m_{\&z}^* & 1/2, 1/2, 1/2 \end{pmatrix}$$

219.2.1589 F&3c1'

219.3.1590	$F\bar{3}c'$	F23	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\bar{y}z}^*0,0,0)$ $(\bar{2}_x^*1/2,1/2,1/2)'$ $(\bar{2}_y^*1/2,1/2,1/2)'$ $(\bar{2}_z^*1/2,1/2,1/2)'$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\bar{y}z}^{-1*}0,0,0)$ $(\bar{2}_x^{-1*}1/2,1/2,1/2)'$ $(\bar{2}_y^{-1*}1/2,1/2,1/2)'$ $(\bar{2}_z^{-1*}1/2,1/2,1/2)'$	$(2_y^*0,0,0)$ $(3_{\bar{x}yz}^*0,0,0)$ $(3_{xy\bar{z}}^*0,0,0)$ $(m_{xy}^*1/2,1/2,1/2)'$ $(m_{xz}^*1/2,1/2,1/2)'$ $(m_{yz}^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(3_{\bar{x}yz}^{-1*}0,0,0)$ $(3_{xy\bar{z}}^{-1*}0,0,0)$ $(m_{\bar{x}y}^*1/2,1/2,1/2)'$ $(m_{\bar{z}x}^*1/2,1/2,1/2)'$ $(m_{\bar{z}y}^*1/2,1/2,1/2)'$
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220.1.1591	$I\bar{3}d$			$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\bar{y}z}^*1/2,0,1/2)$ $(\bar{2}_x^*3/4,3/4,1/4)$ $(\bar{2}_y^*1/4,3/4,3/4)$ $(\bar{2}_z^*3/4,1/4,3/4)$	$(2_x^*1/2,1/2,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\bar{y}z}^{-1*}1/2,1/2,0)$ $(\bar{2}_x^{-1*}1/4,3/4,3/4)$ $(\bar{2}_y^{-1*}3/4,1/4,3/4)$ $(\bar{2}_z^{-1*}3/4,3/4,1/4)$	$(2_y^*0,1/2,1/2)$ $(3_{\bar{x}yz}^*0,1/2,1/2)$ $(3_{xy\bar{z}}^*1/2,1/2,0)$ $(m_{xy}^*1/4,3/4,3/4)$ $(m_{xz}^*3/4,3/4,1/4)$ $(m_{yz}^*3/4,1/4,3/4)$	$(2_z^*1/2,0,1/2)$ $(3_{\bar{x}yz}^{-1*}1/2,0,1/2)$ $(3_{xy\bar{z}}^{-1*}0,1/2,1/2)$ $(m_{\bar{x}y}^*1/4,1/4,1/4)$ $(m_{\bar{z}x}^*1/4,1/4,1/4)$ $(m_{\bar{z}y}^*1/4,1/4,1/4)$
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220.2.1592  $I\bar{3}d1'$

220.3.1593	$I\bar{3}d'$	$I2_3$	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\bar{y}z}^*1/2,0,1/2)$ $(\bar{2}_x^*3/4,3/4,1/4)'$ $(\bar{2}_y^*1/4,3/4,3/4)'$ $(\bar{2}_z^*3/4,1/4,3/4)'$	$(2_x^*1/2,1/2,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\bar{y}z}^{-1*}1/2,1/2,0)$ $(\bar{2}_x^{-1*}1/4,3/4,3/4)'$ $(\bar{2}_y^{-1*}3/4,1/4,3/4)'$ $(\bar{2}_z^{-1*}3/4,3/4,1/4)'$	$(2_y^*0,1/2,1/2)$ $(3_{\bar{x}yz}^*0,1/2,1/2)$ $(3_{xy\bar{z}}^*1/2,1/2,0)$ $(m_{xy}^*1/4,3/4,3/4)'$ $(m_{xz}^*3/4,3/4,1/4)'$ $(m_{yz}^*3/4,1/4,3/4)'$	$(2_z^*1/2,0,1/2)$ $(3_{\bar{x}yz}^{-1*}1/2,0,1/2)$ $(3_{xy\bar{z}}^{-1*}0,1/2,1/2)$ $(m_{\bar{x}y}^*1/4,1/4,1/4)'$ $(m_{\bar{z}x}^*1/4,1/4,1/4)'$ $(m_{\bar{z}y}^*1/4,1/4,1/4)'$
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221.1.1594	$Pm\bar{3}m$			$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\bar{y}z}^*0,0,0)$ $(4_x^*0,0,0)$ $(4_y^*0,0,0)$ $(4_z^*0,0,0)$ $(\bar{2}_x^*0,0,0)$ $(\bar{2}_{xyz}^*0,0,0)$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\bar{y}z}^{-1*}0,0,0)$ $(4_x^{-1*}0,0,0)$ $(4_y^{-1*}0,0,0)$ $(4_z^{-1*}0,0,0)$ $(m_x^*0,0,0)$ $(\bar{2}_{xyz}^{-1*}0,0,0)$	$(2_y^*0,0,0)$ $(3_{\bar{x}yz}^*0,0,0)$ $(3_{xy\bar{z}}^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(2_{xz}^*0,0,0)$ $(2_{yz}^*0,0,0)$ $(m_y^*0,0,0)$ $(\bar{2}_{\bar{x}yz}^*0,0,0)$	$(2_z^*0,0,0)$ $(3_{\bar{x}yz}^{-1*}0,0,0)$ $(3_{xy\bar{z}}^{-1*}0,0,0)$ $(2_{\bar{x}y}^*0,0,0)$ $(2_{\bar{x}z}^*0,0,0)$ $(2_{\bar{x}y}^*0,0,0)$ $(m_z^*0,0,0)$ $(\bar{2}_{\bar{x}yz}^{-1*}0,0,0)$
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$$\begin{array}{cccc}
(\&_{x\&z}^*0,0,0) & (\&_{x\&z}^{-1*}0,0,0) & (\&_{xy\&}^*0,0,0) & (\&_{xy\&}^{-1*}0,0,0) \\
(\&_x^*0,0,0) & (\&_x^{-1*}0,0,0) & (m_{xy}^*0,0,0) & (m_{\&y}^*0,0,0) \\
(\&_y^*0,0,0) & (\&_y^{-1*}0,0,0) & (m_{xz}^*0,0,0) & (m_{\&z}^*0,0,0) \\
(\&_z^*0,0,0) & (\&_z^{-1*}0,0,0) & (m_{yz}^*0,0,0) & (m_{\&z}^*0,0,0)
\end{array}$$

221.2.1595 Pm&m1'

221.3.1596 Pm'&m P&3m (0,0,0;a,b,c)

$$\begin{array}{cccc}
(1^*0,0,0) & (2_x^*0,0,0) & (2_y^*0,0,0) & (2_z^*0,0,0) \\
(3_{xyz}^*0,0,0) & (3_{xyz}^{-1*}0,0,0) & (3_{\&yz}^*0,0,0) & (3_{\&yz}^{-1*}0,0,0) \\
(3_{x\&z}^*0,0,0) & (3_{x\&z}^{-1*}0,0,0) & (3_{xy\&}^*0,0,0) & (3_{xy\&}^{-1*}0,0,0) \\
(4_x^*0,0,0)' & (4_x^{-1*}0,0,0) & (2_{xy}^*0,0,0)' & (2_{\&y}^*0,0,0)' \\
(4_y^*0,0,0)' & (4_y^{-1*}0,0,0)' & (2_{xz}^*0,0,0)' & (2_{\&z}^*0,0,0)' \\
(4_z^*0,0,0)' & (4_z^{-1*}0,0,0)' & (2_{yz}^*0,0,0)' & (2_{\&z}^*0,0,0)' \\
(\&^*0,0,0)' & (m_x^*0,0,0)' & (m_y^*0,0,0)' & (m_z^*0,0,0)' \\
(\&_{xyz}^*0,0,0)' & (\&_{xyz}^{-1*}0,0,0)' & (\&_{\&y}^*0,0,0)' & (\&_{\&y}^{-1*}0,0,0)' \\
(\&_{x\&z}^*0,0,0)' & (\&_{x\&z}^{-1*}0,0,0)' & (\&_{xy\&}^*0,0,0)' & (\&_{xy\&}^{-1*}0,0,0)' \\
(\&_x^*0,0,0) & (\&_x^{-1*}0,0,0) & (m_{xy}^*0,0,0) & (m_{\&y}^*0,0,0) \\
(\&_y^*0,0,0) & (\&_y^{-1*}0,0,0) & (m_{xz}^*0,0,0) & (m_{\&z}^*0,0,0) \\
(\&_z^*0,0,0) & (\&_z^{-1*}0,0,0) & (m_{yz}^*0,0,0) & (m_{\&z}^*0,0,0)
\end{array}$$

221.4.1597 Pm&m' Pm& (0,0,0;a,b,c)

$$\begin{array}{cccc}
(1^*0,0,0) & (2_x^*0,0,0) & (2_y^*0,0,0) & (2_z^*0,0,0) \\
(3_{xyz}^*0,0,0) & (3_{xyz}^{-1*}0,0,0) & (3_{\&y}^*0,0,0) & (3_{\&y}^{-1*}0,0,0) \\
(3_{x\&z}^*0,0,0) & (3_{x\&z}^{-1*}0,0,0) & (3_{xy\&}^*0,0,0) & (3_{xy\&}^{-1*}0,0,0) \\
(4_x^*0,0,0)' & (4_x^{-1*}0,0,0)' & (2_{xy}^*0,0,0)' & (2_{\&y}^*0,0,0)' \\
(4_y^*0,0,0)' & (4_y^{-1*}0,0,0)' & (2_{xz}^*0,0,0)' & (2_{\&z}^*0,0,0)' \\
(4_z^*0,0,0)' & (4_z^{-1*}0,0,0)' & (2_{yz}^*0,0,0)' & (2_{\&z}^*0,0,0)' \\
(\&^*0,0,0) & (m_x^*0,0,0) & (m_y^*0,0,0) & (m_z^*0,0,0) \\
(\&_{xyz}^*0,0,0) & (\&_{xyz}^{-1*}0,0,0) & (\&_{\&y}^*0,0,0) & (\&_{\&y}^{-1*}0,0,0) \\
(\&_{x\&z}^*0,0,0) & (\&_{x\&z}^{-1*}0,0,0) & (\&_{xy\&}^*0,0,0) & (\&_{xy\&}^{-1*}0,0,0) \\
(\&_x^*0,0,0)' & (\&_x^{-1*}0,0,0)' & (m_{xy}^*0,0,0)' & (m_{\&y}^*0,0,0)' \\
(\&_y^*0,0,0)' & (\&_y^{-1*}0,0,0)' & (m_{xz}^*0,0,0)' & (m_{\&z}^*0,0,0)' \\
(\&_z^*0,0,0)' & (\&_z^{-1*}0,0,0)' & (m_{yz}^*0,0,0)' & (m_{\&z}^*0,0,0)'
\end{array}$$

221.5.1598 Pm'&m' P432 (0,0,0;a,b,c)

$$\begin{array}{cccc}
(1^*0,0,0) & (2_x^*0,0,0) & (2_y^*0,0,0) & (2_z^*0,0,0) \\
(3_{xyz}^*0,0,0) & (3_{xyz}^{-1*}0,0,0) & (3_{\&y}^*0,0,0) & (3_{\&y}^{-1*}0,0,0)
\end{array}$$



$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(4_x^*0,0,0)$	$(4_x^{-1*}0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_{\&y}^*0,0,0)$
$(4_y^*0,0,0)$	$(4_y^{-1*}0,0,0)$	$(2_{xz}^*0,0,0)$	$(2_{\&z}^*0,0,0)$
$(4_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$	$(2_{yz}^*0,0,0)$	$(2_{\&z}^*0,0,0)$
$(\&^*0,0,0)'$	$(m_x^*0,0,0)'$	$(m_y^*0,0,0)'$	$(m_z^*0,0,0)'$
$(\&_{xyz}^*0,0,0)'$	$(\&_{xyz}^{-1*}0,0,0)'$	$(\&_{\&yz}^*0,0,0)'$	$(\&_{\&yz}^{-1*}0,0,0)'$
$(\&_{x\&z}^*0,0,0)'$	$(\&_{x\&z}^{-1*}0,0,0)'$	$(\&_{xy\&}^*0,0,0)'$	$(\&_{xy\&}^{-1*}0,0,0)'$
$(\&_x^*0,0,0)'$	$(\&_x^{-1*}0,0,0)'$	$(m_{xy}^*0,0,0)'$	$(m_{\&y}^*0,0,0)'$
$(\&_y^*0,0,0)'$	$(\&_y^{-1*}0,0,0)'$	$(m_{xz}^*0,0,0)'$	$(m_{\&z}^*0,0,0)'$
$(\&_z^*0,0,0)'$	$(\&_z^{-1*}0,0,0)'$	$(m_{yz}^*0,0,0)'$	$(m_{\&z}^*0,0,0)'$

221.6.1599  $P_F m\&m$   $Fm\&m$   $(0,0,0;a,b,c)$

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(4_x^*0,0,0)$	$(4_x^{-1*}0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_{\&y}^*0,0,0)$
$(4_y^*0,0,0)$	$(4_y^{-1*}0,0,0)$	$(2_{xz}^*0,0,0)$	$(2_{\&z}^*0,0,0)$
$(4_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$	$(2_{yz}^*0,0,0)$	$(2_{\&z}^*0,0,0)$

$(\&^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*0,0,0)$	$(m_z^*0,0,0)$
$(\&_{xyz}^*0,0,0)$	$(\&_{xyz}^{-1*}0,0,0)$	$(\&_{\&yz}^*0,0,0)$	$(\&_{\&yz}^{-1*}0,0,0)$
$(\&_{x\&z}^*0,0,0)$	$(\&_{x\&z}^{-1*}0,0,0)$	$(\&_{xy\&}^*0,0,0)$	$(\&_{xy\&}^{-1*}0,0,0)$
$(\&_x^*0,0,0)$	$(\&_x^{-1*}0,0,0)$	$(m_{xy}^*0,0,0)$	$(m_{\&y}^*0,0,0)$
$(\&_y^*0,0,0)$	$(\&_y^{-1*}0,0,0)$	$(m_{xz}^*0,0,0)$	$(m_{\&z}^*0,0,0)$
$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$	$(m_{yz}^*0,0,0)$	$(m_{\&z}^*0,0,0)$

221.7.1600  $P_F m\&m'$   $Fm\&c$   $(0,0,0;2a,2b,2c)$

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(4_x^*1,0,0)$	$(4_x^{-1*}1,0,0)$	$(2_{xy}^*1,0,0)$	$(2_{\&y}^*1,0,0)$
$(4_y^*1,0,0)$	$(4_y^{-1*}1,0,0)$	$(2_{xz}^*1,0,0)$	$(2_{\&z}^*1,0,0)$
$(4_z^*1,0,0)$	$(4_z^{-1*}1,0,0)$	$(2_{yz}^*1,0,0)$	$(2_{\&z}^*1,0,0)$
$(\&^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*0,0,0)$	$(m_z^*0,0,0)$

$(\&_{xyz}^*0,0,0)$	$(\&_{xyz}^{-1*}0,0,0)$	$(\&_{\&yz}^*0,0,0)$	$(\&_{\&yz}^{-1*}0,0,0)$
$(\&_{x\&z}^*0,0,0)$	$(\&_{x\&z}^{-1*}0,0,0)$	$(\&_{xy\&}^*0,0,0)$	$(\&_{xy\&}^{-1*}0,0,0)$
$(\&_x^*1,0,0)$	$(\&_x^{-1*}1,0,0)$	$(m_{xy}^*1,0,0)$	$(m_{\&y}^*1,0,0)$
$(\&_y^*1,0,0)$	$(\&_y^{-1*}1,0,0)$	$(m_{xz}^*1,0,0)$	$(m_{\&z}^*1,0,0)$
$(\&_z^*1,0,0)$	$(\&_z^{-1*}1,0,0)$	$(m_{yz}^*1,0,0)$	$(m_{\&z}^*1,0,0)$

222.1.1601 Pn&n

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(4_x^*0,0,0)$	$(4_x^{-1*}0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_{\&y}^*0,0,0)$
$(4_y^*0,0,0)$	$(4_y^{-1*}0,0,0)$	$(2_{xz}^*0,0,0)$	$(2_{\&z}^*0,0,0)$
$(4_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$	$(2_{yz}^*0,0,0)$	$(2_{\&z}^*0,0,0)$
$(\&^*1/2,1/2,1/2)$	$(m_x^*1/2,1/2,1/2)$	$(m_y^*1/2,1/2,1/2)$	$(m_z^*1/2,1/2,1/2)$
$(\&_{xyz}^*1/2,1/2,1/2)$	$(\&_{xyz}^{-1*}1/2,1/2,1/2)$	$(\&_{\&yz}^*1/2,1/2,1/2)$	$(\&_{\&yz}^{-1*}1/2,1/2,1/2)$
$(\&_{x\&z}^*1/2,1/2,1/2)$	$(\&_{x\&z}^{-1*}1/2,1/2,1/2)$	$(\&_{xy\&}^*1/2,1/2,1/2)$	$(\&_{xy\&}^{-1*}1/2,1/2,1/2)$
$(\&_x^*1/2,1/2,1/2)$	$(\&_x^{-1*}1/2,1/2,1/2)$	$(m_{xy}^*1/2,1/2,1/2)$	$(m_{\&y}^*1/2,1/2,1/2)$
$(\&_y^*1/2,1/2,1/2)$	$(\&_y^{-1*}1/2,1/2,1/2)$	$(m_{xz}^*1/2,1/2,1/2)$	$(m_{\&z}^*1/2,1/2,1/2)$
$(\&_z^*1/2,1/2,1/2)$	$(\&_z^{-1*}1/2,1/2,1/2)$	$(m_{yz}^*1/2,1/2,1/2)$	$(m_{\&z}^*1/2,1/2,1/2)$

222.2.1602 Pn&n1'

222.3.1603 Pn'&n

P&3n (0,0,0;a,b,c)

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(4_x^*0,0,0)'$	$(4_x^{-1*}0,0,0)'$	$(2_{xy}^*0,0,0)'$	$(2_{\&y}^*0,0,0)'$
$(4_y^*0,0,0)'$	$(4_y^{-1*}0,0,0)'$	$(2_{xz}^*0,0,0)'$	$(2_{\&z}^*0,0,0)'$
$(4_z^*0,0,0)'$	$(4_z^{-1*}0,0,0)'$	$(2_{yz}^*0,0,0)'$	$(2_{\&z}^*0,0,0)'$
$(\&^*1/2,1/2,1/2)'$	$(m_x^*1/2,1/2,1/2)'$	$(m_y^*1/2,1/2,1/2)'$	$(m_z^*1/2,1/2,1/2)'$
$(\&_{xyz}^*1/2,1/2,1/2)'$	$(\&_{xyz}^{-1*}1/2,1/2,1/2)'$	$(\&_{\&yz}^*1/2,1/2,1/2)'$	$(\&_{\&yz}^{-1*}1/2,1/2,1/2)'$
$(\&_{x\&z}^*1/2,1/2,1/2)'$	$(\&_{x\&z}^{-1*}1/2,1/2,1/2)'$	$(\&_{xy\&}^*1/2,1/2,1/2)'$	$(\&_{xy\&}^{-1*}1/2,1/2,1/2)'$
$(\&_x^*1/2,1/2,1/2)$	$(\&_x^{-1*}1/2,1/2,1/2)$	$(m_{xy}^*1/2,1/2,1/2)$	$(m_{\&y}^*1/2,1/2,1/2)$
$(\&_y^*1/2,1/2,1/2)$	$(\&_y^{-1*}1/2,1/2,1/2)$	$(m_{xz}^*1/2,1/2,1/2)$	$(m_{\&z}^*1/2,1/2,1/2)$
$(\&_z^*1/2,1/2,1/2)$	$(\&_z^{-1*}1/2,1/2,1/2)$	$(m_{yz}^*1/2,1/2,1/2)$	$(m_{\&z}^*1/2,1/2,1/2)$

222.4.1604	$Pn\bar{3}n'$	$Pn\bar{3}$	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\bar{y}z}^*0,0,0)$ $(4_x^*0,0,0)'$ $(4_y^*0,0,0)'$ $(4_z^*0,0,0)'$ $(\bar{6}_x^*1/2,1/2,1/2)$ $(\bar{6}_{xyz}^*1/2,1/2,1/2)$ $(\bar{6}_{x\bar{y}z}^*1/2,1/2,1/2)$ $(\bar{6}_x^*1/2,1/2,1/2)'$ $(\bar{6}_y^*1/2,1/2,1/2)'$ $(\bar{6}_z^*1/2,1/2,1/2)'$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\bar{y}z}^{-1*}0,0,0)$ $(4_x^{-1*}0,0,0)'$ $(4_y^{-1*}0,0,0)'$ $(4_z^{-1*}0,0,0)'$ $(m_x^*1/2,1/2,1/2)$ $(\bar{6}_{xyz}^{-1*}1/2,1/2,1/2)$ $(\bar{6}_{x\bar{y}z}^{-1*}1/2,1/2,1/2)$ $(\bar{6}_x^{-1*}1/2,1/2,1/2)'$ $(\bar{6}_y^{-1*}1/2,1/2,1/2)'$ $(\bar{6}_z^{-1*}1/2,1/2,1/2)'$	$(2_y^*0,0,0)$ $(3_{\bar{x}yz}^*0,0,0)$ $(3_{xy\bar{z}}^*0,0,0)$ $(2_{xy}^*0,0,0)'$ $(2_{xz}^*0,0,0)'$ $(2_{yz}^*0,0,0)'$ $(m_y^*1/2,1/2,1/2)$ $(\bar{6}_{\bar{y}z}^*1/2,1/2,1/2)$ $(\bar{6}_{xy\bar{z}}^*1/2,1/2,1/2)$ $(m_{xy}^*1/2,1/2,1/2)'$ $(m_{xz}^*1/2,1/2,1/2)'$ $(m_{yz}^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(3_{\bar{x}yz}^{-1*}0,0,0)$ $(3_{xy\bar{z}}^{-1*}0,0,0)$ $(2_{\bar{x}y}^*0,0,0)'$ $(2_{\bar{x}z}^*0,0,0)'$ $(2_{\bar{x}z}^*0,0,0)'$ $(m_z^*1/2,1/2,1/2)$ $(\bar{6}_{\bar{y}z}^{-1*}1/2,1/2,1/2)$ $(\bar{6}_{xy\bar{z}}^{-1*}1/2,1/2,1/2)$ $(m_{\bar{x}y}1/2,1/2,1/2)'$ $(m_{\bar{x}z}^*1/2,1/2,1/2)'$ $(m_{\bar{x}z}^*1/2,1/2,1/2)'$
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222.5.1605	$Pn'\bar{3}n'$	P432	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\bar{y}z}^*0,0,0)$ $(4_x^*0,0,0)$ $(4_y^*0,0,0)$ $(4_z^*0,0,0)$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\bar{y}z}^{-1*}0,0,0)$ $(4_x^{-1*}0,0,0)$ $(4_y^{-1*}0,0,0)$ $(4_z^{-1*}0,0,0)$	$(2_y^*0,0,0)$ $(3_{\bar{x}yz}^*0,0,0)$ $(3_{xy\bar{z}}^*0,0,0)$ $(2_{xy}^*0,0,0)$ $(2_{xz}^*0,0,0)$ $(2_{yz}^*0,0,0)$	$(2_z^*0,0,0)$ $(3_{\bar{x}yz}^{-1*}0,0,0)$ $(3_{xy\bar{z}}^{-1*}0,0,0)$ $(2_{\bar{x}y}^*0,0,0)$ $(2_{\bar{x}z}^*0,0,0)$ $(2_{\bar{x}z}^*0,0,0)$
				$(\bar{6}_x^*1/2,1/2,1/2)'$ $(\bar{6}_{xyz}^*1/2,1/2,1/2)'$ $(\bar{6}_{x\bar{y}z}^*1/2,1/2,1/2)'$ $(\bar{6}_x^*1/2,1/2,1/2)'$ $(\bar{6}_y^*1/2,1/2,1/2)'$ $(\bar{6}_z^*1/2,1/2,1/2)'$	$(m_x^*1/2,1/2,1/2)'$ $(\bar{6}_{xyz}^{-1*}1/2,1/2,1/2)'$ $(\bar{6}_{x\bar{y}z}^{-1*}1/2,1/2,1/2)'$ $(\bar{6}_x^{-1*}1/2,1/2,1/2)'$ $(\bar{6}_y^{-1*}1/2,1/2,1/2)'$ $(\bar{6}_z^{-1*}1/2,1/2,1/2)'$	$(m_y^*1/2,1/2,1/2)'$ $(\bar{6}_{\bar{y}z}^*1/2,1/2,1/2)'$ $(\bar{6}_{xy\bar{z}}^*1/2,1/2,1/2)'$ $(m_{xy}^*1/2,1/2,1/2)'$ $(m_{xz}^*1/2,1/2,1/2)'$ $(m_{yz}^*1/2,1/2,1/2)'$	$(m_z^*1/2,1/2,1/2)'$ $(\bar{6}_{\bar{y}z}^{-1*}1/2,1/2,1/2)'$ $(\bar{6}_{xy\bar{z}}^{-1*}1/2,1/2,1/2)'$ $(m_{\bar{x}y}1/2,1/2,1/2)'$ $(m_{\bar{x}z}^*1/2,1/2,1/2)'$ $(m_{\bar{x}z}^*1/2,1/2,1/2)'$

223.1.1606	$Pm\bar{3}n$			$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\bar{y}z}^*0,0,0)$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\bar{y}z}^{-1*}0,0,0)$	$(2_y^*0,0,0)$ $(3_{\bar{x}yz}^*0,0,0)$ $(3_{xy\bar{z}}^*0,0,0)$	$(2_z^*0,0,0)$ $(3_{\bar{x}yz}^{-1*}0,0,0)$ $(3_{xy\bar{z}}^{-1*}0,0,0)$
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$(4_x^* 1/2, 1/2, 1/2)$	$(4_x^{-1*} 1/2, 1/2, 1/2)$	$(2_{xy}^* 1/2, 1/2, 1/2)$	$(2_{&y}^* 1/2, 1/2, 1/2)$
$(4_y^* 1/2, 1/2, 1/2)$	$(4_y^{-1*} 1/2, 1/2, 1/2)$	$(2_{xz}^* 1/2, 1/2, 1/2)$	$(2_{&z}^* 1/2, 1/2, 1/2)$
$(4_z^* 1/2, 1/2, 1/2)$	$(4_z^{-1*} 1/2, 1/2, 1/2)$	$(2_{yz}^* 1/2, 1/2, 1/2)$	$(2_{&z}^* 1/2, 1/2, 1/2)$
$(\&^* 0, 0, 0)$	$(m_x^* 0, 0, 0)$	$(m_y^* 0, 0, 0)$	$(m_z^* 0, 0, 0)$
$(\&_{xyz}^* 0, 0, 0)$	$(\&_{xyz}^{-1*} 0, 0, 0)$	$(\&_{&yz}^* 0, 0, 0)$	$(\&_{&yz}^{-1*} 0, 0, 0)$
$(\&_{x&z}^* 0, 0, 0)$	$(\&_{x&z}^{-1*} 0, 0, 0)$	$(\&_{xy&}^* 0, 0, 0)$	$(\&_{xy&}^{-1*} 0, 0, 0)$
$(\&_x^* 1/2, 1/2, 1/2)$	$(\&_x^{-1*} 1/2, 1/2, 1/2)$	$(m_{xy}^* 1/2, 1/2, 1/2)$	$(m_{&y}^* 1/2, 1/2, 1/2)$
$(\&_y^* 1/2, 1/2, 1/2)$	$(\&_y^{-1*} 1/2, 1/2, 1/2)$	$(m_{xz}^* 1/2, 1/2, 1/2)$	$(m_{&z}^* 1/2, 1/2, 1/2)$
$(\&_z^* 1/2, 1/2, 1/2)$	$(\&_z^{-1*} 1/2, 1/2, 1/2)$	$(m_{yz}^* 1/2, 1/2, 1/2)$	$(m_{&z}^* 1/2, 1/2, 1/2)$

223.2.1607 Pm&n1'

223.3.1608 Pm'&n P&3n (0,0,0;a,b,c)

$(1^* 0, 0, 0)$	$(2_x^* 0, 0, 0)$	$(2_y^* 0, 0, 0)$	$(2_z^* 0, 0, 0)$
$(3_{xyz}^* 0, 0, 0)$	$(3_{xyz}^{-1*} 0, 0, 0)$	$(3_{&yz}^* 0, 0, 0)$	$(3_{&yz}^{-1*} 0, 0, 0)$
$(3_{x&z}^* 0, 0, 0)$	$(3_{x&z}^{-1*} 0, 0, 0)$	$(3_{xy&}^* 0, 0, 0)$	$(3_{xy&}^{-1*} 0, 0, 0)$
$(4_x^* 1/2, 1/2, 1/2)'$	$(4_x^{-1*} 1/2, 1/2, 1/2)'$	$(2_{xy}^* 1/2, 1/2, 1/2)'$	$(2_{&y}^* 1/2, 1/2, 1/2)'$
$(4_y^* 1/2, 1/2, 1/2)'$	$(4_y^{-1*} 1/2, 1/2, 1/2)'$	$(2_{xz}^* 1/2, 1/2, 1/2)'$	$(2_{&z}^* 1/2, 1/2, 1/2)'$
$(4_z^* 1/2, 1/2, 1/2)'$	$(4_z^{-1*} 1/2, 1/2, 1/2)'$	$(2_{yz}^* 1/2, 1/2, 1/2)'$	$(2_{&z}^* 1/2, 1/2, 1/2)'$
$(\&^* 0, 0, 0)'$	$(m_x^* 0, 0, 0)'$	$(m_y^* 0, 0, 0)'$	$(m_z^* 0, 0, 0)'$
$(\&_{xyz}^* 0, 0, 0)'$	$(\&_{xyz}^{-1*} 0, 0, 0)'$	$(\&_{&yz}^* 0, 0, 0)'$	$(\&_{&yz}^{-1*} 0, 0, 0)'$
$(\&_{x&z}^* 0, 0, 0)'$	$(\&_{x&z}^{-1*} 0, 0, 0)'$	$(\&_{xy&}^* 0, 0, 0)'$	$(\&_{xy&}^{-1*} 0, 0, 0)'$
$(\&_x^* 1/2, 1/2, 1/2)'$	$(\&_x^{-1*} 1/2, 1/2, 1/2)'$	$(m_{xy}^* 1/2, 1/2, 1/2)'$	$(m_{&y}^* 1/2, 1/2, 1/2)'$
$(\&_y^* 1/2, 1/2, 1/2)'$	$(\&_y^{-1*} 1/2, 1/2, 1/2)'$	$(m_{xz}^* 1/2, 1/2, 1/2)'$	$(m_{&z}^* 1/2, 1/2, 1/2)'$
$(\&_z^* 1/2, 1/2, 1/2)'$	$(\&_z^{-1*} 1/2, 1/2, 1/2)'$	$(m_{yz}^* 1/2, 1/2, 1/2)'$	$(m_{&z}^* 1/2, 1/2, 1/2)'$

223.4.1609 Pm&n' Pm& (0,0,0;a,b,c)

$(1^* 0, 0, 0)$	$(2_x^* 0, 0, 0)$	$(2_y^* 0, 0, 0)$	$(2_z^* 0, 0, 0)$
$(3_{xyz}^* 0, 0, 0)$	$(3_{xyz}^{-1*} 0, 0, 0)$	$(3_{&yz}^* 0, 0, 0)$	$(3_{&yz}^{-1*} 0, 0, 0)$
$(3_{x&z}^* 0, 0, 0)$	$(3_{x&z}^{-1*} 0, 0, 0)$	$(3_{xy&}^* 0, 0, 0)$	$(3_{xy&}^{-1*} 0, 0, 0)$
$(4_x^* 1/2, 1/2, 1/2)'$	$(4_x^{-1*} 1/2, 1/2, 1/2)'$	$(2_{xy}^* 1/2, 1/2, 1/2)'$	$(2_{&y}^* 1/2, 1/2, 1/2)'$
$(4_y^* 1/2, 1/2, 1/2)'$	$(4_y^{-1*} 1/2, 1/2, 1/2)'$	$(2_{xz}^* 1/2, 1/2, 1/2)'$	$(2_{&z}^* 1/2, 1/2, 1/2)'$
$(4_z^* 1/2, 1/2, 1/2)'$	$(4_z^{-1*} 1/2, 1/2, 1/2)'$	$(2_{yz}^* 1/2, 1/2, 1/2)'$	$(2_{&z}^* 1/2, 1/2, 1/2)'$
$(\&^* 0, 0, 0)$	$(m_x^* 0, 0, 0)$	$(m_y^* 0, 0, 0)$	$(m_z^* 0, 0, 0)$
$(\&_{xyz}^* 0, 0, 0)$	$(\&_{xyz}^{-1*} 0, 0, 0)$	$(\&_{&yz}^* 0, 0, 0)$	$(\&_{&yz}^{-1*} 0, 0, 0)$
$(\&_{x&z}^* 0, 0, 0)$	$(\&_{x&z}^{-1*} 0, 0, 0)$	$(\&_{xy&}^* 0, 0, 0)$	$(\&_{xy&}^{-1*} 0, 0, 0)$
$(\&_x^* 1/2, 1/2, 1/2)'$	$(\&_x^{-1*} 1/2, 1/2, 1/2)'$	$(m_{xy}^* 1/2, 1/2, 1/2)'$	$(m_{&y}^* 1/2, 1/2, 1/2)'$

$$\begin{array}{cccc}
 (\mathcal{E}_y^* 1/2, 1/2, 1/2)' & (\mathcal{E}_y^{-1*} 1/2, 1/2, 1/2)' & (m_{xz}^* 1/2, 1/2, 1/2)' & (m_{\mathcal{E}z}^* 1/2, 1/2, 1/2)' \\
 (\mathcal{E}_z^* 1/2, 1/2, 1/2)' & (\mathcal{E}_z^{-1*} 1/2, 1/2, 1/2)' & (m_{yz}^* 1/2, 1/2, 1/2)' & (m_{\mathcal{E}z}^* 1/2, 1/2, 1/2)'
 \end{array}$$

223.5.1610 Pm' $\mathcal{E}$ 'n' P4<sub>2</sub>32 (0,0,0;a,b,c)

$$\begin{array}{cccc}
 (1^*0,0,0) & (2_x^*0,0,0) & (2_y^*0,0,0) & (2_z^*0,0,0) \\
 (3_{xyz}^*0,0,0) & (3_{xyz}^{-1*}0,0,0) & (3_{\mathcal{E}yz}^*0,0,0) & (3_{\mathcal{E}yz}^{-1*}0,0,0) \\
 (3_{x\mathcal{E}z}^*0,0,0) & (3_{x\mathcal{E}z}^{-1*}0,0,0) & (3_{xy\mathcal{E}}^*0,0,0) & (3_{xy\mathcal{E}}^{-1*}0,0,0) \\
 (4_x^* 1/2, 1/2, 1/2) & (4_x^{-1*} 1/2, 1/2, 1/2) & (2_{xy}^* 1/2, 1/2, 1/2) & (2_{\mathcal{E}y}^* 1/2, 1/2, 1/2) \\
 (4_y^* 1/2, 1/2, 1/2) & (4_y^{-1*} 1/2, 1/2, 1/2) & (2_{xz}^* 1/2, 1/2, 1/2) & (2_{\mathcal{E}z}^* 1/2, 1/2, 1/2) \\
 (4_z^* 1/2, 1/2, 1/2) & (4_z^{-1*} 1/2, 1/2, 1/2) & (2_{yz}^* 1/2, 1/2, 1/2) & (2_{\mathcal{E}z}^* 1/2, 1/2, 1/2) \\
 (\mathcal{E}^*0,0,0)' & (m_x^*0,0,0)' & (m_y^*0,0,0)' & (m_z^*0,0,0)' \\
 (\mathcal{E}_{xyz}^*0,0,0)' & (\mathcal{E}_{xyz}^{-1*}0,0,0)' & (\mathcal{E}_{\mathcal{E}yz}^*0,0,0)' & (\mathcal{E}_{\mathcal{E}yz}^{-1*}0,0,0)' \\
 (\mathcal{E}_{x\mathcal{E}z}^*0,0,0)' & (\mathcal{E}_{x\mathcal{E}z}^{-1*}0,0,0)' & (\mathcal{E}_{xy\mathcal{E}}^*0,0,0)' & (\mathcal{E}_{xy\mathcal{E}}^{-1*}0,0,0)' \\
 (\mathcal{E}_x^* 1/2, 1/2, 1/2)' & (\mathcal{E}_x^{-1*} 1/2, 1/2, 1/2)' & (m_{xy}^* 1/2, 1/2, 1/2)' & (m_{\mathcal{E}y}^* 1/2, 1/2, 1/2)' \\
 (\mathcal{E}_y^* 1/2, 1/2, 1/2)' & (\mathcal{E}_y^{-1*} 1/2, 1/2, 1/2)' & (m_{xz}^* 1/2, 1/2, 1/2)' & (m_{\mathcal{E}z}^* 1/2, 1/2, 1/2)' \\
 (\mathcal{E}_z^* 1/2, 1/2, 1/2)' & (\mathcal{E}_z^{-1*} 1/2, 1/2, 1/2)' & (m_{yz}^* 1/2, 1/2, 1/2)' & (m_{\mathcal{E}z}^* 1/2, 1/2, 1/2)'
 \end{array}$$

224.1.1611 Pn $\mathcal{E}$ m

$$\begin{array}{cccc}
 (1^*0,0,0) & (2_x^*0,0,0) & (2_y^*0,0,0) & (2_z^*0,0,0) \\
 (3_{xyz}^*0,0,0) & (3_{xyz}^{-1*}0,0,0) & (3_{\mathcal{E}yz}^*0,0,0) & (3_{\mathcal{E}yz}^{-1*}0,0,0) \\
 (3_{x\mathcal{E}z}^*0,0,0) & (3_{x\mathcal{E}z}^{-1*}0,0,0) & (3_{xy\mathcal{E}}^*0,0,0) & (3_{xy\mathcal{E}}^{-1*}0,0,0) \\
 (4_x^* 1/2, 1/2, 1/2) & (4_x^{-1*} 1/2, 1/2, 1/2) & (2_{xy}^* 1/2, 1/2, 1/2) & (2_{\mathcal{E}y}^* 1/2, 1/2, 1/2) \\
 (4_y^* 1/2, 1/2, 1/2) & (4_y^{-1*} 1/2, 1/2, 1/2) & (2_{xz}^* 1/2, 1/2, 1/2) & (2_{\mathcal{E}z}^* 1/2, 1/2, 1/2) \\
 (4_z^* 1/2, 1/2, 1/2) & (4_z^{-1*} 1/2, 1/2, 1/2) & (2_{yz}^* 1/2, 1/2, 1/2) & (2_{\mathcal{E}z}^* 1/2, 1/2, 1/2) \\
 \\
 (\mathcal{E}^* 1/2, 1/2, 1/2) & (m_x^* 1/2, 1/2, 1/2) & (m_y^* 1/2, 1/2, 1/2) & (m_z^* 1/2, 1/2, 1/2) \\
 (\mathcal{E}_{xyz}^* 1/2, 1/2, 1/2) & (\mathcal{E}_{xyz}^{-1*} 1/2, 1/2, 1/2) & (\mathcal{E}_{\mathcal{E}yz}^* 1/2, 1/2, 1/2) & (\mathcal{E}_{\mathcal{E}yz}^{-1*} 1/2, 1/2, 1/2) \\
 (\mathcal{E}_{x\mathcal{E}z}^* 1/2, 1/2, 1/2) & (\mathcal{E}_{x\mathcal{E}z}^{-1*} 1/2, 1/2, 1/2) & (\mathcal{E}_{xy\mathcal{E}}^* 1/2, 1/2, 1/2) & (\mathcal{E}_{xy\mathcal{E}}^{-1*} 1/2, 1/2, 1/2) \\
 (\mathcal{E}_x^*0,0,0) & (\mathcal{E}_x^{-1*}0,0,0) & (m_{xy}^*0,0,0) & (m_{\mathcal{E}y}^*0,0,0) \\
 (\mathcal{E}_y^*0,0,0) & (\mathcal{E}_y^{-1*}0,0,0) & (m_{xz}^*0,0,0) & (m_{\mathcal{E}z}^*0,0,0) \\
 (\mathcal{E}_z^*0,0,0) & (\mathcal{E}_z^{-1*}0,0,0) & (m_{yz}^*0,0,0) & (m_{\mathcal{E}z}^*0,0,0)
 \end{array}$$

224.2.1612 Pn $\mathcal{E}$ m1'

224.3.1613	Pn' $\bar{6}$ m	P $\bar{6}$ 3m	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\bar{y}z}^*0,0,0)$ $(4_x^*1/2,1/2,1/2)'$ $(4_y^*1/2,1/2,1/2)'$ $(4_z^*1/2,1/2,1/2)'$ $(\bar{6}_{xyz}^*1/2,1/2,1/2)'$ $(\bar{6}_{x\bar{y}z}^*1/2,1/2,1/2)'$ $(\bar{6}_x^*0,0,0)$ $(\bar{6}_y^*0,0,0)$ $(\bar{6}_z^*0,0,0)$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\bar{y}z}^{-1*}0,0,0)$ $(4_x^{-1*}1/2,1/2,1/2)'$ $(4_y^{-1*}1/2,1/2,1/2)'$ $(4_z^{-1*}1/2,1/2,1/2)'$ $(m_x^*1/2,1/2,1/2)'$ $(\bar{6}_{xyz}^{-1*}1/2,1/2,1/2)'$ $(\bar{6}_x^{-1*}0,0,0)$ $(\bar{6}_y^{-1*}0,0,0)$ $(\bar{6}_z^{-1*}0,0,0)$	$(2_y^*0,0,0)$ $(3_{\bar{y}yz}^*0,0,0)$ $(3_{xy\bar{z}}^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)'$ $(2_{xz}^*1/2,1/2,1/2)'$ $(2_{yz}^*1/2,1/2,1/2)'$ $(m_y^*1/2,1/2,1/2)'$ $(\bar{6}_{\bar{y}yz}^*1/2,1/2,1/2)'$ $(m_{xy}^*0,0,0)$ $(m_{xz}^*0,0,0)$ $(m_{yz}^*0,0,0)$	$(2_z^*0,0,0)$ $(3_{\bar{y}z}^{-1*}0,0,0)$ $(3_{xy\bar{z}}^{-1*}0,0,0)$ $(2_{\bar{y}y}^*1/2,1/2,1/2)'$ $(2_{\bar{z}z}^*1/2,1/2,1/2)'$ $(2_{\bar{z}z}^*1/2,1/2,1/2)'$ $(m_z^*1/2,1/2,1/2)'$ $(\bar{6}_{\bar{y}z}^{-1*}1/2,1/2,1/2)'$ $(\bar{6}_{xy\bar{z}}^{-1*}1/2,1/2,1/2)'$ $(m_{\bar{y}y}^*0,0,0)$ $(m_{\bar{z}z}^*0,0,0)$ $(m_{\bar{z}z}^*0,0,0)$
224.4.1614	Pn' $\bar{6}$ m'	Pn $\bar{6}$	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\bar{y}z}^*0,0,0)$ $(4_x^*1/2,1/2,1/2)'$ $(4_y^*1/2,1/2,1/2)'$ $(4_z^*1/2,1/2,1/2)'$ $(\bar{6}_{xyz}^*1/2,1/2,1/2)$ $(\bar{6}_{x\bar{y}z}^*1/2,1/2,1/2)$ $(\bar{6}_x^*0,0,0)'$ $(\bar{6}_y^*0,0,0)'$ $(\bar{6}_z^*0,0,0)'$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\bar{y}z}^{-1*}0,0,0)$ $(4_x^{-1*}1/2,1/2,1/2)'$ $(4_y^{-1*}1/2,1/2,1/2)'$ $(4_z^{-1*}1/2,1/2,1/2)'$ $(m_x^*1/2,1/2,1/2)$ $(\bar{6}_{xyz}^{-1*}1/2,1/2,1/2)$ $(\bar{6}_x^{-1*}0,0,0)'$ $(\bar{6}_y^{-1*}0,0,0)'$ $(\bar{6}_z^{-1*}0,0,0)'$	$(2_y^*0,0,0)$ $(3_{\bar{y}yz}^*0,0,0)$ $(3_{xy\bar{z}}^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)'$ $(2_{xz}^*1/2,1/2,1/2)'$ $(2_{yz}^*1/2,1/2,1/2)'$ $(m_y^*1/2,1/2,1/2)$ $(\bar{6}_{\bar{y}yz}^*1/2,1/2,1/2)$ $(m_{xy}^*0,0,0)'$ $(m_{xz}^*0,0,0)'$ $(m_{yz}^*0,0,0)'$	$(2_z^*0,0,0)$ $(3_{\bar{y}z}^{-1*}0,0,0)$ $(3_{xy\bar{z}}^{-1*}0,0,0)$ $(2_{\bar{y}y}^*1/2,1/2,1/2)'$ $(2_{\bar{z}z}^*1/2,1/2,1/2)'$ $(2_{\bar{z}z}^*1/2,1/2,1/2)'$ $(m_z^*1/2,1/2,1/2)$ $(\bar{6}_{\bar{y}z}^{-1*}1/2,1/2,1/2)$ $(\bar{6}_{xy\bar{z}}^{-1*}1/2,1/2,1/2)$ $(m_{\bar{y}y}^*0,0,0)'$ $(m_{\bar{z}z}^*0,0,0)'$ $(m_{\bar{z}z}^*0,0,0)'$
224.5.1615	Pn' $\bar{6}$ m'	P4 <sub>2</sub> 32	(0,0,0;a,b,c)	$(1^*0,0,0)$ $(3_{xyz}^*0,0,0)$ $(3_{x\bar{y}z}^*0,0,0)$ $(4_x^*1/2,1/2,1/2)$ $(4_y^*1/2,1/2,1/2)$ $(4_z^*1/2,1/2,1/2)$ $(\bar{6}_{xyz}^*1/2,1/2,1/2)'$ $(\bar{6}_{x\bar{y}z}^*1/2,1/2,1/2)'$	$(2_x^*0,0,0)$ $(3_{xyz}^{-1*}0,0,0)$ $(3_{x\bar{y}z}^{-1*}0,0,0)$ $(4_x^{-1*}1/2,1/2,1/2)$ $(4_y^{-1*}1/2,1/2,1/2)$ $(4_z^{-1*}1/2,1/2,1/2)$ $(m_x^*1/2,1/2,1/2)'$ $(\bar{6}_{xyz}^{-1*}1/2,1/2,1/2)'$ $(\bar{6}_{x\bar{y}z}^{-1*}1/2,1/2,1/2)'$	$(2_y^*0,0,0)$ $(3_{\bar{y}yz}^*0,0,0)$ $(3_{xy\bar{z}}^*0,0,0)$ $(2_{xy}^*1/2,1/2,1/2)$ $(2_{xz}^*1/2,1/2,1/2)$ $(2_{yz}^*1/2,1/2,1/2)$ $(m_y^*1/2,1/2,1/2)'$ $(\bar{6}_{\bar{y}yz}^*1/2,1/2,1/2)'$	$(2_z^*0,0,0)$ $(3_{\bar{y}z}^{-1*}0,0,0)$ $(3_{xy\bar{z}}^{-1*}0,0,0)$ $(2_{\bar{y}y}^*1/2,1/2,1/2)$ $(2_{\bar{z}z}^*1/2,1/2,1/2)$ $(2_{\bar{z}z}^*1/2,1/2,1/2)$ $(m_z^*1/2,1/2,1/2)'$ $(\bar{6}_{\bar{y}z}^{-1*}1/2,1/2,1/2)'$ $(\bar{6}_{xy\bar{z}}^{-1*}1/2,1/2,1/2)'$

$$\begin{array}{cccc}
(\mathcal{E}_{x\&yz}^* 1/2, 1/2, 1/2)' & (\mathcal{E}_{x\&yz}^{-1*} 1/2, 1/2, 1/2)' & (\mathcal{E}_{xy\&}^* 1/2, 1/2, 1/2)' & (\mathcal{E}_{xy\&}^{-1*} 1/2, 1/2, 1/2)' \\
(\mathcal{E}_x^* 0, 0, 0)' & (\mathcal{E}_x^{-1*} 0, 0, 0)' & (m_{xy}^* 0, 0, 0)' & (m_{\&y}^* 0, 0, 0)' \\
(\mathcal{E}_y^* 0, 0, 0)' & (\mathcal{E}_y^{-1*} 0, 0, 0)' & (m_{xz}^* 0, 0, 0)' & (m_{\&z}^* 0, 0, 0)' \\
(\mathcal{E}_z^* 0, 0, 0)' & (\mathcal{E}_z^{-1*} 0, 0, 0)' & (m_{yz}^* 0, 0, 0)' & (m_{\&z}^* 0, 0, 0)'
\end{array}$$

224.6.1616  $P_{F_n}\mathcal{E}m$   $Fd\mathcal{E}m$  (0,0,0;2a,2b,2c)

$$\begin{array}{cccc}
(1^* 0, 0, 0) & (2_x^* 0, 0, 0) & (2_y^* 0, 0, 0) & (2_z^* 0, 0, 0) \\
(3_{xyz}^* 0, 0, 0) & (3_{xyz}^{-1*} 0, 0, 0) & (3_{\&yz}^* 0, 0, 0) & (3_{\&yz}^{-1*} 0, 0, 0) \\
(3_{x\&z}^* 0, 0, 0) & (3_{x\&z}^{-1*} 0, 0, 0) & (3_{xy\&}^* 0, 0, 0) & (3_{xy\&}^{-1*} 0, 0, 0) \\
(4_x^* 1/2, 1/2, 1/2) & (4_x^{-1*} 1/2, 1/2, 1/2) & (2_{xy}^* 1/2, 1/2, 1/2) & (2_{\&y}^* 1/2, 1/2, 1/2) \\
(4_y^* 1/2, 1/2, 1/2) & (4_y^{-1*} 1/2, 1/2, 1/2) & (2_{xz}^* 1/2, 1/2, 1/2) & (2_{\&z}^* 1/2, 1/2, 1/2) \\
(4_z^* 1/2, 1/2, 1/2) & (4_z^{-1*} 1/2, 1/2, 1/2) & (2_{yz}^* 1/2, 1/2, 1/2) & (2_{\&z}^* 1/2, 1/2, 1/2) \\
(\mathcal{E}^* 1/2, 1/2, 1/2) & (m_x^* 1/2, 1/2, 1/2) & (m_y^* 1/2, 1/2, 1/2) & (m_z^* 1/2, 1/2, 1/2) \\
(\mathcal{E}_{xyz}^* 1/2, 1/2, 1/2) & (\mathcal{E}_{xyz}^{-1*} 1/2, 1/2, 1/2) & (\mathcal{E}_{\&yz}^* 1/2, 1/2, 1/2) & (\mathcal{E}_{\&yz}^{-1*} 1/2, 1/2, 1/2) \\
(\mathcal{E}_{x\&z}^* 1/2, 1/2, 1/2) & (\mathcal{E}_{x\&z}^{-1*} 1/2, 1/2, 1/2) & (\mathcal{E}_{xy\&}^* 1/2, 1/2, 1/2) & (\mathcal{E}_{xy\&}^{-1*} 1/2, 1/2, 1/2) \\
(\mathcal{E}_x^* 0, 0, 0) & (\mathcal{E}_x^{-1*} 0, 0, 0) & (m_{xy}^* 0, 0, 0) & (m_{\&y}^* 0, 0, 0) \\
(\mathcal{E}_y^* 0, 0, 0) & (\mathcal{E}_y^{-1*} 0, 0, 0) & (m_{xz}^* 0, 0, 0) & (m_{\&z}^* 0, 0, 0) \\
(\mathcal{E}_z^* 0, 0, 0) & (\mathcal{E}_z^{-1*} 0, 0, 0) & (m_{yz}^* 0, 0, 0) & (m_{\&z}^* 0, 0, 0)
\end{array}$$

224.7.1617  $P_{F_n}\mathcal{E}m'$   $Fd\mathcal{E}c$  (0,0,0;2a,2b,2c)

$$\begin{array}{cccc}
(1^* 0, 0, 0) & (2_x^* 0, 0, 0) & (2_y^* 0, 0, 0) & (2_z^* 0, 0, 0) \\
(3_{xyz}^* 0, 0, 0) & (3_{xyz}^{-1*} 0, 0, 0) & (3_{\&yz}^* 0, 0, 0) & (3_{\&yz}^{-1*} 0, 0, 0) \\
(3_{x\&z}^* 0, 0, 0) & (3_{x\&z}^{-1*} 0, 0, 0) & (3_{xy\&}^* 0, 0, 0) & (3_{xy\&}^{-1*} 0, 0, 0) \\
(4_x^* 3/2, 1/2, 1/2) & (4_x^{-1*} 3/2, 1/2, 1/2) & (2_{xy}^* 3/2, 1/2, 1/2) & (2_{\&y}^* 3/2, 1/2, 1/2) \\
(4_y^* 3/2, 1/2, 1/2) & (4_y^{-1*} 3/2, 1/2, 1/2) & (2_{xz}^* 3/2, 1/2, 1/2) & (2_{\&z}^* 3/2, 1/2, 1/2) \\
(4_z^* 3/2, 1/2, 1/2) & (4_z^{-1*} 3/2, 1/2, 1/2) & (2_{yz}^* 3/2, 1/2, 1/2) & (2_{\&z}^* 3/2, 1/2, 1/2)
\end{array}$$

$$\begin{array}{cccc}
(\mathcal{E}^* 1/2, 1/2, 1/2) & (m_x^* 1/2, 1/2, 1/2) & (m_y^* 1/2, 1/2, 1/2) & (m_z^* 1/2, 1/2, 1/2) \\
(\mathcal{E}_{xyz}^* 1/2, 1/2, 1/2) & (\mathcal{E}_{xyz}^{-1*} 1/2, 1/2, 1/2) & (\mathcal{E}_{\&yz}^* 1/2, 1/2, 1/2) & (\mathcal{E}_{\&yz}^{-1*} 1/2, 1/2, 1/2) \\
(\mathcal{E}_{x\&z}^* 1/2, 1/2, 1/2) & (\mathcal{E}_{x\&z}^{-1*} 1/2, 1/2, 1/2) & (\mathcal{E}_{xy\&}^* 1/2, 1/2, 1/2) & (\mathcal{E}_{xy\&}^{-1*} 1/2, 1/2, 1/2) \\
(\mathcal{E}_x^* 1, 0, 0) & (\mathcal{E}_x^{-1*} 1, 0, 0) & (m_{xy}^* 1, 0, 0) & (m_{\&y}^* 1, 0, 0) \\
(\mathcal{E}_y^* 1, 0, 0) & (\mathcal{E}_y^{-1*} 1, 0, 0) & (m_{xz}^* 1, 0, 0) & (m_{\&z}^* 1, 0, 0) \\
(\mathcal{E}_z^* 1, 0, 0) & (\mathcal{E}_z^{-1*} 1, 0, 0) & (m_{yz}^* 1, 0, 0) & (m_{\&z}^* 1, 0, 0)
\end{array}$$

225.1.1618 Fm $\bar{2}$ m

(1*0,0,0)	(2 <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)
(3 <sub>xyz</sub> *0,0,0)	(3 <sub>xyz</sub> <sup>-1</sup> *0,0,0)	(3 <sub>xyz</sub> *0,0,0)	(3 <sub>xyz</sub> <sup>-1</sup> *0,0,0)
(3 <sub>x&amp;z</sub> *0,0,0)	(3 <sub>x&amp;z</sub> <sup>-1</sup> *0,0,0)	(3 <sub>xy&amp;</sub> *0,0,0)	(3 <sub>xy&amp;</sub> <sup>-1</sup> *0,0,0)
(4 <sub>x</sub> *0,0,0)	(4 <sub>x</sub> <sup>-1</sup> *0,0,0)	(2 <sub>xy</sub> *0,0,0)	(2 <sub>&amp;y</sub> *0,0,0)
(4 <sub>y</sub> *0,0,0)	(4 <sub>y</sub> <sup>-1</sup> *0,0,0)	(2 <sub>xz</sub> *0,0,0)	(2 <sub>&amp;z</sub> *0,0,0)
(4 <sub>z</sub> *0,0,0)	(4 <sub>z</sub> <sup>-1</sup> *0,0,0)	(2 <sub>yz</sub> *0,0,0)	(2 <sub>&amp;z</sub> *0,0,0)
(&*0,0,0)	(m <sub>x</sub> *0,0,0)	(m <sub>y</sub> *0,0,0)	(m <sub>z</sub> *0,0,0)
(& <sub>xyz</sub> *0,0,0)	(& <sub>xyz</sub> <sup>-1</sup> *0,0,0)	(& <sub>xyz</sub> *0,0,0)	(& <sub>xyz</sub> <sup>-1</sup> *0,0,0)
(& <sub>x&amp;z</sub> *0,0,0)	(& <sub>x&amp;z</sub> <sup>-1</sup> *0,0,0)	(& <sub>xy&amp;</sub> *0,0,0)	(& <sub>xy&amp;</sub> <sup>-1</sup> *0,0,0)
(& <sub>x</sub> *0,0,0)	(& <sub>x</sub> <sup>-1</sup> *0,0,0)	(m <sub>xy</sub> *0,0,0)	(m <sub>&amp;y</sub> *0,0,0)
(& <sub>y</sub> *0,0,0)	(& <sub>y</sub> <sup>-1</sup> *0,0,0)	(m <sub>xz</sub> *0,0,0)	(m <sub>&amp;z</sub> *0,0,0)
(& <sub>z</sub> *0,0,0)	(& <sub>z</sub> <sup>-1</sup> *0,0,0)	(m <sub>yz</sub> *0,0,0)	(m <sub>&amp;z</sub> *0,0,0)

225.2.1619 Fm $\bar{2}$ m1'

225.3.1620 Fm' $\bar{2}$ 'm F $\bar{2}$ 3m (0,0,0;a,b,c)

(1*0,0,0)	(2 <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)
(3 <sub>xyz</sub> *0,0,0)	(3 <sub>xyz</sub> <sup>-1</sup> *0,0,0)	(3 <sub>xyz</sub> *0,0,0)	(3 <sub>xyz</sub> <sup>-1</sup> *0,0,0)
(3 <sub>x&amp;z</sub> *0,0,0)	(3 <sub>x&amp;z</sub> <sup>-1</sup> *0,0,0)	(3 <sub>xy&amp;</sub> *0,0,0)	(3 <sub>xy&amp;</sub> <sup>-1</sup> *0,0,0)
(4 <sub>x</sub> *0,0,0)'	(4 <sub>x</sub> <sup>-1</sup> *0,0,0)'	(2 <sub>xy</sub> *0,0,0)'	(2 <sub>&amp;y</sub> *0,0,0)'
(4 <sub>y</sub> *0,0,0)'	(4 <sub>y</sub> <sup>-1</sup> *0,0,0)'	(2 <sub>xz</sub> *0,0,0)'	(2 <sub>&amp;z</sub> *0,0,0)'
(4 <sub>z</sub> *0,0,0)'	(4 <sub>z</sub> <sup>-1</sup> *0,0,0)'	(2 <sub>yz</sub> *0,0,0)'	(2 <sub>&amp;z</sub> *0,0,0)'
(&*0,0,0)'	(m <sub>x</sub> *0,0,0)'	(m <sub>y</sub> *0,0,0)'	(m <sub>z</sub> *0,0,0)'
(& <sub>xyz</sub> *0,0,0)'	(& <sub>xyz</sub> <sup>-1</sup> *0,0,0)'	(& <sub>xyz</sub> *0,0,0)'	(& <sub>xyz</sub> <sup>-1</sup> *0,0,0)'
(& <sub>x&amp;z</sub> *0,0,0)'	(& <sub>x&amp;z</sub> <sup>-1</sup> *0,0,0)'	(& <sub>xy&amp;</sub> *0,0,0)'	(& <sub>xy&amp;</sub> <sup>-1</sup> *0,0,0)'
(& <sub>x</sub> *0,0,0)	(& <sub>x</sub> <sup>-1</sup> *0,0,0)	(m <sub>xy</sub> *0,0,0)	(m <sub>&amp;y</sub> *0,0,0)
(& <sub>y</sub> *0,0,0)	(& <sub>y</sub> <sup>-1</sup> *0,0,0)	(m <sub>xz</sub> *0,0,0)	(m <sub>&amp;z</sub> *0,0,0)
(& <sub>z</sub> *0,0,0)	(& <sub>z</sub> <sup>-1</sup> *0,0,0)	(m <sub>yz</sub> *0,0,0)	(m <sub>&amp;z</sub> *0,0,0)

225.4.1621 Fm $\bar{2}$ m' Fm $\bar{2}$  (0,0,0;a,b,c)

(1*0,0,0)	(2 <sub>x</sub> *0,0,0)	(2 <sub>y</sub> *0,0,0)	(2 <sub>z</sub> *0,0,0)
(3 <sub>xyz</sub> *0,0,0)	(3 <sub>xyz</sub> <sup>-1</sup> *0,0,0)	(3 <sub>xyz</sub> *0,0,0)	(3 <sub>xyz</sub> <sup>-1</sup> *0,0,0)
(3 <sub>x&amp;z</sub> *0,0,0)	(3 <sub>x&amp;z</sub> <sup>-1</sup> *0,0,0)	(3 <sub>xy&amp;</sub> *0,0,0)	(3 <sub>xy&amp;</sub> <sup>-1</sup> *0,0,0)
(4 <sub>x</sub> *0,0,0)'	(4 <sub>x</sub> <sup>-1</sup> *0,0,0)'	(2 <sub>xy</sub> *0,0,0)'	(2 <sub>&amp;y</sub> *0,0,0)'
(4 <sub>y</sub> *0,0,0)'	(4 <sub>y</sub> <sup>-1</sup> *0,0,0)'	(2 <sub>xz</sub> *0,0,0)'	(2 <sub>&amp;z</sub> *0,0,0)'



$(4_z^*0,0,0)'$	$(4_x^{-1}0,0,0)'$	$(2_y^*0,0,0)'$	$(2_z^*0,0,0)'$
$(\&^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*0,0,0)$	$(m_z^*0,0,0)$
$(\&_{xyz}^*0,0,0)$	$(\&_{xyz}^{-1}0,0,0)$	$(\&_{\&yz}^*0,0,0)$	$(\&_{\&yz}^{-1}0,0,0)$
$(\&_{x\&z}^*0,0,0)$	$(\&_{x\&z}^{-1}0,0,0)$	$(\&_{xy\&}^*0,0,0)$	$(\&_{xy\&}^{-1}0,0,0)$
$(\&_x^*0,0,0)'$	$(\&_x^{-1}0,0,0)'$	$(m_{xy}^*0,0,0)'$	$(m_{\&y}^*0,0,0)'$
$(\&_y^*0,0,0)'$	$(\&_y^{-1}0,0,0)'$	$(m_{xz}^*0,0,0)'$	$(m_{\&z}^*0,0,0)'$
$(\&_z^*0,0,0)'$	$(\&_z^{-1}0,0,0)'$	$(m_{yz}^*0,0,0)'$	$(m_{\&z}^*0,0,0)'$

225.5.1622 Fm' $\&$ 'm' F432 (0,0,0;a,b,c)

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1}0,0,0)$
$(4_x^*0,0,0)$	$(4_x^{-1}0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_{\&y}^*0,0,0)$
$(4_y^*0,0,0)$	$(4_y^{-1}0,0,0)$	$(2_{xz}^*0,0,0)$	$(2_{\&z}^*0,0,0)$
$(4_z^*0,0,0)$	$(4_z^{-1}0,0,0)$	$(2_{yz}^*0,0,0)$	$(2_{\&z}^*0,0,0)$
$(\&^*0,0,0)'$	$(m_x^*0,0,0)'$	$(m_y^*0,0,0)'$	$(m_z^*0,0,0)'$
$(\&_{xyz}^*0,0,0)'$	$(\&_{xyz}^{-1}0,0,0)'$	$(\&_{\&yz}^*0,0,0)'$	$(\&_{\&yz}^{-1}0,0,0)'$
$(\&_{x\&z}^*0,0,0)'$	$(\&_{x\&z}^{-1}0,0,0)'$	$(\&_{xy\&}^*0,0,0)'$	$(\&_{xy\&}^{-1}0,0,0)'$
$(\&_x^*0,0,0)'$	$(\&_x^{-1}0,0,0)'$	$(m_{xy}^*0,0,0)'$	$(m_{\&y}^*0,0,0)'$
$(\&_y^*0,0,0)'$	$(\&_y^{-1}0,0,0)'$	$(m_{xz}^*0,0,0)'$	$(m_{\&z}^*0,0,0)'$
$(\&_z^*0,0,0)'$	$(\&_z^{-1}0,0,0)'$	$(m_{yz}^*0,0,0)'$	$(m_{\&z}^*0,0,0)'$

226.1.1623 Fm $\&$ c

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1}0,0,0)$
$(4_x^*1/2,1/2,1/2)$	$(4_x^{-1}1/2,1/2,1/2)$	$(2_{xy}^*1/2,1/2,1/2)$	$(2_{\&y}^*1/2,1/2,1/2)$
$(4_y^*1/2,1/2,1/2)$	$(4_y^{-1}1/2,1/2,1/2)$	$(2_{xz}^*1/2,1/2,1/2)$	$(2_{\&z}^*1/2,1/2,1/2)$
$(4_z^*1/2,1/2,1/2)$	$(4_z^{-1}1/2,1/2,1/2)$	$(2_{yz}^*1/2,1/2,1/2)$	$(2_{\&z}^*1/2,1/2,1/2)$
$(\&^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*0,0,0)$	$(m_z^*0,0,0)$
$(\&_{xyz}^*0,0,0)$	$(\&_{xyz}^{-1}0,0,0)$	$(\&_{\&yz}^*0,0,0)$	$(\&_{\&yz}^{-1}0,0,0)$
$(\&_{x\&z}^*0,0,0)$	$(\&_{x\&z}^{-1}0,0,0)$	$(\&_{xy\&}^*0,0,0)$	$(\&_{xy\&}^{-1}0,0,0)$
$(\&_x^*1/2,1/2,1/2)$	$(\&_x^{-1}1/2,1/2,1/2)$	$(m_{xy}^*1/2,1/2,1/2)$	$(m_{\&y}^*1/2,1/2,1/2)$

$$\begin{matrix}
 (\mathcal{E}_y^* 1/2, 1/2, 1/2) & (\mathcal{E}_y^{-1*} 1/2, 1/2, 1/2) & (m_{xz}^* 1/2, 1/2, 1/2) & (m_{\mathcal{E}z}^* 1/2, 1/2, 1/2) \\
 (\mathcal{E}_z^* 1/2, 1/2, 1/2) & (\mathcal{E}_z^{-1*} 1/2, 1/2, 1/2) & (m_{yz}^* 1/2, 1/2, 1/2) & (m_{\mathcal{E}z}^* 1/2, 1/2, 1/2)
 \end{matrix}$$

226.2.1624 Fm $\mathcal{E}$ c1'

226.3.1625 Fm' $\mathcal{E}$ 'c F $\mathcal{E}$ 3c (0,0,0;a,b,c)

$$\begin{matrix}
 (1^*0,0,0) & (2_x^*0,0,0) & (2_y^*0,0,0) & (2_z^*0,0,0) \\
 (3_{xyz}^*0,0,0) & (3_{xyz}^{-1*}0,0,0) & (3_{\mathcal{E}yz}^*0,0,0) & (3_{\mathcal{E}yz}^{-1*}0,0,0) \\
 (3_{x\mathcal{E}z}^*0,0,0) & (3_{x\mathcal{E}z}^{-1*}0,0,0) & (3_{xy\mathcal{E}}^*0,0,0) & (3_{xy\mathcal{E}}^{-1*}0,0,0) \\
 (4_x^* 1/2, 1/2, 1/2)' & (4_x^{-1*} 1/2, 1/2, 1/2)' & (2_{xy}^* 1/2, 1/2, 1/2) & (2_{\mathcal{E}y}^* 1/2, 1/2, 1/2)' \\
 (4_y^* 1/2, 1/2, 1/2)' & (4_y^{-1*} 1/2, 1/2, 1/2)' & (2_{xz}^* 1/2, 1/2, 1/2)' & (2_{\mathcal{E}z}^* 1/2, 1/2, 1/2)' \\
 (4_z^* 1/2, 1/2, 1/2)' & (4_z^{-1*} 1/2, 1/2, 1/2)' & (2_{yz}^* 1/2, 1/2, 1/2)' & (2_{\mathcal{E}z}^* 1/2, 1/2, 1/2)' \\
 (\mathcal{E}^*0,0,0)' & (m_x^*0,0,0)' & (m_y^*0,0,0)' & (m_z^*0,0,0)' \\
 (\mathcal{E}_{xyz}^*0,0,0)' & (\mathcal{E}_{xyz}^{-1*}0,0,0)' & (\mathcal{E}_{\mathcal{E}yz}^*0,0,0)' & (\mathcal{E}_{\mathcal{E}yz}^{-1*}0,0,0)' \\
 (\mathcal{E}_{x\mathcal{E}z}^*0,0,0)' & (\mathcal{E}_{x\mathcal{E}z}^{-1*}0,0,0)' & (\mathcal{E}_{xy\mathcal{E}}^*0,0,0)' & (\mathcal{E}_{xy\mathcal{E}}^{-1*}0,0,0)' \\
 (\mathcal{E}_x^* 1/2, 1/2, 1/2) & (\mathcal{E}_x^{-1*} 1/2, 1/2, 1/2) & (m_{xy}^* 1/2, 1/2, 1/2) & (m_{\mathcal{E}y}^* 1/2, 1/2, 1/2) \\
 (\mathcal{E}_y^* 1/2, 1/2, 1/2) & (\mathcal{E}_y^{-1*} 1/2, 1/2, 1/2) & (m_{xz}^* 1/2, 1/2, 1/2) & (m_{\mathcal{E}z}^* 1/2, 1/2, 1/2) \\
 (\mathcal{E}_z^* 1/2, 1/2, 1/2) & (\mathcal{E}_z^{-1*} 1/2, 1/2, 1/2) & (m_{yz}^* 1/2, 1/2, 1/2) & (m_{\mathcal{E}z}^* 1/2, 1/2, 1/2)
 \end{matrix}$$

226.4.1626 Fm $\mathcal{E}$ 'c' Fm $\mathcal{E}$  (0,0,0;a,b,c)

$$\begin{matrix}
 (1^*0,0,0) & (2_x^*0,0,0) & (2_y^*0,0,0) & (2_z^*0,0,0) \\
 (3_{xyz}^*0,0,0) & (3_{xyz}^{-1*}0,0,0) & (3_{\mathcal{E}yz}^*0,0,0) & (3_{\mathcal{E}yz}^{-1*}0,0,0) \\
 (3_{x\mathcal{E}z}^*0,0,0) & (3_{x\mathcal{E}z}^{-1*}0,0,0) & (3_{xy\mathcal{E}}^*0,0,0) & (3_{xy\mathcal{E}}^{-1*}0,0,0) \\
 (4_x^* 1/2, 1/2, 1/2)' & (4_x^{-1*} 1/2, 1/2, 1/2)' & (2_{xy}^* 1/2, 1/2, 1/2)' & (2_{\mathcal{E}y}^* 1/2, 1/2, 1/2)' \\
 (4_y^* 1/2, 1/2, 1/2)' & (4_y^{-1*} 1/2, 1/2, 1/2)' & (2_{xz}^* 1/2, 1/2, 1/2)' & (2_{\mathcal{E}z}^* 1/2, 1/2, 1/2)' \\
 (4_z^* 1/2, 1/2, 1/2)' & (4_z^{-1*} 1/2, 1/2, 1/2)' & (2_{yz}^* 1/2, 1/2, 1/2)' & (2_{\mathcal{E}z}^* 1/2, 1/2, 1/2)' \\
 (\mathcal{E}^*0,0,0) & (m_x^*0,0,0) & (m_y^*0,0,0) & (m_z^*0,0,0) \\
 (\mathcal{E}_{xyz}^*0,0,0) & (\mathcal{E}_{xyz}^{-1*}0,0,0) & (\mathcal{E}_{\mathcal{E}yz}^*0,0,0) & (\mathcal{E}_{\mathcal{E}yz}^{-1*}0,0,0) \\
 (\mathcal{E}_{x\mathcal{E}z}^*0,0,0) & (\mathcal{E}_{x\mathcal{E}z}^{-1*}0,0,0) & (\mathcal{E}_{xy\mathcal{E}}^*0,0,0) & (\mathcal{E}_{xy\mathcal{E}}^{-1*}0,0,0) \\
 (\mathcal{E}_x^* 1/2, 1/2, 1/2)' & (\mathcal{E}_x^{-1*} 1/2, 1/2, 1/2)' & (m_{xy}^* 1/2, 1/2, 1/2)' & (m_{\mathcal{E}y}^* 1/2, 1/2, 1/2)' \\
 (\mathcal{E}_y^* 1/2, 1/2, 1/2)' & (\mathcal{E}_y^{-1*} 1/2, 1/2, 1/2)' & (m_{xz}^* 1/2, 1/2, 1/2)' & (m_{\mathcal{E}z}^* 1/2, 1/2, 1/2)' \\
 (\mathcal{E}_z^* 1/2, 1/2, 1/2)' & (\mathcal{E}_z^{-1*} 1/2, 1/2, 1/2)' & (m_{yz}^* 1/2, 1/2, 1/2)' & (m_{\mathcal{E}z}^* 1/2, 1/2, 1/2)'
 \end{matrix}$$

226.5.1627 Fm' $\mathcal{E}$ 'c' F432 (1/4,1/4,1/4;a,b,c)

$$\begin{matrix}
 (1^*0,0,0) & (2_x^*0,0,0) & (2_y^*0,0,0) & (2_z^*0,0,0) \\
 (3_{xyz}^*0,0,0) & (3_{xyz}^{-1*}0,0,0) & (3_{\mathcal{E}yz}^*0,0,0) & (3_{\mathcal{E}yz}^{-1*}0,0,0)
 \end{matrix}$$

$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(4_x^*1/2,1/2,1/2)$	$(4_x^{-1*}1/2,1/2,1/2)$	$(2_{xy}^*1/2,1/2,1/2)$	$(2_{xy}^{-1*}1/2,1/2,1/2)$
$(4_y^*1/2,1/2,1/2)$	$(4_y^{-1*}1/2,1/2,1/2)$	$(2_{xz}^*1/2,1/2,1/2)$	$(2_{xz}^{-1*}1/2,1/2,1/2)$
$(4_z^*1/2,1/2,1/2)$	$(4_z^{-1*}1/2,1/2,1/2)$	$(2_{yz}^*1/2,1/2,1/2)$	$(2_{yz}^{-1*}1/2,1/2,1/2)$
$(\&^*0,0,0)'$	$(m_x^*0,0,0)'$	$(m_y^*0,0,0)'$	$(m_z^*0,0,0)'$
$(\&_{xyz}^*0,0,0)'$	$(\&_{xyz}^{-1*}0,0,0)'$	$(\&_{\&yz}^*0,0,0)'$	$(\&_{\&yz}^{-1*}0,0,0)'$
$(\&_{x\&z}^*0,0,0)'$	$(\&_{x\&z}^{-1*}0,0,0)'$	$(\&_{xy\&}^*0,0,0)'$	$(\&_{xy\&}^{-1*}0,0,0)'$
$(\&_x^*1/2,1/2,1/2)'$	$(\&_x^{-1*}1/2,1/2,1/2)'$	$(m_{xy}^*1/2,1/2,1/2)'$	$(m_{\&y}^*1/2,1/2,1/2)'$
$(\&_y^*1/2,1/2,1/2)'$	$(\&_y^{-1*}1/2,1/2,1/2)'$	$(m_{xz}^*1/2,1/2,1/2)'$	$(m_{\&z}^*1/2,1/2,1/2)'$
$(\&_z^*1/2,1/2,1/2)'$	$(\&_z^{-1*}1/2,1/2,1/2)'$	$(m_{yz}^*1/2,1/2,1/2)'$	$(m_{\&z}^*1/2,1/2,1/2)'$

227.1.1628 Fd&m

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(4_x^*1/4,3/4,3/4)$	$(4_x^{-1*}3/4,1/4,3/4)$	$(2_{xy}^*3/4,1/4,3/4)$	$(2_{xy}^{-1*}1/4,1/4,1/4)$
$(4_y^*3/4,1/4,3/4)$	$(4_y^{-1*}3/4,3/4,1/4)$	$(2_{xz}^*1/4,3/4,3/4)$	$(2_{xz}^{-1*}1/4,1/4,1/4)$
$(4_z^*3/4,3/4,1/4)$	$(4_z^{-1*}1/4,3/4,3/4)$	$(2_{yz}^*3/4,3/4,1/4)$	$(2_{yz}^{-1*}1/4,1/4,1/4)$
$(\&^*1/4,1/4,1/4)$	$(m_x^*3/4,1/4,3/4)$	$(m_y^*3/4,3/4,1/4)$	$(m_z^*1/4,3/4,3/4)$
$(\&_{xyz}^*1/4,1/4,1/4)$	$(\&_{xyz}^{-1*}1/4,1/4,1/4)$	$(\&_{\&yz}^*3/4,3/4,1/4)$	$(\&_{\&yz}^{-1*}1/4,3/4,3/4)$
$(\&_{x\&z}^*1/4,3/4,3/4)$	$(\&_{x\&z}^{-1*}3/4,1/4,3/4)$	$(\&_{xy\&}^*3/4,1/4,3/4)$	$(\&_{xy\&}^{-1*}3/4,3/4,1/4)$
$(\&_x^*0,0,0)$	$(\&_x^{-1*}0,0,0)$	$(m_{xy}^*0,0,0)$	$(m_{\&y}^*0,0,0)$
$(\&_y^*0,0,0)$	$(\&_y^{-1*}0,0,0)$	$(m_{xz}^*0,0,0)$	$(m_{\&z}^*0,0,0)$
$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$	$(m_{yz}^*0,0,0)$	$(m_{\&z}^*0,0,0)$

227.2.1629 Fd&m1'

227.3.1630 Fd'&'m F&3m (0,0,0;a,b,c)

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(4_x^*1/4,3/4,3/4)'$	$(4_x^{-1*}3/4,1/4,3/4)'$	$(2_{xy}^*3/4,1/4,3/4)'$	$(2_{xy}^{-1*}1/4,1/4,1/4)'$
$(4_y^*3/4,1/4,3/4)'$	$(4_y^{-1*}3/4,3/4,1/4)'$	$(2_{xz}^*1/4,3/4,3/4)'$	$(2_{xz}^{-1*}1/4,1/4,1/4)'$
$(4_z^*3/4,3/4,1/4)'$	$(4_z^{-1*}1/4,3/4,3/4)'$	$(2_{yz}^*3/4,3/4,1/4)'$	$(2_{yz}^{-1*}1/4,1/4,1/4)'$
$(\&^*1/4,1/4,1/4)'$	$(m_x^*3/4,1/4,3/4)'$	$(m_y^*3/4,3/4,1/4)'$	$(m_z^*1/4,3/4,3/4)'$

$(\&_{xyz}^* 1/4, 1/4, 1/4)'$	$(\&_{xyz}^{-1*} 1/4, 1/4, 1/4)'$	$(\&_{\&yz}^* 3/4, 3/4, 1/4)'$	$(\&_{\&yz}^{-1*} 1/4, 3/4, 3/4)'$
$(\&_{x\&z}^* 1/4, 3/4, 3/4)'$	$(\&_{x\&z}^{-1*} 3/4, 1/4, 3/4)'$	$(\&_{xy\&}^* 3/4, 1/4, 3/4)'$	$(\&_{xy\&}^{-1*} 3/4, 3/4, 1/4)'$
$(\&_x^* 0, 0, 0)$	$(\&_x^{-1*} 0, 0, 0)$	$(m_{xy}^* 0, 0, 0)$	$(m_{\&y}^* 0, 0, 0)$
$(\&_y^* 0, 0, 0)$	$(\&_y^{-1*} 0, 0, 0)$	$(m_{xz}^* 0, 0, 0)$	$(m_{\&z}^* 0, 0, 0)$
$(\&_z^* 0, 0, 0)$	$(\&_z^{-1*} 0, 0, 0)$	$(m_{yz}^* 0, 0, 0)$	$(m_{\&z}^* 0, 0, 0)$

227.4.1631 Fd $\&$ m' Fd $\&$  (0,0,0;a,b,c)

$(1^* 0, 0, 0)$	$(2_x^* 0, 0, 0)$	$(2_y^* 0, 0, 0)$	$(2_z^* 0, 0, 0)$
$(3_{xyz}^* 0, 0, 0)$	$(3_{xyz}^{-1*} 0, 0, 0)$	$(3_{\&yz}^* 0, 0, 0)$	$(3_{\&yz}^{-1*} 0, 0, 0)$
$(3_{x\&z}^* 0, 0, 0)$	$(3_{x\&z}^{-1*} 0, 0, 0)$	$(3_{xy\&}^* 0, 0, 0)$	$(3_{xy\&}^{-1*} 0, 0, 0)$
$(4_x^* 1/4, 3/4, 3/4)'$	$(4_x^{-1*} 3/4, 1/4, 3/4)'$	$(2_{xy}^* 3/4, 1/4, 3/4)'$	$(2_{\&y}^* 1/4, 1/4, 1/4)'$
$(4_y^* 3/4, 1/4, 3/4)'$	$(4_y^{-1*} 3/4, 3/4, 1/4)'$	$(2_{xz}^* 1/4, 3/4, 3/4)'$	$(2_{\&z}^* 1/4, 1/4, 1/4)'$
$(4_z^* 3/4, 3/4, 1/4)'$	$(4_z^{-1*} 1/4, 3/4, 3/4)'$	$(2_{yz}^* 3/4, 3/4, 1/4)'$	$(2_{\&z}^* 1/4, 1/4, 1/4)'$
$(\&^* 1/4, 1/4, 1/4)$	$(m_x^* 3/4, 1/4, 3/4)$	$(m_y^* 3/4, 3/4, 1/4)$	$(m_z^* 1/4, 3/4, 3/4)$
$(\&_{xyz}^* 1/4, 1/4, 1/4)$	$(\&_{xyz}^{-1*} 1/4, 1/4, 1/4)$	$(\&_{\&yz}^* 3/4, 3/4, 1/4)$	$(\&_{\&yz}^{-1*} 1/4, 3/4, 3/4)$
$(\&_{x\&z}^* 1/4, 3/4, 3/4)$	$(\&_{x\&z}^{-1*} 3/4, 1/4, 3/4)$	$(\&_{xy\&}^* 3/4, 1/4, 3/4)$	$(\&_{xy\&}^{-1*} 3/4, 3/4, 1/4)$
$(\&_x^* 0, 0, 0)'$	$(\&_x^{-1*} 0, 0, 0)'$	$(m_{xy}^* 0, 0, 0)'$	$(m_{\&y}^* 0, 0, 0)'$
$(\&_y^* 0, 0, 0)'$	$(\&_y^{-1*} 0, 0, 0)'$	$(m_{xz}^* 0, 0, 0)'$	$(m_{\&z}^* 0, 0, 0)'$
$(\&_z^* 0, 0, 0)'$	$(\&_z^{-1*} 0, 0, 0)'$	$(m_{yz}^* 0, 0, 0)'$	$(m_{\&z}^* 0, 0, 0)'$

227.5.1632 Fd' $\&$ 'm' F4 $_1$ 32 (0,0,0;a,b,c)

$(1^* 0, 0, 0)$	$(2_x^* 0, 0, 0)$	$(2_y^* 0, 0, 0)$	$(2_z^* 0, 0, 0)$
$(3_{xyz}^* 0, 0, 0)$	$(3_{xyz}^{-1*} 0, 0, 0)$	$(3_{\&yz}^* 0, 0, 0)$	$(3_{\&yz}^{-1*} 0, 0, 0)$
$(3_{x\&z}^* 0, 0, 0)$	$(3_{x\&z}^{-1*} 0, 0, 0)$	$(3_{xy\&}^* 0, 0, 0)$	$(3_{xy\&}^{-1*} 0, 0, 0)$
$(4_x^* 1/4, 3/4, 3/4)$	$(4_x^{-1*} 3/4, 1/4, 3/4)$	$(2_{xy}^* 3/4, 1/4, 3/4)$	$(2_{\&y}^* 1/4, 1/4, 1/4)$
$(4_y^* 3/4, 1/4, 3/4)$	$(4_y^{-1*} 3/4, 3/4, 1/4)$	$(2_{xz}^* 1/4, 3/4, 3/4)$	$(2_{\&z}^* 1/4, 1/4, 1/4)$
$(4_z^* 3/4, 3/4, 1/4)$	$(4_z^{-1*} 1/4, 3/4, 3/4)$	$(2_{yz}^* 3/4, 3/4, 1/4)$	$(2_{\&z}^* 1/4, 1/4, 1/4)$
$(\&^* 1/4, 1/4, 1/4)'$	$(m_x^* 3/4, 1/4, 3/4)'$	$(m_y^* 3/4, 3/4, 1/4)'$	$(m_z^* 1/4, 3/4, 3/4)'$
$(\&_{xyz}^* 1/4, 1/4, 1/4)'$	$(\&_{xyz}^{-1*} 1/4, 1/4, 1/4)'$	$(\&_{\&yz}^* 3/4, 3/4, 1/4)'$	$(\&_{\&yz}^{-1*} 1/4, 3/4, 3/4)'$
$(\&_{x\&z}^* 1/4, 3/4, 3/4)'$	$(\&_{x\&z}^{-1*} 3/4, 1/4, 3/4)'$	$(\&_{xy\&}^* 3/4, 1/4, 3/4)'$	$(\&_{xy\&}^{-1*} 3/4, 3/4, 1/4)'$
$(\&_x^* 0, 0, 0)'$	$(\&_x^{-1*} 0, 0, 0)'$	$(m_{xy}^* 0, 0, 0)'$	$(m_{\&y}^* 0, 0, 0)'$
$(\&_y^* 0, 0, 0)'$	$(\&_y^{-1*} 0, 0, 0)'$	$(m_{xz}^* 0, 0, 0)'$	$(m_{\&z}^* 0, 0, 0)'$
$(\&_z^* 0, 0, 0)'$	$(\&_z^{-1*} 0, 0, 0)'$	$(m_{yz}^* 0, 0, 0)'$	$(m_{\&z}^* 0, 0, 0)'$

228.1633 Fd&c

$(1^*0,0,0)$	$(2_x^*1/2,1/4,3/4)$	$(2_y^*3/4,1/2,1/4)$	$(2_z^*1/4,3/4,1/2)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{&yz}^*3/4,1/2,1/4)$	$(3_{&yz}^{-1*}1/4,3/4,1/2)$
$(3_{x&z}^*1/4,3/4,1/2)$	$(3_{x&z}^{-1*}1/2,1/4,3/4)$	$(3_{xy&}^*1/2,1/4,3/4)$	$(3_{xy&}^{-1*}3/4,1/2,1/4)$
$(4_x^*1/4,0,3/4)$	$(4_x^{-1*}3/4,1/4,0)$	$(2_{xy}^*3/4,1/4,0)$	$(2_{&y}^*1/2,1/2,1/2)$
$(4_y^*3/4,1/4,0)$	$(4_y^{-1*}0,3/4,1/4)$	$(2_{xz}^*1/4,0,3/4)$	$(2_{&z}^*1/2,1/2,1/2)$
$(4_z^*0,3/4,1/4)$	$(4_z^{-1*}1/4,0,3/4)$	$(2_{yz}^*0,3/4,1/4)$	$(2_{&z}^*1/2,1/2,1/2)$
$(\&^*0,0,0)$	$(m_x^*1/2,3/4,1/4)$	$(m_y^*1/4,1/2,3/4)$	$(m_z^*3/4,1/4,1/2)$
$(\&_{xyz}^*0,0,0)$	$(\&_{xyz}^{-1*}0,0,0)$	$(\&_{&yz}^*1/4,1/2,3/4)$	$(\&_{&yz}^{-1*}3/4,1/4,1/2)$
$(\&_{x&z}^*3/4,1/4,1/2)$	$(\&_{x&z}^{-1*}1/2,3/4,1/4)$	$(\&_{xy&}^*1/2,3/4,1/4)$	$(\&_{xy&}^{-1*}1/4,1/2,3/4)$
$(\&_x^*3/4,0,1/4)$	$(\&_x^{-1*}1/4,3/4,0)$	$(m_{xy}^*1/4,3/4,0)$	$(m_{&y}^*1/2,1/2,1/2)$
$(\&_y^*1/4,3/4,0)$	$(\&_y^{-1*}0,1/4,3/4)$	$(m_{xz}^*3/4,0,1/4)$	$(m_{&z}^*1/2,1/2,1/2)$
$(\&_z^*0,1/4,3/4)$	$(\&_z^{-1*}3/4,0,1/4)$	$(m_{yz}^*0,1/4,3/4)$	$(m_{&z}^*1/2,1/2,1/2)$

228.2.1634 Fd&c1'

228.3.1635 Fd'&'c

F&3c

(1/8,1/8,1/8;a,b,c)

$(1^*0,0,0)$	$(2_x^*1/2,1/4,3/4)$	$(2_y^*3/4,1/2,1/4)$	$(2_z^*1/4,3/4,1/2)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{&yz}^*3/4,1/2,1/4)$	$(3_{&yz}^{-1*}1/4,3/4,1/2)$
$(3_{x&z}^*1/4,3/4,1/2)$	$(3_{x&z}^{-1*}1/2,1/4,3/4)$	$(3_{xy&}^*1/2,1/4,3/4)$	$(3_{xy&}^{-1*}3/4,1/2,1/4)$
$(4_x^*1/4,0,3/4)'$	$(4_x^{-1*}3/4,1/4,0)'$	$(2_{xy}^*3/4,1/4,0)'$	$(2_{&y}^*1/2,1/2,1/2)'$
$(4_y^*3/4,1/4,0)'$	$(4_y^{-1*}0,3/4,1/4)'$	$(2_{xz}^*1/4,0,3/4)'$	$(2_{&z}^*1/2,1/2,1/2)'$
$(4_z^*0,3/4,1/4)'$	$(4_z^{-1*}1/4,0,3/4)'$	$(2_{yz}^*0,3/4,1/4)'$	$(2_{&z}^*1/2,1/2,1/2)'$
$(\&^*0,0,0)'$	$(m_x^*1/2,3/4,1/4)'$	$(m_y^*1/4,1/2,3/4)'$	$(m_z^*3/4,1/4,1/2)'$
$(\&_{xyz}^*0,0,0)'$	$(\&_{xyz}^{-1*}0,0,0)'$	$(\&_{&yz}^*1/4,1/2,3/4)'$	$(\&_{&yz}^{-1*}3/4,1/4,1/2)'$
$(\&_{x&z}^*3/4,1/4,1/2)'$	$(\&_{x&z}^{-1*}1/2,3/4,1/4)'$	$(\&_{xy&}^*1/2,3/4,1/4)'$	$(\&_{xy&}^{-1*}1/4,1/2,3/4)'$
$(\&_x^*3/4,0,1/4)'$	$(\&_x^{-1*}1/4,3/4,0)'$	$(m_{xy}^*1/4,3/4,0)'$	$(m_{&y}^*1/2,1/2,1/2)'$
$(\&_y^*1/4,3/4,0)'$	$(\&_y^{-1*}0,1/4,3/4)'$	$(m_{xz}^*3/4,0,1/4)'$	$(m_{&z}^*1/2,1/2,1/2)'$
$(\&_z^*0,1/4,3/4)'$	$(\&_z^{-1*}3/4,0,1/4)'$	$(m_{yz}^*0,1/4,3/4)'$	$(m_{&z}^*1/2,1/2,1/2)'$

228.4.1636 Fd&c'

Fd&

(-1/8,-1/8,-1/8;a,b,c)

$(1^*0,0,0)$	$(2_x^*1/2,1/4,3/4)$	$(2_y^*3/4,1/2,1/4)$	$(2_z^*1/4,3/4,1/2)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{&yz}^*3/4,1/2,1/4)$	$(3_{&yz}^{-1*}1/4,3/4,1/2)$
$(3_{x&z}^*1/4,3/4,1/2)$	$(3_{x&z}^{-1*}1/2,1/4,3/4)$	$(3_{xy&}^*1/2,1/4,3/4)$	$(3_{xy&}^{-1*}3/4,1/2,1/4)$
$(4_x^*1/4,0,3/4)'$	$(4_x^{-1*}3/4,1/4,0)'$	$(2_{xy}^*3/4,1/4,0)'$	$(2_{&y}^*1/2,1/2,1/2)'$
$(4_y^*3/4,1/4,0)'$	$(4_y^{-1*}0,3/4,1/4)'$	$(2_{xz}^*1/4,0,3/4)'$	$(2_{&z}^*1/2,1/2,1/2)'$
$(4_z^*0,3/4,1/4)'$	$(4_z^{-1*}1/4,0,3/4)'$	$(2_{yz}^*0,3/4,1/4)'$	$(2_{&z}^*1/2,1/2,1/2)'$

$(\&^*0,0,0)$	$(m_x^*1/2,3/4,1/4)$	$(m_y^*1/4,1/2,3/4)$	$(m_z^*3/4,1/4,1/2)$
$(\&_{xyz}^*0,0,0)$	$(\&_{xyz}^{-1*}0,0,0)$	$(\&_{\&yz}^*1/4,1/2,3/4)$	$(\&_{\&yz}^{-1*}3/4,1/4,1/2)$
$(\&_{x\&z}^*3/4,1/4,1/2)$	$(\&_{x\&z}^{-1*}1/2,3/4,1/4)$	$(\&_{xy\&}^*1/2,3/4,1/4)$	$(\&_{xy\&}^{-1*}1/4,1/2,3/4)$
$(\&_x^*3/4,0,1/4)'$	$(\&_x^{-1*}1/4,3/4,0)'$	$(m_{xy}^*1/4,3/4,0)'$	$(m_{\&y}^*1/2,1/2,1/2)'$
$(\&_y^*1/4,3/4,0)'$	$(\&_y^{-1*}0,1/4,3/4)'$	$(m_{xz}^*3/4,0,1/4)'$	$(m_{\&z}^*1/2,1/2,1/2)'$
$(\&_z^*0,1/4,3/4)'$	$(\&_z^{-1*}3/4,0,1/4)'$	$(m_{yz}^*0,1/4,3/4)'$	$(m_{\&z}^*1/2,1/2,1/2)'$

228.5.1637 Fd' $\&c'$  F4<sub>1</sub>32 (1/8,1/8,1/8;a,b,c)

$(1^*0,0,0)$	$(2_x^*1/2,1/4,3/4)$	$(2_y^*3/4,1/2,1/4)$	$(2_z^*1/4,3/4,1/2)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*3/4,1/2,1/4)$	$(3_{\&yz}^{-1*}1/4,3/4,1/2)$
$(3_{x\&z}^*1/4,3/4,1/2)$	$(3_{x\&z}^{-1*}1/2,1/4,3/4)$	$(3_{xy\&}^*1/2,1/4,3/4)$	$(3_{xy\&}^{-1*}3/4,1/2,1/4)$
$(4_x^*1/4,0,3/4)$	$(4_x^{-1*}3/4,1/4,0)$	$(2_{xy}^*3/4,1/4,0)$	$(2_{\&y}^*1/2,1/2,1/2)$
$(4_y^*3/4,1/4,0)$	$(4_y^{-1*}0,3/4,1/4)$	$(2_{xz}^*1/4,0,3/4)$	$(2_{\&z}^*1/2,1/2,1/2)$
$(4_z^*0,3/4,1/4)$	$(4_z^{-1*}1/4,0,3/4)$	$(2_{yz}^*0,3/4,1/4)$	$(2_{\&z}^*1/2,1/2,1/2)$
$(\&^*0,0,0)'$	$(m_x^*1/2,3/4,1/4)'$	$(m_y^*1/4,1/2,3/4)'$	$(m_z^*3/4,1/4,1/2)'$
$(\&_{xyz}^*0,0,0)'$	$(\&_{xyz}^{-1*}0,0,0)'$	$(\&_{\&yz}^*1/4,1/2,3/4)'$	$(\&_{\&yz}^{-1*}3/4,1/4,1/2)'$
$(\&_{x\&z}^*3/4,1/4,1/2)'$	$(\&_{x\&z}^{-1*}1/2,3/4,1/4)'$	$(\&_{xy\&}^*1/2,3/4,1/4)'$	$(\&_{xy\&}^{-1*}1/4,1/2,3/4)'$
$(\&_x^*3/4,0,1/4)'$	$(\&_x^{-1*}1/4,3/4,0)'$	$(m_{xy}^*1/4,3/4,0)'$	$(m_{\&y}^*1/2,1/2,1/2)'$
$(\&_y^*1/4,3/4,0)'$	$(\&_y^{-1*}0,1/4,3/4)'$	$(m_{xz}^*3/4,0,1/4)'$	$(m_{\&z}^*1/2,1/2,1/2)'$
$(\&_z^*0,1/4,3/4)'$	$(\&_z^{-1*}3/4,0,1/4)'$	$(m_{yz}^*0,1/4,3/4)'$	$(m_{\&z}^*1/2,1/2,1/2)'$

229.1.1638 Im $\&m$

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(4_x^*0,0,0)$	$(4_x^{-1*}0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_{\&y}^*0,0,0)$
$(4_y^*0,0,0)$	$(4_y^{-1*}0,0,0)$	$(2_{xz}^*0,0,0)$	$(2_{\&z}^*0,0,0)$
$(4_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$	$(2_{yz}^*0,0,0)$	$(2_{\&z}^*0,0,0)$
$(\&^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*0,0,0)$	$(m_z^*0,0,0)$
$(\&_{xyz}^*0,0,0)$	$(\&_{xyz}^{-1*}0,0,0)$	$(\&_{\&yz}^*0,0,0)$	$(\&_{\&yz}^{-1*}0,0,0)$
$(\&_{x\&z}^*0,0,0)$	$(\&_{x\&z}^{-1*}0,0,0)$	$(\&_{xy\&}^*0,0,0)$	$(\&_{xy\&}^{-1*}0,0,0)$
$(\&_x^*0,0,0)$	$(\&_x^{-1*}0,0,0)$	$(m_{xy}^*0,0,0)$	$(m_{\&y}^*0,0,0)$
$(\&_y^*0,0,0)$	$(\&_y^{-1*}0,0,0)$	$(m_{xz}^*0,0,0)$	$(m_{\&z}^*0,0,0)$
$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$	$(m_{yz}^*0,0,0)$	$(m_{\&z}^*0,0,0)$

229.2.1639  $Im\bar{m}1'$

229.3.1640  $Im'\bar{m}$   $I\bar{3}m$   $(0,0,0;a,b,c)$

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\bar{y}z}^*0,0,0)$	$(3_{\bar{y}z}^{-1*}0,0,0)$
$(3_{x\bar{z}}^*0,0,0)$	$(3_{x\bar{z}}^{-1*}0,0,0)$	$(3_{xy\bar{z}}^*0,0,0)$	$(3_{xy\bar{z}}^{-1*}0,0,0)$
$(4_x^*0,0,0)'$	$(4_x^{-1*}0,0,0)'$	$(2_{xy}^*0,0,0)'$	$(2_{\bar{y}}^*0,0,0)'$
$(4_y^*0,0,0)'$	$(4_y^{-1*}0,0,0)'$	$(2_{xz}^*0,0,0)'$	$(2_{\bar{z}}^*0,0,0)'$
$(4_z^*0,0,0)'$	$(4_z^{-1*}0,0,0)'$	$(2_{yz}^*0,0,0)'$	$(2_{\bar{z}}^*0,0,0)'$
$(\bar{x}^*0,0,0)'$	$(m_x^*0,0,0)'$	$(m_y^*0,0,0)'$	$(m_z^*0,0,0)'$
$(\bar{x}_{yz}^*0,0,0)'$	$(\bar{x}_{yz}^{-1*}0,0,0)'$	$(\bar{x}_{\bar{y}z}^*0,0,0)'$	$(\bar{x}_{\bar{y}z}^{-1*}0,0,0)'$
$(\bar{x}_{x\bar{z}}^*0,0,0)'$	$(\bar{x}_{x\bar{z}}^{-1*}0,0,0)'$	$(\bar{x}_{xy\bar{z}}^*0,0,0)'$	$(\bar{x}_{xy\bar{z}}^{-1*}0,0,0)'$
$(\bar{x}_x^*0,0,0)$	$(\bar{x}_x^{-1*}0,0,0)$	$(m_{xy}^*0,0,0)$	$(m_{\bar{y}}^*0,0,0)$
$(\bar{x}_y^*0,0,0)$	$(\bar{x}_y^{-1*}0,0,0)$	$(m_{xz}^*0,0,0)$	$(m_{\bar{z}}^*0,0,0)$
$(\bar{x}_z^*0,0,0)$	$(\bar{x}_z^{-1*}0,0,0)$	$(m_{yz}^*0,0,0)$	$(m_{\bar{z}}^*0,0,0)$

229.4.1641  $Im\bar{m}'$   $Im\bar{3}$   $(0,0,0;a,b,c)$

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\bar{y}z}^*0,0,0)$	$(3_{\bar{y}z}^{-1*}0,0,0)$
$(3_{x\bar{z}}^*0,0,0)$	$(3_{x\bar{z}}^{-1*}0,0,0)$	$(3_{xy\bar{z}}^*0,0,0)$	$(3_{xy\bar{z}}^{-1*}0,0,0)$
$(4_x^*0,0,0)'$	$(4_x^{-1*}0,0,0)'$	$(2_{xy}^*0,0,0)'$	$(2_{\bar{y}}^*0,0,0)'$
$(4_y^*0,0,0)'$	$(4_y^{-1*}0,0,0)'$	$(2_{xz}^*0,0,0)'$	$(2_{\bar{z}}^*0,0,0)'$
$(4_z^*0,0,0)'$	$(4_z^{-1*}0,0,0)'$	$(2_{yz}^*0,0,0)'$	$(2_{\bar{z}}^*0,0,0)'$
$(\bar{x}^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*0,0,0)$	$(m_z^*0,0,0)$
$(\bar{x}_{yz}^*0,0,0)$	$(\bar{x}_{yz}^{-1*}0,0,0)$	$(\bar{x}_{\bar{y}z}^*0,0,0)$	$(\bar{x}_{\bar{y}z}^{-1*}0,0,0)$
$(\bar{x}_{x\bar{z}}^*0,0,0)'$	$(\bar{x}_{x\bar{z}}^{-1*}0,0,0)'$	$(\bar{x}_{xy\bar{z}}^*0,0,0)'$	$(\bar{x}_{xy\bar{z}}^{-1*}0,0,0)'$
$(\bar{x}_x^*0,0,0)'$	$(\bar{x}_x^{-1*}0,0,0)'$	$(m_{xy}^*0,0,0)'$	$(m_{\bar{y}}^*0,0,0)'$
$(\bar{x}_y^*0,0,0)'$	$(\bar{x}_y^{-1*}0,0,0)'$	$(m_{xz}^*0,0,0)'$	$(m_{\bar{z}}^*0,0,0)'$
$(\bar{x}_z^*0,0,0)'$	$(\bar{x}_z^{-1*}0,0,0)'$	$(m_{yz}^*0,0,0)'$	$(m_{\bar{z}}^*0,0,0)'$

229.5.1642  $Im'\bar{m}'$   $I432$   $(0,0,0;a,b,c)$

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\bar{y}z}^*0,0,0)$	$(3_{\bar{y}z}^{-1*}0,0,0)$
$(3_{x\bar{z}}^*0,0,0)$	$(3_{x\bar{z}}^{-1*}0,0,0)$	$(3_{xy\bar{z}}^*0,0,0)$	$(3_{xy\bar{z}}^{-1*}0,0,0)$
$(4_x^*0,0,0)$	$(4_x^{-1*}0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_{\bar{y}}^*0,0,0)$
$(4_y^*0,0,0)$	$(4_y^{-1*}0,0,0)$	$(2_{xz}^*0,0,0)$	$(2_{\bar{z}}^*0,0,0)$
$(4_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$	$(2_{yz}^*0,0,0)$	$(2_{\bar{z}}^*0,0,0)$

$(\&^*0,0,0)'$	$(m_x^*0,0,0)'$	$(m_y^*0,0,0)'$	$(m_z^*0,0,0)'$
$(\&_{xyz}^*0,0,0)'$	$(\&_{xyz}^{-1*}0,0,0)'$	$(\&_{\&yz}^*0,0,0)'$	$(\&_{\&yz}^{-1*}0,0,0)'$
$(\&_{x\&z}^*0,0,0)'$	$(\&_{x\&z}^{-1*}0,0,0)'$	$(\&_{xy\&}^*0,0,0)'$	$(\&_{xy\&}^{-1*}0,0,0)'$
$(\&_x^*0,0,0)'$	$(\&_x^{-1*}0,0,0)'$	$(m_{xy}^*0,0,0)'$	$(m_{\&y}^*0,0,0)'$
$(\&_y^*0,0,0)'$	$(\&_y^{-1*}0,0,0)'$	$(m_{xz}^*0,0,0)'$	$(m_{\&z}^*0,0,0)'$
$(\&_z^*0,0,0)'$	$(\&_z^{-1*}0,0,0)'$	$(m_{yz}^*0,0,0)'$	$(m_{\&z}^*0,0,0)'$

229.6.1643  $I_p m\&m$   $Pm\&m$  (0,0,0;a,b,c)

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(4_x^*0,0,0)$	$(4_x^{-1*}0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_{\&y}^*0,0,0)$
$(4_y^*0,0,0)$	$(4_y^{-1*}0,0,0)$	$(2_{xz}^*0,0,0)$	$(2_{\&z}^*0,0,0)$
$(4_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$	$(2_{yz}^*0,0,0)$	$(2_{\&z}^*0,0,0)$
$(\&^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*0,0,0)$	$(m_z^*0,0,0)$
$(\&_{xyz}^*0,0,0)$	$(\&_{xyz}^{-1*}0,0,0)$	$(\&_{\&yz}^*0,0,0)$	$(\&_{\&yz}^{-1*}0,0,0)$
$(\&_{x\&z}^*0,0,0)$	$(\&_{x\&z}^{-1*}0,0,0)$	$(\&_{xy\&}^*0,0,0)$	$(\&_{xy\&}^{-1*}0,0,0)$
$(\&_x^*0,0,0)$	$(\&_x^{-1*}0,0,0)$	$(m_{xy}^*0,0,0)$	$(m_{\&y}^*0,0,0)$
$(\&_y^*0,0,0)$	$(\&_y^{-1*}0,0,0)$	$(m_{xz}^*0,0,0)$	$(m_{\&z}^*0,0,0)$
$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$	$(m_{yz}^*0,0,0)$	$(m_{\&z}^*0,0,0)$

229.7.1644  $I_p m'\&'m$   $Pn\&m$  (0,0,0;a,b,c)

$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\&yz}^*0,0,0)$	$(3_{\&yz}^{-1*}0,0,0)$
$(3_{x\&z}^*0,0,0)$	$(3_{x\&z}^{-1*}0,0,0)$	$(3_{xy\&}^*0,0,0)$	$(3_{xy\&}^{-1*}0,0,0)$
$(4_x^*1/2,1/2,1/2)$	$(4_x^{-1*}1/2,1/2,1/2)$	$(2_{xy}^*1/2,1/2,1/2)$	$(2_{\&y}^*1/2,1/2,1/2)$
$(4_y^*1/2,1/2,1/2)$	$(4_y^{-1*}1/2,1/2,1/2)$	$(2_{xz}^*1/2,1/2,1/2)$	$(2_{\&z}^*1/2,1/2,1/2)$
$(4_z^*1/2,1/2,1/2)$	$(4_z^{-1*}1/2,1/2,1/2)$	$(2_{yz}^*1/2,1/2,1/2)$	$(2_{\&z}^*1/2,1/2,1/2)$
$(\&^*1/2,1/2,1/2)$	$(m_x^*1/2,1/2,1/2)$	$(m_y^*1/2,1/2,1/2)$	$(m_z^*1/2,1/2,1/2)$
$(\&_{xyz}^*1/2,1/2,1/2)$	$(\&_{xyz}^{-1*}1/2,1/2,1/2)$	$(\&_{\&yz}^*1/2,1/2,1/2)$	$(\&_{\&yz}^{-1*}1/2,1/2,1/2)$
$(\&_{x\&z}^*1/2,1/2,1/2)$	$(\&_{x\&z}^{-1*}1/2,1/2,1/2)$	$(\&_{xy\&}^*1/2,1/2,1/2)$	$(\&_{xy\&}^{-1*}1/2,1/2,1/2)$
$(\&_x^*0,0,0)$	$(\&_x^{-1*}0,0,0)$	$(m_{xy}^*0,0,0)$	$(m_{\&y}^*0,0,0)$
$(\&_y^*0,0,0)$	$(\&_y^{-1*}0,0,0)$	$(m_{xz}^*0,0,0)$	$(m_{\&z}^*0,0,0)$
$(\&_z^*0,0,0)$	$(\&_z^{-1*}0,0,0)$	$(m_{yz}^*0,0,0)$	$(m_{\&z}^*0,0,0)$



229.8.1645	$I_p m \bar{2} m'$	$Pm \bar{2} n$	(0,0,0;a,b,c)	$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
				$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\bar{2}yz}^*0,0,0)$	$(3_{\bar{2}yz}^{-1*}0,0,0)$
				$(3_{x\bar{2}z}^*0,0,0)$	$(3_{x\bar{2}z}^{-1*}0,0,0)$	$(3_{xy\bar{2}}^*0,0,0)$	$(3_{xy\bar{2}}^{-1*}0,0,0)$
				$(4_x^*1/2,1/2,1/2)$	$(4_x^{-1*}1/2,1/2,1/2)$	$(2_{xy}^*1/2,1/2,1/2)$	$(2_{\bar{2}y}^*1/2,1/2,1/2)$
				$(4_y^*1/2,1/2,1/2)$	$(4_y^{-1*}1/2,1/2,1/2)$	$(2_{xz}^*1/2,1/2,1/2)$	$(2_{\bar{2}z}^*1/2,1/2,1/2)$
				$(4_z^*1/2,1/2,1/2)$	$(4_z^{-1*}1/2,1/2,1/2)$	$(2_{yz}^*1/2,1/2,1/2)$	$(2_{\bar{2}z}^*1/2,1/2,1/2)$
				$(\bar{2}^*0,0,0)$	$(m_x^*0,0,0)$	$(m_y^*0,0,0)$	$(m_z^*0,0,0)$
				$(\bar{2}_{xyz}^*0,0,0)$	$(\bar{2}_{xyz}^{-1*}0,0,0)$	$(\bar{2}_{\bar{2}yz}^*0,0,0)$	$(\bar{2}_{\bar{2}yz}^{-1*}0,0,0)$
				$(\bar{2}_{x\bar{2}z}^*0,0,0)$	$(\bar{2}_{x\bar{2}z}^{-1*}0,0,0)$	$(\bar{2}_{xy\bar{2}}^*0,0,0)$	$(\bar{2}_{xy\bar{2}}^{-1*}0,0,0)$
				$(\bar{2}_x^*1/2,1/2,1/2)$	$(\bar{2}_x^{-1*}1/2,1/2,1/2)$	$(m_{xy}^*1/2,1/2,1/2)$	$(m_{\bar{2}y}^*1/2,1/2,1/2)$
				$(\bar{2}_y^*1/2,1/2,1/2)$	$(\bar{2}_y^{-1*}1/2,1/2,1/2)$	$(m_{xz}^*1/2,1/2,1/2)$	$(m_{\bar{2}z}^*1/2,1/2,1/2)$
				$(\bar{2}_z^*1/2,1/2,1/2)$	$(\bar{2}_z^{-1*}1/2,1/2,1/2)$	$(m_{yz}^*1/2,1/2,1/2)$	$(m_{\bar{2}z}^*1/2,1/2,1/2)$

229.9.1646	$I_p m' \bar{2} m'$	$Pn \bar{2} n$	(0,0,0;a,b,c)	$(1^*0,0,0)$	$(2_x^*0,0,0)$	$(2_y^*0,0,0)$	$(2_z^*0,0,0)$
				$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\bar{2}yz}^*0,0,0)$	$(3_{\bar{2}yz}^{-1*}0,0,0)$
				$(3_{x\bar{2}z}^*0,0,0)$	$(3_{x\bar{2}z}^{-1*}0,0,0)$	$(3_{xy\bar{2}}^*0,0,0)$	$(3_{xy\bar{2}}^{-1*}0,0,0)$
				$(4_x^*0,0,0)$	$(4_x^{-1*}0,0,0)$	$(2_{xy}^*0,0,0)$	$(2_{\bar{2}y}^*0,0,0)$
				$(4_y^*0,0,0)$	$(4_y^{-1*}0,0,0)$	$(2_{xz}^*0,0,0)$	$(2_{\bar{2}z}^*0,0,0)$
				$(4_z^*0,0,0)$	$(4_z^{-1*}0,0,0)$	$(2_{yz}^*0,0,0)$	$(2_{\bar{2}z}^*0,0,0)$
				$(\bar{2}^*1/2,1/2,1/2)$	$(m_x^*1/2,1/2,1/2)$	$(m_y^*1/2,1/2,1/2)$	$(m_z^*1/2,1/2,1/2)$
				$(\bar{2}_{xyz}^*1/2,1/2,1/2)$	$(\bar{2}_{xyz}^{-1*}1/2,1/2,1/2)$	$(\bar{2}_{\bar{2}yz}^*1/2,1/2,1/2)$	$(\bar{2}_{\bar{2}yz}^{-1*}1/2,1/2,1/2)$
				$(\bar{2}_{x\bar{2}z}^*1/2,1/2,1/2)$	$(\bar{2}_{x\bar{2}z}^{-1*}1/2,1/2,1/2)$	$(\bar{2}_{xy\bar{2}}^*1/2,1/2,1/2)$	$(\bar{2}_{xy\bar{2}}^{-1*}1/2,1/2,1/2)$
				$(\bar{2}_x^*1/2,1/2,1/2)$	$(\bar{2}_x^{-1*}1/2,1/2,1/2)$	$(m_{xy}^*1/2,1/2,1/2)$	$(m_{\bar{2}y}^*1/2,1/2,1/2)$
				$(\bar{2}_y^*1/2,1/2,1/2)$	$(\bar{2}_y^{-1*}1/2,1/2,1/2)$	$(m_{xz}^*1/2,1/2,1/2)$	$(m_{\bar{2}z}^*1/2,1/2,1/2)$
				$(\bar{2}_z^*1/2,1/2,1/2)$	$(\bar{2}_z^{-1*}1/2,1/2,1/2)$	$(m_{yz}^*1/2,1/2,1/2)$	$(m_{\bar{2}z}^*1/2,1/2,1/2)$

230.1.1647	$Ia \bar{2} d$			$(1^*0,0,0)$	$(2_x^*1/2,1/2,0)$	$(2_y^*0,1/2,1/2)$	$(2_z^*1/2,0,1/2)$
				$(3_{xyz}^*0,0,0)$	$(3_{xyz}^{-1*}0,0,0)$	$(3_{\bar{2}yz}^*0,1/2,1/2)$	$(3_{\bar{2}yz}^{-1*}1/2,0,1/2)$
				$(3_{x\bar{2}z}^*1/2,0,1/2)$	$(3_{x\bar{2}z}^{-1*}1/2,1/2,0)$	$(3_{xy\bar{2}}^*1/2,1/2,0)$	$(3_{xy\bar{2}}^{-1*}0,1/2,1/2)$
				$(4_x^*1/4,1/4,3/4)$	$(4_x^{-1*}3/4,1/4,1/4)$	$(2_{xy}^*3/4,1/4,1/4)$	$(2_{\bar{2}y}^*3/4,3/4,3/4)$
				$(4_y^*3/4,1/4,1/4)$	$(4_y^{-1*}1/4,3/4,1/4)$	$(2_{xz}^*1/4,1/4,3/4)$	$(2_{\bar{2}z}^*3/4,3/4,3/4)$

$$(4_z^* 1/4, 3/4, 1/4) \quad (4_z^{-1*} 1/4, 1/4, 3/4) \quad (2_{yz}^* 1/4, 3/4, 1/4) \quad (2_{yz}^* 3/4, 3/4, 3/4)$$

$$\begin{aligned} & (\&^* 0, 0, 0) & (m_x^* 1/2, 1/2, 0) & (m_y^* 0, 1/2, 1/2) & (m_z^* 1/2, 0, 1/2) \\ & (\&_{xyz}^* 0, 0, 0) & (\&_{xyz}^{-1*} 0, 0, 0) & (\&_{&yz}^* 0, 1/2, 1/2) & (\&_{&yz}^{-1*} 1/2, 0, 1/2) \\ & (\&_{x&yz}^* 1/2, 0, 1/2) & (\&_{x&yz}^{-1*} 1/2, 1/2, 0) & (\&_{xy&}^* 1/2, 1/2, 0) & (\&_{xy&}^{-1*} 0, 1/2, 1/2) \\ & (\&_x^* 1/4, 1/4, 3/4) & (\&_x^{-1*} 3/4, 1/4, 1/4) & (m_{xy}^* 3/4, 1/4, 1/4) & (m_{&y}^* 3/4, 3/4, 3/4) \\ & (\&_y^* 3/4, 1/4, 1/4) & (\&_y^{-1*} 1/4, 3/4, 1/4) & (m_{xz}^* 1/4, 1/4, 3/4) & (m_{&z}^* 3/4, 3/4, 3/4) \\ & (\&_z^* 1/4, 3/4, 1/4) & (\&_z^{-1*} 1/4, 1/4, 3/4) & (m_{yz}^* 1/4, 3/4, 1/4) & (m_{&z}^* 3/4, 3/4, 3/4) \end{aligned}$$

230.2.1648  $la\&d1'$

230.3.1649  $la'\&d$   $l\&3d$   $(0,0,0;a,b,c)$

$$\begin{aligned} & (1^* 0, 0, 0) & (2_x^* 1/2, 1/2, 0) & (2_y^* 0, 1/2, 1/2) & (2_z^* 1/2, 0, 1/2) \\ & (3_{xyz}^* 0, 0, 0) & (3_{xyz}^{-1*} 0, 0, 0) & (3_{&yz}^* 0, 1/2, 1/2) & (3_{&yz}^{-1*} 1/2, 0, 1/2) \\ & (3_{x&yz}^* 1/2, 0, 1/2) & (3_{x&yz}^{-1*} 1/2, 1/2, 0) & (3_{xy&}^* 1/2, 1/2, 0) & (3_{xy&}^{-1*} 0, 1/2, 1/2) \\ & (4_x^* 1/4, 1/4, 3/4)' & (4_x^{-1*} 3/4, 1/4, 1/4)' & (2_{xy}^* 3/4, 1/4, 1/4)' & (2_{&y}^* 3/4, 3/4, 3/4)' \\ & (4_y^* 3/4, 1/4, 1/4)' & (4_y^{-1*} 1/4, 3/4, 1/4)' & (2_{xz}^* 1/4, 1/4, 3/4)' & (2_{&z}^* 3/4, 3/4, 3/4)' \\ & (4_z^* 1/4, 3/4, 1/4)' & (4_z^{-1*} 1/4, 1/4, 3/4)' & (2_{yz}^* 1/4, 3/4, 1/4)' & (2_{&z}^* 3/4, 3/4, 3/4)' \\ & (\&^* 0, 0, 0)' & (m_x^* 1/2, 1/2, 0)' & (m_y^* 0, 1/2, 1/2)' & (m_z^* 1/2, 0, 1/2)' \\ & (\&_{xyz}^* 0, 0, 0)' & (\&_{xyz}^{-1*} 0, 0, 0)' & (\&_{&yz}^* 0, 1/2, 1/2)' & (\&_{&yz}^{-1*} 1/2, 0, 1/2)' \\ & (\&_{x&yz}^* 1/2, 0, 1/2)' & (\&_{x&yz}^{-1*} 1/2, 1/2, 0)' & (\&_{xy&}^* 1/2, 1/2, 0)' & (\&_{xy&}^{-1*} 0, 1/2, 1/2)' \\ & (\&_x^* 1/4, 1/4, 3/4)' & (\&_x^{-1*} 3/4, 1/4, 1/4)' & (m_{xy}^* 3/4, 1/4, 1/4)' & (m_{&y}^* 3/4, 3/4, 3/4)' \\ & (\&_y^* 3/4, 1/4, 1/4)' & (\&_y^{-1*} 1/4, 3/4, 1/4)' & (m_{xz}^* 1/4, 1/4, 3/4)' & (m_{&z}^* 3/4, 3/4, 3/4)' \\ & (\&_z^* 1/4, 3/4, 1/4)' & (\&_z^{-1*} 1/4, 1/4, 3/4)' & (m_{yz}^* 1/4, 3/4, 1/4)' & (m_{&z}^* 3/4, 3/4, 3/4)' \end{aligned}$$

230.4.1650  $la\&d'$   $la\&$   $(0,0,0;a,b,c)$

$$\begin{aligned} & (1^* 0, 0, 0) & (2_x^* 1/2, 1/2, 0) & (2_y^* 0, 1/2, 1/2) & (2_z^* 1/2, 0, 1/2) \\ & (3_{xyz}^* 0, 0, 0) & (3_{xyz}^{-1*} 0, 0, 0) & (3_{&yz}^* 0, 1/2, 1/2) & (3_{&yz}^{-1*} 1/2, 0, 1/2) \\ & (3_{x&yz}^* 1/2, 0, 1/2) & (3_{x&yz}^{-1*} 1/2, 1/2, 0) & (3_{xy&}^* 1/2, 1/2, 0) & (3_{xy&}^{-1*} 0, 1/2, 1/2) \\ & (4_x^* 1/4, 1/4, 3/4)' & (4_x^{-1*} 3/4, 1/4, 1/4)' & (2_{xy}^* 3/4, 1/4, 1/4)' & (2_{&y}^* 3/4, 3/4, 3/4)' \\ & (4_y^* 3/4, 1/4, 1/4)' & (4_y^{-1*} 1/4, 3/4, 1/4)' & (2_{xz}^* 1/4, 1/4, 3/4)' & (2_{&z}^* 3/4, 3/4, 3/4)' \\ & (4_z^* 1/4, 3/4, 1/4)' & (4_z^{-1*} 1/4, 1/4, 3/4)' & (2_{yz}^* 1/4, 3/4, 1/4)' & (2_{&z}^* 3/4, 3/4, 3/4)' \\ & (\&^* 0, 0, 0) & (m_x^* 1/2, 1/2, 0) & (m_y^* 0, 1/2, 1/2) & (m_z^* 1/2, 0, 1/2) \\ & (\&_{xyz}^* 0, 0, 0) & (\&_{xyz}^{-1*} 0, 0, 0) & (\&_{&yz}^* 0, 1/2, 1/2) & (\&_{&yz}^{-1*} 1/2, 0, 1/2) \\ & (\&_{x&yz}^* 1/2, 0, 1/2) & (\&_{x&yz}^{-1*} 1/2, 1/2, 0) & (\&_{xy&}^* 1/2, 1/2, 0) & (\&_{xy&}^{-1*} 0, 1/2, 1/2) \\ & (\&_x^* 1/4, 1/4, 3/4)' & (\&_x^{-1*} 3/4, 1/4, 1/4)' & (m_{xy}^* 3/4, 1/4, 1/4)' & (m_{&y}^* 3/4, 3/4, 3/4)' \end{aligned}$$

$$\begin{array}{cccc}
 (\mathfrak{g}_y^* 3/4, 1/4, 1/4)' & (\mathfrak{g}_y^{-1*} 1/4, 3/4, 1/4)' & (m_{xz}^* 1/4, 1/4, 3/4)' & (m_{\mathfrak{g}z}^* 3/4, 3/4, 3/4)' \\
 (\mathfrak{g}_z^* 1/4, 3/4, 1/4)' & (\mathfrak{g}_z^{-1*} 1/4, 1/4, 3/4)' & (m_{yz}^* 1/4, 3/4, 1/4)' & (m_{\mathfrak{g}z}^* 3/4, 3/4, 3/4)'
 \end{array}$$

230.5.1651 la'&d'

I4<sub>32</sub>

(0,0,0;a,b,c)

$$\begin{array}{cccc}
 (1^* 0, 0, 0) & (2_x^* 1/2, 1/2, 0) & (2_y^* 0, 1/2, 1/2) & (2_z^* 1/2, 0, 1/2) \\
 (3_{xyz}^* 0, 0, 0) & (3_{xyz}^{-1*} 0, 0, 0) & (3_{\mathfrak{g}yz}^* 0, 1/2, 1/2) & (3_{\mathfrak{g}yz}^{-1*} 1/2, 0, 1/2) \\
 (3_{x\mathfrak{g}z}^* 1/2, 0, 1/2) & (3_{x\mathfrak{g}z}^{-1*} 1/2, 1/2, 0) & (3_{xy\mathfrak{g}}^* 1/2, 1/2, 0) & (3_{xy\mathfrak{g}}^{-1*} 0, 1/2, 1/2) \\
 (4_x^* 1/4, 1/4, 3/4) & (4_x^{-1*} 3/4, 1/4, 1/4) & (2_{xy}^* 3/4, 1/4, 1/4) & (2_{\mathfrak{g}y}^* 3/4, 3/4, 3/4) \\
 (4_y^* 3/4, 1/4, 1/4) & (4_y^{-1*} 1/4, 3/4, 1/4) & (2_{xz}^* 1/4, 1/4, 3/4) & (2_{\mathfrak{g}z}^* 3/4, 3/4, 3/4) \\
 (4_z^* 1/4, 3/4, 1/4) & (4_z^{-1*} 1/4, 1/4, 3/4) & (2_{yz}^* 1/4, 3/4, 1/4) & (2_{\mathfrak{g}z}^* 3/4, 3/4, 3/4) \\
 (\mathfrak{g}^* 0, 0, 0)' & (m_x^* 1/2, 1/2, 0)' & (m_y^* 0, 1/2, 1/2)' & (m_z^* 1/2, 0, 1/2)' \\
 (\mathfrak{g}_{xyz}^* 0, 0, 0)' & (\mathfrak{g}_{xyz}^{-1*} 0, 0, 0)' & (\mathfrak{g}_{\mathfrak{g}yz}^* 0, 1/2, 1/2)' & (\mathfrak{g}_{\mathfrak{g}yz}^{-1*} 1/2, 0, 1/2)' \\
 (\mathfrak{g}_{x\mathfrak{g}z}^* 1/2, 0, 1/2)' & (\mathfrak{g}_{x\mathfrak{g}z}^{-1*} 1/2, 1/2, 0)' & (\mathfrak{g}_{xy\mathfrak{g}}^* 1/2, 1/2, 0)' & (\mathfrak{g}_{xy\mathfrak{g}}^{-1*} 0, 1/2, 1/2)' \\
 (\mathfrak{g}_x^* 1/4, 1/4, 3/4)' & (\mathfrak{g}_x^{-1*} 3/4, 1/4, 1/4)' & (m_{xy}^* 3/4, 1/4, 1/4)' & (m_{\mathfrak{g}y}^* 3/4, 3/4, 3/4)' \\
 (\mathfrak{g}_y^* 3/4, 1/4, 1/4)' & (\mathfrak{g}_y^{-1*} 1/4, 3/4, 1/4)' & (m_{xz}^* 1/4, 1/4, 3/4)' & (m_{\mathfrak{g}z}^* 3/4, 3/4, 3/4)' \\
 (\mathfrak{g}_z^* 1/4, 3/4, 1/4)' & (\mathfrak{g}_z^{-1*} 1/4, 1/4, 3/4)' & (m_{yz}^* 1/4, 3/4, 1/4)' & (m_{\mathfrak{g}z}^* 3/4, 3/4, 3/4)'
 \end{array}$$

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Superfamilies of Two-Dimensional Magnetic Space Groups

Serial Number	Symbol	Non-Magnetic Subgroup of Index Two		Standard Set of Coset Representatives	
1.1.1	p1			(1 00)	
1.2.2	p11'				
1.3.3	p <sub>2a</sub> 1	p1	(00;2a,b)	(1 00)	
2.1.4	p211			(1 00)	(2 <sub>z</sub>  00)
2.2.5	p2111'				
2.3.6	p2'11	p1	(00;a,b)	(1 00)	(2 <sub>z</sub>  00)'
2.4.7	p <sub>2a</sub> 211	p211	(00;2a,b)	(1 00)	(2 <sub>z</sub>  00)
3.1.8	p1m1			(1 00)	(m <sub>x</sub>  00)
3.2.9	p1m11'				
3.3.10	p1m'1	p1	(00;a,b)	(1 00)	(m <sub>x</sub>  00)'
3.4.11	p <sub>2a</sub> 1m1	p1m1	(00;2a,b)	(1 00)	(m <sub>x</sub>  00)
3.5.12	p <sub>2b</sub> 1m1	p1m1	(00;a,2b)	(1 00)	(m <sub>x</sub>  00)
3.6.13	p <sub>2b</sub> 1m'1	p1g1	(00;a,2b)	(1 00)	(m <sub>x</sub>  01)
3.7.14	p <sub>c</sub> 1m1	c1m1	(00;2a,2b)	(1 00)	(m <sub>x</sub>  00)
4.1.15	p1g1			(1 00)	(m <sub>x</sub>  0½)
4.2.16	p1g11'				
4.3.17	p1g'1	p1	(00;a,b)	(1 00)	(m <sub>x</sub>  0½)'
4.4.18	p <sub>2a</sub> 1g1	p1g1	(000;2a,b)	(1 00)	(m <sub>x</sub>  0½)
5.1.19	c1m1			(1 00)	(m <sub>x</sub>  00)
5.2.20	c1m11'				
5.3.21	c1m'1	p1	(00;a,(a+b)/2)	(1 00)	(m <sub>x</sub>  00)'
5.4.22	c <sub>p</sub> 1m1	p1m1	(00;a,b)	(1 00)	(m <sub>x</sub>  00)
5.5.23	c <sub>p</sub> 1m'1	p1g1	(¼00;a,b)	(1 00)	(m <sub>x</sub>  ½½)

6.1.24	p2mm			(1 00)	(m <sub>x</sub>  00)	(m <sub>y</sub>  00)	(2 <sub>z</sub>  00)
6.2.25	p2mm1'						
6.3.26	p2m'm'	p211	(00;a,b)	(1 00)	(m <sub>x</sub>  00)'	(m <sub>y</sub>  00)'	(2 <sub>z</sub>  00)
6.4.27	p2'mm'	p1m1	(00;a,b)	(1 00)	(m <sub>x</sub>  00)	(m <sub>y</sub>  00)'	(2 <sub>z</sub>  00)'
6.5.28	p <sub>2a</sub> 2m'm'	p2mg	(00;2a,b)	(1 00)	(m <sub>x</sub>  10)	(m <sub>y</sub>  10)	(2 <sub>z</sub>  00)
6.6.29	p <sub>c</sub> 2mm	c2mm	(00;2a,2b)	(1 00)	(m <sub>x</sub>  00)	(m <sub>y</sub>  00)	(2 <sub>z</sub>  00)
6.7.30	p <sub>2a</sub> 2mm	p2mm	(00;2a,b)	(1 00)	(m <sub>x</sub>  00)	(m <sub>y</sub>  00)	(2 <sub>z</sub>  00)
7.1.31	p2mg			(1 00)	(m <sub>x</sub>  ½0)	(m <sub>y</sub>  ½0)	(2 <sub>z</sub>  00)
7.2.32	p2mg1'						
7.3.33	p2m'g'	p211	(00;a,b)	(1 00)	(m <sub>x</sub>  ½0)'	(m <sub>y</sub>  ½0)'	(2 <sub>z</sub>  00)
7.4.34	p2'm'g	p1g1	(00;b,ā)	(1 00)	(m <sub>x</sub>  ½0)'	(m <sub>y</sub>  ½0)	(2 <sub>z</sub>  00)'
7.5.35	p2'mg'	p1m1	(¼0;a,b)	(1 00)	(m <sub>x</sub>  ½0)	(m <sub>y</sub>  ½0)'	(2 <sub>z</sub>  00)'
7.6.36	p <sub>2b</sub> 2m'g'	p2gg	(00;a,2b)	(1 00)	(m <sub>x</sub>  ½1)	(m <sub>y</sub>  ½1)	(2 <sub>z</sub>  00)
7.7.37	p <sub>2b</sub> 2mg	p2mg	(00;a,2b)	(1 00)	(m <sub>x</sub>  ½0)	(m <sub>y</sub>  ½0)	(2 <sub>z</sub>  00)
8.1.38	p2gg			(1 00)	(m <sub>x</sub>  ½½)	(m <sub>y</sub>  ½½)	(2 <sub>z</sub>  00)
8.2.39	p2gg1'						
8.3.40	p2g'g'	p211	(00;a,b)	(1 00)	(m <sub>x</sub>  ½½)'	(m <sub>y</sub>  ½½)'	(2 <sub>z</sub>  00)
8.4.41	p2'gg'	p1g1	(¼0;a,b)	(1 00)	(m <sub>x</sub>  ½½)	(m <sub>y</sub>  ½½)'	(2 <sub>z</sub>  00)'
9.1.42	c2mm			(1 00)	(m <sub>x</sub>  00)	(m <sub>y</sub>  00)	(2 <sub>z</sub>  00)
9.2.43	c2mm1'						
9.3.44	c2m'm'	p211	(00;a,(a+b)/2)	(1 00)	(m <sub>x</sub>  00)'	(m <sub>y</sub>  00)'	(2 <sub>z</sub>  00)
9.4.45	c2'mm'	p1m1	(00;a,(a+b)/2)	(1 00)	(m <sub>x</sub>  00)	(m <sub>y</sub>  00)'	(2 <sub>z</sub>  00)'
9.5.46	c <sub>p</sub> 2mm	pmm2	(00;a,b)	(1 00)	(m <sub>x</sub>  00)	(m <sub>y</sub>  00)	(2 <sub>z</sub>  00)
9.6.47	c <sub>p</sub> 2m'm'	p2gg	(00;a,b)	(1 00)	(m <sub>x</sub>  ½½)	(m <sub>y</sub>  ½½)	(2 <sub>z</sub>  00)
9.7.48	c <sub>p</sub> 2'mm'	p2mg	(¼¼;a,b)	(1 00)	(m <sub>x</sub>  00)	(m <sub>y</sub>  ½½)	(2 <sub>z</sub>  ½½)

10.1.49	p4			$(1 00)$	$(4_z 00)$	$(2_z 00)$	$(4_z^{-1} 00)$
10.2.50	p41'						
10.3.51	p4'	p211	(00;a,b)	$(1 00)$	$(4_z 00)'$	$(2_z 00)$	$(4_z^{-1} 00)'$
10.4.52	p <sub>p</sub> 4	p4	(00;a-b,a+b)	$(1 00)$	$(4_z 00)$	$(2_z 00)$	$(4_z^{-1} 00)$
11.1.53	p4mm			$(1 00)$ $(m_x 00)$	$(4_z 00)$ $(m_y 00)$	$(2_z 00)$ $(m_{xy} 00)$	$(4_z^{-1} 00)$ $(m_{\bar{xy}} 00)$
11.2.54	p4mm1'						
11.3.55	p4m'm'	p4	(00;a,b)	$(1 00)$ $(m_x 00)'$	$(4_z 00)$ $(m_y 00)'$	$(2_z 00)$ $(m_{xy} 00)'$	$(4_z^{-1} 00)$ $(m_{\bar{xy}} 00)'$
11.4.56	p4'mm'	p2mm	(00;a,b)	$(1 00)$ $(m_x 00)$	$(4_z 00)'$ $(m_y 00)$	$(2_z 00)$ $(m_{xy} 00)'$	$(4_z^{-1} 00)'$ $(m_{\bar{xy}} 00)'$
11.5.57	p4'm'm	c2mm	(00;a-b,a+b)	$(1 00)$ $(m_x 00)'$	$(4_z 00)'$ $(m_y 00)'$	$(2_z 00)$ $(m_{xy} 00)$	$(4_z^{-1} 00)'$ $(m_{\bar{xy}} 00)$
11.6.58	p <sub>p</sub> 4m'm'	p4gm	(00;a-b,a+b)	$(1 00)$ $(m_x 10)$	$(4_z 00)$ $(m_y 10)$	$(2_z 00)$ $(m_{xy} 10)$	$(4_z^{-1} 00)$ $(m_{\bar{xy}} 10)$
11.7.59	p <sub>p</sub> 4mm	p4mm	(00;a-b,a+b)	$(1 00)$ $(m_x 00)$	$(4_z 00)$ $(m_y 00)$	$(2_z 00)$ $(m_{xy} 00)$	$(4_z^{-1} 00)$ $(m_{\bar{xy}} 00)$
12.1.60	p4gm			$(1 00)$ $(m_x \frac{1}{2}\frac{1}{2})$	$(4_z 00)$ $(m_y \frac{1}{2}\frac{1}{2})$	$(2_z 00)$ $(m_{xy} \frac{1}{2}\frac{1}{2})$	$(4_z^{-1} 00)$ $(m_{\bar{xy}} \frac{1}{2}\frac{1}{2})$

12.2.61	p4gm1'						
12.3.62	p4g'm'	p4	(00;a,b)	$(1 00)$ $(m_x \frac{1}{2}\frac{1}{2})'$	$(4_z 00)$ $(m_y \frac{1}{2}\frac{1}{2})'$	$(2_z 00)$ $(m_{xy} \frac{1}{2}\frac{1}{2})'$	$(4_z^{-1} 00)$ $(m_{\bar{xy}} \frac{1}{2}\frac{1}{2})'$
12.4.63	p4'gm'	p2gg	(00;a,b)	$(1 00)$ $(m_x \frac{1}{2}\frac{1}{2})'$	$(4_z 00)'$ $(m_y \frac{1}{2}\frac{1}{2})'$	$(2_z 00)$ $(m_{xy} \frac{1}{2}\frac{1}{2})'$	$(4_z^{-1} 00)'$ $(m_{\bar{xy}} \frac{1}{2}\frac{1}{2})'$
12.5.64	p4'g'm	c2mm	( $\frac{1}{2}0$ ;a-b,a+b)	$(1 00)$ $(m_x \frac{1}{2}\frac{1}{2})'$	$(4_z 00)'$ $(m_y \frac{1}{2}\frac{1}{2})'$	$(2_z 00)$ $(m_{xy} \frac{1}{2}\frac{1}{2})'$	$(4_z^{-1} 00)'$ $(m_{\bar{xy}} \frac{1}{2}\frac{1}{2})'$
13.1.65	p3			$(1 00)$	$(3_z 00)$	$(3_z^{-1} 00)$	
13.2.66	p31'						
14.1.67	p3m1			$(1 00)$ $(m_x 00)$	$(3_z 00)$ $(m_y 00)$	$(3_z^{-1} 00)$ $(m_{xy} 00)$	
14.2.68	p3m11'						
14.3.69	p3m'1	p3	(00;a,b)	$(1 00)$ $(m_x 00)'$	$(3_z 00)$ $(m_y 00)'$	$(3_z^{-1} 00)$ $(m_{xy} 00)'$	
15.1.70	p31m			$(1 00)$ $(m_1 00)$	$(3_z 00)$ $(m_2 00)$	$(3_z^{-1} 00)$ $(m_3 00)$	
15.2.71	p31m1'						



15.3.72	p31m'	p3	(00;a,b)	$(1 00)$ $(m_1 00)'$	$(3_z 00)$ $(m_2 00)'$	$(3_z^{-1} 00)$ $(m_3 00)'$
16.1.73	p6			$(1 00)$ $(6_z 00)$	$(3_z 00)$ $(2_z 00)$	$(3_z^{-1} 00)$ $(6_z^{-1} 00)$
16.2.74	p61'					
16.3.75	p6'	p3	(00;a,b)	$(1 00)$ $(6_z 00)'$	$(3_z 00)$ $(2_z 00)'$	$(3_z^{-1} 00)$ $(6_z^{-1} 00)'$
17.1.76	p6mm			$(1 00)$ $(6_z 00)$ $(m_x 00)$ $(m_1 00)$	$(3_z 00)$ $(2_z 00)$ $(m_y 00)$ $(m_2 00)$	$(3_z^{-1} 00)$ $(6_z^{-1} 00)$ $(m_{xy} 00)$ $(m_3 00)$
17.2.77	p6mm1'					
17.3.78	p6m'm'	p6	(000;a,b)	$(1 00)$ $(6_z 00)$ $(m_x 00)'$ $(m_1 00)'$	$(3_z 00)$ $(2_z 00)$ $(m_y 00)'$ $(m_2 00)'$	$(3_z^{-1} 00)$ $(6_z^{-1} 00)$ $(m_{xy} 00)'$ $(m_3 00)'$
17.4.79	p6'mm'	p3m1	(00;a,b)	$(1 00)$	$(3_z 00)$	$(3_z^{-1} 00)$

				$(6_z 00)'$	$(2_z 00)'$	$(6_z^{-1} 00)'$
				$(m_x 00)$	$(m_y 00)$	$(m_{xy} 00)$
				$(m_1 00)'$	$(m_2 00)'$	$(m_3 00)'$
17.5.80	p6'm'm	p31m	(00;a,b)	$(1 00)$	$(3_z 00)$	$(3_z^{-1} 00)$
				$(6_z 00)'$	$(2_z 00)'$	$(6_z^{-1} 00)'$
				$(m_x 00)'$	$(m_y 00)'$	$(m_{xy} 00)'$
				$(m_1 00)$	$(m_2 00)$	$(m_3 00)$

Superfamilies of One-Dimensional Magnetic Space Groups

Serial Number	Symbol	Non-Magnetic Subgroup of Index Two	Standard Set of Coset Representatives
1.1.1	$p1$		(0;a) (1 0)
1.2.2	$p11'$		
1.3.3	$p_{2a}1$	$p1$	(0;2a) (1 0)
2.1.4	$pm$		(0;a) (1 0) (m 0)
2.2.5	$pm1'$		
2.3.6	$pm'$	$p1$	(0;a) (1 0) (m 0)'
2.4.7	$p_{2a}m$	$pm$	(0;2a) (1 0) (m 0)

**Table 1.2: Relative Lengths and Mutual Orientations of Translation Vectors**

<b>Three-Dimensional</b>		
Conventional Coordinate System		
Crystal system	Restrictions on cell parameter	Parameters to be determined
-----	-----	-----
Triclinic	None	a,b,c; $\alpha, \beta, \gamma$
Monoclinic	$\alpha = \gamma = 90^\circ$	a,b,c; $\gamma$
Orthorhombic	$\alpha = \beta = \gamma = 90^\circ$	a,b,c
Tetragonal	$a = b; \alpha = \beta = \gamma = 90^\circ$	a,c
Trigonal	Hexagonal axes: $a = b;$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$	a,c
	Rhombohedral axes: $a = b = c; \alpha = \beta = \gamma$	a, $\alpha$
Hexagonal	$a = b;$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$	a,c
Cubic	$a = b = c; \alpha = \beta = \gamma = 90^\circ$	a
<b>Two-Dimensional</b>		
Oblique	None	a,b, $\gamma$
Rectangular	$\gamma = 90^\circ$	a,b
Square	$a = b$ $\gamma = 90^\circ$	a
Hexagonal	$a = b$ $\gamma = 120^\circ$	a
<b>One Dimensional</b>		
-----	None	a

**Table 1.3.1 : Symmetry directions and position in Hermann-Mauguin symbols**

Directions which belong to the same set of equivalent symmetry directions are given between braces. The first entry in each set is taken as the representative of that set.

**Three-Dimensional**

Symmetry direction  
(position in Hermann-Mauguin symbol)

Lattice	Primary	Secondary	Tertiary
Triclinic	None		
Monoclinic	$[010]$ unique axis b		
Orthorhombic	$[100]$	$[010]$	$[001]$
Tetragonal		$\begin{Bmatrix} [100] \\ [010] \end{Bmatrix}$	$\begin{Bmatrix} [1\bar{1}0] \\ [110] \end{Bmatrix}$
Hexagonal	$[001]$	$\begin{Bmatrix} [100] \\ [010] \\ [\bar{1}\bar{1}0] \end{Bmatrix}$	$\begin{Bmatrix} [1\bar{1}0] \\ [120] \\ [2\bar{1}0] \end{Bmatrix}$
Rhombohedral (hexagonal axes)	$[001]$	$\begin{Bmatrix} [100] \\ [010] \\ [\bar{1}\bar{1}0] \end{Bmatrix}$	
Cubic	$\begin{Bmatrix} [100] \\ [010] \\ [001] \end{Bmatrix}$	$\begin{Bmatrix} [111] \\ [1\bar{1}\bar{1}] \\ [\bar{1}1\bar{1}] \\ [\bar{1}\bar{1}1] \end{Bmatrix}$	$\begin{Bmatrix} [1\bar{1}0] & [110] \\ [01\bar{1}] & [011] \\ [\bar{1}01] & [101] \end{Bmatrix}$

## Two-Dimensional

Symmetry direction  
(position in Hermann-Mauguin symbol)

Lattice	Primary	Secondary	Tertiary
Oblique	Rotation Point in Plane		
Rectangular	Rotation Point in Plane	$[10]$	$[01]$
Square	Rotation Point in Plane	$\left\{ \begin{array}{l} [10] \\ [01] \end{array} \right\}$	$\left\{ \begin{array}{l} [1\bar{1}] \\ [11] \end{array} \right\}$
Hexagonal	Rotation Point in Plane	$\left\{ \begin{array}{l} [10] \\ [01] \\ [\bar{1}\bar{1}] \end{array} \right\}$	$\left\{ \begin{array}{l} [1\bar{1}] \\ [12] \\ [2\bar{1}] \end{array} \right\}$

TABLE 1.3.1 - 2

**Table 1.3.2 : Symmetry direction subindex symbols**

<b>Three-Dimensional</b>		
Lattice	Symmetry direction	Subindex symbol
Monoclinic	[010]	y
Orthorhombic	[100]	x
	[010]	y
	[001]	z
Tetragonal	[001]	z
	[100]	x
	[010]	$\bar{y}$
	$[\bar{1}10]$	$\overline{xy}$
	[110]	xy
Hexagonal	[001]	z
	[100]	x
	[010]	y
	[110]	xy
	[210]	1
	[120]	2
	$[\bar{1}10]$	3
Rhombohedral (hexagonal axes)	[001]	z
	[100]	x
	[010]	y
	[110]	xy
Cubic	[100]	x
	[010]	y
	[001]	z
	[111]	xyz
	$[\bar{1}11]$	$\overline{xyz}$
	$[1\bar{1}1]$	$x\bar{y}z$
	$[11\bar{1}]$	$xy\bar{z}$
	[110]	xy
	$[\bar{1}10]$	$\overline{xy}$
	[011]	yz
	$[0\bar{1}1]$	$\overline{yz}$
	[101]	xz
	$[\bar{1}01]$	$\overline{xz}$

TABLE 1.3.2 - 1

## Two-dimensional

Lattice	Symmetry direction	Subindex symbol
Oblique	[10]	x
	[01]	y
Rectangular	[10]	x
	[01]	y
Square	[10]	x
	[01]	y
	[11]	xy
	$\bar{1}\bar{1}$	$\bar{x}\bar{y}$
Hexagonal	[10]	x
	[01]	y
	[11]	xy
	[21]	1
	[12]	2
	$\bar{1}\bar{1}$	3

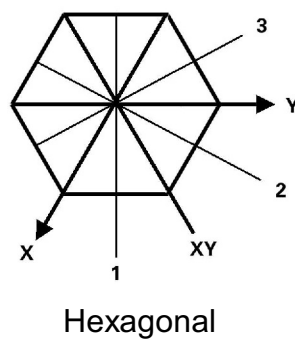
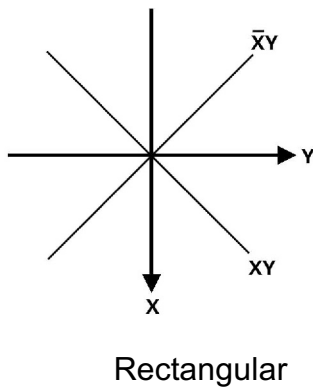
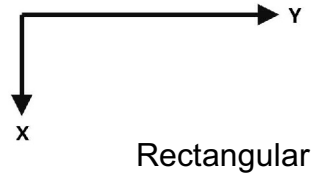
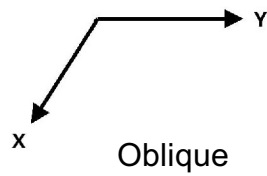


TABLE 1.3.2 - 2



**Tables 1.4: Comparison of Magnetic Space Group and Black and White Space Group Symbols**

**Table 1.4 - 3D**

**Three-dimensional:** Opechowski and Guccione (OG) symbols, Table 1.1-3D, compared with Belov, Neronova and Smirnova (BNS) symbols (1955, 1957). If the symbols are the same, no symbol is given in the BNS column.

	<b>OG</b>	<b>BNS</b>		<b>OG</b>	<b>BNS</b>
<b>TRICLINIC SYSTEM</b>					
1.1.1	<b>P1</b>		<b>4.1.15</b>	<b>P<sub>2</sub><sub>1</sub></b>	
1.2.2	P11'		4.2.16	P2 <sub>1</sub> 1'	
1.3.3	P <sub>2s</sub> 1	P <sub>s</sub> 1	4.3.17	P2 <sub>1</sub> '	
			4.4.18	P <sub>2a</sub> 2 <sub>1</sub>	P <sub>a</sub> 2 <sub>1</sub>
<b>2.1.4</b>	<b>P<math>\bar{1}</math></b>				
2.2.5	P $\bar{1}$ 1'		<b>5.1.19</b>	<b>C2</b>	
2.3.6	P $\bar{1}$ '		5.2.20	C21'	
2.4.7	P <sub>2s</sub> $\bar{1}$	P <sub>s</sub> $\bar{1}$	5.3.21	C2'	
			5.4.22	C <sub>2c</sub> 2	C <sub>c</sub> 2
			5.5.23	C <sub>p</sub> 2	P <sub>C</sub> 2
			5.6.24	C <sub>p</sub> 2'	P <sub>C</sub> 2 <sub>1</sub>
<b>MONOCLINIC SYSTEM</b>					
<b>3.1.8</b>	<b>P2</b>				
3.2.9	P21'		<b>6.1.25</b>	<b>Pm</b>	
3.3.10	P2'		6.2.26	Pm1'	
3.4.11	P <sub>2a</sub> 2	P <sub>a</sub> 2	6.3.27	Pm'	
3.5.12	P <sub>2b</sub> 2	P <sub>b</sub> 2	6.4.28	P <sub>2a</sub> m	P <sub>a</sub> m
3.6.13	P <sub>C</sub> 2	C <sub>a</sub> 2	6.5.29	P <sub>2b</sub> m	P <sub>b</sub> m
3.7.14	P <sub>2b</sub> 2'	P <sub>b</sub> 2 <sub>1</sub>			

6.6.30	$P_C m$	$C_a m$	10.3.51	$P2'/m$	
6.7.31	$P_{2c} m'$	$P_c c$	10.4.52	$P2/m'$	
<b>7.1.32</b>	<b><math>Pc</math></b>		10.5.53	$P2'/m'$	
7.2.33	$Pc1'$		10.6.54	$P_{2a} 2/m$	$P_a 2/m$
7.3.34	$Pc'$		10.7.55	$P_{2b} 2/m$	$P_b 2/m$
7.4.35	$P_{2a} c$	$P_a c$	10.8.56	$P_C 2/m$	$C_a 2/m$
7.5.36	$P_{2b} c$	$P_b c$	10.9.57	$P_{2b} 2'/m$	$P_b 2_1/m$
7.6.37	$P_C c$	$C_a c$	10.10.58	$P_{2c} 2/m'$	$P_c 2/c$
<b>8.1.38</b>	<b><math>Cm</math></b>		<b>11.1.59</b>	<b><math>P2_1/m</math></b>	
8.2.39	$Cm1'$		11.2.60	$P2_1/m1'$	
8.3.40	$Cm'$		11.3.61	$P2_1'/m$	
8.4.41	$C_{2c} m$	$C_c m$	11.4.62	$P2_1/m'$	
8.5.42	$C_P m$	$P_C m$	11.5.63	$P2_1'/m'$	
8.6.43	$C_{2c} m'$	$C_c c$	11.6.64	$P_{2a} 2_1/m$	$P_a 2_1/m$
8.7.44	$C_P m'$	$P_A c$	11.7.65	$P_{2c} 2_1/m'$	$P_c 2_1/c$
<b>9.1.45</b>	<b><math>Cc</math></b>		<b>12.1.66</b>	<b><math>C2/m</math></b>	
9.2.46	$Cc1'$		12.2.67	$C2/m1'$	
9.3.47	$Cc'$		12.3.68	$C2'/m$	
9.4.48	$C_P c$	$P_C c$	12.4.69	$C2/m'$	
<b>10.1.49</b>	<b><math>P2/m</math></b>		12.5.70	$C2'/m'$	
10.2.50	$P2/m1'$		12.6.71	$C_{2c} 2/m$	$C_c 2/m$
			12.7.72	$C_P 2/m$	$P_C 2/m$

TABLE 1.4 - 3D - 2

12.8.73	$C_{2c} 2/m'$	$C_c 2/c$	15.3.94	$C2'/c$	
12.9.74	$C_p 2'/m$	$P_c 2_1/m$	15.4.95	$C2/c'$	
12.10.75	$C_p 2/m'$	$P_A 2/c$	15.5.96	$C2'/c'$	
12.11.76	$C_p 2'/m'$	$P_A 2_1/c$	15.6.97	$C_p 2/c$	$P_c 2/c$
			15.7.98	$C_p 2'/c$	$P_c 2_1/c$
<b>13.1.77</b>	<b><math>P2/c</math></b>				
13.2.78	$P2/c1'$		<b>ORTHORHOMBIC SYSTEM</b>		
13.3.79	$P2'/c$		<b>16.1.99</b>	<b><math>P222</math></b>	
13.4.80	$P2/c'$		16.2.100	$P2221'$	
13.5.81	$P2'/c'$		16.3.101	$P2'2'2$	
13.6.82	$P_{2a} 2/c$	$P_a 2/c$	16.4.102	$P_{2a} 222$	$P_a 222$
13.7.83	$P_{2b} 2/c$	$P_b 2/c$	16.5.103	$P_c 222$	$C_a 222$
13.8.84	$P_c 2/c$	$C_a 2/c$	16.6.104	$P_F 222$	$F_s 222$
13.9.85	$P_{2b} 2'/c$	$P_b 2_1/c$	16.7.105	$P_{2c} 22'2'$	$P_c 222_1$
<b>14.1.86</b>	<b><math>P2_1/c</math></b>		<b>17.1.106</b>	<b><math>P222_1</math></b>	
14.2.87	$P2_1/c1'$		17.2.107	$P222_11'$	
14.3.88	$P2_1'/c$		17.3.108	$P2'2'2_1$	
14.4.89	$P2_1/c'$		17.4.109	$P22'2_1'$	
14.5.90	$P2_1'/c'$		17.5.110	$P_{2a} 222_1$	$P_a 222_1$
14.6.91	$P_{2a} 2_1/c$	$P_a 2_1/c$	17.6.111	$P_c 222_1$	$C_a 222_1$
<b>15.1.92</b>	<b><math>C2/c</math></b>		17.7.112	$P_{2a} 2'2'2_1$	$P_a 2_1 2_1 2$
15.2.93	$C2/c1'$		<b>18.1.113</b>	<b><math>P2_1 2_1 2</math></b>	

TABLE 1.4 - 3D - 3

18.2.114	P <sub>2</sub> 2 <sub>1</sub> 2 <sub>1</sub> '		21.7.135	C <sub>1</sub> 222	I <sub>c</sub> 222
18.3.115	P <sub>2</sub> 1'2 <sub>1</sub> '2		21.8.136	C <sub>2c</sub> 22'2'	C <sub>c</sub> 222 <sub>1</sub>
18.4.116	P <sub>2</sub> 2 <sub>1</sub> '2'		21.9.137	C <sub>p</sub> 2'2'2	P <sub>C</sub> 2 <sub>1</sub> 2 <sub>1</sub> 2
18.5.117	P <sub>2c</sub> 2 <sub>1</sub> 2 <sub>1</sub> 2	P <sub>c</sub> 2 <sub>1</sub> 2 <sub>1</sub> 2	21.10.138	C <sub>p</sub> 22'2'	P <sub>A</sub> 222 <sub>1</sub>
18.6.118	P <sub>2c</sub> 2 <sub>1</sub> 2 <sub>1</sub> '2'	P <sub>a</sub> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	21.11.139	C <sub>1</sub> 2'22'	I <sub>c</sub> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
<b>19.1.119</b>	<b>P<sub>2</sub>1,2,1</b>		<b>22.1.140</b>	<b>F222</b>	
19.2.120	P <sub>2</sub> 1,2,1,1'		22.2.141	F2221'	
19.3.121	P <sub>2</sub> 1'2 <sub>1</sub> '2 <sub>1</sub>		22.3.142	F2'2'2	
<b>20.1.122</b>	<b>C222<sub>1</sub></b>		22.4.143	F <sub>C</sub> 222	C <sub>A</sub> 222
20.2.123	C222 <sub>1</sub> 1'		22.5.144	F <sub>C</sub> 22'2'	C <sub>A</sub> 222 <sub>1</sub>
20.3.124	C2'2'2 <sub>1</sub>		<b>23.1.145</b>	<b>I222</b>	
20.4.125	C22'2 <sub>1</sub> '		23.2.146	I2221'	
20.5.126	C <sub>p</sub> 222 <sub>1</sub>	P <sub>C</sub> 222 <sub>1</sub>	23.3.147	I2'2'2	
20.6.127	C <sub>p</sub> 2'2'2 <sub>1</sub>	P <sub>C</sub> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	23.4.148	I <sub>p</sub> 222	P <sub>1</sub> 222
20.7.128	C <sub>p</sub> 22'2 <sub>1</sub> '	P <sub>A</sub> 2 <sub>1</sub> 2 <sub>1</sub> 2	23.5.149	I <sub>p</sub> 2'2'2	P <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> 2
<b>21.1.129</b>	<b>C222</b>		<b>24.1.150</b>	<b>I2,2,2<sub>1</sub></b>	
21.2.130	C2221'		24.2.151	I2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> 1'	
21.3.131	C2'2'2		24.3.152	I2 <sub>1</sub> '2 <sub>1</sub> '2 <sub>1</sub>	
21.4.132	C22'2'		24.4.153	I <sub>p</sub> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	P <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
21.5.133	C <sub>2c</sub> 222	C <sub>c</sub> 222	24.5.154	I <sub>p</sub> 2 <sub>1</sub> '2 <sub>1</sub> '2 <sub>1</sub>	P <sub>1</sub> 222 <sub>1</sub>
21.6.134	C <sub>p</sub> 222	P <sub>C</sub> 222	<b>25.1.155</b>	<b>Pmm2</b>	

TABLE 1.4 - 3D - 4

25.2.156	Pmm21'		<b>27.1.178</b>	<b>Pcc2</b>	
25.3.157	Pm'm2'		27.2.179	Pcc21'	
25.4.158	Pm'm'2		27.3.180	Pc'c'2'	
25.5.159	P <sub>2c</sub> mm2	P <sub>c</sub> mm2	27.4.181	Pc'c'2	
25.6.160	P <sub>2a</sub> mm2	P <sub>a</sub> mm2	27.5.182	P <sub>2a</sub> cc2	P <sub>a</sub> cc2
25.7.161	P <sub>C</sub> mm2	C <sub>a</sub> mm2	27.6.183	P <sub>C</sub> cc2	C <sub>a</sub> cc2
25.8.162	P <sub>A</sub> mm2	A <sub>c</sub> mm2	27.7.184	P <sub>2b</sub> c'c'2'	P <sub>b</sub> nc2
25.9.163	P <sub>F</sub> mm2	F <sub>s</sub> mm2			
25.10.164	P <sub>2c</sub> mm'2'	P <sub>c</sub> mc2 <sub>1</sub>	<b>28.1.185</b>	<b>Pma2</b>	
25.11.165	P <sub>2c</sub> m'm'2	P <sub>c</sub> cc2	28.2.186	Pma21'	
25.12.166	P <sub>2a</sub> m'm'2	P <sub>a</sub> ma2	28.3.187	Pm'a2'	
25.13.167	P <sub>A</sub> m'm'2	A <sub>c</sub> bm2	28.4.188	Pma'2'	
			28.5.189	Pm'a'2	
<b>26.1.168</b>	<b>Pmc2<sub>1</sub></b>		28.6.190	P <sub>2b</sub> ma2	P <sub>b</sub> ma2
26.2.169	Pmc2 <sub>1</sub> '		28.7.191	P <sub>2c</sub> ma2	P <sub>c</sub> ma2
26.3.170	Pm'c2 <sub>1</sub> '		28.8.192	P <sub>A</sub> ma2	A <sub>c</sub> ma2
26.4.171	Pmc'2 <sub>1</sub> '		28.9.193	P <sub>2b</sub> m'a2'	P <sub>a</sub> ba2
26.5.172	Pm'c'2 <sub>1</sub>		28.10.194	P <sub>2c</sub> m'a2'	P <sub>c</sub> ca2 <sub>1</sub>
26.6.173	P <sub>2a</sub> mc2 <sub>1</sub>	P <sub>a</sub> mc2 <sub>1</sub>	28.11.195	P <sub>2c</sub> ma'2'	P <sub>c</sub> mn2 <sub>1</sub>
26.7.174	P <sub>2b</sub> mc2 <sub>1</sub>	P <sub>b</sub> mc2 <sub>1</sub>	28.12.196	P <sub>2c</sub> m'a'2	P <sub>c</sub> nc2
26.8.175	P <sub>C</sub> mc2 <sub>1</sub>	C <sub>a</sub> mc2 <sub>1</sub>	28.13.197	P <sub>A</sub> m'a'2	A <sub>c</sub> ba2
26.9.176	P <sub>2a</sub> mc'2 <sub>1</sub> '	P <sub>a</sub> mn2 <sub>1</sub>			
26.10.177	P <sub>2b</sub> m'c'2 <sub>1</sub>	P <sub>a</sub> ca2 <sub>1</sub>	<b>29.1.198</b>	<b>Pca2<sub>1</sub></b>	
			29.2.199	Pca2 <sub>1</sub> '	

TABLE 1.4 - 3D - 5

29.3.200	Pc'a2 <sub>1</sub> '		32.3.221	Pb'a2'	
29.4.201	Pca'2 <sub>1</sub> '		32.4.222	Pb'a'2	
29.5.202	Pc'a'2 <sub>1</sub>		32.5.223	P <sub>2c</sub> ba2	P <sub>c</sub> ba2
29.6.203	P <sub>2b</sub> ca2 <sub>1</sub>	P <sub>b</sub> ca2 <sub>1</sub>	32.6.224	P <sub>2c</sub> b'a2'	P <sub>c</sub> na2 <sub>1</sub>
29.7.204	P <sub>2b</sub> c'a'2 <sub>1</sub>	P <sub>b</sub> na2 <sub>1</sub>	32.7.225	P <sub>2c</sub> b'a'2	P <sub>c</sub> nn2
<b>30.1.205</b>	<b>Pnc2</b>		<b>33.1.226</b>	<b>Pna2<sub>1</sub></b>	
30.2.206	Pnc21'		33.2.227	Pna2 <sub>1</sub> 1'	
30.3.207	Pn'c2'		33.3.228	Pn'a2 <sub>1</sub> '	
30.4.208	Pnc'2'		33.4.229	Pna'2 <sub>1</sub> '	
30.5.209	Pn'c'2		33.5.230	Pn'a'2 <sub>1</sub>	
30.6.210	P <sub>2a</sub> nc2	P <sub>a</sub> nc2	<b>34.1.231</b>	<b>Pnn2</b>	
30.7.211	P <sub>2a</sub> nc'2'	P <sub>a</sub> nn2	34.2.232	Pnn21'	
<b>31.1.212</b>	<b>Pmn2<sub>1</sub></b>		34.3.233	Pn'n2'	
31.2.213	Pmn2 <sub>1</sub> 1'		34.4.234	Pn'n'2	
31.3.214	Pm'n2 <sub>1</sub> '		34.5.235	P <sub>F</sub> nn2	F <sub>s</sub> dd2
31.4.215	Pmn'2 <sub>1</sub> '		<b>35.1.236</b>	<b>Cmm2</b>	
31.5.216	Pm'n'2 <sub>1</sub>		35.2.237	Cmm21'	
31.6.217	P <sub>2b</sub> mn2 <sub>1</sub>	P <sub>b</sub> mn2 <sub>1</sub>	35.3.238	Cm'm2'	
31.7.218	P <sub>2b</sub> m'n'2 <sub>1</sub> '	P <sub>a</sub> na2 <sub>1</sub>	35.4.239	Cm'm'2	
<b>32.1.219</b>	<b>Pba2</b>		35.5.240	C <sub>2c</sub> mm2	C <sub>c</sub> mm2
32.2.220	Pba21'		35.6.241	C <sub>p</sub> mm2	P <sub>c</sub> mm2

TABLE 1.4 - 3D - 6

35.7.242	$C_1mm2$	$I_cmm2$	37.7.264	$C_Pc'c'2$	$P_Cnn2$
35.8.243	$C_{2c}m'm2'$	$C_cmc2_1$	<b>38.1.265</b>	<b><math>Amm2</math></b>	
35.9.244	$C_{2c}m'm'2$	$C_ccc2$	38.2.266	$Amm21'$	
35.10.245	$C_Pm'm2'$	$P_Cma2$	38.3.267	$Am'm2'$	
35.11.246	$C_Pm'm'2$	$P_Cba2$	38.4.268	$Amm'2'$	
35.12.247	$C_1m'm2'$	$I_cma2$	38.5.269	$Am'm'2$	
35.13.248	$C_1m'm'2$	$I_cba2$	38.6.270	$A_{2a}mm2$	$A_a mm2$
<b>36.1.249</b>	<b><math>Cmc2_1</math></b>		38.7.271	$A_Pmm2$	$P_A mm2$
36.2.250	$Cmc2_11'$		38.8.272	$A_1mm2$	$I_a mm2$
36.3.251	$Cm'c2_1'$		38.9.273	$A_{2a}mm'2'$	$A_a ma2$
36.4.252	$Cmc'2_1'$		38.10.274	$A_Pm'm2'$	$P_B mn2_1$
36.5.253	$Cm'c'2_1$		38.11.275	$A_Pmm'2'$	$P_A mc2_1$
36.6.254	$C_Pmc2_1$	$P_Cmc2_1$	38.12.276	$A_Pm'm'2$	$P_A nc2$
36.7.255	$C_Pm'c2_1'$	$P_Cca2_1$	38.13.277	$A_1m'm'2$	$I_a ma2$
36.8.256	$C_Pmc'2_1'$	$P_Cmn2_1$	<b>39.1.278</b>	<b><math>Abm2</math></b>	
36.9.257	$C_Pm'c'2_1$	$P_Cna2_1$	39.2.279	$Abm21'$	
<b>37.1.258</b>	<b><math>Ccc2</math></b>		39.3.280	$Ab'm2'$	
37.2.259	$Ccc21'$		39.4.281	$Abm'2'$	
37.3.260	$Cc'c2'$		39.5.282	$Ab'm'2$	
37.4.261	$Cc'c'2$		39.6.283	$A_{2a}bm2$	$A_a bm2$
37.5.262	$C_Pcc2$	$P_Ccc2$	39.7.284	$A_Pbm2$	$P_B ma2$
37.6.263	$C_Pc'c'2'$	$P_Cnc2$	39.8.285	$A_1bm2$	$I_b ma2$

TABLE 1.4 - 3D - 7

39.9.286	$A_{2a} b'm'2$	$A_a ba2$	41.9.308	$A_p b'a'2$	$P_B nc2$
39.10.287	$A_p b'm'2'$	$P_B mc2_1$	<b>42.1.309</b>	<b>Fmm2</b>	
39.11.288	$A_p bm'2'$	$P_B ca2_1$	42.2.310	Fmm21'	
39.12.289	$A_p b'm'2$	$P_A cc2$	42.3.311	Fm'm'2'	
39.13.290	$A_l b'm'2$	$I_a ba2$	42.4.312	Fm'm'2	
<b>40.1.291</b>	<b>Ama2</b>		42.5.313	$F_C mm2$	$C_A mm2$
40.2.292	Ama21'		42.6.314	$F_A mm2$	$A_C mm2$
40.3.293	Am'a'2'		42.7.315	$F_C mm'2'$	$C_A mc2_1$
40.4.294	Ama'2'		42.8.316	$F_C m'm'2$	$C_A cc2$
40.5.295	Am'a'2		42.9.317	$F_A m'm'2'$	$A_C bm2$
40.6.296	$A_p ma2$	$P_A ma2$	42.10.318	$F_A mm'2'$	$A_C ma2$
40.7.297	$A_p m'a'2'$	$P_A na2_1$	42.11.319	$F_A m'm'2$	$A_C ba2$
40.8.298	$A_p ma'2'$	$P_A mn2_1$	<b>43.1.320</b>	<b>Fdd2</b>	
40.9.299	$A_p m'a'2$	$P_A nn2$	43.2.321	Fdd21'	
<b>41.1.300</b>	<b>Aba2</b>		43.3.322	Fd'd'2'	
41.2.301	Aba21'		43.4.323	Fd'd'2	
41.3.302	Ab'a'2'		<b>44.1.324</b>	<b>Imm2</b>	
41.4.303	Aba'2'		44.2.325	Imm21'	
41.5.304	Ab'a'2		44.3.326	Im'm'2'	
41.6.305	$A_p ba2$	$P_A ba2$	44.4.327	Im'm'2	
41.7.306	$A_p b'a'2'$	$P_A ca2_1$	44.5.328	$I_p mm2$	$P_l mm2$
41.8.307	$A_p ba'2'$	$P_B na2_1$			

TABLE 1.4 - 3D - 8



44.6.329	$I_p mm'2'$	$P_1 mm2_1$	47.4.350	$Pm'm'm$	
44.7.330	$I_p m'm'2$	$P_1 nn2$	47.5.351	$Pm'm'm'$	
<b>45.1.331</b>	<b><math>Iba2</math></b>		47.6.352	$P_{2a} mmm$	$P_a mmm$
45.2.332	$Iba21'$		47.7.353	$P_C mmm$	$C_a mmm$
45.3.333	$Ib'a2'$		47.8.354	$P_F mmm$	$F_s mmm$
45.4.334	$Ib'a'2$		47.9.355	$P_{2a} mmm'$	$P_a mma$
45.5.335	$I_p ba2$	$P_1 cc2$	47.10.356	$P_{2c} m'm'm$	$P_c ccm$
45.6.336	$I_p ba'2'$	$P_1 ca2_1$	47.11.357	$P_C mmm'$	$C_a mma$
45.7.337	$I_p b'a'2$	$P_1 ba2$	<b>48.1.358</b>	<b><math>Pnnn</math></b>	
<b>46.1.338</b>	<b><math>Ima2</math></b>		48.2.359	$Pnnn1'$	
46.2.339	$Ima21'$		48.3.360	$Pn'nn$	
46.3.340	$Im'a2'$		48.4.361	$Pn'n'n$	
46.4.341	$Ima'2'$		48.5.362	$Pn'n'n'$	
46.5.342	$Im'a'2$		48.6.363	$P_F nnn$	$F_s ddd$
46.6.343	$I_p ma2$	$P_1 ma2$	<b>49.1.364</b>	<b><math>Pccm</math></b>	
46.7.344	$I_p m'a2'$	$P_1 na2_1$	49.2.365	$Pccm1'$	
46.8.345	$I_p ma'2'$	$P_1 mc2_1$	49.3.366	$Pc'cm$	
46.9.346	$I_p m'a'2$	$P_1 nc2$	49.4.367	$Pccm'$	
<b>47.1.347</b>	<b><math>Pmmm</math></b>		49.5.368	$Pc'c'm$	
47.2.348	$Pmmm1'$		49.6.369	$Pc'cm'$	
47.3.349	$Pm'mm$		49.7.370	$Pc'c'm'$	
			49.8.371	$P_{2a} ccm$	$P_a ccm$

TABLE 1.4 - 3D - 9

49.9.372	$P_C ccm$	$C_a ccm$	51.8.394	$Pm'ma'$	
49.10.373	$P_{2a} ccm'$	$P_a cca$	51.9.395	$Pm'm'a'$	
49.11.374	$P_{2a} c'c'm$	$P_c mna$	51.10.396	$P_{2b} mma$	$P_b mma$
49.12.375	$P_{2a} c'c'm'$	$P_a ban$	51.11.397	$P_{2c} mma$	$P_c mma$
49.13.376	$P_C ccm'$	$C_a cca$	51.12.398	$P_A mma$	$C_a mcm$
<b>50.1.377</b>	<b>Pban</b>		51.13.399	$P_{2b} m'ma$	$P_c bcm$
50.2.378	$Pban1'$		51.14.400	$P_{2b} mma'$	$P_a mmn$
50.3.379	$Pb'an$		51.15.401	$P_{2b} m'ma'$	$P_a mna$
50.4.380	$Pban'$		51.16.402	$P_{2c} m'ma$	$P_a bam$
50.5.381	$Pb'a'n$		51.17.403	$P_{2c} mm'a$	$P_b bcm$
50.6.382	$Pb'an'$		51.18.404	$P_{2c} m'm'a$	$P_c cca$
50.7.383	$Pb'a'n'$		51.19.405	$P_A m'ma$	$C_a mca$
50.8.384	$P_{2c} ban$	$P_c ban$	<b>52.1.406</b>	<b>Pnna</b>	
50.9.385	$P_{2c} b'an$	$P_b nna$	52.2.407	$Pnna1'$	
50.10.386	$P_{2c} b'a'n$	$P_a nnn$	52.3.408	$Pn'na$	
<b>51.1.387</b>	<b>Pmma</b>		52.4.409	$Pnn'a$	
51.2.388	$Pmma1'$		52.5.410	$Pnna'$	
51.3.389	$Pm'ma$		52.6.411	$Pn'n'a$	
51.4.390	$Pmm'a$		52.7.412	$Pnn'a'$	
51.5.391	$Pmma'$		52.8.413	$Pn'na'$	
51.6.392	$Pm'm'a$		52.9.414	$Pn'n'a'$	
51.7.393	$Pmm'a'$		<b>53.1.415</b>	<b>Pmna</b>	

53.2.416	Pmna1'		54.11.438	P <sub>2b</sub> c'ca	P <sub>a</sub> bcn
53.3.417	Pm'n'a		54.12.439	P <sub>2b</sub> cca'	P <sub>a</sub> ccn
53.4.418	Pmn'a		54.13.440	P <sub>2b</sub> c'ca'	P <sub>c</sub> nna
53.5.419	Pmna'		<b>55.1.441</b>	<b>Pbam</b>	
53.6.420	Pm'n'a		55.2.442	Pbam1'	
53.7.421	Pmn'a'		55.3.443	Pb'am	
53.8.422	Pm'n'a'		55.4.444	Pbam'	
53.9.423	Pm'n'a'		55.5.445	Pb'a'm	
53.10.424	P <sub>2b</sub> mna	P <sub>b</sub> mna	55.6.446	Pb'am'	
53.11.425	P <sub>2b</sub> m'n'a	P <sub>c</sub> bcn	55.7.447	Pb'a'm'	
53.12.426	P <sub>2b</sub> mna'	P <sub>a</sub> nnm	55.8.448	P <sub>2c</sub> bam	P <sub>c</sub> bam
53.13.427	P <sub>2b</sub> m'n'a'	P <sub>a</sub> nna	55.9.449	P <sub>2c</sub> b'am	P <sub>b</sub> nma
<b>54.1.428</b>	<b>Pcca</b>		55.10.450	P <sub>2c</sub> b'a'm	P <sub>c</sub> nnm
54.2.429	Pcca1'		<b>56.1.451</b>	<b>Pccn</b>	
54.3.430	Pc'ca		56.2.452	Pccn1'	
54.4.431	Pcc'a		56.3.453	Pc'cn	
54.5.432	Pcca'		56.4.454	Pccn'	
54.6.433	Pc'c'a		56.5.455	Pc'c'n	
54.7.434	Pcc'a'		56.6.456	Pc'cn'	
54.8.435	Pc'ca'		56.7.457	Pc'c'n'	
54.9.436	Pc'c'a'		<b>57.1.458</b>	<b>Pbcm</b>	
54.10.437	P <sub>2b</sub> cca	P <sub>b</sub> cca			

TABLE 1.4 - 3D - 11

57.2.459	Pbcm1'			59.4.481	Pmmn'	
57.3.460	Pb'cm			59.5.482	Pm'm'n	
57.4.461	Pbc'm			59.6.483	Pmm'n'	
57.5.462	Pbcm'			59.7.484	Pm'm'n'	
57.6.463	Pb'c'm			59.8.485	P <sub>2c</sub> mmn	P <sub>c</sub> mmn
57.7.464	Pbc'm'			59.9.486	P <sub>2c</sub> m'mn	P <sub>a</sub> nma
57.8.465	Pb'cm'			59.10.487	P <sub>2c</sub> m'm'n	P <sub>c</sub> ccn
57.9.466	Pb'c'm'					
57.10.467	P <sub>2a</sub> bcm	P <sub>a</sub> bcm	<b>60.1.488</b>	<b>Pbcn</b>		
57.11.468	P <sub>2a</sub> bc'm	P <sub>c</sub> nma	60.2.489	Pbcn1'		
57.12.469	P <sub>2a</sub> bcm'	P <sub>a</sub> bca	60.3.490	Pb'cn		
57.13.470	P <sub>2a</sub> bc'm'	P <sub>b</sub> bcn	60.4.491	Pbc'n		
			60.5.492	Pbcn'		
<b>58.1.471</b>	<b>Pnnm</b>		60.6.493	Pb'c'n		
58.2.472	Pnnm1'		60.7.494	Pbc'n'		
58.3.473	Pn'nm		60.8.495	Pb'cn'		
58.4.474	Pnnm'		60.9.496	Pb'c'n'		
58.5.475	Pn'n'm					
58.6.476	Pnn'm'		<b>61.1.497</b>	<b>Pbca</b>		
58.7.477	Pn'n'm'		61.2.498	Pbca1'		
			61.3.499	Pb'ca		
<b>59.1.478</b>	<b>Pmmn</b>		61.4.500	Pb'c'a		
59.2.479	Pmmn1'		61.5.501	Pb'c'a'		
59.3.480	Pm'mn					

TABLE 1.4 - 3D - 12

<b>62.1.502</b>	<b>Pnma</b>		63.14.524	$C_P m'c'm$	$P_B nma$
62.2.503	$Pnma1'$		63.15.525	$C_P mc'm'$	$P_A nnm$
62.3.504	$Pn'ma$		63.16.526	$C_P m'cm'$	$P_C bcn$
62.4.505	$Pnm'a$		63.17.527	$C_P m'c'm'$	$P_C nna$
62.5.506	$Pnma'$				
62.6.507	$Pn'm'a$		<b>64.1.528</b>	<b>Cmca</b>	
62.7.508	$Pnm'a'$		64.2.529	$Cmca1'$	
62.8.509	$Pn'ma'$		64.3.530	$Cm'ca$	
62.9.510	$Pn'm'a'$		64.4.531	$Cmc'a$	
			64.5.532	$Cmca'$	
<b>63.1.511</b>	<b>Cmcm</b>		64.6.533	$Cm'c'a$	
63.2.512	$Cmcm1'$		64.7.534	$Cmc'a'$	
63.3.513	$Cm'cm$		64.8.535	$Cm'ca'$	
63.4.514	$Cmc'm$		64.9.536	$Cm'c'a'$	
63.5.515	$Cmcm'$				
63.6.516	$Cm'c'm$		64.10.537	$C_P mca$	$P_A bam$
63.7.517	$Cmc'm'$		64.11.538	$C_P m'ca$	$P_A cca$
63.8.518	$Cm'cm'$		64.12.539	$C_P mc'a$	$P_C nma$
63.9.519	$Cm'c'm'$		64.13.540	$C_P mca'$	$P_B bcm$
63.10.520	$C_P mcm$	$P_A mma$	64.14.541	$C_P m'c'a$	$P_A ccn$
63.11.521	$C_P m'cm$	$P_C bcm$	64.15.542	$C_P mc'a'$	$P_C mna$
63.12.522	$C_P mc'm$	$P_A mmn$	64.16.543	$C_P m'ca'$	$P_C bca$
63.13.523	$C_P mcm'$	$P_A nma$	64.17.544	$C_P m'c'a'$	$P_A bcn$

TABLE 1.4 - 3D - 13

<b>65.1.545</b>	<b>Cmmm</b>		66.4.567	Cccm'	
65.2.546	Cmmm1'		66.5.568	Cc'c'm	
65.3.547	Cm'mm		66.6.569	Ccc'm'	
65.4.548	Cmmm'		66.7.570	Cc'c'm'	
65.5.549	Cm'm'm		66.8.571	C <sub>P</sub> ccm	P <sub>C</sub> ccm
65.6.550	Cmm'm'		66.9.572	C <sub>P</sub> c'cm	P <sub>A</sub> mna
65.7.551	Cm'm'm'		66.10.573	C <sub>P</sub> ccm'	P <sub>C</sub> ccn
65.8.552	C <sub>2c</sub> mmm	C <sub>c</sub> mmm	66.11.574	C <sub>P</sub> c'c'm	P <sub>C</sub> nnm
65.9.553	C <sub>P</sub> mmm	P <sub>C</sub> mmm	66.12.575	C <sub>P</sub> cc'm'	P <sub>A</sub> nna
65.10.554	C <sub>1</sub> mmm	I <sub>c</sub> mmm	66.13.576	C <sub>P</sub> c'c'm'	P <sub>C</sub> nnn
65.11.555	C <sub>2c</sub> m'm'm	C <sub>c</sub> ccm	<b>67.1.577</b>	<b>Cmma</b>	
65.12.556	C <sub>2c</sub> mm'm'	C <sub>c</sub> mcm	67.2.578	Cmma1'	
65.13.557	C <sub>P</sub> m'mm	P <sub>B</sub> mma	67.3.579	Cm'ma	
65.14.558	C <sub>P</sub> mmm'	P <sub>C</sub> mmn	67.4.580	Cmma'	
65.15.559	C <sub>P</sub> m'm'm	P <sub>C</sub> bam	67.5.581	Cm'm'a	
65.16.560	C <sub>P</sub> mm'm'	P <sub>B</sub> mna	67.6.582	Cmm'a'	
65.17.561	C <sub>P</sub> m'm'm'	P <sub>C</sub> ban	67.7.583	Cm'm'a'	
65.18.562	C <sub>1</sub> m'mm	I <sub>a</sub> mma	67.8.584	C <sub>2c</sub> mma	C <sub>c</sub> mma
65.19.563	C <sub>1</sub> m'm'm	I <sub>c</sub> bam	67.9.585	C <sub>P</sub> mma	P <sub>A</sub> ccm
<b>66.1.564</b>	<b>Cccm</b>		67.10.586	C <sub>1</sub> mma	I <sub>a</sub> bam
66.2.565	Cccm1'		67.11.587	C <sub>2c</sub> m'ma	C <sub>c</sub> mca
66.3.566	Cc'cm		67.12.588	C <sub>2c</sub> m'm'a	C <sub>c</sub> cca

67.13.589	$C_P m'ma$	$P_B cca$	69.7.611	$F_C m'mm$	$C_A mcm$
67.14.590	$C_P mm'a$	$P_C mma$	69.8.612	$F_C mmm'$	$C_A mma$
67.15.591	$C_P mma'$	$P_A bcm$	69.9.613	$F_C m'm'm$	$C_A ccm$
67.16.592	$C_I mm'a$	$I_C mma$	69.10.614	$F_C mm'm'$	$C_A mca$
67.17.593	$C_I m'ma'$	$I_C bca$	69.11.615	$F_C m'm'm'$	$C_A cca$
<b>68.1.594</b>	<b>Ccca</b>		<b>70.1.616</b>	<b>Fddd</b>	
68.2.595	$Ccca1'$		70.2.617	$Fddd1'$	
68.3.596	$Cc'ca$		70.3.618	$Fd'dd$	
68.4.597	$Ccca'$		70.4.619	$Fd'd'd$	
68.5.598	$Cc'c'a$		70.5.620	$Fd'd'd'$	
68.6.599	$Ccc'a'$		<b>71.1.621</b>	<b>Immm</b>	
68.7.600	$Cc'c'a'$		71.2.622	$Immm1'$	
68.8.601	$C_P cca$	$P_A ban$	71.3.623	$Im'mm$	
68.9.602	$C_P c'ca$	$P_C cca$	71.4.624	$Im'm'm$	
68.10.603	$C_P cca'$	$P_B bcn$	71.5.625	$Im'm'm'$	
68.11.604	$C_P cc'a'$	$P_C nna$	71.6.626	$I_P mmm$	$P_I mmm$
<b>69.1.605</b>	<b>Fmmm</b>		71.7.627	$I_P m'mm$	$P_I mmn$
69.2.606	$Fmmm1'$		71.8.628	$I_P m'm'm$	$P_I nnm$
69.3.607	$Fm'mm$		71.9.629	$I_P m'm'm'$	$P_I nnn$
69.4.608	$Fm'm'm$		<b>72.1.630</b>	<b>Ibam</b>	
69.5.609	$Fm'm'm'$		72.2.631	$Ibam1'$	
69.6.610	$F_C mmm$	$C_A mmm$			

TABLE 1.4 - 3D - 15

72.3.632	lb'am		74.5.654	Im'm'a	
72.4.633	lbam'		74.6.655	Imm'a'	
72.5.634	lb'a'm		74.7.656	Im'm'a'	
72.6.635	lba'm'		74.8.657	I <sub>p</sub> mma	P <sub>1</sub> mma
72.7.636	lb'a'm'		74.9.658	I <sub>p</sub> m'm'a	P <sub>1</sub> nna
72.8.637	I <sub>p</sub> bam	P <sub>1</sub> ccm	74.10.659	I <sub>p</sub> mm'a'	P <sub>1</sub> mna
72.9.638	I <sub>p</sub> b'am	P <sub>1</sub> bcm	74.11.660	I <sub>p</sub> m'ma'	P <sub>1</sub> nma
72.10.639	I <sub>p</sub> bam'	P <sub>1</sub> ccn			
72.11.640	I <sub>p</sub> b'a'm	P <sub>1</sub> bam			
72.12.641	I <sub>p</sub> b'am'	P <sub>1</sub> bcn	<b>75.1.661</b>	<b>P4</b>	
72.13.642	I <sub>p</sub> b'a'm'	P <sub>1</sub> ban	75.2.662	P4 <sub>1</sub> '	
			75.3.663	P4'	
<b>73.1.643</b>	<b>lbca</b>		75.4.664	P <sub>2c</sub> 4	P <sub>c</sub> 4
73.2.644	lbca1'		75.5.665	P <sub>p</sub> 4	P <sub>c</sub> 4
73.3.645	lb'ca		75.6.666	P <sub>1</sub> 4	I <sub>c</sub> 4
73.4.646	lb'c'a		75.7.667	P <sub>2c</sub> 4'	P <sub>c</sub> 4 <sub>2</sub>
73.5.647	lb'c'a'				
73.6.648	I <sub>p</sub> bca	P <sub>1</sub> bca	<b>76.1.668</b>	<b>P4<sub>1</sub></b>	
73.7.649	I <sub>p</sub> b'ca	P <sub>1</sub> cca	76.2.669	P4 <sub>1</sub> 1'	
			76.3.670	P4 <sub>1</sub> '	
<b>74.1.650</b>	<b>Imma</b>		76.4.671	P <sub>p</sub> 4 <sub>1</sub>	P <sub>c</sub> 4 <sub>1</sub>
74.2.651	Imma1'				
74.3.652	Im'ma		<b>77.1.672</b>	<b>P4<sub>2</sub></b>	
74.4.653	Imma'		77.2.673	P4 <sub>2</sub> 1'	

**TETRAGONAL SYSTEM**



77.3.674	$P4_2'$		81.3.695	$P\bar{4}'$	
77.4.675	$P_{2c}4_2$	$P_c4_1$	81.4.696	$P_{2c}\bar{4}$	$P_c\bar{4}$
77.5.676	$P_p4_2$	$P_c4_2$	81.5.697	$P_p\bar{4}$	$P_c\bar{4}$
77.6.677	$P_l4_2$	$I_c4_1$	81.6.698	$P_l\bar{4}$	$I_c\bar{4}$
77.7.678	$P_{2c}4_2'$	$P_c4_3$	<b>82.1.699</b>	<b><math>I\bar{4}</math></b>	
<b>78.1.679</b>	<b><math>P4_3</math></b>		82.2.700	$I\bar{4}1'$	
78.2.680	$P4_31'$		82.3.701	$I\bar{4}'$	
78.3.681	$P4_3'$		82.4.702	$I_p\bar{4}$	$P_l\bar{4}$
78.4.682	$P_p4_3$	$P_c4_3$	<b>83.1.703</b>	<b><math>P4/m</math></b>	
<b>79.1.683</b>	<b><math>I4</math></b>		83.2.704	$P4/m1'$	
79.2.684	$I41'$		$\bar{4}$		
79.3.685	$I4'$		83.3.705	$P4'/m$	
79.4.686	$I_p4$	$P_l4$	83.4.706	$P4'/m'$	
79.5.687	$I_p4'$	$P_l4_2$	83.5.707	$P4'/m'$	
<b>80.1.688</b>	<b><math>I4_1</math></b>		83.6.708	$P_{2c}4/m$	$P_c4/m$
80.2.689	$I4_11'$		83.7.709	$P_p4/m$	$P_c4/m$
80.3.690	$I4_1'$		83.8.710	$P_l4/m$	$I_c4/m$
80.4.691	$I_p4_1$	$P_l4_1$	83.9.711	$P_{2c}4'/m$	$P_c4_2/m$
80.5.692	$I_p4_1'$	$P_l4_3$	83.10.712	$P_p4'/m'$	$P_c4/n$
<b>81.1.693</b>	<b><math>P\bar{4}</math></b>		<b>84.1.713</b>	<b><math>P4_2/m</math></b>	
81.2.694	$P\bar{4}1'$		84.2.714	$P4_2'/m1'$	
			84.3.715	$P4_2'/m$	
			84.4.716	$P4_2'/m'$	

TABLE 1.4 - 3D - 17

84.5.717	$P_{4_2}/m'$		87.6.738	$I_p 4/m$	$P_1 4/m$
84.6.718	$P_p 4_2/m$	$P_c 4_2/m$	87.7.739	$I_p 4'/m$	$P_1 4_2/m$
84.7.719	$P_p 4_2/m'$	$P_c 4_2/n$	87.8.740	$I_p 4/m'$	$P_1 4/n$
<b>85.1.720</b>	<b><math>P4/n</math></b>		87.9.741	$I_p 4'/m'$	$P_1 4_2/n$
85.2.721	$P4/n1'$		<b>88.1.742</b>	<b><math>I4_1/a</math></b>	
85.3.722	$P4'/n$		88.2.743	$I4_1/a1'$	
85.4.723	$P4/n'$		88.3.744	$I4_1/a$	
85.5.724	$P4'/n'$		88.4.745	$I4_1/a'$	
85.6.725	$P_{2c} 4/n$	$P_c 4/n$	88.5.746	$I4_1/a'$	
85.7.726	$P_{2c} 4'/n$	$P_c 4_2/n$	<b>89.1.747</b>	<b><math>P422</math></b>	
<b>86.1.727</b>	<b><math>P4_2/n</math></b>		89.2.748	$P4221'$	
86.2.728	$P4_2/n1'$		89.3.749	$P4'22'$	
86.3.729	$P4_2'/n$		89.4.750	$P42'2'$	
86.4.730	$P4_2/n'$		89.5.751	$P4'2'2$	
86.5.731	$P4_2'/n'$		89.6.752	$P_{2c} 422$	$P_c 422$
86.6.732	$P_1 4_2/n$	$I_c 4_1/a$	89.7.753	$P_p 422$	$P_c 422$
<b>87.1.733</b>	<b><math>I4/m</math></b>		89.8.754	$P_1 422$	$I_c 422$
87.2.734	$I4/m1'$		89.9.755	$P_{2c} 4'22'$	$P_c 4_2 22$
87.3.735	$I4'/m$		89.10.756	$P_p 4'22'$	$P_c 42_1 2$
87.4.736	$I4/m'$		<b>90.1.757</b>	<b><math>P42_1 2</math></b>	
87.5.737	$I4'/m'$		90.2.758	$P42_1 21'$	

TABLE 1.4 - 3D - 18

90.3.759	P4'2 <sub>1</sub> '2'		93.5.780	P4 <sub>2</sub> '2'2	
90.4.760	P4 <sub>2</sub> '1'2'		93.6.781	P <sub>2c</sub> 4 <sub>2</sub> '22	P <sub>c</sub> 4 <sub>1</sub> '22
90.5.761	P4'2 <sub>1</sub> '2		93.7.782	P <sub>p</sub> 4 <sub>2</sub> '22	P <sub>c</sub> 4 <sub>2</sub> '22
90.6.762	P <sub>2c</sub> 4 <sub>2</sub> '2	P <sub>c</sub> 4 <sub>2</sub> '2	93.8.783	P <sub>1</sub> 4 <sub>2</sub> '22	I <sub>c</sub> 4 <sub>1</sub> '22
90.7.763	P <sub>2c</sub> 4'2 <sub>1</sub> '2	P <sub>c</sub> 4 <sub>2</sub> '2 <sub>1</sub> '2	93.9.784	P <sub>2c</sub> 4 <sub>2</sub> '22'	P <sub>c</sub> 4 <sub>3</sub> '22
<b>91.1.764</b>	<b>P4<sub>1</sub>'22</b>		93.10.785	P <sub>p</sub> 4 <sub>2</sub> '22'	P <sub>c</sub> 4 <sub>2</sub> '2 <sub>1</sub> '2
91.2.765	P4 <sub>1</sub> '221'		<b>94.1.786</b>	<b>P4<sub>2</sub>'2<sub>1</sub>'2</b>	
91.3.766	P4 <sub>1</sub> '22'		94.2.787	P4 <sub>2</sub> '2 <sub>1</sub> '21'	
91.4.767	P4 <sub>1</sub> '2'2'		94.3.788	P4 <sub>2</sub> '2 <sub>1</sub> '2'	
91.5.768	P4 <sub>1</sub> '2'2		94.4.789	P4 <sub>2</sub> '2 <sub>1</sub> '2'	
91.6.769	P <sub>p</sub> 4 <sub>1</sub> '22	P <sub>c</sub> 4 <sub>1</sub> '22	94.5.790	P4 <sub>2</sub> '2 <sub>1</sub> '2	
91.7.770	P <sub>p</sub> 4 <sub>1</sub> '22'	P <sub>c</sub> 4 <sub>1</sub> '2 <sub>1</sub> '2	94.6.791	P <sub>2c</sub> 4 <sub>2</sub> '2 <sub>1</sub> '2	P <sub>c</sub> 4 <sub>1</sub> '2 <sub>1</sub> '2
<b>92.1.771</b>	<b>P4<sub>1</sub>'2<sub>1</sub>'2</b>		94.7.792	P <sub>2c</sub> 4 <sub>2</sub> '2 <sub>1</sub> '2	P <sub>c</sub> 4 <sub>3</sub> '2 <sub>1</sub> '2
92.2.772	P4 <sub>1</sub> '2 <sub>1</sub> '21'		<b>95.1.793</b>	<b>P4<sub>3</sub>'22</b>	
92.3.773	P4 <sub>1</sub> '2 <sub>1</sub> '2'		95.2.794	P4 <sub>3</sub> '221'	
92.4.774	P4 <sub>1</sub> '2 <sub>1</sub> '2'		95.3.795	P4 <sub>3</sub> '22'	
92.5.775	P4 <sub>1</sub> '2 <sub>1</sub> '2		95.4.796	P4 <sub>3</sub> '2'2'	
<b>93.1.776</b>	<b>P4<sub>2</sub>'22</b>		95.5.797	P4 <sub>3</sub> '2'2	
93.2.777	P4 <sub>2</sub> '221'		95.6.798	P <sub>p</sub> 4 <sub>3</sub> '22	P <sub>c</sub> 4 <sub>3</sub> '22
93.3.778	P4 <sub>2</sub> '22'		95.7.799	P <sub>p</sub> 4 <sub>3</sub> '22'	P <sub>c</sub> 4 <sub>3</sub> '2 <sub>1</sub> '2
93.4.779	P4 <sub>2</sub> '2'2'		<b>96.1.800</b>	<b>P4<sub>3</sub>'2<sub>1</sub>'2</b>	

96.2.801	$P4_3 2_1 21'$		<b>99.1.823</b>	<b>P4mm</b>	
96.3.802	$P4_3' 2_1 2'$		99.2.824	P4mm1'	
96.4.803	$P4_3 2_1' 2'$		99.3.825	P4'm'm	
96.5.804	$P4_3' 2_1' 2'$		99.4.826	P4'mm'	
<b>97.1.805</b>	<b>I422</b>		99.5.827	P4m'm'	
97.2.806	I422		99.6.828	$P_{2c} 4mm$	$P_c 4mm$
97.3.807	I4'22'		99.7.829	$P_p 4mm$	$P_c 4mm$
97.4.808	I42'2'		99.8.830	$P_1 4mm$	$I_c 4mm$
97.5.809	I4'2'2		99.9.831	$P_{2c} 4'm'm$	$P_c 4_2 cm$
97.6.810	$I_p 422$	$P_1 422$	99.10.832	$P_{2c} 4'mm'$	$P_c 4_2 mc$
97.7.811	$I_p 4'22'$	$P_1 4_2 22$	99.11.833	$P_{2c} 4m'm'$	$P_c 4cc$
97.8.812	$I_p 42'2'$	$P_1 42_1 2$	99.12.834	$P_p 4'mm'$	$P_c 4bm$
97.9.813	$I_p 4'2'2$	$P_1 4_2 2_1 2$	99.13.835	$P_1 4m'm'$	$I_c 4cm$
<b>98.1.814</b>	<b>I4<sub>1</sub>22</b>		<b>100.1.836</b>	<b>P4bm</b>	
98.2.815	I4 <sub>1</sub> 221'		100.2.837	P4bm1'	
98.3.816	I4 <sub>1</sub> '22'		100.3.838	P4'b'm	
98.4.817	I4 <sub>1</sub> 2'2'		100.4.839	P4'bm'	
98.5.818	I4 <sub>1</sub> '2'2		100.5.840	P4b'm'	
98.6.819	$I_p 4_1 22$	$P_1 4_1 22$	100.6.841	$P_{2c} 4bm$	$P_c 4bm$
98.7.820	$I_p 4_1' 22'$	$P_1 4_3 22$	100.7.842	$P_{2c} 4'b'm$	$P_c 4_2 nm$
98.8.821	$I_p 4_1 2' 2'$	$P_1 4_1 2_1 2$	100.8.843	$P_{2c} 4'bm'$	$P_c 4_2 bc$
98.9.822	$I_p 4_1' 2' 2'$	$P_1 4_3 2_1 2$	100.9.844	$P_{2c} 4b'm'$	$P_c 4nc$

TABLE 1.4 - 3D - 20

<b>101.1.845</b>	<b>P<sub>4</sub><sub>2</sub> cm</b>		<b>104.1.866</b>	<b>P4nc</b>	
101.2.846	P <sub>4</sub> <sub>2</sub> cm1'		104.2.867	P4nc1'	
101.3.847	P <sub>4</sub> <sub>2</sub> 'c'm		104.3.868	P4'n'c	
101.4.848	P <sub>4</sub> <sub>2</sub> 'cm'		104.4.869	P4'nc'	
101.5.849	P <sub>4</sub> <sub>2</sub> c'm'		104.5.870	P4n'c'	
101.6.850	P <sub>p</sub> 4 <sub>2</sub> cm	P <sub>c</sub> 4 <sub>2</sub> mc	<b>105.1.871</b>	<b>P<sub>4</sub><sub>2</sub> mc</b>	
101.7.851	P <sub>p</sub> 4 <sub>2</sub> 'cm'	P <sub>c</sub> 4 <sub>2</sub> bc	105.2.872	P <sub>4</sub> <sub>2</sub> mc1'	
<b>102.1.852</b>	<b>P<sub>4</sub><sub>2</sub> nm</b>		105.3.873	P <sub>4</sub> <sub>2</sub> 'm'c	
102.2.853	P <sub>4</sub> <sub>2</sub> nm1'		105.4.874	P <sub>4</sub> <sub>2</sub> 'mc'	
102.3.854	P <sub>4</sub> <sub>2</sub> 'n'm		105.5.875	P <sub>4</sub> <sub>2</sub> m'c'	
102.4.855	P <sub>4</sub> <sub>2</sub> 'nm'		105.6.876	P <sub>p</sub> 4 <sub>2</sub> mc	P <sub>c</sub> 4 <sub>2</sub> cm
102.5.856	P <sub>4</sub> <sub>2</sub> n'm'		105.7.877	P <sub>p</sub> 4 <sub>2</sub> 'mc'	P <sub>c</sub> 4 <sub>2</sub> nm
102.6.857	P <sub>1</sub> 4 <sub>2</sub> nm	I <sub>c</sub> 4 <sub>1</sub> md	<b>106.1.878</b>	<b>P<sub>4</sub><sub>2</sub> bc</b>	
102.7.858	P <sub>1</sub> 4 <sub>2</sub> n'm'	I <sub>c</sub> 4 <sub>1</sub> cd	106.2.879	P <sub>4</sub> <sub>2</sub> bc1'	
<b>103.1.859</b>	<b>P4cc</b>		106.3.880	P <sub>4</sub> <sub>2</sub> 'b'c	
103.2.860	P4cc1'		106.4.881	P <sub>4</sub> <sub>2</sub> 'bc'	
103.3.861	P4'c'c		106.5.882	P <sub>4</sub> <sub>2</sub> b'c'	
103.4.862	P4'cc'		<b>107.1.883</b>	<b>I4mm</b>	
103.5.863	P4c'c'		107.2.884	I4mm1'	
103.6.864	P <sub>p</sub> 4cc	P <sub>c</sub> 4cc	107.3.885	I4'm'm	
103.7.865	P <sub>p</sub> 4'cc'	P <sub>c</sub> 4nc	107.4.886	I4'mm'	

TABLE 1.4 - 3D - 21

107.5.887	$I_4m'm'$		110.3.908	$I_4_1'c'd$	
107.6.888	$I_p 4mm$	$P_1 4mm$	110.4.909	$I_4_1'cd'$	
107.7.889	$I_p 4'm'm'$	$P_1 4_2 nm$	110.5.910	$I_4_1c'd'$	
107.8.890	$I_p 4'mm'$	$P_1 4_2 mc$	<b>111.1.911</b>	<b><math>P\bar{4}2m</math></b>	
107.9.891	$I_p 4m'm'$	$P_1 4nc$	111.2.912	$P\bar{4}2m1'$	
<b>108.1.892</b>	<b><math>I_4cm</math></b>		111.3.913	$P\bar{4}'2'm$	
108.2.893	$I_4cm1'$		111.4.914	$P\bar{4}'2m'$	
108.3.894	$I_4'c'm$		111.5.915	$P\bar{4}2'm'$	
108.4.895	$I_4'cm'$		111.6.916	$P_{2c}\bar{4}2m$	$P_c\bar{4}2m$
108.5.896	$I_4c'm'$		111.7.917	$P_p\bar{4}2m$	$P_c\bar{4}m2$
108.6.897	$I_p 4cm$	$P_1 4bm$	111.8.918	$P_1\bar{4}2m$	$I_c\bar{4}m2$
108.7.898	$I_p 4'c'm$	$P_1 4_2 cm$	111.9.919	$P_{2c}\bar{4}2'm'$	$P_c\bar{4}2c$
108.8.899	$I_p 4'cm'$	$P_1 4_2 bc$	111.10.920	$P_p\bar{4}'2m'$	$P_c\bar{4}b2$
108.9.900	$I_p 4c'm'$	$P_1 4cc$	111.11.921	$P_1\bar{4}'2m'$	$I_c\bar{4}c2$
<b>109.1.901</b>	<b><math>I_4_1md</math></b>		<b>112.1.922</b>	<b><math>P\bar{4}2c</math></b>	
109.2.902	$I_4_1md1'$		112.2.923	$P\bar{4}2c1'$	
109.3.903	$I_4_1'm'd$		112.3.924	$P\bar{4}'2'c$	
109.4.904	$I_4_1'md'$		112.4.925	$P\bar{4}'2c'$	
109.5.905	$I_4_1m'd'$		112.5.926	$P\bar{4}2'c'$	
			112.6.927	$P_p\bar{4}2c$	$P_c\bar{4}c2$
<b>110.1.906</b>	<b><math>I_4_1cd</math></b>		112.7.928	$P_p\bar{4}'2c'$	$P_c\bar{4}n2$
110.2.907	$I_4_1cd1'$				

TABLE 1.4 - 3D - 22

<b>113.1.929</b>	<b><math>P\bar{4}2_1m</math></b>			<b>116.1.951</b>	<b><math>P\bar{4}c2</math></b>		
113.2.930	$P\bar{4}2_1m1'$			116.2.952	$P\bar{4}c21'$		
113.3.931	$P\bar{4}'2_1'm$			116.3.953	$P\bar{4}'c'2$		
113.4.932	$P\bar{4}'2_1'm'$			116.4.954	$P\bar{4}'c'2'$		
113.5.933	$P\bar{4}2_1'm'$			116.5.955	$P\bar{4}c'2'$		
113.6.934	$P_{2c}\bar{4}2_1m$	$P_c\bar{4}2_1m$		116.6.956	$P_p\bar{4}c2$	$P_c\bar{4}2c$	
113.7.935	$P_{2c}\bar{4}'2_1'm'$	$P_c\bar{4}2_1c$		116.7.957	$P_p\bar{4}'c'2'$	$P_c\bar{4}2_1c$	
<b>114.1.936</b>	<b><math>P\bar{4}2_1c</math></b>			<b>117.1.958</b>	<b><math>P\bar{4}b2</math></b>		
114.2.937	$P\bar{4}2_1c1'$			117.2.959	$P\bar{4}b21'$		
114.3.938	$P\bar{4}'2_1'c$			117.3.960	$P\bar{4}'b'2$		
114.4.939	$P\bar{4}'2_1'c'$			117.4.961	$P\bar{4}'b'2'$		
114.5.940	$P\bar{4}2_1'c'$			117.5.962	$P\bar{4}b'2'$		
<b>115.1.941</b>	<b><math>P\bar{4}m2</math></b>			117.6.963	$P_{2c}\bar{4}b2$	$P_c\bar{4}b2$	
115.2.942	$P\bar{4}m21'$			117.7.964	$P_{2c}\bar{4}'b'2$	$P_c\bar{4}n2$	
115.3.943	$P\bar{4}'m'2$			<b>118.1.965</b>	<b><math>P\bar{4}n2</math></b>		
115.4.944	$P\bar{4}'m'2'$			118.2.966	$P\bar{4}n21'$		
115.5.945	$P\bar{4}m'2'$			118.3.967	$P\bar{4}'n'2$		
115.6.946	$P_{2c}\bar{4}m2$	$P_c\bar{4}m2$		118.4.968	$P\bar{4}'n'2'$		
115.7.947	$P_p\bar{4}m2$	$P_c\bar{4}2m$		118.5.969	$P\bar{4}n'2'$		
115.8.948	$P_1\bar{4}m2$	$I_c\bar{4}2m$		118.6.970	$P_1\bar{4}n2$	$I_c\bar{4}2d$	
115.9.949	$P_{2c}\bar{4}'m'2$	$P_c\bar{4}c2$		<b>119.1.971</b>	<b><math>I\bar{4}m2</math></b>		
115.10.950	$P_p\bar{4}'m'2'$	$P_c\bar{4}2_1m$					

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119.2.972	$\bar{I}4m21'$		121.9.993	$I_p \bar{4}2'm'$	$P_1 \bar{4}2_1c$
119.3.973	$\bar{I}4'm'2$		<b>122.1.994</b>	<b><math>\bar{I}42d</math></b>	
119.4.974	$\bar{I}4'm'2'$		122.2.995	$\bar{I}42d1'$	
119.5.975	$\bar{I}4m'2'$		122.3.996	$\bar{I}4'2'd$	
119.6.976	$I_p \bar{4}m2$	$P_1 \bar{4}m2$	122.4.997	$\bar{I}4'2d'$	
119.7.977	$I_p \bar{4}'m'2$	$P_1 \bar{4}n2$	122.5.998	$\bar{I}42'd'$	
<b>120.1.978</b>	<b><math>\bar{I}4c2</math></b>		<b>123.1.999</b>	<b><math>P4/mmm</math></b>	
120.2.979	$\bar{I}4c21'$		123.2.1000	$P4/mmm1'$	
120.3.980	$\bar{I}4'c'2$		123.3.1001	$P4/m'mm$	
120.4.981	$\bar{I}4'c'2'$		123.4.1002	$P4'/mm'm$	
120.5.982	$\bar{I}4c'2'$		123.5.1003	$P4'/mmm'$	
120.6.983	$I_p \bar{4}c2$	$P_1 \bar{4}c2$	123.6.1004	$P4'/m'm'm$	
120.7.984	$I_p \bar{4}c'2'$	$P_1 \bar{4}b2$	123.7.1005	$P4/mm'm'$	
<b>121.1.985</b>	<b><math>\bar{I}42m</math></b>		123.8.1006	$P4'/m'mm'$	
121.2.986	$\bar{I}42m1'$		123.9.1007	$P4/m'm'm'$	
121.3.987	$\bar{I}4'2'm$		123.10.1008	$P_{2c} 4/mmm$	$P_c 4/mmm$
121.4.988	$\bar{I}4'2m'$		123.11.1009	$P_p 4/mmm$	$P_c 4/mmm$
121.5.989	$\bar{I}42'm'$		123.12.1010	$P_1 4/mmm$	$I_c 4/mmm$
121.6.990	$I_p \bar{4}2m$	$P_1 \bar{4}2m$	123.13.1011	$P_{2c} 4'/mm'm'$	$P_c 4_2/mcm$
121.7.991	$I_p \bar{4}'2'm$	$P_1 \bar{4}2_1m$	123.14.1012	$P_{2c} 4'/mmm'$	$P_c 4_2/mmc$
121.8.992	$I_p \bar{4}'2m'$	$P_1 \bar{4}2c$	123.15.1013	$P_{2c} 4/mm'm'$	$P_c 4/mcc$
			123.16.1014	$P_p 4/m'mm$	$P_c 4/nmm$

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123.17.1015	$P_4/mmm'$	$P_4/mbm$	125.7.1037	$P_4/nb'm'$	
123.18.1016	$P_4/m'mm'$	$P_4/nbm$	125.8.1038	$P_4/n'bm'$	
123.19.1017	$P_4/mm'm'$	$I_4/mcm$	125.9.1039	$P_4/n'b'm'$	
<b>124.1.1018</b>	<b><math>P_4/mcc</math></b>		125.10.1040	$P_4/nbm$	$P_4/nbm$
124.2.1019	$P_4/mcc1'$		125.11.1041	$P_4/nb'm$	$P_4/nm$
124.3.1020	$P_4/m'cc$		125.12.1042	$P_4/nbm'$	$P_4/nbc$
124.4.1021	$P_4/mc'c$		125.13.1043	$P_4/nb'm'$	$P_4/nnc$
124.5.1022	$P_4/mcc'$		<b>126.1.1044</b>	<b><math>P_4/nnc</math></b>	
124.6.1023	$P_4/m'c'c$		126.2.1045	$P_4/nnc1'$	
124.7.1024	$P_4/mc'c'$		126.3.1046	$P_4/n'nc$	
124.8.1025	$P_4/m'cc'$		126.4.1047	$P_4/nn'c$	
124.9.1026	$P_4/m'c'c'$		126.5.1048	$P_4/nnc'$	
124.10.1027	$P_4/mcc$	$P_4/mcc$	126.6.1049	$P_4/n'n'c$	
124.11.1028	$P_4/m'cc$	$P_4/ncc$	126.7.1050	$P_4/nn'c'$	
124.12.1029	$P_4/mcc'$	$P_4/mnc$	126.8.1051	$P_4/n'nc'$	
124.13.1030	$P_4/m'cc'$	$P_4/nnc$	126.9.1052	$P_4/n'n'c'$	
<b>125.1.1031</b>	<b><math>P_4/nbm</math></b>		<b>127.1.1053</b>	<b><math>P_4/mbm</math></b>	
125.2.1032	$P_4/nbm1'$		127.2.1054	$P_4/mbm1'$	
125.3.1033	$P_4/n'bm$		127.3.1055	$P_4/m'bm$	
125.4.1034	$P_4/nb'm$		127.4.1056	$P_4/mb'm$	
125.5.1035	$P_4/nbm'$		127.5.1057	$P_4/mbm'$	
125.6.1036	$P_4/n'b'm$		127.6.1058	$P_4/m'b'm$	

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127.7.1059	P4/mb'm'		129.7.1081	P4/nm'm'	
127.8.1060	P4'/m'bm'		129.8.1082	P4'/n'mm'	
127.9.1061	P4/m'b'm'		129.9.1083	P4/n'm'm'	
127.10.1062	P <sub>2c</sub> 4/mbm	P <sub>c</sub> 4/mbm	129.10.1084	P <sub>2c</sub> 4/nmm	P <sub>c</sub> 4/nmm
127.11.1063	P <sub>2c</sub> 4'/mb'm	P <sub>c</sub> 4 <sub>2</sub> /mnm	129.11.1085	P <sub>2c</sub> 4'/nm'm	P <sub>c</sub> 4 <sub>2</sub> /ncm
127.12.1064	P <sub>2c</sub> 4'/mbm'	P <sub>c</sub> 4 <sub>2</sub> /mbc	129.12.1086	P <sub>2c</sub> 4'/nmm'	P <sub>c</sub> 4 <sub>2</sub> /nmc
127.13.1065	P <sub>2c</sub> 4/mb'm'	P <sub>c</sub> 4/mnc	129.13.1087	P <sub>2c</sub> 4/nm'm'	P <sub>c</sub> 4/ncc
<b>128.1.1066</b>	<b>P4/mnc</b>		<b>130.1.1088</b>	<b>P4/ncc</b>	
128.2.1067	P4/mnc1'		130.2.1089	P4/ncc1'	
128.3.1068	P4/m'nc		130.3.1090	P4/n'cc	
128.4.1069	P4'/mn'c		130.4.1091	P4'/nc'c	
128.5.1070	P4'/mnc'		130.5.1092	P4'/ncc'	
128.6.1071	P4'/m'n'c		130.6.1093	P4'/n'c'c	
128.7.1072	P4/mn'c'		130.7.1094	P4/nc'c'	
128.8.1073	P4'/m'nc'		130.8.1095	P4'/n'cc'	
128.9.1074	P4/m'n'c'		130.9.1096	P4/n'c'c'	
<b>129.1.1075</b>	<b>P4/nmm</b>		<b>131.1.1097</b>	<b>P4<sub>2</sub>/mmc</b>	
129.2.1076	P4/nmm1'		131.2.1098	P4 <sub>2</sub> /mmc1'	
129.3.1077	P4/n'mm		131.3.1099	P4 <sub>2</sub> /m'mc	
129.4.1078	P4'/nm'm		131.4.1100	P4 <sub>2</sub> '/mm'c	
129.5.1079	P4'/nmm'		131.5.1101	P4 <sub>2</sub> '/mmc'	
129.6.1080	P4'/n'm'm		131.6.1102	P4 <sub>2</sub> '/m'm'c	

131.7.1103	$P4_2/mm'c'$		133.3.1125	$P4_2/n'bc$	
131.8.1104	$P4_2'/m'mc'$		133.4.1126	$P4_2'/nb'c$	
131.9.1105	$P4_2/m'm'c'$		133.5.1127	$P4_2'/nbc'$	
131.10.1106	$P_P4_2/mmc$	$P_C4_2/mcm$	133.6.1128	$P4_2'/n'b'c$	
131.11.1107	$P_P4_2/m'mc$	$P_C4_2/ncm$	133.7.1129	$P4_2/nb'c'$	
131.12.1108	$P_P4_2/mm'c'$	$P_C4_2/mnm$	133.8.1130	$P4_2'/n'bc'$	
131.13.1109	$P_P4_2'/m'mc'$	$P_C4_2/nnm$	133.9.1131	$P4_2'/n'b'c'$	
132.1.1110	$P4_2/mcm$		<b>134.1.1132</b>	<b><math>P4_2/nnm</math></b>	
132.2.1111	$P4_2/mcm1'$		134.2.1133	$P4_2/nnm1'$	
132.3.1112	$P4_2/m'cm$		134.3.1134	$P4_2/n'nm$	
132.4.1113	$P4_2'/mc'm$		134.4.1135	$P4_2'/nn'm$	
132.5.1114	$P4_2'/mcm'$		134.5.1136	$P4_2'/nnm'$	
132.6.1115	$P4_2'/m'c'm$		134.6.1137	$P4_2'/n'n'm$	
132.7.1116	$P4_2/mc'm'$		134.7.1138	$P4_2/nn'm'$	
132.8.1117	$P4_2'/m'cm'$		134.8.1139	$P4_2'/n'nm'$	
132.9.1118	$P4_2/m'c'm'$		134.9.1140	$P4_2'/n'n'm'$	
132.10.1119	$P_P4_2/mcm$	$P_C4_2/mmc$	134.10.1141	$P_14_2/nnm$	$I_c4_1/amd$
132.11.1120	$P_P4_2/m'cm$	$P_C4_2/nmc$	134.11.1142	$P_14_2/nn'm'$	$I_c4_1/acd$
132.12.1121	$P_P4_2'/mcm'$	$P_C4_2/mbc$	<b>135.1.1143</b>	<b><math>P4_2/mbc</math></b>	
132.13.1122	$P_P4_2'/m'cm'$	$P_C4_2/nbc$	135.2.1144	$P4_2/mbc1'$	
<b>133.1.1123</b>	<b><math>P4_2/nbc</math></b>		135.3.1145	$P4_2/m'bc$	
133.2.1124	$P4_2/nbc1'$		135.4.1146	$P4_2'/mb'c$	

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135.5.1147	$P4_2/mbc'$	137.9.1169	$P4_2/n'm'c'$	
135.6.1148	$P4_2/m'b'c$	<b>138.1.1170</b>	<b><math>P4_2/ncm</math></b>	
135.7.1149	$P4_2/mb'c'$	138.2.1171	$P4_2/ncm1'$	
135.8.1150	$P4_2/m'bc'$	138.3.1172	$P4_2/n'cm$	
135.9.1151	$P4_2/m'b'c'$	138.4.1173	$P4_2/nc'm$	
<b>136.1.1152</b>	<b><math>P4_2/mnm</math></b>	138.5.1174	$P4_2/ncm'$	
136.2.1153	$P4_2/mnm1'$	138.6.1175	$P4_2/n'c'm$	
136.3.1154	$P4_2/m'nm$	138.7.1176	$P4_2/nc'm'$	
136.4.1155	$P4_2/mn'm$	138.8.1177	$P4_2/n'cm'$	
136.5.1156	$P4_2/mnm'$	138.9.1178	$P4_2/n'c'm'$	
136.6.1157	$P4_2/m'n'm$	<b>139.1.1179</b>	<b><math>I4/mmm</math></b>	
136.7.1158	$P4_2/mn'm'$	139.2.1180	$I4/mmm1'$	
136.8.1159	$P4_2/m'nm'$	139.3.1181	$I4/m'mm$	
136.9.1160	$P4_2/m'n'm'$	139.4.1182	$I4'/mm'm$	
<b>137.1.1161</b>	<b><math>P4_2/nmc</math></b>	139.5.1183	$I4'/mmm'$	
137.2.1162	$P4_2/nmc1'$	139.6.1184	$I4'/m'm'm$	
137.3.1163	$P4_2/n'mc$	139.7.1185	$I4/mm'm'$	
137.4.1164	$P4_2/nm'c$	139.8.1186	$I4'/m'mm'$	
137.5.1165	$P4_2/nmc'$	139.9.1187	$I4/m'm'm'$	
137.6.1166	$P4_2/n'm'c$	139.10.1188	$I_p 4/mmm$	$P_1 4/mmm$
137.7.1167	$P4_2/nm'c'$	139.11.1189	$I_p 4/m'mm$	$P_1 4/nmm$
137.8.1168	$P4_2/n'mc'$	139.12.1190	$I_p 4'/mm'm$	$P_1 4_2/mnm$

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139.13.1191	$I_p 4'/mmm'$	$P_1 4_2/mmc$	<b>141.1.1213</b>	<b><math>I4_1/amd</math></b>
139.14.1192	$I_p 4'/m'm'm$	$P_1 4_2/nnc$	141.2.1214	$I4_1/amd1'$
139.15.1193	$I_p 4'/mm'm'$	$P_1 4/mnc$	141.3.1215	$I4_1/a'md$
139.16.1194	$I_p 4'/m'mm'$	$P_1 4_2/nmc$	141.4.1216	$I4_1'/am'd$
139.17.1195	$I_p 4'/m'm'm'$	$P_1 4/nnc$	141.5.1217	$I4_1'/amd'$
			141.6.1218	$I4_1'/a'm'd$
			141.7.1219	$I4_1/am'd'$
			141.8.1220	$I4_1'/a'md'$
			141.9.1221	$I4_1/a'm'd'$
<b>140.1.1196</b>	<b><math>I4/mcm</math></b>			
140.2.1197	$I4/mcm1'$			
140.3.1198	$I4/m'cm$			
140.4.1199	$I4'/mc'm$			
140.5.1200	$I4'/mcm'$		<b>142.1.1222</b>	<b><math>I4_1/acd</math></b>
140.6.1201	$I4'/m'c'm$		142.2.1223	$I4_1/acd1'$
140.7.1202	$I4/mc'm'$		142.3.1224	$I4_1/a'cd$
140.8.1203	$I4'/m'cm'$		142.4.1225	$I4_1'/ac'd$
140.9.1204	$I4/m'c'm'$		142.5.1226	$I4_1'/acd'$
140.10.1205	$I_p 4/mcm$	$P_1 4/mcc$	142.6.1227	$I4_1'/a'c'd$
140.11.1206	$I_p 4/m'cm$	$P_1 4/ncc$	142.7.1228	$I4_1'/ac'd'$
140.12.1207	$I_p 4'/mc'm$	$P_1 4_2/mbc$	142.8.1229	$I4_1'/a'cd'$
140.13.1208	$I_p 4'/mcm'$	$P_1 4_2/mcm$	142.9.1230	$I4_1/a'c'd'$
140.14.1209	$I_p 4'/m'c'm$	$P_1 4_2/nbc$		
140.15.1210	$I_p 4/mc'm'$	$P_1 4/mbm$		
140.16.1211	$I_p 4'/m'cm'$	$P_1 4_2/ncm$	<b>143.1.1231</b>	<b><math>P3</math></b>
140.17.1212	$I_p 4/m'c'm'$	$P_1 4/nbm$	143.2.1232	$P31'$

**TRIGONAL SYSTEM**

143.3.1233	$P_{2c} 3$	$P_c 3$	149.3.1253	$P312'$	
<b>144.1.1234</b>	<b><math>P3_1</math></b>		149.4.1254	$P_{2c} 312$	$P_c 312$
144.2.1235	$P3_11'$		<b>150.1.1255</b>	<b><math>P321</math></b>	
144.3.1236	$P_{2c} 3_2$	$P_c 3_2$	150.2.1256	$P3211'$	
<b>145.1.1237</b>	<b><math>P3_2</math></b>		150.3.1257	$P32'1$	
145.2.1238	$P3_21'$		150.4.1258	$P_{2c} 321$	$P_c 321$
145.3.1239	$P_{2c} 3_1$	$P_c 3_1$	<b>151.1.1259</b>	<b><math>P3_112</math></b>	
<b>146.1.1240</b>	<b><math>R3</math></b>		151.2.1260	$P3_1121'$	
146.2.1241	$R31'$		151.3.1261	$P3_112'$	
146.3.1242	$R_R 3$	$R_1 3$	151.4.1262	$P_{2c} 3_212$	$P_c 3_212$
<b>147.1.1243</b>	<b><math>P\bar{3}</math></b>		<b>152.1.1263</b>	<b><math>P3_121</math></b>	
147.2.1244	$P\bar{3}1'$		152.2.1264	$P3_1211'$	
147.3.1245	$P\bar{3}'$		152.3.1265	$P3_12'1$	
147.4.1246	$P_{2c}\bar{3}$	$P_c\bar{3}$	152.4.1266	$P_{2c} 3_221$	$P_c 3_221$
<b>148.1.1247</b>	<b><math>R\bar{3}</math></b>		<b>153.1.1267</b>	<b><math>P3_212</math></b>	
148.2.1248	$R\bar{3}1'$		153.2.1268	$P3_2121'$	
148.3.1249	$R\bar{3}'$		153.3.1269	$P3_212'$	
148.4.1250	$R_R\bar{3}$	$R_1\bar{3}$	153.4.1270	$P_{2c} 3_112$	$P_c 3_112$
<b>149.1.1251</b>	<b><math>P312</math></b>		<b>154.1.1271</b>	<b><math>P3_221</math></b>	
149.2.1252	$P3121'$		154.2.1272	$P3_2211'$	

154.3.1273	$P3_2 2'1$		159.2.1293	$P31c1'$	
154.4.1274	$P_{2c} 3_1 2'1$	$P_c 3_1 2'1$	159.3.1294	$P31c'$	
<b>155.1.1275</b>	<b>R32</b>		<b>160.1.1295</b>	<b>R3m</b>	
155.2.1276	$R321'$		160.2.1296	$R3m1'$	
155.3.1277	$R32'$		160.3.1297	$R3m'$	
155.4.1278	$R_R 32$	$R_I 32$	160.4.1298	$R_R 3m$	$R_I 3m$
<b>156.1.1279</b>	<b>P3m1</b>		160.5.1299	$R_R 3m'$	$R_I 3c$
156.2.1280	$P3m11'$		<b>161.1.1300</b>	<b>R3c</b>	
156.3.1281	$P3m'1$		161.2.1301	$R3c1'$	
156.4.1282	$P_{2c} 3m1$	$P_c 3m1$	161.3.1302	$R3c'$	
156.5.1283	$P_{2c} 3m'1$	$P_c 3c1$	<b>162.1.1303</b>	<b><math>P\bar{3}1m</math></b>	
<b>157.1.1284</b>	<b>P31m</b>		162.2.1304	$P\bar{3}1m1'$	
157.2.1285	$P31m1'$		162.3.1305	$P\bar{3}'1m$	
157.3.1286	$P31m'$		162.4.1306	$P\bar{3}'1m'$	
157.4.1287	$P_{2c} 31m$	$P_c 31m$	162.5.1307	$P\bar{3}1m'$	
157.5.1288	$P_{2c} 31m'$	$P_c 31c$	162.6.1308	$P_{2c} \bar{3}1m$	$P_c \bar{3}1m$
<b>158.1.1289</b>	<b>P3c1</b>		162.7.1309	$P_{2c} \bar{3}1m'$	$P_c \bar{3}1c$
158.2.1290	$P3c11'$		<b>163.1.1310</b>	<b><math>P\bar{3}1c</math></b>	
158.3.1291	$P3c'1$		163.2.1311	$P\bar{3}1c1'$	
<b>159.1.1292</b>	<b>P31c</b>		163.3.1312	$P\bar{3}'1c$	
			163.4.1313	$P\bar{3}'1c'$	

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163.5.1314  $P\bar{3}1c'$

**164.1.1315  $P\bar{3}m1$**

164.2.1316  $P\bar{3}m11'$

164.3.1317  $P\bar{3}'m1$

164.4.1318  $P\bar{3}'m'1$

164.5.1319  $P\bar{3}m'1$

164.6.1320  $P_{2c}\bar{3}m1$   $P_c\bar{3}m1$

164.7.1321  $P_{2c}\bar{3}m'1$   $P_c\bar{3}c1$

**165.1.1322  $P\bar{3}c1$**

165.2.1323  $P\bar{3}c11'$

165.3.1324  $P\bar{3}'c1$

165.4.1325  $P\bar{3}'c'1$

165.5.1326  $P\bar{3}c'1$

**166.1.1327  $R\bar{3}m$**

166.2.1328  $R\bar{3}m1'$

166.3.1329  $R\bar{3}'m$

166.4.1330  $R\bar{3}'m'$

166.5.1331  $R\bar{3}m'$

166.6.1332  $R_R\bar{3}m$   $R_1\bar{3}m$

166.7.1333  $R_R\bar{3}m'$   $R_1\bar{3}c$

**167.1.1334  $R\bar{3}c$**

167.2.1335  $R\bar{3}c1'$

167.3.1336  $R\bar{3}'c$

167.4.1337  $R\bar{3}'c'$

167.5.1338  $R\bar{3}c'$

**HEXAGONAL SYSTEM**

**168.1.1339  $P6$**

168.2.1340  $P61'$

168.3.1341  $P6'$

168.4.1342  $P_{2c}6$   $P_c6$

168.5.1343  $P_{2c}6'$   $P_c6_3$

**169.1.1344  $P6_1$**

169.2.1345  $P6_11'$

169.3.1346  $P6_1'$

**170.1.1347  $P6_5$**

170.2.1348  $P6_51'$

170.3.1349  $P6_5'$

**171.1.1350  $P6_2$**

171.2.1351  $P6_21'$

171.3.1352  $P6_2'$

171.4.1353  $P_{2c}6_2$   $P_c6_1$

171.5.1354  $P_{2c}6_2'$   $P_c6_4$



<b>172.1.1355</b>	<b>P6<sub>4</sub></b>		176.2.1375	P6 <sub>3</sub> /m1'	
172.2.1356	P6 <sub>4</sub> 1'		176.3.1376	P6 <sub>3</sub> '/m	
172.3.1357	P6 <sub>4</sub> '		176.4.1377	P6 <sub>3</sub> /m'	
172.4.1358	P <sub>2c</sub> 6 <sub>4</sub>	P <sub>c</sub> 6 <sub>2</sub>	176.5.1378	P6 <sub>3</sub> '/m'	
172.5.1359	P <sub>2c</sub> 6 <sub>4</sub> '	P <sub>c</sub> 6 <sub>5</sub>	<b>177.1.1379</b>	<b>P622</b>	
<b>173.1.1360</b>	<b>P6<sub>3</sub></b>		177.2.1380	P6221'	
173.2.1361	P6 <sub>3</sub> 1'		177.3.1381	P6'2'2	
173.3.1362	P6 <sub>3</sub> '		177.4.1382	P6'22'	
<b>174.1.1363</b>	<b>P6̄</b>		177.5.1383	P62'2'	
174.2.1364	P6̄1'		177.6.1384	P <sub>2c</sub> 622	P <sub>c</sub> 622
174.3.1365	P6̄'		177.7.1385	P <sub>2c</sub> 6'22'	P <sub>c</sub> 6 <sub>3</sub> 22
174.4.1366	P <sub>2c</sub> 6̄	P <sub>c</sub> 6̄	<b>178.1.1386</b>	<b>P6<sub>1</sub>22</b>	
<b>175.1.1367</b>	<b>P6/m</b>		178.2.1387	P6 <sub>1</sub> 221'	
175.2.1368	P6/m1'		178.3.1388	P6 <sub>1</sub> '2'2	
175.3.1369	P6'/m		178.4.1389	P6 <sub>1</sub> '22'	
175.4.1370	P6/m'		178.5.1390	P6 <sub>1</sub> 2'2'	
175.5.1371	P6'/m'		<b>179.1.1391</b>	<b>P6<sub>5</sub>22</b>	
175.6.1372	P <sub>2c</sub> 6/m	P <sub>c</sub> 6/m	179.2.1392	P6 <sub>5</sub> 221'	
175.7.1373	P <sub>2c</sub> 6'/m	P <sub>c</sub> 6 <sub>3</sub> /m	179.3.1393	P6 <sub>5</sub> '2'2	
<b>176.1.1374</b>	<b>P6<sub>3</sub>/m</b>		179.4.1394	P6 <sub>5</sub> '22'	
			179.5.1395	P6 <sub>5</sub> 2'2'	

<b>180.1.1396</b>	<b>P6<sub>2</sub>22</b>			183.3.1417	P6'm'm	
180.2.1397	P6 <sub>2</sub> 221'			183.4.1418	P6'mm'	
180.3.1398	P6 <sub>2</sub> '2'2			183.5.1419	P6m'm'	
180.4.1399	P6 <sub>2</sub> '22'			183.6.1420	P <sub>2c</sub> 6mm	P <sub>c</sub> 6mm
180.5.1400	P6 <sub>2</sub> 2'2'			183.7.1421	P <sub>2c</sub> 6'm'm	P <sub>c</sub> 6 <sub>3</sub> cm
180.6.1401	P <sub>2c</sub> 6 <sub>2</sub> 22	P <sub>c</sub> 6 <sub>1</sub> 22		183.8.1422	P <sub>2c</sub> 6'mm'	P <sub>c</sub> 6 <sub>3</sub> mc
180.7.1402	P <sub>2c</sub> 6 <sub>2</sub> '22'	P <sub>c</sub> 6 <sub>4</sub> 22		183.9.1423	P <sub>2c</sub> 6m'm'	P <sub>c</sub> 6cc
<b>181.1.1403</b>	<b>P6<sub>4</sub>22</b>			<b>184.1.1424</b>	<b>P6cc</b>	
181.2.1404	P6 <sub>4</sub> 221'			184.2.1425	P6cc1'	
181.3.1405	P6 <sub>4</sub> '2'2			184.3.1426	P6'c'c	
181.4.1406	P6 <sub>4</sub> '22'			184.4.1427	P6'cc'	
181.5.1407	P6 <sub>4</sub> 2'2'			184.5.1428	P6c'c'	
181.6.1408	P <sub>2c</sub> 6 <sub>4</sub> 22	P <sub>c</sub> 6 <sub>2</sub> 22		<b>185.1.1429</b>	<b>P6<sub>3</sub>cm</b>	
181.7.1409	P <sub>2c</sub> 6 <sub>4</sub> '2'2	P <sub>c</sub> 6 <sub>5</sub> 22		185.2.1430	P6 <sub>3</sub> cm1'	
<b>182.1.1410</b>	<b>p6<sub>3</sub>22</b>			185.3.1431	P6 <sub>3</sub> 'c'm	
182.2.1411	p6 <sub>3</sub> 221'			185.4.1432	P6 <sub>3</sub> 'cm'	
182.3.1412	p6 <sub>3</sub> '2'2			185.5.1433	P6 <sub>3</sub> c'm'	
182.4.1413	p6 <sub>3</sub> '22'			<b>186.1.1434</b>	<b>P6<sub>3</sub>mc</b>	
182.5.1414	p6 <sub>3</sub> 2'2'			186.2.1435	P6 <sub>3</sub> mc1'	
<b>183.1.1415</b>	<b>p6mm</b>			186.3.1436	P6 <sub>3</sub> 'm'c	
183.2.1416	P6mm1'			186.4.1437	P6 <sub>3</sub> 'mc'	

186.5.1438	$P6_3m'c'$			190.2.1459	$P\bar{6}2c1'$		
<b>187.1.1439</b>	<b><math>P\bar{6}m2</math></b>			190.3.1460	$P\bar{6}'2'c$		
187.2.1440	$P\bar{6}m21'$			190.4.1461	$P\bar{6}'2c'$		
187.3.1441	$P\bar{6}'m'2$			190.5.1462	$P\bar{6}2'c'$		
187.4.1442	$P\bar{6}'m'2'$			<b>191.1.1463</b>	<b><math>P6/mmm</math></b>		
187.5.1443	$P\bar{6}m'2'$			191.2.1464	$P6/mmm1'$		
187.6.1444	$P_{2c}\bar{6}m2$	$P_c\bar{6}m2$		191.3.1465	$P6/m'mm$		
187.7.1445	$P_{2c}\bar{6}'m'2$	$P_c\bar{6}c2$		191.4.1466	$P6'/mm'm$		
<b>188.1.1446</b>	<b><math>P\bar{6}c2</math></b>			191.5.1467	$P6'/mmm'$		
188.2.1447	$P\bar{6}c21'$			191.6.1468	$P6'/m'm'm$		
188.3.1448	$P\bar{6}'c'2$			191.7.1469	$P6'/m'mm'$		
188.4.1449	$P\bar{6}'c'2'$			191.8.1470	$P6/mm'm'$		
188.5.1450	$P\bar{6}c'2'$			191.9.1471	$P6/m'm'm'$		
<b>189.1.1451</b>	<b><math>P\bar{6}2m</math></b>			191.10.1472	$P_{2c}6/mmm$	$P_c6/mmm$	
189.2.1452	$P\bar{6}2m1'$			191.11.1473	$P_{2c}6'/mm'm$	$P_c6_3/mcm$	
189.3.1453	$P\bar{6}'2'm$			191.12.1474	$P_{2c}6'/mmm'$	$P_c6_3/mmc$	
189.4.1454	$P\bar{6}'2m'$			191.13.1475	$P_{2c}6/mm'm'$	$P_c6/mcc$	
189.5.1455	$P\bar{6}2'm'$			<b>192.1.1476</b>	<b><math>P6/mcc</math></b>		
189.6.1456	$P_{2c}\bar{6}2m$	$P_c\bar{6}2m$		192.2.1477	$P6/mcc1'$		
189.7.1457	$P_{2c}\bar{6}'2m'$	$P_c\bar{6}2c$		192.3.1478	$P6/m'cc$		
<b>190.1.1458</b>	<b><math>P\bar{6}2c</math></b>			192.4.1479	$P6'/mc'c$		

192.5.1480	$P6'/mcc'$	194.9.1502	$P6_3/m'm'c'$	
192.6.1481	$P6'/m'c'c'$			
192.7.1482	$P6'/m'cc'$			
192.8.1483	$P6/mc'c'$			
192.9.1484	$P6/m'c'c'$			
<b>193.1.1485</b>	<b><math>P6_3/mcm</math></b>			
193.2.1486	$P6_3/mcm1'$			
193.3.1487	$P6_3/m'cm$			
193.4.1488	$P6_3'/mc'm$			
193.5.1489	$P6_3'/mcm'$			
193.6.1490	$P6_3'/m'c'm$			
193.7.1491	$P6_3'/m'cm'$			
193.8.1492	$P6_3/mc'm'$			
193.9.1493	$P6_3/m'c'm'$			
<b>194.1.1494</b>	<b><math>P6_3/mmc</math></b>			
194.2.1495	$P6_3/mmc1'$			
194.3.1496	$P6_3/m'mc$			
194.4.1497	$P6_3'/mm'c$			
194.5.1498	$P6_3'/mmc'$			
194.6.1499	$P6_3'/m'm'c$			
194.7.1500	$P6_3'/m'mc'$			
194.8.1501	$P6_3'/mm'c'$			
		<b>CUBIC SYSTEM</b>		
		<b>195.1.1503</b>	<b>P23</b>	
		195.2.1504	P231'	
		195.3.1505	$P_F23$	$F_s23$
		<b>196.1.1506</b>	<b>F23</b>	
		196.2.1507	F231'	
		<b>197.1.1508</b>	<b>I23</b>	
		197.2.1509	I231'	
		197.3.1510	$I_P23$	$P_I23$
		<b>198.1.1511</b>	<b>P2<sub>1</sub>3</b>	
		198.2.1512	P2 <sub>1</sub> 31'	
		<b>199.1.1513</b>	<b>I2<sub>1</sub>3</b>	
		199.2.1514	I2 <sub>1</sub> 31'	
		199.3.1515	$I_P2_13$	$P_I2_13$
		<b>200.1.1516</b>	<b><math>Pm\bar{3}</math></b>	
		200.2.1517	$Pm\bar{3}1'$	
		200.3.1518	$Pm'\bar{3}'$	
		200.4.1519	$P_Fm\bar{3}$	$F_s m\bar{3}$

<b>201.1.1520</b>	<b><math>Pn\bar{3}</math></b>		206.3.1540	$Ia'\bar{3}'$	
201.2.1521	$Pn\bar{3}1'$		206.4.1541	$I_p a\bar{3}$	$P_1 a\bar{3}$
201.3.1522	$Pn'\bar{3}'$		<b>207.1.1542</b>	<b><math>P432</math></b>	
201.4.1523	$P_F n\bar{3}$	$F_s d\bar{3}$	207.2.1543	$P4321'$	
<b>202.1.1524</b>	<b><math>Fm\bar{3}</math></b>		207.3.1544	$P4'32'$	
202.2.1525	$Fm\bar{3}1'$		207.4.1545	$P_F 432$	$F_s 432$
202.3.1526	$Fm'\bar{3}'$		<b>208.1.1546</b>	<b><math>P4_2 32</math></b>	
<b>203.1.1527</b>	<b><math>Fd\bar{3}</math></b>		208.2.1547	$P4_2 321'$	
203.2.1528	$Fd\bar{3}1'$		208.3.1548	$P4_2'32'$	
203.3.1529	$Fd'\bar{3}'$		208.4.1549	$P_F 4_2 32$	$F_s 4_1 32$
<b>204.1.1530</b>	<b><math>Im\bar{3}</math></b>		<b>209.1.1550</b>	<b><math>F432</math></b>	
204.2.1531	$Im\bar{3}1'$		209.2.1551	$F4321'$	
204.3.1532	$Im'\bar{3}'$		209.3.1552	$F4'32'$	
204.4.1533	$I_p m\bar{3}$	$P_1 m\bar{3}$	<b>210.1.1553</b>	<b><math>F4_1 32</math></b>	
204.5.1534	$I_p m'\bar{3}'$	$P_1 n\bar{3}$	210.2.1554	$F4_1 321'$	
<b>205.1.1535</b>	<b><math>Pa\bar{3}</math></b>		210.3.1555	$F4_1'32'$	
205.2.1536	$Pa\bar{3}$		<b>211.1.1556</b>	<b><math>I432</math></b>	
205.3.1537	$Pa'\bar{3}'$		211.2.1557	$I4321'$	
<b>206.1.1538</b>	<b><math>Ia\bar{3}</math></b>		211.3.1558	$I4'32'$	
206.2.1539	$Ia\bar{3}1'$		211.4.1559	$I_p 432$	$P_1 432$

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211.5.1560	$I_p \bar{4}'32'$	$P_1 \bar{4}_2 32$	<b>217.1.1580</b>	$I\bar{4}3m$	
<b>212.1.1561</b>	<b><math>P\bar{4}_3 32</math></b>		217.2.1581	$I\bar{4}3m1'$	
212.2.1562	$P\bar{4}_3 321'$		217.3.1582	$I\bar{4}'3m'$	
212.3.1563	$P\bar{4}_3'32'$		217.4.1583	$I_p \bar{4}3m$	$P_1 \bar{4}3m$
<b>213.1.1564</b>	<b><math>P\bar{4}_1 32</math></b>		217.5.1584	$I_p \bar{4}'3m'$	$P_1 \bar{4}3n$
213.2.1565	$P\bar{4}_1 321'$		<b>218.1.1585</b>	<b><math>P\bar{4}3n</math></b>	
213.3.1566	$P\bar{4}_1'32'$		218.2.1586	$P\bar{4}3n1'$	
<b>214.1.1567</b>	<b><math>I\bar{4}_1 32</math></b>		218.3.1587	$P\bar{4}'3n'$	
214.2.1568	$I\bar{4}_1 321'$		<b>219.1.1588</b>	<b><math>F\bar{4}3c</math></b>	
214.3.1569	$I\bar{4}_1'32'$		219.2.1589	$F\bar{4}3c1'$	
214.4.1570	$I_p \bar{4}_1 32$	$P_1 \bar{4}_3 32$	219.3.1590	$F\bar{4}'3c'$	
214.5.1571	$I_p \bar{4}_1'32'$	$P_1 \bar{4}_1 32$	<b>220.1.1591</b>	<b><math>I\bar{4}3d</math></b>	
<b>215.1.1572</b>	<b><math>P\bar{4}3m</math></b>		220.2.1592	$I\bar{4}3d1'$	
215.2.1573	$P\bar{4}3m1'$		220.3.1593	$I\bar{4}'3d'$	
215.3.1574	$P\bar{4}'3m'$		<b>221.1.1594</b>	<b><math>Pm\bar{3}m</math></b>	
215.4.1575	$P_F \bar{4}3m$	$F_s \bar{4}3m$	221.2.1595	$Pm\bar{3}m1'$	
215.5.1576	$P_F \bar{4}'3m'$	$F_s \bar{4}3c$	221.3.1596	$Pm'\bar{3}'m$	
<b>216.1.1577</b>	<b><math>F\bar{4}3m</math></b>		221.4.1597	$Pm\bar{3}m'$	
216.2.1578	$F\bar{4}3m1'$		221.5.1598	$Pm'\bar{3}'m'$	
216.3.1579	$F\bar{4}'3m'$		221.6.1599	$P_F m\bar{3}m$	$F_s m\bar{3}m$
			221.7.1600	$P_F m\bar{3}m'$	$F_s m\bar{3}c$

<b>222.1.1601</b>	<b><math>Pn\bar{3}n</math></b>			225.5.1622	$Fm'\bar{3}'m'$
222.2.1602	$Pn\bar{3}n1'$			<b>226.1.1623</b>	<b><math>Fm\bar{3}c</math></b>
222.3.1603	$Pn'\bar{3}'n$			226.2.1624	$Fm\bar{3}c1'$
222.4.1604	$Pn\bar{3}n'$			226.3.1625	$Fm'\bar{3}'c$
222.5.1605	$Pn'\bar{3}'n'$			226.4.1626	$Fm\bar{3}c'$
<b>223.1.1606</b>	<b><math>Pm\bar{3}n</math></b>			226.5.1627	$Fm'\bar{3}'c'$
223.2.1607	$Pm\bar{3}n1'$			<b>227.1.1628</b>	<b><math>Fd\bar{3}m</math></b>
223.3.1608	$Pm'\bar{3}'n$			227.2.1629	$Fd\bar{3}m1'$
223.4.1609	$Pm\bar{3}n'$			227.3.1630	$Fd'\bar{3}'m$
223.5.1610	$Pm'\bar{3}'n'$			227.4.1631	$Fd\bar{3}m'$
<b>224.1.1611</b>	<b><math>Pn\bar{3}m</math></b>			227.5.1632	$Fd'\bar{3}'m'$
224.2.1612	$Pn\bar{3}m1'$			<b>228.1633</b>	<b><math>Fd\bar{3}c</math></b>
224.3.1613	$Pn'\bar{3}'m$			228.2.1634	$Fd\bar{3}c1'$
224.4.1614	$Pn\bar{3}m'$			228.3.1635	$Fd'\bar{3}'c$
224.5.1615	$Pn'\bar{3}'m'$			228.4.1636	$Fd\bar{3}c'$
224.6.1616	$P_F n\bar{3}m$	$F_s d\bar{3}m$		228.5.1637	$Fd'\bar{3}'c'$
224.7.1617	$P_F n\bar{3}m'$	$F_s d\bar{3}m'$		<b>229.1.1638</b>	<b><math>Im\bar{3}m</math></b>
<b>225.1.1618</b>	<b><math>Fm\bar{3}m</math></b>			229.2.1639	$Im\bar{3}m1'$
225.2.1619	$Fm\bar{3}m1'$			229.3.1640	$Im'\bar{3}'m$
225.3.1620	$Fm'\bar{3}'m$			229.4.1641	$Im\bar{3}m'$
225.4.1621	$Fm\bar{3}m'$			229.5.1642	$Im'\bar{3}'m'$

229.6.1643	$I_p m \bar{3}m$	$P_1 m \bar{3}m$
229.7.1644	$I_p m' \bar{3}'m$	$P_1 n \bar{3}m$
229.8.1645	$I_p m \bar{3}m'$	$P_1 m \bar{3}n$
229.9.1646	$I_p m' \bar{3}'m'$	$P_1 n \bar{3}n$

**230.1.1647**  $Ia \bar{3}d$

230.2.1648	$Ia \bar{3}d1'$
230.3.1649	$Ia' \bar{3}'d$
230.4.1650	$Ia \bar{3}d'$
230.5.1651	$Ia' \bar{3}'d'$



**Table 1.4 - 2D**

**Two-dimensional:** Magnetic space group symbols of Table 1.1-2D compared with the one-dimensional black and white symbols given by Belov and Tarkhova (BT) (1956).

Table 1.1-2D		BT	Table 1.1-2D		BT
1.1.1	$p1$	$p1$	7.3.33	$p2m'g'$	$pm'g'$
1.2.2	$p11'$	$p11'$	7.4.34	$p2'm'g$	$pm'g$
1.3.3	$p_{2a}1$	$p'_b1$	7.5.35	$p2'mg'$	$pmg'$
			7.6.36	$p_{2b}2m'g'$	$p'_b gg$
2.1.4	$p211$	$p2$	7.7.37	$p_{2b}2mg$	$p'_b mg$
2.2.5	$p2111'$	$p21'$			
2.3.6	$p2'11$	$p2'$	8.1.38	$p2gg$	$pgg2$
2.4.7	$p_{2a}211$		8.2.39	$p2gg1'$	$pgg21'$
			8.3.40	$p2g'g'$	$pg'g'$
3.1.8	$p1m1$	$pm$	8.4.41	$p2'gg'$	$pgg'$
3.2.9	$p1m11'$	$pm1'$			
3.3.10	$p1m'1$	$pm'$	9.1.42	$c2mm$	$cmm2$
3.4.11	$p_{2a}1m1$	$p'_b1m$	9.2.43	$c2mm1'$	$cmm21'$
3.5.12	$p_{2b}1m1$	$p'_b m$	9.3.44	$c2m'm'$	$cm'm'$
3.6.13	$p_{2b}1m'1$	$p'_b g$	9.4.45	$c2'mm'$	$cmm'$
3.7.14	$p_c1m1$	$c'm$	9.5.46	$c_p2mm$	$p'_c mm$
			9.6.47	$c_p2m'm'$	$p'_c gg$
4.1.15	$p1g1$	$pg$	9.7.48	$c_p2'mm'$	$p'_c mg$
4.2.16	$p1g11'$	$pg1'$			
4.3.17	$p1g'1$	$pg'$	10.1.49	$p4$	$p4$
4.4.18	$p_{2a}1g1$	$p'_b1g$	10.2.50	$p41'$	$p41'$
			10.3.51	$p4'$	$p4'$
5.1.19	$c1m1$	$cm$	10.4.52	$p_p4$	$p'_c 4$
5.2.20	$c1m11'$	$cm1'$			
5.3.21	$c1m'1$	$cm'$	11.1.53	$p4mm$	$p4mm$
5.4.22	$c_p1m1$	$p'_c m$	11.2.54	$p4mm1'$	$p4mm1'$
5.5.23	$c_p1m'1$	$p'_c g$	11.3.55	$p4m'm'$	$p4m'm'$
			11.4.56	$p4'mm'$	$p4'mm'$
6.1.24	$p2mm$	$pmm2$	11.5.57	$p4'm'm$	$p4'm'm$
6.2.25	$p2mm1'$	$pmm21'$	11.6.58	$p_p4m'm'$	$p'_c 4gm$
6.3.26	$p2m'm'$	$pm'm'$	11.7.59	$p_p4mm$	$p'_c 4mm$
6.4.27	$p2'mm'$	$pmm'$			
6.5.28	$p_{2a}2m'm'$	$p'_b gm$	12.1.60	$p4gm$	$p4gm$
6.6.29	$p_c2mm$	$c'mm$	12.2.61	$p4gm1'$	$p4gm1'$
6.7.30	$p_{2a}2mm$	$p'_b mm$	12.3.62	$p4g'm'$	$p4g'm'$
			12.4.63	$p4'gm'$	$p4'gm'$
7.1.31	$p2mg$	$pmg2$	12.5.64	$p4'g'm$	$p4'g'm$
7.2.32	$p2mg1'$	$pmg21'$			

Table 1.1-2D		BT
13.1.65	p3	<i>p3</i>
13.2.66	p31'	<i>p31'</i>
14.1.67	p3m1	<i>p3m</i>
14.2.68	p3m11'	<i>p3m1'</i>
14.3.69	p3m'1	<i>p3m'</i>
15.1.70	p31m	<i>p31m</i>
15.2.71	p31m1'	<i>p31m1'</i>
15.3.72	p31m'	<i>p31m'</i>
16.1.73	p6	<i>p6</i>
16.2.74	p61'	<i>p61'</i>
16.3.75	p6'	<i>p6'</i>
17.1.76	p6mm	<i>p6mm</i>
17.2.77	p6mm1'	<i>p6mm1'</i>
17.3.78	p6m'm'	<i>p6m'm'</i>
17.4.79	p6'mm'	<i>p6'mm'</i>
17.5.80	p6'm'm	<i>p6'm'm</i>

**Table 1.4 - 1D**

**One-Dimensional:** Magnetic space group symbols of Table 1.1-1D compared with the one-dimensional black and white symbols given by Niggli (1964).

	Table 1.1-1D	Niggli
1.1.1	$p1$	P1
1.2.2	$p11'$	(P1')
1.3.3	$p_{2a}1$	C'1
2.1.4	$pm$	Pm
2.2.5	$pm1'$	(P'm)
2.3.6	$pm'$	Pm'
2.3.7	$p_{2a}m$	C'm

**Table 2.2.3-3D Graphical Symbols**

Three-Dimensional Magnetic Space Groups

**2.2.3.1 Symmetry axes parallel to the plane of projection**





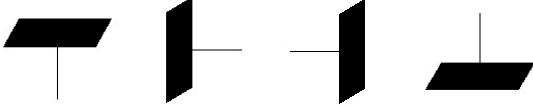
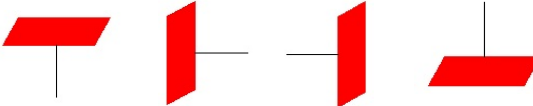
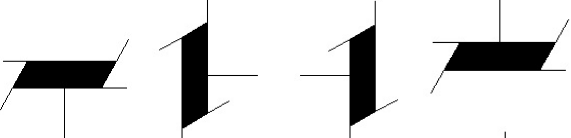
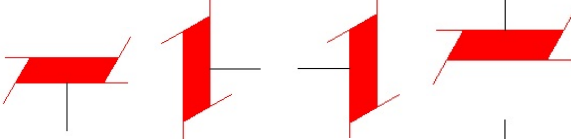
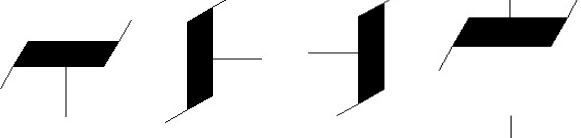
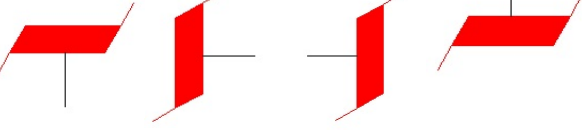
Symmetry Axis	Graphical symbol	Screw vector of a right-handed screw rotation in units of the shortest non-primed translation vector parallel to the axis.	Printed symbol
Twofold unprimed rotation axis,		None	2
Twofold primed rotation axis		None	2'
Twofold unprimed screw axis, 2 sub 1		1/2	2 <sub>1</sub>
Twofold primed screw axis, 2 sub 1 primed		1/2	2' <sub>1</sub>
Fourfold unprimed rotation axis		None	4
Fourfold primed rotation axis		None	4'
Fourfold unprimed screw axis, 4 sub 1		1/4	4 <sub>1</sub>
Fourfold primed screw axis, 4 sub 1 primed		1/4	4' <sub>1</sub>
Fourfold unprimed screw axis, 4 sub 2		1/2	4 <sub>2</sub>
Fourfold primed screw axis, 4 sub 2 primed		1/2	4' <sub>2</sub>

Table 2.2.3 - 1

Fourfold unprim screw axis, 4 sub 3		3/4	$4_3$
Fourfold unprim screw axis, 4 sub 3		3/4	$4_3$
unprimed Inversion axis, 4 bar		None	$\bar{4}$
primed inversion axis, 4 bar primed		None	$\bar{4}'$
Fourfold primed screw axis 4 sub1 prime and fourfold unprimed screw axis 4 sub 3		1/4,3/4	$4_1',4_3$

### 2.2.3.2 Symmetry axes normal to the plane of projection

Symmetry Axis or symmetry point	Graphical symbol	Screw vector of a right-handed screw rotation in units of the shortest non-primed translation vector parallel to the axis.	Printed symbol
Identity	None	None	1
Twofold unprimed rotation axis, 2		None	2
Twofold primed rotation axis, 2 primed		None	2'
Twofold unprimed screw axis, 2 sub 1		1/2	2 <sub>1</sub>
Twofold primed screw axis, 2 sub 1 primed		1/2	2' <sub>1</sub>

Table 2.2.3 - 2







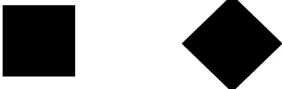

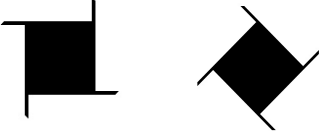

Threefold unprimed rotation axis, 3		None	3
Threefold primed rotation axis, 3 primed		None	3'
Threefold unprimed screw axis, 3 sub 1		1/3	3 <sub>1</sub>
Threefold primed screw axis, 3 sub 1 primed		1/3	3' <sub>1</sub>
Threefold unprimed screw axis, 3 sub 2		2/3	3 <sub>2</sub>
Threefold primed screw axis, 3 sub 2 primed		2/3	3' <sub>2</sub>
Fourfold unprimed rotation axis, 4		None	4
Fourfold primed rotation axis, 4 prime		None	4'
Fourfold unprimed screw axis, 4 sub 1		1/4	4 <sub>1</sub>
Fourfold primed screw axis, 4 sub 1 prime		1/4	4' <sub>1</sub>

Table 2.2.3 - 3






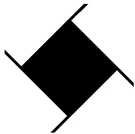








Fourfold unprimed screw axis, 4 sub 2			1/2	$4_2$
Fourfold primed screw axis, 4 sub 2 primed			1/2	$4_2'$
Fourfold unprimed screw axis, 4 sub 3			3/4	$4_3$
Fourfold primed screw axis, 4 sub 3 primed			3/4	$4_3'$
Sixfold unprimed rotation axis, 6			None	6
Sixfold primed rotation axis, 6 primed			None	6'
Sixfold unprimed screw axis, 6 sub 1			1/6	$6_1$
Sixfold primed screw axis, 6 sub 1 primed			1/6	$6_1'$
Sixfold unprimed screw axis, 6 sub 2			1/3	$6_2$
Sixfold primed screw axis, 6 sub 2 primed			1/3	$6_2'$

Table 2.2.3 - 4











Sixfold unprimed screw axis, 6 sub 3		1/2	$6_3$
Sixfold primed screw axis, 6 sub 3 primed		1/2	$6_3'$
Sixfold unprimed screw axis, 6 sub 4		2/3	$6_4$
Sixfold primed screw axis, 6 sub 4 primed		2/3	$6_4'$
Sixfold unprimed screw axis, 6 sub 5		5/6	$6_5$
Sixfold primed screw axis, 6 sub 5 primed		5/6	$6_5'$
Unprimed center of symmetry, unprimed inversion center, 1 bar		None	$\bar{1}$
Primed center of symmetry, primed inversion center, 1 bar primed		None	$\bar{1}'$
Twofold unprimed rotation axis with unprimed center of symmetry		None	$2, \bar{1} = 2/m$
Twofold primed rotation axis with unprimed center of symmetry		None	$2', \bar{1} = 2'/m'$

Table 2.2.3 - 5













Twofold unprimed rotation axis with primed center of symmetry		None	$2, \bar{1}' = 2/m'$
Twofold primed rotation axis with primed center of symmetry		None	$2', \bar{1}' = 2'/m'$
Twofold unprimed screw axis with unprimed center of symmetry		1/2	$2_1, \bar{1}$
Twofold primed screw axis with unprimed center of symmetry		1/2	$2_1', \bar{1}$
Twofold unprimed screw axis with primed center of symmetry		1/2	$2_1, \bar{1}'$
Twofold primed screw axis with primed center of symmetry		1/2	$2_1', \bar{1}'$
Twofold primed screw axis with unprimed twofold rotation axis		1/2	$2_1', 2$
Twofold unprimed screw axis with primed twofold rotation axis		1/2	$2_1, 2'$
Twofold primed screw axis, twofold unprimed rotation axis, and primed and unprimed centers of symmetry		1/2	$2_1', 2, \bar{1}, \bar{1}'$
Twofold unprimed screw axis, twofold primed rotation axis, and primed and unprimed centers of symmetry		1/2	$2_1, 2', \bar{1}', \bar{1}$

Table 2.2.3 - 6


















Threefold unprimed rotation axis with unprimed center of symmetry, inversion axis 3 bar		None	$3, \bar{1} = \bar{3}$	
Threefold unprimed rotation axis with primed center of symmetry, inversion axis 3 bar prime		None	$3, \bar{1}' = \bar{3}'$	
Threefold unprimed rotation axis with primed and unprimed centers of symmetry		None	$3, \bar{1}', \bar{1}$	
Fourfold unprimed rotation axis with unprimed center of symmetry			None	$4, \bar{1} = 4/m$
Fourfold primed rotation axis with unprimed center of symmetry			None	$4', \bar{1} = 4'/m$
Fourfold unprimed rotation axis with primed center of symmetry			None	$4, \bar{1}' = 4'/m'$
Fourfold primed rotation axis with primed center of symmetry			None	$4, \bar{1}' = 4'/m'$
Fourfold unprimed screw axis with unprimed center of symmetry			1/2	$4_2, \bar{1}$
Fourfold primed screw axis with unprimed center of symmetry			1/2	$4_2', \bar{1}$
Fourfold unprimed screw axis with primed center of symmetry			1/2	$4_2, \bar{1}'$

Table 2.2.3 - 7

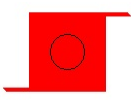
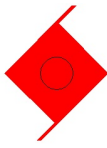


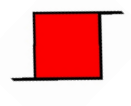
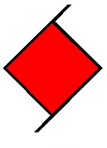


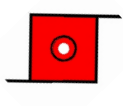
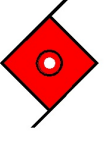
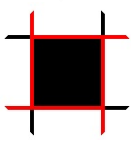
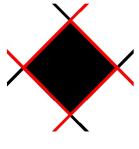
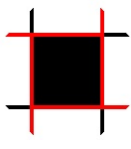







Fourfold primed screw axis with primed center of symmetry			1/2	$4_2', \bar{1}'$
Fourfold primed screw axis with fourfold unprimed rotation axis			1/2	$4_2', 4$
Fourfold unprimed screw axis with fourfold primed rotation axis			1/2	$4_2, 4'$
Fourfold primed screw axis, fourfold unprimed rotation axis and primed and unprimed center of symmetry			1/2	$4_2', 4, \bar{1}', \bar{1}$
Fourfold unprimed screw axis, fourfold primed rotation axis, and primed and unprimed center of symmetry			1/2	$4_2, 4', \bar{1}', \bar{1}$
Fourfold unprimed screw axis 4 sub1 and fourfold primed screw axis 4 sub 3 prime			1/4, 3/4	$4_1, 4_3'$
Fourfold primed screw axis 4 sub1 prime and fourfold unprimed screw axis 4 sub 3			1/4, 3/4	$4_1', 4_3$
Unprimed inversion axis 4 bar			None	$\bar{4}, 2 = \bar{4}$
Primed inversion axis 4 bar prime			None	$\bar{4}', 2 = \bar{4}'$
Primed and unprimed inversion axes 4 bar and 4 bar prime, and primed twofold screw axis			1/2	$\bar{4}, 2 = \bar{4}$ $\bar{4}', 2 = \bar{4}'$ $2_1'$

Table 2.2.3 - 8




















Sixfold unprimed rotation axis with unprimed center of symmetry		None	$6, \bar{1} = 6/m$
Sixfold primed rotation axis with unprimed center of symmetry		None	$6', \bar{1} = 6'/m$
Sixfold unprimed rotation axis with primed center of symmetry		None	$6, \bar{1}' = 6/m'$
Sixfold primed rotation axis with primed center of symmetry		None	$6', \bar{1}' = 6'/m'$
Sixfold unprimed screw axis 6 sub 3 with unprimed center of symmetry		1/2	$6_3, \bar{1}$
Sixfold primed screw axis 6 sub 3 prime with unprimed center of symmetry		1/2	$6_3', \bar{1}$
Sixfold unprimed screw axis 6 sub 3 with primed center of symmetry		1/2	$6_3, \bar{1}'$
Sixfold primed screw axis 6 sub 3 prime with primed center of symmetry		1/2	$6_3', \bar{1}'$
Sixfold unprimed rotation axis, sixfold primed screw axis 6 sub 3 prime		1/2	$6_3', 6$
Sixfold primed rotation axis, sixfold unprimed screw axis 6 sub 3		1/2	$6_3, 6'$

Table 2.2.3 - 9

Sixfold unprimed rotation axis, sixfold primed screw axis 6 sub 3 prime, with primed and unprimed centers of symmetry		1/2	$\frac{6_3', 6}{\bar{1}, \bar{1}'}$
Sixfold primed rotation axis, sixfold unprimed screw axis 6 sub 3, with primed and unprimed centers of symmetry		1/2	$\frac{6_3', 6}{\bar{1}, \bar{1}'}$
Unprimed inversion axis 6 bar		None	$\bar{6}$
Primed inversion axis 6 bar prime		None	$\bar{6}'$
Primed and unprimed inversion axes, 6 bar prime and 6 bar		None	$\bar{6}', \bar{6}$
Primed and unprimed centers of symmetry		None	$\bar{1}, \bar{1}'$

### 2.2.3.3 Symmetry planes normal to the plane of projection

Symmetry plane	Graphical symbol	Glide vector in units of unprimed lattice translation parallel and normal to the projection plane	Printed symbol
Unprimed reflection plane		None	m
Primed reflection plane		None	m'
Unprimed axial glide plane		1/2 along line parallel to projection plane	a,b






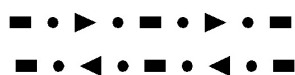
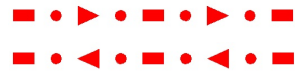
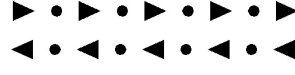
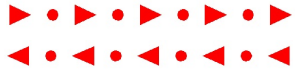








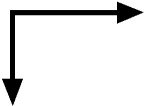
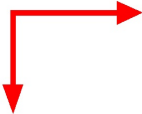
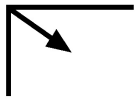

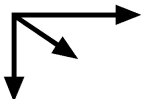
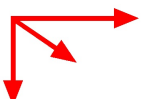
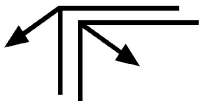
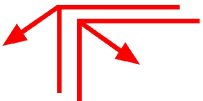
Primed axial glide plane		1/2 along line parallel to projection plane	a',b'
Unprimed axial glide plane		1/2 along line normal to projection plane	c
Primed axial glide plane		1/2 along line normal to projection plane	c'
Unprimed diagonal glide plane		One glide plane with two components: 1/2 along line parallel to projection plane <i>and</i> 1/2 normal to projection plane	n
Primed diagonal glide plane		One glide plane with two components: 1/2 along line parallel to projection plane <i>and</i> 1/2 normal to projection plane	n'
Unprimed diamond glide plane		One glide plane with two components: 1/4 along line parallel to projection plane in direction of arrow <i>and</i> 1/4 up normal to projection plane	d
Primed diamond glide plane		One glide plane with two components: 1/4 along line parallel to projection plane in direction of arrow <i>and</i> 1/4 up normal to projection plane	d'
Unprimed diamond glide plane		One glide plane with two components: 1/4 along line parallel to projection plane in direction of arrow <i>and</i> 3/4 up normal to projection plane	d
Primed diamond glide plane		One glide plane with two components: 1/4 along line parallel to projection plane in direction of arrow <i>and</i> 3/4 up normal to projection plane	d'
Unprimed axial glide planes		Two glide planes each with one component: 1/2 along line parallel to projection plane; 1/2 normal to projection plane	a,b; c

Table 2.2.3 - 11

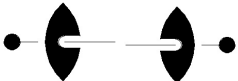
Primed axial glide planes		Two glide planes each with one $a, b, c$ component: $1/2$ along line parallel to projection plane; $1/2$ normal to projection plane
Unprimed axial glide plane and primed axial glide plane		Two glide planes each with one $a', b', c$ component: $1/2$ along line parallel to projection plane; $1/2$ normal to projection plane
Unprimed axial glide plane and primed axial glide plane		Two glide planes each with one $a, b, c'$ component: $1/2$ along line parallel to projection plane; $1/2$ normal to projection plane

#### 2.2.3.4 Symmetry planes parallel to the plane of projection

Symmetry plane	Graphical symbol	Glide vector in units of unprimed lattice translation parallel to the projection plane	Printed symbol
Unprimed reflection plane		None	$m$
Primed reflection plane		None	$m'$
Unprimed axial glide plane		$1/2$ along direction parallel to arrow	$a, b$
Primed axial glide plane		$1/2$ along direction parallel to arrow	$a', b'$
Unprimed double glide plane		Two glide planes each with one component $1/2$ along directions parallel to the two arrows	$a, b$

Primed double glide plane		Two glide planes each with one component 1/2 along directions parallel to the two arrows	a',b'
Unprimed diagonal glide plane		1/2 along direction parallel to arrow	n
Primed diagonal glide plane		1/2 along direction parallel to arrow	n'
Unprimed double glide plane and unprimed diagonal glide plane		Three glide planes each with one component 1/2 along directions parallel to the three arrows	a,b,n
Primed double glide plane and primed diagonal glide plane		Three glide planes each with one component 1/2 along directions parallel to the three arrows	a',b',n'
Unprimed double diagonal glide planes		Two glide planes each with one component 1/2 along directions parallel to the two arrows	d
Primed double diagonal glide planes		Two glide planes each with one component 1/2 along directions parallel to the two arrows	d'

### 2.2.3.5 Symmetry axes inclined to the plane of projection (in cubic magnetic space groups only)

Symmetry plane	Graphical symbol	Screw vector of a right-handed screw rotation in units of the shortest unprimed lattice translation parallel to the axis	Printed symbol
Unprimed twofold rotation axis parallel to a face diagonal of the cube		None	2






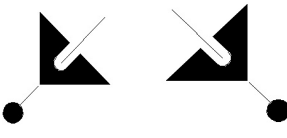
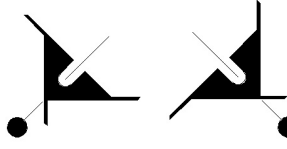
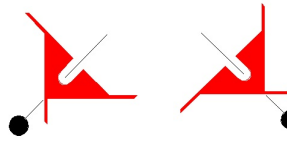
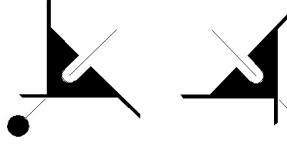
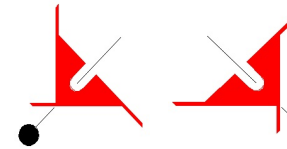
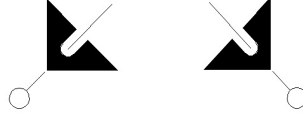
Primed twofold rotation axis parallel to a face diagonal of the cube		None	$2'$
Unprimed twofold screw axis 2 sub 1 parallel to a face diagonal of the cube		$1/2$	$2_1$
Primed twofold screw axis 2 sub 1 prime parallel to a face diagonal of the cube		$1/2$	$2_1'$
Unprimed threefold rotation axis parallel to a body diagonal of the cube		None	$3$
Unprimed threefold screw axis 3 sub 1 parallel to a body diagonal of the cube		$1/3$	$3_1$
Primed threefold screw axis 3 sub 1 prime parallel to a body diagonal of the cube		$1/3$	$3_1'$
Unprimed threefold screw axis 3 sub 2 parallel to a body diagonal of the cube		$2/3$	$3_2$
Primed threefold screw axis 3 sub 2 prime parallel to a body diagonal of the cube		$2/3$	$3_2'$
Unprimed inversion axis 3 bar parallel to a body diagonal of the cube		None	$3, \bar{1} = \bar{3}$

Table 2.2.3 - 14

### 2.2.3.6 Symmetry planes inclined to the plane of projection (in cubic magnetic space groups only)

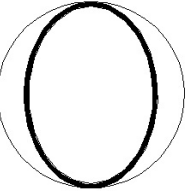
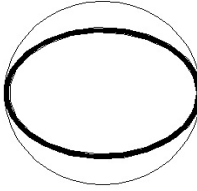
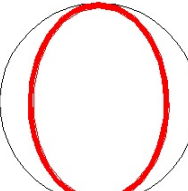
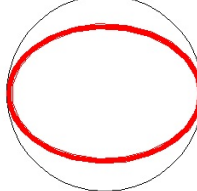
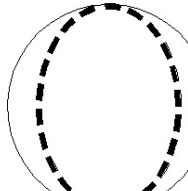
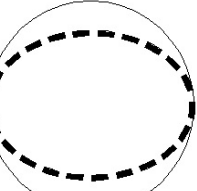
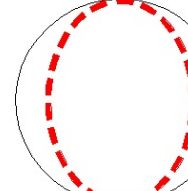
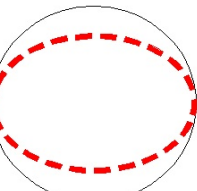
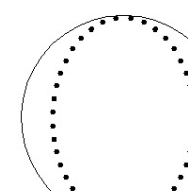
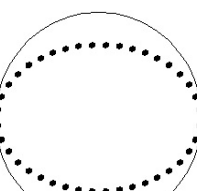
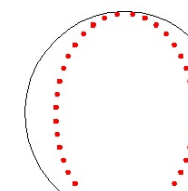
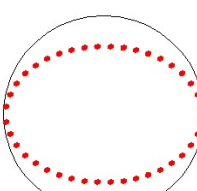
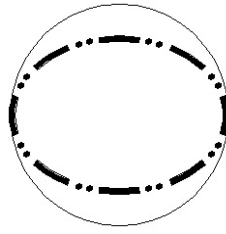
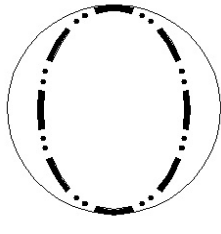
Symmetry Plane Symbol	Graphical symbol for planes normal to [011] and $[0\bar{1}\bar{1}]$ ; [101] and $[10\bar{1}]$	Glide vectors in units of unprimed lattice translation for planes normal to [011] and $[0\bar{1}\bar{1}]$ ; [101] and $[10\bar{1}]$	Printed		
Unprimed Reflection plane			None	None	m
Primed Reflection plane			None	None	m'
Unprimed axial glide plane			1/2 along [100]	1/2 along [010]	a,b
Primed axial glide plane			1/2 along [100]	1/2 along [010]	a',b'
Unprimed axial glide plane			1/2 along $[0\bar{1}\bar{1}]$ or [011]	1/2 along $[10\bar{1}]$ or [101]	
Unprimed axial glide plane			1/2 along $[0\bar{1}\bar{1}]$ or [011]	1/2 along $[10\bar{1}]$ or [101]	

Table 2.2.3 - 15

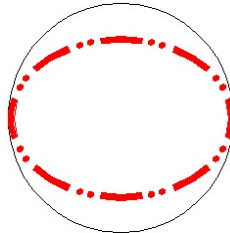
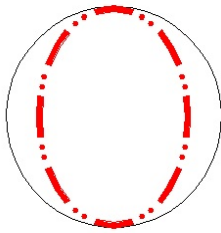
Unprimed double glide plane



Two glide vectors: 1/2 along [100] and 1/2 along  $[0\bar{1}\bar{1}]$  or  $[011]$

Two glide vectors: 1/2 along [010] and 1/2 along  $[10\bar{1}]$  or  $[101]$

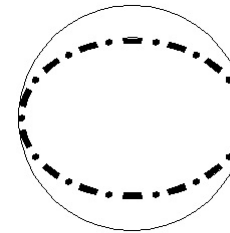
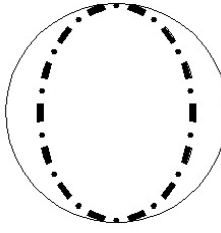
Primed double glide plane



Two glide vectors: 1/2 along [100] and 1/2 along  $[0\bar{1}\bar{1}]$  or  $[011]$

Two glide vectors: 1/2 along [010] and 1/2 along  $[10\bar{1}]$  or  $[101]$

Unprimed diagonal glide plane

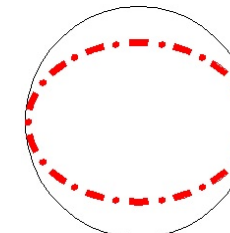
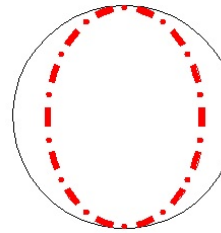


1/2 along  $[1\bar{1}\bar{1}]$  or  $[111]$

1/2 along  $[1\bar{1}\bar{1}]$  or  $[111]$

n

Primed diagonal glide plane

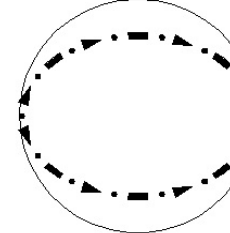
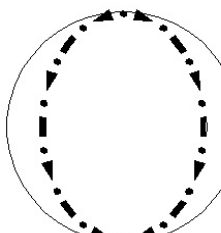


1/2 along  $[1\bar{1}\bar{1}]$  or  $[111]$

1/2 along  $[1\bar{1}\bar{1}]$  or  $[111]$

n'

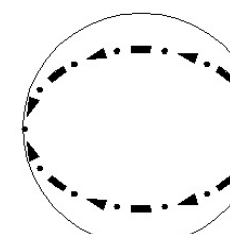
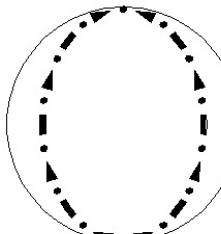
Unprimed diamond glide plane



1/2 along  $[1\bar{1}\bar{1}]$  or  $[111]$

1/2 along  $[\bar{1}11]$  or  $[111]$

d



1/2 along  $[\bar{1}11]$  or  $[\bar{1}\bar{1}\bar{1}]$

1/2 along  $[\bar{1}11]$  or  $[\bar{1}\bar{1}\bar{1}]$

d

Table 2.2.3 - 16

Primed diamond glide plane			1/2 along $[\bar{1}\bar{1}1]$ or $[111]$	1/2 along $[\bar{1}11]$ or $[1\bar{1}1]$	d'
			1/2 along $[\bar{1}\bar{1}1]$ or $[\bar{1}11]$	1/2 along $[\bar{1}\bar{1}1]$ or $[\bar{1}11]$	d'
Unprimed axial glide planes			Two glide vectors: 1/2 along $[100]$ and 1/2 along $[011]$	Two glide vectors: 1/2 along $[010]$ and 1/2 along $[101]$	
Unprimed axial glide planes			Two glide vectors: 1/2 along $[100]$ and 1/2 along $[01\bar{1}]$	Two glide vectors: 1/2 along $[010]$ and 1/2 along $[10\bar{1}]$	
Primed axial glide planes			Two glide vectors: 1/2 along $[100]$ and 1/2 along $[011]$	Two glide vectors: 1/2 along $[010]$ and 1/2 along $[101]$	
Primed axial glide planes			Two glide vectors: 1/2 along $[100]$ and 1/2 along $[01\bar{1}]$	Two glide vectors: 1/2 along $[010]$ and 1/2 along $[10\bar{1}]$	

Table 2.2.3 - 17

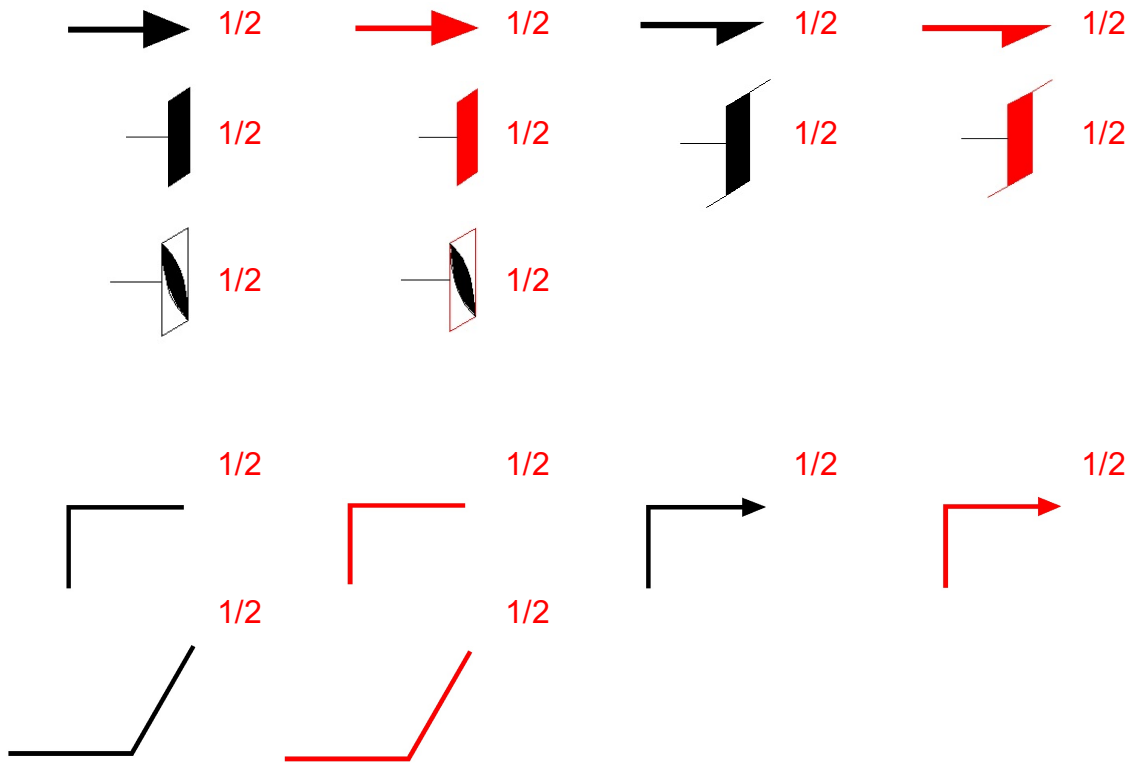
Unprimed diamond glide plane			1/2 along $[\bar{1}\bar{1}1]$ or $[\bar{1}11]$	1/2 along $[\bar{1}\bar{1}1]$ or $[111]$	d
			1/2 along $[\bar{1}\bar{1}1]$ or $[111]$	1/2 along $[\bar{1}\bar{1}1]$ or $[\bar{1}\bar{1}1]$	d
Primed diamond glide plane			1/2 along $[\bar{1}\bar{1}1]$ or $[\bar{1}11]$	1/2 along $[\bar{1}\bar{1}1]$ or $[111]$	d'
			1/2 along $[\bar{1}\bar{1}1]$ or $[111]$	1/2 along $[\bar{1}\bar{1}1]$ or $[\bar{1}\bar{1}1]$	d'

Table 2.2.3 - 18

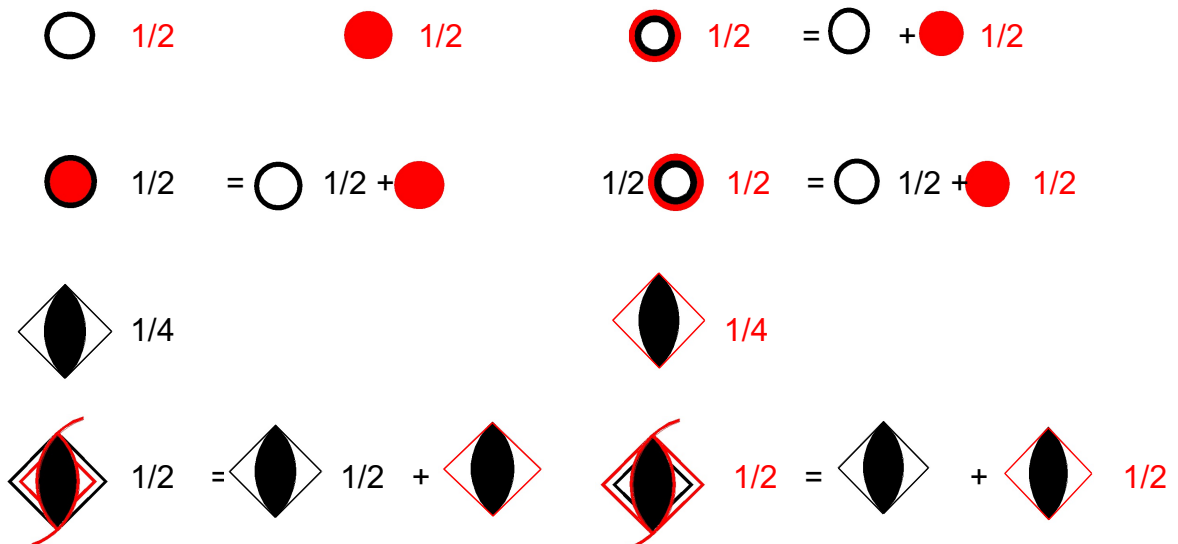
### 2.2.3.7 Height of symmetry operations above plane of projection

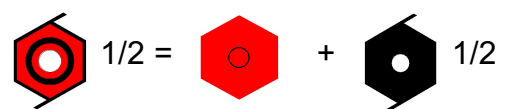
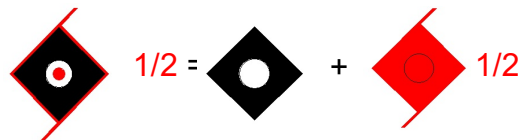
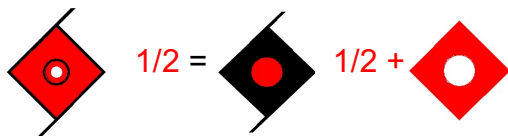
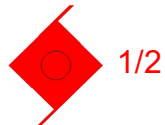
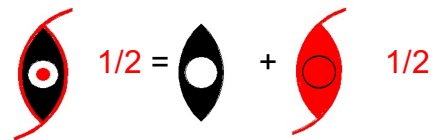
Heights are given as a fraction of the shortest primed or unprimed translation perpendicular to the plane of projection. Fractions are color coded black and red corresponding to related unprimed and primed operations, respectively. Examples are as follows:

#### 2.2.3.7a Rotation axes, screw axes, inversion axes and reflection and glide planes parallel to the plane of projection















#### 2.2.3.7b Inversion centers and inversion axes perpendicular to the plane of projection (i.e. height of inversion center of rotation-inversion)





**Table 2.2.3-2D Graphical Symbols**



Two-Dimensional Magnetic Space Groups

Symmetry	Graphical Symbol	Printed Symbol
Unprimed reflection line, mirror line		m
Primed reflection line, mirror line		m'
Unprimed glide line, 1/2 lattice vector along line in plane		g
Primed glide line, 1/2 lattice vector along line in plane		g'
Unprimed two-fold rotation point		2
Primed two-fold rotation point		2'
Unprimed three-fold rotation point		3
Primed three-fold rotation point		3'
Unprimed four-fold rotation point		4
Primed four-fold rotation point		4'
Unprimed six-fold rotation point		6
Primed six-fold rotation point		6'



### Table 2.2.3-1D Graphical Symbols

#### One-Dimensional Magnetic Space Groups

Symmetry	Graphical Symbol	Printed Symbol
Unprimed point of reflection		m
Primed point of reflection		m'

## **Table 3 - 1D:**

# **One-Dimensional Magnetic Space Group Tables**

ONE-DIMENSIONAL MAGNETIC SPACE GROUP INDEX

Figures 1.1-3D: Three-dimensional Magnetic Space Group Lattices  
Figures 1.1-2D: Two-dimensional Magnetic Space Group Lattices

## Index of One-Dimensional Magnetic Space Groups

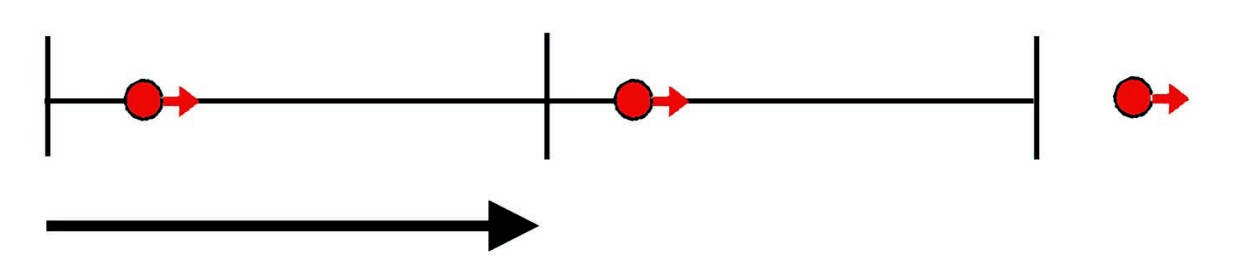
1.1.1	$p1$
1.2.2	$p11'$
1.3.3	$p_{2a}1$
2.1.4	$pm$
2.2.5	$pm1'$
2.3.6	$pm'$
2.4.7	$p_{2a}m$

$p1$

1

No. 1.1.1

$p1$



**Origin** arbitrary

**Asymmetric unit**  $0 \leq z \leq 1$

**Symmetry operations**

(1) 1  
(1|0,0,0)

**Generators selected** (1); t(1)

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site symmetry

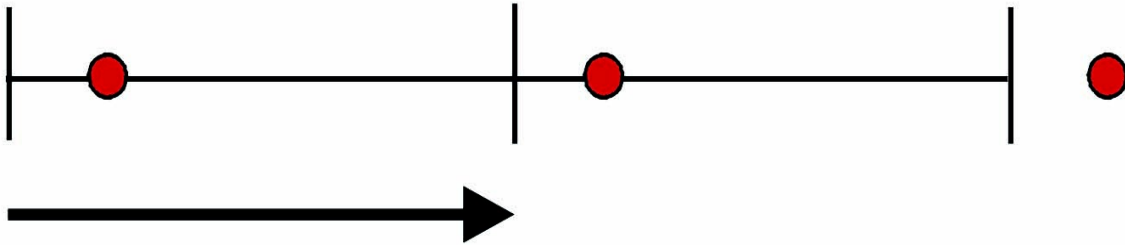
1 a 1 (1) x [u]

$p11'$

$1'$

No. 1.2.2

$p11'$



**Origin** arbitrary

**Asymmetric unit**  $0 \leq x \leq 1$

**Symmetry operations**

For  $1 +$  set  
 (1)  $1$   
 (1|0)

For  $1' +$  set  
 (1)  $1'$   
 (1|0)'

**Generators selected** (1);  $t(1)$ ;  $1'$

**Positions**

Coordinates

Multiplicity,  
 Wyckoff letter,  
 Site symmetry

$1+$      $1'+$

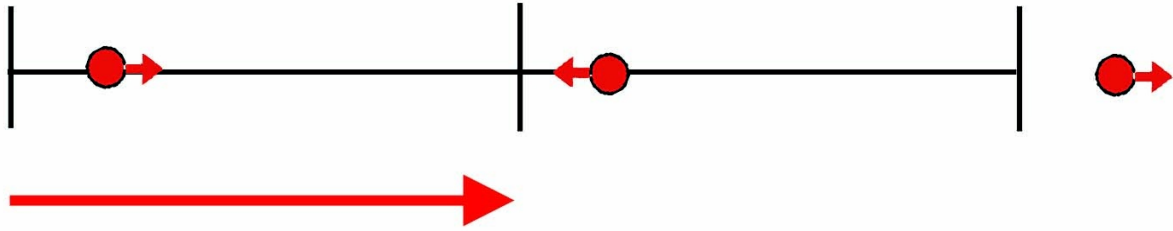
$1$  a  $11'$  (1) x [0]

$\rho_{2a}1$

$1'$

No. 1.3.3

$\rho_{2a}1$



**Origin** arbitrary

**Asymmetric unit**  $0 \leq x \leq 1$

**Symmetry operations**

For (0) + set  
 (1) 1  
 (1|0)

For (1)' + set  
 (1) t' (1)  
 (1|1)'

**Generators selected** (1); t(1)'

**Positions**

Coordinates

Multiplicity,  
 Wyckoff letter,  
 Site symmetry

(0)+ (1)' +

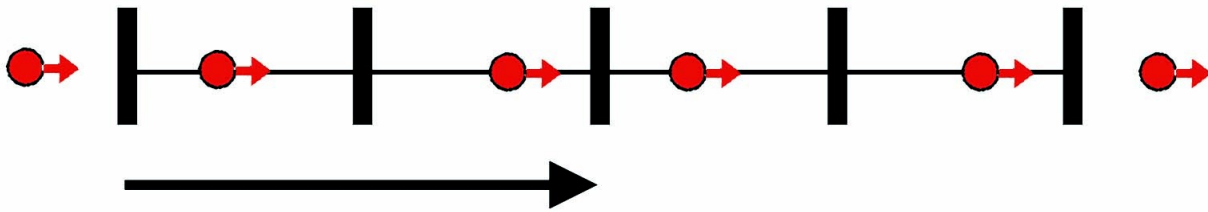
1 a 1 (1) x [u]

$\rho m$

$m$

No. 2.1.4

$\rho m$



**Origin** on mirror  $m$

**Asymmetric unit**  $0 \leq x \leq \frac{1}{2}$

**Symmetry operations**

(1) 1	(2) $m \ 0$
(1 0)	(m 0)

**Generators selected** (1);  $t(1)$ ; (2)

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site symmetry

2	c	1	(1) $x \ [u]$	(2) $\bar{x} \ [u]$
---	---	---	---------------	---------------------

1	b	$m$	$\frac{1}{2} \ [u]$
---	---	-----	---------------------

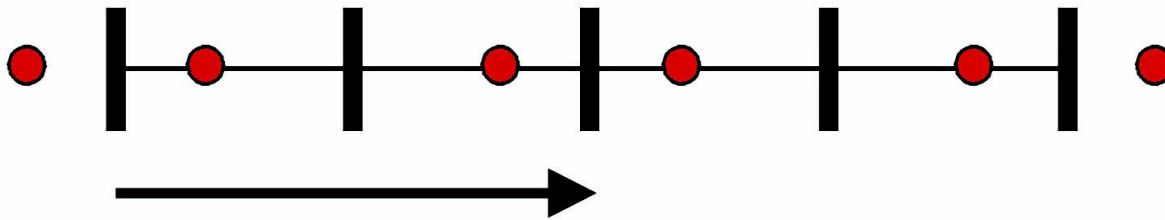
1	a	$m$	$0 \ [u]$
---	---	-----	-----------

$pm1'$

$m1'$

No. 2.2.5

$pm1'$



**Origin** on mirror  $m1'$

**Asymmetric unit**  $0 \leq x \leq \frac{1}{2}$

**Symmetry operations**

For  $1 +$  set

(1) $1$	(2) $m \ 0$
(1 0)	(m 0)

For  $1' +$  set

(1) $1'$	(2) $m' \ 0$
(1 0)'	(m 0)'

**Generators selected** (1);  $t(1)$ ; (2);  $1'$

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site symmetry

$1+$	$1'+$
------	-------

2	c	$11'$	(1) $x \ [0]$	(2) $\bar{x} \ [0]$
---	---	-------	---------------	---------------------

1	b	$m1'$	$1/2 \ [0]$
---	---	-------	-------------

1	a	$m1'$	$0 \ [0]$
---	---	-------	-----------

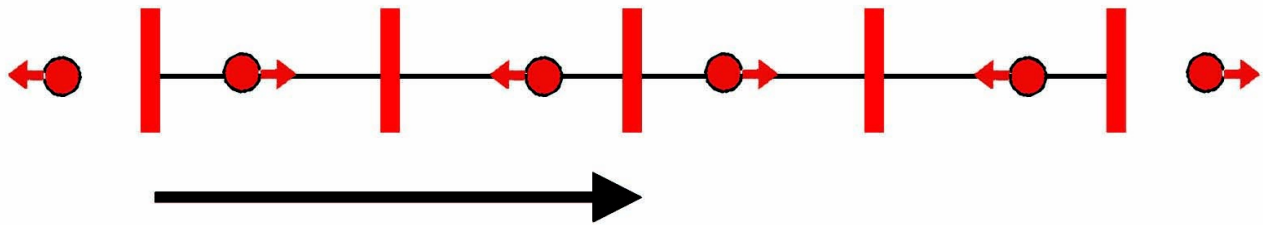


$\rho m'$

$m'$

No. 2.3.6

$\rho m'$



**Origin** on mirror  $m'$

**Asymmetric unit**  $0 \leq x \leq \frac{1}{2}$

**Symmetry operations**

(1) 1	(2) $m' \ 0$
(1 0)	( $m 0$ )'

**Generators selected** (1);  $t(1)$ ; (2)

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site symmetry

2	c	1	(1) $x [u]$	(2) $\bar{x} [\bar{u}]$
---	---	---	-------------	-------------------------

1	b	$m'$	$\frac{1}{2} [0]$
---	---	------	-------------------

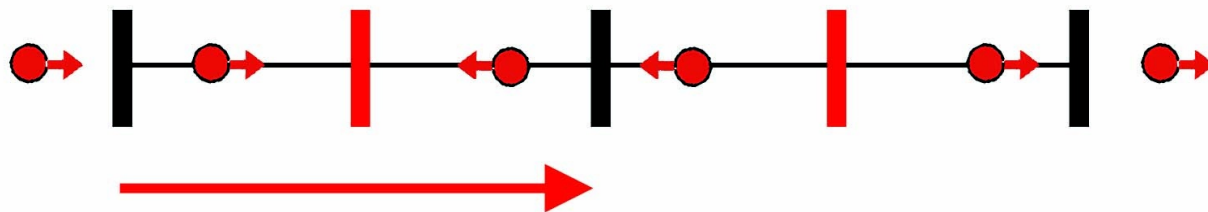
1	a	$m'$	$0 [0]$
---	---	------	---------

$p_{2a}m$

$m1'$

No. 2.4.7

$p_{2a}m$



**Origin** on mirror  $m$

**Asymmetric unit**  $0 \leq x \leq \frac{1}{2}$

### Symmetry operations

For (0) + set

(1) 1  
(1|0)

(2)  $m \ 0$   
( $m|0$ )

For (1)' + set

(1)  $t' \ (1)$   
( $1|1'$ )

(2)  $m' \ 1/2$   
( $m|1'$ )

**Generators selected** (1);  $t(1)'$ ; (2)

### Positions

#### Coordinates

Multiplicity,  
Wyckoff letter,  
Site symmetry

(0)+

(1)' +

2 c 1 (1)  $x [u]$

(2)  $\bar{x} [u]$

1 b  $m'$   $1/2 [0]$

1 a  $m$   $0 [u]$

## **Table 3 - 2D:**

# **Two-Dimensional Magnetic Space Group Tables**

TWO-DIMENSIONAL MAGNETIC SPACE GROUP INDEX

Table 3 - 3D: Three-Dimensional Magnetic Space Group Tables

Table 3 - 1D: One-Dimensional Magnetic Space Group Tables

## Index of Two-Dimensional Magnetic Space Groups

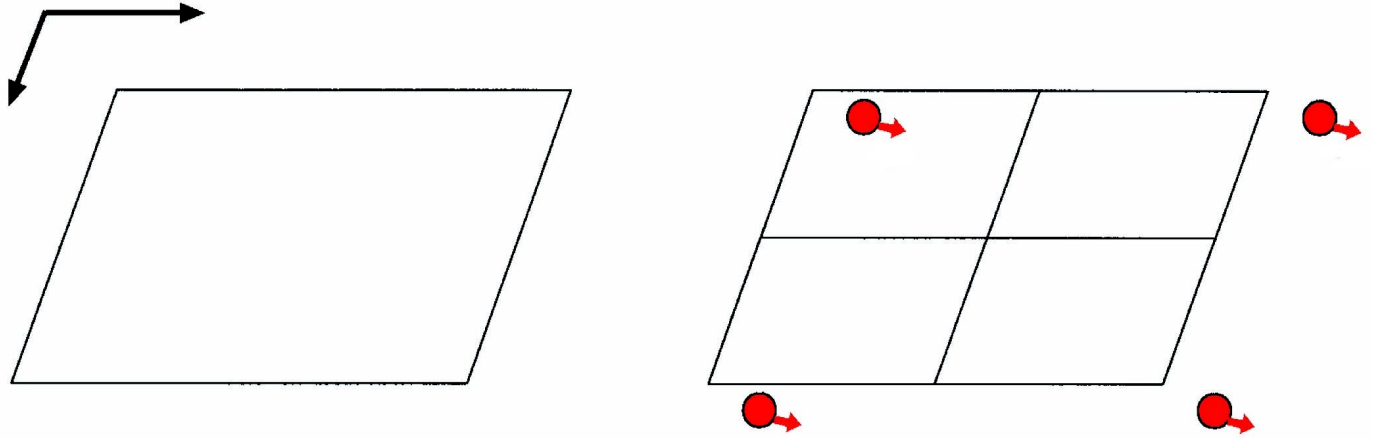
1.1.1	p1	8.1.38	p2gg	17.1.76	p6mm
1.2.2	p11'	8.2.39	p2gg1'	17.2.77	p6mm1'
1.3.3	p <sub>2a</sub> 1	8.3.40	p2g'g'	17.3.78	p6m'm'
		8.4.41	p2'gg'	17.4.79	p6'mm'
2.1.4	p211			17.5.80	p6'm'm
2.2.5	p2111'	9.1.42	c2mm		
2.3.6	p2'11	9.2.43	c2mm1'		
2.4.7	p <sub>2a</sub> 211	9.3.44	c2m'm'		
		9.4.45	c2'mm'		
3.1.8	p1m1	9.5.46	c <sub>p</sub> 2mm		
3.2.9	p1m11'	9.6.47	c <sub>p</sub> 2m'm'		
3.3.10	p1m'1	9.7.48	c <sub>p</sub> 2'mm'		
3.4.11	p <sub>2a</sub> 1m1				
3.5.12	p <sub>2b</sub> 1m1	10.1.49	p4		
3.6.13	p <sub>2b</sub> 1m'1	10.2.50	p41'		
3.7.14	p <sub>c</sub> 1m1	10.3.51	p4'		
		10.4.52	p <sub>p</sub> 4		
4.1.15	p1g1				
4.2.16	p1g11'	11.1.53	p4mm		
4.3.17	p1g'1	11.2.54	p4mm1'		
4.4.18	p <sub>2a</sub> 1g1	11.3.55	p4m'm'		
		11.4.56	p4'mm'		
5.1.19	c1m1	11.5.57	p4'm'm		
5.2.20	c1m11'	11.6.58	p <sub>p</sub> 4m'm'		
5.3.21	c1m'1	11.7.59	p <sub>p</sub> 4mm		
5.4.22	c <sub>p</sub> 1m1				
5.5.23	c <sub>p</sub> 1m'1	12.1.60	p4gm		
		12.2.61	p4gm1'		
6.1.24	p2mm	12.3.62	p4g'm'		
6.2.25	p2mm1'	12.4.63	p4'gm'		
6.3.26	p2m'm'	12.5.64	p4'g'm		
6.4.27	p2'mm'				
6.5.28	p <sub>2a</sub> 2m'm'	13.1.65	p3		
6.6.29	p <sub>c</sub> 2mm	13.2.66	p31'		
6.7.30	p <sub>2a</sub> 2mm				
		14.1.67	p3m1		
7.1.31	p2mg	14.2.68	p3m11'		
7.2.32	p2mg1'	14.3.69	p3m'1		
7.3.33	p2m'g'				
7.4.34	p2'm'g	15.1.70	p31m		
7.5.35	p2'mg'	15.2.71	p31m1'		
7.6.36	p <sub>2b</sub> 2m'g'	15.3.72	p31m'		
7.7.37	p <sub>2b</sub> 2mg				
		16.1.73	p6		
		16.2.74	p61'		
		16.3.75	p6'		

p1

1

No. 1.1.1

p1



**Origin** arbitrary

**Asymmetric unit**  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$

**Symmetry operations**

(1) 1  
(1|0,0)

**Generators selected** (1); t(1,0); t(0,1)

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site symmetry

1 a 1 (1) x,y [u,v]

**Symmetry of special projections**

Along [10] p1

$\mathbf{a}^* = \mathbf{b}_p$

Origin at x,0

Along [01] p1

$\mathbf{a}^* = \mathbf{a}_p$

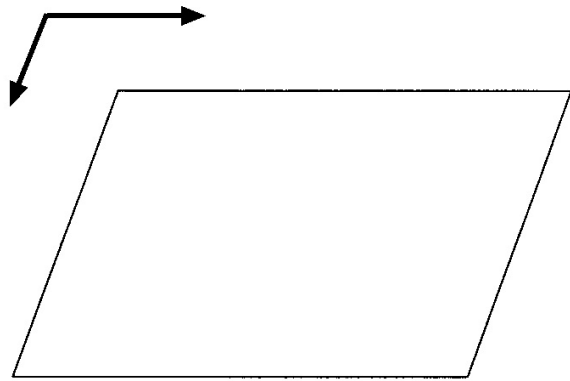
Origin at 0,y

p11'

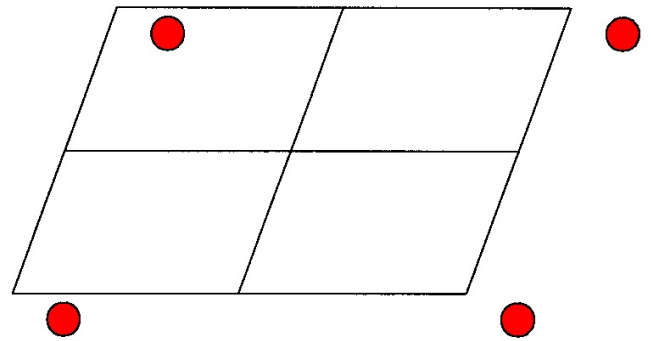
11'

No. 1.2.2

p11'



1'



**Origin** arbitrary 1'

**Asymmetric unit**  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$

**Symmetry operations**

For 1 + set  
(1) 1  
(1|0,0)

For 1' + set  
(1) 1'  
(1|0,0)'

**Generators selected** (1); t(1,0); t(0,1); 1'

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	1+	1' +
1 a 11'	(1) x,y	[0,0]

**Symmetry of special projections**

Along [10] p11'	Along [01] p11'
$\mathbf{a}^* = \mathbf{b}_p$	$\mathbf{a}^* = \mathbf{a}_p$
Origin at x,0	Origin at 0,y

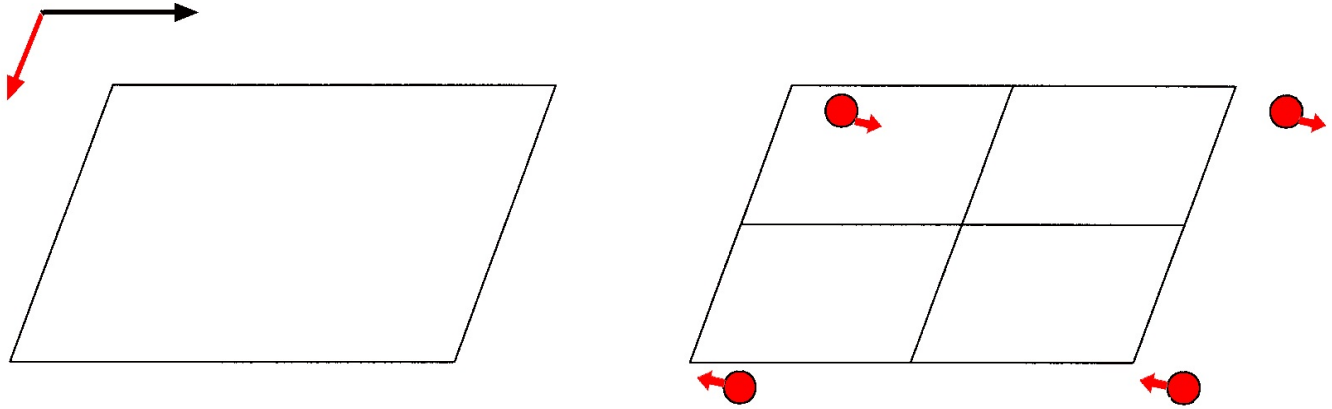


p<sub>2a</sub>1

11'

No. 1.3.3

p<sub>2a</sub>1



**Origin arbitrary**

**Asymmetric unit**  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$

**Symmetry operations**

For (0,0) + set  
(1) 1  
(1|0,0)

For (1,0)' + set  
(1) t' (1,0)  
(1|1,0)'

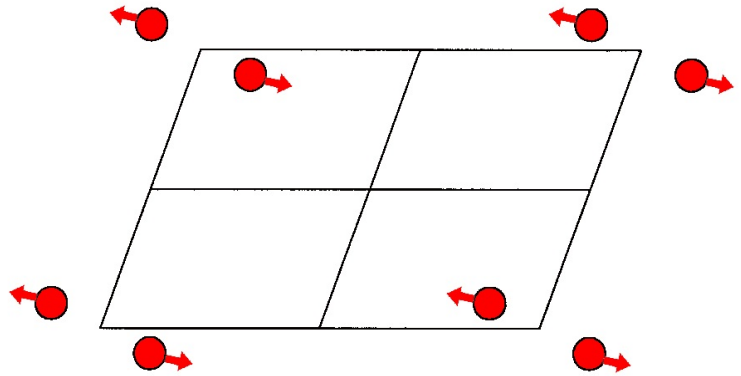
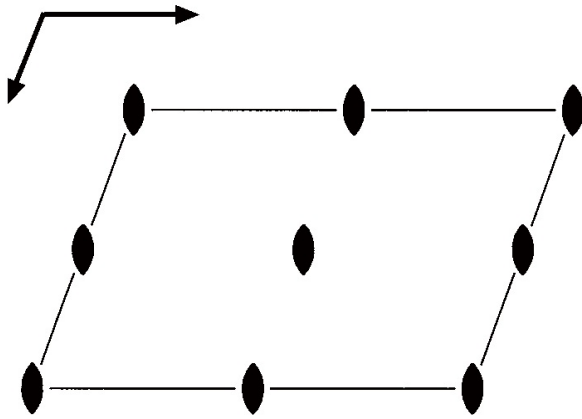
**Generators selected** (1);  $t(1,0)'$ ;  $t(0,1)$

**Positions**

	Coordinates
Multiplicity, Wyckoff letter, Site symmetry	$(0,0)+ (1,0)'$ +
1 a 1	(1) x,y [u,v]

**Symmetry of special projections**

Along [10] $p11'$	Along [01] $p_{2a}1$
$\mathbf{a}^* = \mathbf{b}_p$	$\mathbf{a}^* = \mathbf{a}_p$
Origin at x,0	Origin at 0,y



**Origin on 2**

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1$

**Symmetry operations**

- |         |                       |
|---------|-----------------------|
| (1) 1   | (2) 2 0,0             |
| (1 0,0) | (2 <sub>z</sub>  0,0) |

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ; (2)

**Positions**

Multiplicity,  
Wyckoff letter,  
Site symmetry

2 e 1 (1)  $x,y$   $[u,v]$  (2)  $\bar{x},\bar{y}$   $[\bar{u},\bar{v}]$

1 d 2  $1/2,1/2$   $[0,0]$

1 c 2  $1/2,0$   $[0,0]$

1 b 2  $0,1/2$   $[0,0]$

1 a 2  $0,0$   $[0,0]$

**Symmetry of special projections**

Along  $[10]$   $p1m'1$

$\mathbf{a}^* = \mathbf{b}_p$

Origin at  $x,0$

Along  $[01]$   $p1m'1$

$\mathbf{a}^* = \mathbf{a}_p$

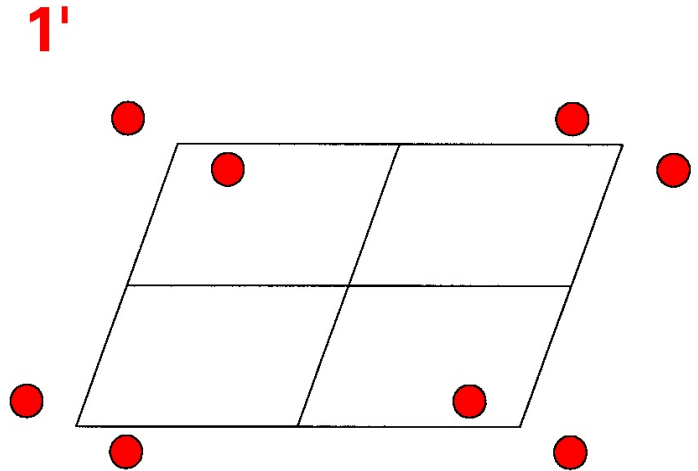
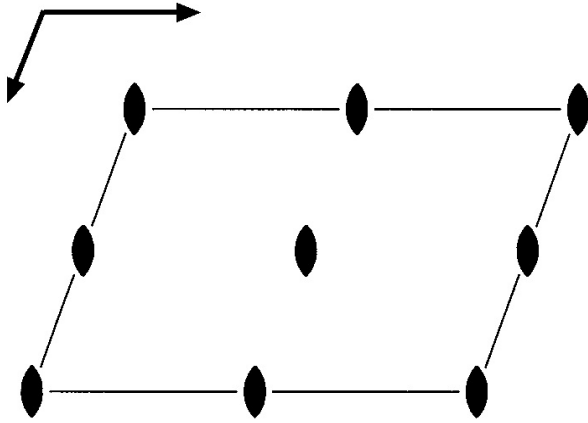
Origin at  $0,y$

p2111'

No. 2.2.5

21'

p1121'



Origin on 21'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$

Symmetry operations

For 1 + set

- |         |                       |
|---------|-----------------------|
| (1) 1   | (2) 2 0,0             |
| (1 0,0) | (2 <sub>z</sub>  0,0) |

For 1' + set

- |          |                        |
|----------|------------------------|
| (1) 1'   | (2) 2' 0,0             |
| (1 0,0)' | (2 <sub>z</sub>  0,0)' |

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ; (2);  $1'$

**Positions**

Multiplicity,  
Wyckoff letter,  
Site symmetry

		1+	1' +
2	e 11'	(1) x,y [0,0]	(2) $\bar{x},\bar{y}$ [0,0]
1	d 21'	1/2,1/2 [0,0]	
1	c 21'	1/2,0 [0,0]	
1	b 21'	0,1/2 [0,0]	
1	a 21'	0,0 [0,0]	

**Symmetry of special projections**

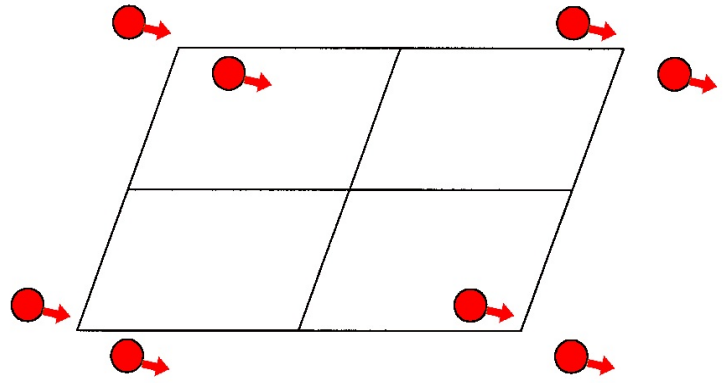
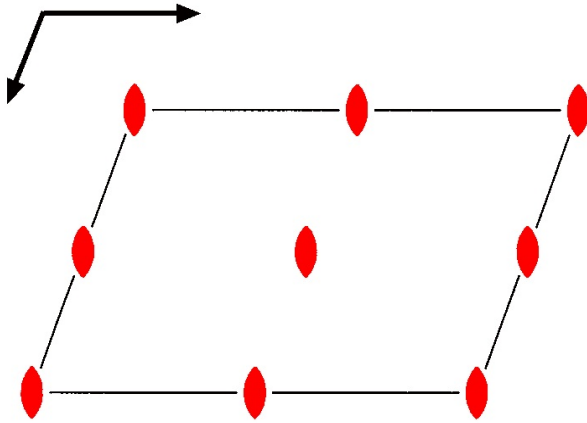
Along [10] $\rho m 1'$	Along [01] $\rho m 1'$
$\mathbf{a}^* = \mathbf{b}_p$	$\mathbf{a}^* = \mathbf{a}_p$
Origin at x,0	Origin at 0,y

p2'11

No. 2.3.6

2'

p2'11



Origin on 2'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$

Symmetry operations

(1) 1  
(1|0,0)

(2) 2' 0,0  
(2<sub>z</sub>|0,0)'

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ; (2)

**Positions**

Multiplicity,  
Wyckoff letter,  
Site symmetry

2 e 1 (1)  $x,y [u,v]$  (2)  $\bar{x},\bar{y} [u,v]$

1 d 2'  $1/2,1/2 [u,v]$

1 c 2'  $1/2,0 [u,v]$

1 b 2'  $0,1/2 [u,v]$

1 a 2'  $0,0 [u,v]$

**Symmetry of special projections**

Along  $[10] \rho m$

$\mathbf{a}^* = \mathbf{b}_p$

Origin at  $x,0$

Along  $[01] \rho m$

$\mathbf{a}^* = \mathbf{a}_p$

Origin at  $0,y$

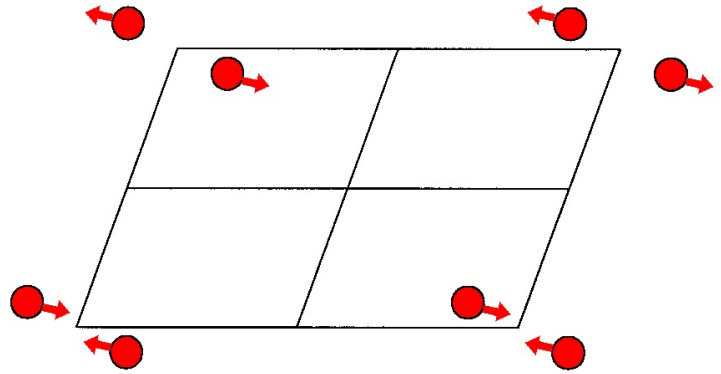
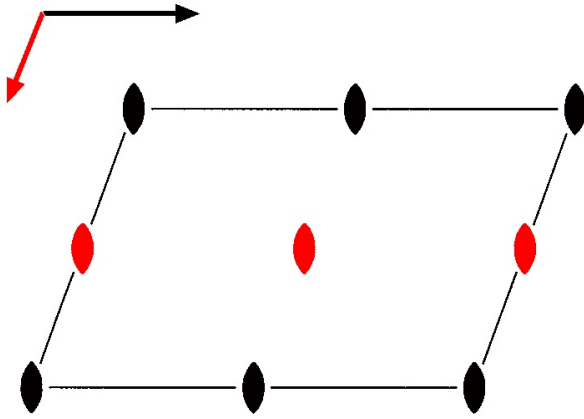


$p_{2a}211$

No. 2.4.7

$21'$

$p_{2a}211$



**Origin on 2**

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1$

**Symmetry operations**

For  $(0,0) +$  set

(1) 1	(2) 2 <sub>0,0</sub>
(1 0,0)	(2 <sub>z</sub>  0,0)

For  $(1,0)' +$  set

(1) t' (1,0)	(2) 2' 1/2,0
(1 1,0)'	(2 <sub>z</sub>  1,0)'

**Generators selected** (1);  $t(1,0)'$ ;  $t(0,1)$ ; (2)

**Positions**

Multiplicity,  
Wyckoff letter,  
Site symmetry

		(0,0) +	(1,0)' +
2	e 1	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [ $\bar{u},\bar{v}$ ]
1	d 2'	1/2,1/2 [u,v]	
1	c 2'	1/2,0 [u,v]	
1	b 2	0,1/2 [0,0]	
1	a 2	0,0 [0,0]	

**Symmetry of special projections**

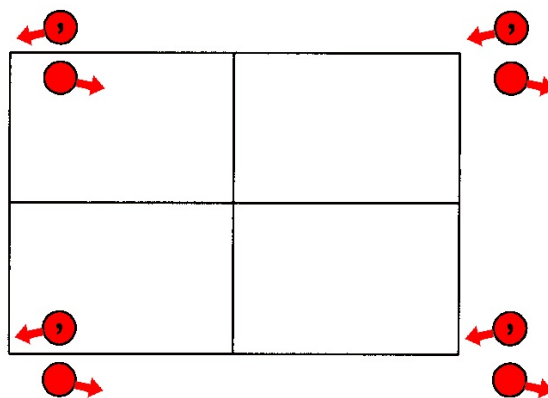
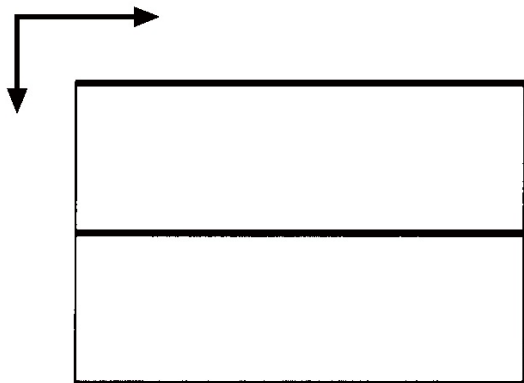
Along [10] $\rho m1'$	Along [01] $\rho_{2a}m'$
$\mathbf{a}^* = \mathbf{b}_p$	$\mathbf{a}^* = \mathbf{a}_p$
Origin at x,0	Origin at 0,y

p1m1

No. 3.1.8

m

p1m1



**Origin** on mirror line  $m$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1$

**Symmetry operations**

(1) 1  
(1|0,0)

(2)  $m \ 0,y$   
( $m_x|0,0$ )

**Generators selected** (1); t(1,0); t(0,1); (2)

**Positions**

			Coordinates	
Multiplicity,				
Wyckoff letter,				
Site symmetry				
2	c	1	(1) x,y [u,v]	(2) $\bar{x}$ ,y [u, $\bar{v}$ ]
1	b	m	1/2,y [u,0]	
1	a	m	0,y [u,0]	

**Symmetry of special projections**

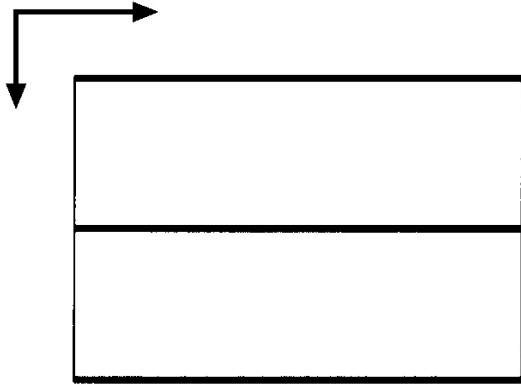
Along [10] $p11'$	Along [01] $pm$
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = \mathbf{a}$
Origin at x,0	Origin at 0,y

p1m11'

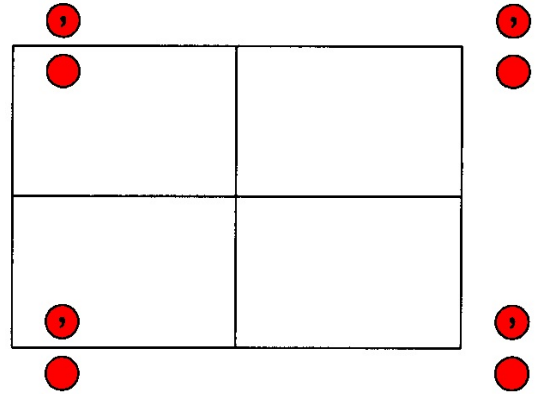
No. 3.2.9

m1'

p1m11'



1'



**Origin** on mirror line  $m1'$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1$

**Symmetry operations**

For 1 + set

- |         |               |
|---------|---------------|
| (1) 1   | (2) $m \ 0,y$ |
| (1 0,0) | ( $m_x 0,0$ ) |

For 1' + set

- |          |                |
|----------|----------------|
| (1) 1'   | (2) $m' \ 0,y$ |
| (1 0,0)' | ( $m_x 0,0$ )' |

**Generators selected** (1); t(1,0); t(0,1); (2); 1'

**Positions**

		Coordinates	
Multiplicity, Wyckoff letter, Site symmetry		1+	1' +
2 c 11'	(1) x,y [0,0]		(2) $\bar{x}$ ,y [0,0]
1 b m1'	1/2,y [0,0]		
1 a m1'	0,y [0,0]		

**Symmetry of special projections**

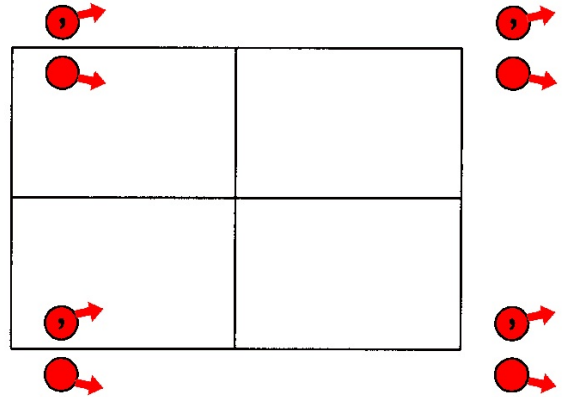
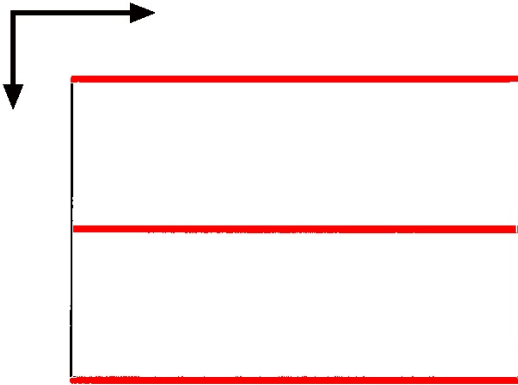
Along [10] p11'	Along [01] pm1'
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = \mathbf{a}$
Origin at x,0	Origin at 0,y

p1m'1

No. 3.3.10

m'

pm'11



**Origin** on mirror line  $m'$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1$

**Symmetry operations**

- |         |                 |
|---------|-----------------|
| (1) 1   | (2) $m' \ 0, y$ |
| (1 0,0) | ( $m_x$  0,0)'  |

**Generators selected** (1); t(1,0); t(0,1); (2)

**Positions**

		Coordinates	
Multiplicity, Wyckoff letter, Site symmetry			
2	c 1	(1) x,y [u,v]	(2) $\bar{x}$ ,y [ $\bar{u}$ ,v]
1	b m'	1/2,y [0,v]	
1	a m'	0,y [0,v]	

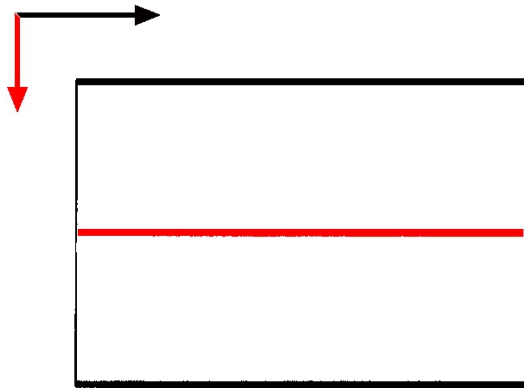
**Symmetry of special projections**

Along [10] p1	Along [01] pm'
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = \mathbf{a}$
Origin at x,0	Origin at 0,y



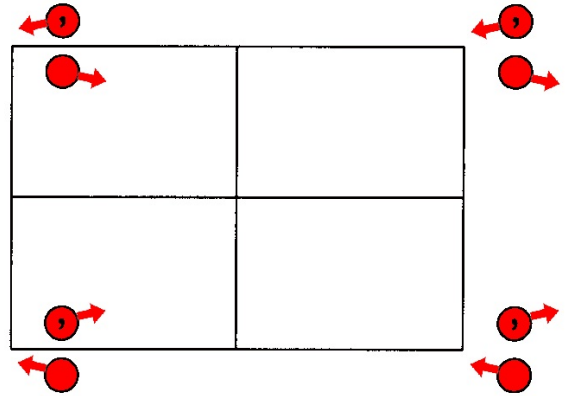
$p_{2a}1m1$

No. 3.4.11



$m1'$

$p_{2a}1m1$



**Origin** on mirror line  $m$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1$

**Symmetry operations**

For  $(0,0) +$  set

(1) 1	(2) $m \ 0,y$
$(1 0,0)$	$(m_x 0,0)$

For  $(1,0)' +$  set

(1) $t' \ (1,0)$	(2) $m' \ 1/2,y$
$(1 1,0)'$	$(m_x 1,0)'$

**Generators selected** (1);  $t(1,0)'$ ;  $t(0,1)$ ; (2)

**Positions**

		Coordinates	
Multiplicity, Wyckoff letter, Site symmetry		(0,0)+	(1,0)' +
2	c 1	(1) $x,y [u,v]$	(2) $\bar{x},y [u,\bar{v}]$
1	b $m'$	$1/2,y [0,v]$	
1	a $m$	$0,y [u,0]$	

**Symmetry of special projections**

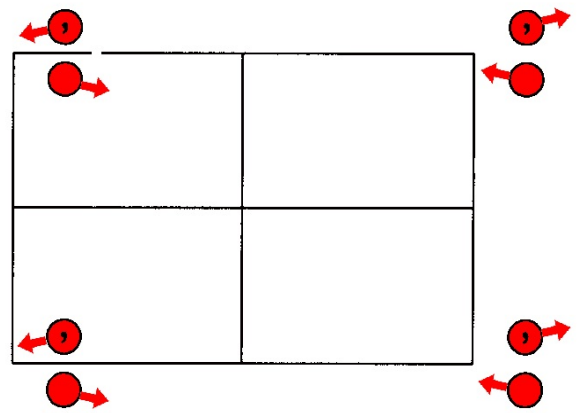
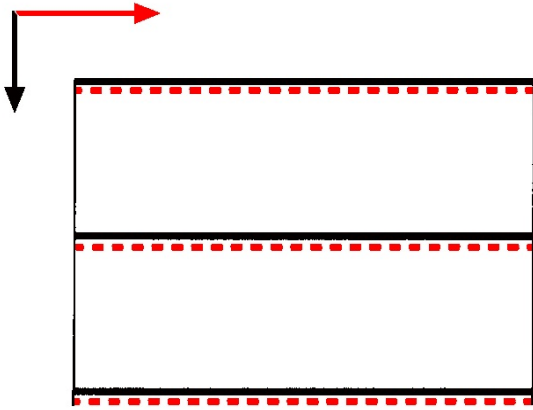
Along [10] $p11'$	Along [01] $p_{2a}m$
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = \mathbf{a}$
Origin at $x,0$	Origin at $0,y$

$p_{2b}1m1$

No. 3.5.12

$m1'$

$p_{2b}1m1$



**Origin** on mirror line  $m$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1$

**Symmetry operations**

For  $(0,0) +$  set

(1) 1	(2) $m \ 0,y$
$(1 0,0)$	$(m_x 0,0)$

For  $(0,1)' +$  set

(1) $t' \ (0,1)$	(2) $g' \ (0,1) \ 0,y$
$(1 0,1)'$	$(m_x 0,1)'$

**Generators selected** (1); t(1,0); t(0,1)' ; (2)

**Positions**

			Coordinates	
Multiplicity, Wyckoff letter, Site symmetry			(0,0)+	(0,1)' +
2	c	1	(1) x,y [u,v]	(2) $\bar{x},y$ [u, $\bar{v}$ ]
1	b	m	1/2,y [u,0]	
1	a	m	0,y [u,0]	

**Symmetry of special projections**

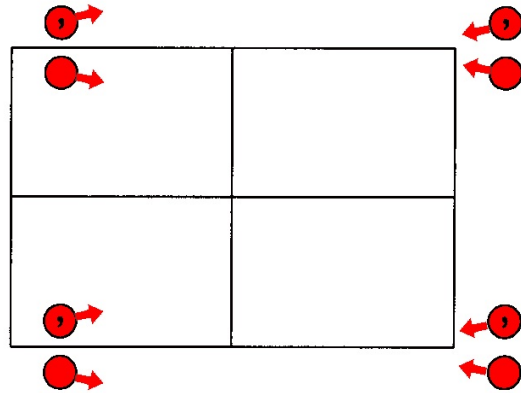
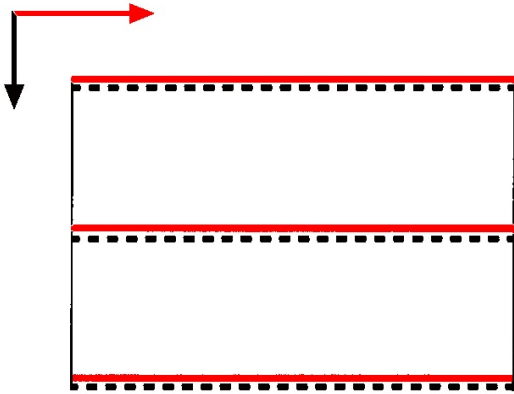
Along [10] p11'	Along [01] pm1'
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = \mathbf{a}$
Origin at x,0	Origin at 0,y

$p_{2b}1m'1$

No. 3.6.13

$m1'$

$p_{2b}1m'1$



**Origin** on mirror line  $m'$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1$

**Symmetry operations**

For  $(0,0) +$  set

(1) 1	(2) $m' \ 0,y$
$(1 0,0)$	$(m_x 0,0)'$

For  $(0,1) +$  set

(1) $t' \ (0,1)$	(2) $g \ (0,1) \ 0,y$
$(1 0,1)'$	$(m_x 0,1)$

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)'$ ; (2)

**Positions**

		Coordinates	
Multiplicity, Wyckoff letter, Site symmetry		(0,0)+	(0,1)' +
2	c 1	(1) $x,y [u,v]$	(2) $\bar{x},y [\bar{u},v]$
1	b $m'$	$1/2,y [0,v]$	
1	a $m'$	$0,y [0,v]$	

**Symmetry of special projections**

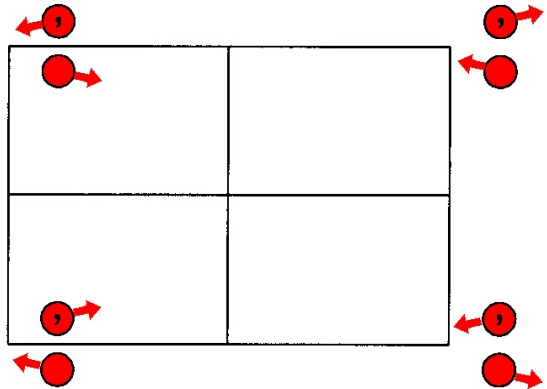
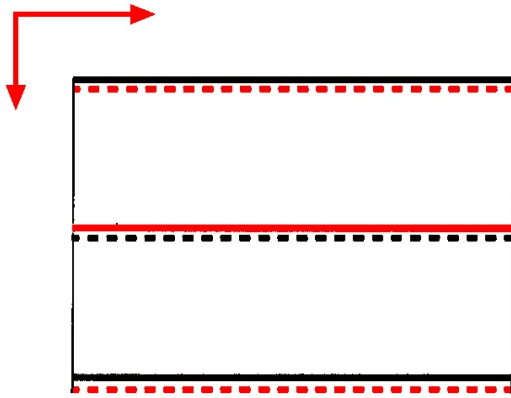
Along [10] $p_{2a}1$	Along [01] $pm1'$
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = \mathbf{a}$
Origin at $x,0$	Origin at $0,y$

$p_c1m1$

No. 3.7.14

$m1'$

$p_c m11$



**Origin** on mirror line  $m$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1$

**Symmetry operations**

For  $(0,0) +$  set

(1) 1	(2) $m \ 0,y$
$(1 0,0)$	$(m_x 0,0)$

For  $(0,1)'$  + set

(1) $t' \ (0,1)$	(2) $g' \ (0,1) \ 0,y$
$(1 0,1)'$	$(m_x 0,1)'$

**Generators selected** (1);  $t(1,0)'$ ;  $t(0,1)'$ ; (2)

**Positions**

		Coordinates	
Multiplicity, Wyckoff letter, Site symmetry		(0,0)+	(0,1)' +
2	c 1	(1) $x,y [u,v]$	(2) $\bar{x},y [u,\bar{v}]$
1	b $m'$	$1/2,y [0,v]$	
1	a $m$	$0,y [u,0]$	

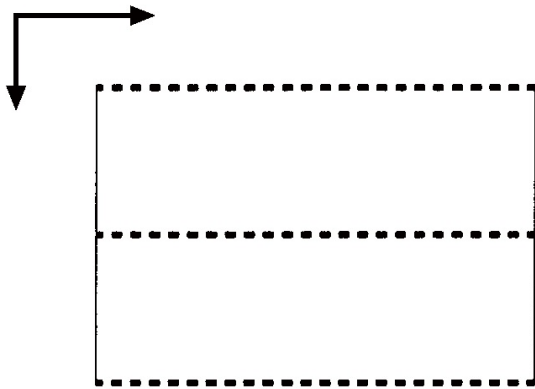
**Symmetry of special projections**

Along [10] $p11'$	Along [01] $pm1'$
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = \mathbf{a}$
Origin at $x,0$	Origin at $0,y$



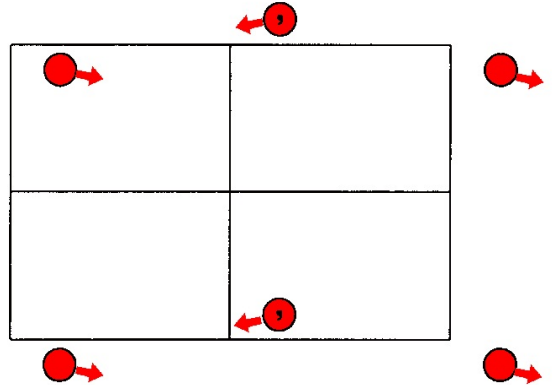
p1g1

No. 4.1.15



m

p1g1



**Origin** on glide line  $g$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1$

**Symmetry operations**

- (1) 1  
(1|0,0)
- (2)  $g$  (0,1/2) 0,y  
( $m_x$ |0,1/2)

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ; (2)

**Positions**

	Coordinates	
Multiplicity, Wyckoff letter, Site symmetry		
2 a 1	(1) $x,y [u,v]$	(2) $\bar{x},y+1/2 [u,\bar{v}]$

**Symmetry of special projections**

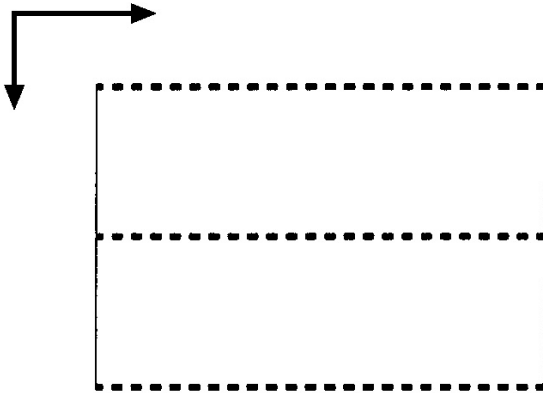
Along [10] $p_{2a^*}11$	Along [01] $pm$
$\mathbf{a}^* = \mathbf{b}/2$	$\mathbf{a}^* = \mathbf{a}$
Origin at $x,0$	Origin at $0,y$

p1g11'

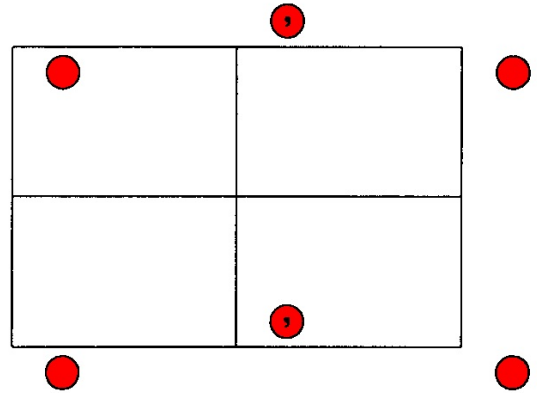
No. 4.2.16

m1'

p1g11'



1'



**Origin** on glide line  $g1'$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1$

**Symmetry operations**

For 1 + set

- |         |                         |
|---------|-------------------------|
| (1) 1   | (2) g (0,1/2) 0,y       |
| (1 0,0) | (m <sub>x</sub>  0,1/2) |

For 1' + set

- |          |                          |
|----------|--------------------------|
| (1) 1'   | (2) g' (0,1/2) 0,y       |
| (1 0,0)' | (m <sub>x</sub>  0,1/2)' |

**Generators selected** (1); t(1,0); t(0,1); (2); 1'

**Positions**

	Coordinates	
Multiplicity, Wyckoff letter, Site symmetry	1+	1' +
2 a 11'	(1) x,y [0,0]	(2) $\bar{x},y+1/2$ [0,0]

**Symmetry of special projections**

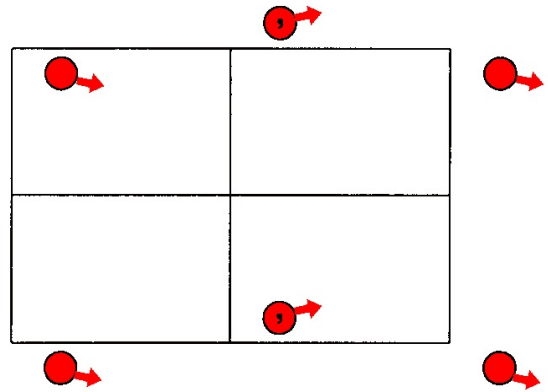
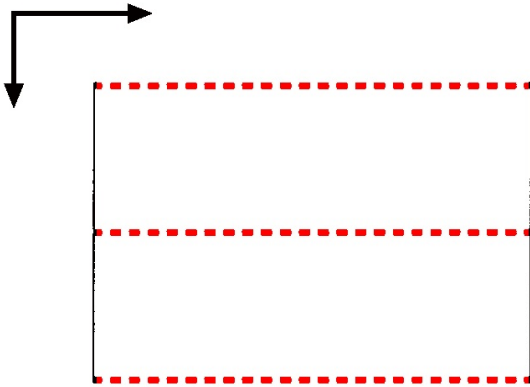
Along [10] p11'	Along [01] pm1'
$\mathbf{a}^* = \mathbf{b}/2$	$\mathbf{a}^* = \mathbf{a}$
Origin at x,0	Origin at 0,y

p1g'1

No. 4.3.17

m'

p1g'1



**Origin** on glide line  $g'$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1$

**Symmetry operations**

- (1) 1  
(1|0,0)
- (2)  $g'$  (0,1/2) 0,y  
( $m_x$ |0,1/2)'

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ; (2)

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site symmetry

2 a 1 (1)  $x,y$   $[u,v]$  (2)  $\bar{x},y+1/2$   $[\bar{u},v]$

**Symmetry of special projections**

Along  $[10]$   $p1$  Along  $[01]$   $pm'$

$\mathbf{a}^* = \mathbf{b}/2$

$\mathbf{a}^* = \mathbf{a}$

Origin at  $x,0$

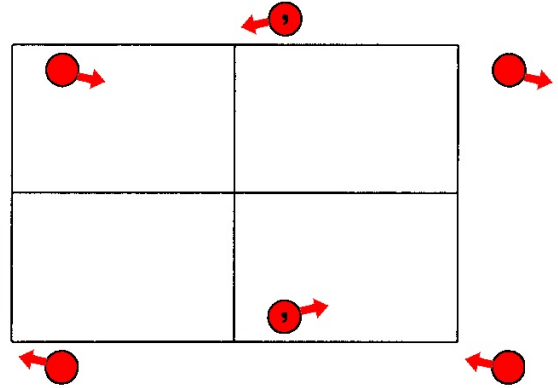
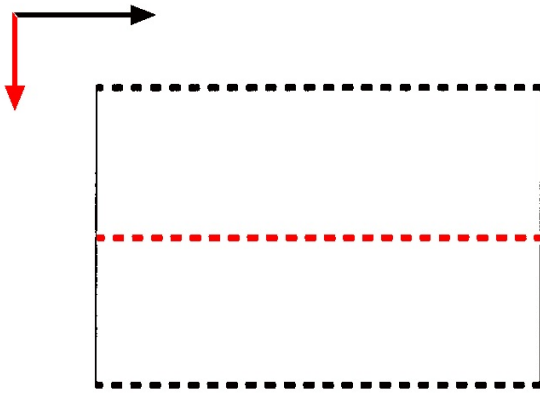
Origin at  $0,y$

$p_{2a}1g1$

No. 4.4.18

$m1'$

$p_{2a}1g1$



**Origin** on glide line  $g$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1$

**Symmetry operations**

For  $(0,0) +$  set

(1) 1	(2) $g (0,1/2) 0,y$
$(1 0,0)$	$(m_x 0,1/2)$

For  $(1,0)' +$  set

(1) $t' (1,0)$	(2) $g' (0,1/2) 1/2,y$
$(1 1,0)'$	$(m_x 1,1/2)'$

**Generators selected** (1);  $t(1,0)1'$ ;  $t(0,1)$ ; (2)

**Positions**

		Coordinates	
Multiplicity, Wyckoff letter, Site symmetry		(0,0)+	(1,0)' +
2	a 1	(1) $x,y [u,v]$	(2) $\bar{x},y+ 1/2 [u,\bar{v}]$

**Symmetry of special projections**

Along [10] $p11'$	Along [01] $p_{2a^*}m$
$\mathbf{a}^* = \mathbf{b}/2$	$\mathbf{a}^* = \mathbf{a}$
Origin at $x,0$	Origin at $0,y$

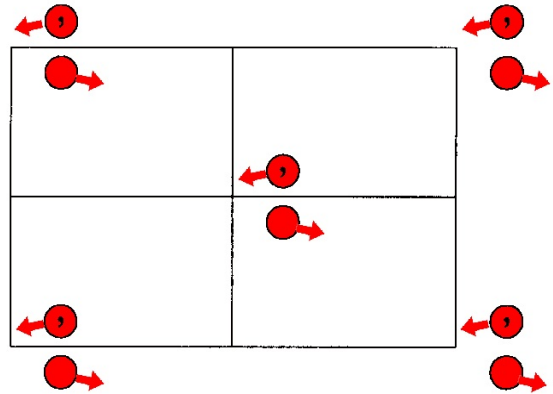
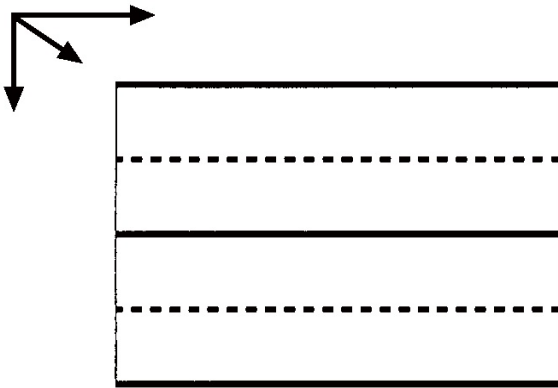


c1m11

No. 5.1.19

m

c1m1



**Origin** on mirror line  $m$

**Asymmetric unit**  $0 \leq x \leq 1/4; 0 \leq y \leq 1$

**Symmetry operations**

For  $(0,0)$  + set

(1) 1	(2) $m \ 0,y$
(1 0,0)	( $m_x$  0,0)

For  $(1/2,1/2)$  + set

(1) $t \ (1/2,1/2)$	(2) $g \ (0,1/2) \ 1/4,y$
(1 1/2,1/2)	( $m_x$  1/2,1/2)

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ;  $t(1/2,1/2)$ ; (2)

**Positions**

		Coordinates	
Multiplicity, Wyckoff letter, Site symmetry		(0,0) +	(1/2,1/2) +
4	b 1	(1) $x,y [u,v]$	(2) $\bar{x},y [u,\bar{v}]$
2	a m	0,y [u,0]	

**Symmetry of special projections**

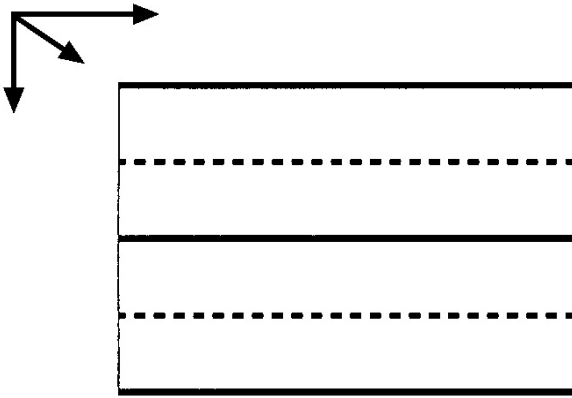
Along [10] $p11'$	Along [01] $pm$
$\mathbf{a}^* = \mathbf{b}/2$	$\mathbf{a}^* = \mathbf{a}/2$
Origin at $x,0$	Origin at $0,y$

c1m11'

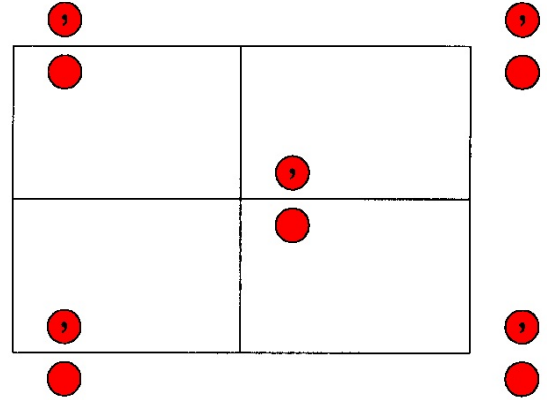
m1'

No. 5.2.20

c1m11'



1'



Origin on mirror line m1'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$

Symmetry operations

For (0,0) + set  
 (1) 1 (2) m 0,y  
 (1|0,0) (m\_x|0,0)

For (1/2,1/2) + set  
 (1) t (1/2,1/2) (2) g (0,1/2) 1/4,y  
 (1|1/2,1/2) (m\_x|1/2,1/2)

For (0,0)' + set  
 (1) 1' (2) m' 0,y  
 (1|0,0)' (m\_x|0,0)'

For (1/2,1/2)' + set  
 (1) t' (1/2,1/2) (2) g' (0,1/2) 1/4,y  
 (1|1/2,1/2)' (m\_x|1/2,1/2)'

**Generators selected** (1); t(1,0); t(0,1); t(1/2,1/2); (2); 1'

**Positions**

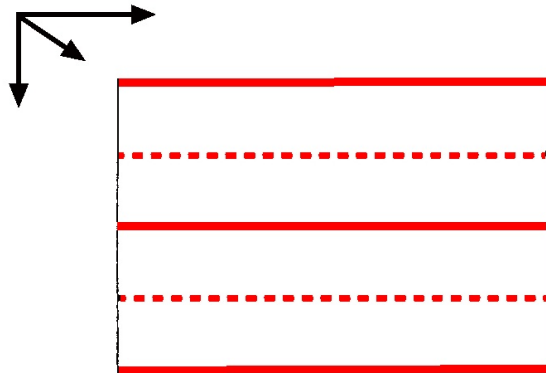
		Coordinates	
Multiplicity,			
Wyckoff letter,			
Site symmetry			
		(0,0) +	(1/2,1/2) +
		(0,0)' +	(1/2,1/2)' +
4	b 11'	(1) x,y [0,0]	(2) $\bar{x}$ ,y [0,0]
2	a m1'	0,y [0,0]	

**Symmetry of special projections**

Along [10] p11'	Along [01] pm1'
$\mathbf{a}^* = \mathbf{b}/2$	$\mathbf{a}^* = \mathbf{a}/2$
Origin at x,0	Origin at 0,y

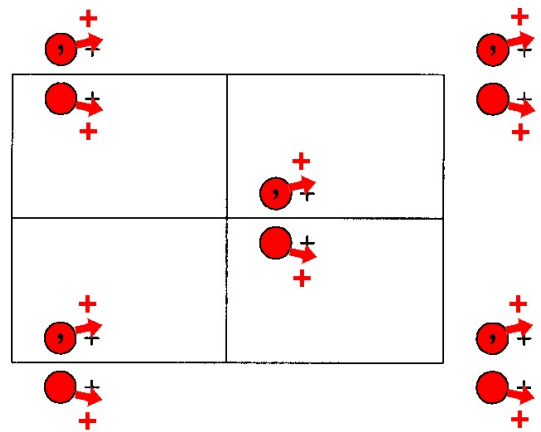
c1m'1

No. 5.3.21



m'

c1m'1



**Origin** on mirror line  $m'$

**Asymmetric unit**  $0 \leq x \leq 1/4; 0 \leq y \leq 1$

**Symmetry operations**

For  $(0,0) +$  set

(1) 1	(2) $m' \quad 0,y$
$(1 0,0)$	$(m_x 0,0)'$

For  $(1/2,1/2) +$  set

(1) $t \quad (1/2,1/2)$	(2) $g' \quad (0,1/2) \quad 1/4,y$
$(1 1/2,1/2)$	$(m_x 1/2,1/2)'$

**Generators selected** (1); t(1,0); t(0,1); t(1/2,1/2); (2)

**Positions**

		Coordinates	
Multiplicity, Wyckoff letter, Site symmetry		(0,0) +	(1/2,1/2) +
4	b 1	(1) x,y [u,v]	(2) $\bar{x}$ ,y [ $\bar{u}$ ,v]
2	a m'	0,y [0,v]	

**Symmetry of special projections**

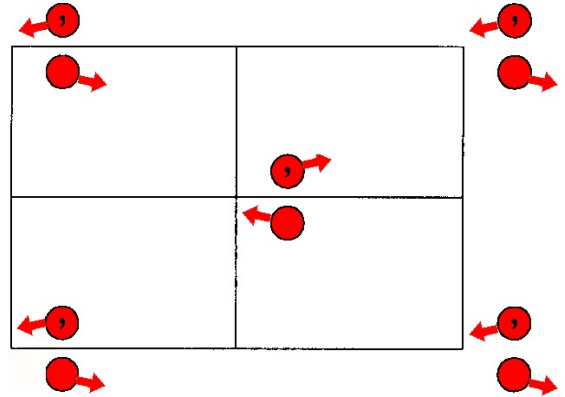
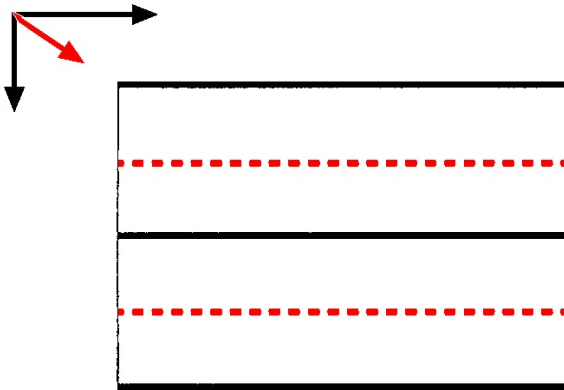
Along [10] p1	Along [01] pm'
$\mathbf{a}^* = \mathbf{b}/2$	$\mathbf{a}^* = \mathbf{a}/2$
Origin at x,0	Origin at 0,y

$c_p1m1$

No. 5.4.22

$m1'$

$c_p1m1$



**Origin** on mirror line  $m$

**Asymmetric unit**  $0 \leq x \leq 1/4; 0 \leq y \leq 1$

**Symmetry operations**

For  $(0,0) +$  set

(1) 1	(2) $m \ 0,y$
$(1 0,0)$	$(m_x 0,0)$

For  $(1/2,1/2)'$  + set

(1) $t' \ (1/2,1/2)$	(2) $g' \ (0,1/2) \ 1/4,y$
$(1 1/2,1/2)'$	$(m_x 1/2,1/2)'$

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ;  $t(1/2,1/2)'$ ; (2)

**Positions**

		Coordinates	
Multiplicity, Wyckoff letter, Site symmetry			
		(0,0) +	(1/2,1/2)' +
4	b 1	(1) $x,y [u,v]$	(2) $\bar{x},y [u,\bar{v}]$
2	a m	0,y [u,0]	

**Symmetry of special projections**

Along [10] $p11'$	Along [01] $p_{2a^*}m$
$\mathbf{a}^* = \mathbf{b}/2$	$\mathbf{a}^* = \mathbf{a}/2$
Origin at $x,0$	Origin at $0,y$

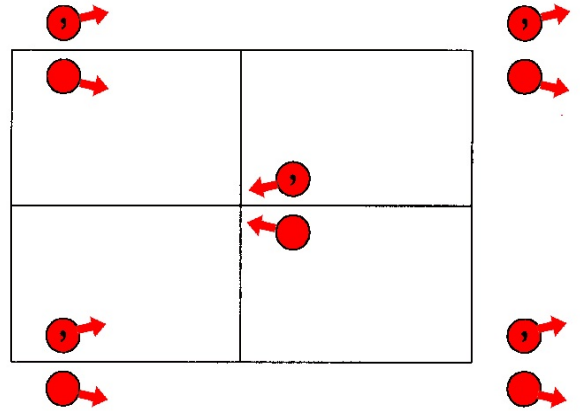
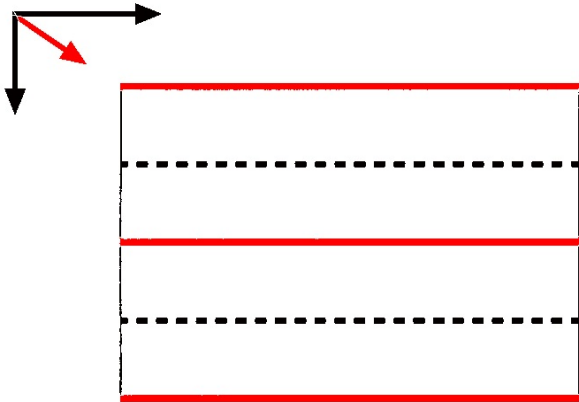


$c_p1m'1$

No. 5.5.23

$m1'$

$c_p1m'1$



**Origin** on mirror line  $m'$

**Asymmetric unit**  $0 \leq x \leq 1/4; 0 \leq y \leq 1$

**Symmetry operations**

For  $(0,0) +$  set

(1) 1	(2) $m' \ 0,y$
$(1 0,0)$	$(m_x 0,0)'$

For  $(1/2,1/2)'$  + set

(1) $t' \ (1/2,1/2)$	(2) $g \ (0,1/2) \ 1/4,y$
$(1 1/2,1/2)'$	$(m_x 1/2,1/2)$

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ;  $t(1/2,1/2)'$ ; (2)

**Positions**

		Coordinates	
Multiplicity, Wyckoff letter, Site symmetry			
		(0,0) +	(1/2,1/2)' +
4	b 1	(1) x,y [u,v]	(2) $\bar{x},y [\bar{u},v]$
2	a m'	0,y [0,v]	

**Symmetry of special projections**

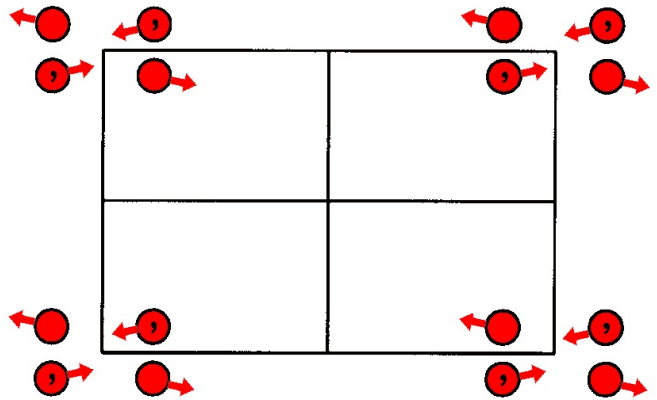
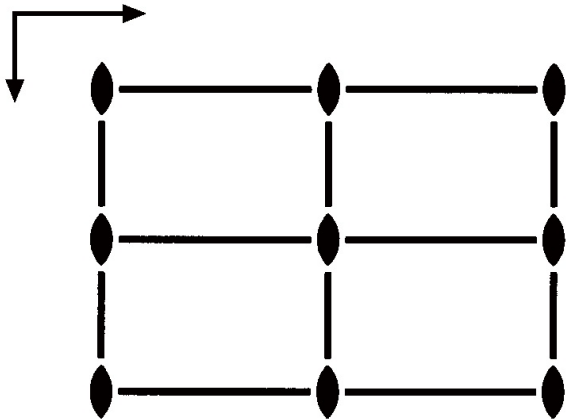
Along [10] $p_{2a^*}1$	Along [01] $p_{2a^*}m$
$\mathbf{a}^* = \mathbf{b}/2$	$\mathbf{a}^* = \mathbf{a}/2$
Origin at x,0	Origin at 1/4,y

p2mm

No. 6.1.24

2mm

p2mm



Origin on 2mm

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$

Symmetry operations

(1) 1  
(1|0,0)

(2) 2 0,0  
(2<sub>z</sub>|0,0)

(3) m x,0  
(m<sub>y</sub>|0,0)

(4) m 0,y  
(m<sub>x</sub>|0,0)

**Generators selected** (1); t(1,0); t(0,1); (2); (3)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(1) $x, y$ [u,v]	(2) $\bar{x}, \bar{y}$ [ $\bar{u}, \bar{v}$ ]
4 i 1	(3) $x, \bar{y}$ [ $\bar{u}, v$ ]	(4) $\bar{x}, y$ [ $u, \bar{v}$ ]
2 h .m.	$1/2, y$ [u,0]	$1/2, \bar{y}$ [ $\bar{u}, 0$ ]
2 g .m.	$0, y$ [u,0]	$0, \bar{y}$ [ $\bar{u}, 0$ ]
2 f ..m	$x, 1/2$ [0,v]	$\bar{x}, 1/2$ [0, $\bar{v}$ ]
2 e ..m	$x, 0$ [0,v]	$\bar{x}, 0$ [0, $\bar{v}$ ]
1 d 2mm	$1/2, 1/2$ [0,0]	
1 c 2mm	$1/2, 0$ [0,0]	
1 b 2mm	$0, 1/2$ [0,0]	
1 a 2mm	$0, 0$ [0,0]	

**Symmetry of special projections**

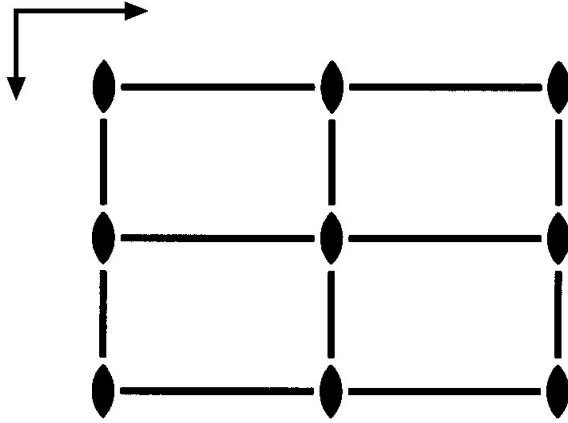
Along [10] $\rho m 1'$	Along [01] $\rho m 1'$
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = \mathbf{a}$
Origin at x,0	Origin at 0,y

p2mm1'

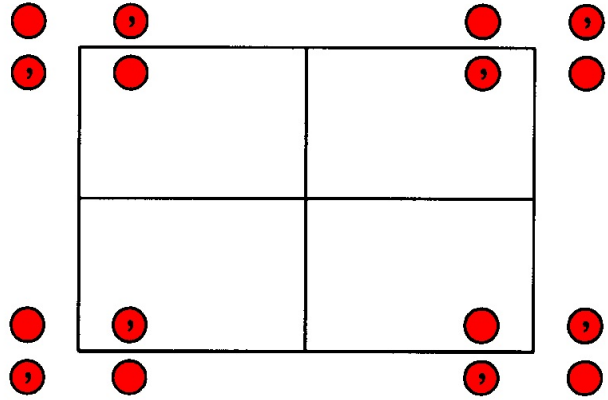
No. 6.2.25

2mm1'

p2mm1'



1'



Origin on 2mm1'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2$

Symmetry operations

For 1 + set			
(1) 1 (1 0,0)	(2) 2 0,0 (2 <sub>z</sub>  0,0)	(3) m x,0 (m <sub>y</sub>  0,0)	(4) m 0,y (m <sub>x</sub>  0,0)
For 1' + set			
(1) 1' (1 0,0)'	(2) 2' 0,0 (2 <sub>z</sub>  0,0)'	(3) m' x,0 (m <sub>y</sub>  0,0)'	(4) m' 0,y (m <sub>x</sub>  0,0)'

**Generators selected** (1); t(1,0); t(0,1); (2); (3); 1'

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	1+	1' +
4 i 11'	(1) x,y [0,0]	(2) $\bar{x},\bar{y}$ [0,0]
	(3) x, $\bar{y}$ [0,0]	(4) $\bar{x},y$ [0,0]
2 h .m.1'	1/2,y [0,0]	1/2, $\bar{y}$ [0,0]
2 g .m.1'	0,y [0,0]	0, $\bar{y}$ [0,0]
2 f ..m1'	x,1/2 [0,0]	$\bar{x},1/2$ [0,0]
2 e ..m1'	x,0 [0,0]	$\bar{x},0$ [0,0]
1 d 2mm1'	1/2,1/2 [0,0]	
1 c 2mm1'	1/2,0 [0,0]	
1 b 2mm1'	0,1/2 [0,0]	
1 a 2mm1'	0,0 [0,0]	

**Symmetry of special projections**

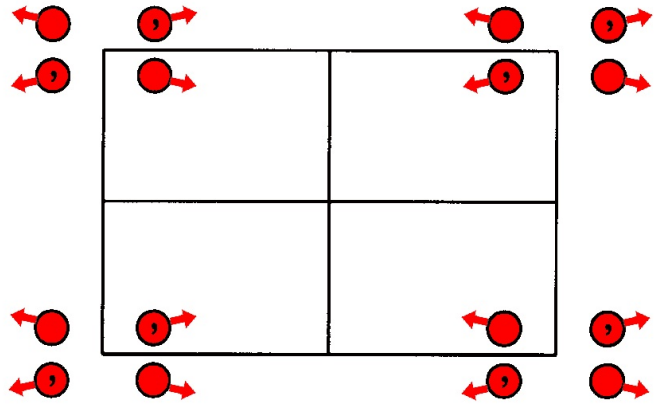
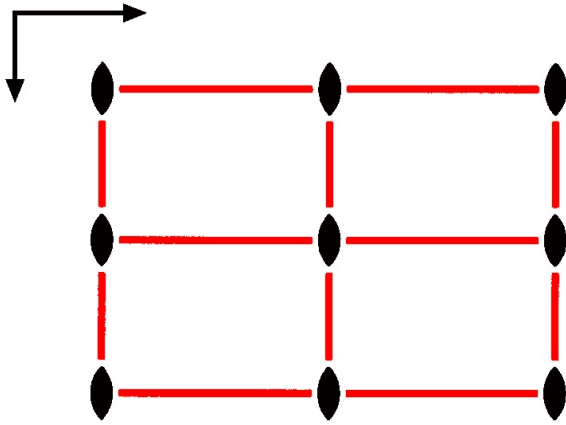
Along [10] $\rho m 1'$	Along [01] $\rho m 1'$
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = \mathbf{a}$
Origin at x,0	Origin at 0,y

p2m'm'

No. 6.3.26

2m'm'

p2m'm'



Origin on 2m'm'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$

Symmetry operations

(1) 1  
(1|0,0)

(2) 2 0,0  
(2<sub>z</sub>|0,0)

(3) m' x,0  
(m<sub>y</sub>|0,0)'

(4) m' 0,y  
(m<sub>x</sub>|0,0)'

**Generators selected** (1); t(1,0); t(0,1); (2); (3)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [ $\bar{u},\bar{v}$ ]
4 i 1	(3) $x,\bar{y}$ [u, $\bar{v}$ ]	(4) $\bar{x},y$ [ $\bar{u},v$ ]
2 h .m'	1/2,y [0,v]	1/2, $\bar{y}$ [0, $\bar{v}$ ]
2 g .m'	0,y [0,v]	0, $\bar{y}$ [0, $\bar{v}$ ]
2 f ..m'	x,1/2 [u,0]	$\bar{x},1/2$ [ $\bar{u},0$ ]
2 e ..m'	x,0 [u,0]	$\bar{x},0$ [ $\bar{u},0$ ]
1 d 2m'm'	1/2,1/2 [0,0]	
1 c 2m'm'	1/2,0 [0,0]	
1 b 2m'm'	0,1/2 [0,0]	
1 a m'm'2	0,0 [0,0]	

**Symmetry of special projections**

Along [10]  $\rho m'$   
 $\mathbf{a}^* = \mathbf{b}$   
 Origin at x,0

Along [01]  $\rho m'$   
 $\mathbf{a}^* = \mathbf{a}$   
 Origin at 0,y

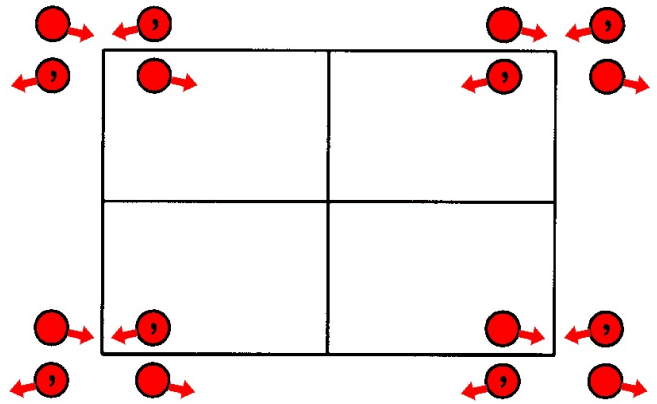
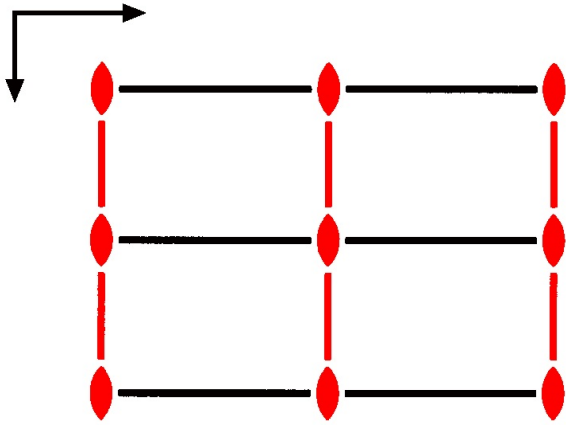


p2'mm'

No. 6.4.27

2'mm'

p2'mm'



Origin on 2'mm'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2$

Symmetry operations

(1) 1  
(1|0,0)

(2) 2' 0,0  
(2<sub>z</sub>|0,0)'

(3) m' x,0  
(m<sub>y</sub>|0,0)'

(4) m 0,y  
(m<sub>x</sub>|0,0)

**Generators selected** (1); t(1,0); t(0,1); (2); (3)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [u,v]
4 i 1	(3) x, $\bar{y}$ [u, $\bar{v}$ ]	(4) $\bar{x},y$ [u, $\bar{v}$ ]
2 h .m.	1/2,y [u,0]	1/2, $\bar{y}$ [u,0]
2 g .m.	0,y [u,0]	0, $\bar{y}$ [u,0]
2 f ..m'	x,1/2 [u,0]	$\bar{x},1/2$ [u,0]
2 e ..m'	x,0 [u,0]	$\bar{x},0$ [u,0]
1 d 2'mm'	1/2,1/2 [u,0]	
1 c 2'mm'	1/2,0 [u,0]	
1 b 2'mm'	0,1/2 [u,0]	
1 a 2'mm'	0,0 [u,0]	

**Symmetry of special projections**

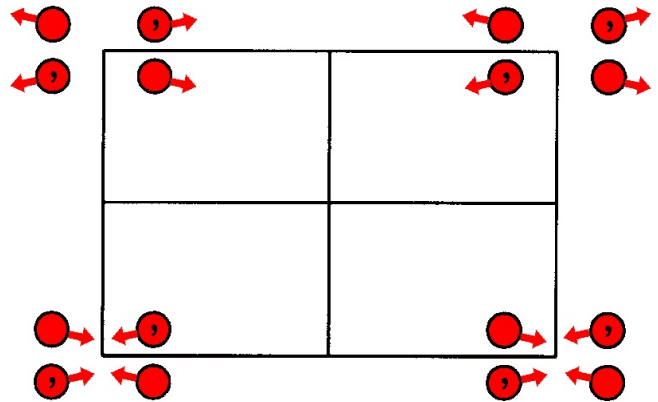
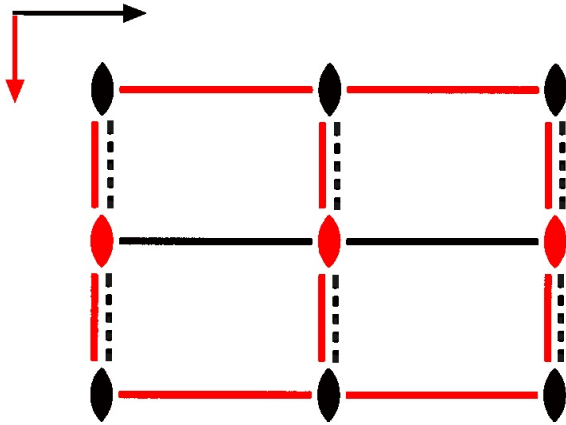
Along [10] $\rho m 1'$ $\mathbf{a}^* = \mathbf{b}$ Origin at x,0	Along [01] $\rho m$ $\mathbf{a}^* = \mathbf{a}$ Origin at 0,y
--	---

$p_{2a}2m'm'$

No. 6.5.28

$2mm1'$

$p_{2a}2m'm'$



Origin on  $2m'm'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2$

**Symmetry operations**

- For  $(0,0)$  + set
- |                  |                                    |                                      |                                      |
|------------------|------------------------------------|--------------------------------------|--------------------------------------|
| (1) 1<br>(1 0,0) | (2) 2 0,0<br>(2 <sub>z</sub>  0,0) | (3) m' x,0<br>(m <sub>y</sub>  0,0)' | (4) m' 0,y<br>(m <sub>x</sub>  0,0)' |
|------------------|------------------------------------|--------------------------------------|--------------------------------------|
- For  $(1,0)$ ' + set
- |                          |  |  |                                      |
|--------------------------|--|--|--------------------------------------|
| (1) t' (1,0)<br>(1 1,0)' | (2) 2' 1/2,0<br>(2 <sub>z</sub>  1,0)' | (3) g (1,0) x,0<br>(m <sub>y</sub>  1,0) | (4) m 1/2,y<br>(m <sub>x</sub>  1,0) |
|--------------------------|--|--|--------------------------------------|

**Generators selected** (1);  $t(1,0)'$ ;  $t(0,1)$ ; (2); (3)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(0,0)+	(1,0)'+
4 i 1	(1) $x,y [u,v]$ (3) $x,\bar{y} [u,\bar{v}]$	(2) $\bar{x},\bar{y} [\bar{u},\bar{v}]$ (4) $\bar{x},y [\bar{u},v]$
2 h .m.	$1/2,y [u,0]$	$1/2,\bar{y} [u,0]$
2 g .m'	$0,y [0,v]$	$0,\bar{y} [0,\bar{v}]$
2 f ..m'	$x,1/2 [u,0]$	$\bar{x},1/2 [\bar{u},0]$
2 e .'m'	$x,0 [u,0]$	$\bar{x},0 [\bar{u},0]$
1 d 2'mm'	$1/2,1/2 [u,0]$	
1 c 2'mm'	$1/2,0 [u,0]$	
1 b 2m'm'	$0,1/2 [0,0]$	
1 a 2m'm'	$0,0 [0,0]$	

**Symmetry of special projections**

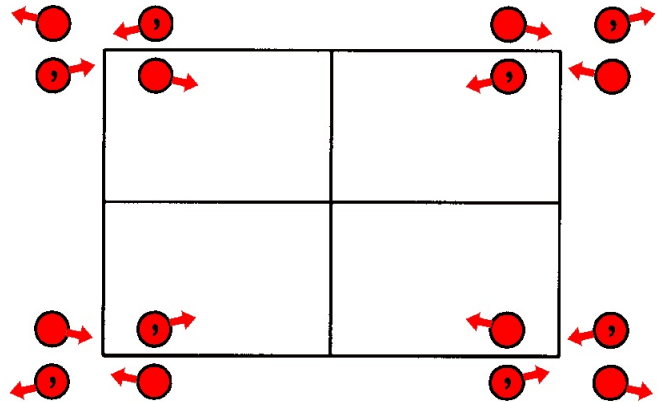
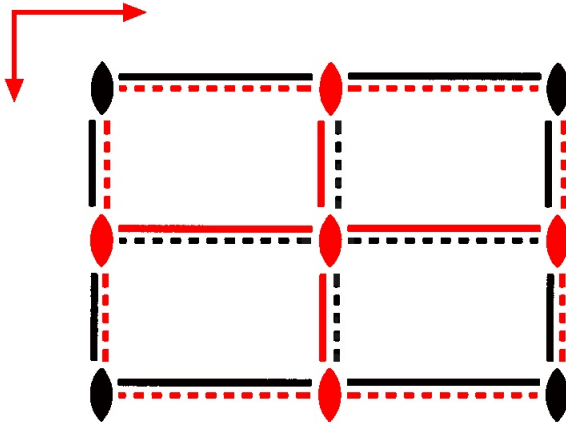
Along [10] $pm1'$ $\mathbf{a}^* = \mathbf{b}$ Origin at $x,0$	Along [01] $p_{2a}m$ $\mathbf{a}^* = \mathbf{a}$ Origin at $1/2,y$
---	--

$p_c 2mm$

No. 6.6.29

$2mm 1'$

$p_c 2mm$



**Origin** on  $2mm$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2$

**Symmetry operations**

For  $(0,0)$  + set

- |                  |                                      |                                      |                                      |
|------------------|--------------------------------------|--------------------------------------|--------------------------------------|
| (1) 1<br>(1 0,0) | (2) 2 $0,0$<br>(2 <sub>z</sub>  0,0) | (3) m $x,0$<br>(m <sub>y</sub>  0,0) | (4) m $0,y$<br>(m <sub>x</sub>  0,0) |
|------------------|--------------------------------------|--------------------------------------|--------------------------------------|

For  $(0,1)'$  + set

- |                            |  |  |  |
|----------------------------|--|--|--|
| (1) t' $(0,1)$<br>(1 0,1)' | (2) 2' $0,1/2$<br>(2 <sub>z</sub>  0,1)' | (3) m' $x,1/2$<br>(m <sub>y</sub>  0,1)' | (4) g' $(0,1) 0,y$<br>(m <sub>x</sub>  0,1)' |
|----------------------------|--|--|--|

**Generators selected** (1);  $t(1,0)'$ ;  $t(0,1)'$ ; (2); (3)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(0,0)+	(0,1)' +
4 i 1	(1) $x,y [u,v]$	(2) $\bar{x},\bar{y} [\bar{u},\bar{v}]$
	(3) $x,\bar{y} [\bar{u},v]$	(4) $\bar{x},y [u,\bar{v}]$
2 h .m'	$1/2,y [0,v]$	$1/2,\bar{y} [0,v]$
2 g .m	$0,y [u,0]$	$0,\bar{y} [\bar{u},0]$
2 f ..m'	$x,1/2 [u,0]$	$\bar{x},1/2 [u,0]$
2 e ..m	$x,0 [0,v]$	$\bar{x},0 [0,\bar{v}]$
1 d 2m'm'	$1/2,1/2 [0,0]$	
1 c 2'm'm	$1/2,0 [0,v]$	
1 b 2'mm'	$0,1/2 [u,0]$	
1 a 2mm	$0,0 [0,0]$	

**Symmetry of special projections**

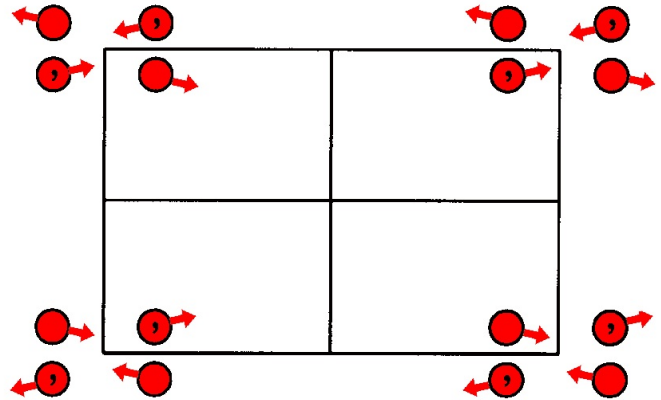
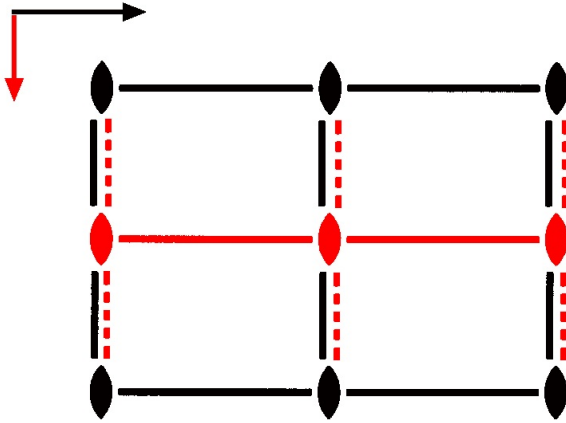
Along [10] $\rho m 1'$ $\mathbf{a}^* = \mathbf{b}$ Origin at $x,0$	Along [01] $\rho m 1'$ $\mathbf{a}^* = \mathbf{a}$ Origin at $0,y$
--	--

$p_{2a}2mm$

No. 6.7.30

$2mm1'$

$p_{2a}2mm$



Origin on  $2mm$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2$

Symmetry operations

For  $(0,0) +$  set

(1) 1

$(1|0,0)$

(2) 2  $0,0$

$(2_z|0,0)$

(3) m  $x,0$

$(m_y|0,0)$

(4) m  $0,y$

$(m_x|0,0)$

For  $(1,0)' +$  set

(1)  $t' (1,0)$

$(1|1,0)'$

(2)  $2' 1/2,0$

$(2_z|1,0)'$

(3)  $g' (1,0) x,0$

$(m_y|1,0)'$

(4)  $m' 1/2,y$

$(m_x|1,0)'$

**Generators selected** (1);  $t(1,0)'$ ;  $t(0,1)$ ; (2); (3)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(0,0)+	(1,0)' +
4 i 1	(1) $x,y [u,v]$	(2) $\bar{x},\bar{y} [\bar{u},\bar{v}]$
	(3) $x,\bar{y} [\bar{u},v]$	(4) $\bar{x},y [u,\bar{v}]$
2 h .m'	$1/2,y [0,v]$	$1/2,\bar{y} [0,v]$
2 g .m	$0,y [u,0]$	$0,\bar{y} [\bar{u},0]$
2 f ..m	$x,1/2 [0,v]$	$\bar{x},1/2 [0,\bar{v}]$
2 e ..m	$x,0 [0,v]$	$\bar{x},0 [0,\bar{v}]$
1 d 2'm'm	$1/2,1/2 [0,v]$	
1 c 2'm'm	$1/2,0 [0,v]$	
1 b 2mm	$0,1/2 [0,0]$	
1 a 2mm	$0,0 [0,0]$	

**Symmetry of special projections**

Along [10] $p1m11'$	Along [01] $p1m11'$
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = \mathbf{a}$
Origin at $x,0,0$	Origin at $0,y,0$

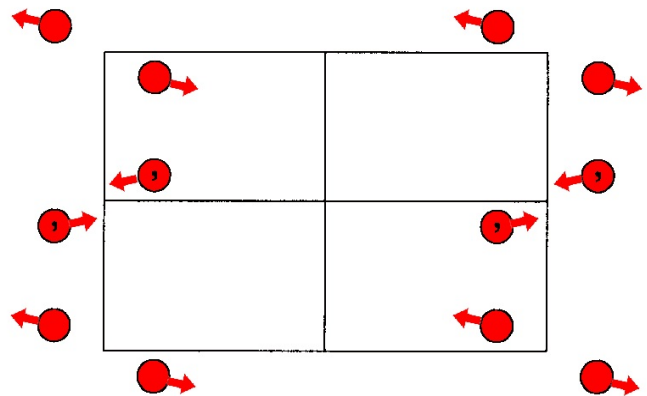
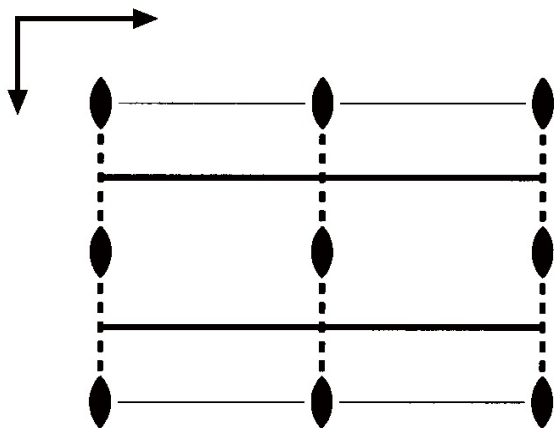


p2mg

2mm

No. 7.1.31

p2mg



Origin on 21g

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$

Symmetry operations

(1) 1  
(1|0,0)

(2) 2 0,0  
(2<sub>z</sub>|0,0)

(3) g (1/2,0) x,0  
(m<sub>y</sub>|1/2,0)

(4) m 1/4,y  
(m<sub>x</sub>|1/2,0)

**Generators selected** (1); t(1,0); t(0,1); (2); (3)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(1) $x, y$ $[u, v]$	(2) $\bar{x}, \bar{y}$ $[\bar{u}, \bar{v}]$
4 d 1	(3) $x+1/2, \bar{y}$ $[\bar{u}, v]$	(4) $\bar{x}+1/2, y$ $[u, \bar{v}]$
2 c .m.	1/4, $y$ $[u, 0]$	3/4, $\bar{y}$ $[\bar{u}, 0]$
2 b 2..	0, 1/2 $[0, 0]$	1/2, 1/2 $[0, 0]$
2 a 2..	0, 0 $[0, 0]$	1/2, 0 $[0, 0]$

**Symmetry of special projections**

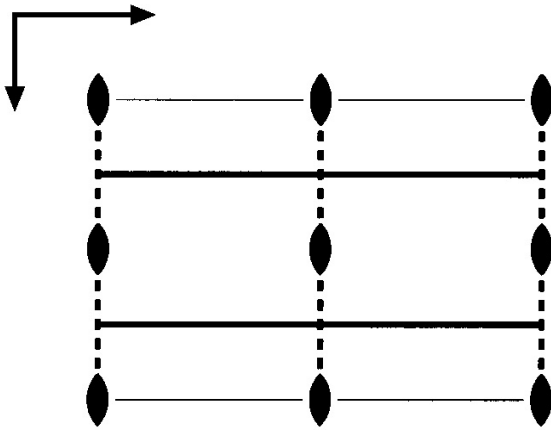
Along $[10]$ $pm1'$ $\mathbf{a}^* = \mathbf{b}$ Origin at $x, 0$	Along $[01]$ $p_{2a}m$ $\mathbf{a}^* = \mathbf{a}/2$ Origin at $1/4, y$
--	---

p2mg1'

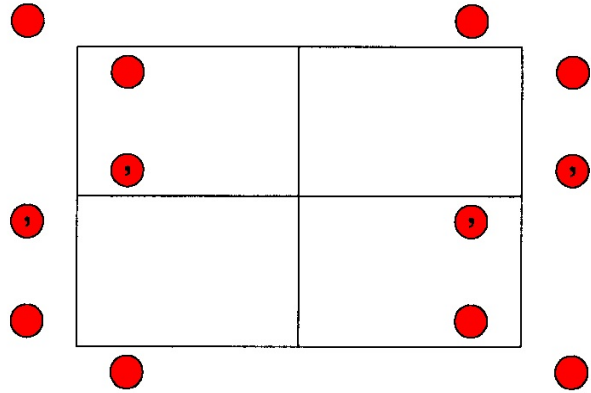
No. 7.2.32

2mm1'

p2ma1'



1'



Origin on 21g1'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$

Symmetry operations

For 1 + set

(1) 1

(1|0,0)

(2) 2 0,0

(2<sub>z</sub>|0,0)

(3) g (1/2,0) x,0

(m<sub>y</sub>|1/2,0)

(4) m 1/4,y

(m<sub>x</sub>|1/2,0)

For 1' + set

(1) 1'

(1|0,0)'

(2) 2' 0,0

(2<sub>z</sub>|0,0)'

(3) g' (1/2,0) x,0

(m<sub>y</sub>|1/2,0)'

(4) m' 1/4,y

(m<sub>x</sub>|1/2,0)'

**Generators selected** (1); t(1,0); t(0,1); (2); (3); 1'

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	1+	1' +
4 d 11'	(1) x,y [0,0]	(2) $\bar{x},\bar{y}$ [0,0]
	(3) $x+1/2,\bar{y}$ [0,0]	(4) $\bar{x}+1/2,y$ [0,0]
2 c .m.1'	1/4,y [0,0]	3/4, $\bar{y}$ [0,0]
2 b 2..1'	0,1/2 [0,0]	1/2,1/2 [0,0]
2 a 2..1'	0,0 [0,0]	1/2,0 [0,0]

**Symmetry of special projections**

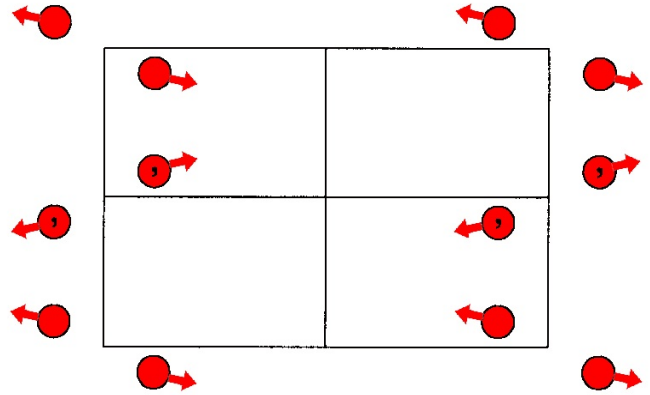
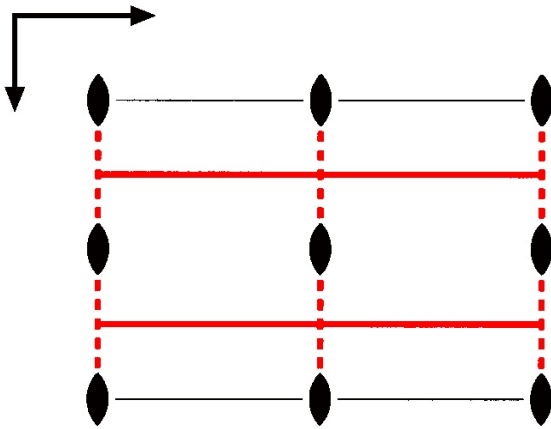
Along [10] $pm1'$	Along [01] $pm1'$
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = \mathbf{a}/2$
Origin at x,0	Origin at 0,y

p2m'g'

No. 7.3.33

2m'm'

p2m'g'



Origin on 21g'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$

Symmetry operations

(1) 1  
(1|0,0)

(2) 2 0,0  
(2<sub>z</sub>|0,0)

(3) g' (1/2,0) x,0  
(m<sub>y</sub>|1/2,0)'

(4) m' 1/4,y  
(m<sub>x</sub>|1/2,0)'

**Generators selected** (1); t(1,0); t(0,1); (2); (3)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [ $\bar{u},\bar{v}$ ]
4 d 1	(3) $x+1/2,\bar{y}$ [u, $\bar{v}$ ]	(4) $\bar{x}+1/2,y$ [ $\bar{u},v$ ]
2 c .m'	1/4,y [u,v]	3/4, $\bar{y}$ [0, $\bar{v}$ ]
2 b 2..	0,1/2 [0,0]	1/2,1/2 [0,0]
2 a 2..	0,0 [0,0]	1/2,0 [0,0]

**Symmetry of special projections**

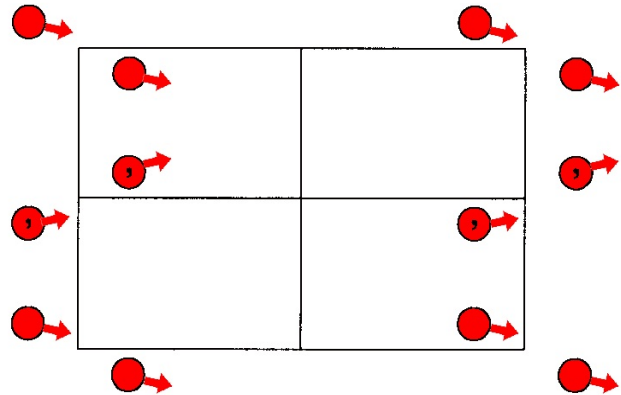
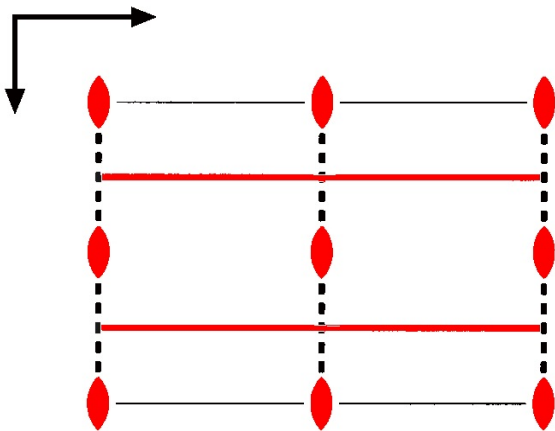
Along [10] $\rho m'$ $\mathbf{a}^* = \mathbf{b}$ Origin at x,0	Along [01] $\rho m'$ $\mathbf{a}^* = \mathbf{a}/2$ Origin at 0,y

p2'm'g

No. 7.4.34

2'm'm

p2'm'g



Origin on 2'1g

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$

Symmetry operations

(1) 1  
(1|0,0)

(2) 2' 0,0  
(2<sub>z</sub>|0,0)'

(3) g (1/2,0) x,0  
(m<sub>y</sub>|1/2,0)

(4) m' 1/4,y  
(m<sub>x</sub>|1/2,0)'

**Generators selected** (1); t(1,0); t(0,1); (2); (3)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [u,v]
4 d 1	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [u,v]
	(3) $x+1/2,\bar{y}$ [ $\bar{u}$ ,v]	(4) $\bar{x}+1/2,y$ [ $\bar{u}$ ,v]
2 c .m'	1/4,y [0,v]	3/4, $\bar{y}$ [0,v]
2 b 2'..	0,1/2 [u,v]	1/2,1/2 [ $\bar{u}$ ,v]
2 a 2'..	0,0 [u,v]	1/2,0 [ $\bar{u}$ ,v]

**Symmetry of special projections**

Along [10] $pm$ $\mathbf{a}^* = \mathbf{b}$ Origin at x,0	Along [01] $p_{2a}\cdot m$ $\mathbf{a}^* = \mathbf{a}/2$ Origin at 0,y
---	--

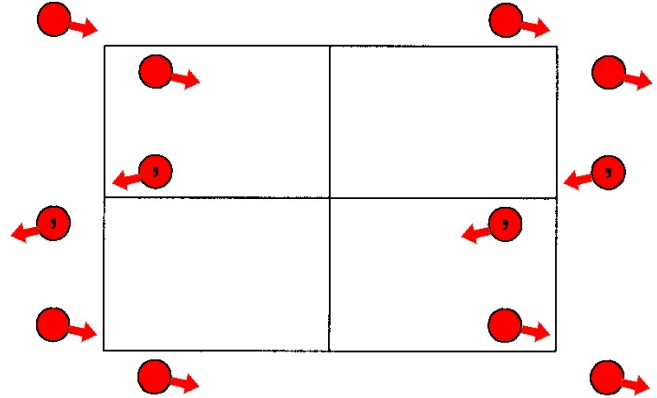
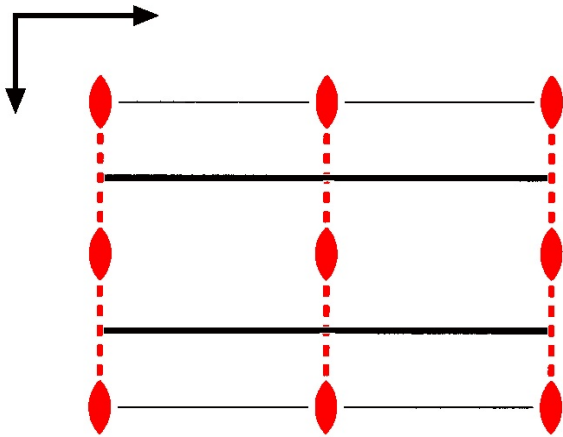


$p2'mg'$

No. 7.5.35

$2'mm'$

$p2'mg'$



Origin on  $2'1g'$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1$

Symmetry operations

(1) 1  
(1|0,0)

(2)  $2' \ 0,0$   
( $2_z$ |0,0)'

(3)  $g' \ (1/2,0) \ x,0$   
( $m_y$ | $1/2,0$ )'

(4)  $m \ 1/4,y$   
( $m_x$ | $1/2,0$ )

**Generators selected** (1); t(1,0); t(0,1); (2); (3)

**Positions**

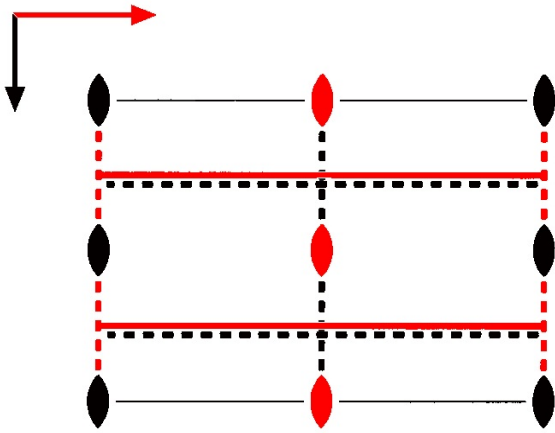
Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [u,v]
4 d 1	(3) $x+1/2,\bar{y}$ [u, $\bar{v}$ ]	(4) $\bar{x}+1/2,y$ [u, $\bar{v}$ ]
2 c .m.	1/4,y [u,0]	3/4, $\bar{y}$ [u,0]
2 b 2'..	0,1/2 [u,v]	1/2,1/2 [u, $\bar{v}$ ]
2 a 2'..	0,0 [u,v]	1/2,0 [u, $\bar{v}$ ]

**Symmetry of special projections**

Along [10] $pm1'$	Along [01] $pm$
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = \mathbf{a}/2$
Origin at x,0	Origin at 0,y

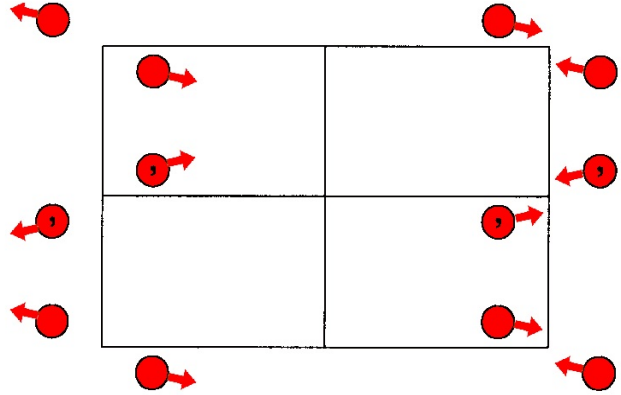
$p_{2b}2m'g'$

No. 7.6.36



$2mm1'$

$p_{2b}2m'g'$



Origin on  $21g'$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1$

Symmetry operations

For  $(0,0)$  + set

- |           |                   |
|-----------|-------------------|
| (1) 1     | (2) $2 \quad 0,0$ |
| $(1 0,0)$ | $(2_z 0,0)$       |

- |                                  |
|----------------------------------|
| (3) $g' \quad (1/2,0) \quad x,0$ |
| $(m_y 1/2,0)'$                   |

- |                      |
|----------------------|
| (4) $m' \quad 1/4,y$ |
| $(m_x 1/2,0)'$       |

For  $(0,1)'$  + set

- |                      |                      |
|----------------------|----------------------|
| (1) $t' \quad (0,1)$ | (2) $2' \quad 0,1/2$ |
| $(1 0,1)'$           | $(2_z 0,1)'$         |

- |                                   |
|-----------------------------------|
| (3) $g \quad (1/2,0) \quad x,1/2$ |
| $(m_y 1/2,1)$                     |

- |                                 |
|---------------------------------|
| (4) $g \quad (0,1) \quad 1/4,y$ |
| $(m_x 1/2,1)$                   |

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)'$ ; (2); (3)

**Positions**

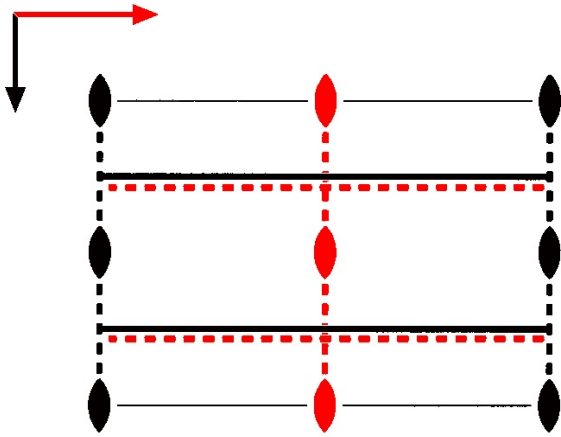
Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(0,0)+	(0,1)' +
4 d 1	(1) $x,y [u,v]$	(2) $\bar{x},\bar{y} [\bar{u},\bar{v}]$
	(3) $x+1/2,\bar{y} [u,\bar{v}]$	(4) $\bar{x}+1/2,y [\bar{u},v]$
2 c .m'	$1/4,y [0,v]$	$3/4,\bar{y} [0,\bar{v}]$
2 b 2'..	$0,1/2 [u,v]$	$1/2,1/2 [\bar{u},v]$
2 a 2..	$0,0 [0,0]$	$1/2,0 [0,0]$

**Symmetry of special projections**

Along [10] $p_{2a}m$	Along [01] $pm1'$
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = \mathbf{a}/2$
Origin at $x,1/2$	Origin at $0,y$

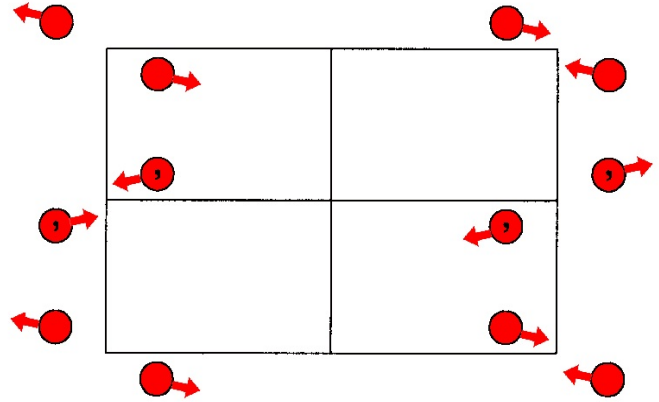
$p_{2b}2mg$

No. 7.7.37



$2mm1'$

$p_{2b}2mg$



Origin on  $21g$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1$

Symmetry operations

For  $(0,0)$  + set

- |         |                       |
|---------|-----------------------|
| (1) 1   | (2) 2 $0,0$           |
| (1 0,0) | (2 <sub>z</sub>  0,0) |

- |                         |                         |
|-------------------------|-------------------------|
| (3) g $(1/2,0)$ $x,0$   | (4) m $1/4,y$           |
| (m <sub>y</sub>  1/2,0) | (m <sub>x</sub>  1/2,0) |

- |                         |
|-------------------------|
| (4) m $1/4,y$           |
| (m <sub>x</sub>  1/2,0) |

For  $(0,1)'$  + set

- |                |                        |
|----------------|------------------------|
| (1) t' $(0,1)$ | (2) 2' $0,1/2$         |
| (1 0,1)'       | (2 <sub>z</sub>  0,1)' |

- |                          |                          |
|--------------------------|--------------------------|
| (3) g' $(1/2,0)$ $x,1/2$ | (4) g' $(0,1)$ $1/4,y$   |
| (m <sub>y</sub>  1/2,1)' | (m <sub>x</sub>  1/2,1)' |

- |                          |
|--------------------------|
| (4) g' $(0,1)$ $1/4,y$   |
| (m <sub>x</sub>  1/2,1)' |

**Generators selected** (1); t(1,0); t(0,1)'; (2); (3)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(0,0)+	(0,1)' +
4 d 1	(1) x,y [u,v] (3) x+1/2,ȳ [ū,v]	(2) x̄,ȳ [ū,v̄] (4) x̄+1/2,y [u,v̄]
2 c .m.	1/4,y [u,0]	3/4,ȳ [ū,0]
2 b 2'..	0,1/2 [u,v]	1/2,1/2 [u,v̄]
2 a 2..	0,0 [0,0]	1/2,0 [0,0]

**Symmetry of special projections**

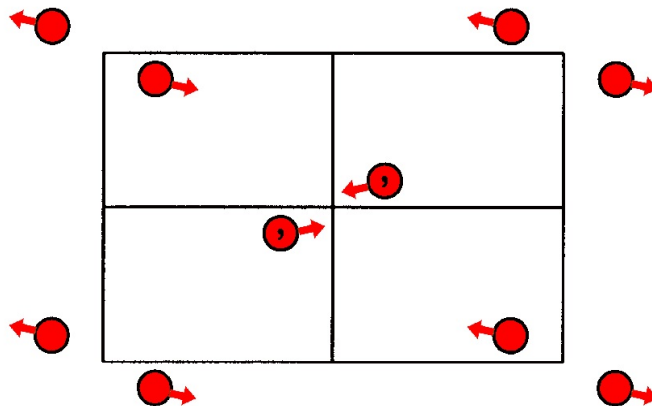
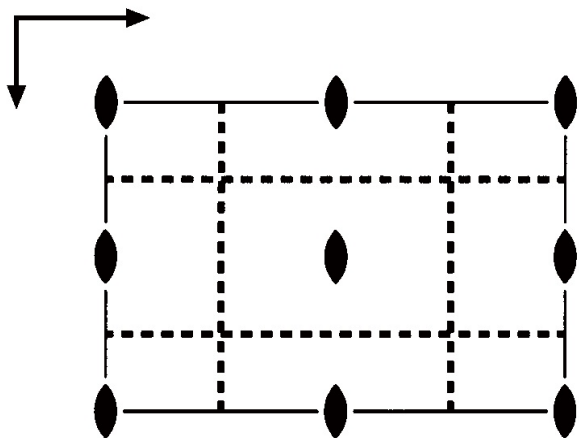
Along [10] p m 1'	Along [01] p m 1'
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = \mathbf{a}/2$
Origin at x,0	Origin at 0,y

p2gg

2mm

No. 8.1.38

p2gg



Origin on 211

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$

Symmetry operations

(1) 1  
(1|0,0)

(2) 2 0,0  
(2<sub>z</sub>|0,0)

(3) g (1/2,0) x,1/4  
(m<sub>y</sub>|1/2,1/2)

(4) g (0,1/2) 1/4,y  
(m<sub>x</sub>|1/2,1/2)

**Generators selected** (1); t(1,0); t(0,1); (2); (3)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(1) $x, y$ $[u, v]$	(2) $\bar{x}, \bar{y}$ $[\bar{u}, \bar{v}]$
4 c 1	(3) $x+1/2, \bar{y}+1/2$ $[\bar{u}, v]$	(4) $\bar{x}+1/2, y+1/2$ $[u, \bar{v}]$
2 b 2..	0, 1/2 [0,0]	1/2, 0 [0,0]
2 a 2..	0, 0 [0,0]	1/2, 1/2 [0,0]

**Symmetry of special projections**

Along [10] $p_{2a \cdot m}$ $\mathbf{a}^* = \mathbf{b}/2$ Origin at $x, 1/4$	Along [01] $p_{2a \cdot m}$ $\mathbf{a}^* = \mathbf{a}/2$ Origin at $1/4, y$
--	--

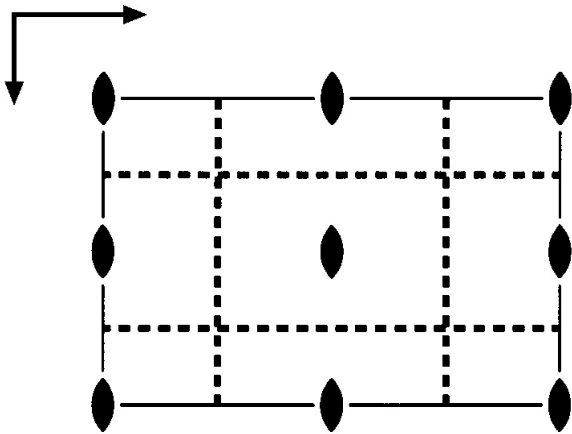


p2gg1'

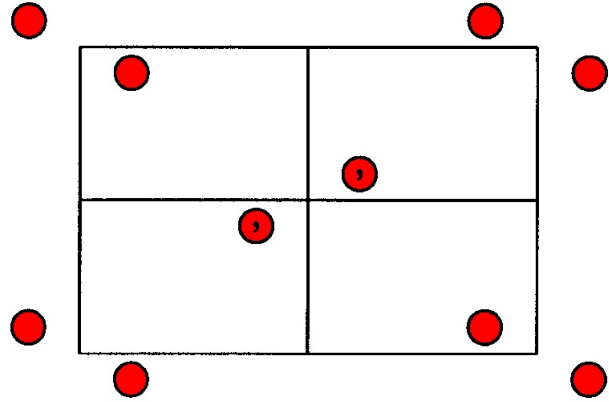
No. 8.2.39

2mm1'

p2gg1'



1'



Origin on 2111'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$

Symmetry operations

For 1 + set

(1) 1

(1|0,0)

(2) 2 0,0

(2<sub>z</sub>|0,0)

(3) g (1/2,0) x,1/4

(m<sub>y</sub>|1/2,1/2)

(4) g (0,1/2) 1/4,y

(m<sub>x</sub>|1/2,1/2)

For 1' + set

(1) 1'

(1|0,0)'

(2) 2' 0,0

(2<sub>z</sub>|0,0)'

(3) g' (1/2,0) x,1/4

(m<sub>y</sub>|1/2,1/2)'

(4) g' (0,1/2) 1/4,y

(m<sub>x</sub>|1/2,1/2)'

**Generators selected** (1); t(1,0); t(0,1); (2); (3); 1'

**Positions**

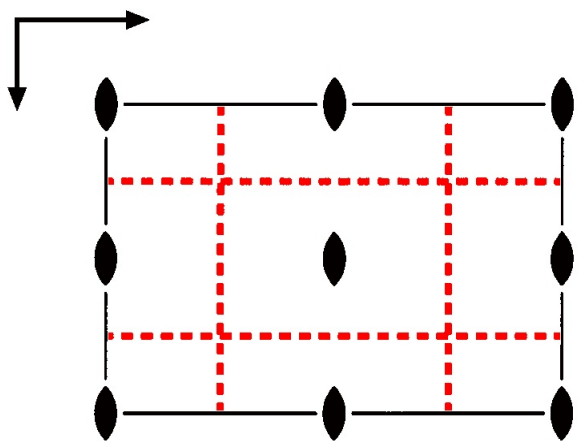
Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	1+	1' +
4 c 11'	(1) x,y [0,0]	(2) $\bar{x},\bar{y}$ [0,0]
	(3) $x+1/2,\bar{y}+1/2$ [0,0]	(4) $\bar{x}+1/2,y+1/2$ [0,0]
2 b 2..1'	0,1/2 [0,0]	1/2,0 [0,0]
2 a 2..1'	0,0 [0,0]	1/2,1/2 [0,0]

**Symmetry of special projections**

Along [10] $pm1'$	Along [01] $pm1'$
$\mathbf{a}^* = \mathbf{b}/2$	$\mathbf{a}^* = \mathbf{a}/2$
Origin at x,0	Origin at 0,y

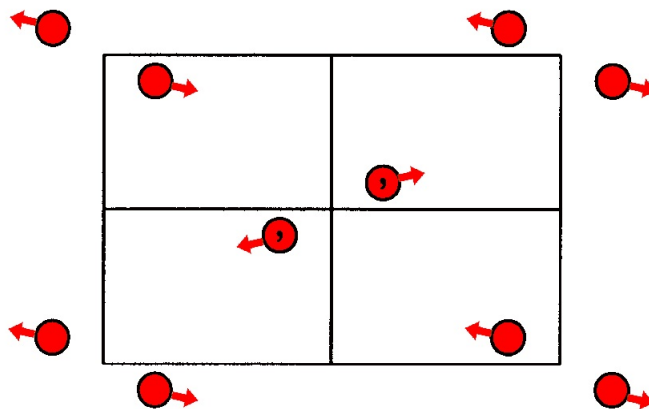
p2g'g'

No. 8.3.40



2m'm'

p2g'g'



Origin on 211

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$

Symmetry operations

(1) 1  
(1|0,0)

(2) 2 0,0  
(2<sub>z</sub>|0,0)

(3) g' (1/2,0) x,1/4  
(m<sub>y</sub>|1/2,1/2)'

(4) g' (0,1/2) 1/4,y  
(m<sub>x</sub>|1/2,1/2)'

**Generators selected** (1); t(1,0); t(0,1); (2); (3)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(1) $x, y$ [u, v]	(2) $\bar{x}, \bar{y}$ [ $\bar{u}, \bar{v}$ ]
4 c 1	(3) $x+1/2, \bar{y}+1/2$ [u, $\bar{v}$ ]	(4) $\bar{x}+1/2, y+1/2$ [ $\bar{u}, v$ ]
2 b 2..	0, 1/2 [0, 0]	1/2, 0 [0, 0]
2 a 2..	0, 0 [0, 0]	1/2, 1/2 [0, 0]

**Symmetry of special projections**

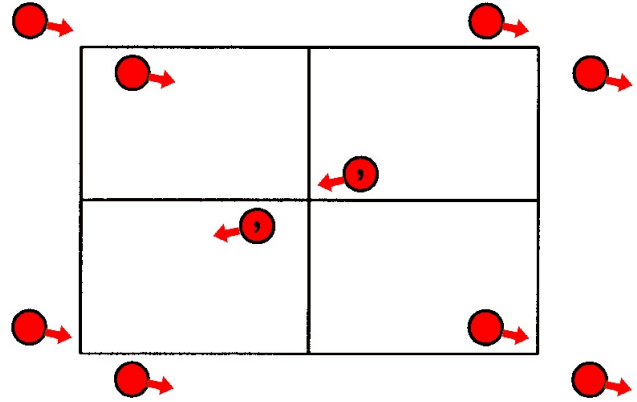
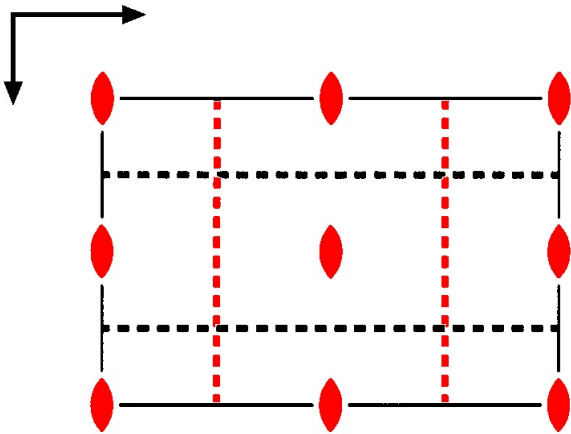
Along [10] $pm'$ $a^* = b/2$ Origin at x, 0	Along [01] $pm'$ $a^* = a/2$ Origin at 0, y

p2'gg'

2'mm'

No. 8.4.41

p2'gg'



Origin on 2'11

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$

Symmetry operations

(1) 1  
(1|0,0)

(2) 2' 0,0  
(2<sub>z</sub>|0,0)'

(3) g' (1/2,0) x,1/4  
(m<sub>y</sub>|1/2,1/2)'

(4) g (0,1/2) 1/4,y  
(m<sub>x</sub>|1/2,1/2)

**Generators selected** (1); t(1,0); t(0,1); (2); (3)

**Positions**

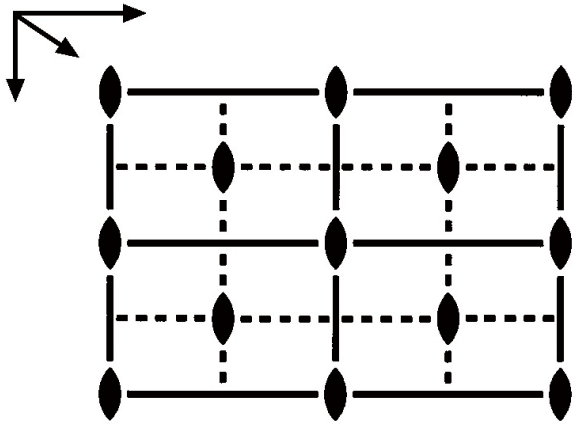
Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [u,v]
4 c 1	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [u,v]
	(3) $x+1/2,\bar{y}+1/2$ [u, $\bar{v}$ ]	(4) $\bar{x}+1/2,y+1/2$ [u, $\bar{v}$ ]
2 b 2'..	0,1/2 [u,v]	1/2,0 [u, $\bar{v}$ ]
2 a 2'..	0,0 [u,v]	1/2,1/2 [u, $\bar{v}$ ]

**Symmetry of special projections**

Along [10] $p_{2a'm}$	Along [01] $pm$
$\mathbf{a}^* = \mathbf{b}/2$	$\mathbf{a}^* = \mathbf{a}/2$
Origin at x,0	Origin at 0,y

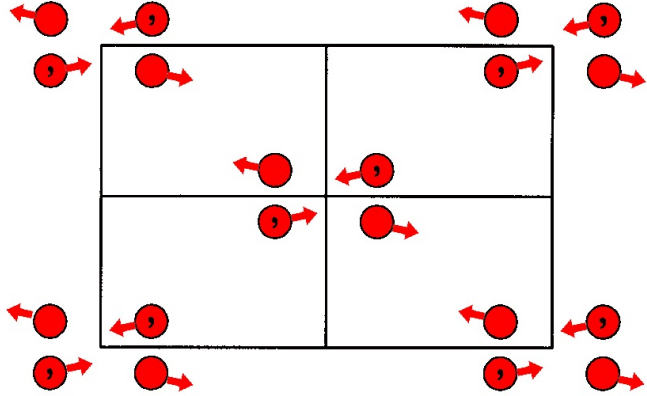
c2mm

No. 9.1.42



2mm

c2mm



Origin on 2mm

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$

Symmetry operations

For (0,0) + set

(1) 1

(1|0,0)

(2) 2 0,0

(2<sub>z</sub>|0,0)

(3) m x,0  
(m<sub>y</sub>|0,0)

(4) m 0,y  
(m<sub>x</sub>|0,0)

For (1/2,1/2) + set

(1) t (1/2,1/2)

(1|1/2,1/2)

(2) 2 1/4,1/4

(2<sub>z</sub>|1/2,1/2)

(3) g (1/2,0) x,1/4  
(m<sub>y</sub>|1/2,1/2)

(4) g (0,1/2) 1/4,y  
(m<sub>x</sub>|1/2,1/2)

**Generators selected** (1); t(1,0); t(0,1); t(1/2,1/2); (2); (3)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(0,0) +	(1/2,1/2) +
8 f 1	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [ $\bar{u},\bar{v}$ ]
	(3) $x,\bar{y}$ [ $\bar{u},v$ ]	(4) $\bar{x},y$ [u, $\bar{v}$ ]
4 e .m.	0,y [u,0]	0, $\bar{y}$ [ $\bar{u},0$ ]
4 d ..m	x,0 [0,v]	$\bar{x},0$ [0,v]
4 c 2..	1/4,1/4 [0,0]	1/4,3/4 [0,0]
2 b 2mm	0,1/2 [0,0]	
2 a 2mm	0,0 [0,0]	

**Symmetry of special projections**

Along [10] $pm1'$ $\mathbf{a}^* = \mathbf{b}/2$ Origin at x,0	Along [01] $pm1'$ $\mathbf{a}^* = \mathbf{a}/2$ Origin at 0,y
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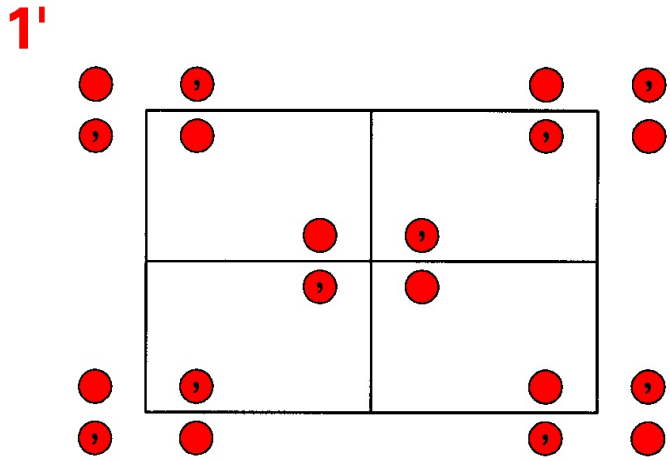
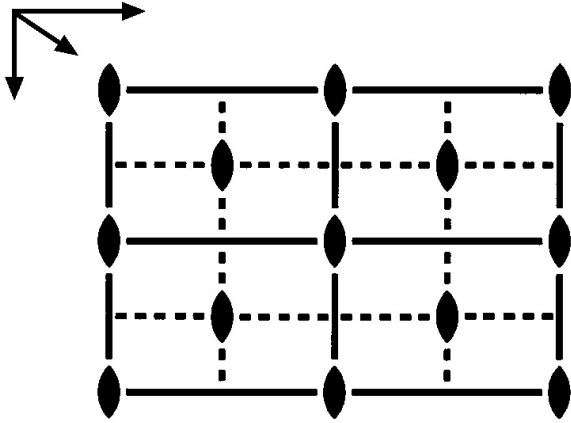


c2mm 1'

No. 9.2.43

2mm 1'

2cmm 1'



Origin on 2mm 1'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$

**Symmetry operations**

For (0,0) + set			
(1) 1	(2) 2	(3) m	(4) m
(1 0,0)	0,0 (2 <sub>z</sub>  0,0)	x,0 (m <sub>y</sub>  0,0)	0,y (m <sub>x</sub>  0,0)
For (1/2,1/2) + set			
(1) t	(2) 2	(3) g	(4) g
(1 1/2,1/2)	1/4,1/4 (2 <sub>z</sub>  1/2,1/2)	(1/2,0) x,1/4 (m <sub>y</sub>  1/2,1/2)	(0,1/2) 1/4,y (m <sub>x</sub>  1/2,1/2)
For (0,0)' + set			
(1) 1'	(2) 2'	(3) m'	(4) m'
(1 0,0)'	0,0 (2 <sub>z</sub>  0,0)'	x,0 (m <sub>y</sub>  0,0)'	0,y (m <sub>x</sub>  0,0)'
For (1/2,1/2)' + set			
(1) t'	(2) 2'	(3) g'	(4) g'
(1 1/2,1/2)'	1/4,1/4 (2 <sub>z</sub>  1/2,1/2)'	(1/2,0) x,1/4 (m <sub>y</sub>  1/2,1/2)'	(0,1/2) 1/4,y (m <sub>x</sub>  1/2,1/2)'

**Generators selected** (1); t(1,0); t(0,1); t(1/2,1/2); (2); (3); 1'

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(0,0) +	(1/2,1/2) +
	(0,0)' +	(1/2,1/2)' +
8 f 11'	(1) x,y [0,0]	(2) $\bar{x},\bar{y}$ [0,0]
	(3) $x,\bar{y}$ [0,0]	(4) $\bar{x},y$ [0,0]
4 e .m.1'	0,y [0,0]	0, $\bar{y}$ [0,0]
4 d ..m1'	x,0 [0,0]	$\bar{x},0$ [0,0]
4 c 2..1'	1/4,1/4 [0,0]	1/4,3/4 [0,0]
2 b 2mm1'	0,1/2 [0,0]	
2 a 2mm1'	0,0 [0,0]	

**Symmetry of special projections**

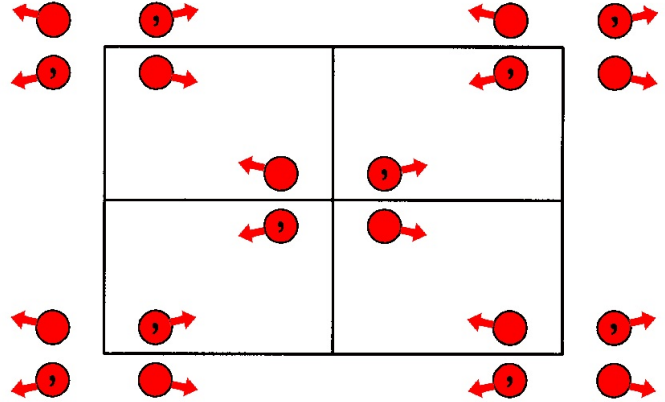
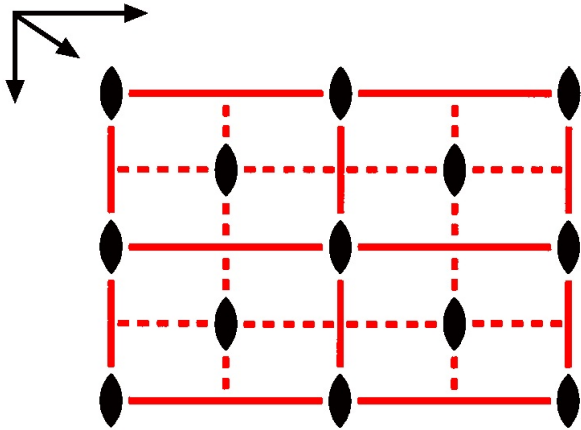
Along [10] $\rho m 1'$	Along [01] $\rho m 1'$
$\mathbf{a}^* = \mathbf{b}/2$	$\mathbf{a}^* = \mathbf{a}/2$
Origin at x,0	Origin at 0,y

c2m'm'

No. 9.3.44

2m'm'

c2m'm'



Origin on 2m'm'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$

Symmetry operations

For (0,0) + set

- (1) 1  
(1|0,0)
- (2) 2 0,0  
(2<sub>z</sub>|0,0)

- (3) m' x,0  
(m<sub>y</sub>|0,0)'

- (4) m' 0,y  
(m<sub>x</sub>|0,0)'

For (1/2,1/2) + set

- (1) t (1/2,1/2)  
(1|1/2,1/2)
- (2) 2 1/4,1/4  
(2<sub>z</sub>|1/2,1/2)

- (3) g' (1/2,0) x,1/4  
(m<sub>y</sub>|1/2,1/2)'

- (4) g' (0,1/2) 1/4,y  
(m<sub>x</sub>|1/2,1/2)'

**Generators selected** (1); t(1,0); t(0,1); t(1/2,1/2); (2); (3)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(0,0) +	(1/2,1/2) +
8 f 1	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [ $\bar{u},\bar{v}$ ]
	(3) $x,\bar{y}$ [u, $\bar{v}$ ]	(4) $\bar{x},y$ [ $\bar{u},v$ ]
4 e .m'	0,y [0,v]	0, $\bar{y}$ [0, $\bar{v}$ ]
4 d ...m'	x,0 [u,0]	$\bar{x},0$ [ $\bar{u},0$ ]
4 c 2..	1/4,1/4 [0,0]	1/4,3/4 [0,0]
2 b 2m'm'	0,1/2 [0,0]	
2 a 2m'm'	0,0 [0,0]	

**Symmetry of special projections**

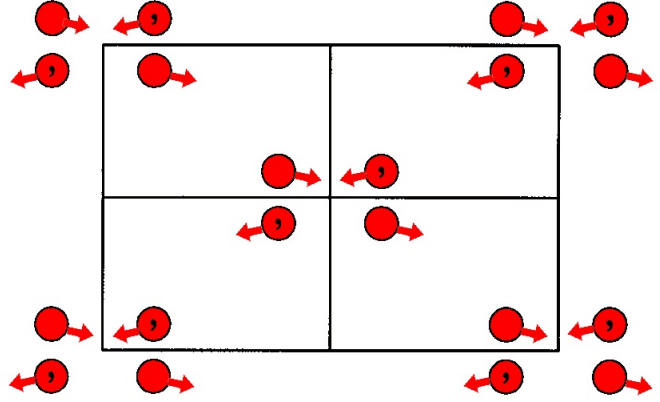
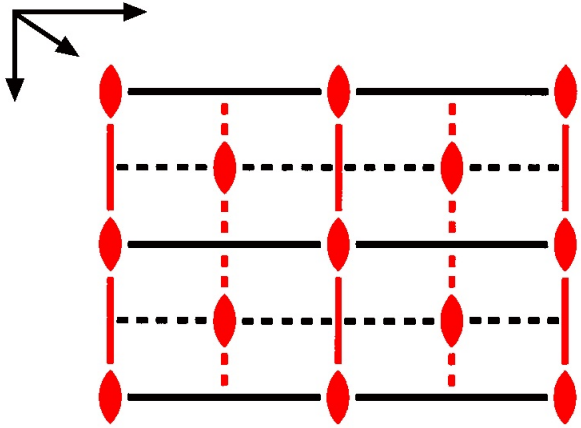
Along [10] $\rho m'$ $\mathbf{a}^* = \mathbf{b}/2$ Origin at x,0	Along [01] $\rho m'$ $\mathbf{a}^* = \mathbf{a}/2$ Origin at 0,y

c2'mm'

No. 9.4.45

2'mm'

2'cmm'



Origin on 2'mm'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$

Symmetry operations

For (0,0) + set

(1) 1

(1|0,0)

(2) 2' 0,0

(2<sub>z</sub>|0,0)'

(3) m' x,0

(m<sub>y</sub>|0,0)'

(4) m 0,y

(m<sub>x</sub>|0,0)

For (1/2,1/2) + set

(1) t (1/2,1/2)

(1|1/2,1/2)

(2) 2' 1/4,1/4

(2<sub>z</sub>|1/2,1/2)'

(3) g' (1/2,0) x,1/4

(m<sub>y</sub>|1/2,1/2)'

(4) g (0,1/2) 1/4,y

(m<sub>x</sub>|1/2,1/2)

**Generators selected** (1); t(1,0); t(0,1); t(1/2,1/2); (2); (3)

**Positions**

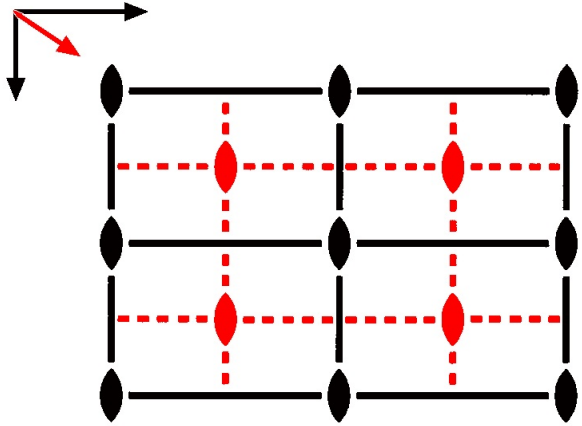
Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(0,0) +	(1/2,1/2) +
8 f 1	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [u,v]
	(3) $x,\bar{y}$ [u, $\bar{v}$ ]	(4) $\bar{x},y$ [u, $\bar{v}$ ]
4 e .m.	0,y [u,0]	0, $\bar{y}$ [u,0]
4 d ..m'	x,0 [u,0]	$\bar{x}$ ,0 [u,0]
4 c 2'..	1/4,1/4 [u,v]	1/4,3/4 [u, $\bar{v}$ ]
2 b 2'mm'	0,1/2 [u,0]	
2 a 2'mm'	0,0 [u,0]	

**Symmetry of special projections**

Along [10] $\rho m 1'$ $\mathbf{a}^* = \mathbf{b}/2$ Origin at x,0	Along [01] $\rho m$ $\mathbf{a}^* = \mathbf{a}/2$ Origin at 0,y
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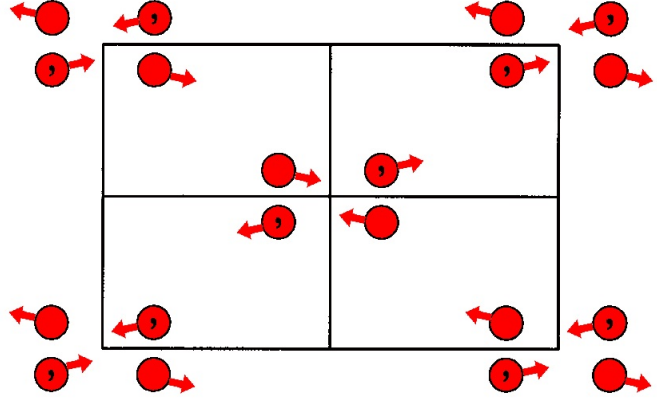
$c_p 2mm$

No. 9.5.46



$2mm 1'$

$c_p 2mm$



**Origin on  $2mm$**

**Asymmetric unit**  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2$

**Symmetry operations**

For  $(0,0) + \text{set}$

(1) 1

$(1|0,0)$

(2)  $2_{0,0}$

$(2_z|0,0)$

(3)  $m_{x,0}$

$(m_y|0,0)$

(4)  $m_{0,y}$

$(m_x|0,0)$

For  $(1/2,1/2)' + \text{set}$

(1)  $t'_{(1/2,1/2)}$

$(1|1/2,1/2)'$

(2)  $2'_{1/4,1/4}$

$(2_z|1/2,1/2)'$

(3)  $g'_{(1/2,0) x,1/4}$

$(m_y|1/2,1/2)'$

(4)  $g'_{(0,1/2) 1/4,y}$

$(m_x|1/2,1/2)'$

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ;  $t(1/2,1/2)'$ ; (2); (3)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(0,0) +	$(1/2,1/2)'$ +
8 f 1	(1) $x,y [u,v]$	(2) $\bar{x},\bar{y} [\bar{u},\bar{v}]$
	(3) $x,\bar{y} [\bar{u},v]$	(4) $\bar{x},y [u,\bar{v}]$
4 e .m.	$0,y [u,0]$	$0,\bar{y} [\bar{u},0]$
4 d ..m	$x,0 [0,v]$	$\bar{x},0 [0,\bar{v}]$
4 c 2'..	$1/4,1/4 [u,v]$	$1/4,3/4 [\bar{u},v]$
2 b 2mm	$0,1/2 [0,0]$	
2 a 2mm	$0,0 [0,0]$	

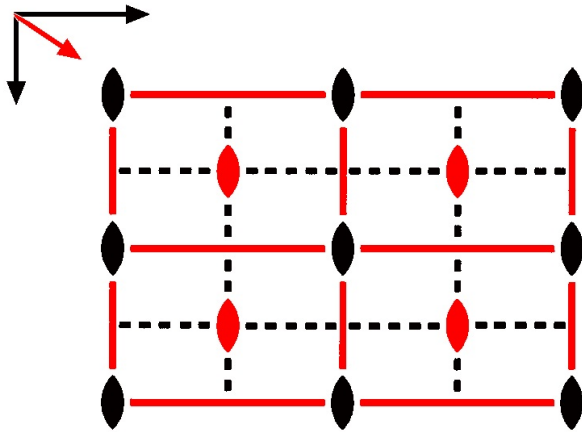
**Symmetry of special projections**

Along $[10] pm1'$	Along $[01] pm1'$
$\mathbf{a}^* = \mathbf{b}/2$	$\mathbf{a}^* = \mathbf{a}/2$
Origin at $x,0$	Origin at $0,y$



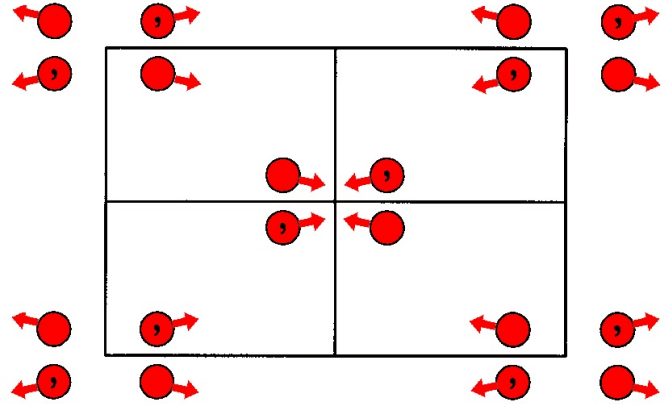
$c_p 2m'm'$

No. 8.6.47



$2mm1'$

$c_p 2m'm'$



**Origin** on  $2m'm'$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$

**Symmetry operations**

For  $(0,0)$  + set

(1) 1

$(1|0,0)$

(2)  $2 \quad 0,0$

$(2_z|0,0)$

(3)  $m' \quad x,0$   
 $(m_y|0,0)'$

(4)  $m' \quad 0,y$   
 $(m_x|0,0)'$

For  $(1/2,1/2)'$  + set

(1)  $t' \quad (1/2,1/2)$

$(1|1/2,1/2)'$

(2)  $2' \quad 1/4,1/4$

$(2_z|1/2,1/2)'$

(3)  $g \quad (1/2,0) \quad x,1/4$   
 $(m_y|1/2,1/2)$

(4)  $g \quad (0,1/2) \quad 1/4,y$   
 $(m_x|1/2,1/2)$

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ;  $t(1/2,1/2)'$ ; (2); (3)

**Positions**

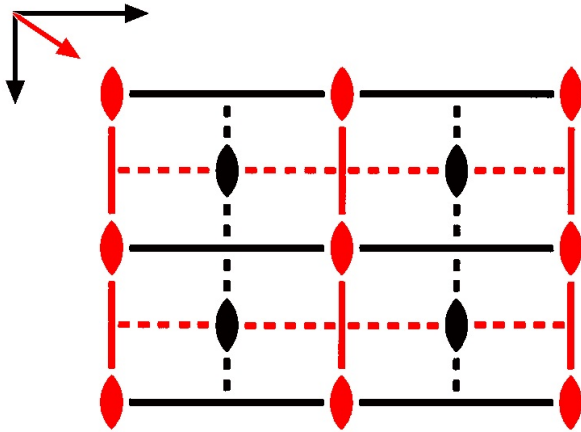
Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(0,0) +	$(1/2,1/2)'$ +
8 f 1	(1) $x,y [u,v]$	(2) $\bar{x},\bar{y} [\bar{u},\bar{v}]$
	(3) $x,\bar{y} [u,\bar{v}]$	(4) $\bar{x},y [\bar{u},v]$
4 e $.m'$	$0,y [0,v]$	$0,\bar{y} [0,\bar{v}]$
4 d $..m'$	$x,0 [u,0]$	$\bar{x},0 [\bar{u},0]$
4 c $2'..$	$1/4,1/4 [u,v]$	$1/4,3/4 [u,\bar{v}]$
2 b $2m'm'$	$0,1/2 [0,0]$	
2 a $2m'm'$	$0,0 [0,0]$	

**Symmetry of special projections**

Along [10] $p_{2a'm}$	Along [01] $p_{2a'm}$
$\mathbf{a}^* = \mathbf{b}/2$	$\mathbf{a}^* = \mathbf{a}/2$
Origin at $x,1/4$	Origin at $1/4,y$

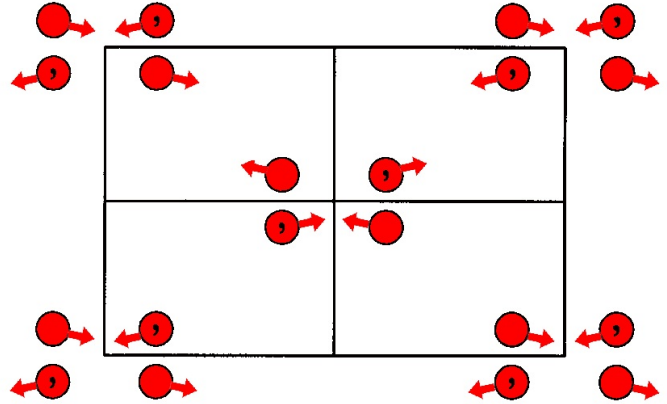
$c_p 2'mm'$

No. 9.7.48



$2mm1'$

$c_p 2'mm'$



Origin on  $2'mm'$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2$

**Symmetry operations**

For  $(0,0)$  + set

- |         |                    |                    |                   |
|---------|--------------------|--------------------|-------------------|
| (1) 1   | (2) $2' \quad 0,0$ | (3) $m' \quad x,0$ | (4) $m \quad 0,y$ |
| (1 0,0) | ( $2_z$  0,0)'     | ( $m_y$  0,0)'     | ( $m_x$  0,0)     |

For  $(1/2,1/2)'$  + set

- |                          |                       |                                   |                                    |
|--------------------------|-----------------------|-----------------------------------|------------------------------------|
| (1) $t' \quad (1/2,1/2)$ | (2) $2 \quad 1/4,1/4$ | (3) $g \quad (1/2,0) \quad x,1/4$ | (4) $g' \quad (0,1/2) \quad 1/4,y$ |
| (1  $1/2,1/2$ )'         | ( $2_z$   $1/2,1/2$ ) | ( $m_y$   $1/2,1/2$ )             | ( $m_x$   $1/2,1/2$ )'             |

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ;  $t(1/2,1/2)'$ ; (2); (3)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	
	(0,0) +	$(1/2,1/2)'$ +
8 f 1	(1) $x,y [u,v]$ (3) $x,\bar{y} [u,\bar{v}]$	(2) $\bar{x},\bar{y} [u,v]$ (4) $\bar{x},y [u,\bar{v}]$
4 e .m.	$0,y [u,0]$	$0,\bar{y} [u,0]$
4 d ..m'	$x,0 [u,0]$	$\bar{x},0 [u,0]$
4 c 2..	$1/4,1/4 [0,0]$	$1/4,3/4 [0,0]$
2 b 2'mm'	$0,1/2 [u,0]$	
2 a 2'mm'	$0,0 [u,0]$	

**Symmetry of special projections**

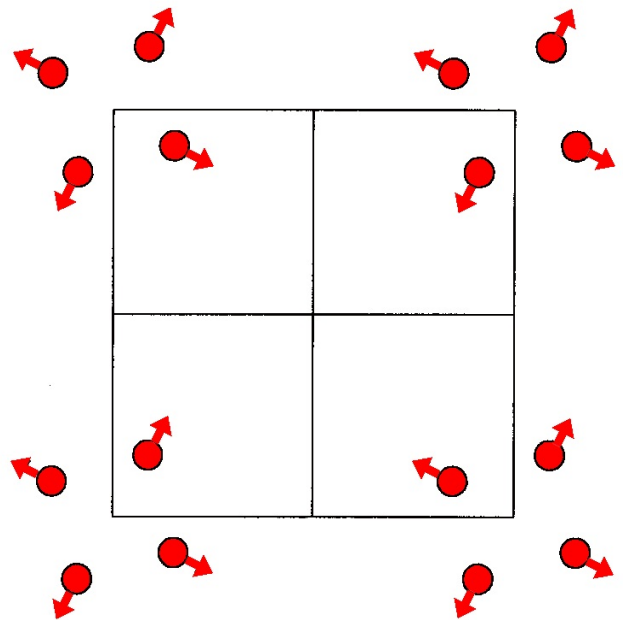
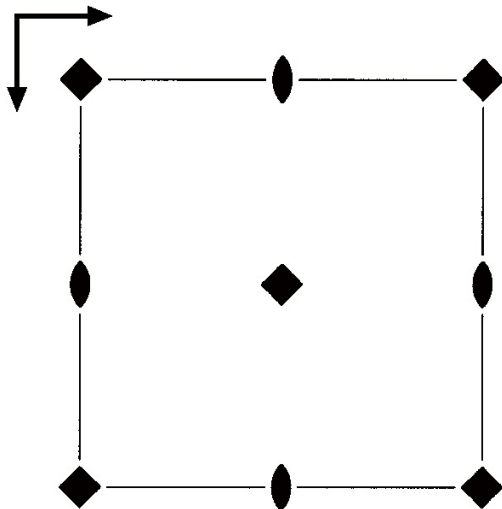
Along [10] $pm1'$ $\mathbf{a}^* = \mathbf{b}/2$ Origin at $x,0$	Along [01] $p_{2a}m$ $\mathbf{a}^* = \mathbf{a}/2$ Origin at $0,y$
---	--

p4

4

No. 10.1.49

p4



Origin on 4

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2$

Symmetry operations

(1) 1  
(1|0,0)

(2) 2 0,0  
(2<sub>z</sub>|0,0)

(3) 4<sup>+</sup> 0,0  
(4<sub>z</sub><sup>+</sup>|0,0)

(4) 4<sup>-</sup> 0,0  
(4<sub>z</sub><sup>-</sup>|0,0)

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ; (2); (3)

**Positions**

		Coordinates			
Multiplicity, Wyckoff letter, Site symmetry					
4	d 1	(1) $x,y [u,v]$	(2) $\bar{x},\bar{y} [\bar{u},\bar{v}]$	(3) $\bar{y},x [\bar{v},u]$	(4) $y,\bar{x} [v,\bar{u}]$
2	c 2..	$0,1/2 [0,0]$	$1/2,0 [0,0]$		
1	b 4..	$1/2,1/2 [0,0]$			
1	a 4..	$0,0 [0,0]$			

**Symmetry of special projections**

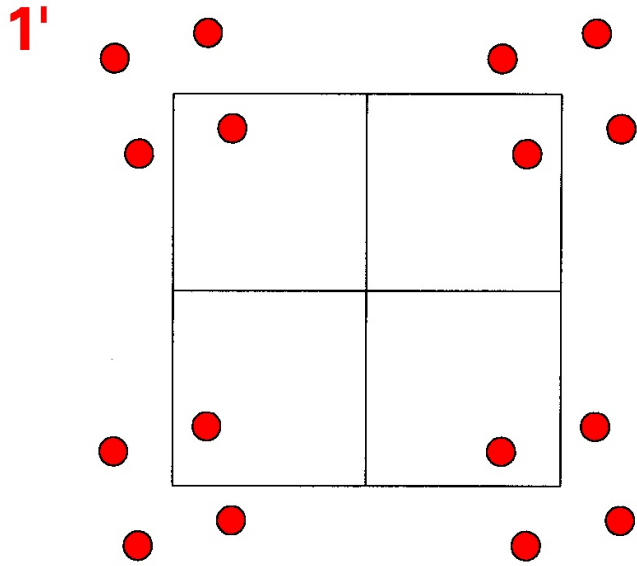
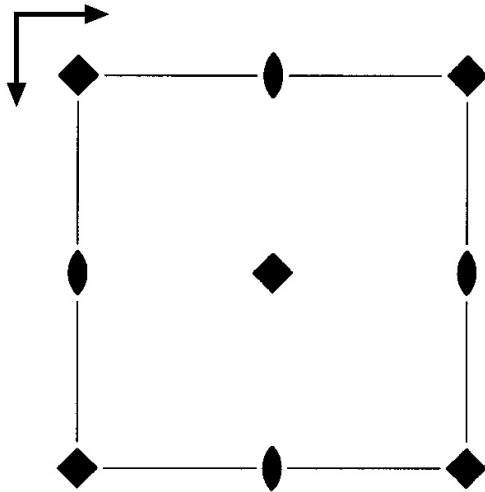
Along $[10] \rho m'$	Along $[11] \rho m'$
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$
Origin at $x,0$	Origin at $x,x$

P4

4

No. 10.2.50

p41'



Origin on 41'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2$

**Symmetry operations**

- |              |                        |                          |                                      |
|--------------|------------------------|--------------------------|--------------------------------------|
| For 1 + set  |                        |                          |                                      |
| (1) 1        | (2) 2 0,0              | (3) 4 <sup>+</sup> 0,0   | (4) 4 <sup>-</sup> 0,0               |
| (1 0,0)      | (2 <sub>z</sub>  0,0)  | (4 <sub>z</sub>  0,0)    | (4 <sub>z</sub> <sup>-1</sup>  0,0)  |
| For 1' + set |                        |                          |                                      |
| (1) 1'       | (2) 2' 0,0             | (3) 4 <sup>+</sup> ' 0,0 | (4) 4 <sup>-</sup> ' 0,0             |
| (1 0,0)'     | (2 <sub>z</sub>  0,0)' | (4 <sub>z</sub>  0,0)'   | (4 <sub>z</sub> <sup>-1</sup>  0,0)' |

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ; (2); (3);  $1'$

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
		1+	1' +	
4 d 11'	(1) $x,y [0,0]$	(2) $\bar{x},\bar{y} [0,0]$	(3) $\bar{y},x [0,0]$	(4) $y,\bar{x} [0,0]$
2 c 2..1'	$0,1/2 [0,0]$	$1/2,0 [0,0]$		
1 b 4..1'	$1/2,1/2 [0,0]$			
1 a 4..1'	$0,0 [0,0]$			

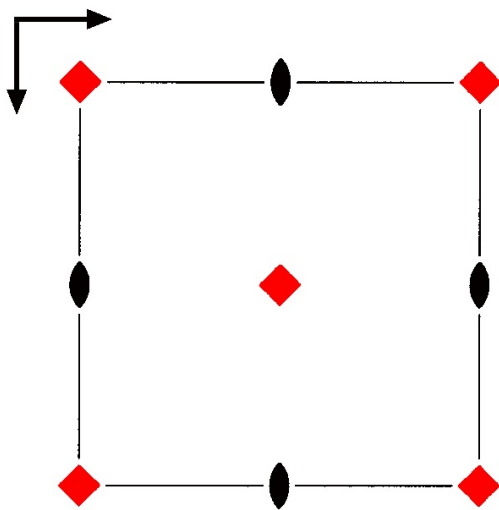
**Symmetry of special projections**

Along $[10] \rho m 1'$	Along $[11] \rho m 1'$
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$
Origin at $x,0$	Origin at $x,x$



p4'

No. 10.3.51



Origin on 4'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2$

Symmetry operations

$$(1) 1$$

$$(1|0,0)$$

$$(2) 2 \quad 0,0$$

$$(2_z|0,0)$$

$$(3) 4^{+'} \quad 0,0$$

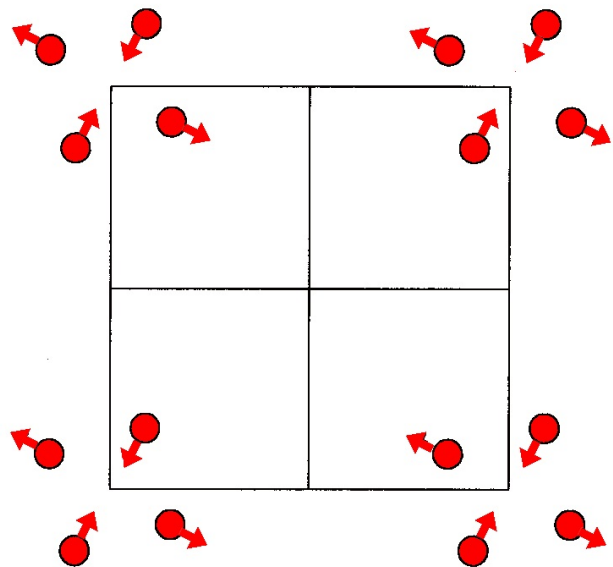
$$(4_z|0,0)'$$

$$(4) 4^{-'} \quad 0,0$$

$$(4_z^{-1}|0,0)'$$

4'

p4'



**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ; (2); (3)

**Positions**

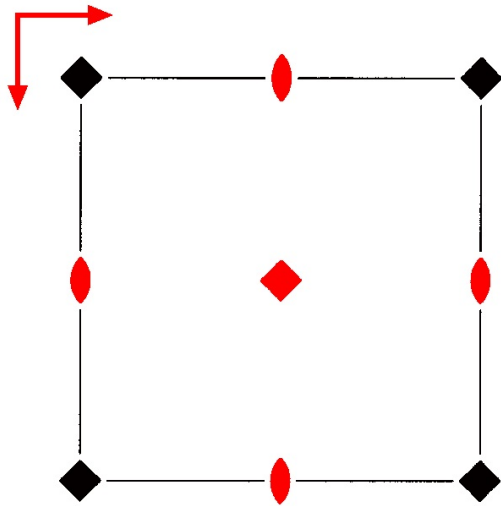
		Coordinates			
Multiplicity, Wyckoff letter, Site symmetry					
4	d 1	(1) $x,y [u,v]$	(2) $\bar{x},\bar{y} [\bar{u},\bar{v}]$	(3) $\bar{y},x [v,\bar{u}]$	(4) $y,\bar{x} [\bar{v},u]$
2	c 2..	$0,1/2 [0,0]$	$1/2,0 [0,0]$		
1	b 4'..	$1/2,1/2 [0,0]$			
1	a 4'..	$0,0 [0,0]$			

**Symmetry of special projections**

Along $[10] \rho m$	Along $[11] \rho m$
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$
Origin at $x,0$	Origin at $x,x$

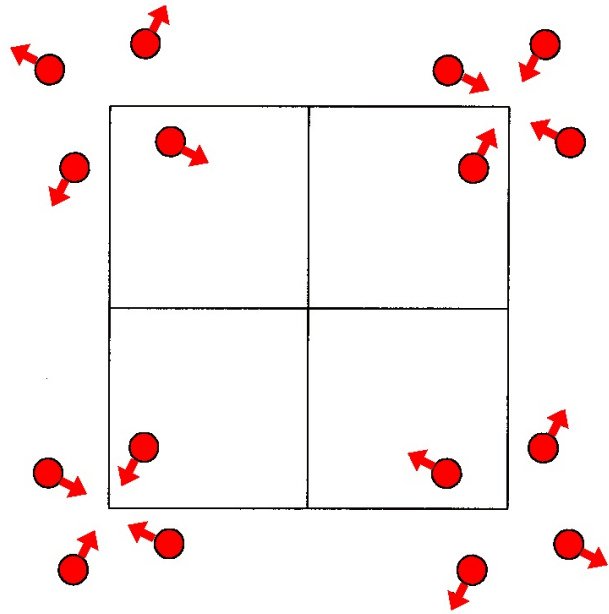
$p_p4$

No. 10.4.52



$41'$

$p_p4$



Origin on 4

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2$

**Symmetry operations**

For (0,0) + set

- |                  |                                    |   |   |
|------------------|------------------------------------|---|---|
| (1) 1<br>(1 0,0) | (2) 2 0,0<br>(2 <sub>z</sub>  0,0) | (3) 4 <sup>+</sup> 0,0<br>(4 <sub>z</sub>  0,0) | (4) 4 <sup>-</sup> 0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0) |
|------------------|------------------------------------|---|---|

For (1,0)' + set

- |                          |  |  |  |
|--------------------------|--|--|--|
| (1) t' (1,0)<br>(1 1,0)' | (2) 2' 1/2,0<br>(2 <sub>z</sub>  1,0)' | (3) 4 <sup>+</sup> ' 1/2,1/2<br>(4 <sub>z</sub>  1,0)' | (4) 4 <sup>-</sup> ' 1/2,1/2<br>(4 <sub>z</sub> <sup>-1</sup>  1,0)' |
|--------------------------|--|--|--|

**Generators selected** (1); t(1,0)'; t(0,1)'; (2); (3)

**Positions**

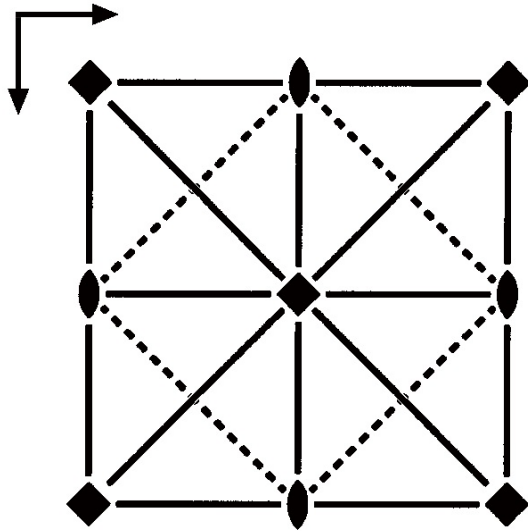
Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
	(0,0)+	(1,0)' +		
4 d 1	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [ $\bar{u},\bar{v}$ ]	(3) $\bar{y},x$ [ $\bar{v},u$ ]	(4) $y,\bar{x}$ [ $v,\bar{u}$ ]
2 c 2'..	0,1/2 [u,v]	1/2,0 [v, $\bar{u}$ ]		
1 b 4'..	1/2,1/2 [0,0]			
1 a 4..	0,0 [0,0]			

**Symmetry of special projections**

Along [10] $p_{2a,m}$	Along [11] $pm$
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$
Origin at x, 1/2	Origin at x-1/4, x+1/4

p4mm

No. 11.1.53



Origin on 4mm

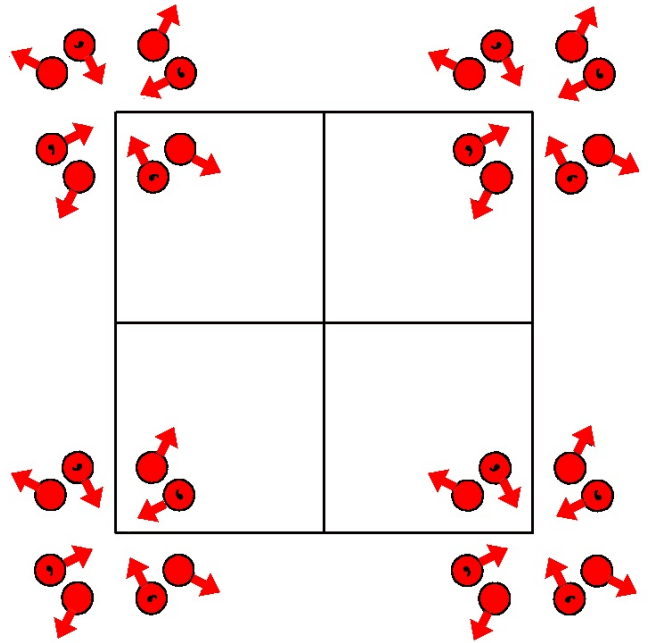
Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; x \leq y$

Symmetry operations

- |                                    |                                    |  |  |
|------------------------------------|------------------------------------|--|--|
| (1) 1<br>(1 0,0)                   | (2) 2 0,0<br>(2 <sub>z</sub>  0,0) | (3) 4 <sup>+</sup> 0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0) | (4) 4 <sup>-</sup> 0,0<br>(4 <sub>z</sub> <sup>-</sup>  0,0) |
| (5) m x,0<br>(m <sub>y</sub>  0,0) | (6) m 0,y<br>(m <sub>x</sub>  0,0) | (7) m x, $\bar{x}$<br>(m <sub>xy</sub>  0,0)                 | (8) m x,x<br>(m <sub><math>\bar{xy}</math></sub>  0,0)       |

4mm

p4mm



**Generators selected** (1); t(1,0); t(0,1); (2); (3); (5)

**Positions**

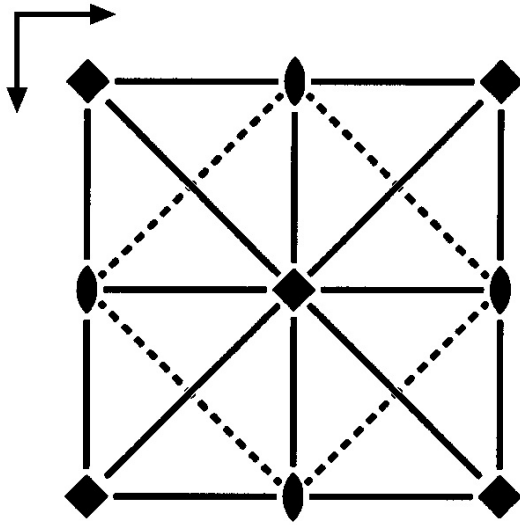
Wyckoff letter, Site symmetry	Coordinates			
	(1) $x, y$ $[u, v]$	(2) $\bar{x}, \bar{y}$ $[\bar{u}, \bar{v}]$	(3) $\bar{y}, x$ $[\bar{v}, u]$	(4) $y, \bar{x}$ $[v, \bar{u}]$
8 g 1	(5) $x, \bar{y}$ $[\bar{u}, v]$	(6) $\bar{x}, y$ $[u, \bar{v}]$	(7) $\bar{y}, \bar{x}$ $[v, u]$	(8) $y, x$ $[v, \bar{u}]$
4 f .m.	$x, 1/2$ $[0, v]$	$\bar{x}, 1/2$ $[0, \bar{v}]$	$1/2, x$ $[\bar{v}, 0]$	$1/2, \bar{x}$ $[v, 0]$
4 e .m.	$x, 0$ $[0, v]$	$\bar{x}, 0$ $[0, \bar{v}]$	$0, x$ $[\bar{v}, 0]$	$0, \bar{x}$ $[v, 0]$
4 d ..m	$x, x$ $[\bar{u}, u]$	$\bar{x}, \bar{x}$ $[u, \bar{u}]$	$\bar{x}, x$ $[\bar{u}, \bar{u}]$	$x, \bar{x}$ $[u, u]$
2 c 2mm.	$1/2, 0$ $[0, 0]$	$0, 1/2$ $[0, 0]$		
1 b 4mm	$1/2, 1/2$ $[0, 0]$			
1 a 4mm	$0, 0$ $[0, 0]$			

**Symmetry of special projections**

Along $[10]$ $\rho m 1'$ $\mathbf{a}^* = \mathbf{b}$ Origin at $x, 0$	Along $[11]$ $\rho m 1'$ $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$ Origin at $x, x$
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p4mm1'

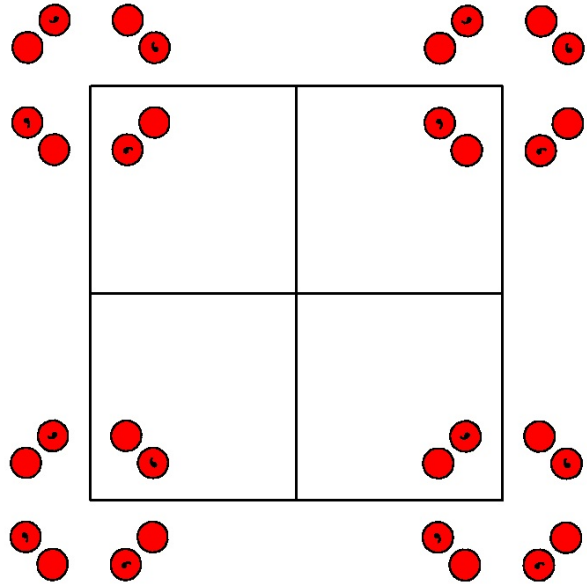
No. 11.2.54



4mm1'

p4mm1'

1'



Origin on 4mm1'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; x \leq y$

**Symmetry operations**

For 1 + set

- |                                    |                                    |   |   |
|------------------------------------|------------------------------------|---|---|
| (1) 1<br>(1 0,0)                   | (2) 2 0,0<br>(2 <sub>z</sub>  0,0) | (3) 4 <sup>+</sup> 0,0<br>(4 <sub>z</sub>  0,0) | (4) 4 <sup>-</sup> 0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0) |
| (5) m x,0<br>(m <sub>y</sub>  0,0) | (6) m 0,y<br>(m <sub>x</sub>  0,0) | (7) m x, $\bar{x}$<br>(m <sub>xy</sub>  0,0)    | (8) m x,x<br>(m $\bar{xy}$  0,0)                              |

For 1' + set

- |                                      |                                      |  |  |
|--------------------------------------|--------------------------------------|--|--|
| (1) 1'<br>(1 0,0)'                   | (2) 2' 0,0<br>(2 <sub>z</sub>  0,0)' | (3) 4 <sup>+</sup> ' 0,0<br>(4 <sub>z</sub>  0,0)' | (4) 4 <sup>-</sup> ' 0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0)' |
| (5) m' x,0<br>(m <sub>y</sub>  0,0)' | (6) m' 0,y<br>(m <sub>x</sub>  0,0)' | (7) m' x, $\bar{x}$<br>(m <sub>xy</sub>  0,0)'     | (8) m' x,x<br>(m $\bar{xy}$  0,0)'                               |

**Generators selected** (1); t(1,0); t(0,1); (2); (3); (5); 1'

**Positions**

Wyckoff letter, Site symmetry	Coordinates			
	1+	1' +		
8 g 11'	(1) x,y [0,0]	(2) $\bar{x},\bar{y}$ [0,0]	(3) $\bar{y},x$ [0,0]	(4) $y,\bar{x}$ [0,0]
	(5) $x,\bar{y}$ [0,0]	(6) $\bar{x},y$ [0,0]	(7) $\bar{y},\bar{x}$ [0,0]	(8) $y,x$ [0,0]
4 f .m.1'	x,1/2 [0,0]	$\bar{x},1/2$ [0,0]	1/2,x [0,0]	1/2, $\bar{x}$ [0,0]
4 e .m.1'	x,0 [0,0]	$\bar{x},0$ [0,0]	0,x [0,0]	0, $\bar{x}$ [0,0]
4 d ..m1'	x,x [0,0]	$\bar{x},\bar{x}$ [0,0]	$\bar{x},x$ [0,0]	x, $\bar{x}$ [0,0]
2 c 2mm.1'	1/2,0 [0,0]	0,1/2 [0,0]		
1 b 4mm1'	1/2,1/2 [0,0]			
1 a 4mm1'	0,0 [0,0]			

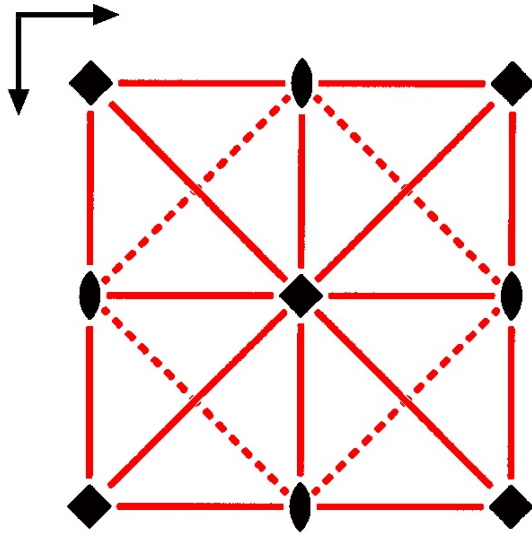
**Symmetry of special projections**

Along [10] p m 1'	Along [11] p m 1'
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$
Origin at x,0	Origin at x,x



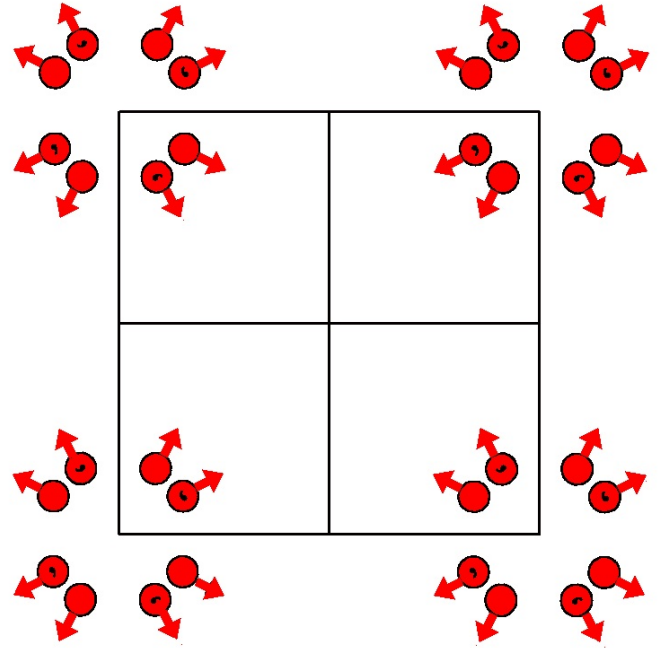
p4m'm'

No. 11.3.55



4m'm'

p4m'm'



Origin on 4m'm'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; x \leq y$

**Symmetry operations**

- |                                      |   |  |  |
|--------------------------------------|---|--|--|
| (1) 1<br>(1 0,0)                     | (2) 2 <sub>z</sub> 0,0<br>(2 <sub>z</sub>  0,0) | (3) 4 <sup>+</sup> 0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0) | (4) 4 <sup>-</sup> 0,0<br>(4 <sub>z</sub> <sup>-</sup>  0,0) |
| (5) m' x,0<br>(m <sub>y</sub>  0,0)' | (6) m' 0,y<br>(m <sub>x</sub>  0,0)'            | (7) m' x,x̄<br>(m <sub>xy</sub>  0,0)'                       | (8) m' x,x<br>(m <sub>xȳ</sub>  0,0)'                       |

**Generators selected** (1); t(1,0); t(0,1); (2); (3); (5)

**Positions**

Wyckoff letter, Site symmetry	Coordinates			
	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [ $\bar{u},\bar{v}$ ]	(3) $\bar{y},x$ [ $\bar{v},u$ ]	(4) $y,\bar{x}$ [ $v,\bar{u}$ ]
8 g 1	(5) $x,\bar{y}$ [ $u,\bar{v}$ ]	(6) $\bar{x},y$ [ $\bar{u},v$ ]	(7) $\bar{y},\bar{x}$ [ $\bar{v},\bar{u}$ ]	(8) $y,x$ [ $v,u$ ]
4 f .m'	x,1/2 [u,0]	$\bar{x},1/2$ [ $\bar{u},0$ ]	1/2,x [0,u]	1/2, $\bar{x}$ [0, $\bar{u}$ ]
4 e .m'	x,0 [u,0]	$\bar{x},0$ [ $\bar{u},0$ ]	0,x [0,u]	0, $\bar{x}$ [0, $\bar{u}$ ]
4 d ..m'	x,x [u,u]	$\bar{x},\bar{x}$ [ $\bar{u},\bar{u}$ ]	$\bar{x},x$ [ $\bar{u},u$ ]	$x,\bar{x}$ [ $u,\bar{u}$ ]
2 c 2mm'	1/2,0 [0,0]	0,1/2 [0,0]		
1 b 4m'm'	1/2,1/2 [0,0]			
1 a 4m'm'	0,0 [0,0]			

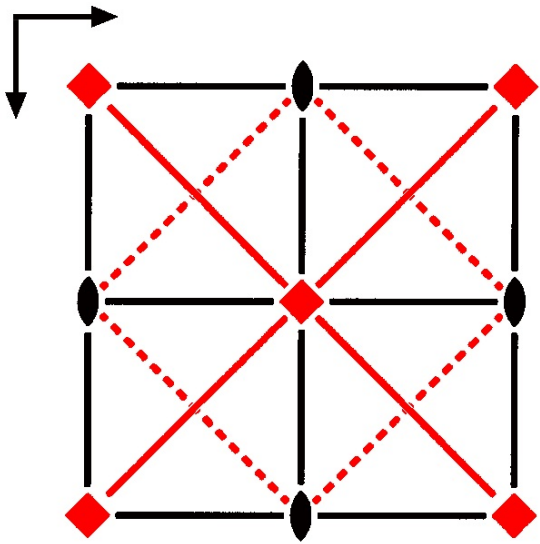
**Symmetry of special projections**

Along [10]  $\rho m'$   
 $\mathbf{a}^* = \mathbf{b}$   
 Origin at x,0

Along [11]  $\rho m'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x

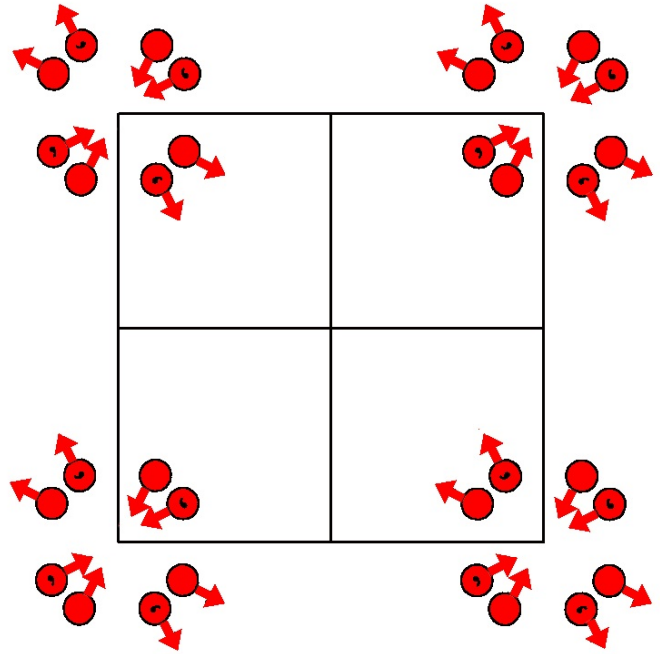
p4'mm'

No. 11.4.56



4'mm'

p4'mm'



Origin on 4'mm'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $x \leq y$

**Symmetry operations**

- |                                    |                                    |  |  |
|------------------------------------|------------------------------------|--|--|
| (1) 1<br>(1 0,0)                   | (2) 2 0,0<br>(2 <sub>z</sub>  0,0) | (3) 4 <sup>+</sup> 0,0<br>(4 <sub>z</sub>  0,0)' | (4) 4 <sup>-</sup> 0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0)' |
| (5) m x,0<br>(m <sub>y</sub>  0,0) | (6) m 0,y<br>(m <sub>x</sub>  0,0) | (7) m' x, $\bar{x}$<br>(m <sub>xy</sub>  0,0)'   | (8) m' x,x<br>(m $\bar{xy}$  0,0)'                             |

**Generators selected** (1); t(1,0); t(0,1); (2); (3); (5)

**Positions**

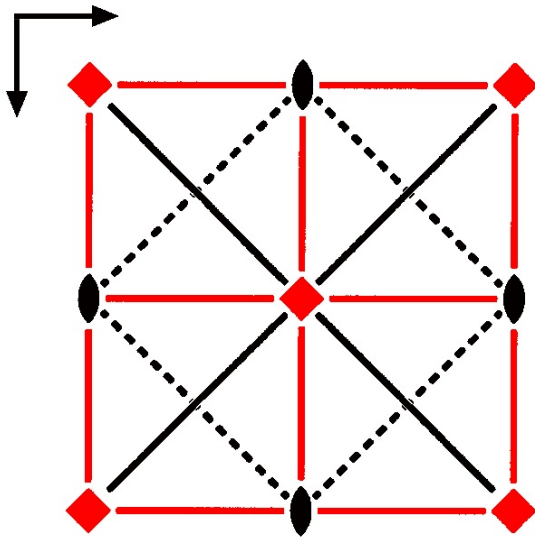
Wyckoff letter, Site symmetry	Coordinates			
	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [ $\bar{u},\bar{v}$ ]	(3) $\bar{y},x$ [v, $\bar{u}$ ]	(4) $y,\bar{x}$ [ $\bar{v},u$ ]
8 g 1	(5) $x,\bar{y}$ [ $\bar{u},v$ ]	(6) $\bar{x},y$ [u, $\bar{v}$ ]	(7) $\bar{y},\bar{x}$ [ $\bar{v},\bar{u}$ ]	(8) $y,x$ [v,u]
4 f .m.	x,1/2 [0,v]	$\bar{x},1/2$ [0, $\bar{v}$ ]	1/2,x [v,0]	1/2, $\bar{x}$ [ $\bar{v},0$ ]
4 e .m.	x,0 [0,v]	$\bar{x},0$ [0, $\bar{v}$ ]	0,x [v,0]	0, $\bar{x}$ [ $\bar{v},0$ ]
4 d ..m'	x,x [u,u]	$\bar{x},\bar{x}$ [ $\bar{u},\bar{u}$ ]	$\bar{x},x$ [u, $\bar{u}$ ]	$x,\bar{x}$ [ $\bar{u},u$ ]
2 c 2mm.	1/2,0 [0,0]	0,1/2 [0,0]		
1 b 4'mm'	1/2,1/2 [0,0]			
1 a 4'mm'	0,0 [0,0]			

**Symmetry of special projections**

Along [10] $\rho m 1'$ $\mathbf{a}^* = \mathbf{b}$ Origin at x,0	Along [11] $\rho m$ $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$ Origin at x,x
--	---

p4'm'm

No. 11.5.57



Origin on 4'm'm

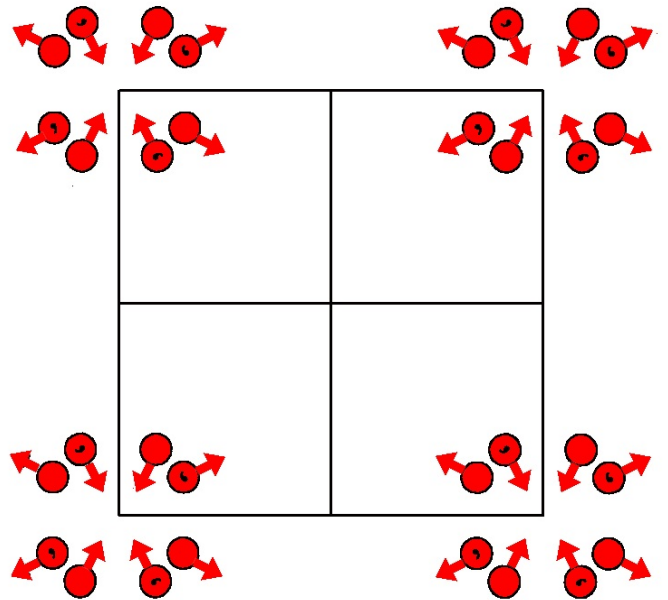
Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; x \leq y$

Symmetry operations

- |                                      |                                      |  |  |
|--------------------------------------|--------------------------------------|--|--|
| (1) 1<br>(1 0,0)                     | (2) 2 0,0<br>(2 <sub>z</sub>  0,0)   | (3) 4 <sup>+</sup> 0,0<br>(4 <sub>z</sub>  0,0)' | (4) 4 <sup>-</sup> 0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0)' |
| (5) m' x,0<br>(m <sub>y</sub>  0,0)' | (6) m' 0,y<br>(m <sub>x</sub>  0,0)' | (7) m x,x̄<br>(m <sub>xy</sub>  0,0)             | (8) m x,x<br>(m <sub>x̄y</sub>  0,0)                           |

4'm'm

p4'm'm



**Generators selected** (1); t(1,0); t(0,1); (2); (3); (5)

**Positions**

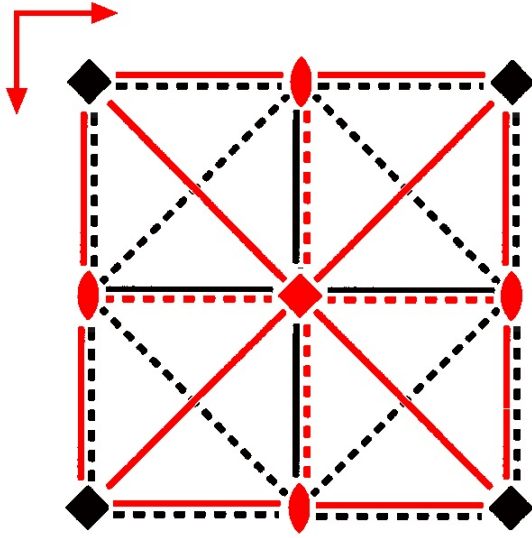
Wyckoff letter, Site symmetry	Coordinates			
	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [ $\bar{u},\bar{v}$ ]	(3) $\bar{y},x$ [v, $\bar{u}$ ]	(4) y, $\bar{x}$ [ $\bar{v},u$ ]
8 g 1	(5) x, $\bar{y}$ [u, $\bar{v}$ ]	(6) $\bar{x},y$ [ $\bar{u},v$ ]	(7) $\bar{y},\bar{x}$ [v,u]	(8) y,x [ $\bar{v},\bar{u}$ ]
4 f .m'	x,1/2 [u,0]	$\bar{x},1/2$ [ $\bar{u},0$ ]	1/2,x [0, $\bar{u}$ ]	1/2, $\bar{x}$ [0,u]
4 e .m'	x,0 [u,0]	$\bar{x},0$ [ $\bar{u},0$ ]	0,x [0, $\bar{u}$ ]	0, $\bar{x}$ [0,u]
4 d ..m	x,x [u,u]	$\bar{x},\bar{x}$ [ $\bar{u},\bar{u}$ ]	$\bar{x},x$ [u, $\bar{u}$ ]	x, $\bar{x}$ [ $\bar{u},u$ ]
2 c 2m'm'	1/2,0 [0,0]	0,1/2 [0,0]		
1 b 4'm'm	1/2,1/2 [0,0]			
1 a 4'm'm	0,0 [0,0]			

**Symmetry of special projections**

Along [10] $\rho m$ $\mathbf{a}^* = \mathbf{b}$ Origin at x,0	Along [11] $\rho m 1'$ $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$ Origin at x,x
---	--

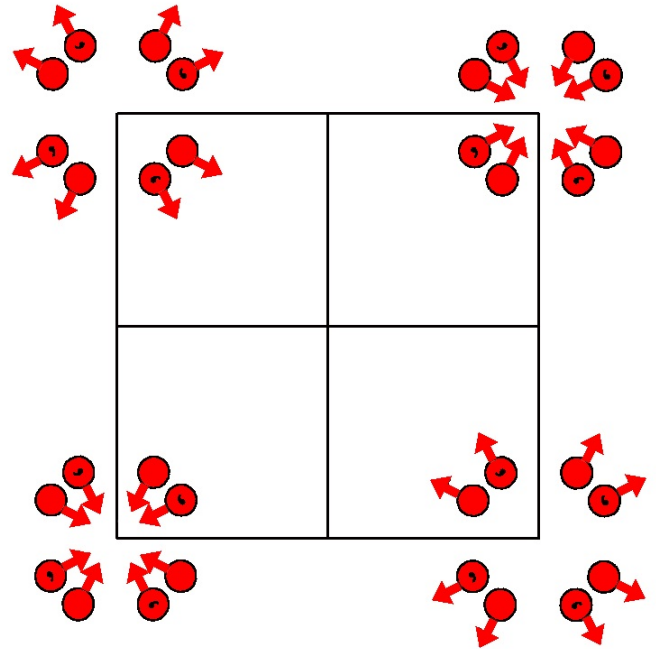
$p_p4m'm'$

No. 11.6.58



$4mm1'$

$p_p4m'm'$



Origin on  $4m'm'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; x \leq y$

**Symmetry operations**

For  $(0,0)$  + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0)                         | (2) 2 0,0<br>(2 <sub>z</sub>  0,0)     | (3) 4 <sup>+</sup> 0,0<br>(4 <sub>z</sub>  0,0)             | (4) 4 <sup>-</sup> 0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0)        |
| (5) m' x,0<br>(m <sub>y</sub>  0,0)'     | (6) m' 0,y<br>(m <sub>x</sub>  0,0)'   | (7) m' x, $\bar{x}$<br>(m <sub>xy</sub>  0,0)'              | (8) m' x,x<br>(m <sub><math>\bar{xy}</math></sub>  0,0)'             |
| For $(1,0)$ ' + set                      |  |   |  |
| (1) t' (1,0)<br>(1 1,0)'                 | (2) 2' 1/2,0<br>(2 <sub>z</sub>  1,0)' | (3) 4 <sup>+</sup> ' 1/2,1/2<br>(4 <sub>z</sub>  1,0)'      | (4) 4 <sup>-</sup> ' 1/2,1/2<br>(4 <sub>z</sub> <sup>-1</sup>  1,0)' |
| (5) g (1,0) x,0<br>(m <sub>y</sub>  1,0) | (6) m 1/2,y<br>(m <sub>x</sub>  1,0)   | (7) g (1/2,-1/2) x+1/2, $\bar{x}$<br>(m <sub>xy</sub>  1,0) | (8) g (1/2,1/2) x+1/2,x<br>(m <sub><math>\bar{xy}</math></sub>  1,0) |

**Generators selected** (1);  $t(1,0)'$ ;  $t(0,1)'$ ; (2); (3); (5)

**Positions**

Wyckoff letter, Site symmetry	Coordinates			
	(0,0)+	(1,0)' +		
8 g 1	(1) $x, y [u, v]$	(2) $\bar{x}, \bar{y} [\bar{u}, \bar{v}]$	(3) $\bar{y}, x [\bar{v}, u]$	(4) $y, \bar{x} [v, \bar{u}]$
	(5) $x, \bar{y} [u, \bar{v}]$	(6) $\bar{x}, y [\bar{u}, v]$	(7) $\bar{y}, \bar{x} [\bar{v}, \bar{u}]$	(8) $y, x [v, u]$
4 f .m.	$x, 1/2 [0, v]$	$\bar{x}, 1/2 [0, v]$	$1/2, x [v, 0]$	$1/2, \bar{x} [v, 0]$
4 e .m'	$x, 0 [u, 0]$	$\bar{x}, 0 [\bar{u}, 0]$	$0, x [0, u]$	$0, \bar{x} [0, \bar{u}]$
4 d ..m'	$x, x [u, u]$	$\bar{x}, \bar{x} [\bar{u}, \bar{u}]$	$\bar{x}, x [\bar{u}, u]$	$x, \bar{x} [u, \bar{u}]$
2 c 2'mm'	$1/2, 0 [u, 0]$	$0, 1/2 [0, u]$		
1 b 4'm'm	$1/2, 1/2 [0, 0]$			
1 a 4m'm'	$0, 0 [0, 0]$			

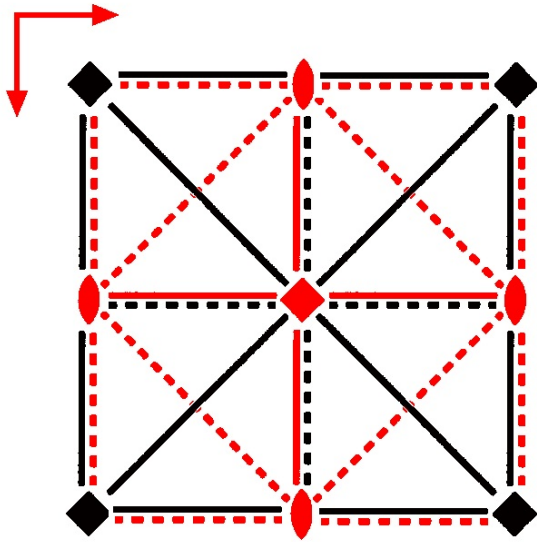
**Symmetry of special projections**

Along [10] $p_{2a \cdot m}$	Along [11] $p_{2a \cdot m}$
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$
Origin at $x, 1/2$	Origin at $x-1/4, x+1/4$



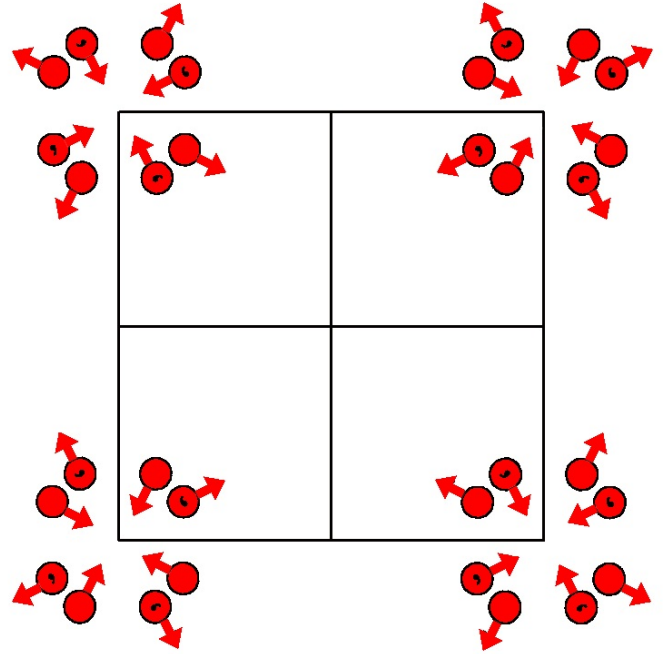
$p_4mm$

No. 11.7.59



$4mm1'$

$p_4mm$



Origin on  $4mm$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; x \leq y$

**Symmetry operations**

For  $(0,0) + \text{set}$

- |                                    |                                    |   |   |
|------------------------------------|------------------------------------|---|---|
| (1) 1<br>(1 0,0)                   | (2) 2 0,0<br>(2 <sub>z</sub>  0,0) | (3) 4 <sup>+</sup> 0,0<br>(4 <sub>z</sub>  0,0) | (4) 4 <sup>-</sup> 0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0) |
| (5) m x,0<br>(m <sub>y</sub>  0,0) | (6) m 0,y<br>(m <sub>x</sub>  0,0) | (7) m x, $\bar{x}$<br>(m <sub>xy</sub>  0,0)    | (8) m x,x<br>(m <sub><math>\bar{xy}</math></sub>  0,0)        |

For  $(1,0)' + \text{set}$

- |  |  |   |  |
|--|--|---|--|
| (1) t' (1,0)<br>(1 1,0)'                   | (2) 2' 1/2,0<br>(2 <sub>z</sub>  1,0)' | (3) 4 <sup>+</sup> ' 1/2,1/2<br>(4 <sub>z</sub>  1,0)'        | (4) 4 <sup>-</sup> ' 1/2,1/2<br>(4 <sub>z</sub> <sup>-1</sup>  1,0)'   |
| (5) g' (1,0) x,0<br>(m <sub>y</sub>  1,0)' | (6) m' 1/2,y<br>(m <sub>x</sub>  1,0)' | (7) g' (1/2,-1/2) x+1/2, $\bar{x}$<br>(m <sub>xy</sub>  1,0)' | (8) g' (1/2,1/2) x+1/2,x<br>(m <sub><math>\bar{xy}</math></sub>  1,0)' |

**Generators selected** (1);  $t(1,0)'$ ;  $t(0,1)'$ ; (2); (3); (5)

**Positions**

Wyckoff letter, Site symmetry	Coordinates			
	(0,0)+	(1,0)' +		
8 g 1	(1) $x, y [u, v]$	(2) $\bar{x}, \bar{y} [\bar{u}, \bar{v}]$	(3) $\bar{y}, x [\bar{v}, u]$	(4) $y, \bar{x} [v, \bar{u}]$
	(5) $x, \bar{y} [\bar{u}, v]$	(6) $\bar{x}, y [u, \bar{v}]$	(7) $\bar{y}, \bar{x} [v, u]$	(8) $y, x [\bar{v}, \bar{u}]$
4 f .m'	$x, 1/2 [u, 0]$	$\bar{x}, 1/2 [u, 0]$	$1/2, x [0, \bar{u}]$	$1/2, \bar{x} [0, \bar{u}]$
4 e .m.	$x, 0 [0, v]$	$\bar{x}, 0 [0, \bar{v}]$	$0, x [\bar{v}, 0]$	$0, \bar{x} [v, 0]$
4 d ..m	$x, x [\bar{u}, u]$	$\bar{x}, \bar{x} [u, \bar{u}]$	$\bar{x}, x [\bar{u}, \bar{u}]$	$x, \bar{x} [u, u]$
2 c 2'm'm.	$1/2, 0 [0, v]$	$0, 1/2 [\bar{v}, 0]$		
1 b 4'm'm	$1/2, 1/2 [0, 0]$			
1 a 4mm	$0, 0 [0, 0]$			

**Symmetry of special projections**

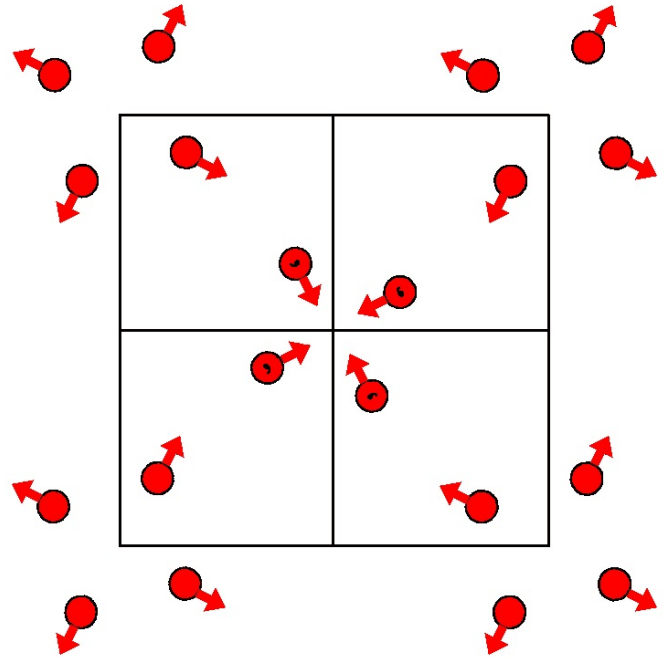
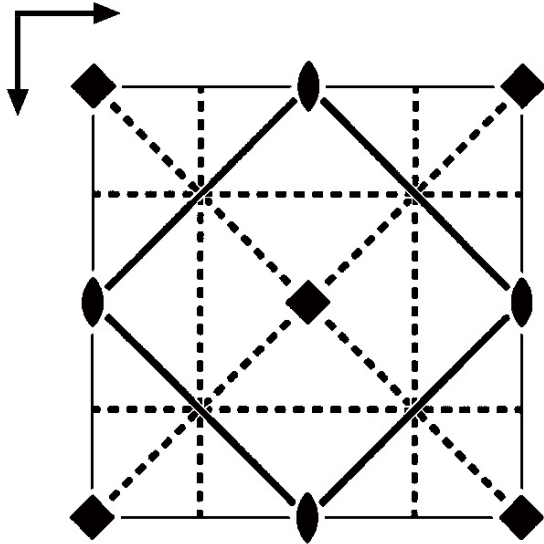
Along $[10] \rho m 1'$	Along $[11] \rho m 1'$
$\mathbf{a}^* = \mathbf{b}$	$\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$
Origin at $x, 0$	Origin at $x, x$

p4gm

4mm

No. 12.1.60

p4gm



Origin on 41g

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $y \leq 1/2 - x$

**Symmetry operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0)                                 | (2) 2 0,0<br>(2 <sub>z</sub>  0,0)               | (3) 4 <sup>+</sup> 0,0<br>(4 <sub>z</sub>  0,0) | (4) 4 <sup>-</sup> 0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0) |
| (5) g (1/2,0) x,1/4<br>(m <sub>y</sub>  1/2,1/2) | (6) g (0,1/2) 1/4,y<br>(m <sub>x</sub>  1/2,1/2) | (7) m x+1/2,x̄<br>(m <sub>xy</sub>  1/2,1/2)    | (8) g (1/2,1/2) x,x<br>(m <sub>xy</sub>  1/2,1/2)             |

**Generators selected** (1); t(1,0); t(0,1); (2); (3); (5)

**Positions**

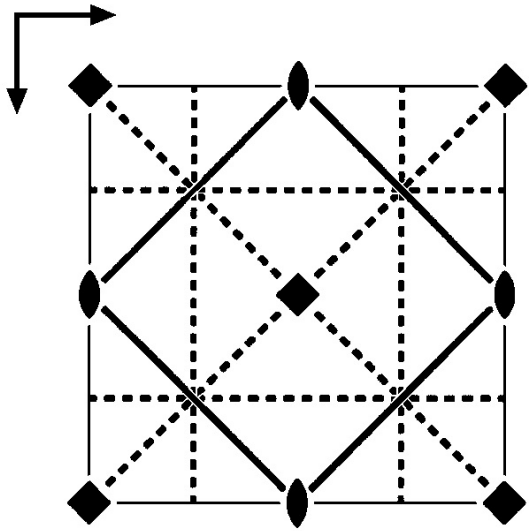
Multiplicity, Wyckoff letter, Site symmetry	Coordinates				
8 d 1	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [ $\bar{u},\bar{v}$ ]			
	(3) $\bar{y},x$ [ $\bar{v},u$ ]	(4) $y,\bar{x}$ [v, $\bar{u}$ ]			
	(5) $x+1/2,\bar{y}+1/2$ [ $\bar{u},v$ ]	(6) $\bar{x}+1/2,y+1/2$ [u, $\bar{v}$ ]			
	(7) $\bar{y}+1/2,\bar{x}+1/2$ [v,u]	(8) $y+1/2,x+1/2$ [ $\bar{v},\bar{u}$ ]			
	4 c ..m	$x,x+1/2$ [ $\bar{u},u$ ]	$\bar{x},\bar{x}+1/2$ [u, $\bar{u}$ ]	$\bar{x}+1/2,x$ [ $\bar{u},\bar{u}$ ]	$x+1/2,\bar{x}$ [u,u]
	2 b 2.mm	1/2,0 [0,0]	0,1/2 [0,0]		
	2 a 4..	0,0 [0,0]	1/2,1/2 [0,0]		

**Symmetry of special projections**

Along [10] $p_{2a^*m}$	Along [11] $pm1'$
$\mathbf{a}^* = \mathbf{b}/2$	$\mathbf{a}^* = (-\mathbf{a}+\mathbf{b})/2$
Origin at x,1/2	Origin at x,x

p4gm1'

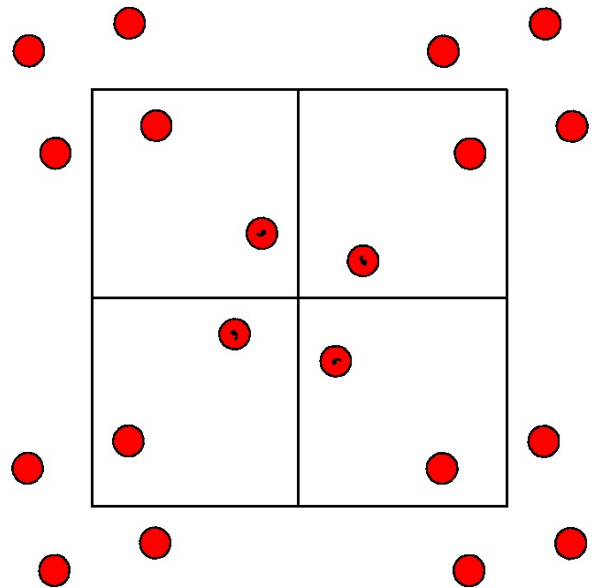
No. 12.2.61



4mm1'

p4gm1'

1'



Origin on 41g1'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $y \leq 1/2 - x$

**Symmetry operations**

For 1 + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0)                                 | (2) 2 0,0<br>(2 <sub>z</sub>  0,0)               | (3) 4 <sup>+</sup> 0,0<br>(4 <sub>z</sub>  0,0) | (4) 4 <sup>-</sup> 0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0) |
| (5) g (1/2,0) x,1/4<br>(m <sub>y</sub>  1/2,1/2) | (6) g (0,1/2) 1/4,y<br>(m <sub>x</sub>  1/2,1/2) | (7) m x+1/2,x̄<br>(m <sub>xy</sub>  1/2,1/2)    | (8) g (1/2,1/2) x,x<br>(m <sub>xy</sub>  1/2,1/2)             |

For 1' + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1'<br>(1 0,0)'                                 | (2) 2' 0,0<br>(2 <sub>z</sub>  0,0)'               | (3) 4 <sup>+</sup> ' 0,0<br>(4 <sub>z</sub>  0,0)' | (4) 4 <sup>-</sup> ' 0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (5) g' (1/2,0) x,1/4<br>(m <sub>y</sub>  1/2,1/2)' | (6) g' (0,1/2) 1/4,y<br>(m <sub>x</sub>  1/2,1/2)' | (7) m' x+1/2,x̄<br>(m <sub>xy</sub>  1/2,1/2)'     | (8) g' (1/2,1/2) x,x<br>(m <sub>xy</sub>  1/2,1/2)'                |

**Generators selected** (1); t(1,0); t(0,1); (2); (3); (5); 1'

**Positions**

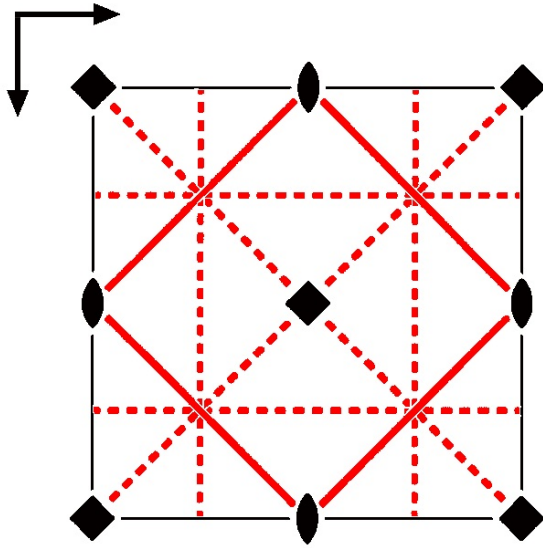
Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
	1+	1' +		
8 d 11'	(1) x,y [0,0]	(2) $\bar{x},\bar{y}$ [0,0]		
	(3) $\bar{y},x$ [0,0]	(4) $y,\bar{x}$ [0,0]		
	(5) $x+1/2,\bar{y}+1/2$ [0,0]	(6) $\bar{x}+1/2,y+1/2$ [0,0]		
	(7) $\bar{y}+1/2,\bar{x}+1/2$ [0,0]	(8) $y+1/2,x+1/2$ [0,0]		
4 c ..m1'	$x,x+1/2$ [0,0]	$\bar{x},\bar{x}+1/2$ [0,0]	$\bar{x}+1/2,x$ [0,0]	$x+1/2,\bar{x}$ [0,0]
2 b 2.mm1'	$1/2,0$ [0,0]	$0,1/2$ [0,0]		
2 a 4..1'	$0,0$ [0,0]	$1/2,1/2$ [0,0]		

**Symmetry of special projections**

Along [10] $\rho m 1'$	Along [11] $\rho m 1'$
$\mathbf{a}^* = \mathbf{b}/2$	$\mathbf{a}^* = (-\mathbf{a}+\mathbf{b})/2$
Origin at x,0	Origin at x,x

p4g'm'

No. 12.3.62



Origin on 41g'

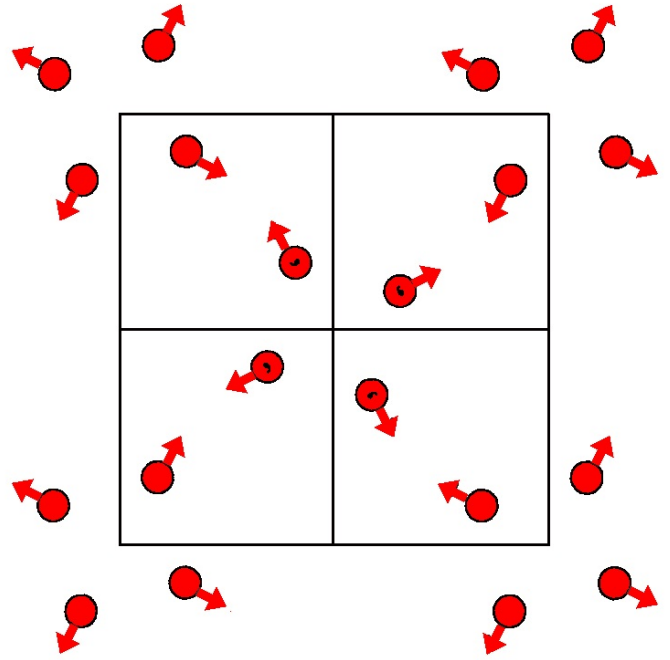
Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $y \leq 1/2 - x$

Symmetry operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0)                                   | (2) 2 0,0<br>(2 <sub>z</sub>  0,0)                 | (3) 4 <sup>+</sup> 0,0<br>(4 <sub>z</sub>  0,0) | (4) 4 <sup>-</sup> 0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0) |
| (5) g' (1/2,0) x,1/4<br>(m <sub>y</sub>  1/2,1/2)' | (6) g' (0,1/2) 1/4,y<br>(m <sub>x</sub>  1/2,1/2)' | (7) m' x+1/2,x̄<br>(m <sub>xy</sub>  1/2,1/2)'  | (8) g' (1/2,1/2) x,x<br>(m <sub>xy</sub>  1/2,1/2)'           |

4m'm'

p4g'm'



**Generators selected** (1); t(1,0); t(0,1); (2); (3); (5)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
	(1) x,y [u,v]	(2) $\bar{x},\bar{y}$ [ $\bar{u},\bar{v}$ ]	(3) $\bar{y},x$ [ $\bar{v},u$ ]	(4) $y,\bar{x}$ [v, $\bar{u}$ ]
8 d 1	(5) $x+1/2,\bar{y}+1/2$ [u, $\bar{v}$ ]	(6) $\bar{x}+1/2,y+1/2$ [ $\bar{u},v$ ]	(7) $\bar{y}+1/2,\bar{x}+1/2$ [ $\bar{v},\bar{u}$ ]	(8) $y+1/2,x+1/2$ [v,u]
4 c ..m'	$x,x+1/2$ [u,u]	$\bar{x},\bar{x}+1/2$ [ $\bar{u},\bar{u}$ ]	$\bar{x}+1/2,x$ [ $\bar{u},u$ ]	$x+1/2,\bar{x}$ [u, $\bar{u}$ ]
2 b 2.m'm'	$1/2,0$ [0,0]	$0,1/2$ [0,0]		
2 a 4..	$0,0$ [0,0]	$1/2,1/2$ [0,0]		

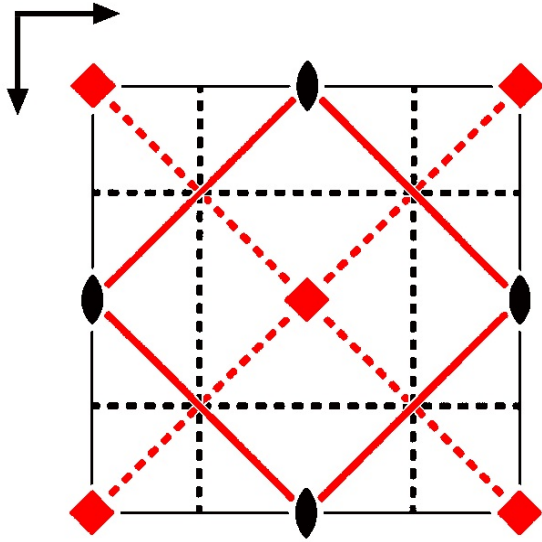
**Symmetry of special projections**

Along [10] $\rho m'$ $\mathbf{a}^* = \mathbf{b}/2$ Origin at x,0	Along [11] $\rho m'$ $\mathbf{a}^* = (-\mathbf{a}+\mathbf{b})/2$ Origin at x,x
--	--



p4'gm'

No. 12.4.63



Origin on 4'1g'

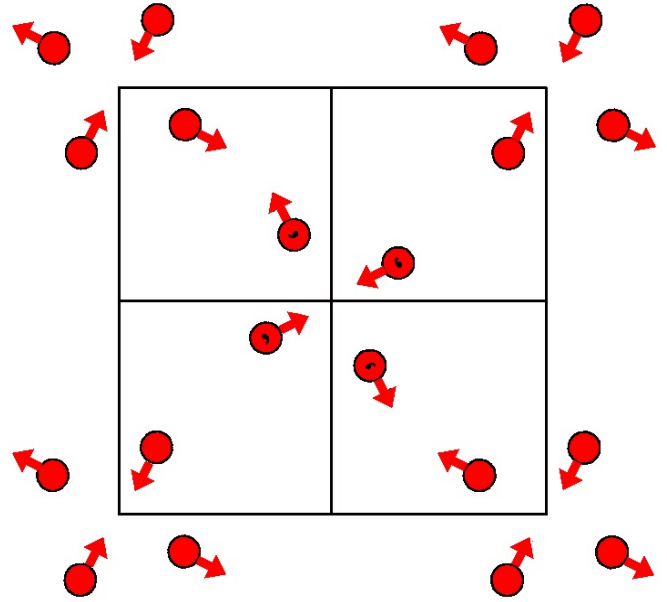
Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; y \leq 1/2 - x$

Symmetry operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0)                                 | (2) 2 <sub>z</sub> 0,0<br>(2 <sub>z</sub>  0,0)  | (3) 4 <sup>+</sup> 0,0<br>(4 <sub>z</sub>  0,0)' | (4) 4 <sup>-</sup> 0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0)' |
| (5) g (1/2,0) x,1/4<br>(m <sub>y</sub>  1/2,1/2) | (6) g (0,1/2) 1/4,y<br>(m <sub>x</sub>  1/2,1/2) | (7) m' x+1/2,x̄<br>(m <sub>xy</sub>  1/2,1/2)'   | (8) g' (1/2,1/2,0) x,x<br>(m <sub>xy</sub>  1/2,1/2)'          |

4'mm'

p4'gm'



**Generators selected** (1); t(1,0); t(0,1); (2); (3); (5)

**Positions**

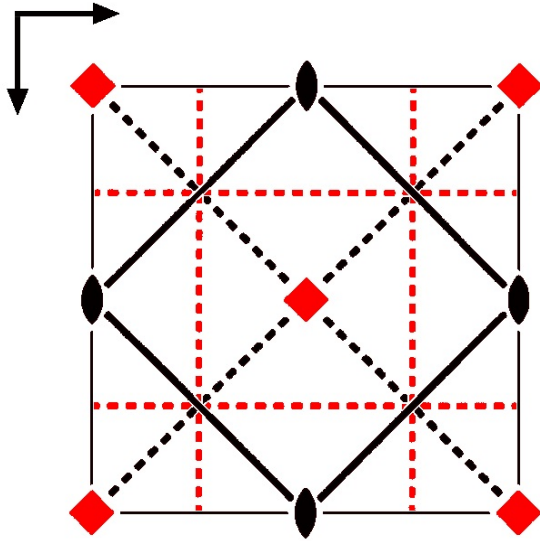
Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
	(1) $x, y$ [u, v]	(2) $\bar{x}, \bar{y}$ [ $\bar{u}, \bar{v}$ ]	(3) $\bar{y}, x$ [v, $\bar{u}$ ]	(4) $y, \bar{x}$ [ $\bar{v}, u$ ]
8 d 1	(5) $x+1/2, \bar{y}+1/2$ [ $\bar{u}, v$ ]	(6) $\bar{x}+1/2, y+1/2$ [u, $\bar{v}$ ]	(7) $\bar{y}+1/2, \bar{x}+1/2$ [ $\bar{v}, \bar{u}$ ]	(8) $y+1/2, x+1/2$ [v, u]
4 c ..m'	$x, x+1/2$ [u, u]	$\bar{x}, \bar{x}+1/2$ [ $\bar{u}, \bar{u}$ ]	$\bar{x}+1/2, x$ [u, $\bar{u}$ ]	$x+1/2, \bar{x}$ [ $\bar{u}, u$ ]
2 b 2.mm	$1/2, 0$ [0, 0]	$0, 1/2$ [0, 0]		
2 a 4'..	$0, 0$ [0, 0]	$1/2, 1/2$ [0, 0]		

**Symmetry of special projections**

Along [10] $p_{2a^*m}$ $\mathbf{a}^* = \mathbf{b}/2$ Origin at x, 0	Along [11] $pm$ $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$ Origin at x, x
---	--

p4'g'm

No. 12.5.64



Origin on 4'1g

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $y \leq 1/2 - x$

Symmetry operations

(1) 1  
(1|0,0)

(2) 2 0,0  
(2<sub>z</sub>|0,0)

(3) 4<sup>+</sup> 0,0  
(4<sub>z</sub><sup>+</sup>|0,0)'

(4) 4<sup>-</sup> 0,0  
(4<sub>z</sub><sup>-</sup>|0,0)'

(5) g' (1/2,0) x,1/4  
(m<sub>y</sub>|1/2,1/2)'

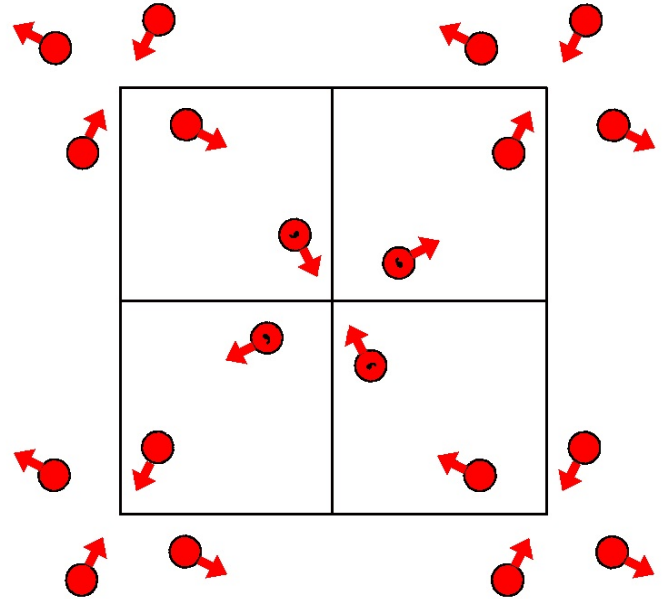
(6) g' (0,1/2) 1/4,y  
(m<sub>x</sub>|1/2,1/2)'

(7) m x+1/2,x̄  
(m<sub>xy</sub>|1/2,1/2)

(8) g (1/2,1/2) x,x  
(m<sub>xy</sub>|1/2,1/2)

4'm'm

p4'g'm



**Generators selected** (1); t(1,0); t(0,1); (2); (3); (5)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
	(1) $x, y$ [u, v]	(2) $\bar{x}, \bar{y}$ [ $\bar{u}, \bar{v}$ ]	(3) $\bar{y}, x$ [v, $\bar{u}$ ]	(4) $y, \bar{x}$ [ $\bar{v}, u$ ]
8 d 1	(5) $x+1/2, \bar{y}+1/2$ [u, $\bar{v}$ ]	(6) $\bar{x}+1/2, y+1/2$ [ $\bar{u}, v$ ]	(7) $\bar{y}+1/2, \bar{x}+1/2$ [v, u]	(8) $y+1/2, x+1/2$ [ $\bar{v}, \bar{u}$ ]
4 c ..m	$x, x+1/2$ [ $\bar{u}, u$ ]	$\bar{x}, \bar{x}+1/2$ [u, $\bar{u}$ ]	$\bar{x}+1/2, x$ [u, u]	$x+1/2, \bar{x}$ [ $\bar{u}, \bar{u}$ ]
2 b 2.mm	$1/2, 0$ [0, 0]	$0, 1/2$ [0, 0]		
2 a 4'..	$0, 0$ [0, 0]	$1/2, 1/2$ [0, 0]		

**Symmetry of special projections**

Along [10] $\rho m$ $\mathbf{a}^* = \mathbf{b}/2$ Origin at x, 0	Along [11] $\rho m 1'$ $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$ Origin at x, x
--	---

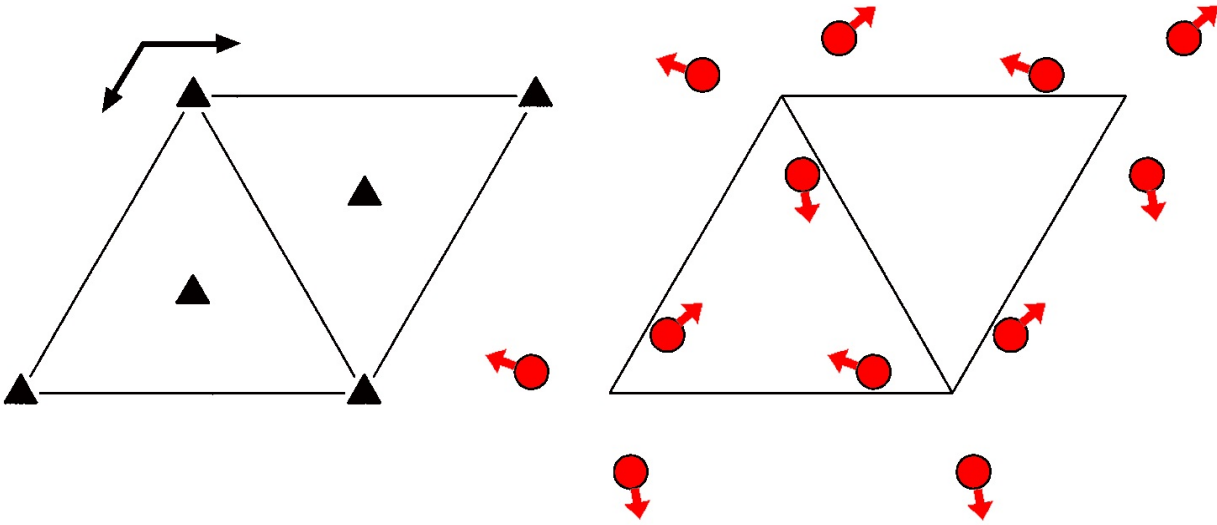
p3

No. 13.1.65

3

1

p3



**Origin on 3**

**Asymmetric unit**  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $x \leq (1 + y)/2$ ;

$$y \leq \min(1 - x, (1 + x)/2)$$

**Vertices** 0,0; 1/2,0; 2/3,1/3; 1/3,2/3; 0,1/2

**Symmetry operations**

(1) 1  
(1|0,0)

(2)  $3^+$  0,0  
( $3_z$ |0,0)

(3)  $3^-$  0,0  
( $3_z^{-1}$ |0,0)

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ; (2)

**Positions**

		Coordinates		
Wyckoff letter, Site symmetry				
3	d 1	(1) $x,y [u,v]$	(2) $\bar{y},x-y [\bar{v},u-v]$	(3) $\bar{x}+y,\bar{x} [\bar{u}+v,\bar{u}]$
1	c 3..	$2/3,1/3 [0,0]$		
1	b 3..	$1/3,2/3 [0,0]$		
1	a 3..	$0,0 [0,0]$		

**Symmetry of special projections**

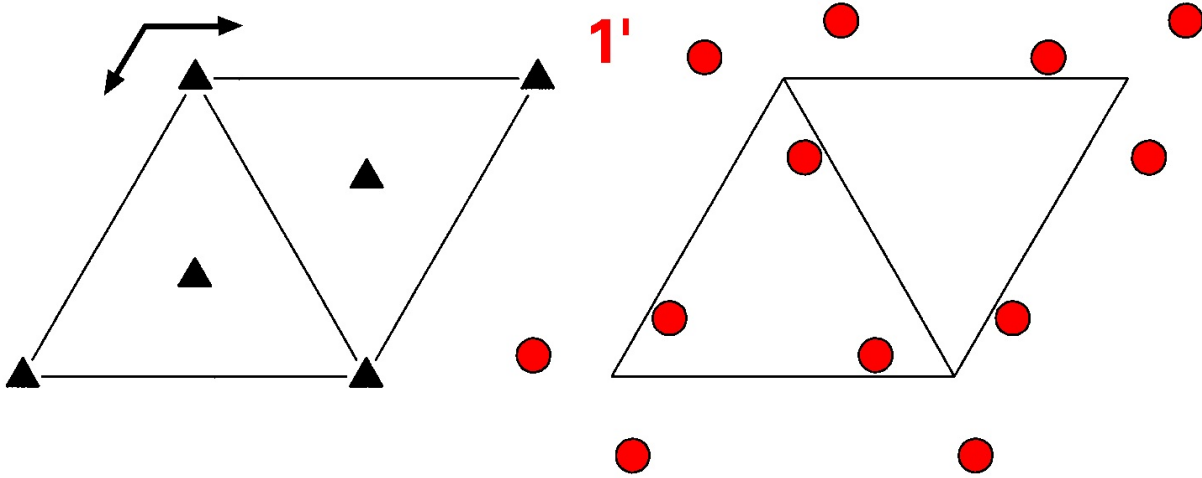
Along $[10] p1$	Along $[21] p1$
$\mathbf{a}^* = (\mathbf{a}+2\mathbf{b})/2$	$\mathbf{a}^* = \mathbf{b}/2$
Origin at $x,0$	Origin at $x,x/2$

p31'

No. 13.2.66

31'

p31'



Origin on 31'

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $x \leq (1 + y)/2$ ;

$$y \leq \min(1 - x, (1 + x)/2)$$

Vertices  $0,0$ ;  $1/2,0$ ;  $2/3,1/3$ ;  $1/3,2/3$ ;  $0,1/2$

**Symmetry operations**

For 1 + set

(1) 1

$$(1|0,0)$$

(2)  $3^+$  0,0

$$(3_z|0,0)$$

(3)  $3^-$  0,0

$$(3_z^{-1}|0,0)$$

For 1' + set

(1) 1'

$$(1|0,0)'$$

(2)  $3^{+'}$  0,0

$$(3_z|0,0)'$$

(3)  $3^{-'}$  0,0

$$(3_z^{-1}|0,0)'$$

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ; (2);  $1'$

**Positions**

Wyckoff letter, Site symmetry	Coordinates		
		1+	1' +
3 d 11'	(1) $x,y [0,0]$	(2) $\bar{y},x-y [0,0]$	(3) $\bar{x}+y,\bar{x} [0,0]$
1 c 3..1	$2/3,1/3 [0,0]$		
1 b 3..1'	$1/3,2/3 [0,0]$		
1 a 3..1'	$0,0 [0,0]$		

**Symmetry of special projections**

Along [10] $p11'$	Along [21] $p11'$
$\mathbf{a}^* = (\mathbf{a}+2\mathbf{b})/2$	$\mathbf{a}^* = \mathbf{b}/2$
Origin at $x,0$	Origin at $x,x/2$

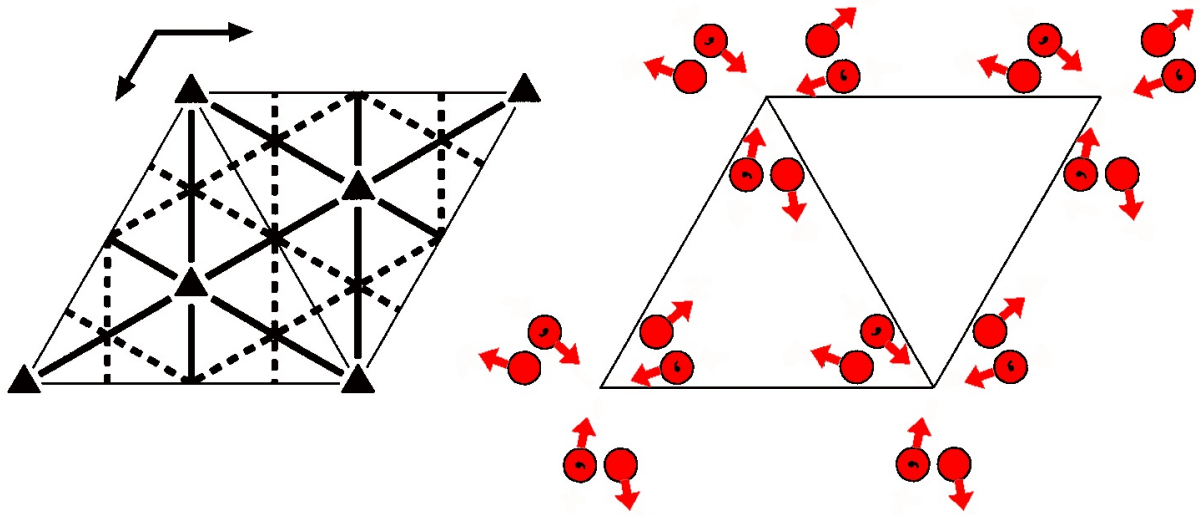


p3m1

3m1

No. 14.1.67

p3m1



**Origin on 3m1**

**Asymmetric unit**  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $x \leq 2y$ ;

$$y \leq \min(1 - x, 2x)$$

**Vertices**  $0,0$ ;  $2/3,1/3$ ;  $1/3,2/3$

**Symmetry operations**

(1) 1  
(1|0,0)

(2)  $3^+$  0,0  
( $3_z$ |0,0)

(3)  $3^-$  0,0  
( $3_z^{-1}$ |0,0)

(4) m  $x, \bar{x}$   
( $m_{xy}$ |0,0)

(5) m  $x, 2x$   
( $m_x$ |0,0)

(6) m  $2x, x$   
( $m_y$ |0,0)

**Generators selected** (1); t(1,0); t(0,1); (2); (4)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
	(1) $x, y$ [u,v]	(2) $\bar{y}, x-y$ [ $\bar{v}, u-v$ ]	(3) $\bar{x}+y, \bar{x}$ [ $\bar{u}+v, \bar{u}$ ]
6 e 1	(4) $\bar{y}, \bar{x}$ [v,u]	(5) $\bar{x}+y, y$ [u-v, $\bar{v}$ ]	(6) $x, x-y$ [ $\bar{u}, \bar{u}+v$ ]
3 d .m.	$x, \bar{x}$ [u,u]	$x, 2x$ [ $\bar{u}, 0$ ]	$2\bar{x}, \bar{x}$ , [0, $\bar{u}, 0$ ]
1 c 3m.	$2/3, 1/3$ [0,0]		
1 b 3m.	$1/3, 2/3$ [0,0]		
1 a 3m.	0,0 [0,0]		

**Symmetry of special projections**

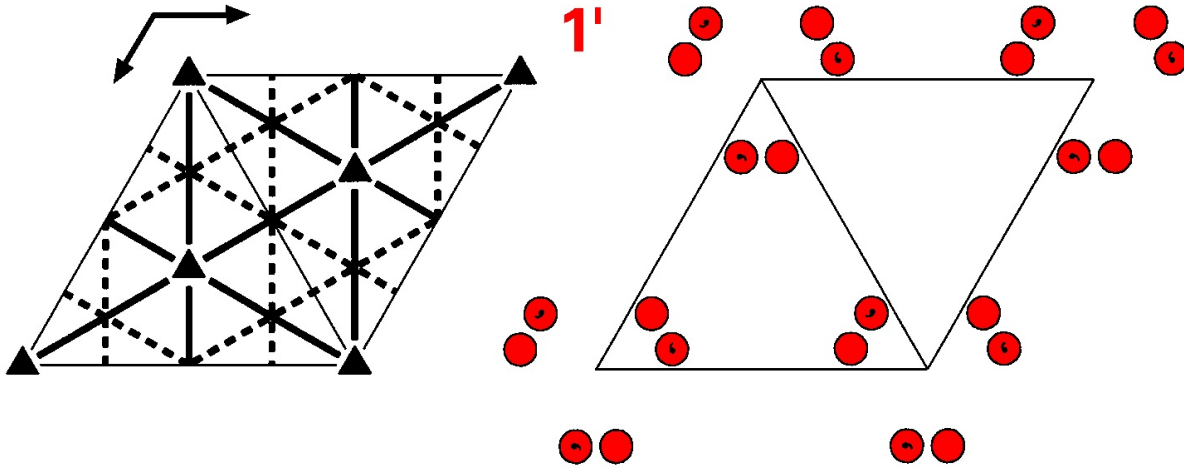
Along [10] $p11'$ $\mathbf{a}^* = (\mathbf{a}+2\mathbf{b})/2$ Origin at x,0	Along [21] $\rho m$ $\mathbf{a}^* = \mathbf{b}/2$ Origin at x,x/2
---	---

p3m11'

3m11'

No. 14.2.68

p3m11'



Origin on 3m11'

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $x \leq 2y$ ;

$$y \leq \min(1 - x, 2x)$$

Vertices  $0,0$ ;  $2/3,1/3$ ;  $1/3,2/3$

### Symmetry operations

For 1 + set

(1) 1

$$(1|0,0)$$

(2)  $3^+$  0,0

$$(3_z|0,0)$$

(3)  $3^-$  0,0

$$(3_z^{-1}|0,0)$$

(4) m  $x, \bar{x}$

$$(m_{xy}|0,0)$$

(5) m  $x, 2x$

$$(m_x|0,0)$$

(6) m  $2x, x$

$$(m_y|0,0)$$

For 1' + set

(1) 1'

$$(1|0,0)'$$

(2)  $3^{+'}$  0,0

$$(3_z|0,0)'$$

(3)  $3^{-'}$  0,0

$$(3_z^{-1}|0,0)'$$

(4) m'  $x, \bar{x}$

$$(m_{xy}|0,0)'$$

(5) m'  $x, 2x$

$$(m_x|0,0)'$$

(6) m'  $2x, x$

$$(m_y|0,0)'$$

**Generators selected** (1); t(1,0); t(0,1); (2); (4); 1'

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
	1+	1' +	
6 e 11'	(1) x,y [0,0]	(2) $\bar{y}$ ,x-y [0,0]	(3) $\bar{x}$ +y, $\bar{x}$ [0,0]
	(4) $\bar{y}$ , $\bar{x}$ [0,0]	(5) $\bar{x}$ +y,y [0,0]	(6) x,x-y [0,0]
3 d .m.1'	x, $\bar{x}$ [0,0]	x,2x [0,0]	2 $\bar{x}$ , $\bar{x}$ [0,0]
1 c 3m.1'	2/3,1/3 [0,0]		
1 b 3m.1'	1/3,2/3 [0,0]		
1 a 3m.1'	0,0 [0,0]		

**Symmetry of special projections**

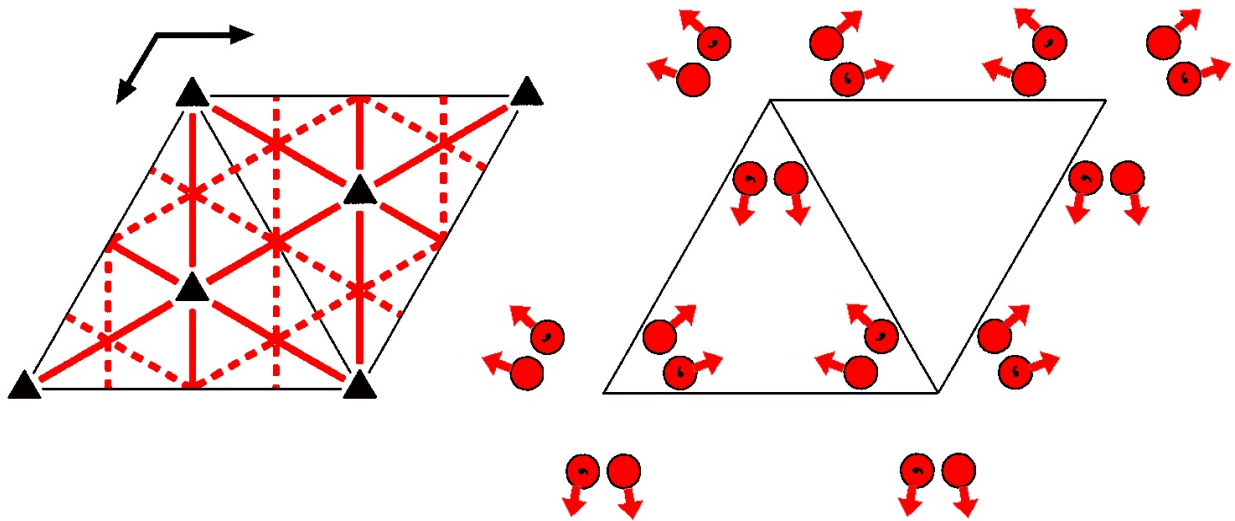
Along [10] $p11'$	Along [21] $\rho m1'$
$\mathbf{a}^* = (\mathbf{a}+2\mathbf{b})/2$	$\mathbf{a}^* = \mathbf{b}/2$
Origin at x,0	Origin at x,x/2

p3m'1

3m'1

No. 14.3.69

p3m'1



Origin on 3m'1

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $x \leq 2y$ ;

$$y \leq \min(1 - x, 2x)$$

Vertices  $0,0$ ;  $2/3,1/3$ ;  $1/3,2/3$

Symmetry operations

(1) 1  
(1|0,0)

(2)  $3^+$  0,0  
( $3_z$ |0,0)

(3)  $3^-$  0,0  
( $3_z^{-1}$ |0,0)

(4)  $m'$   $x, \bar{x}$   
( $m_{xy}$ |0,0)'

(5)  $m'$   $x, 2x$   
( $m_x$ |0,0)'

(6)  $m'$   $2x, x$   
( $m_y$ |0,0)'

**Generators selected** (1); t(1,0); t(0,1); (2); (4)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
	(1) $x, y$ [u, v]	(2) $\bar{y}, x-y$ [ $\bar{v}, u-v$ ]	(3) $\bar{x}+y, \bar{x}$ [ $\bar{u}+v, \bar{u}$ ]
6 e 1	(4) $\bar{y}, \bar{x}$ [ $\bar{v}, \bar{u}$ ]	(5) $\bar{x}+y, y$ [ $\bar{u}+v, v$ ]	(6) $x, x-y$ [u, u-v]
3 d .m'	$x, \bar{x}$ [u, $\bar{u}$ ]	$x, 2x$ [u, 2u]	$2\bar{x}, \bar{x}$ [2 $\bar{u}$ , $\bar{u}$ ]
1 c 3m'	$2/3, 1/3$ [0, 0]		
1 b 3m'	$1/3, 2/3$ [0, 0]		
1 a 3m'	0, 0 [0, 0]		

**Symmetry of special projections**

Along [10]  $\rho 1$   
 $\mathbf{a}^* = (\mathbf{a}+2\mathbf{b})/2$   
 Origin at x, 0

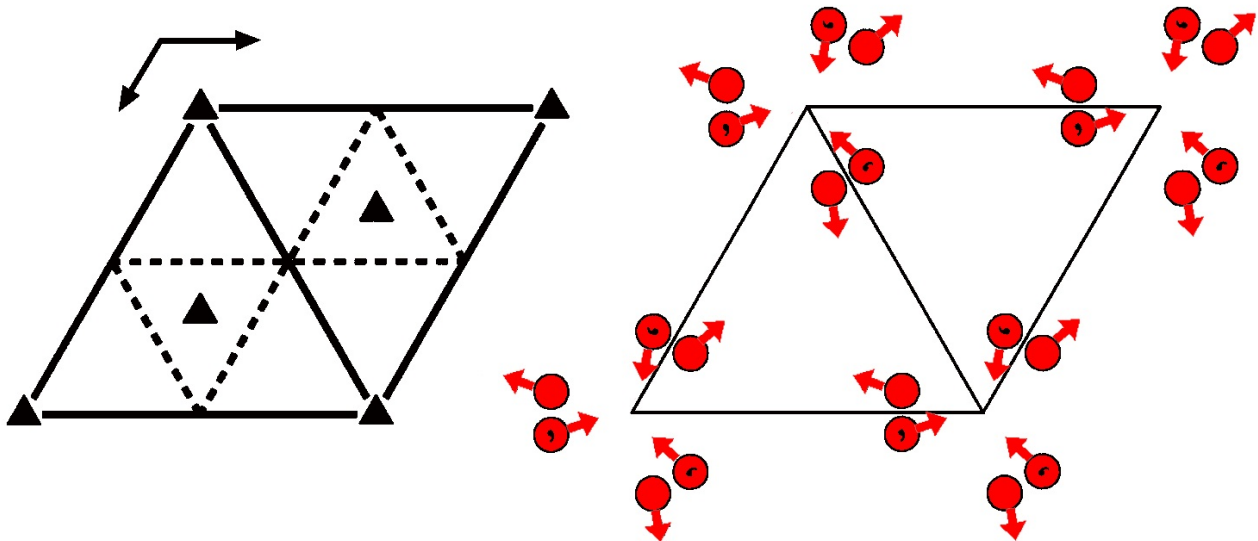
Along [21]  $\rho m'$   
 $\mathbf{a}^* = \mathbf{b}/2$   
 Origin at x, x/2

p31m

31m

No. 15.1.70

p31m



**Origin** on 31m

**Asymmetric unit**  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/2$ ;  $x \leq (y + 1)/2$ ;

$$y \leq \min(1 - x, x)$$

**Vertices**  $0,0$ ;  $1/2,0$ ;  $2/3,1/3$ ;  $1/2,1/2$

**Symmetry operations**

- |                            |                                |                                     |
|----------------------------|--------------------------------|-------------------------------------|
| (1) 1<br>(1 0,0)           | (2) $3^+$ 0,0<br>( $3_z$  0,0) | (3) $3^-$ 0,0<br>( $3_z^{-1}$  0,0) |
| (4) m x,x<br>( $m_3$  0,0) | (5) m x,0<br>( $m_2$  0,0)     | (6) m 0,y<br>( $m_1$  0,0)          |

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ; (2); (4)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
	(1) $x,y$ [ $u,v$ ]	(2) $\bar{y},x-y$ [ $\bar{v},u-v$ ]	(3) $\bar{x}+y,\bar{x}$ [ $\bar{u}+v,\bar{u}$ ]
6 d 1	(4) $y,x$ [ $\bar{v},\bar{u}$ ]	(5) $x-y,\bar{y}$ [ $\bar{u}+v,v$ ]	(6) $\bar{x},\bar{x}+y$ [ $u,u-v$ ]
3 c ..m	$x,0$ [ $u,2u$ ]	$0,x$ [ $2\bar{u},\bar{u}$ ]	$\bar{x},\bar{x}$ [ $u,\bar{u}$ ]
2 b 3..	$1/3,2/3$ [ $0,0$ ]	$2/3,1/3$ [ $0,0$ ]	
1 a 3.m	$0,0$ [ $0,0$ ]		

**Symmetry of special projections**

Along $[10]$ $pm$ $\mathbf{a}^* = (\mathbf{a}+2\mathbf{b})/2$ Origin at $x,0$	Along $[21]$ $p11'$ $\mathbf{a}^* = \mathbf{b}/2$ Origin at $x,x/2$
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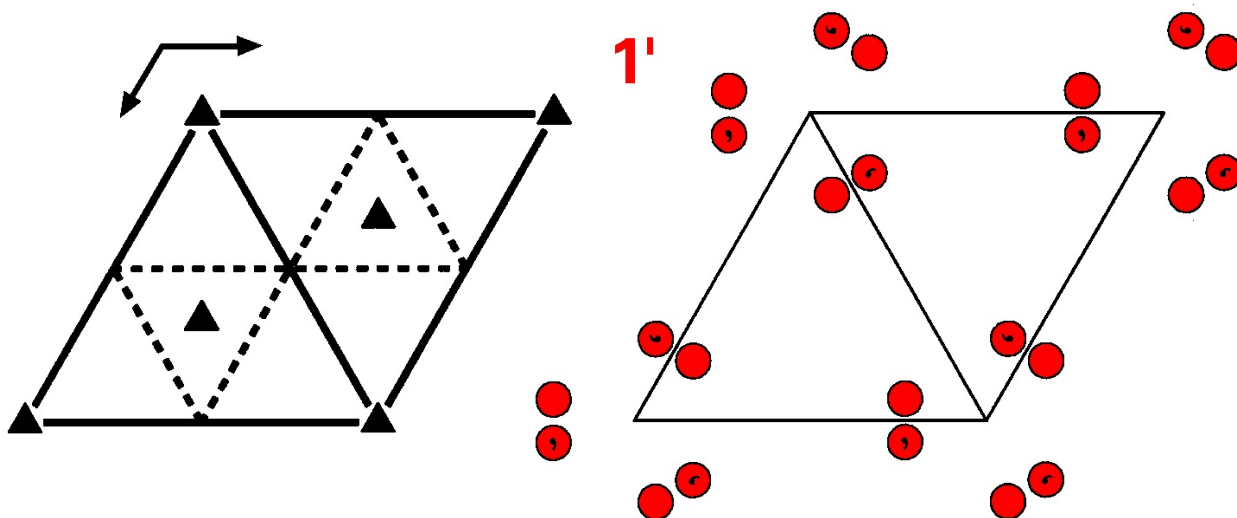


p31m1'

31m1'

No. 15.2.71

p31m1'



**Origin** on 31m1'

**Asymmetric unit**  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/2$ ;  $x \leq (y + 1)/2$ ;

$$y \leq \min(1 - x, x)$$

**Vertices** 0,0; 1/2,0; 2/3,1/3; 1/2,1/2

**Symmetry operations**

For 1 + set

(1) 1

$$(1|0,0)$$

(2)  $3^+$  0,0

$$(3_z|0,0)$$

(3)  $3^-$  0,0

$$(3_z^{-1}|0,0)$$

(4) m x,x

$$(m_3|0,0)$$

(5) m x,0

$$(m_2|0,0)$$

(6) m 0,y

$$(m_1|0,0)$$

For 1' + set

(1) 1'

$$(1|0,0)'$$

(2)  $3^{+'}$  0,0

$$(3_z|0,0)'$$

(3)  $3^{-'}$  0,0

$$(3_z^{-1}|0,0)'$$

(4) m' x,x

$$(m_3|0,0)'$$

(5) m' x,0

$$(m_2|0,0)'$$

(6) m' 0,y

$$(m_1|0,0)'$$

**Generators selected** (1); t(1,0); t(0,1); (2); (4); 1'

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
	1+	1' +	
6 d 11'	(1) x,y [0,0]	(2) $\bar{y},x-y$ [0,0]	(3) $\bar{x}+y,\bar{x}$ [0,0]
	(4) y,x [0,0]	(5) x-y, $\bar{y}$ [0,0]	(6) $\bar{x},\bar{x}+y$ [0,0]
3 c ..m1'	x,0 [0,0]	0,x [0,0]	$\bar{x},\bar{x}$ [0,0]
2 b 3..1'	1/3,2/3 [0,0]	2/3,1/3 [0,0]	
1 a 3.m1'	0,0 [0,0]		

**Symmetry of special projections**

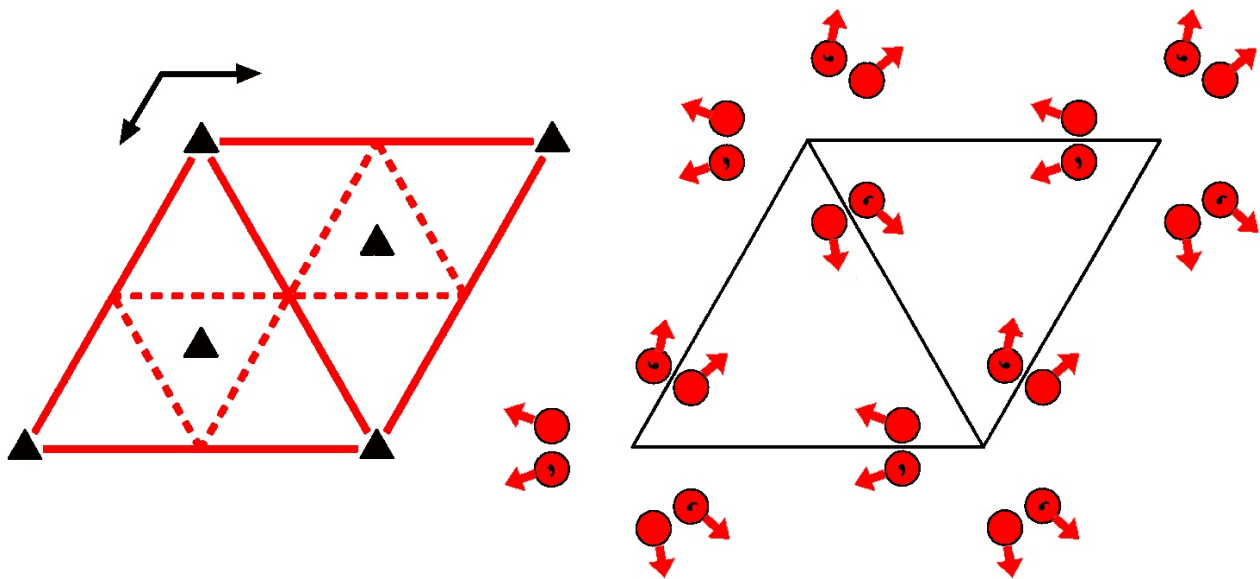
Along [10] $\rho m 1'$	Along [21] $\rho 11'$
$\mathbf{a}^* = (\mathbf{a}+2\mathbf{b})/2$	$\mathbf{a}^* = \mathbf{b}/2$
Origin at x,0	Origin at x,x/2

p31m'

No. 15.3.72

31m'

p31m'



Origin on 31m'

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/2$ ;  $x \leq (y + 1)/2$ ;

$$y \leq \min(1 - x, x)$$

Vertices  $0,0$ ;  $1/2,0$ ;  $2/3,1/3$ ;  $1/2,1/2$

Symmetry operations

(1) 1  
(1|0,0)

(2)  $3^+$  0,0  
( $3_z$ |0,0)

(3)  $3^-$  0,0  
( $3_z^{-1}$ |0,0)

(4)  $m'$  x,x  
( $m_3$ |0,0)'

(5)  $m'$  x,0  
( $m_2$ |0,0)'

(6)  $m'$  0,y  
( $m_1$ |0,0)'

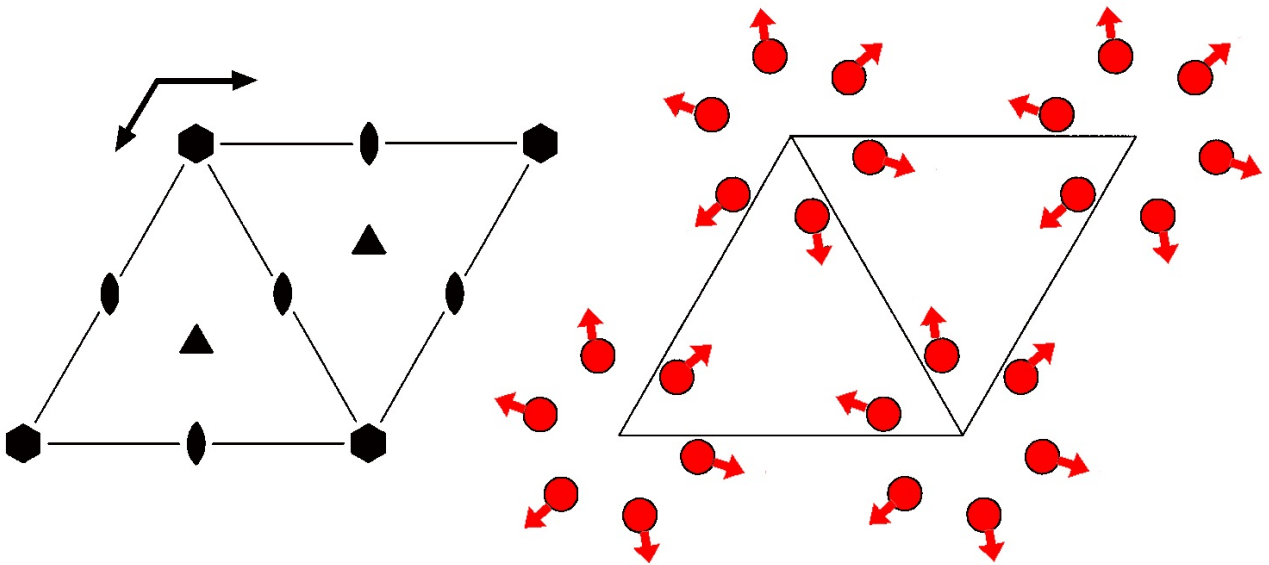
**Generators selected** (1); t(1,0); t(0,1); (2); (4)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
	(1) x,y [u,v]	(2) $\bar{y},x-y$ [ $\bar{v},u-v$ ]	(3) $\bar{x}+y,\bar{x}$ [ $\bar{u}+v,\bar{u}$ ]
6 d 1	(4) y,x [v,u]	(5) x-y, $\bar{y}$ [u-v, $\bar{v}$ ]	(6) $\bar{x},\bar{x}+y$ [ $\bar{u},\bar{u}+v$ ]
3 c ..m'	x,0 [u,0]	0,x [0,u]	$\bar{x},\bar{x}$ [ $\bar{u},\bar{u}$ ]
2 b 3..	1/3,2/3 [0,0]	2/3,1/3 [0,0]	
1 a 3.m'	0,0 [0,0]		

**Symmetry of special projections**

Along [10] $\rho m'$	Along [21] $\rho 1$
$\mathbf{a}^* = (\mathbf{a}+2\mathbf{b})/2$	$\mathbf{a}^* = \mathbf{b}/2$
Origin at x,0	Origin at x,x/2



**Origin** on 6

**Asymmetric unit**  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/2$ ;  $x \leq (1+y)/2$ ;

$$y \leq \min(1-x, x)$$

**Vertices** 0,0; 1/2,0; 2/3,1/3; 1/2,1/2

**Symmetry operations**

(1) 1  
(1|0,0)

(2)  $3^+$  0,0  
( $3_z$ |0,0)

(3)  $3^-$  0,0  
( $3_z^{-1}$ |0,0)

(4) 2 0,0  
( $2_z$ |0,0)

(5)  $6^-$  0,0  
( $6_z^{-1}$ |0,0)

(6)  $6^+$  0,0  
( $6_z$ |0,0)

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ; (2); (4)

**Positions**

		Coordinates		
Multiplicity, Wyckoff letter, Site symmetry				
6	d 1	(1) $x,y [u,v]$	(2) $\bar{y},x-y [\bar{v},u-v]$	(3) $\bar{x}+y,\bar{x} [\bar{u}+v,\bar{u}]$
		(4) $\bar{x},\bar{y} [\bar{u},\bar{v}]$	(5) $y,\bar{x}+y [v,\bar{u}+v]$	(6) $x-y,x [u-v,u]$
3	c 2..	$1/2,0 [0,0]$	$0,1/2 [0,0]$	$1/2,1/2 [0,0]$
2	b 3..	$1/3,2/3 [0,0]$	$2/3,1/3 [0,0]$	
1	a 6..	$0,0 [0,0]$		

**Symmetry of special projections**

Along  $[10] \rho m'$   
 $\mathbf{a}^* = (\mathbf{a}+2\mathbf{b})/2$   
 Origin at  $x,0$

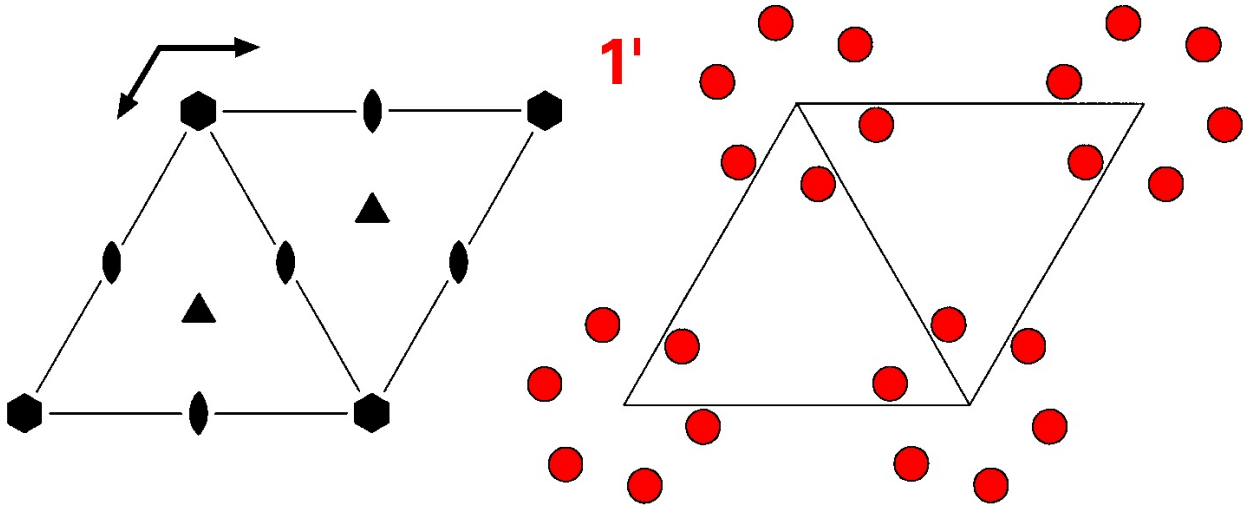
Along  $[21] \rho m'$   
 $\mathbf{a}^* = \mathbf{b}/2$   
 Origin at  $x,x/2$

p61'

61'

No. 16.2.74

p61'



Origin on 61'

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/2$ ;  $x \leq (1+y)/2$ ;

$$y \leq \min(1-x, x)$$

Vertices  $0,0$ ;  $1/2,0$ ;  $2/3,1/3$ ;  $1/2,1/2$

### Symmetry operations

For 1 + set

(1) 1 (1 0,0)	(2) $3^+$ 0,0 ( $3_z$  0,0)	(3) $3^-$ 0,0 ( $3_z^{-1}$  0,0)
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(4) 2 0,0 ( $2_z$  0,0)	(5) $6^-$ 0,0 ( $6_z^{-1}$  0,0)	(6) $6^+$ 0,0 ( $6_z$  0,0)
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For 1' + set

(1) 1' (1 0,0)'	(2) $3^{+'}$ 0,0 ( $3_z$  0,0)'	(3) $3^{-'}$ 0,0 ( $3_z^{-1}$  0,0)'
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(4) $2'$ 0,0 ( $2_z$  0,0)'	(5) $6^{-'}$ 0,0 ( $6_z^{-1}$  0,0)'	(6) $6^{+'}$ 0,0 ( $6_z$  0,0)'
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**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ; (2); (4);  $1'$

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
	1+	1' +	
6 d 11'	(1) $x,y$ [0,0]	(2) $\bar{y},x-y$ [0,0]	(3) $\bar{x}+y,\bar{x}$ [0,0]
	(4) $\bar{x},\bar{y}$ [0,0]	(5) $y,\bar{x}+y$ [0,0]	(6) $x-y,x$ [0,0]
3 c 2..1'	$1/2,0$ [0,0]	$0,1/2$ [0,0]	$1/2,1/2$ [0,0]
2 b 3..1'	$1/3,2/3$ [0,0]	$2/3,1/3$ [0,0]	
1 a 6..1'	$0,0$ [0,0]		

**Symmetry of special projections**

Along $[10]$ $\rho m 1'$ $\mathbf{a}^* = (\mathbf{a}+2\mathbf{b})/2$ Origin at $x,0$	Along $[21]$ $\rho m 1'$ $\mathbf{a}^* = \mathbf{b}/2$ Origin at $x,x/2$
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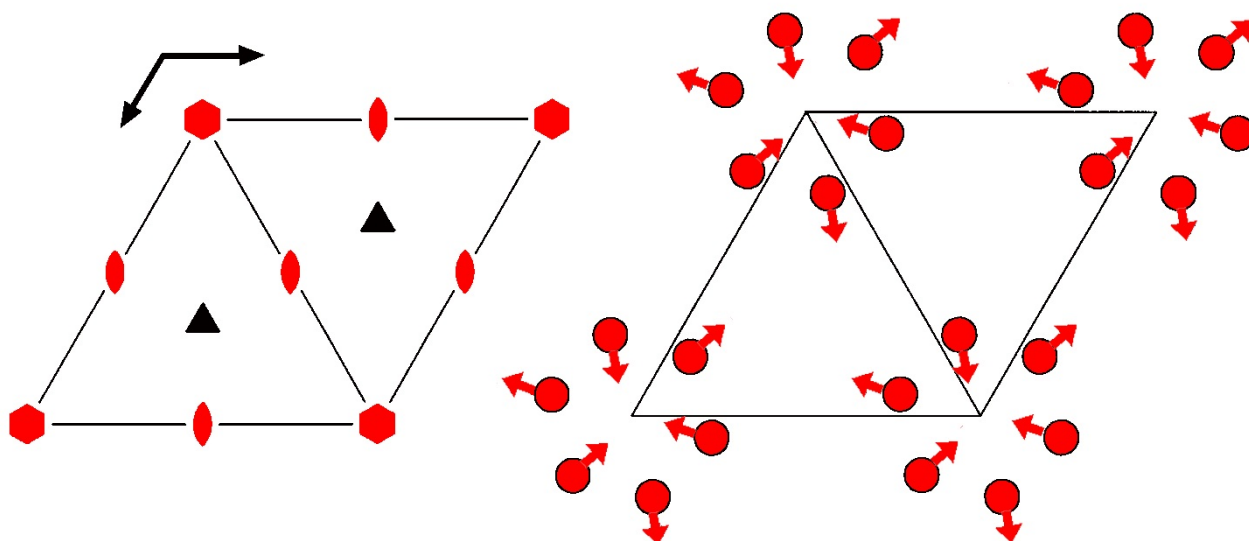


p6'

6'

No. 16.3.75

p6'



Origin on 6'

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/2$ ;  $x \leq (1+y)/2$ ;

$$y \leq \min(1-x, x)$$

Vertices  $0,0$ ;  $1/2,0$ ;  $2/3,1/3$ ;  $1/2,1/2$

Symmetry operations

(1) 1  
(1|0,0)

(2)  $3^+$  0,0  
( $3_z$ |0,0)

(3)  $3^-$  0,0  
( $3_z^{-1}$ |0,0)

(4)  $2'$  0,0  
( $2_z$ |0,0)'

(5)  $6^-$  0,0  
( $6_z^{-1}$ |0,0)'

(6)  $6^+$  0,0  
( $6_z$ |0,0)'

**Generators selected** (1); t(1,0); t(0,1); (2); (4)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
	(1) $x, y$ [u,v]	(2) $\bar{y}, x-y$ [ $\bar{v}, u-v$ ]	(3) $\bar{x}+y, \bar{x}$ [ $\bar{u}+v, \bar{u}$ ]
6 d 1	(4) $\bar{x}, \bar{y}$ [u,v]	(5) $y, \bar{x}+y$ [ $\bar{v}, u-v$ ]	(6) $x-y, x$ [ $\bar{u}+v, \bar{u}$ ]
3 c 2'..	1/2,0 [u,v]	0,1/2 [ $\bar{v}, u-v$ ]	1/2,1/2 [ $\bar{u}+v, \bar{u}$ ]
2 b 3..	1/3,2/3 [0,0]	2/3,1/3 [0,0]	
1 a 6'..	0,0 [0,0]		

**Symmetry of special projections**

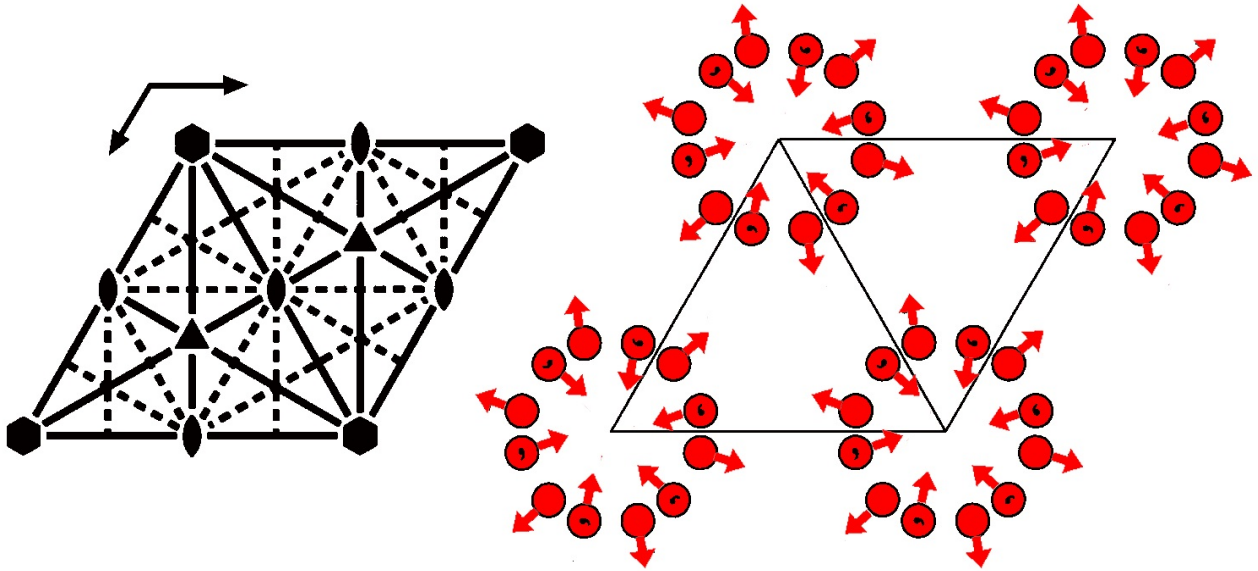
Along [10] $\rho m$ $\mathbf{a}^* = (\mathbf{a}+2\mathbf{b})/2$ Origin at x,0	Along [21] $\rho m$ $\mathbf{a}^* = \mathbf{b}/2$ Origin at x,x/2
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p6mm

6mm

No. 17.1.76

p6mm



Origin on 6mm

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/3$ ;  $x \leq (1 + y)/2$ ;  $y \leq x/2$

Vertices  $0,0$ ;  $1/2,0$ ;  $2/3,1/3$

**Symmetry operations**

- |  |                                     |                                     |
|--|-------------------------------------|-------------------------------------|
| (1) 1<br>(1 0,0)                       | (2) $3^+$ 0,0<br>( $3_z$  0,0)      | (3) $3^-$ 0,0<br>( $3_z^{-1}$  0,0) |
| (4) 2 0,0<br>( $2_z$  0,0)             | (5) $6^-$ 0,0<br>( $6_z^{-1}$  0,0) | (6) $6^+$ 0,0<br>( $6_z$  0,0)      |
| (7) m $x, \bar{x}$<br>( $m_{xy}$  0,0) | (8) m $x, 2x$<br>( $m_x$  0,0)      | (9) m $2x, x$<br>( $m_y$  0,0)      |
| (10) m $x, x$<br>( $m_3$  0,0)         | (11) m $x, 0$<br>( $m_2$  0,0)      | (12) m $0, y$<br>( $m_1$  0,0)      |

**Generators selected** (1); t(1,0,0); t(0,1,0); (2); (4); (7)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
	(1) $x, y$ [u, v]	(2) $\bar{y}, x-y$ [ $\bar{v}, u-v$ ]	(3) $\bar{x}+y, \bar{x}$ [ $\bar{u}+v, \bar{u}$ ]
12 f 1	(4) $\bar{x}, \bar{y}$ [ $\bar{u}, \bar{v}$ ]	(5) $y, \bar{x}+y$ [ $v, \bar{u}+v$ ]	(6) $x-y, x$ [ $u-v, u$ ]
	(7) $\bar{y}, \bar{x}$ [ $v, u$ ]	(8) $\bar{x}+y, y$ [ $u-v, \bar{v}$ ]	(9) $x, x-y$ [ $\bar{u}, \bar{u}+v$ ]
	(10) $y, x$ [ $\bar{v}, \bar{u}$ ]	(11) $x-y, \bar{y}$ [ $\bar{u}+v, v$ ]	(12) $\bar{x}, \bar{x}+y$ [ $u, u-v$ ]
6 e .m.	$x, \bar{x}$ [u, u]	$x, 2x$ [ $\bar{u}, 0$ ]	$2\bar{x}, \bar{x}$ [0, $\bar{u}$ ]
	$\bar{x}, x$ [ $\bar{u}, \bar{u}$ ]	$\bar{x}, 2\bar{x}$ [u, 0]	$2x, x$ [0, u]
6 d ..m	$x, 0$ [u, 2u]	$0, x$ [ $2\bar{u}, \bar{u}$ ]	$\bar{x}, \bar{x}$ [u, $\bar{u}$ ]
	$\bar{x}, 0$ [ $\bar{u}, 2\bar{u}$ ]	$0, \bar{x}$ [2u, u]	$x, x$ [ $\bar{u}, u$ ]
3 c 2mm	$1/2, 0$ [0, 0]	$0, 1/2$ [0, 0]	$1/2, 1/2$ [0, 0]
2 b 3m.	$1/3, 2/3$ [0, 0]	$2/3, 1/3$ [0, 0]	
1 a 6mm	$0, 0$ [0, 0]		

**Symmetry of special projections**

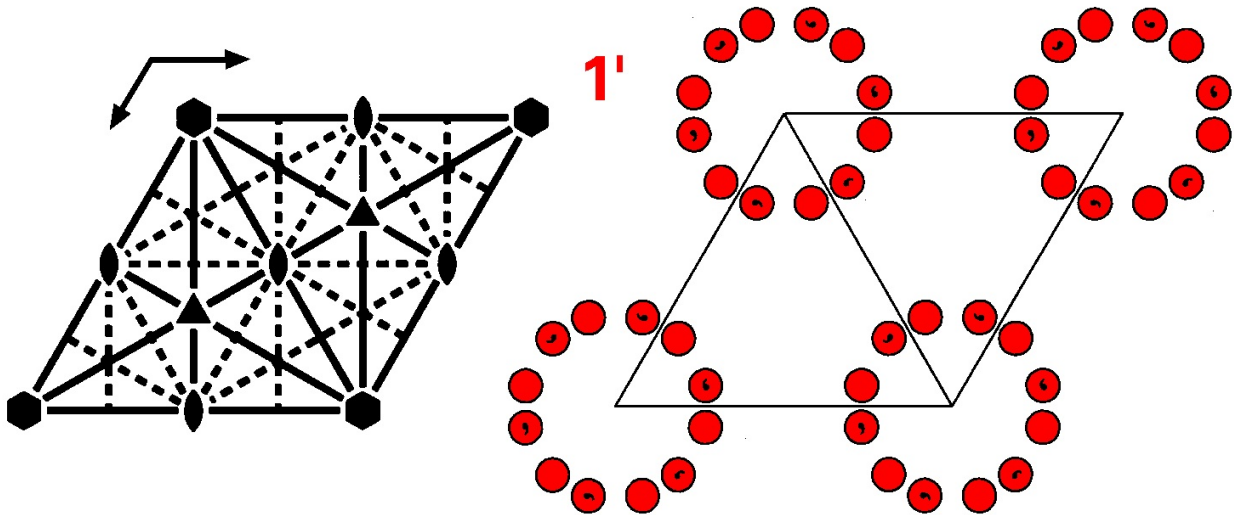
Along [10] $\rho m 1'$ $\mathbf{a}^* = (\mathbf{a}+2\mathbf{b})/2$ Origin at x, 0	Along [21] $\rho m 1'$ $\mathbf{a}^* = \mathbf{b}/2$ Origin at x, x/2
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p6mm1'

No. 17.2.77

6mm1'

p6mm1'



Origin on 6mm1'

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/3$ ;  $x \leq (1 + y)/2$ ;  $y \leq x/2$

Vertices  $0,0$ ;  $1/2,0$ ;  $2/3,1/3$

### Symmetry operations

For 1 + set		
(1) 1 (1 0,0)	(2) $3^+$ 0,0 ( $3_z$  0,0)	(3) $3^-$ 0,0 ( $3_z^{-1}$  0,0)
(4) 2 0,0 ( $2_z$  0,0)	(5) $6^-$ 0,0 ( $6_x^{-1}$  0,0)	(6) $6^+$ 0,0 ( $6_z$  0,0)
(7) m $x, \bar{x}$ ( $m_{xy}$  0,0)	(8) m $x, 2x$ ( $m_x$  0,0)	(9) m $2x, x$ ( $m_y$  0,0)
(10) m $x, x$ ( $m_3$  0,0)	(11) m $x, 0$ ( $m_2$  0,0)	(12) m $0, y$ ( $m_1$  0,0)

## For 1' + set

(1) 1' (1 0,0)'	(2) 3 <sup>+</sup> 0,0 (3 <sub>z</sub>  0,0)'	(3) 3 <sup>-</sup> 0,0 (3 <sub>z</sub> <sup>-1</sup>  0,0)'
(4) 2' 0,0 (2 <sub>z</sub>  0,0)'	(5) 6 <sup>-</sup> 0,0 (6 <sub>z</sub> <sup>-1</sup>  0,0)'	(6) 6 <sup>+</sup> 0,0 (6 <sub>z</sub>  0,0)'
(7) m' x, $\bar{x}$ (m <sub>xy</sub>  0,0)'	(8) m' x,2x (m <sub>x</sub>  0,0)'	(9) m' 2x,x (m <sub>y</sub>  0,0)'
(10) m' x,x (m <sub>3</sub>  0,0)'	(11) m' x,0 (m <sub>2</sub>  0,0)'	(12) m' 0,y (m <sub>1</sub>  0,0)'

**Generators selected** (1); t(1,0); t(0,1); (2); (4); (7); 1'

**Positions**

	Coordinates		
		1+	1' +
12 f 11'	(1) x,y [0,0] (4) $\bar{x},\bar{y}$ [0,0] (7) $\bar{y},\bar{x}$ [0,0] (10) y,x [0,0]	(2) $\bar{y},x-y$ [0,0] (5) y, $\bar{x}+y$ [0,0] (8) $\bar{x}+y,y$ [0,0] (11) x-y, $\bar{y}$ [0,0]	(3) $\bar{x}+y,\bar{x}$ [0,0] (6) x-y,x [0,0] (9) x,x-y [0,0] (12) $\bar{x},\bar{x}+y$ [0,0]
6 e .m.1'	x, $\bar{x}$ [0,0] $\bar{x},x$ [0,0]	x,2x [0,0] $\bar{x},2\bar{x}$ [0,0]	2 $\bar{x},\bar{x}$ [0,0] 2x,x [0,0]
6 d ..m1'	x,0 [0,0] $\bar{x},0$ [0,0]	0,x [0,0] 0, $\bar{x}$ [0,0]	$\bar{x},\bar{x}$ [0,0] x,x [0,0]
3 c 2mm1'	1/2,0 [0,0]	0,1/2 [0,0]	1/2,1/2 [0,0]
2 b 3m.1'	1/3,2/3 [0,0]	2/3,1/3 [0,0]	
1 a 6mm1'	0,0 [0,0]		

**Symmetry of special projections**Along [10]  $\rho m 1'$ 

$$\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$$

Origin at  $x, 0$ Along [21]  $\rho m 1'$ 

$$\mathbf{a}^* = \mathbf{b}/2$$

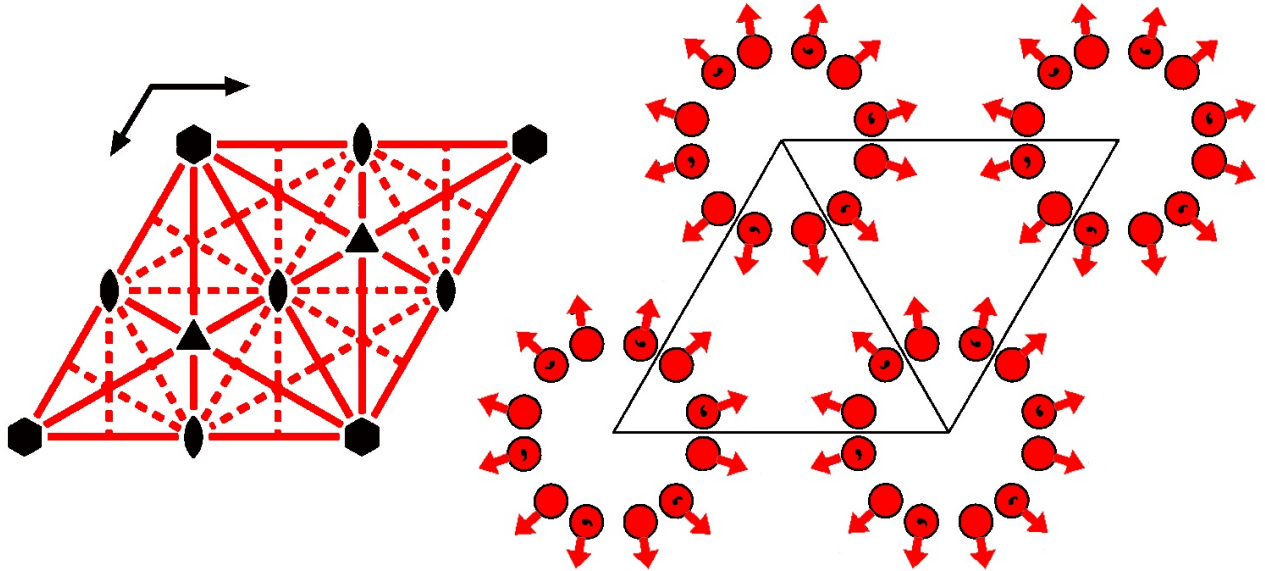
Origin at  $x, x/2$

p6m'm'

6m'm'

No. 17.3.78

p6m'm'



Origin on 6m'm'

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/3$ ;  $x \leq (1 + y)/2$ ;  $y \leq x/2$

Vertices  $0,0$ ;  $1/2,0$ ;  $2/3,1/3$

**Symmetry operations**

- |  |                                     |                                     |
|--|-------------------------------------|-------------------------------------|
| (1) 1<br>(1 0,0)                           | (2) $3^+$ 0,0<br>( $3_z$  0,0)      | (3) $3^-$ 0,0<br>( $3_z^{-1}$  0,0) |
| (4) 2 0,0<br>( $2_z$  0,0)                 | (5) $6^-$ 0,0<br>( $6_z^{-1}$  0,0) | (6) $6^+$ 0,0<br>( $6_z$  0,0)      |
| (7) $m'$ $x, \bar{x}$<br>( $m_{xy}$  0,0)' | (8) $m'$ $x, 2x$<br>( $m_x$  0,0)'  | (9) $m'$ $2x, x$<br>( $m_y$  0,0)'  |
| (10) $m'$ $x, x$<br>( $m_3$  0,0)'         | (11) $m'$ $x, 0$<br>( $m_2$  0,0)'  | (12) $m'$ $0, y$<br>( $m_1$  0,0)'  |



**Generators selected** (1); t(1,0); t(0,1); (2); (4); (7)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
	(1)	(2)	(3)
12 f 1	(1) x,y [u,v] (4) $\bar{x},\bar{y}$ [ $\bar{u},\bar{v}$ ] (7) $\bar{y},\bar{x}$ [ $\bar{v},\bar{u}$ ] (10) y,x [v,u]	(2) $\bar{y},x-y$ [ $\bar{v},u-v$ ] (5) y, $\bar{x}+y$ [v, $\bar{u}+v$ ] (8) $\bar{x}+y,y$ [ $\bar{u}+v,v$ ] (11) x-y, $\bar{y}$ [u-v, $\bar{v}$ ]	(3) $\bar{x}+y,\bar{x}$ [ $\bar{u}+v,\bar{u}$ ] (6) x-y,x [u-v,u] (9) x,x-y [u,u-v] (12) $\bar{x},\bar{x}+y$ [ $\bar{u},\bar{u}+v$ ]
6 e .m'	x, $\bar{x}$ [u, $\bar{u}$ ] $\bar{x},x$ [ $\bar{u},u$ ]	x,2x [u,2u] $\bar{x},2\bar{x}$ [ $\bar{u},2\bar{u}$ ]	2 $\bar{x},\bar{x}$ [2 $\bar{u},\bar{u}$ ] 2x,x [2u,u]
6 d ..m'	x,0 [u,0] $\bar{x},0$ [ $\bar{u},0$ ]	0,x [0,u] 0, $\bar{x}$ [0, $\bar{u}$ ]	$\bar{x},\bar{x}$ [ $\bar{u},\bar{u}$ ] x,x [u,u]
3 c 2m'm'	1/2,0 [0,0]	0,1/2 [0,0]	1/2,1/2 [0,0]
2 b 3m'	1/3,2/3 [0,0]	2/3,1/3 [0,0]	
1 a 6m'm'	0,0 [0,0]		

**Symmetry of special projections**

Along [10]  $\rho m'$   
 $\mathbf{a}^* = (\mathbf{a}+2\mathbf{b})/2$   
 Origin at x,0

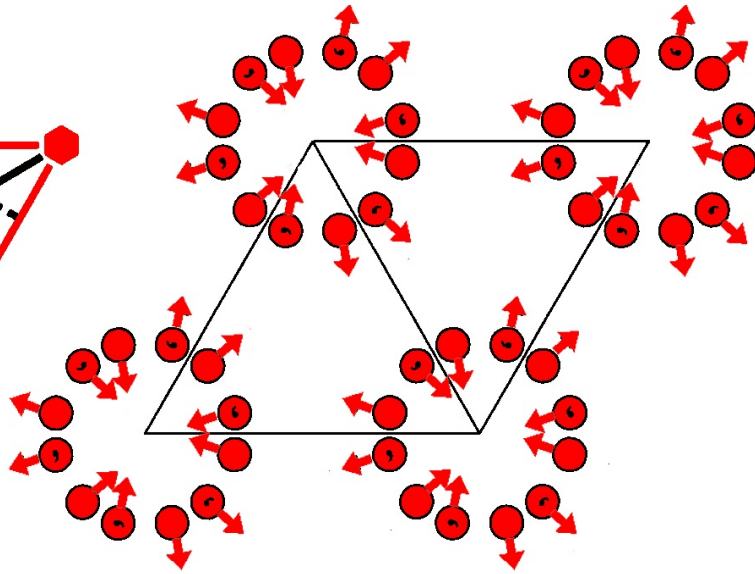
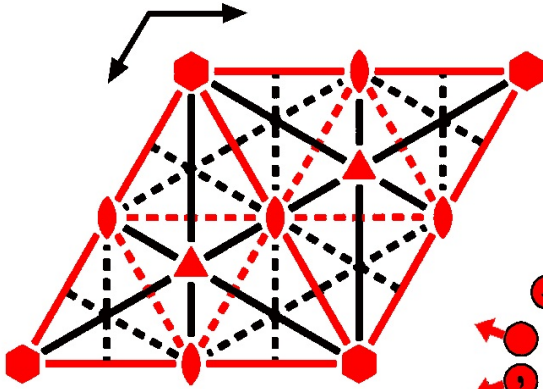
Along [21]  $\rho m'$   
 $\mathbf{a}^* = \mathbf{b}/2$   
 Origin at x,x/2

p6'mm'

No. 17.4.79

6'mm'

p6'mm'



Origin on 6'mm'

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/3$ ;  $x \leq (1 + y)/2$ ;  $y \leq x/2$

Vertices  $0,0$ ;  $1/2,0$ ;  $2/3,1/3$

**Symmetry operations**

- |  |                                      |                                     |
|--|--------------------------------------|-------------------------------------|
| (1) 1<br>(1 0,0)                       | (2) $3^+$ 0,0<br>( $3_z$  0,0)       | (3) $3^-$ 0,0<br>( $3_z^{-1}$  0,0) |
| (4) $2'$ 0,0<br>( $2_z$  0,0)'         | (5) $6^-$ 0,0<br>( $6_z^{-1}$  0,0)' | (6) $6^+$ 0,0<br>( $6_z$  0,0)'     |
| (7) m $x, \bar{x}$<br>( $m_{xy}$  0,0) | (8) m $x, 2x$<br>( $m_x$  0,0)       | (9) m $2x, x$<br>( $m_y$  0,0)      |
| (10) $m'$ $x, x$<br>( $m_3$  0,0)'     | (11) $m'$ $x, 0$<br>( $m_2$  0,0)'   | (12) $m'$ $0, y$<br>( $m_1$  0,0)'  |

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ; (2); (4); (7)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
	(1) $x,y [u,v]$	(2) $\bar{y},x-y [\bar{v},u-v]$	(3) $\bar{x}+y,\bar{x} [\bar{u}+v,\bar{u}]$
12 f 1	(4) $\bar{x},\bar{y} [u,v]$	(5) $y,\bar{x}+y [\bar{v},u-v]$	(6) $x-y,x [\bar{u}+v,\bar{u}]$
	(7) $\bar{y},\bar{x} [v,u]$	(8) $\bar{x}+y,y [u-v,\bar{v}]$	(9) $x,x-y [\bar{u},\bar{u}+v]$
	(10) $y,x [v,u]$	(11) $x-y,\bar{y} [u-v,\bar{v}]$	(12) $\bar{x},\bar{x}+y [\bar{u},\bar{u}+v]$
6 e .m.	$x,\bar{x} [u,u]$	$x,2x [\bar{u},0]$	$2\bar{x},\bar{x} [0,\bar{u}]$
	$\bar{x},x [u,u]$	$\bar{x},2\bar{x} [\bar{u},0]$	$2x,x [0,\bar{u}]$
6 d ..m'	$x,0 [u,0]$	$0,x [0,u]$	$\bar{x},\bar{x} [\bar{u},\bar{u}]$
	$\bar{x},0 [u,0]$	$0,\bar{x} [0,u]$	$x,x [\bar{u},\bar{u}]$
3 c 2'mm'	$1/2,0 [u,0]$	$0,1/2 [0,u]$	$1/2,1/2 [\bar{u},\bar{u}]$
2 b 3m.	$1/3,2/3 [0,0]$	$2/3,1/3 [0,0]$	
1 a 6'mm'	$0,0 [0,0]$		

**Symmetry of special projections**

Along [10]  $\rho m 1'$   
 $\mathbf{a}^* = (\mathbf{a}+2\mathbf{b})/2$   
 Origin at  $x,0$

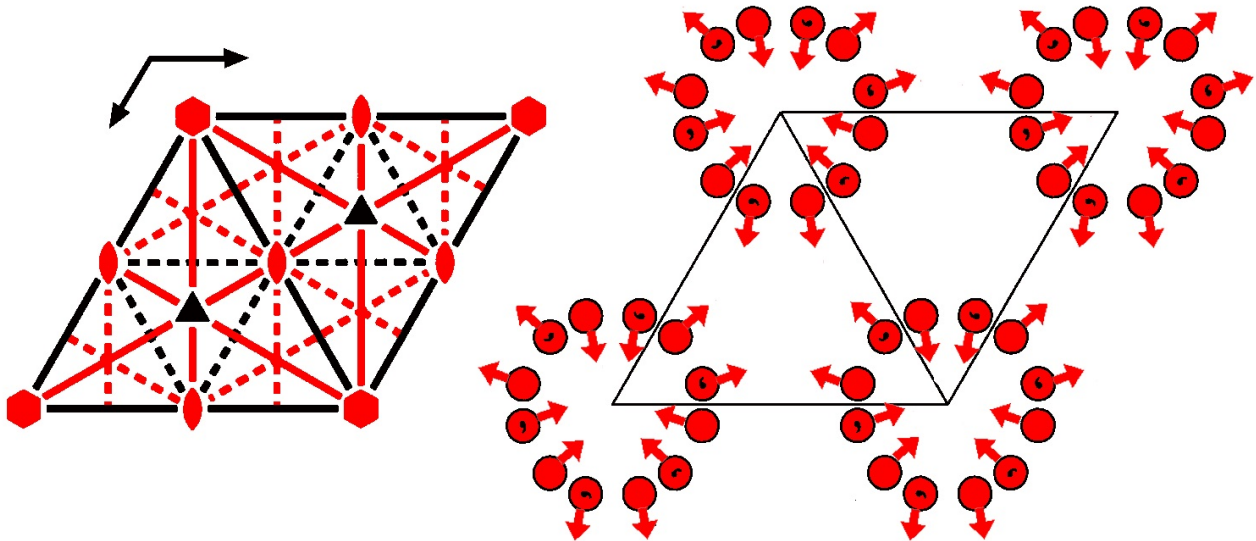
Along [21]  $\rho m$   
 $\mathbf{a}^* = \mathbf{b}/2$   
 Origin at  $x,x/2$

p6'm'm

6'm'm

No. 17.5.80

p6'm'm



Origin on 6'm'm

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/3$ ;  $x \leq (1 + y)/2$ ;  $y \leq x/2$

Vertices  $0,0$ ;  $1/2,0$ ;  $2/3,1/3$

Symmetry operations

- |  |                                      |                                     |
|--|--------------------------------------|-------------------------------------|
| (1) 1<br>(1 0,0)                           | (2) $3^+$ 0,0<br>( $3_z$  0,0)       | (3) $3^-$ 0,0<br>( $3_z^{-1}$  0,0) |
| (4) $2'$ 0,0<br>( $2_z$  0,0)'             | (5) $6^-$ 0,0<br>( $6_z^{-1}$  0,0)' | (6) $6^+$ 0,0<br>( $6_z$  0,0)'     |
| (7) $m'$ $x, \bar{x}$<br>( $m_{xy}$  0,0)' | (8) $m'$ $x, 2x$<br>( $m_x$  0,0)'   | (9) $m'$ $2x, x$<br>( $m_y$  0,0)'  |
| (10) $m$ $x, x$<br>( $m_3$  0,0)           | (11) $m$ $x, 0$<br>( $m_2$  0,0)     | (12) $m$ $0, y$<br>( $m_1$  0,0)    |

**Generators selected** (1); t(1,0); t(0,1); (2); (4); (7)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
	(1) $x, y$ [u, v]	(2) $\bar{y}, x-y$ [ $\bar{v}, u-v$ ]	(3) $\bar{x}+y, \bar{x}$ [ $\bar{u}+v, \bar{u}$ ]
12 f 1	(4) $\bar{x}, \bar{y}$ [u, v]	(5) $y, \bar{x}+y$ [ $\bar{v}, u-v$ ]	(6) $x-y, x$ [ $\bar{u}+v, \bar{u}$ ]
	(7) $\bar{y}, \bar{x}$ [ $\bar{v}, \bar{u}$ ]	(8) $\bar{x}+y, y$ [ $\bar{u}+v, v$ ]	(9) $x, x-y$ [u, u-v]
	(10) $y, x$ [ $\bar{v}, \bar{u}$ ]	(11) $x-y, \bar{y}$ [ $\bar{u}+v, v$ ]	(12) $\bar{x}, \bar{x}+y$ [u, u-v]
6 e .m'	$x, \bar{x}$ [u, $\bar{u}$ ]	$x, 2x$ [u, 2u]	$2\bar{x}, \bar{x}$ [2 $\bar{u}$ , $\bar{u}$ ]
	$\bar{x}, x$ [u, $\bar{u}$ ]	$\bar{x}, 2\bar{x}$ [u, 2u]	$2x, x$ [2 $\bar{u}$ , $\bar{u}$ ]
6 d ..m	$x, 0$ [u, 2u]	$0, x$ [2 $\bar{u}$ , $\bar{u}$ ]	$\bar{x}, \bar{x}$ [u, $\bar{u}$ ]
	$\bar{x}, 0$ [u, 2u]	$0, \bar{x}$ [2 $\bar{u}$ , $\bar{u}$ ]	$x, x$ [u, $\bar{u}$ ]
3 c 2'm'm	$1/2, 0$ [u, 2u]	$0, 1/2$ [2 $\bar{u}$ , $\bar{u}$ ]	$1/2, 1/2$ [u, $\bar{u}$ ]
2 b 3m'	$1/3, 2/3$ [0, 0]	$2/3, 1/3$ [0, 0]	
1 a 6'm'm	$0, 0$ [0, 0]		

**Symmetry of special projections**

Along [10] $\rho m$ $\mathbf{a}^* = (\mathbf{a}+2\mathbf{b})/2$ Origin at x, 0	Along [21] $\rho m 1'$ $\mathbf{a}^* = \mathbf{b}/2$ Origin at x, x/2
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## **Table 3 - 3D:**

### **Three-Dimensional Magnetic Space Group Tables**

HIERARCHAL THREE DIMENSIONAL MAGNETIC SPACE GROUP SUPERFAMILY INDEX

THREE DIMENSIONAL MAGNETIC SPACE GROUP INDEX

Table 3 - 2D: Two-Dimensional Magnetic Space Group Tables

Table 3 - 1D: One-Dimensional Magnetic Space Group Tables

**TRICLINIC SYSTEM**

1 P1

2 P $\bar{1}$ **MONOCLINIC SYSTEM**

3 P2

4 P2<sub>1</sub>

5 C2

6 Pm

7 Pc

8 Cm

9 Cc

10 P2/m

11 P2<sub>1</sub>/m

12 C2/m

13 P2/c

14 P2<sub>1</sub>/c

15 C2/c

**ORTHORHOMBIC SYSTEM**

16 P222

17 P222<sub>1</sub>18 P2<sub>1</sub>2<sub>1</sub>219 P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>20 C222<sub>1</sub>

21 C222

22 F222

23 I222

24 I2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>

25 Pmm2

26 Pmc2<sub>1</sub>

27 Pcc2

28 Pma2

29 Pca2<sub>1</sub>

30 Pnc2

31 Pmn2<sub>1</sub>

32 Pba2

33 Pna2<sub>1</sub>

34 Pnn2

35 Cmm2

36 Cmc2<sub>1</sub>

37 Ccc2

38 Amm2

39 Abm2

40 Ama2

41 Aba2

42 Fmm2

43 Fdd2

44 Imm2

45 Iba2

46 Ima2

47 Pmmm

48 Pnnn

49 Pccm

50 Pban

51 Pmma

52 Pnna

53 Pmna

54 Pcca

55 Pbam

56 Pccn

57 Pbcm

58 Pnnm

59 Pmmn

60 Pbcn

61 Pbca

62 Pnma

63 Cmcm

64 Cmca

65 Cmnm

66 Cccm

67 Cmma

68 Ccca

69 Fmmm

70 Fddd

71 Immm

72 Ibam

73 Ibca

74 Imma

**TETRAGONAL SYSTEM**

75 P4

76 P4<sub>1</sub>77 P4<sub>2</sub>78 P4<sub>3</sub>

79 I4

80 I4<sub>1</sub>81 P $\bar{4}$ 82 I $\bar{4}$ 

83 P4/m

84 P4<sub>2</sub>/m

85 P4/n

86 P4<sub>2</sub>/n

87 I4/m

88 I4<sub>1</sub>/a

89 P422

90 P4<sub>2</sub>291 P4<sub>1</sub>2292 P4<sub>1</sub>2<sub>1</sub>293 P4<sub>2</sub>2294 P4<sub>2</sub>2<sub>1</sub>295 P4<sub>3</sub>2296 P4<sub>3</sub>2<sub>1</sub>2

97 I422

98 I4<sub>1</sub>22

99	P4mm	125	P4/nbm	150	P321	175	P6/m
100	P4bm	126	P4/nnc	151	P3 <sub>1</sub> 12	176	P6 <sub>3</sub> /m
101	P4 <sub>2</sub> cm	127	P4/mbm	152	P3 <sub>1</sub> 21	177	P622
102	P4 <sub>2</sub> nm	128	P4/mnc	153	P3 <sub>2</sub> 12	178	P6 <sub>1</sub> 22
103	P4cc	129	P4/nmm	154	P3 <sub>2</sub> 21	179	P6 <sub>5</sub> 22
104	P4nc	130	P4/ncc	155	R32	180	P6 <sub>2</sub> 22
105	P4 <sub>2</sub> mc	131	P4 <sub>2</sub> /mmc	156	P3m1	181	P6 <sub>4</sub> 22
106	P4 <sub>2</sub> bc	132	P4 <sub>2</sub> /mcm	157	P31m	182	p6 <sub>3</sub> 22
107	I4mm	133	P4 <sub>2</sub> /nbc	158	P3c1	183	p6mm
108	I4cm	134	P4 <sub>2</sub> /nnm	159	P31c	184	P6cc
109	I4 <sub>1</sub> md	135	P4 <sub>2</sub> /mbc	160	R3m	185	P6 <sub>3</sub> cm
110	I4 <sub>1</sub> cd	136	P4 <sub>2</sub> /mnm	161	R3c	186	P6 <sub>3</sub> mc
111	P <del>4</del> 2m	137	P4 <sub>2</sub> /nmc	162	P <del>3</del> 1m	187	P <del>6</del> m2
112	P <del>4</del> 2c	138	P4 <sub>2</sub> /ncm	163	P <del>3</del> 1c	188	P <del>6</del> c2
113	P <del>4</del> 2 <sub>1</sub> m	139	I4/mmm	164	P <del>3</del> m1	189	P <del>6</del> 2m
114	P <del>4</del> 2 <sub>1</sub> c	140	I4/mcm	165	P <del>3</del> c1	190	P <del>6</del> 2c
115	P <del>4</del> m2	141	I4 <sub>1</sub> /amd	166	R <del>3</del> m	191	P6/mmm
116	P <del>4</del> c2	142	I4 <sub>1</sub> /acd	167	R <del>3</del> c	192	P6/mcc
117	P <del>4</del> b2		<b>TRIGONAL SYSTEM</b>		<b>HEXAGONAL SYSTEM</b>	193	P6 <sub>3</sub> /mcm
118	P <del>4</del> n2					194	P6 <sub>3</sub> /mmc
119	I <del>4</del> m2	143	P3	168	P6		<b>CUBIC SYSTEM</b>
120	I <del>4</del> c2	144	P3 <sub>1</sub>	169	P6 <sub>1</sub>	195	P23
121	I <del>4</del> 2m	145	P3 <sub>2</sub>	170	P6 <sub>5</sub>	196	F23
122	I <del>4</del> 2d	146	R3	171	P6 <sub>2</sub>	197	I23
123	P4/mmm	147	P <del>3</del>	172	P6 <sub>4</sub>	198	P2 <sub>1</sub> 3
124	P4/mcc	148	R <del>3</del>	173	P6 <sub>3</sub>	199	I2 <sub>1</sub> 3
		149	P312	174	P <del>3</del>		



200	$Pm\bar{2}$	226	$Fm\bar{2}c$
201	$Pn\bar{2}$	227	$Fd\bar{2}m$
202	$Fm\bar{2}$	228	$Fd\bar{2}c$
203	$Fd\bar{2}$	229	$Im\bar{2}m$
204	$Im\bar{2}$	230	$Ia\bar{2}d$
205	$Pa\bar{2}$		
206	$Ia\bar{2}$		
207	$P4_32$		
208	$P4_232$		
209	$F4_32$		
210	$F4_132$		
211	$I4_32$		
212	$P4_332$		
213	$P4_132$		
214	$I4_132$		
215	$P\bar{4}3m$		
216	$F\bar{4}3m$		
217	$I\bar{4}3m$		
218	$P\bar{4}3n$		
219	$F\bar{4}3c$		
220	$I\bar{4}3d$		
221	$Pm\bar{2}m$		
222	$Pn\bar{2}n$		
223	$Pm\bar{2}n$		
224	$Pn\bar{2}m$		
225	$Fm\bar{2}m$		

**TRICLINIC SYSTEM**

		5.5.23	$C_P 2$	9.3.47	$Cc'$
<b>1.1.1</b>	<b>P1</b>	5.6.24	$C_P 2'$	9.4.48	$C_P c$
1.2.2	$P11'$				
1.3.3	$P_{2s} 1$	<b>6.1.25</b>	<b>Pm</b>	<b>10.1.49</b>	<b>P2/m</b>
		6.2.26	$Pm1'$	10.2.50	$P2/m1'$
<b>2.1.4</b>	<b>P&amp;</b>	6.3.27	$Pm'$	10.3.51	$P2'/m$
2.2.5	$P&1'$	6.4.28	$P_{2a} m$	10.4.52	$P2/m'$
2.3.6	$P&'$	6.5.29	$P_{2b} m$	10.5.53	$P2'/m'$
2.4.7	$P_{2s} \&$	6.6.30	$P_C m$	10.6.54	$P_{2a} 2/m$

**MONOCLINIC SYSTEM**

		6.7.31	$P_{2c} m'$	10.7.55	$P_{2b} 2/m$
				10.8.56	$P_C 2/m$
<b>3.1.8</b>	<b>P2</b>	<b>7.1.32</b>	<b>Pc</b>	10.9.57	$P_{2b} 2'/m$
3.2.9	$P21'$	7.2.33	$Pc1'$	10.10.58	$P_{2c} 2/m'$
3.3.10	$P2'$	7.3.34	$Pc'$		
3.4.11	$P_{2a} 2$	7.4.35	$P_{2a} c$	<b>11.1.59</b>	<b>P2<sub>1</sub>/m</b>
3.5.12	$P_{2b} 2$	7.5.36	$P_{2b} c$	11.2.60	$P2_1/m1'$
3.6.13	$P_C 2$	7.6.37	$P_C c$	11.3.61	$P2_1'/m$
3.7.14	$P_{2b} 2'$	<b>8.1.38</b>	<b>Cm</b>	11.4.62	$P2_1/m'$
		8.2.39	$Cm1'$	11.5.63	$P2_1'/m'$
<b>4.1.15</b>	<b>P2<sub>1</sub></b>	8.3.40	$Cm'$	11.6.64	$P_{2a} 2_1/m$
4.2.16	$P2_1 1'$	8.4.41	$C_{2c} m$	11.7.65	$P_{2c} 2_1/m'$
4.3.17	$P2_1'$	8.5.42	$C_P m$	<b>12.1.66</b>	<b>C2/m</b>
4.4.18	$P_{2a} 2_1$	8.6.43	$C_{2c} m'$	12.2.67	$C2/m1'$
<b>5.1.19</b>	<b>C2</b>	8.7.44	$C_P m'$	12.3.68	$C2'/m$
5.2.20	$C21'$			12.4.69	$C2/m'$
5.3.21	$C2'$	<b>9.1.45</b>	<b>Cc</b>	12.5.70	$C2'/m'$
5.4.22	$C_{2c} 2$	9.2.46	$Cc1'$	12.6.71	$C_{2c} 2/m$

12.7.72	$C_P 2/m$	15.5.96	$C2'/c'$	<b>19.1.119</b>	<b><math>P2_1 2_1 2_1</math></b>
12.8.73	$C_{2c} 2/m'$	15.6.97	$C_P 2/c$	19.2.120	$P2_1 2_1 2_1 1'$
12.9.74	$C_P 2'/m$	15.7.98	$C_P 2'/c$	19.3.121	$P2_1' 2_1' 2_1$
12.10.75	$C_P 2/m'$	<b>ORTHORHOMBIC SYSTEM</b>			
12.11.76	$C_P 2'/m'$			<b>20.1.122</b>	<b><math>C222_1</math></b>
<b>13.1.77</b>	<b><math>P2/c</math></b>	<b>16.1.99</b>	<b><math>P222</math></b>	20.2.123	$C222_1 1'$
13.2.78	$P2/c1'$	16.2.100	$P2221'$	20.3.124	$C2' 2' 2_1$
13.3.79	$P2'/c$	16.3.101	$P2' 2' 2$	20.4.125	$C22' 2_1'$
13.4.80	$P2/c'$	16.4.102	$P_{2a} 222$	20.5.126	$C_P 222_1$
13.5.81	$P2'/c'$	16.5.103	$P_C 222$	20.6.127	$C_P 2' 2' 2_1$
13.6.82	$P_{2a} 2/c$	16.6.104	$P_F 222$	20.7.128	$C_P 22' 2_1'$
13.7.83	$P_{2b} 2/c$	16.7.105	$P_{2c} 22' 2'$	<b>21.1.129</b>	<b><math>C222</math></b>
13.8.84	$P_C 2/c$	<b>17.1.106</b>	<b><math>P222_1</math></b>	21.2.130	$C2221'$
13.9.85	$P_{2b} 2'/c$	17.2.107	$P222_1 1'$	21.3.131	$C2' 2' 2$
<b>14.1.86</b>	<b><math>P2_1/c</math></b>	17.3.108	$P2' 2' 2_1$	21.4.132	$C22' 2'$
14.2.87	$P2_1/c1'$	17.4.109	$P22' 2_1'$	21.5.133	$C_{2c} 222$
14.3.88	$P2_1'/c$	17.5.110	$P_{2a} 222_1$	21.6.134	$C_P 222$
14.4.89	$P2_1/c'$	17.6.111	$P_C 222_1$	21.7.135	$C_1 222$
14.5.90	$P2_1'/c'$	17.7.112	$P_{2a} 2' 2' 2_1$	21.8.136	$C_{2c} 22' 2'$
14.6.91	$P_{2a} 2_1/c$	<b>18.1.113</b>	<b><math>P2_1 2_1 2</math></b>	21.9.137	$C_P 2' 2' 2$
<b>15.1.92</b>	<b><math>C2/c</math></b>	18.2.114	$P2_1 2_1 21'$	21.10.138	$C_P 22' 2'$
15.2.93	$C2/c1'$	18.3.115	$P2_1' 2_1' 2$	21.11.139	$C_1 2' 22'$
15.3.94	$C2'/c$	18.4.116	$P2_1 2_1' 2'$	<b>22.1.140</b>	<b><math>F222</math></b>
15.4.95	$C2/c'$	18.5.117	$P_{2c} 2_1 2_1 2$	22.2.141	$F2221'$
		18.6.118	$P_{2c} 2_1 2_1' 2'$	22.3.142	$F2' 2' 2$

22.4.143	$F_C 222$	25.13.167	$P_A m'm'2$	28.7.191	$P_{2c} ma2$
22.5.144	$F_C 22'2'$	<b>26.1.168</b>	<b><math>Pmc2_1</math></b>	28.8.192	$P_A ma2$
<b>23.1.145</b>	<b><math>I222</math></b>	26.2.169	$Pmc2_1 1'$	28.9.193	$P_{2b} m'a2'$
23.2.146	$I2221'$	26.3.170	$Pm'c2_1'$	28.10.194	$P_{2c} m'a2'$
23.3.147	$I2'2'2$	26.4.171	$Pmc'2_1'$	28.11.195	$P_{2c} ma'2'$
23.4.148	$I_p 222$	26.5.172	$Pm'c'2_1$	28.12.196	$P_{2c} m'a'2$
23.5.149	$I_p 2'2'2$	26.6.173	$P_{2a} mc2_1$	28.13.197	$P_A m'a'2$
<b>24.1.150</b>	<b><math>I2_1 2_1 2_1</math></b>	26.7.174	$P_{2b} mc2_1$	<b>29.1.198</b>	<b><math>Pca2_1</math></b>
24.2.151	$I2_1 2_1 2_1 1'$	26.8.175	$P_C mc2_1$	29.2.199	$Pca2_1 1'$
24.3.152	$I2_1' 2_1' 2_1$	26.9.176	$P_{2a} mc'2_1'$	29.3.200	$Pc'a2_1'$
24.4.153	$I_p 2_1 2_1 2_1$	26.10.177	$P_{2b} m'c'2_1$	29.4.201	$Pca'2_1'$
24.5.154	$I_p 2_1' 2_1' 2_1$	<b>27.1.178</b>	<b><math>Pcc2</math></b>	29.5.202	$Pc'a'2_1$
<b>25.1.155</b>	<b><math>Pmm2</math></b>	27.2.179	$Pcc21'$	29.6.203	$P_{2b} ca2_1$
25.2.156	$Pmm21'$	27.3.180	$Pc'c2'$	29.7.204	$P_{2b} c'a'2_1$
25.3.157	$Pm'm2'$	27.4.181	$Pc'c'2$	<b>30.1.205</b>	<b><math>Pnc2</math></b>
25.4.158	$Pm'm'2$	27.5.182	$P_{2a} cc2$	30.2.206	$Pnc21'$
25.5.159	$P_{2c} mm2$	27.6.183	$P_C cc2$	30.3.207	$Pn'c2'$
25.6.160	$P_{2a} mm2$	27.7.184	$P_{2b} c'c2'$	30.4.208	$Pnc'2'$
25.7.161	$P_C mm2$	<b>28.1.185</b>	<b><math>Pma2</math></b>	30.5.209	$Pn'c'2$
25.8.162	$P_A mm2$	28.2.186	$Pma21'$	30.6.210	$P_{2a} nc2$
25.9.163	$P_F mm2$	28.3.187	$Pm'a2'$	30.7.211	$P_{2a} nc'2'$
25.10.164	$P_{2c} mm'2'$	28.4.188	$Pma'2'$	<b>31.1.212</b>	<b><math>Pmn2_1</math></b>
25.11.165	$P_{2c} m'm'2$	28.5.189	$Pm'a'2$	31.2.213	$Pmn2_1 1'$
25.12.166	$P_{2a} m'm'2$	28.6.190	$P_{2b} ma2$	31.3.214	$Pm'n2_1'$

31.4.215	Pmn'2 <sub>1</sub> '	35.4.239	Cm'm'2	37.7.264	C <sub>p</sub> c'c'2
31.5.216	Pm'n'2 <sub>1</sub>	35.5.240	C <sub>2c</sub> mm2	<b>38.1.265</b>	<b>Amm2</b>
31.6.217	P <sub>2b</sub> mn2 <sub>1</sub>	35.6.241	C <sub>p</sub> mm2	38.2.266	Amm21'
31.7.218	P <sub>2b</sub> m'n'2 <sub>1</sub> '	35.7.242	C <sub>1</sub> mm2	38.3.267	Am'm'2'
<b>32.1.219</b>	<b>Pba2</b>	35.8.243	C <sub>2c</sub> m'm'2'	38.4.268	Amm'2'
32.2.220	Pba21'	35.9.244	C <sub>2c</sub> m'm'2	38.5.269	Am'm'2
32.3.221	Pb'a2'	35.10.245	C <sub>p</sub> m'm'2'	38.6.270	A <sub>2a</sub> mm2
32.4.222	Pb'a'2	35.11.246	C <sub>p</sub> m'm'2	38.7.271	A <sub>p</sub> mm2
32.5.223	P <sub>2c</sub> ba2	35.12.247	C <sub>1</sub> m'm'2'	38.8.272	A <sub>1</sub> mm2
32.6.224	P <sub>2c</sub> b'a2'	35.13.248	C <sub>1</sub> m'm'2	38.9.273	A <sub>2a</sub> mm'2'
32.7.225	P <sub>2c</sub> b'a'2	<b>36.1.249</b>	<b>Cmc2<sub>1</sub></b>	38.10.274	A <sub>p</sub> m'm'2'
<b>33.1.226</b>	<b>Pna2<sub>1</sub></b>	36.2.250	Cmc2 <sub>1</sub> 1'	38.11.275	A <sub>p</sub> mm'2'
33.2.227	Pna2 <sub>1</sub> 1'	36.3.251	Cm'c'2 <sub>1</sub> '	38.12.276	A <sub>p</sub> m'm'2
33.3.228	Pn'a2 <sub>1</sub> '	36.4.252	Cmc'2 <sub>1</sub> '	38.13.277	A <sub>1</sub> m'm'2
33.4.229	Pna'2 <sub>1</sub> '	36.5.253	Cm'c'2 <sub>1</sub>	<b>39.1.278</b>	<b>Abm2</b>
33.5.230	Pn'a'2 <sub>1</sub>	36.6.254	C <sub>p</sub> mc2 <sub>1</sub>	39.2.279	Abm21'
<b>34.1.231</b>	<b>Pnn2</b>	36.7.255	C <sub>p</sub> m'c'2 <sub>1</sub> '	39.3.280	Ab'm'2'
34.2.232	Pnn21'	36.8.256	C <sub>p</sub> mc'2 <sub>1</sub> '	39.4.281	Abm'2'
34.3.233	Pn'n'2'	36.9.257	C <sub>p</sub> m'c'2 <sub>1</sub>	39.5.282	Ab'm'2
34.4.234	Pn'n'2	<b>37.1.258</b>	<b>Ccc2</b>	39.6.283	A <sub>2a</sub> bm2
34.5.235	P <sub>F</sub> nn2	37.2.259	Ccc21'	39.7.284	A <sub>p</sub> bm2
<b>35.1.236</b>	<b>Cmm2</b>	37.3.260	Cc'c'2'	39.8.285	A <sub>1</sub> bm2
35.2.237	Cmm21'	37.4.261	Cc'c'2	39.9.286	A <sub>2a</sub> b'm'2
35.3.238	Cm'm'2'	37.5.262	C <sub>p</sub> cc2	39.10.287	A <sub>p</sub> b'm'2'
		37.6.263	C <sub>p</sub> c'c'2'	39.11.288	A <sub>p</sub> bm'2'

39.12.289	$A_p b'm^2$	42.5.313	$F_C mm^2$	45.7.337	$I_p b'a^2$
39.13.290	$A_l b'm^2$	42.6.314	$F_A mm^2$	<b>46.1.338</b>	<b>Ima2</b>
<b>40.1.291</b>	<b>Ama2</b>	42.7.315	$F_C mm^2'$	46.2.339	Ima21'
40.2.292	Ama21'	42.8.316	$F_C m'm^2$	46.3.340	Im'a2'
40.3.293	Am'a2'	42.9.317	$F_A m'm^2'$	46.4.341	Ima'2'
40.4.294	Ama'2'	42.10.318	$F_A mm^2'$	46.5.342	Im'a'2
40.5.295	Am'a'2	42.11.319	$F_A m'm^2$	46.6.343	$I_p ma^2$
40.6.296	$A_p ma^2$	<b>43.1.320</b>	<b>Fdd2</b>	46.7.344	$I_p m'a^2'$
40.7.297	$A_p m'a^2'$	43.2.321	Fdd21'	46.8.345	$I_p ma^2'$
40.8.298	$A_p ma^2'$	43.3.322	Fd'd2'	46.9.346	$I_p m'a^2$
40.9.299	$A_p m'a^2$	43.4.323	Fd'd'2	<b>47.1.347</b>	<b>Pmmm</b>
<b>41.1.300</b>	<b>Aba2</b>	<b>44.1.324</b>	<b>Imm2</b>	47.2.348	Pmmm1'
41.2.301	Aba21'	44.2.325	Imm21'	47.3.349	Pm'mm
41.3.302	Ab'a2'	44.3.326	Im'm2'	47.4.350	Pm'm'm
41.4.303	Aba'2'	44.4.327	Im'm'2	47.5.351	Pm'm'm'
41.5.304	Ab'a'2	44.5.328	$I_p mm^2$	47.6.352	$P_{2a} mmm$
41.6.305	$A_p ba^2$	44.6.329	$I_p mm^2'$	47.7.353	$P_C mmm$
41.7.306	$A_p b'a^2'$	44.7.330	$I_p m'm^2$	47.8.354	$P_F mmm$
41.8.307	$A_p ba^2'$	<b>45.1.331</b>	<b>Iba2</b>	47.9.355	$P_{2a} mmm'$
41.9.308	$A_p b'a^2$	45.2.332	Iba21'	47.10.356	$P_{2c} m'm'm$
<b>42.1.309</b>	<b>Fmm2</b>	45.3.333	Ib'a2'	47.11.357	$P_C mmm'$
42.2.310	Fmm21'	45.4.334	Ib'a'2	<b>48.1.358</b>	<b>Pnnn</b>
42.3.311	Fm'm2'	45.5.335	$I_p ba^2$	48.2.359	Pnnn1'
42.4.312	Fm'm'2	45.6.336	$I_p ba^2'$	48.3.360	Pn'nn

48.4.361	Pn'n'n	50.10.386	P <sub>2c</sub> b'a'n	52.6.411	Pn'n'a
48.5.362	Pn'n'n'			52.7.412	Pnn'a'
48.6.363	P <sub>F</sub> nnn	<b>51.1.387</b>	<b>Pmma</b>	52.8.413	Pn'na'
		51.2.388	Pmma1'	52.9.414	Pn'n'a'
<b>49.1.364</b>	<b>Pccm</b>	51.3.389	Pm'ma		
49.2.365	Pccm1'	51.4.390	Pmm'a	<b>53.1.415</b>	<b>Pmna</b>
49.3.366	Pc'cm	51.5.391	Pmma'	53.2.416	Pmna1'
49.4.367	Pccm'	51.6.392	Pm'm'a	53.3.417	Pm'na
49.5.368	Pc'c'm	51.7.393	Pmm'a'	53.4.418	Pmn'a
49.6.369	Pc'cm'	51.8.394	Pm'ma'	53.5.419	Pmna'
49.7.370	Pc'c'm'	51.9.395	Pm'm'a'	53.6.420	Pm'n'a
49.8.371	P <sub>2a</sub> ccm	51.10.396	P <sub>2b</sub> mma	53.7.421	Pmn'a'
49.9.372	P <sub>C</sub> ccm	51.11.397	P <sub>2c</sub> mma	53.8.422	Pm'na'
49.10.373	P <sub>2a</sub> ccm'	51.12.398	P <sub>A</sub> mma	53.9.423	Pm'n'a'
49.11.374	P <sub>2a</sub> c'c'm	51.13.399	P <sub>2b</sub> m'ma	53.10.424	P <sub>2b</sub> mna
49.12.375	P <sub>2a</sub> c'c'm'	51.14.400	P <sub>2b</sub> mma'	53.11.425	P <sub>2b</sub> m'na
49.13.376	P <sub>C</sub> ccm'	51.15.401	P <sub>2b</sub> m'ma'	53.12.426	P <sub>2b</sub> mna'
		51.16.402	P <sub>2c</sub> m'ma	53.13.427	P <sub>2b</sub> m'na'
<b>50.1.377</b>	<b>Pban</b>	51.17.403	P <sub>2c</sub> mm'a	<b>54.1.428</b>	<b>Pcca</b>
50.2.378	Pban1'	51.18.404	P <sub>2c</sub> m'm'a	54.2.429	Pcca1'
50.3.379	Pb'an	51.19.405	P <sub>A</sub> m'ma	54.3.430	Pc'ca
50.4.380	Pban'			54.4.431	Pcc'a
50.5.381	Pb'a'n	<b>52.1.406</b>	<b>Pnna</b>	54.5.432	Pcca'
50.6.382	Pb'an'	52.2.407	Pnna1'	54.6.433	Pc'c'a
50.7.383	Pb'a'n'	52.3.408	Pn'na	54.7.434	Pcc'a'
50.8.384	P <sub>2c</sub> ban	52.4.409	Pnn'a	54.8.435	Pc'ca'
50.9.385	P <sub>2c</sub> b'an	52.5.410	Pnna'		

54.9.436	Pc'c'a'	57.3.460	Pb'cm	59.8.485	P <sub>2c</sub> mmn
54.10.437	P <sub>2b</sub> cca	57.4.461	Pbc'm	59.9.486	P <sub>2c</sub> m'mn
54.11.438	P <sub>2b</sub> c'ca	57.5.462	Pbcm'	59.10.487	P <sub>2c</sub> m'm'n
54.12.439	P <sub>2b</sub> cca'	57.6.463	Pb'c'm	<b>60.1.488</b>	<b>Pbcn</b>
54.13.440	P <sub>2b</sub> c'ca'	57.7.464	Pbc'm'	60.2.489	Pbcn1'
<b>55.1.441</b>	<b>Pbam</b>	57.8.465	Pb'cm'	60.3.490	Pb'cn
55.2.442	Pbam1'	57.9.466	Pb'c'm'	60.4.491	Pbc'n
55.3.443	Pb'am	57.10.467	P <sub>2a</sub> bcm	60.5.492	Pbcn'
55.4.444	Pbam'	57.11.468	P <sub>2a</sub> bc'm	60.6.493	Pb'c'n
55.5.445	Pb'a'm	57.12.469	P <sub>2a</sub> bcm'	60.7.494	Pbc'n'
55.6.446	Pb'am'	57.13.470	P <sub>2a</sub> bc'm'	60.8.495	Pb'cn'
55.7.447	Pb'a'm'	<b>58.1.471</b>	<b>Pnnm</b>	60.9.496	Pb'c'n'
55.8.448	P <sub>2c</sub> bam	58.2.472	Pnnm1'	<b>61.1.497</b>	<b>Pbca</b>
55.9.449	P <sub>2c</sub> b'am	58.3.473	Pn'nm	61.2.498	Pbca1'
55.10.450	P <sub>2c</sub> b'a'm	58.4.474	Pnnm'	61.3.499	Pb'ca
<b>56.1.451</b>	<b>Pccn</b>	58.5.475	Pn'n'm	61.4.500	Pb'c'a
56.2.452	Pccn1'	58.6.476	Pnn'm'	61.5.501	Pb'c'a'
56.3.453	Pc'cn	58.7.477	Pn'n'm'	<b>62.1.502</b>	<b>Pnma</b>
56.4.454	Pccn'	<b>59.1.478</b>	<b>Pmmn</b>	62.2.503	Pnma1'
56.5.455	Pc'c'n	59.2.479	Pmmn1'	62.3.504	Pn'ma
56.6.456	Pc'cn'	59.3.480	Pm'mn	62.4.505	Pnm'a
56.7.457	Pc'c'n'	59.4.481	Pmmn'	62.5.506	Pnma'
<b>57.1.458</b>	<b>Pbcm</b>	59.5.482	Pm'm'n	62.6.507	Pn'm'a
57.2.459	Pbcm1'	59.6.483	Pmm'n'	62.7.508	Pnm'a'
		59.7.484	Pm'm'n'		



62.8.509	Pn'ma'	64.7.534	Cmc'a'	65.15.559	C <sub>p</sub> m'm'm
62.9.510	Pn'm'a'	64.8.535	Cm'ca'	65.16.560	C <sub>p</sub> mm'm'
<b>63.1.511</b>	<b>Cmcm</b>	64.9.536	Cm'c'a'	65.17.561	C <sub>p</sub> m'm'm'
63.2.512	Cmcm1'	64.10.537	C <sub>p</sub> mca	65.18.562	C <sub>1</sub> m'mm
63.3.513	Cm'cm	64.11.538	C <sub>p</sub> m'ca	65.19.563	C <sub>1</sub> m'm'm
63.4.514	Cmc'm	64.12.539	C <sub>p</sub> mc'a	<b>66.1.564</b>	<b>Cccm</b>
63.5.515	Cmcm'	64.13.540	C <sub>p</sub> mca'	66.2.565	Cccm1'
63.6.516	Cm'c'm	64.14.541	C <sub>p</sub> m'c'a	66.3.566	Cc'cm
63.7.517	Cmc'm'	64.15.542	C <sub>p</sub> mc'a'	66.4.567	Cccm'
63.8.518	Cm'cm'	64.16.543	C <sub>p</sub> m'ca'	66.5.568	Cc'c'm
63.9.519	Cm'c'm'	64.17.544	C <sub>p</sub> m'c'a'	66.6.569	Ccc'm'
63.10.520	C <sub>p</sub> mcm	<b>65.1.545</b>	<b>Cmmm</b>	66.7.570	Cc'c'm'
63.11.521	C <sub>p</sub> m'cm	65.2.546	Cmmm1'	66.8.571	C <sub>p</sub> ccm
63.12.522	C <sub>p</sub> mc'm	65.3.547	Cm'mm	66.9.572	C <sub>p</sub> c'cm
63.13.523	C <sub>p</sub> mcm'	65.4.548	Cmmm'	66.10.573	C <sub>p</sub> ccm'
63.14.524	C <sub>p</sub> m'c'm	65.5.549	Cm'm'm	66.11.574	C <sub>p</sub> c'c'm
63.15.525	C <sub>p</sub> mc'm'	65.6.550	Cmm'm'	66.12.575	C <sub>p</sub> cc'm'
63.16.526	C <sub>p</sub> m'cm'	65.7.551	Cm'm'm'	66.13.576	C <sub>p</sub> c'c'm'
63.17.527	C <sub>p</sub> m'c'm'	65.8.552	C <sub>2c</sub> mmm	<b>67.1.577</b>	<b>Cmma</b>
<b>64.1.528</b>	<b>Cmca</b>	65.9.553	C <sub>p</sub> mmm	67.2.578	Cmma1'
64.2.529	Cmca1'	65.10.554	C <sub>1</sub> mmm	67.3.579	Cm'ma
64.3.530	Cm'ca	65.11.555	C <sub>2c</sub> m'm'm	67.4.580	Cmma'
64.4.531	Cmc'a	65.12.556	C <sub>2c</sub> mm'm'	67.5.581	Cm'm'a
64.5.532	Cmca'	65.13.557	C <sub>p</sub> m'mm	67.6.582	Cmm'a'
64.6.533	Cm'c'a	65.14.558	C <sub>p</sub> mmm'	67.7.583	Cm'm'a'

67.8.584	$C_{2c}mma$	69.5.609	$Fm'm'm'$	72.4.633	$lbam'$
67.9.585	$C_p mma$	69.6.610	$F_C mmm$	72.5.634	$lb'a'm$
67.10.586	$C_1 mma$	69.7.611	$F_C m'mm$	72.6.635	$lba'm'$
67.11.587	$C_{2c} m'ma$	69.8.612	$F_C mmm'$	72.7.636	$lb'a'm'$
67.12.588	$C_{2c} m'm'a$	69.9.613	$F_C m'm'm$	72.8.637	$l_p bam$
67.13.589	$C_p m'ma$	69.10.614	$F_C mm'm'$	72.9.638	$l_p b'am$
67.14.590	$C_p mm'a$	69.11.615	$F_C m'm'm'$	72.10.639	$l_p bam'$
67.15.591	$C_p mma'$	<b>70.1.616</b>	<b>Fddd</b>	72.11.640	$l_p b'a'm$
67.16.592	$C_1 mm'a$	70.2.617	$Fddd1'$	72.12.641	$l_p b'am'$
67.17.593	$C_1 m'ma'$	70.3.618	$Fd'dd$	72.13.642	$l_p b'a'm'$
<b>68.1.594</b>	<b>Ccca</b>	70.4.619	$Fd'd'd$	<b>73.1.643</b>	<b>lbca</b>
68.2.595	$Ccca1'$	70.5.620	$Fd'd'd'$	73.2.644	$lbca1'$
68.3.596	$Cc'ca$	<b>71.1.621</b>	<b>Immm</b>	73.3.645	$lb'ca$
68.4.597	$Ccca'$	71.2.622	$Immm1'$	73.4.646	$lb'c'a$
68.5.598	$Cc'c'a$	71.3.623	$Im'mm$	73.5.647	$lb'c'a'$
68.6.599	$Ccc'a'$	71.4.624	$Im'm'm$	73.6.648	$l_p bca$
68.7.600	$Cc'c'a'$	71.5.625	$Im'm'm'$	73.7.649	$l_p b'ca$
68.8.601	$C_p cca$	71.6.626	$l_p mmm$	<b>74.1.650</b>	<b>Imma</b>
68.9.602	$C_p c'ca$	71.7.627	$l_p m'mm$	74.2.651	$Imma1'$
68.10.603	$C_p cca'$	71.8.628	$l_p m'm'm$	74.3.652	$Im'ma$
68.11.604	$C_p cc'a'$	71.9.629	$l_p m'm'm'$	74.4.653	$Imma'$
<b>69.1.605</b>	<b>Fmmm</b>	<b>72.1.630</b>	<b>lbam</b>	74.5.654	$Im'm'a$
69.2.606	$Fmmm1'$	72.2.631	$lbam1'$	74.6.655	$Imm'a'$
69.3.607	$Fm'mm$	72.3.632	$lb'am$	74.7.656	$Im'm'a'$
69.4.608	$Fm'm'm$			74.8.657	$l_p mma$

74.9.658	$I_p m'm'a$	78.2.680	$P4_3 1'$	83.2.704	$P4/m1'$
74.10.659	$I_p mm'a'$	78.3.681	$P4_3'$	83.3.705	$P4'/m$
74.11.660	$I_p m'ma'$	78.4.682	$P_p 4_3$	83.4.706	$P4/m'$
<b>TETRAGONAL SYSTEM</b>		<b>79.1.683</b>	<b><math>I4</math></b>	83.5.707	$P4'/m'$
<b>75.1.661</b>	<b><math>P4</math></b>	79.2.684	$I41'$	83.6.708	$P_{2c} 4/m$
75.2.662	$P41'$	79.3.685	$I4'$	83.7.709	$P_p 4/m$
75.3.663	$P4'$	79.4.686	$I_p 4$	83.8.710	$P_1 4/m$
75.4.664	$P_{2c} 4$	79.5.687	$I_p 4'$	83.9.711	$P_{2c} 4'/m$
75.5.665	$P_p 4$	<b>80.1.688</b>	<b><math>I4_1</math></b>	83.10.712	$P_p 4/m'$
75.6.666	$P_1 4$	80.2.689	$I4_1 1'$	<b>84.1.713</b>	<b><math>P4_2/m</math></b>
75.7.667	$P_{2c} 4'$	80.3.690	$I4_1'$	84.2.714	$P4_2/m1'$
<b>76.1.668</b>	<b><math>P4_1</math></b>	80.4.691	$I_p 4_1$	84.3.715	$P4_2'/m$
76.2.669	$P4_1 1'$	80.5.692	$I_p 4_1'$	84.4.716	$P4_2/m'$
76.3.670	$P4_1'$	<b>81.1.693</b>	<b><math>P\&amp;</math></b>	84.5.717	$P4_2'/m'$
76.4.671	$P_p 4_1$	81.2.694	$P\& 1'$	84.6.718	$P_p 4_2/m$
<b>77.1.672</b>	<b><math>P4_2</math></b>	81.3.695	$P\&'$	84.7.719	$P_p 4_2'/m'$
77.2.673	$P4_2 1'$	81.4.696	$P_{2c} \&$	<b>85.1.720</b>	<b><math>P4/n</math></b>
77.3.674	$P4_2'$	81.5.697	$P_p \&$	85.2.721	$P4/n1'$
77.4.675	$P_{2c} 4_2$	81.6.698	$P_1 \&$	85.3.722	$P4'/n$
77.5.676	$P_p 4_2$	<b>82.1.699</b>	<b><math>I\&amp;</math></b>	85.4.723	$P4/n'$
77.6.677	$P_1 4_2$	82.2.700	$I\& 1'$	85.5.724	$P4'/n'$
77.7.678	$P_{2c} 4_2'$	82.3.701	$I\&'$	85.6.725	$P_{2c} 4/n$
<b>78.1.679</b>	<b><math>P4_3</math></b>	82.4.702	$I_p \&$	85.7.726	$P_{2c} 4'/n$
		<b>83.1.703</b>	<b><math>P4/m</math></b>	<b>86.1.727</b>	<b><math>P4_2/n</math></b>

86.2.728	$P4_2/n1'$	89.6.752	$P_{2c}422$	<b>93.1.776</b>	<b><math>P4_222</math></b>
86.3.729	$P4_2'/n$	89.7.753	$P_P422$	93.2.777	$P4_2221'$
86.4.730	$P4_2/n'$	89.8.754	$P_1422$	93.3.778	$P4_2'22'$
86.5.731	$P4_2'/n'$	89.9.755	$P_{2c}4'22'$	93.4.779	$P4_22'2'$
86.6.732	$P_14_2/n$	89.10.756	$P_P4'22'$	93.5.780	$P4_2'2'2$
<b>87.1.733</b>	<b><math>I4/m</math></b>	<b>90.1.757</b>	<b><math>P42_12</math></b>	93.6.781	$P_{2c}4_222$
87.2.734	$I4/m1'$	90.2.758	$P42_121'$	93.7.782	$P_P4_222$
87.3.735	$I4'/m$	90.3.759	$P4'2_12'$	93.8.783	$P_14_222$
87.4.736	$I4/m'$	90.4.760	$P42_1'2'$	93.9.784	$P_{2c}4_2'22'$
87.5.737	$I4'/m'$	90.5.761	$P4'2_1'2$	93.10.785	$P_P4_2'22'$
87.6.738	$I_P4/m$	90.6.762	$P_{2c}42_12$	<b>94.1.786</b>	<b><math>P4_22_12</math></b>
87.7.739	$I_P4'/m$	90.7.763	$P_{2c}4'2_1'2$	94.2.787	$P4_22_121'$
87.8.740	$I_P4/m'$	<b>91.1.764</b>	<b><math>P4_122</math></b>	94.3.788	$P4_2'2_12'$
87.9.741	$I_P4'/m'$	91.2.765	$P4_1221'$	94.4.789	$P4_22_1'2'$
<b>88.1.742</b>	<b><math>I4_1/a</math></b>	91.3.766	$P4_1'22'$	94.5.790	$P4_2'2_1'2$
88.2.743	$I4_1/a1'$	91.4.767	$P4_12'2'$	94.6.791	$P_{2c}4_22_12$
88.3.744	$I4_1'/a$	91.5.768	$P4_1'2'2$	94.7.792	$P_{2c}4_2'2_1'2$
88.4.745	$I4_1/a'$	91.6.769	$P_P4_122$	<b>95.1.793</b>	<b><math>P4_322</math></b>
88.5.746	$I4_1'/a'$	91.7.770	$P_P4_1'22'$	95.2.794	$P4_3221'$
<b>89.1.747</b>	<b><math>P422</math></b>	<b>92.1.771</b>	<b><math>P4_12_12</math></b>	95.3.795	$P4_3'22'$
89.2.748	$P4221'$	92.2.772	$P4_12_121'$	95.4.796	$P4_32'2'$
89.3.749	$P4'22'$	92.3.773	$P4_1'2_12'$	95.5.797	$P4_3'2'2$
89.4.750	$P42'2'$	92.4.774	$P4_12_1'2'$	95.6.798	$P_P4_322$
89.5.751	$P4'2'2$	92.5.775	$P4_1'2_1'2$	95.7.799	$P_P4_3'22'$

<b>96.1.800</b>	<b>P<sub>4</sub>2<sub>1</sub>2</b>	99.2.824	P4mm1'	101.5.849	P <sub>4</sub> 2c'm'
96.2.801	P <sub>4</sub> 2 <sub>1</sub> 21'	99.3.825	P4'm'm	101.6.850	P <sub>p</sub> 4 <sub>2</sub> cm
96.3.802	P <sub>4</sub> 2 <sub>1</sub> 2'2'	99.4.826	P4'mmm'	101.7.851	P <sub>p</sub> 4 <sub>2</sub> 'cm'
96.4.803	P <sub>4</sub> 2 <sub>1</sub> 2'	99.5.827	P4m'm'm'	<b>102.1.852</b>	<b>P<sub>4</sub>2nm</b>
96.5.804	P <sub>4</sub> 2 <sub>1</sub> 2'2	99.6.828	P <sub>2c</sub> 4mm	102.2.853	P <sub>4</sub> 2nm1'
<b>97.1.805</b>	<b>I422</b>	99.7.829	P <sub>p</sub> 4mm	102.3.854	P <sub>4</sub> 2'n'm
97.2.806	I422	99.8.830	P <sub>1</sub> 4mm	102.4.855	P <sub>4</sub> 2'nm'
97.3.807	I4'22'	99.9.831	P <sub>2c</sub> 4'm'm	102.5.856	P <sub>4</sub> 2n'm'
97.4.808	I42'2'	99.10.832	P <sub>2c</sub> 4'mm'	102.6.857	P <sub>1</sub> 4 <sub>2</sub> nm
97.5.809	I4'2'2	99.11.833	P <sub>2c</sub> 4m'm'm'	102.7.858	P <sub>1</sub> 4 <sub>2</sub> n'm'
97.6.810	I <sub>p</sub> 422	99.12.834	P <sub>p</sub> 4'mm'	<b>103.1.859</b>	<b>P4cc</b>
97.7.811	I <sub>p</sub> 4'22'	99.13.835	P <sub>1</sub> 4m'm'	103.2.860	P4cc1'
97.8.812	I <sub>p</sub> 42'2'	<b>100.1.836</b>	<b>P4bm</b>	103.3.861	P4'c'c
97.9.813	I <sub>p</sub> 4'2'2	100.2.837	P4bm1'	103.4.862	P4'cc'
<b>98.1.814</b>	<b>I4<sub>1</sub>22</b>	100.3.838	P4'b'm	103.5.863	P4c'c'
98.2.815	I4 <sub>1</sub> 221'	100.4.839	P4'bm'	103.6.864	P <sub>p</sub> 4cc
98.3.816	I4 <sub>1</sub> '22'	100.5.840	P4b'm'	103.7.865	P <sub>p</sub> 4'cc'
98.4.817	I4 <sub>1</sub> 2'2'	100.6.841	P <sub>2c</sub> 4bm	<b>104.1.866</b>	<b>P4nc</b>
98.5.818	I4 <sub>1</sub> '2'2	100.7.842	P <sub>2c</sub> 4'b'm	104.2.867	P4nc1'
98.6.819	I <sub>p</sub> 4 <sub>1</sub> 22	100.8.843	P <sub>2c</sub> 4'bm'	104.3.868	P4'n'c
98.7.820	I <sub>p</sub> 4 <sub>1</sub> '22'	100.9.844	P <sub>2c</sub> 4b'm'	104.4.869	P4'nc'
98.8.821	I <sub>p</sub> 4 <sub>1</sub> 2'2'	<b>101.1.845</b>	<b>P<sub>4</sub>2cm</b>	104.5.870	P4n'c'
98.9.822	I <sub>p</sub> 4 <sub>1</sub> '2'2	101.2.846	P <sub>4</sub> 2cm1'	<b>105.1.871</b>	<b>P<sub>4</sub>2mc</b>
<b>99.1.823</b>	<b>P4mm</b>	101.3.847	P <sub>4</sub> 2'c'm	105.2.872	P <sub>4</sub> 2mc1'
		101.4.848	P <sub>4</sub> 2'cm'		

105.3.873	$P4_2'm'c$	108.6.897	$I_p 4cm$	111.11.921	$P_1 \&'2m'$
105.4.874	$P4_2'mc'$	108.7.898	$I_p 4'c'm$	<b>112.1.922</b>	<b><math>P\&amp;2c</math></b>
105.5.875	$P4_2'm'c'$	108.8.899	$I_p 4'cm'$	112.2.923	$P\&2c1'$
105.6.876	$P_p 4_2 mc$	108.9.900	$I_p 4c'm'$	112.3.924	$P\&'2'c$
105.7.877	$P_p 4_2'mc'$	<b>109.1.901</b>	<b><math>I4_1md</math></b>	112.4.925	$P\&'2c'$
<b>106.1.878</b>	<b><math>P4_2 bc</math></b>	109.2.902	$I4_1md1'$	112.5.926	$P\&'2c'$
106.2.879	$P4_2 bc1'$	109.3.903	$I4_1'm'd$	112.6.927	$P_p \&2c$
106.3.880	$P4_2'b'c$	109.4.904	$I4_1'md'$	112.7.928	$P_p \&'2c'$
106.4.881	$P4_2'bc'$	109.5.905	$I4_1m'd'$	<b>113.1.929</b>	<b><math>P\&amp;2_1m</math></b>
106.5.882	$P4_2 b'c'$	<b>110.1.906</b>	<b><math>I4_1cd</math></b>	113.2.930	$P\&2_1m1'$
<b>107.1.883</b>	<b><math>I4mm</math></b>	110.2.907	$I4_1cd1'$	113.3.931	$P\&'2_1'm$
107.2.884	$I4mm1'$	110.3.908	$I4_1'c'd$	113.4.932	$P\&'2_1m'$
107.3.885	$I4'm'm$	110.4.909	$I4_1'cd'$	113.5.933	$P\&2_1'm'$
107.4.886	$I4'mm'$	110.5.910	$I4_1c'd'$	113.6.934	$P_{2c} \&2_1m$
107.5.887	$I4m'm'$	<b>111.1.911</b>	<b><math>P\&amp;2m</math></b>	113.7.935	$P_{2c} \&'2_1m'$
107.6.888	$I_p 4mm$	111.2.912	$P\&2m1'$	<b>114.1.936</b>	<b><math>P\&amp;2_1c</math></b>
107.7.889	$I_p 4'm'm$	111.3.913	$P\&'2'm$	114.2.937	$P\&2_1c1'$
107.8.890	$I_p 4'mm'$	111.4.914	$P\&'2m'$	114.3.938	$P\&'2_1'c$
107.9.891	$I_p 4m'm'$	111.5.915	$P\&'2'm'$	114.4.939	$P\&'2_1c'$
<b>108.1.892</b>	<b><math>I4cm</math></b>	111.6.916	$P_{2c} \&2m$	114.5.940	$P\&2_1'c'$
108.2.893	$I4cm1'$	111.7.917	$P_p \&2m$	<b>115.1.941</b>	<b><math>P\&amp;m2</math></b>
108.3.894	$I4'c'm$	111.8.918	$P_1 \&2m$	115.2.942	$P\&m21'$
108.4.895	$I4'cm'$	111.9.919	$P_{2c} \&'2'm'$	115.3.943	$P\&'m'2$
108.5.896	$I4c'm'$	111.10.920	$P_p \&'2m'$	115.4.944	$P\&'m'2'$

115.5.945	$P\bar{2}m'$	118.5.969	$P\bar{2}n'$	121.9.993	$I\bar{4}2m'$
115.6.946	$P_{2c}\bar{2}m2$	118.6.970	$P_1\bar{2}n2$	<b>122.1.994</b>	<b><math>I\bar{4}2d</math></b>
115.7.947	$P_p\bar{2}m2$	<b>119.1.971</b>	<b><math>I\bar{4}m2</math></b>	122.2.995	$I\bar{4}2d1'$
115.8.948	$P_1\bar{2}m2$	119.2.972	$I\bar{4}m21'$	122.3.996	$I\bar{4}'2'd$
115.9.949	$P_{2c}\bar{2}'m'2$	119.3.973	$I\bar{4}'m'2$	122.4.997	$I\bar{4}'2d'$
115.10.950	$P_p\bar{2}'m'2$	119.4.974	$I\bar{4}'m'2'$	122.5.998	$I\bar{4}'2d'$
<b>116.1.951</b>	<b><math>P\bar{4}c2</math></b>	119.5.975	$I\bar{4}m'2'$	<b>123.1.999</b>	<b><math>P4/mmm</math></b>
116.2.952	$P\bar{4}c21'$	119.6.976	$I_p\bar{4}m2$	123.2.1000	$P4/mmm1'$
116.3.953	$P\bar{4}'c'2$	119.7.977	$I_p\bar{4}'m'2$	123.3.1001	$P4/m'mm$
116.4.954	$P\bar{4}'c'2'$	<b>120.1.978</b>	<b><math>I\bar{4}c2</math></b>	123.4.1002	$P4'/mm'm$
116.5.955	$P\bar{4}c'2'$	120.2.979	$I\bar{4}c21'$	123.5.1003	$P4'/mmm'$
116.6.956	$P_p\bar{4}c2$	120.3.980	$I\bar{4}'c'2$	123.6.1004	$P4'/m'm'm$
116.7.957	$P_p\bar{4}'c'2'$	120.4.981	$I\bar{4}'c'2'$	123.7.1005	$P4/mm'm'$
<b>117.1.958</b>	<b><math>P\bar{4}b2</math></b>	120.5.982	$I\bar{4}c'2'$	123.8.1006	$P4'/m'mm'$
117.2.959	$P\bar{4}b21'$	120.6.983	$I_p\bar{4}c2$	123.9.1007	$P4/m'm'm'$
117.3.960	$P\bar{4}'b'2$	120.7.984	$I_p\bar{4}'c'2'$	123.10.1008	$P_{2c}4/mmm$
117.4.961	$P\bar{4}'b'2'$	<b>121.1.985</b>	<b><math>I\bar{4}2m</math></b>	123.11.1009	$P_p4/mmm$
117.5.962	$P\bar{4}b'2'$	121.2.986	$I\bar{4}2m1'$	123.12.1010	$P_14/mmm$
117.6.963	$P_{2c}\bar{4}b2$	121.3.987	$I\bar{4}'2'm$	123.13.1011	$P_{2c}4'/mm'm$
117.7.964	$P_{2c}\bar{4}'b'2$	121.4.988	$I\bar{4}'2m'$	123.14.1012	$P_{2c}4'/mmm'$
<b>118.1.965</b>	<b><math>P\bar{4}n2</math></b>	121.5.989	$I\bar{4}'2m'$	123.15.1013	$P_{2c}4/mm'm'$
118.2.966	$P\bar{4}n21'$	121.6.990	$I_p\bar{4}2m$	123.16.1014	$P_p4/m'mm$
118.3.967	$P\bar{4}'n'2$	121.7.991	$I_p\bar{4}'2'm$	123.17.1015	$P_p4'/mmm'$
118.4.968	$P\bar{4}'n'2'$	121.8.992	$I_p\bar{4}'2m'$	123.18.1016	$P_p4'/m'mm'$
				123.19.1017	$P_14/mm'm'$

	125.12.1042	$P_{2c}4'/nbm'$	<b>128.1.1066</b>	<b>P4/mnc</b>
<b>124.1.1018</b>		<b>P4/mcc</b>	128.2.1067	P4/mnc1'
124.2.1019		P4/mcc1'	128.3.1068	P4/m'nc
124.3.1020		P4/m'cc	128.4.1069	P4'/mn'c
124.4.1021		P4'/mc'c	128.5.1070	P4'/mnc'
124.5.1022		P4'/mcc'	128.6.1071	P4'/m'n'c
124.6.1023		P4'/m'c'c	128.7.1072	P4/mn'c'
124.7.1024		P4/mc'c'	128.8.1073	P4'/m'nc'
124.8.1025		P4'/m'cc'	128.9.1074	P4/m'n'c'
124.9.1026		P4/m'c'c'	<b>129.1.1075</b>	<b>P4/nmm</b>
124.10.1027		$P_p4/mcc$	129.2.1076	P4/nmm1'
124.11.1028		$P_p4/m'cc$	129.3.1077	P4/n'mm
124.12.1029		$P_p4'/mcc'$	129.4.1078	P4'/nm'm
124.13.1030		$P_p4'/m'cc'$	129.5.1079	P4'/nmm'
<b>125.1.1031</b>		<b>P4/nbm</b>	129.6.1080	P4'/n'm'm
125.2.1032		P4/nbm1'	129.7.1081	P4/nm'm'
125.3.1033		P4/n'bm	129.8.1082	P4'/n'mm'
125.4.1034		P4'/nb'm	129.9.1083	P4/n'm'm'
125.5.1035		P4'/nbm'	129.10.1084	$P_{2c}4/nmm$
125.6.1036		P4'/n'b'm	129.11.1085	$P_{2c}4'/nm'm$
125.7.1037		P4/nb'm'	129.12.1086	$P_{2c}4'/nmm'$
125.8.1038		P4'/n'bm'	129.13.1087	$P_{2c}4/nm'm'$
125.9.1039		P4/n'b'm'	<b>130.1.1088</b>	<b>P4/ncc</b>
125.10.1040		$P_{2c}4/nbm$	130.2.1089	P4/ncc1'
125.11.1041		$P_{2c}4'/nb'm$	130.3.1090	P4/n'cc
	125.13.1043	$P_{2c}4/nb'm'$		
	<b>126.1.1044</b>	<b>P4/nnc</b>		
	126.2.1045	P4/nnc1'		
	126.3.1046	P4/n'nc		
	126.4.1047	P4'/nn'c		
	126.5.1048	P4'/nnc'		
	126.6.1049	P4'/n'n'c		
	126.7.1050	P4/nn'c'		
	126.8.1051	P4'/n'nc'		
	126.9.1052	P4/n'n'c'		
	<b>127.1.1053</b>	<b>P4/mbm</b>		
	127.2.1054	P4/mbm1'		
	127.3.1055	P4/m'bm		
	127.4.1056	P4'/mb'm		
	127.5.1057	P4'/mbm'		
	127.6.1058	P4'/m'b'm		
	127.7.1059	P4/mb'm'		
	127.8.1060	P4'/m'bm'		
	127.9.1061	P4/m'b'm'		
	127.10.1062	$P_{2c}4/mbm$		
	127.11.1063	$P_{2c}4'/mb'm$		
	127.12.1064	$P_{2c}4'/mbm'$		
	127.13.1065	$P_{2c}4/mb'm'$		



130.4.1091	$P4'/nc'c$	132.7.1116	$P4_2/mc'm'$	134.10.1141	$P_14_2/nnm$
130.5.1092	$P4'/ncc'$	132.8.1117	$P4_2'/m'cm'$	134.11.1142	$P_14_2/nn'm'$
130.6.1093	$P4'/n'c'c$	132.9.1118	$P4_2/m'c'm'$	<b>135.1.1143</b>	<b><math>P4_2/mbc</math></b>
130.7.1094	$P4/nc'c'$	132.10.1119	$P_P4_2/mcm$	135.2.1144	$P4_2/mbc1'$
130.8.1095	$P4'/n'cc'$	132.11.1120	$P_P4_2/m'cm$	135.3.1145	$P4_2/m'bc$
130.9.1096	$P4/n'c'c'$	132.12.1121	$P_P4_2'/mcm'$	135.4.1146	$P4_2'/mb'c$
<b>131.1.1097</b>	<b><math>P4_2/mmc</math></b>	132.13.1122	$P_P4_2'/m'cm'$	135.5.1147	$P4_2'/mbc'$
131.2.1098	$P4_2/mmc1'$	<b>133.1.1123</b>	<b><math>P4_2/nbc</math></b>	135.6.1148	$P4_2'/m'b'c$
131.3.1099	$P4_2/m'mc$	133.2.1124	$P4_2/nbc1'$	135.7.1149	$P4_2/mb'c'$
131.4.1100	$P4_2'/mm'c$	133.3.1125	$P4_2/n'bc$	135.8.1150	$P4_2'/m'bc'$
131.5.1101	$P4_2'/mmc'$	133.4.1126	$P4_2'/nb'c$	135.9.1151	$P4_2/m'b'c'$
131.6.1102	$P4_2'/m'm'c$	133.5.1127	$P4_2'/nbc'$	<b>136.1.1152</b>	<b><math>P4_2/mnm</math></b>
131.7.1103	$P4_2/mm'c'$	133.6.1128	$P4_2'/n'b'c$	136.2.1153	$P4_2/mnm1'$
131.8.1104	$P4_2'/m'mc'$	133.7.1129	$P4_2/nb'c'$	136.3.1154	$P4_2/m'nm$
131.9.1105	$P4_2/m'm'c'$	133.8.1130	$P4_2'/n'bc'$	136.4.1155	$P4_2'/mn'm$
131.10.1106	$P_P4_2/mmc$	133.9.1131	$P4_2/n'b'c'$	136.5.1156	$P4_2'/mnm'$
131.11.1107	$P_P4_2/m'mc$	<b>134.1.1132</b>	<b><math>P4_2/nnm</math></b>	136.6.1157	$P4_2'/m'n'm$
131.12.1108	$P_P4_2/mm'c'$	134.2.1133	$P4_2/nnm1'$	136.7.1158	$P4_2/mn'm'$
131.13.1109	$P_P4_2'/m'mc'$	134.3.1134	$P4_2/n'nm$	136.8.1159	$P4_2'/m'nm'$
<b>132.1.1110</b>	<b><math>P4_2/mcm</math></b>	134.4.1135	$P4_2'/nn'm$	136.9.1160	$P4_2/m'n'm'$
132.2.1111	$P4_2/mcm1'$	134.5.1136	$P4_2'/nmm'$	<b>137.1.1161</b>	<b><math>P4_2/nmc</math></b>
132.3.1112	$P4_2/m'cm$	134.6.1137	$P4_2'/n'n'm$	137.2.1162	$P4_2/nmc1'$
132.4.1113	$P4_2'/mc'm$	134.7.1138	$P4_2/nn'm'$	137.3.1163	$P4_2/n'mc$
132.5.1114	$P4_2'/mcm'$	134.8.1139	$P4_2'/n'nm'$	137.4.1164	$P4_2'/nm'c$
132.6.1115	$P4_2'/m'c'm$	134.9.1140	$P4_2/n'n'm'$		

137.5.1165	$P4_2/nmc'$	139.12.1190	$I_p 4'/mm'm$	141.3.1215	$I4_1/a'md$
137.6.1166	$P4_2/n'm'c$	139.13.1191	$I_p 4'/mmm'$	141.4.1216	$I4_1'/am'd$
137.7.1167	$P4_2/nm'c'$	139.14.1192	$I_p 4'/m'm'm$	141.5.1217	$I4_1'/amd'$
137.8.1168	$P4_2/n'mc'$	139.15.1193	$I_p 4/mm'm'$	141.6.1218	$I4_1'/a'm'd$
137.9.1169	$P4_2/n'm'c'$	139.16.1194	$I_p 4'/m'mm'$	141.7.1219	$I4_1/am'd'$
<b>138.1.1170</b>	<b><math>P4_2/ncm</math></b>	139.17.1195	$I_p 4/m'm'm'$	141.8.1220	$I4_1'/a'md'$
138.2.1171	$P4_2/ncm1'$	<b>140.1.1196</b>	<b><math>I4/mcm</math></b>	141.9.1221	$I4_1/a'm'd'$
138.3.1172	$P4_2/n'cm$	140.2.1197	$I4/mcm1'$	<b>142.1.1222</b>	<b><math>I4_1/acd</math></b>
138.4.1173	$P4_2/nc'm$	140.3.1198	$I4/m'cm$	142.2.1223	$I4_1/acd1'$
138.5.1174	$P4_2'/ncm'$	140.4.1199	$I4'/mc'm$	142.3.1224	$I4_1/a'cd$
138.6.1175	$P4_2'/n'c'm$	140.5.1200	$I4'/mcm'$	142.4.1225	$I4_1'/ac'd$
138.7.1176	$P4_2/nc'm'$	140.6.1201	$I4'/m'c'm$	142.5.1226	$I4_1'/acd'$
138.8.1177	$P4_2'/n'cm'$	140.7.1202	$I4/mc'm'$	142.6.1227	$I4_1'/a'c'd$
138.9.1178	$P4_2/n'c'm'$	140.8.1203	$I4'/m'cm'$	142.7.1228	$I4_1/ac'd'$
<b>139.1.1179</b>	<b><math>I4/mmm</math></b>	140.9.1204	$I4/m'c'm'$	142.8.1229	$I4_1'/a'cd'$
139.2.1180	$I4/mmm1'$	140.10.1205	$I_p 4/mcm$	142.9.1230	$I4_1/a'c'd'$
139.3.1181	$I4/m'mm$	140.11.1206	$I_p 4/m'cm$		
139.4.1182	$I4'/mm'm$	140.12.1207	$I_p 4'/mc'm$		
139.5.1183	$I4'/mmm'$	140.13.1208	$I_p 4'/mcm'$	<b>143.1.1231</b>	<b><math>P3</math></b>
139.6.1184	$I4'/m'm'm$	140.14.1209	$I_p 4'/m'c'm$	143.2.1232	$P31'$
139.7.1185	$I4/mm'm'$	140.15.1210	$I_p 4/mc'm'$	143.3.1233	$P_{2c} 3$
139.8.1186	$I4'/m'mm'$	140.16.1211	$I_p 4'/m'cm'$	<b>144.1.1234</b>	<b><math>P3_1</math></b>
139.9.1187	$I4/m'm'm'$	140.17.1212	$I_p 4/m'c'm'$	144.2.1235	$P3_11'$
139.10.1188	$I_p 4/mmm$	<b>141.1.1213</b>	<b><math>I4_1/amd</math></b>	144.3.1236	$P_{2c} 3_2$
139.11.1189	$I_p 4/m'mm$	141.2.1214	$I4_1/amd1'$		

## TRIGONAL SYSTEM

<b>145.1.1237</b>	<b>P<sub>3</sub><sub>2</sub></b>				
145.2.1238	P <sub>3</sub> <sub>2</sub> 1'	151.2.1260	P <sub>3</sub> <sub>1</sub> 121'	156.5.1283	P <sub>2c</sub> 3m'1
145.3.1239	P <sub>2c</sub> 3 <sub>1</sub>	151.3.1261	P <sub>3</sub> <sub>1</sub> 12'	<b>157.1.1284</b>	<b>P<sub>3</sub>1m</b>
<b>146.1.1240</b>	<b>R<sub>3</sub></b>	151.4.1262	P <sub>2c</sub> 3 <sub>2</sub> 12	157.2.1285	P <sub>3</sub> 1m1'
146.2.1241	R <sub>3</sub> 1'	<b>152.1.1263</b>	<b>P<sub>3</sub><sub>1</sub>21</b>	157.3.1286	P <sub>3</sub> 1m'
146.3.1242	R <sub>R</sub> 3	152.2.1264	P <sub>3</sub> <sub>1</sub> 211'	157.4.1287	P <sub>2c</sub> 31m
<b>147.1.1243</b>	<b>P<sub>3</sub><sub>2</sub></b>	152.3.1265	P <sub>3</sub> <sub>1</sub> 2'1	157.5.1288	P <sub>2c</sub> 31m'
147.2.1244	P <sub>3</sub> <sub>2</sub> 1'	152.4.1266	P <sub>2c</sub> 3 <sub>2</sub> 21	<b>158.1.1289</b>	<b>P<sub>3</sub>c1</b>
147.3.1245	P <sub>3</sub> <sub>2</sub> '	<b>153.1.1267</b>	<b>P<sub>3</sub><sub>2</sub>12</b>	158.2.1290	P <sub>3</sub> c11'
147.4.1246	P <sub>2c</sub> <sub>3</sub>	153.2.1268	P <sub>3</sub> <sub>2</sub> 121'	158.3.1291	P <sub>3</sub> c'1
<b>148.1.1247</b>	<b>R<sub>3</sub><sub>2</sub></b>	153.3.1269	P <sub>3</sub> <sub>2</sub> 12'	<b>159.1.1292</b>	<b>P<sub>3</sub>1c</b>
148.2.1248	R <sub>3</sub> <sub>2</sub> 1'	153.4.1270	P <sub>2c</sub> 3 <sub>1</sub> 12	159.2.1293	P <sub>3</sub> 1c1'
148.3.1249	R <sub>3</sub> <sub>2</sub> '	<b>154.1.1271</b>	<b>P<sub>3</sub><sub>2</sub>21</b>	159.3.1294	P <sub>3</sub> 1c'
148.4.1250	R <sub>R</sub> <sub>3</sub>	154.2.1272	P <sub>3</sub> <sub>2</sub> 211'	<b>160.1.1295</b>	<b>R<sub>3</sub>m</b>
<b>149.1.1251</b>	<b>P<sub>3</sub>12</b>	154.3.1273	P <sub>3</sub> <sub>2</sub> 2'1	160.2.1296	R <sub>3</sub> m1'
149.2.1252	P <sub>3</sub> 121'	154.4.1274	P <sub>2c</sub> 3 <sub>1</sub> 21	160.3.1297	R <sub>3</sub> m'
149.3.1253	P <sub>3</sub> 12'	<b>155.1.1275</b>	<b>R<sub>3</sub>2</b>	160.4.1298	R <sub>R</sub> 3m
149.4.1254	P <sub>2c</sub> 312	155.2.1276	R <sub>3</sub> 21'	160.5.1299	R <sub>R</sub> 3m'
<b>150.1.1255</b>	<b>P<sub>3</sub>21</b>	155.3.1277	R <sub>3</sub> 2'	<b>161.1.1300</b>	<b>R<sub>3</sub>c</b>
150.2.1256	P <sub>3</sub> 211'	155.4.1278	R <sub>R</sub> 32	161.2.1301	R <sub>3</sub> c1'
150.3.1257	P <sub>3</sub> 2'1	<b>156.1.1279</b>	<b>P<sub>3</sub>m1</b>	161.3.1302	R <sub>3</sub> c'
150.4.1258	P <sub>2c</sub> 321	156.2.1280	P <sub>3</sub> m11'	<b>162.1.1303</b>	<b>P<sub>3</sub><sub>1</sub>m</b>
<b>151.1.1259</b>	<b>P<sub>3</sub><sub>1</sub>12</b>	156.3.1281	P <sub>3</sub> m'1	162.2.1304	P <sub>3</sub> <sub>1</sub> m1'
		156.4.1282	P <sub>2c</sub> 3m1		

162.3.1305	$P\bar{6}1m$	166.3.1329	$R\bar{6}m$	171.2.1351	$P6_21'$
162.4.1306	$P\bar{6}1m'$	166.4.1330	$R\bar{6}m'$	171.3.1352	$P6_2'$
162.5.1307	$P\bar{6}1m'$	166.5.1331	$R\bar{6}m'$	171.4.1353	$P_{2c}6_2$
162.6.1308	$P_{2c}\bar{6}1m$	166.6.1332	$R_R\bar{6}m$	171.5.1354	$P_{2c}6_2'$
162.7.1309	$P_{2c}\bar{6}1m'$	166.7.1333	$R_R\bar{6}m'$	<b>172.1.1355</b>	<b><math>P6_4</math></b>
<b>163.1.1310</b>	<b><math>P\bar{6}1c</math></b>	<b>167.1.1334</b>	<b><math>R\bar{6}c</math></b>	172.2.1356	$P6_4 1'$
163.2.1311	$P\bar{6}1c1'$	167.2.1335	$R\bar{6}c1'$	172.3.1357	$P6_4'$
163.3.1312	$P\bar{6}1c$	167.3.1336	$R\bar{6}'c$	172.4.1358	$P_{2c}6_4$
163.4.1313	$P\bar{6}'1c'$	167.4.1337	$R\bar{6}'c'$	172.5.1359	$P_{2c}6_4'$
163.5.1314	$P\bar{6}1c'$	167.5.1338	$R\bar{6}c'$	<b>173.1.1360</b>	<b><math>P6_3</math></b>
<b>164.1.1315</b>	<b><math>P\bar{6}m1</math></b>	<b>HEXAGONAL SYSTEM</b>		173.2.1361	$P6_31'$
164.2.1316	$P\bar{6}m11'$	<b>168.1.1339</b>	<b><math>P6</math></b>	173.3.1362	$P6_3'$
164.3.1317	$P\bar{6}'m1$	168.2.1340	$P61'$	<b>174.1.1363</b>	<b><math>P\bar{6}</math></b>
164.4.1318	$P\bar{6}'m1'$	168.3.1341	$P6'$	174.2.1364	$P\bar{6}1'$
164.5.1319	$P\bar{6}m'1$	168.4.1342	$P_{2c}6$	174.3.1365	$P\bar{6}'$
164.6.1320	$P_{2c}\bar{6}m1$	168.5.1343	$P_{2c}6'$	174.4.1366	$P_{2c}\bar{6}$
164.7.1321	$P_{2c}\bar{6}m'1$	<b>169.1.1344</b>	<b><math>P6_1</math></b>	<b>175.1.1367</b>	<b><math>P6/m</math></b>
<b>165.1.1322</b>	<b><math>P\bar{6}c1</math></b>	169.2.1345	$P6_11'$	175.2.1368	$P6/m1'$
165.2.1323	$P\bar{6}c11'$	169.3.1346	$P6_1'$	175.3.1369	$P6'/m$
165.3.1324	$P\bar{6}'c1$	<b>170.1.1347</b>	<b><math>P6_5</math></b>	175.4.1370	$P6/m'$
165.4.1325	$P\bar{6}'c'1$	170.2.1348	$P6_51'$	175.5.1371	$P6'/m'$
165.5.1326	$P\bar{6}c'1$	170.3.1349	$P6_5'$	175.6.1372	$P_{2c}6/m$
<b>166.1.1327</b>	<b><math>R\bar{6}m</math></b>	<b>171.1.1350</b>	<b><math>P6_2</math></b>	175.7.1373	$P_{2c}6'/m$
166.2.1328	$R\bar{6}m1'$				

<b>176.1.1374</b>	<b><math>P6_3/m</math></b>	180.3.1398	$P6_2'2'2'$	183.8.1422	$P_{2c}6'mm'$
176.2.1375	$P6_3/m1'$	180.4.1399	$P6_2'22'$	183.9.1423	$P_{2c}6m'm'$
176.3.1376	$P6_3'/m$	180.5.1400	$P6_2'2'2'$	<b>184.1.1424</b>	<b><math>P6cc</math></b>
176.4.1377	$P6_3/m'$	180.6.1401	$P_{2c}6_2'22'$	184.2.1425	$P6cc1'$
176.5.1378	$P6_3'/m'$	180.7.1402	$P_{2c}6_2'22'$	184.3.1426	$P6'c'c$
<b>177.1.1379</b>	<b><math>P622</math></b>	<b>181.1.1403</b>	<b><math>P6_4'22</math></b>	184.4.1427	$P6'cc'$
177.2.1380	$P6221'$	181.2.1404	$P6_4'221'$	184.5.1428	$P6c'c'$
177.3.1381	$P6'2'2'$	181.3.1405	$P6_4'2'2'$	<b>185.1.1429</b>	<b><math>P6_3'cm</math></b>
177.4.1382	$P6'22'$	181.4.1406	$P6_4'22'$	185.2.1430	$P6_3'cm1'$
177.5.1383	$P6'2'2'$	181.5.1407	$P6_4'2'2'$	185.3.1431	$P6_3'c'm$
177.6.1384	$P_{2c}622$	181.6.1408	$P_{2c}6_4'22$	185.4.1432	$P6_3'cm'$
177.7.1385	$P_{2c}6'22'$	181.7.1409	$P_{2c}6_4'2'2'$	185.5.1433	$P6_3'c'm'$
<b>178.1.1386</b>	<b><math>P6_1'22</math></b>	<b>182.1.1410</b>	<b><math>p6_3'22</math></b>	<b>186.1.1434</b>	<b><math>P6_3'mc</math></b>
178.2.1387	$P6_1'221'$	182.2.1411	$p6_3'221'$	186.2.1435	$P6_3'mc1'$
178.3.1388	$P6_1'2'2'$	182.3.1412	$p6_3'2'2'$	186.3.1436	$P6_3'm'c$
178.4.1389	$P6_1'22'$	182.4.1413	$p6_3'22'$	186.4.1437	$P6_3'mc'$
178.5.1390	$P6_1'2'2'$	182.5.1414	$p6_3'2'2'$	186.5.1438	$P6_3'm'c'$
<b>179.1.1391</b>	<b><math>P6_5'22</math></b>	<b>183.1.1415</b>	<b><math>p6mm</math></b>	<b>187.1.1439</b>	<b><math>P\&amp;m2</math></b>
179.2.1392	$P6_5'221'$	183.2.1416	$P6mm1'$	187.2.1440	$P\&m21'$
179.3.1393	$P6_5'2'2'$	183.3.1417	$P6'm'm$	187.3.1441	$P\&m'2$
179.4.1394	$P6_5'22'$	183.4.1418	$P6'mm'$	187.4.1442	$P\&m'2'$
179.5.1395	$P6_5'2'2'$	183.5.1419	$P6m'm'$	187.5.1443	$P\&m'2'$
<b>180.1.1396</b>	<b><math>P6_2'22</math></b>	183.6.1420	$P_{2c}6mm$	187.6.1444	$P_{2c}\&m2$
180.2.1397	$P6_2'221'$	183.7.1421	$P_{2c}6'm'm$	187.7.1445	$P_{2c}\&m'2$

**188.1.1446**  **$P\bar{6}c2$**

188.2.1447  $P\bar{6}c21'$

188.3.1448  $P\bar{6}'c'2$

188.4.1449  $P\bar{6}'c'2'$

188.5.1450  $P\bar{6}c'2'$

**189.1.1451**  **$P\bar{6}2m$**

189.2.1452  $P\bar{6}2m1'$

189.3.1453  $P\bar{6}'2'm$

189.4.1454  $P\bar{6}'2m'$

189.5.1455  $P\bar{6}2'm'$

189.6.1456  $P_{2c}\bar{6}2m$

189.7.1457  $P_{2c}\bar{6}'2m'$

**190.1.1458**  **$P\bar{6}2c$**

190.2.1459  $P\bar{6}2c1'$

190.3.1460  $P\bar{6}'2'c$

190.4.1461  $P\bar{6}'2c'$

190.5.1462  $P\bar{6}2'c'$

**191.1.1463**  **$P6/mmm$**

191.2.1464  $P6/mmm1'$

191.3.1465  $P6/m'mm$

191.4.1466  $P6'/mm'm$

191.5.1467  $P6'/mmm'$

191.6.1468  $P6'/m'm'm$

191.7.1469  $P6'/m'mm'$

191.8.1470  $P6/mm'm'$

191.9.1471  $P6/m'm'm'$

191.10.1472  $P_{2c}6/mmm$

191.11.1473  $P_{2c}6'/mm'm$

191.12.1474  $P_{2c}6'/mmm'$

191.13.1475  $P_{2c}6/mm'm'$

**192.1.1476**  **$P6/mcc$**

192.2.1477  $P6/mcc1'$

192.3.1478  $P6/m'cc$

192.4.1479  $P6'/mc'c$

192.5.1480  $P6'/mcc'$

192.6.1481  $P6'/m'c'c$

192.7.1482  $P6'/m'cc'$

192.8.1483  $P6/mc'c'$

192.9.1484  $P6/m'c'c'$

**193.1.1485**  **$P6_3/mcm$**

193.2.1486  $P6_3/mcm1'$

193.3.1487  $P6_3/m'cm$

193.4.1488  $P6_3'/mc'm$

193.5.1489  $P6_3'/mcm'$

193.6.1490  $P6_3'/m'c'm$

193.7.1491  $P6_3'/m'cm'$

193.8.1492  $P6_3/mc'm'$

193.9.1493  $P6_3/m'c'm'$

**194.1.1494**  **$P6_3/mmc$**

194.2.1495  $P6_3/mmc1'$

194.3.1496  $P6_3/m'mc$

194.4.1497  $P6_3'/mm'c$

194.5.1498  $P6_3'/mmc'$

194.6.1499  $P6_3'/m'm'c$

194.7.1500  $P6_3'/m'mc'$

194.8.1501  $P6_3/mm'c'$

194.9.1502  $P6_3/m'm'c'$

## CUBIC SYSTEM

**195.1.1503**  **$P23$**

195.2.1504  $P231'$

195.3.1505  $P_F23$

**196.1.1506**  **$F23$**

196.2.1507  $F231'$

**197.1.1508**  **$I23$**

197.2.1509  $I231'$

197.3.1510  $I_P23$

**198.1.1511**  **$P2_13$**

198.2.1512  $P2_131'$

**199.1.1513**  **$I2_13$**

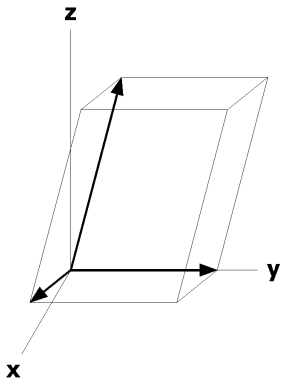
199.2.1514  $I2_131'$

199.3.1515  $I_P2_13$

		<b>206.1.1538</b>	<b>la</b>		<b>212.1.1561</b>	<b>P<sub>4</sub>32</b>
<b>200.1.1516</b>	<b>Pm</b>	206.2.1539	la <sub>1</sub> '		212.2.1562	P <sub>4</sub> 321'
200.2.1517	Pm <sub>1</sub> '	206.3.1540	la' <sub>1</sub>		212.3.1563	P <sub>4</sub> 3'32'
200.3.1518	Pm' <sub>1</sub>	206.4.1541	l <sub>p</sub> a			
200.4.1519	P <sub>F</sub> m			<b>213.1.1564</b>	<b>P<sub>4</sub>32</b>	
		<b>207.1.1542</b>	<b>P432</b>		213.2.1565	P <sub>4</sub> 321'
<b>201.1.1520</b>	<b>Pn</b>	207.2.1543	P4321'		213.3.1566	P <sub>4</sub> 1'32'
201.2.1521	Pn <sub>1</sub> '	207.3.1544	P4'32'			
201.3.1522	Pn' <sub>1</sub>	207.4.1545	P <sub>F</sub> 432	<b>214.1.1567</b>	<b>I<sub>4</sub>32</b>	
201.4.1523	P <sub>F</sub> n			214.2.1568	I <sub>4</sub> 321'	
		<b>208.1.1546</b>	<b>P<sub>4</sub>232</b>	214.3.1569	I <sub>4</sub> 1'32'	
<b>202.1.1524</b>	<b>Fm</b>	208.2.1547	P <sub>4</sub> 2321'	214.4.1570	l <sub>p</sub> 4 <sub>1</sub> 32	
202.2.1525	Fm <sub>1</sub> '	208.3.1548	P <sub>4</sub> 2'32'	214.5.1571	l <sub>p</sub> 4 <sub>1</sub> '32'	
202.3.1526	Fm' <sub>1</sub>	208.4.1549	P <sub>F</sub> 4 <sub>2</sub> 32			
				<b>215.1.1572</b>	<b>P<sub>4</sub>3m</b>	
<b>203.1.1527</b>	<b>Fd</b>	<b>209.1.1550</b>	<b>F432</b>	215.2.1573	P <sub>4</sub> 3m1'	
203.2.1528	Fd <sub>1</sub> '	209.2.1551	F4321'	215.3.1574	P <sub>4</sub> 1'3m'	
203.3.1529	Fd' <sub>1</sub>	209.3.1552	F4'32'	215.4.1575	P <sub>F</sub> 43m	
				215.5.1576	P <sub>F</sub> 4'3m'	
<b>204.1.1530</b>	<b>Im</b>	<b>210.1.1553</b>	<b>F<sub>4</sub>32</b>			
204.2.1531	Im <sub>1</sub> '	210.2.1554	F <sub>4</sub> 321'	<b>216.1.1577</b>	<b>F<sub>4</sub>3m</b>	
204.3.1532	Im' <sub>1</sub>	210.3.1555	F <sub>4</sub> 1'32'	216.2.1578	F <sub>4</sub> 3m1'	
204.4.1533	l <sub>p</sub> m			216.3.1579	F <sub>4</sub> 1'3m'	
204.5.1534	l <sub>p</sub> m' <sub>1</sub>	<b>211.1.1556</b>	<b>I<sub>4</sub>32</b>			
		211.2.1557	I <sub>4</sub> 321'	<b>217.1.1580</b>	<b>I<sub>4</sub>3m</b>	
<b>205.1.1535</b>	<b>Pa</b>	211.3.1558	I <sub>4</sub> '32'	217.2.1581	I <sub>4</sub> 3m1'	
205.2.1536	Pa	211.4.1559	l <sub>p</sub> 432	217.3.1582	I <sub>4</sub> 1'3m'	
205.3.1537	Pa' <sub>1</sub>	211.5.1560	l <sub>p</sub> 4'32'	217.4.1583	l <sub>p</sub> 43m	

217.5.1584	$I_p \overline{4}3m'$	223.2.1607	$Pm\overline{3}n1'$	227.3.1630	$Fd'\overline{3}'m$
<b>218.1.1585</b>	<b><math>P\overline{4}3n</math></b>	223.3.1608	$Pm'\overline{3}'n$	227.4.1631	$Fd\overline{3}m'$
218.2.1586	$P\overline{4}3n1'$	223.4.1609	$Pm\overline{3}n'$	227.5.1632	$Fd'\overline{3}'m'$
218.3.1587	$P\overline{4}'3n'$	223.5.1610	$Pm'\overline{3}'n'$	<b>228.1633</b>	<b><math>Fd\overline{3}c</math></b>
<b>219.1.1588</b>	<b><math>F\overline{4}3c</math></b>	<b>224.1.1611</b>	<b><math>Pn\overline{3}m</math></b>	228.2.1634	$Fd\overline{3}c1'$
219.2.1589	$F\overline{4}3c1'$	224.2.1612	$Pn\overline{3}m1'$	228.3.1635	$Fd'\overline{3}'c$
219.3.1590	$F\overline{4}'3c'$	224.3.1613	$Pn'\overline{3}'m$	228.4.1636	$Fd\overline{3}c'$
<b>220.1.1591</b>	<b><math>I\overline{4}3d</math></b>	224.4.1614	$Pn\overline{3}m'$	228.5.1637	$Fd'\overline{3}'c'$
220.2.1592	$I\overline{4}3d1'$	224.5.1615	$Pn'\overline{3}'m'$	<b>229.1.1638</b>	<b><math>Im\overline{3}m</math></b>
220.3.1593	$I\overline{4}'3d'$	224.6.1616	$P_F n\overline{3}m$	229.2.1639	$Im\overline{3}m1'$
<b>221.1.1594</b>	<b><math>Pm\overline{3}m</math></b>	224.7.1617	$P_F n\overline{3}m'$	229.3.1640	$Im'\overline{3}'m$
221.2.1595	$Pm\overline{3}m1'$	<b>225.1.1618</b>	<b><math>Fm\overline{3}m</math></b>	229.4.1641	$Im\overline{3}m'$
221.3.1596	$Pm'\overline{3}'m$	225.2.1619	$Fm\overline{3}m1'$	229.5.1642	$Im'\overline{3}'m'$
221.4.1597	$Pm\overline{3}m'$	225.3.1620	$Fm'\overline{3}'m$	229.6.1643	$I_p m\overline{3}m$
221.5.1598	$Pm'\overline{3}'m'$	225.4.1621	$Fm\overline{3}m'$	229.7.1644	$I_p m'\overline{3}'m$
221.6.1599	$P_F m\overline{3}m$	225.5.1622	$Fm'\overline{3}'m'$	229.8.1645	$I_p m\overline{3}m'$
221.7.1600	$P_F m\overline{3}m'$	<b>226.1.1623</b>	<b><math>Fm\overline{3}c</math></b>	229.9.1646	$I_p m'\overline{3}'m'$
<b>222.1.1601</b>	<b><math>Pn\overline{3}n</math></b>	226.2.1624	$Fm\overline{3}c1'$	<b>230.1.1647</b>	<b><math>la\overline{3}d</math></b>
222.2.1602	$Pn\overline{3}n1'$	226.3.1625	$Fm'\overline{3}'c$	230.2.1648	$la\overline{3}d1'$
222.3.1603	$Pn'\overline{3}'n$	226.4.1626	$Fm\overline{3}c'$	230.3.1649	$la'\overline{3}'d$
222.4.1604	$Pn\overline{3}n'$	226.5.1627	$Fm'\overline{3}'c'$	230.4.1650	$la\overline{3}d'$
222.5.1605	$Pn'\overline{3}'n'$	<b>227.1.1628</b>	<b><math>Fd\overline{3}m</math></b>	230.5.1651	$la'\overline{3}'d'$
<b>223.1.1606</b>	<b><math>Pm\overline{3}n</math></b>	227.2.1629	$Fd\overline{3}m1'$		

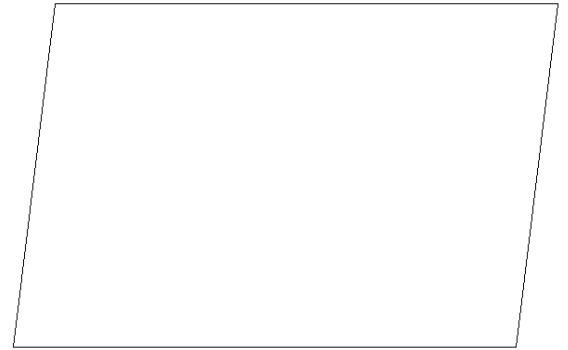
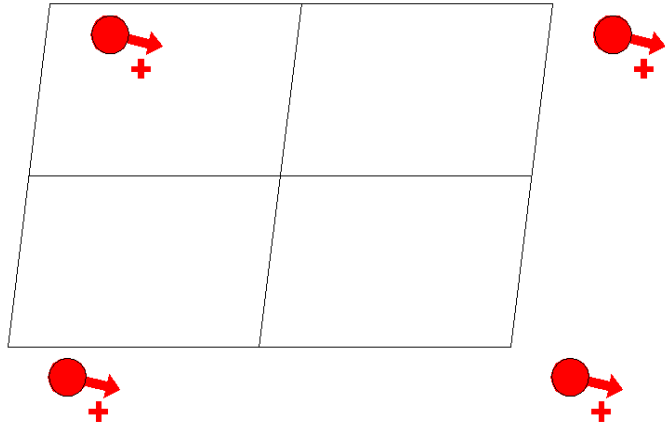




P1  
1.1.1

1  
P1

Triclinic



Origin arbitrary

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

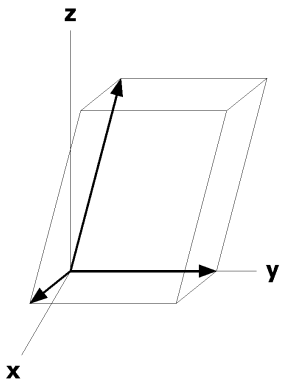
1 a 1 (1) x,y,z [u,v,w]

**Symmetry of Special Projections**

Along [0,0,1] p1  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}_p$   
Origin at 0,0,z

Along [1,0,0] p1  
 $\mathbf{a}^* = \mathbf{b}_p$   $\mathbf{b}^* = \mathbf{c}_p$   
Origin at x,0,0

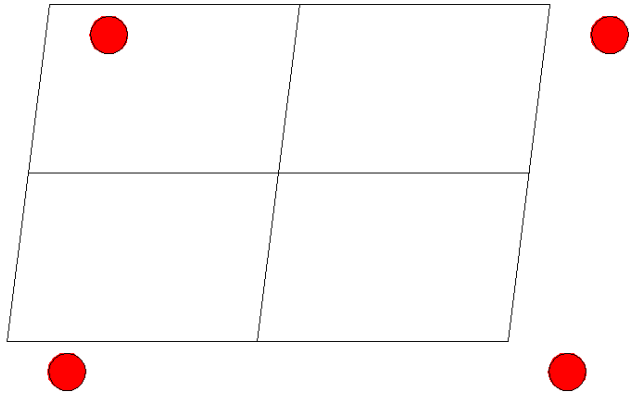
Along [0,1,0] p1  
 $\mathbf{a}^* = \mathbf{c}_p$   $\mathbf{b}^* = \mathbf{a}_p$   
Origin at 0,y,0



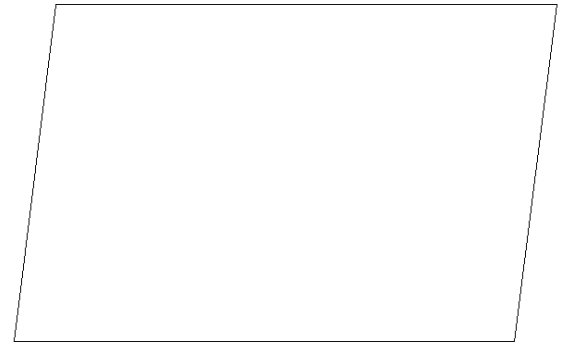
P11'  
1.2.2

11'  
P11'

Triclinic



1'



Origin arbitrary

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1$

Symmetry Operations

For 1 + set

(1) 1  
(1|0,0,0)

For 1' + set

(1) 1'  
(1|0,0,0)'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); 1'.

Positions

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

1+

1'+

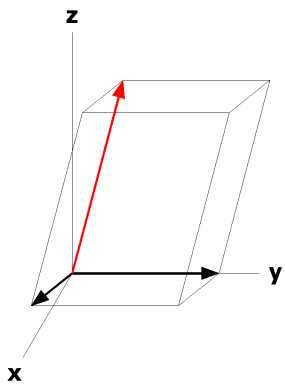
1 a 11' (1) x,y,z [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p11'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}_p$   
Origin at 0,0,z

Along [1,0,0] p11'  
 $\mathbf{a}^* = \mathbf{b}_p$   $\mathbf{b}^* = \mathbf{c}_p$   
Origin at x,0,0

Along [0,1,0] p11'  
 $\mathbf{a}^* = \mathbf{c}_p$   $\mathbf{b}^* = \mathbf{a}_p$   
Origin at 0,y,0



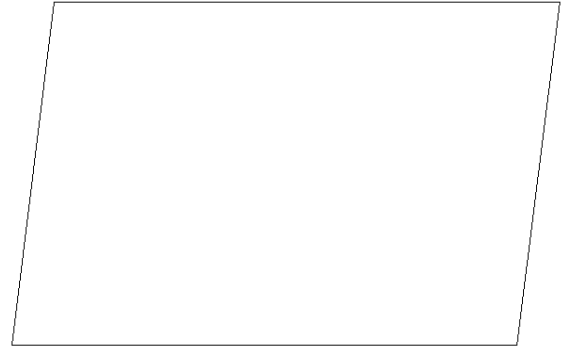
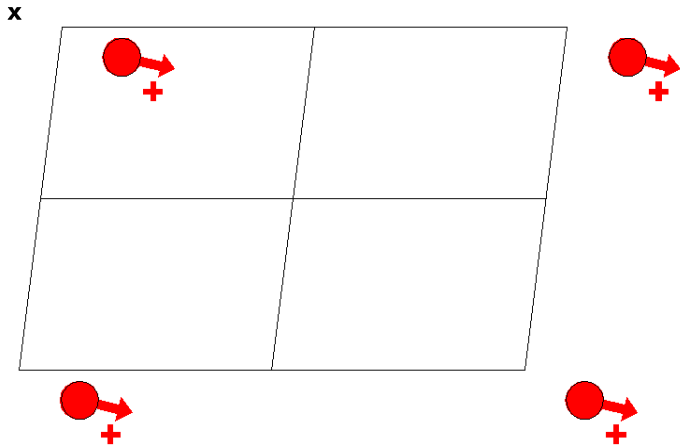
$P_{2s}1$

$11'$

Triclinic

1.3.3

$P_{2s}1$



Origin arbitrary

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0) +$  set

(1) 1  
(1|0,0,0)

For  $(0,0,1)'$  + set

(1)  $t'$  (0,0,1)  
(1|0,0,1)'

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)'$ .

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

$(0,0,0) +$   $(0,0,1)'$  +

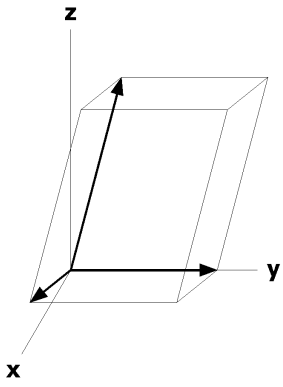
2 a 1 (1) x,y,z [u,v,w]

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p11'$   
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}_p$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a}1$   
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}_p$   
Origin at  $x,0,0$

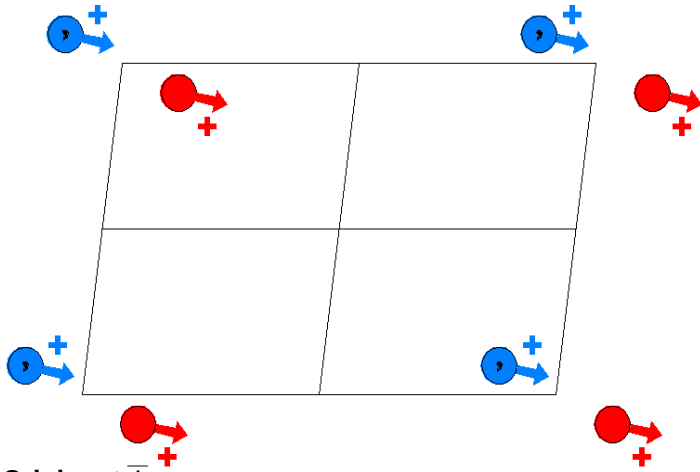
Along  $[0,1,0]$   $p_{2a}1$   
 $\mathbf{a}^* = \mathbf{c}_p$   $\mathbf{b}^* = \mathbf{a}_p$   
Origin at  $0,y,0$



$P\bar{1}$   
2.1.4

$\bar{1}$   
 $P\bar{1}$

Triclinic

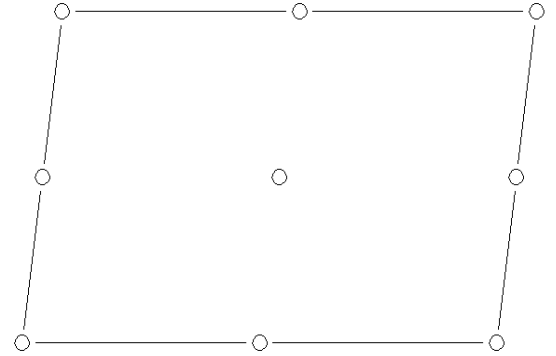


Origin at  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1$

Symmetry Operations

- (1)  $1$   
 $(1|0,0,0)$
- (2)  $\bar{1}$   $0,0,0$   
 $(\bar{1}|0,0,0)$



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

**Positions**

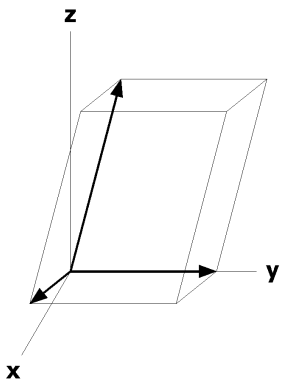
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates	
2	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]
1	h	$\bar{1}$	1/2,1/2,1/2 [u,v,w]	
1	g	$\bar{1}$	0,1/2,1/2 [u,v,w]	
1	f	$\bar{1}$	1/2,0,1/2 [u,v,w]	
1	e	$\bar{1}$	1/2,1/2,0 [u,v,w]	
1	d	$\bar{1}$	1/2,0,0 [u,v,w]	
1	c	$\bar{1}$	0,1/2,0 [u,v,w]	
1	b	$\bar{1}$	0,0,1/2 [u,v,w]	
1	a	$\bar{1}$	0,0,0 [u,v,w]	

**Symmetry of Special Projections**

Along [0,0,1] p2'11  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}_p$   
 Origin at 0,0,z

Along [1,0,0] p2'11  
 $\mathbf{a}^* = \mathbf{b}_p$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

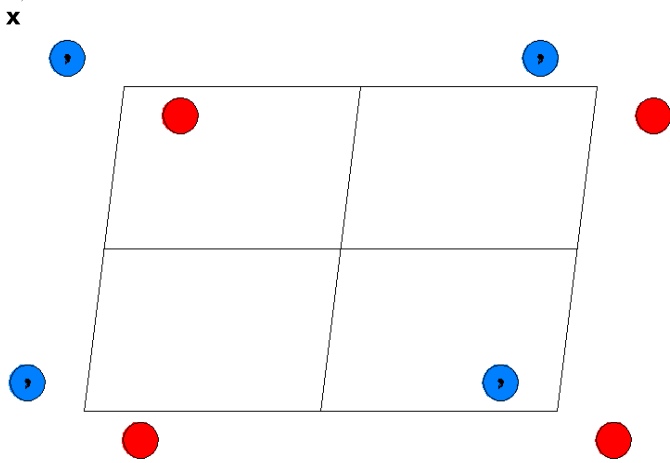
Along [0,1,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}_p$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,y,0



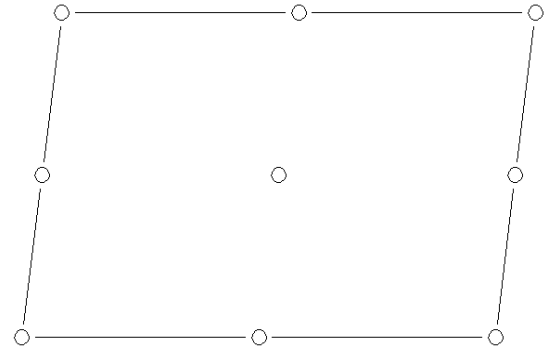
$P\bar{1}1'$   
2.2.5

$\bar{1}1'$   
 $P\bar{1}1'$

Triclinic



$1'$



Origin at  $\bar{1}1'$

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1$

Symmetry Operations

For 1 + set

(1) 1  
(1|0,0,0)      (2)  $\bar{1}$  0,0,0  
( $\bar{1}$ |0,0,0)

For  $1'$  + set

(1)  $1'$   
(1|0,0,0)'      (2)  $\bar{1}'$  0,0,0  
( $\bar{1}'$ |0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); 1'.

**Positions**

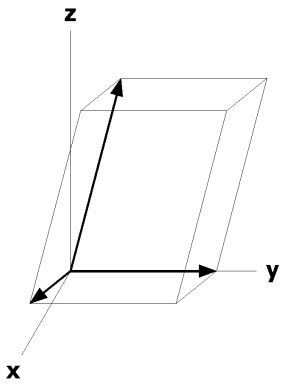
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates	
	1 +	1' +
2 i $\bar{1}1'$	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]
1 h $\bar{1}1'$	1/2, 1/2, 1/2 [0,0,0]	
1 g $\bar{1}1'$	0, 1/2, 1/2 [0,0,0]	
1 f $\bar{1}1'$	1/2, 0, 1/2 [0,0,0]	
1 e $\bar{1}1'$	1/2, 1/2, 0 [0,0,0]	
1 d $\bar{1}1'$	1/2, 0, 0 [0,0,0]	
1 c $\bar{1}1'$	0, 1/2, 0 [0,0,0]	
1 b $\bar{1}1'$	0, 0, 1/2 [0,0,0]	
1 a $\bar{1}1'$	0, 0, 0 [0,0,0]	

**Symmetry of Special Projections**

Along [0,0,1]  $p2111'$   
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}_p$   
 Origin at 0,0,z

Along [1,0,0]  $p2111'$   
 $\mathbf{a}^* = \mathbf{b}_p$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

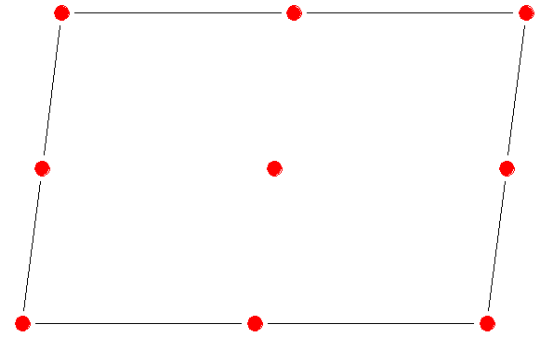
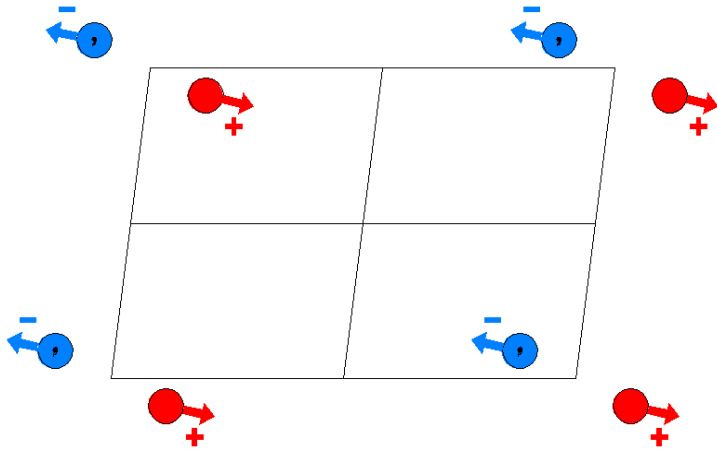
Along [0,1,0]  $p2111'$   
 $\mathbf{a}^* = \mathbf{c}_p$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,y,0



$P\bar{1}'$   
2.3.6

$\bar{1}'$   
 $P\bar{1}'$

Triclinic



Origin at  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1$

Symmetry Operations

- (1)  $1$   
 $(1|0,0,0)$
- (2)  $\bar{1}'$   $0,0,0$   
 $(\bar{1}'|0,0,0)'$



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

**Positions**

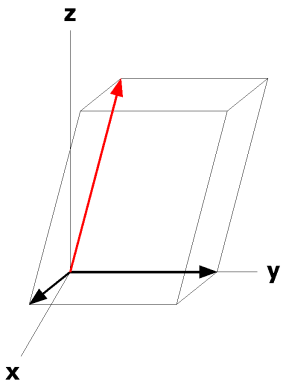
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates	
2	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]
1	h	$\bar{1}$ '	1/2,1/2,1/2 [0,0,0]	
1	g	$\bar{1}$ '	0,1/2,1/2 [0,0,0]	
1	f	$\bar{1}$ '	1/2,0,1/2 [0,0,0]	
1	e	$\bar{1}$ '	1/2,1/2,0 [0,0,0]	
1	d	$\bar{1}$ '	1/2,0,0 [0,0,0]	
1	c	$\bar{1}$ '	0,1/2,0 [0,0,0]	
1	b	$\bar{1}$ '	0,0,1/2 [0,0,0]	
1	a	$\bar{1}$ '	0,0,0 [0,0,0]	

**Symmetry of Special Projections**

Along [0,0,1] p211  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}_p$   
 Origin at 0,0,z

Along [1,0,0] p211  
 $\mathbf{a}^* = \mathbf{b}_p$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

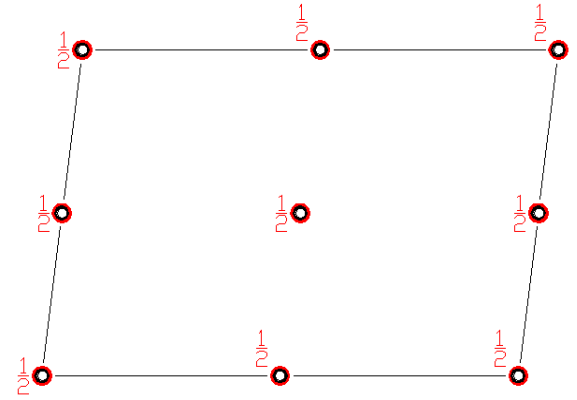
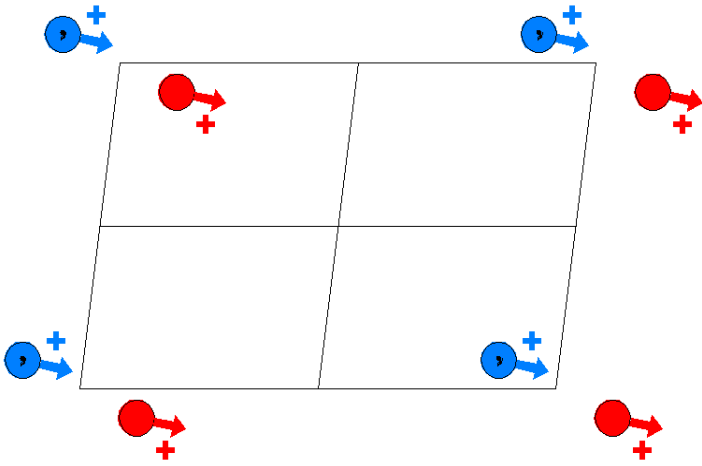
Along [0,1,0] p211  
 $\mathbf{a}^* = \mathbf{c}_p$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,y,0



$P_{2s}\bar{1}$   
2.4.7

$\bar{1}1'$   
 $P_{2s}\bar{1}$

Triclinic



Origin at  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

- (1)  $1$   
 $(1|0,0,0)$
- (2)  $\bar{1}$   $0,0,0$   
 $(\bar{1}|0,0,0)$

For (0,0,1)' + set

- (1)  $t'$   $(0,0,1)$   
 $(1|0,0,1)'$
- (2)  $\bar{1}'$   $0,0,1/2$   
 $(\bar{1}'|0,0,1)'$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2).

**Positions**

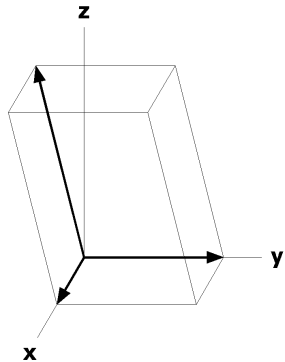
			Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(0,0,1)' +
4	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]
2	h	$\bar{1}'$	1/2,1/2,1/2 [0,0,0]	
2	g	$\bar{1}'$	0,1/2,1/2 [0,0,0]	
2	f	$\bar{1}'$	1/2,0,1/2 [0,0,0]	
2	e	$\bar{1}$	1/2,1/2,0 [u,v,w]	
2	d	$\bar{1}$	1/2,0,0 [u,v,w]	
2	c	$\bar{1}$	0,1/2,0 [u,v,w]	
2	b	$\bar{1}'$	0,0,1/2 [0,0,0]	
2	a	$\bar{1}$	0,0,0 [u,v,w]	

**Symmetry of Special Projections**

Along [0,0,1]  $p2111'$   
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}_p$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}211$   
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}_p$   
 Origin at x,0,1/2

Along [0,1,0]  $p_{2a}211$   
 $\mathbf{a}^* = \mathbf{c}_p$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,y,1/2



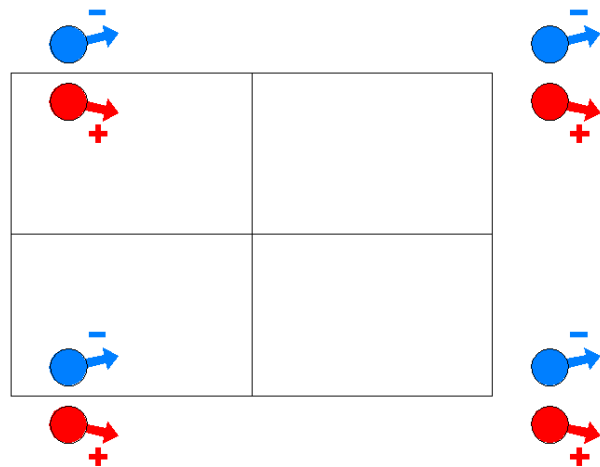
P2

2

Monoclinic

3.1.8

P121



Origin on 2

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- (1) 1 (2) 2  $0, y, 0$   
 (1|0,0,0) (2<sub>y</sub>|0,0,0)

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

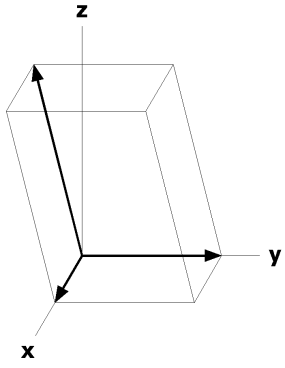
2	e	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]
1	d	2	$1/2, y, 1/2$ [0,v,0]	
1	c	2	$1/2, y, 0$ [0,v,0]	
1	b	2	$0, y, 1/2$ [0,v,0]	
1	a	2	$0, y, 0$ [0,v,0]	

**Symmetry of Special Projections**

Along [0,0,1] p1m'1  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0

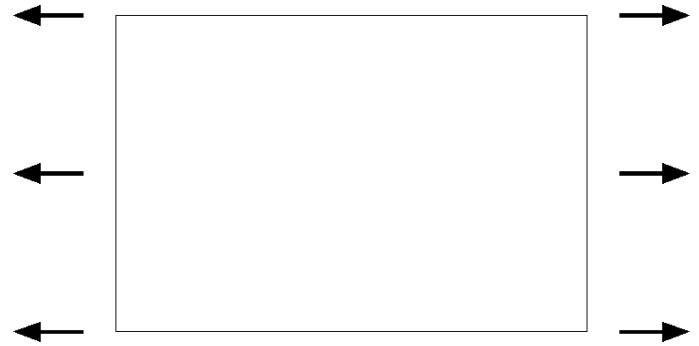
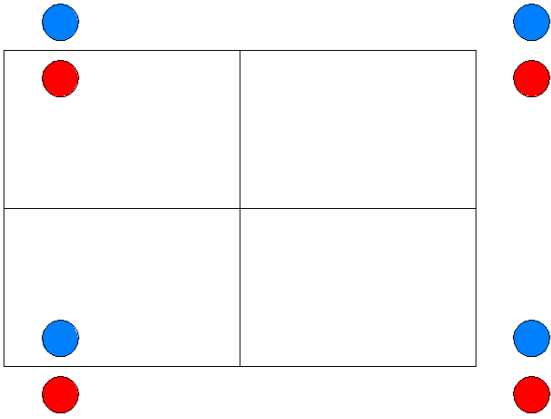


P21'  
3.2.9

21'  
P1211'

Monoclinic

1'



Origin on 21'

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/2$

Symmetry Operations

For 1 + set

(1) 1  
(1|0,0,0)      (2) 2 0,y,0  
(2y|0,0,0)

For 1' + set

(1) 1'  
(1|0,0,0)'      (2) 2' 0,y,0  
(2y|0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); 1'.

**Positions**

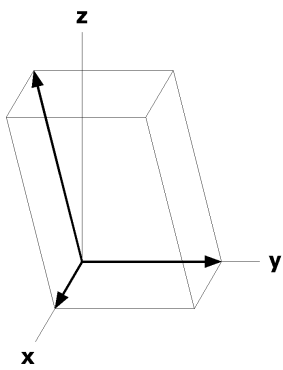
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates	
	1+	1' +
2 e 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},y,\bar{z}$ [0,0,0]
1 d 21'	1/2,y,1/2 [0,0,0]	
1 c 21'	1/2,y,0 [0,0,0]	
1 b 21'	0,y,1/2 [0,0,0]	
1 a 21'	0,y,0 [0,0,0]	

**Symmetry of Special Projections**

Along [0,0,1] p1m11'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



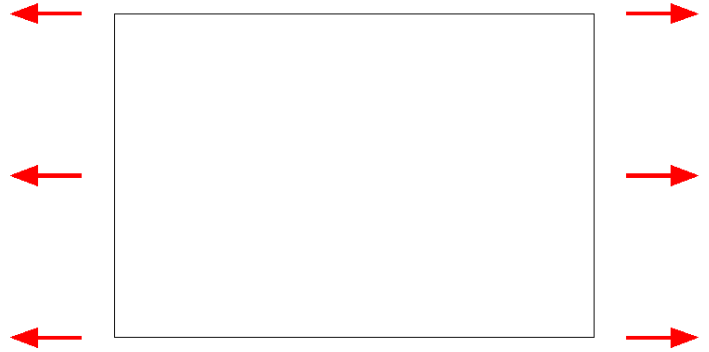
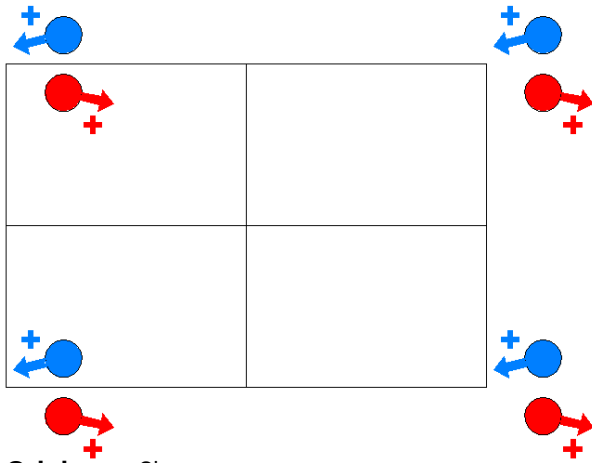
P2'

2'

Monoclinic

3.2.10

P12'1



Origin on 2'

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- (1) 1 (2) 2' 0,y,0  
 (1|0,0,0) (2<sub>y</sub>|0,0,0)'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

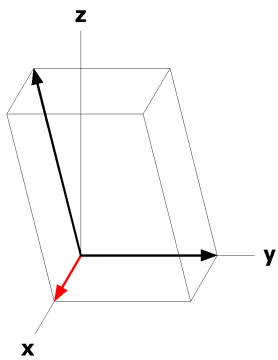
2	e	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, \bar{z}$ [u, $\bar{v}$ , w]
1	d	2'	1/2,y,1/2 [u,0,w]	
1	c	2'	1/2,y,0 [u,0,w]	
1	b	2'	0,y,1/2 [u,0,w]	
1	b	2'	0,y,0 [u,0,w]	

**Symmetry of Special Projections**

Along [0,0,1] p1m1  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



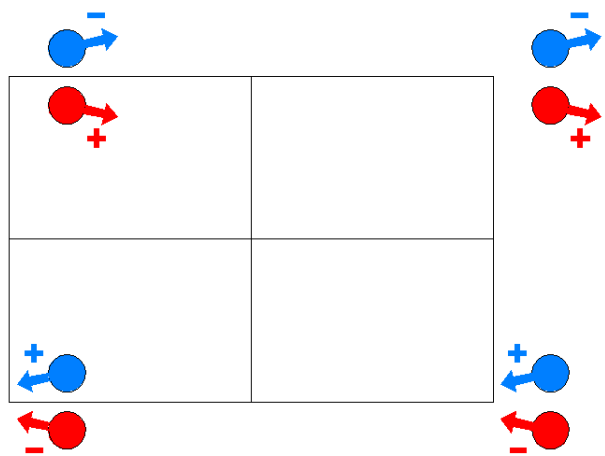
$P_{2a}2$

$21'$

Monoclinic

3.4.11

$P_{2a}121$



Origin on 2

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/2$

Symmetry Operations

For  $(0,0,0) +$

- (1) 1  $(1|0,0,0)$
- (2) 2  $(2|0,y,0)$   $(2_y|0,0,0)$

For  $(1,0,0)' +$

- (1)  $t' (1,0,0)$   $(1|1,0,0)'$
- (2)  $2' (1/2,y,0)$   $(2_y|1,0,0)'$



**Generators selected** (1); t(1,0,0)<sup>'</sup>; t(0,1,0); t(0,0,1); (2).

### Positions

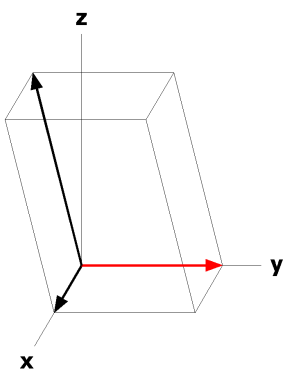
			Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1,0,0) <sup>'</sup> +
4	e	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]
2	d	2'	1/2,y,1/2 [u,0,w]	
2	c	2'	1/2,y,0 [u,0,w]	
2	b	2	0,y,1/2 [0,v,0]	
2	a	2	0,y,0 [0,v,0]	

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>·1m1  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/2,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>·211  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



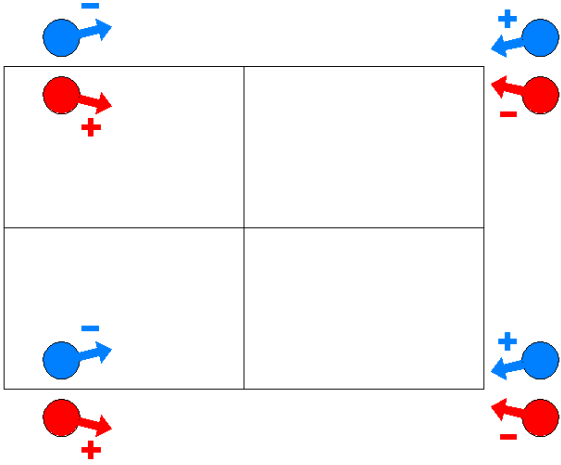
$P_{2b} 2$

3.5.12

$21'$

$P_{2b} 121$

Monoclinic



Origin on 2

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

(1) 1  $(1|0,0,0)$  (2) 2  $(2|0,y,0)$   $(2_y|0,0,0)$

For  $(0,0,0) +$

(1)  $t' (0,1,0)$   $(1|0,1,0)'$  (2)  $2' (0,1,0) 0,y,0$   $(2_y|0,1,0)'$

For  $(0,1,0)' +$



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

**Positions**

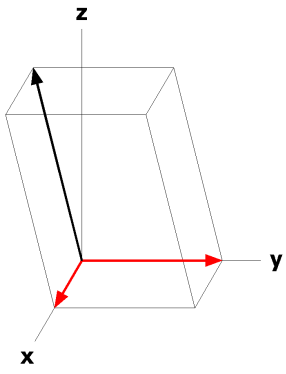
			Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(0,1,0)' +
4	e	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]
2	d	2	1/2,y,1/2 [0,v,0]	
2	c	2	1/2,y,0 [0,v,0]	
2	b	2	0,y,1/2 [0,v,0]	
2	a	2	0,y,0 [0,v,0]	

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2b</sub>.1m'1  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>.1m1  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,1/2,0

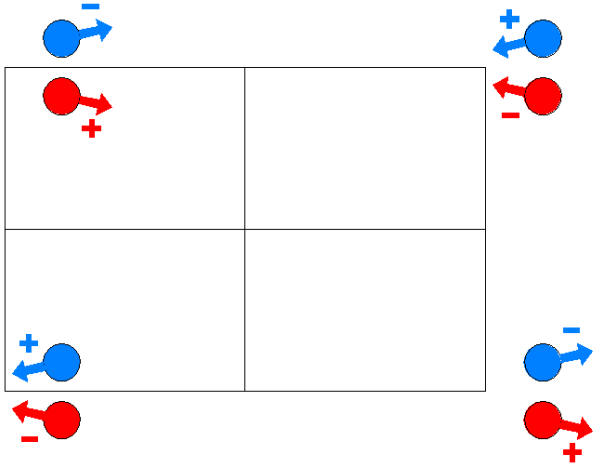
Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



$P_C 2$   
3.6.13

$21'$   
 $P_C 121$

Monoclinic



Origin on 2

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/2$

Symmetry Operations

For  $(0,0,0) +$

(1) 1  
(1|0,0,0)      (2) 2  $0,y,0$   
(2<sub>y</sub>|0,0,0)

For  $(1,0,0)' +$

(1)  $t' (1,0,0)$   
(1|1,0,0)'      (2) 2'  $1/2,y,0$   
(2<sub>y</sub>|1,0,0)'

**Generators selected** (1); t(1,0,0)<sup>'</sup>; t(0,1,0)<sup>'</sup>; t(0,0,1); (2).

### Positions

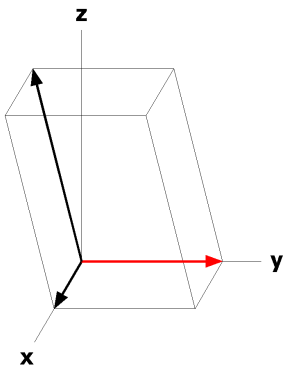
			Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1,0,0) <sup>'</sup> +
4	e	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]
2	d	2'	1/2,y,1/2 [u,0,w]	
2	c	2'	1/2,y,0 [u,0,w]	
2	b	2	0,y,1/2 [0,v,0]	
2	a	2	0,y,0 [0,v,0]	

### Symmetry of Special Projections

Along [0,0,1] p<sub>c</sub>1m1  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/2,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

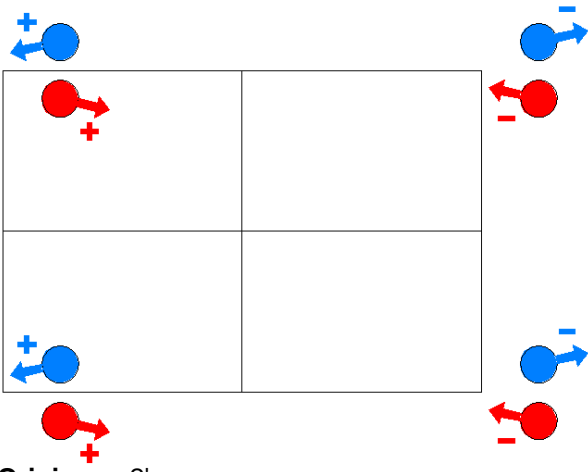
Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



$P_{2b} 2'$   
3.7.14

$21'$   
 $P_{2b} 12'1$

Monoclinic



Origin on  $2'$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

(1) 1  
(1|0,0,0)      (2)  $2'_y$  0,y,0  
(2\_y|0,0,0)'

For (0,0,0) +

(1)  $t'_y$  (0,1,0)  
(1|0,1,0)'      (2) 2 (0,1,0) 0,y,0  
(2\_y|0,1,0)

For (0,1,0)' +

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

**Positions**

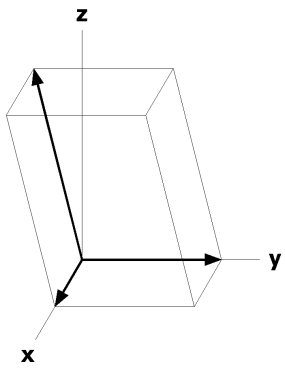
			Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(0,1,0)' +
4	e	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]
2	d	2'	1/2,y,1/2 [u,0,w]	
2	c	2'	1/2,y,0 [u,0,w]	
2	b	2'	0,y,1/2 [u,0,w]	
2	a	2'	0,y,0 [u,0,w]	

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2b</sub>.1m1  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>.1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



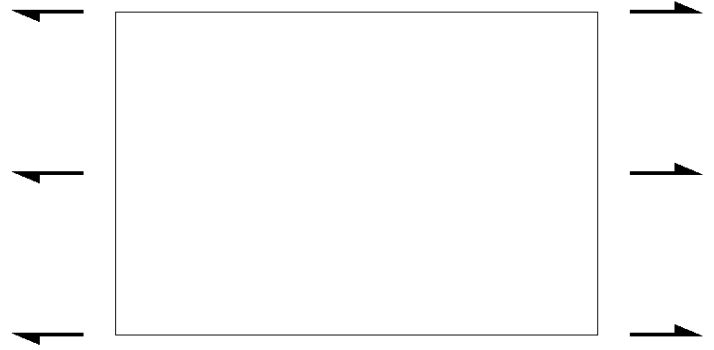
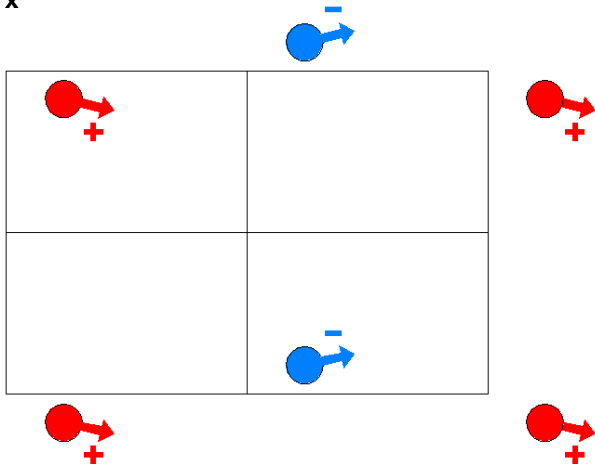
P2<sub>1</sub>

2

Monoclinic

4.1.15

P12<sub>1</sub>1



Origin on 2<sub>1</sub>

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- (1) 1 (2) 2 (0,1/2,0) 0,y,0  
 (1|0,0,0) (2<sub>y</sub>|0,1/2,0)

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

2 a 1 (1) x,y,z [u,v,w] (2)  $\bar{x}, y+1/2, \bar{z}$  [ $\bar{u}, v, \bar{w}$ ]

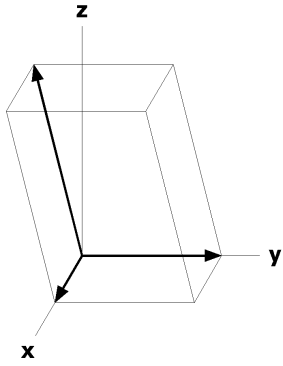
**Symmetry of Special Projections**

Along [0,0,1] p1g'1  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g'1  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0





P21'

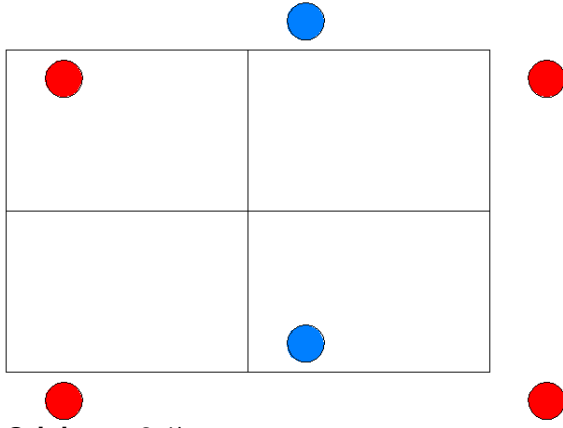
21'

Monoclinic

4.2.16

P1211'

1'



Origin on  $2_11'$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $1 +$

- (1) 1 (1|0,0,0)
- (2) 2 (0,1/2,0) 0,y,0 (2<sub>y</sub>|0,1/2,0)

For  $1' +$

- (1) 1' (1|0,0,0)'
- (2) 2' (0,1/2,0) 0,y,0 (2<sub>y</sub>|0,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); 1'.

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

1+

1' +

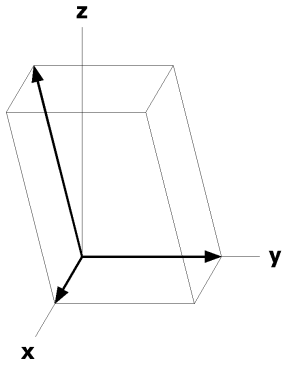
- 1 a 11' (1) x,y,z [0,0,0] (2)  $\bar{x}, y+1/2, \bar{z}$  [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p1g11'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
Origin at 0,y,0



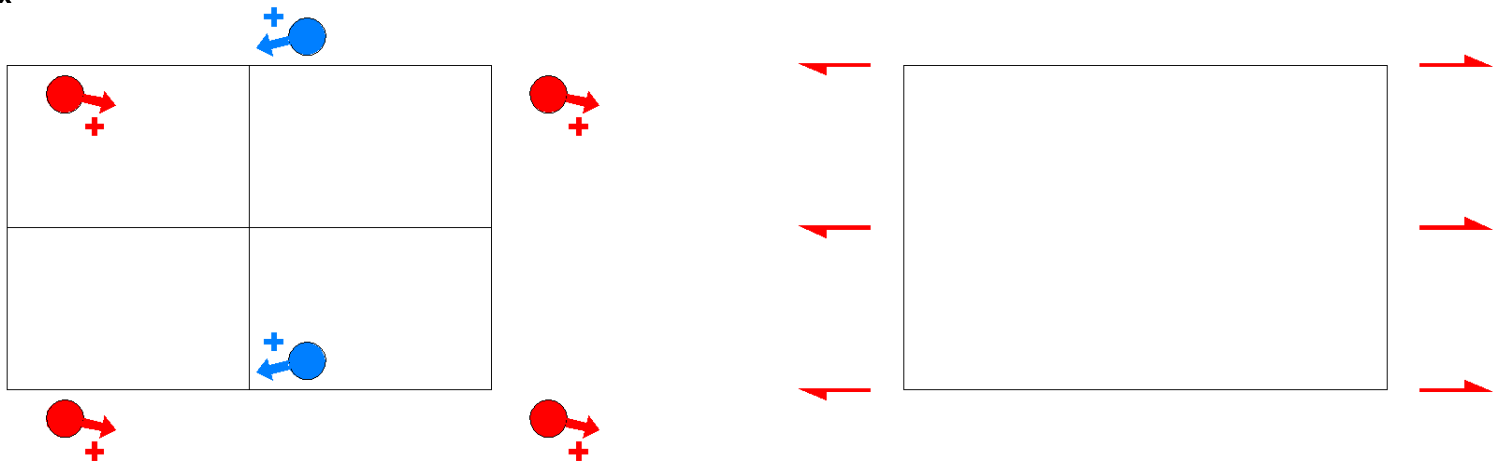
$P2_1'$

4.3.17

$2'$

$P12_1'1$

Monoclinic



Origin on  $2_1'$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- (1) 1  $(1|0,0,0)$
- (2)  $2'$   $(0,1/2,0) 0,y,0$   
 $(2_y|0,1/2,0)'$

Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

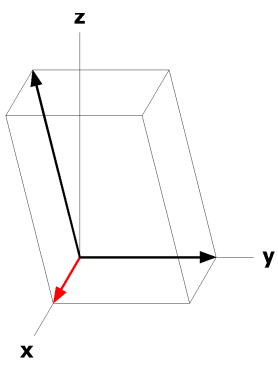
- 2 a 1 (1)  $x,y,z [u,v,w]$  (2)  $\bar{x},y+1/2,\bar{z} [u,\bar{v},w]$

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p1g1$   
 $a^* = a_p$   $b^* = b$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p1g1$   
 $a^* = -c_p$   $b^* = b$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $p2'11$   
 $a^* = c$   $b^* = a$   
 Origin at  $0,y,0$



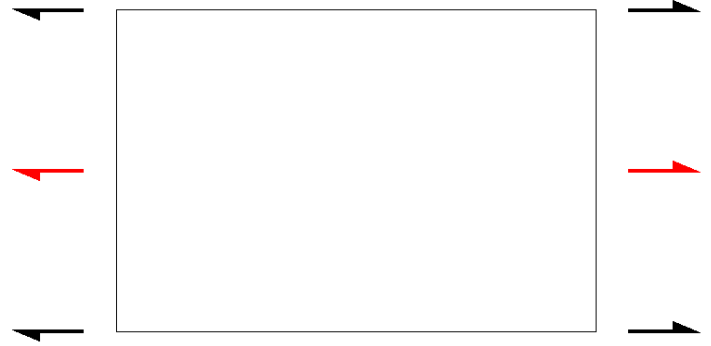
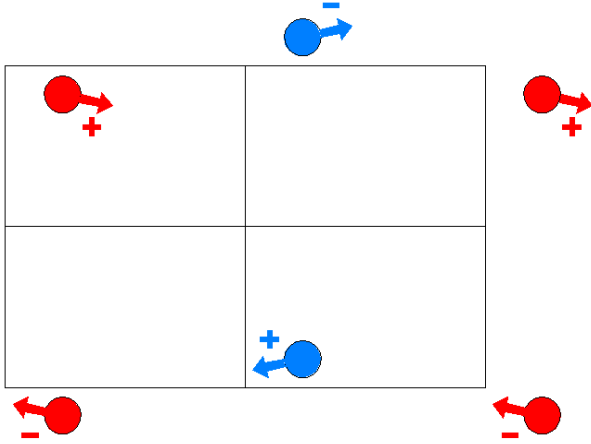
$P_{2a} 2_1$

$21'$

Monoclinic

4.4.18

$P_{2a} 12_1 1$



Origin on  $2_1$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0) +$

- (1) 1  $(1 | 0,0,0)$
- (2) 2  $(0, 1/2, 0) 0, y, 0$   
 $(2_y | 0, 1/2, 0)$

For  $(1,0,0)' +$

- (1)  $t'$   $(1, 0, 0)$   
 $(1 | 1, 0, 0)'$
- (2)  $2'$   $(0, 1/2, 0) 1/2, y, 0$   
 $(2_y | 1, 1/2, 0)'$

Generators selected (1);  $t(1,0,0)'$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

$(0,0,0) +$   $(1,0,0)' +$

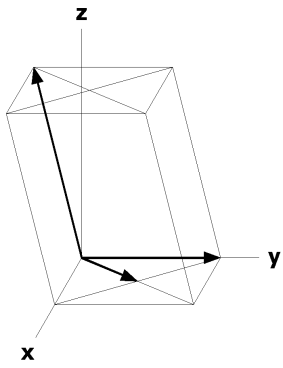
4 a 1 (1)  $x, y, z [u, v, w]$  (2)  $\bar{x}, y+1/2, \bar{z} [\bar{u}, v, \bar{w}]$

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_{2a} 1g1$   
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $1/2, 0, z$

Along  $[1,0,0]$   $p1g11'$   
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $x, 0, 0$

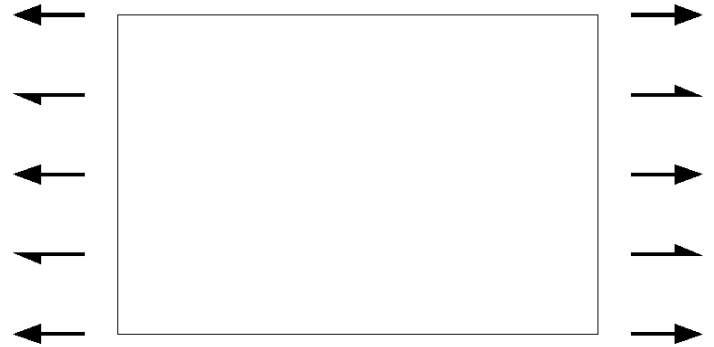
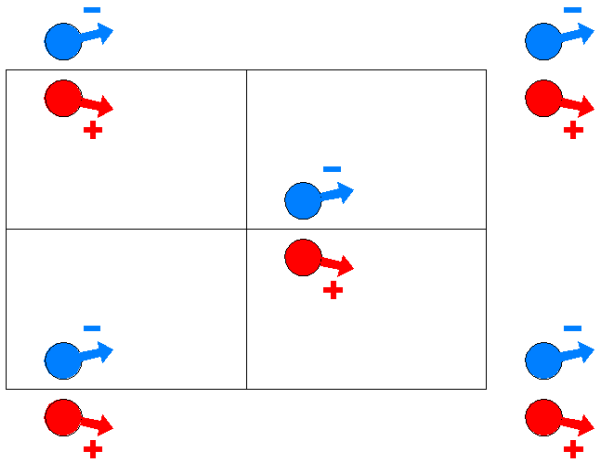
Along  $[0,1,0]$   $p_{2a} 211$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $0, y, 0$



C2  
5.1.19

2  
C121

Monoclinic



Origin on 2

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)      (2) 2 0,y,0  
(2<sub>y</sub>|0,0,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)      (2) 2 (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,0)$ ; (2).

**Positions**

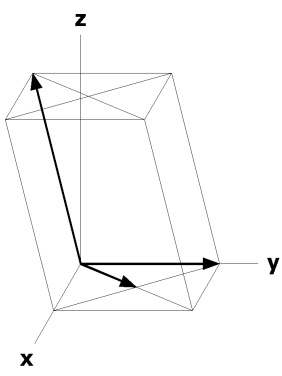
			Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1/2,1/2,0) +
4	c	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]
2	b	2	$0,y,1/2$ [0,v,0]	
2	a	2	$0,y,0$ [0,v,0]	

**Symmetry of Special Projections**

Along  $[0,0,1]$   $c1m'1$   
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p1m'1$   
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $p211$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at  $0,y,0$



C21'

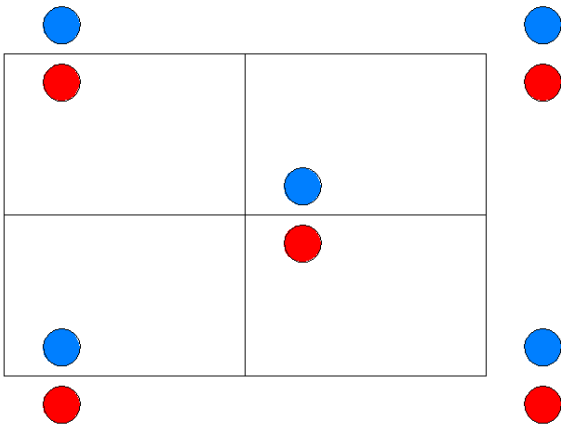
21'

Monoclinic

5.2.20

C1211'

1'



Origin on 21'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1 (1|0,0,0) (2) 2 0,y,0 (2<sub>y</sub>|0,0,0)

For (0,0,0) + set

(1) t (1/2,1/2,0) (1|1/2,1/2,0) (2) 2 (0,1/2,0) 1/4,y,0 (2<sub>y</sub>|1/2,1/2,0)

For (1/2,1/2,0) + set

(1) 1' (1|0,0,0)' (2) 2' 0,y,0 (2<sub>y</sub>|0,0,0)'

For (0,0,0)' + set

(1) t' (1/2,1/2,0)' (1|1/2,1/2,0) (2) 2' (0,1/2,0) 1/4,y,0 (2<sub>y</sub>|1/2,1/2,0)'

For (1/2,1/2,0)' + set

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); 1'.

### Positions

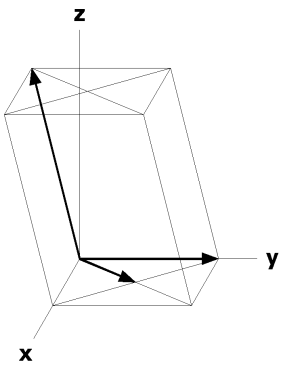
		Coordinates	
Multiplicity,			
Wyckoff letter,			
Site Symmetry.			
		(0,0,0) +	(1/2,1/2,0) +
		(0,0,0)' +	(1/2,1/2,0)' +
4	c 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]
2	b 21'	0,y,1/2 [0,0,0]	
2	a 21'	0,y,0 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] c1m11'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



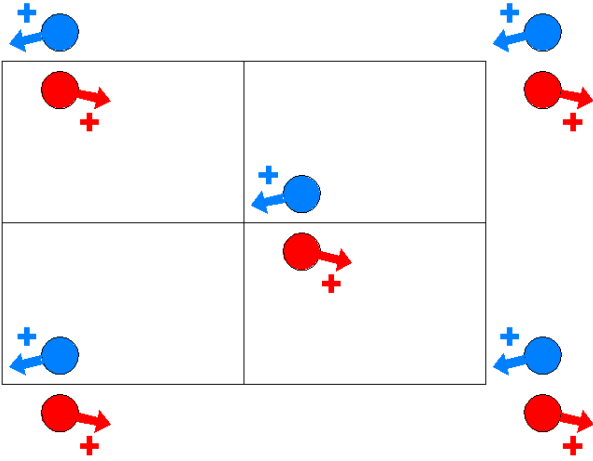
C2'

5.3.21

2'

C12'1

Monoclinic



Origin on 2'

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)      (2) 2' 0,y,0  
(2<sub>y</sub>|0,0,0)'

For (0,0,0) + set

(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)      (2) 2' (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)'

For (1/2,1/2,0) + set





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (1/2,1/2,0) +

4 c 1 (1) x,y,z [u,v,w] (2)  $\bar{x}, \bar{y}, \bar{z}$  [u,  $\bar{v}$ , w]

2 b 2' 0,y,1/2 [u,0,w]

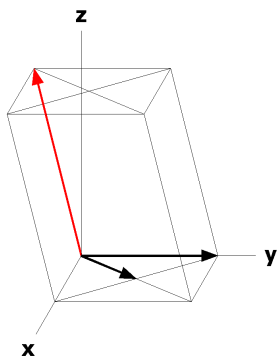
2 a 2' 0,y,0 [u,0,w]

**Symmetry of Special Projections**

Along [0,0,1] c1m1  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,0,0

Along [0,1,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
Origin at 0,y,0



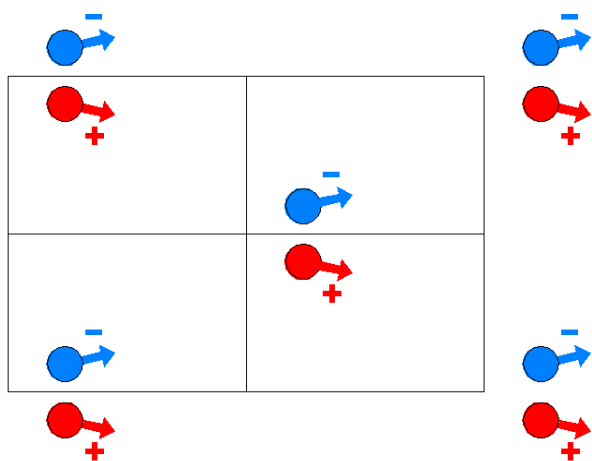
$C_{2c}2$

5.4.22

$21'$

$C_{2c}121$

Monoclinic



Origin on 2

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)      (2) 2 0,y,0  
(2<sub>y</sub>|0,0,0)

For (0,0,0) + set

(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)      (2) 2 (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)

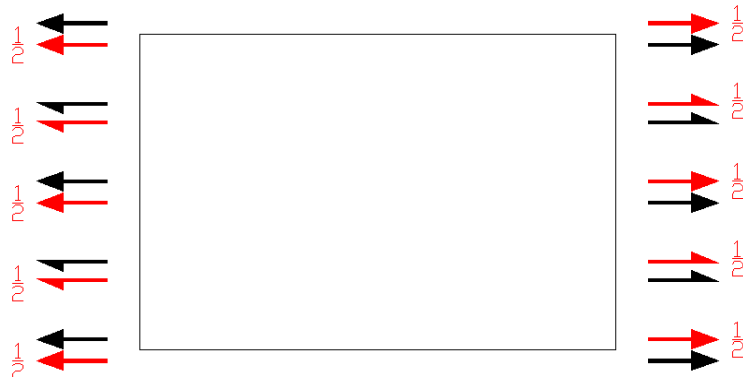
For (1/2,1/2,0) + set

(1) t' (0,0,1)  
(1|0,0,1)'      (2) 2' 0,y,1/2  
(2<sub>y</sub>|0,0,1)'

For (0,0,1)' + set

(1) t' (1/2,1/2,1)  
(1|1/2,1/2,1)'      (2) 2' (0,1/2,0) 1/4,y,1/2  
(2<sub>y</sub>|1/2,1/2,1)'

For (1/2,1/2,1)' + set



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; t(1/2,1/2,0);(2).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates	
	(0,0,0) + (0,0,1)'	(1/2,1/2,0) + (1/2,1/2,1)'

8 c 1 (1) x,y,z [u,v,w] (2)  $\bar{x}, \bar{y}, \bar{z}$  [ $\bar{u}, \bar{v}, \bar{w}$ ]

4 b 2' 0,y,1/2 [u,0,w]

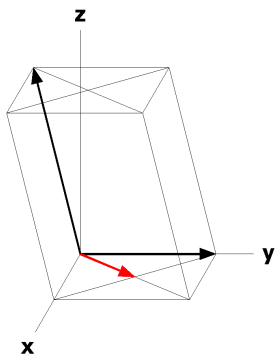
4 a 2 0,y,0 [0,v,0]

### Symmetry of Special Projections

Along [0,0,1] c1m11'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>\*1m1  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,1/2

Along [0,1,0] p<sub>2a</sub>\*211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



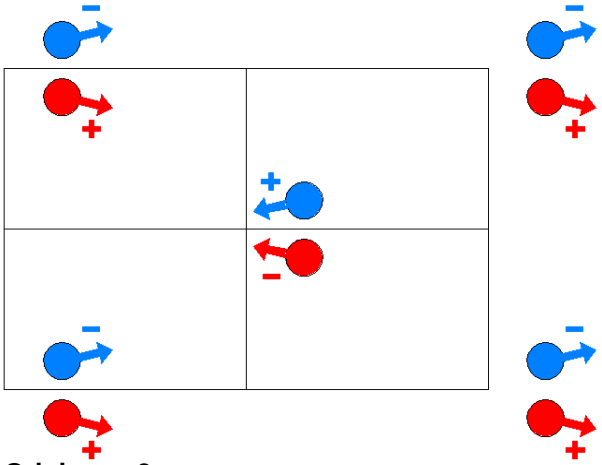
$C_{p2}$

$21'$

Monoclinic

5.5.23

$C_{p121}$



Origin on 2

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0)$  + set

- (1) 1  $(1|0,0,0)$
- (2) 2  $(2|0,y,0)$   $(2_y|0,0,0)$

For  $(1/2,1/2,0)'$  + set

- (1)  $t'$   $(1/2,1/2,0)$   $(1|1/2,1/2,0)'$
- (2)  $2'$   $(0,1/2,0)$   $1/4,y,0$   $(2_y|1/2,1/2,0)'$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)<sup>'</sup>; (2).

### Positions

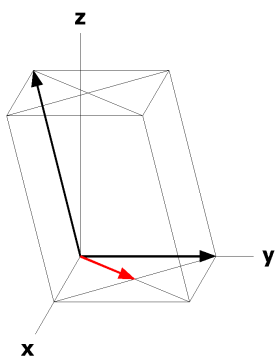
			Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1/2,1/2,0) <sup>'</sup> +
4	c	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]
2	b	2	0,y,1/2 [0,v,0]	
2	a	2	0,y,0 [0,v,0]	

### Symmetry of Special Projections

Along [0,0,1]  $c_p 1m'1$   
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b} 1m'1$   
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a} 211$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



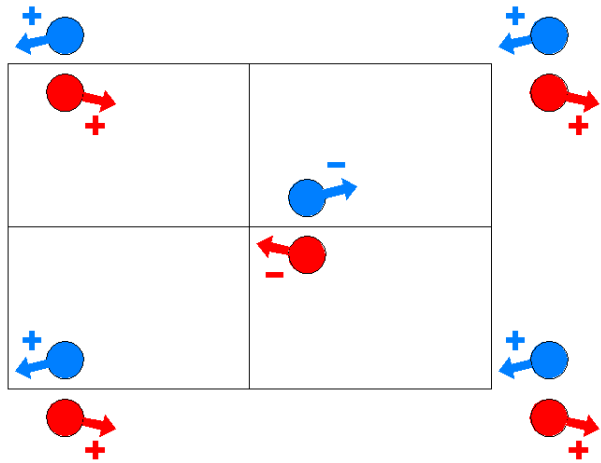
$C_p 2'$

5.6.24

$21'$

$C_p 12'1$

Monoclinic



Origin on  $2'$

Asymmetric unit

$$0 \leq x \leq 1/2;$$

$$0 \leq y \leq 1/2;$$

$$0 \leq z \leq 1$$

Symmetry Operations

For  $(0,0,0)$  + set

$$(1) 1$$

$$(1 | 0,0,0)$$

$$(2) 2' \quad 0,y,0$$

$$(2_y | 0,0,0)'$$

For  $(1/2,1/2,0)'$  + set

$$(1) t' \quad (1/2,1/2,0)$$

$$(1 | 1/2,1/2,0)'$$

$$(2) 2 \quad (0,1/2,0) \quad 1/4,y,0$$

$$(2_y | 1/2,1/2,0)$$

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,0)'$ ; (2).

### Positions

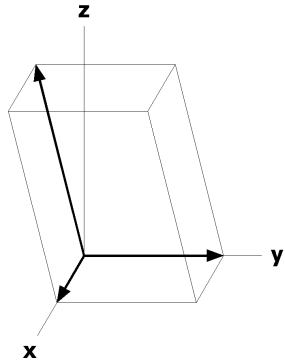
			Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1/2,1/2,0)' +
4	c	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},y,\bar{z}$ [u, $\bar{v}$ ,w]
2	b	2'	0,y,1/2 [u,0,w]	
2	a	2'	0,y,0 [u,0,w]	

### Symmetry of Special Projections

Along [0,0,1]  $c_p 1m1$   
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b} 1m1$   
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a} 211$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



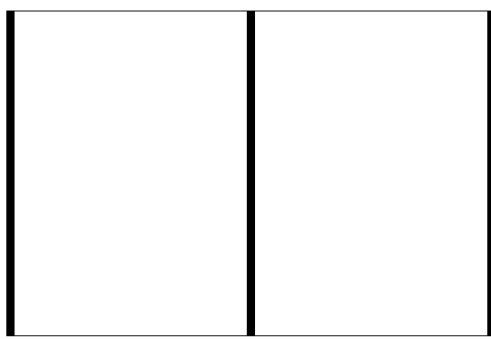
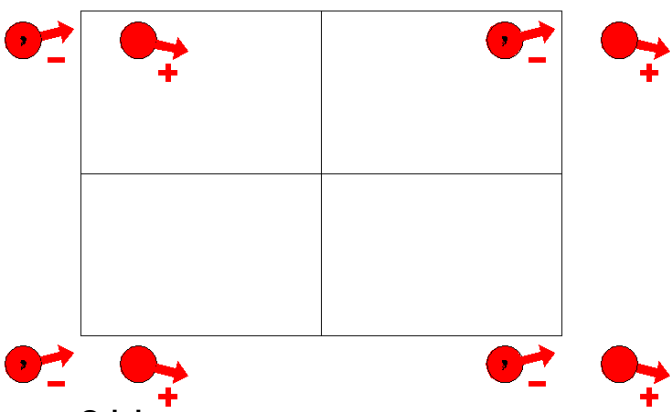
Pm

m

Monoclinic

6.1.25

P1m1



Origin on m

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

- (1) 1  $(1|0,0,0)$
- (2) m  $x,0,z$   $(m_y|0,0,0)$

Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

2	c	1	(1) $x,y,z$ $[u,v,w]$	(2) $x,\bar{y},z$ $[\bar{u},v,\bar{w}]$
1	b	m	$x,1/2,z$ $[0,v,0]$	
1	a	m	$x,0,z$ $[0,v,0]$	

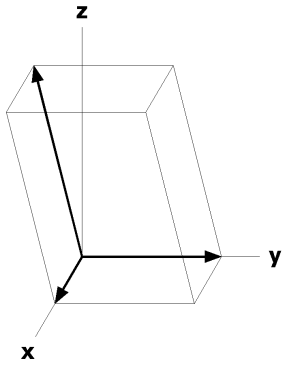
**Symmetry of Special Projections**

Along  $[0,0,1]$   $p1m1$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p1m1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $p11'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at  $0,y,0$





Pm1'

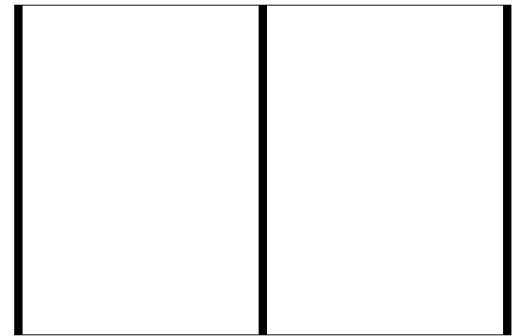
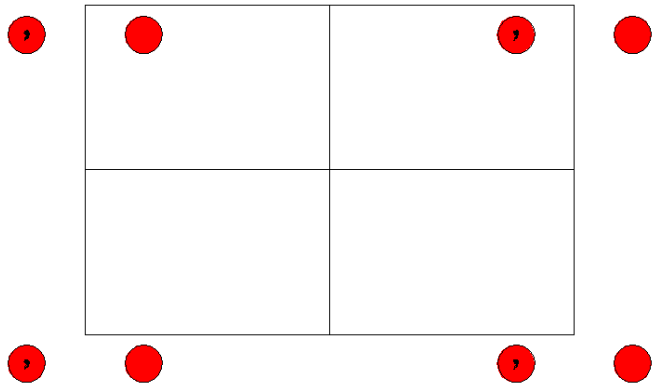
6.2.26

m1'

P1m11'

Monoclinic

1'



Origin on m1'

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

For 1 + set

(1) 1  
(1|0,0,0)      (2) m x,0,z  
(m<sub>y</sub>|0,0,0)

For 1' + set

(1) 1'  
(1|0,0,0)'      (2) m' x,0,z  
(m<sub>y</sub>'|0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); 1'

**Positions**

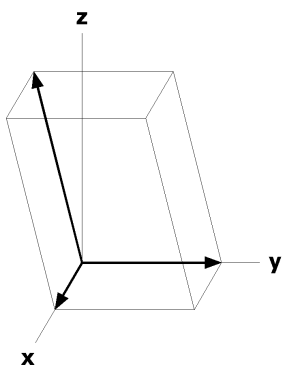
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates	
	1 +	1' +
2 c 11'	(1) x,y,z [0,0,0]	(2) x, $\bar{y}$ ,z [0,0,0]
1 b m1'	x,1/2,z [0,0,0]	
1 a m1'	x,0,z [0,0,0]	

**Symmetry of Special Projections**

Along [0,0,1] p1m11'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



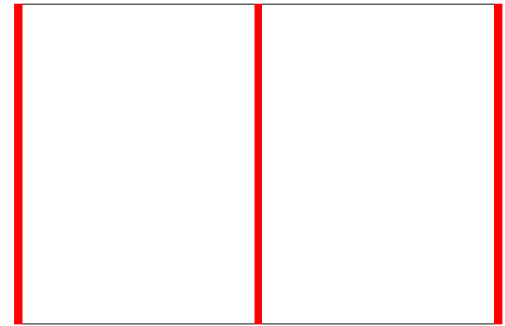
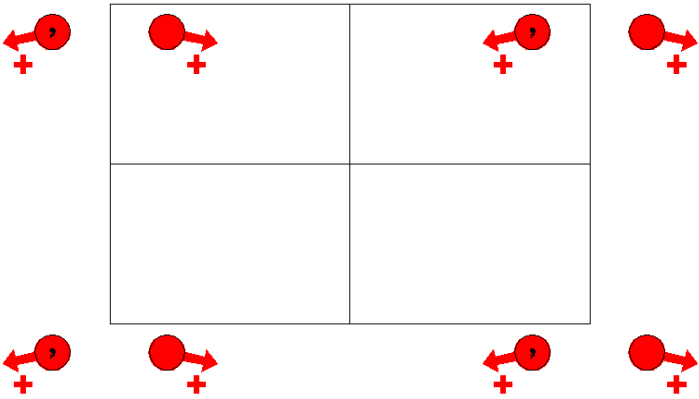
Pm'

6.3.27

m'

P1m'1

Monoclinic



Origin on m'

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

- (1) 1  $(1|0,0,0)$
- (2) m' x,0,z  $(m_y|0,0,0)'$

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

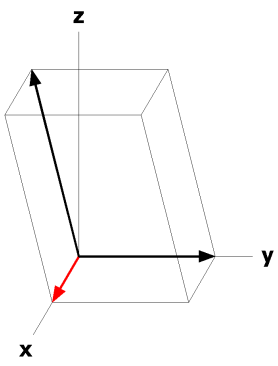
2	c	1	(1) x,y,z [u,v,w]	(2) x, $\bar{y}$ , z [u, $\bar{v}$ , w]
1	b	m'	x, 1/2, z [u, 0, w]	
1	a	m'	x, 0, z [u, 0, w]	

**Symmetry of Special Projections**

Along [0,0,1] p1m'1  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



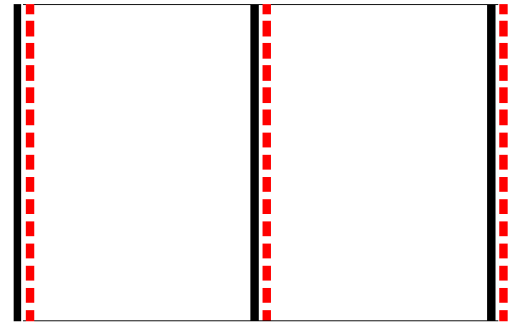
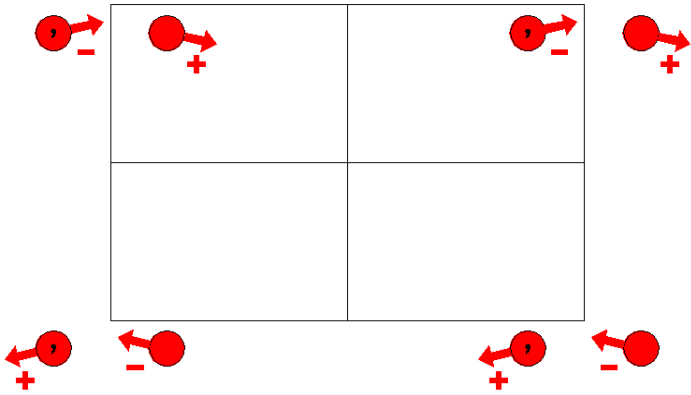
$P_{2a}m$

6.4.28

$m1'$

$P_{2a}1m1$

Monoclinic



**Origin** on  $m$

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1 | 0,0,0)

(2)  $m_x, 0, z$   
( $m_y$  | 0,0,0)

For  $(1,0,0)'$  + set

(1)  $t'$  (1,0,0)  
(1 | 1,0,0)'

(2)  $a'$  (1,0,0)  $x, 0, z$   
( $m_y$  | 1,0,0)'

**Generators selected** (1); t(1,0,0)'; t(0,1,0); t(0,0,1); (2).

**Positions**

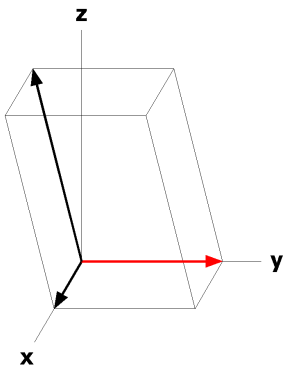
			Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1,0,0)' +
4	c	1	(1) x,y,z [u,v,w]	(2) x, $\bar{y}$ , z [ $\bar{u}$ , v, $\bar{w}$ ]
2	b	m	x, 1/2, z [0,v,0]	
2	a	m	x, 0, z [0,v,0]	

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2b</sub>-1m1  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



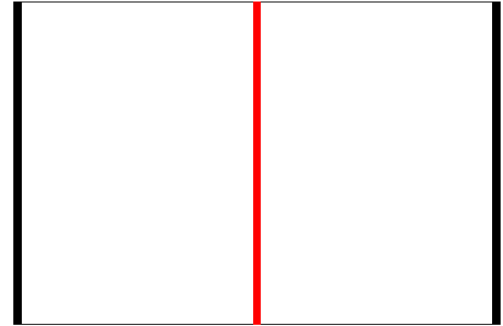
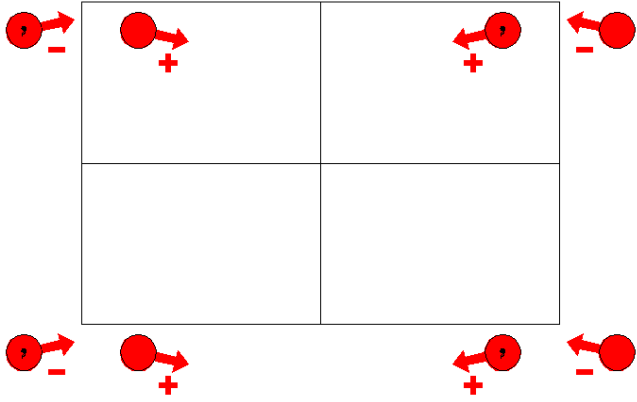
$P_{2b}m$

6.5.29

$m1'$

$P_{2b}1m1$

Monoclinic



Origin on  $m$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0)$  + set

(1)  $1$   
 $(1|0,0,0)$       (2)  $m \quad x,0,z$   
 $(m_y|0,0,0)$

For  $(0,1,0)'$  + set

(1)  $t' \quad (0,1,0)$   
 $(1|0,1,0)'$       (2)  $m' \quad x,1/2,z$   
 $(m_y|0,1,0)'$

**Generators selected** (1); t(1,0,0)<sup>l</sup>; t(0,1,0)<sup>l</sup>; t(0,0,1); (2).

**Positions**

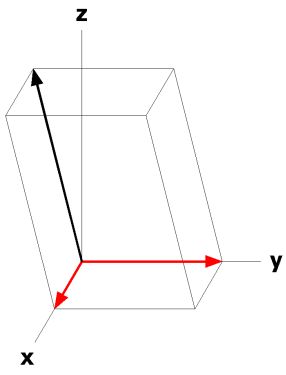
			Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(0,1,0) <sup>l</sup> +
4	c	1	(1) x,y,z [u,v,w]	(2) x, $\bar{y}$ ,z [ $\bar{u}$ ,v, $\bar{w}$ ]
2	b	m'	x,1/2,z [u,0,w]	
2	a	m	x,0,z [0,v,0]	

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>·1m1  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>·1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

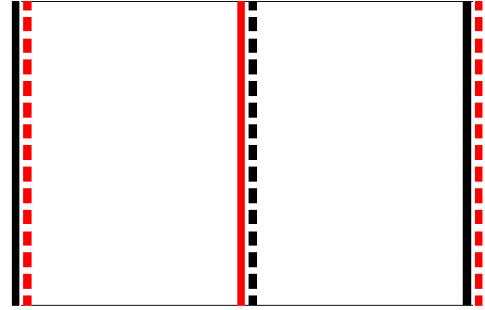
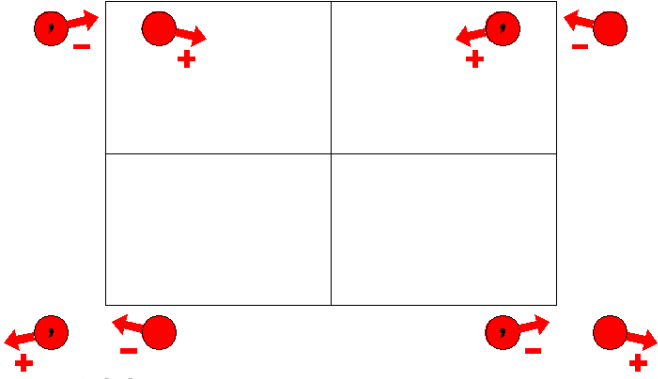
Along [0,1,0] p11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



$P_Cm$   
6.6.30

$m1'$   
 $P_C1m1$

Monoclinic



Origin on m

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) m  $x,0,z$   
( $m_y$ |0,0,0)

For (0,0,0) + set

(1)  $t'$  (1,0,0)  
(1|1,0,0)'

(2)  $a'$  (1,0,0)  $x,0,z$   
( $m_y$ |1,0,0)'

For (1,0,0)' + set



**Generators selected** (1); t(1,0,0)<sup>'</sup>; t(0,1,0)<sup>'</sup>; t(0,0,1); (2).

**Positions**

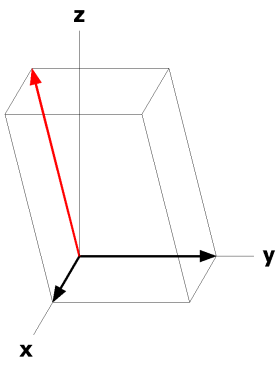
			Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1,0,0) <sup>'</sup> +
4	c	1	(1) x,y,z [u,v,w]	(2) x, $\bar{y}$ ,z [ $\bar{u}$ ,v, $\bar{w}$ ]
2	b	m'	x,1/2,z [u,0,w]	
2	a	m	x,0,z [0,v,0]	

**Symmetry of Special Projections**

Along [0,0,1] p<sub>c</sub>1m1  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

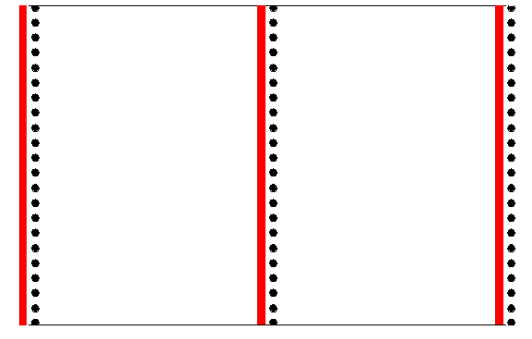
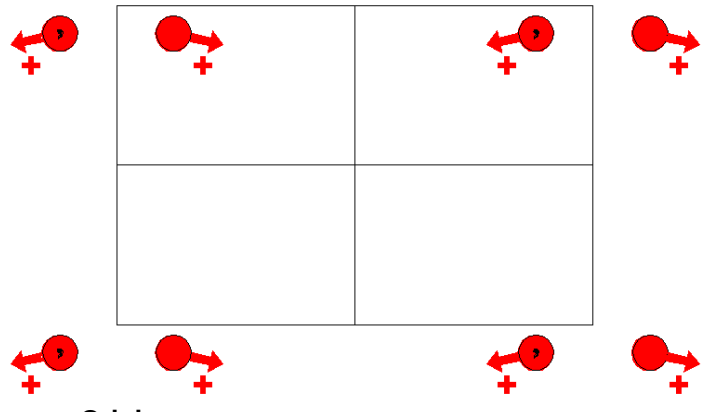
Along [0,1,0] p11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



$P_{2c}m'$   
6.7.31

$m1'$   
 $P_{2c}1m'1$

Monoclinic



Origin on m

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0)$  + set

- (1) 1  $(1|0,0,0)$
- (2)  $m'$   $x,0,z$   $(m_y|0,0,0)'$

For  $(0,0,1)'$  + set

- (1)  $t'$   $(0,0,1)$   $(1|0,0,1)'$
- (2)  $c$   $(0,0,1)$   $x,0,z$   $(m_y|0,0,1)$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2).

**Positions**

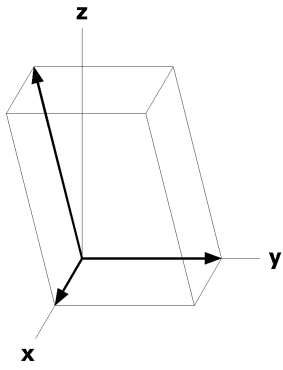
			Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(0,0,1)' +
4	c	1	(1) x,y,z [u,v,w]	(2) x, $\bar{y}$ , z [u, $\bar{v}$ , w]
2	b	m	x, 1/2, z [0,v,0]	
2	a	m'	x, 0, z [u, 0, v]	

**Symmetry of Special Projections**

Along [0,0,1] p1m11'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>'1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

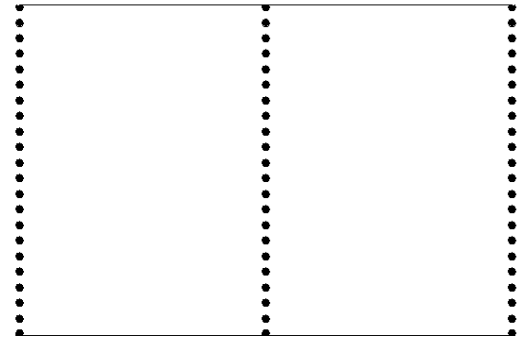
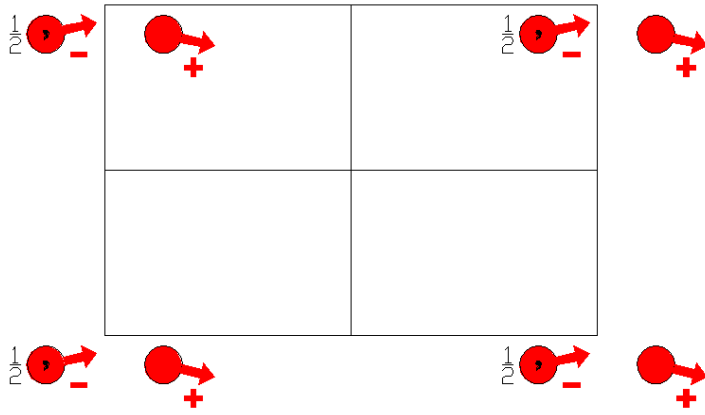
Along [0,1,0] p11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pc  
7.1.32

m  
P1c1

Monoclinic



**Origin** on glide plane c

**Asymmetric unit**  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

- (1) 1
- (1)  $(1|0,0,0)$
- (2) c  $(0,0,1/2)$  x,0,z
- (2)  $(m_y|0,0,1/2)$

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

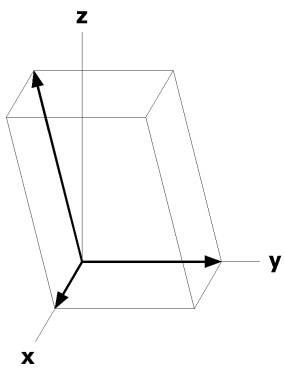
- 2 a 1 (1) x,y,z [u,v,w]
- (2)  $x, \bar{y}, z+1/2$  [ $\bar{u}, v, \bar{w}$ ]

**Symmetry of Special Projections**

Along  $[0,0,1]$  p1m1  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
Origin at 0,0,z

Along  $[1,0,0]$  p1g1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
Origin at x,0,0

Along  $[0,1,0]$  p<sub>2a</sub>-1  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
Origin at 0,y,0

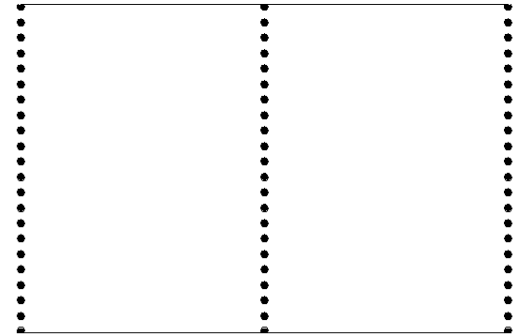
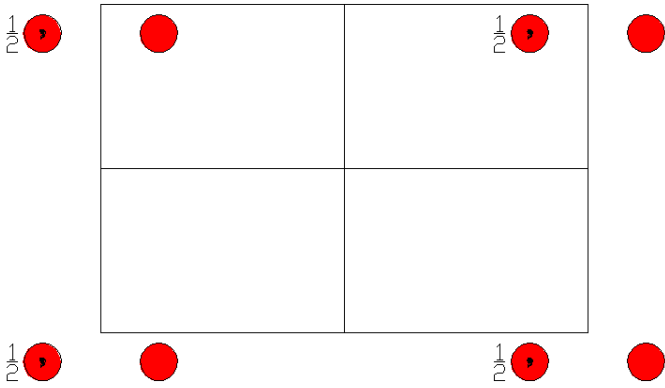


Pc1'  
7.2.33

m1'  
P1c11'

Monoclinic

1'



Origin on glide plane c1'

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

For 1 + set

- (1) 1  $(1|0,0,0)$
- (2) c  $(0,0,1/2)$  x,0,z  $(m_y|0,0,1/2)$

For 1' + set

- (1) 1'  $(1|0,0,0)'$
- (2) c'  $(0,0,1/2)$  x,0,z  $(m_y|0,0,1/2)'$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); 1'.

**Positions**

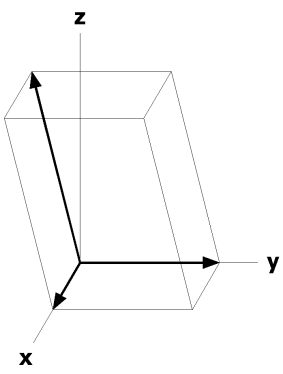
		Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.		1 +	1' +
2	a 11'	(1) x,y,z [0,0,0]	(2) $x, \bar{y}, z+1/2$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p1m11'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p11'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



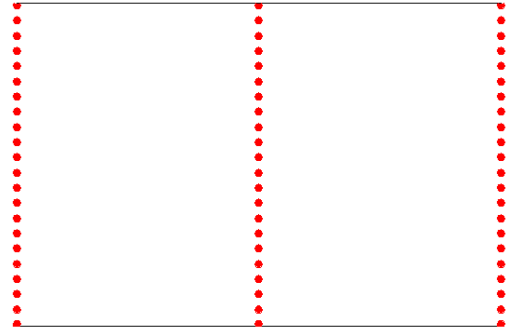
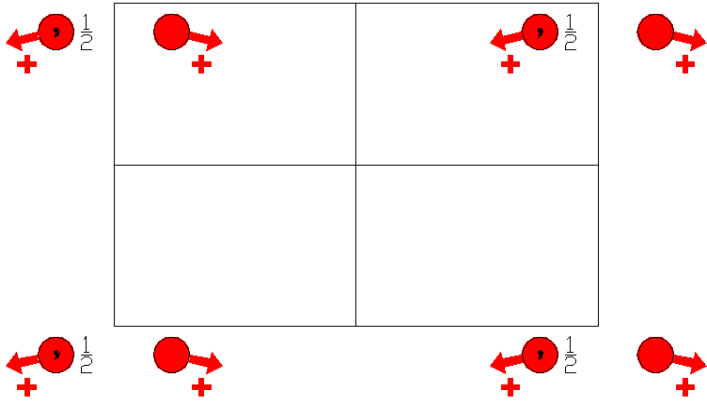
Pc'

7.3.34

m'

P1c'1

Monoclinic



Origin on glide plane  $c'$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

- (1) 1  $(1|0,0,0)$
- (2)  $c'$   $(0,0,1/2) \ x,0,z$   
 $(m_y|0,0,1/2)'$

Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

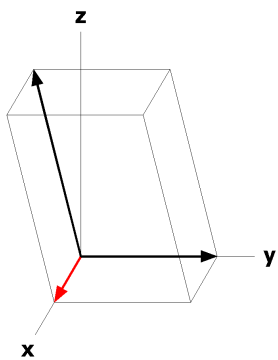
- 2 a 1 (1)  $x,y,z \ [u,v,w]$  (2)  $x,\bar{y},z+1/2 \ [u,\bar{v},w]$

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p1m'1$   
 $a^* = -b \ b^* = a_p$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p1g'1$   
 $a^* = b \ b^* = c_p$   
Origin at  $x,0,0$

Along  $[0,1,0]$   $p1$   
 $a^* = c/2 \ b^* = a$   
Origin at  $0,y,0$



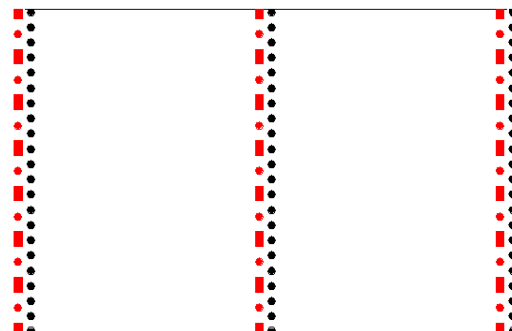
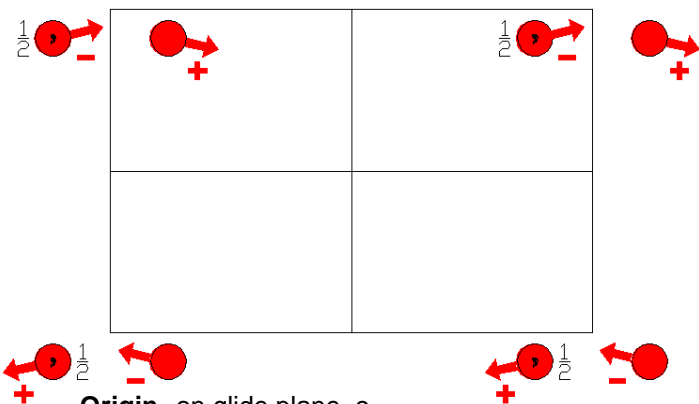
$P_{2a}c$

7.4.35

$m1'$

$P_{2a}1c1$

Monoclinic



Origin on glide plane  $c$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0) +$  set

(1) 1  $(1 | 0,0,0)$  (2)  $c$   $(0,0,1/2) \ x,0,z$   
 $(m_y | 0,0,1/2)$

For  $(1,0,0)' +$  set

(1)  $t'$   $(1,0,0)$   $(1 | 1,0,0)'$  (2)  $n'$   $(1,0,1/2) \ x,0,z$   
 $(m_y | 1,0,1/2)'$

Generators selected (1);  $t(1,0,0)'$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

$(0,0,0) +$   $(1,0,0)' +$

4 a 1 (1)  $x,y,z [u,v,w]$  (2)  $x,\bar{y},z+1/2 [\bar{u},v,\bar{w}]$

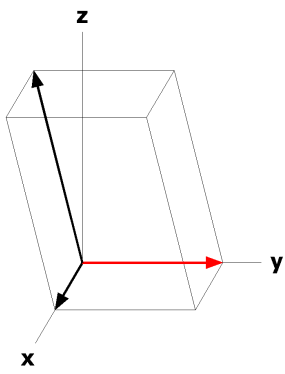
**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_{2b}1m1$   
 $a^* = -b$   $b^* = a_p$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p1g11'$   
 $a^* = b$   $b^* = c_p$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $p_{2a}1$   
 $a^* = -a$   $b^* = c/2$   
 Origin at  $0,y,0$





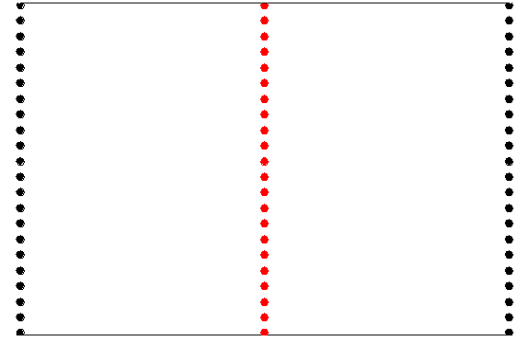
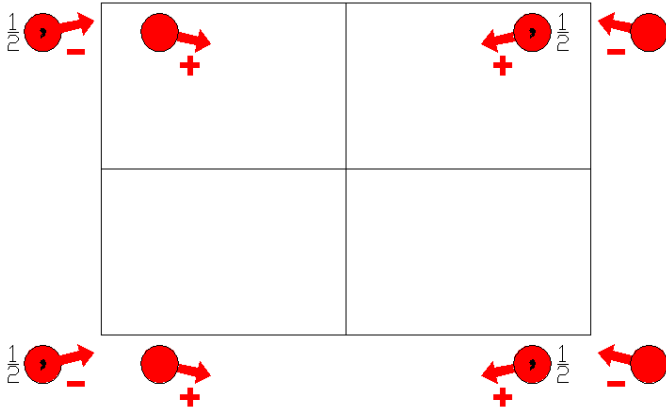
$P_{2b}c$

7.5.36

$m1'$

$P_{2b}1c1$

Monoclinic



Origin on glide plane  $c$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0) +$  set

- (1) 1  $(1 | 0,0,0)$
- (2)  $c$   $(0,0,1/2) \ x,0,z$   
 $(m_y | 0,0,1/2)$

For  $(0,1,0)'$  + set

- (1)  $t'$   $(0,1,0)$   $(1 | 0,1,0)'$
- (2)  $c'$   $(0,0,1/2) \ x,1/2,z$   
 $(m_y | 0,1,1/2)'$

Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)'$ ;  $t(0,0,1)$ ; (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

$(0,0,0) +$   $(0,1,0)'$  +

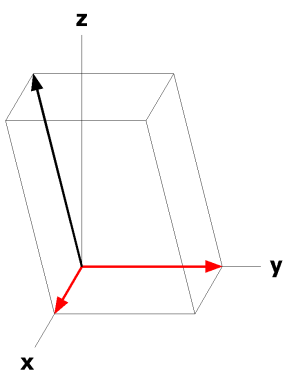
4  $a$  1 (1)  $x,y,z$   $[u,v,w]$  (2)  $x,\bar{y},z+1/2$   $[\bar{u},v,\bar{w}]$

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_{2a}1m1$   
 $a^* = -b$   $b^* = a_p$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a}1g1$   
 $a^* = b$   $b^* = c_p$   
Origin at  $x,0,0$

Along  $[0,1,0]$   $p11'$   
 $a^* = c/2$   $b^* = a$   
Origin at  $0,y,0$



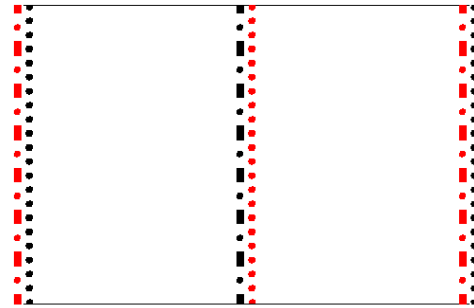
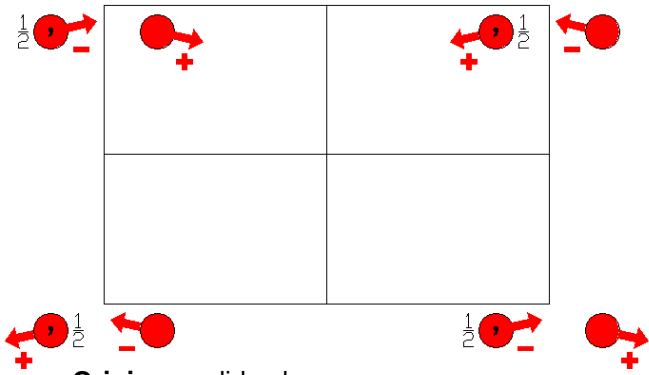
$P_c c$

7.6.37

$m1'$

$P_c 1c1$

Monoclinic



**Origin** on glide plane  $c$

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0) +$  set

- (1) 1  $(1 | 0,0,0)$
- (2)  $c$   $(0,0,1/2) \quad x,0,z$   
 $(m_y | 0,0,1/2)$

For  $(1,0,0)' +$  set

- (1)  $t'$   $(1,0,0)$   
 $(1 | 1,0,0)'$
- (2)  $n'$   $(1,0,1/2) \quad x,0,z$   
 $(m_y | 1,0,1/2)'$

**Generators selected** (1);  $t(1,0,0)'$ ;  $t(0,1,0)'$ ;  $t(0,0,1)$ ; (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

$(0,0,0) +$        $(1,0,0)' +$

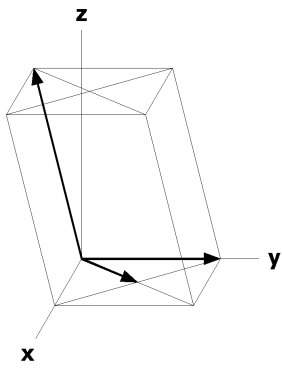
4   a   1      (1)  $x,y,z [u,v,w]$       (2)  $x,\bar{y},z+1/2 [\bar{u},v,\bar{w}]$

**Symmetry of Special Projections**

Along  $[0,0,1]$      $p_c 1m1$   
 $\mathbf{a}^* = -\mathbf{b}$     $\mathbf{b}^* = \mathbf{a}_p$   
Origin at  $0,0,z$

Along  $[1,0,0]$      $p1g11'$   
 $\mathbf{a}^* = \mathbf{b}$     $\mathbf{b}^* = \mathbf{c}_p$   
Origin at  $x,0,0$

Along  $[0,1,0]$      $p11'$   
 $\mathbf{a}^* = \mathbf{a}$     $\mathbf{b}^* = \mathbf{c}/2$   
Origin at  $0,y,0$



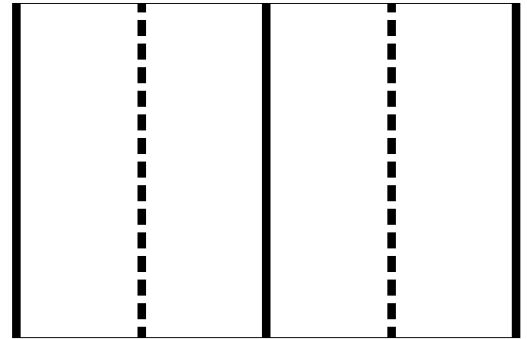
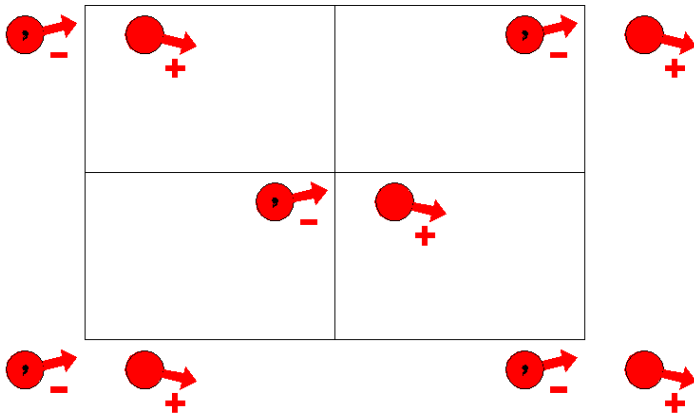
Cm

m

Monoclinic

8.1.38

C1m1



**Origin** on mirror plane *m*

**Asymmetric unit**  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1 | 0,0,0)      (2) *m* *x*,0,*z*  
(*m<sub>y</sub>* | 0,0,0)

For (1/2,1/2,0) + set

(1) *t* (1/2,1/2,0)  
(1 | 1/2,1/2,0)      (2) *a* (1/2,0,0) *x*,1/4,*z*  
(*m<sub>y</sub>* | 1/2,1/2,0)

**Generators selected** (1); *t*(1,0,0); *t*(0,1,0); *t*(0,0,1); *t*(1/2,1/2,0); (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

(0,0,0) +      (1/2,1/2,0) +

4 *b* 1      (1) *x*,*y*,*z* [*u*,*v*,*w*]      (2) *x*,*y*,*z* [*u*,*v*,*w*]

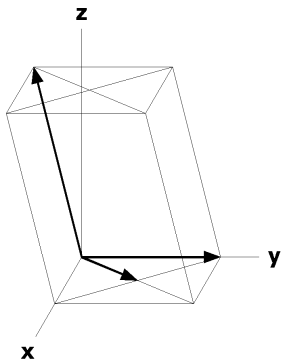
2 *a* *m*      *x*,0,*z* [0,*v*,0]

**Symmetry of Special Projections**

Along [0,0,1] *c*1*m*1  
**a\*** = -**b** **b\*** = **a<sub>p</sub>**  
Origin at 0,0,*z*

Along [1,0,0] *p*1*m*1  
**a\*** = **b**/2 **b\*** = **c<sub>p</sub>**  
Origin at *x*,0,0

Along [0,1,0] *p*11'  
**a\*** = **c** **b\*** = **a**/2  
Origin at 0,*y*,0



Cm1'

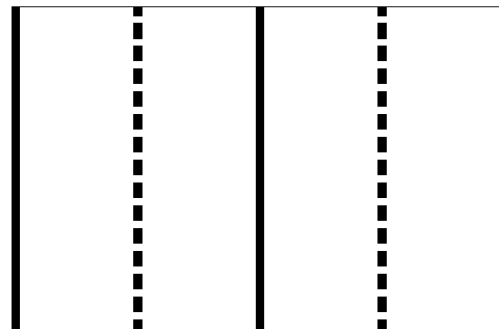
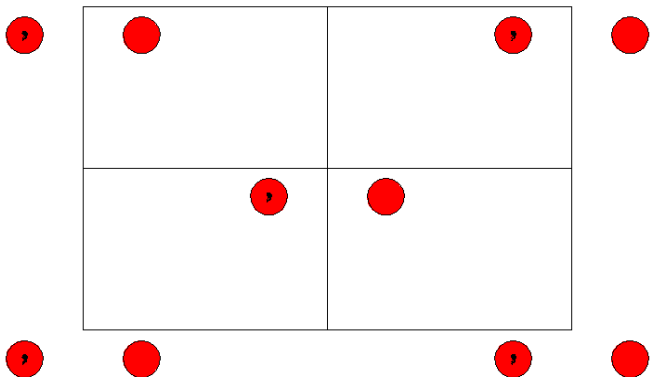
8.2.39

m1'

C1m11'

Monoclinic

1'



**Origin** on mirror plane m1'

**Asymmetric unit**  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1 | 0,0,0)

(2) m x,0,z  
(m<sub>y</sub> | 0,0,0)

For (0,0,0) + set

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1 | 1/2,1/2,0)

(2) a (1/2,0,0) x,1/4,z  
(m<sub>y</sub> | 1/2,1/2,0)

For (0,0,0)' + set

(1) 1'  
(1 | 0,0,0)'

(2) m' x,0,z  
(m<sub>y</sub> | 0,0,0)'

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0)  
(1 | 1/2,1/2,0)'

(2) a' (1/2,0,0) x,1/4,z  
(m<sub>y</sub> | 1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); 1'.

### Positions

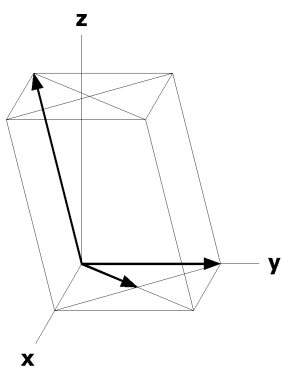
		Coordinates	
Multiplicity,			
Wyckoff letter,			
Site Symmetry.			
		(0,0,0) +	(1/2,1/2,0) +
		(0,0,0)' +	(1/2,1/2,0)' +
4	b 11'	(1) x,y,z [0,0,0]	(2) x, $\bar{y}$ ,z [0,0,0]
2	a m1'	x,0,z [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] c1m11'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



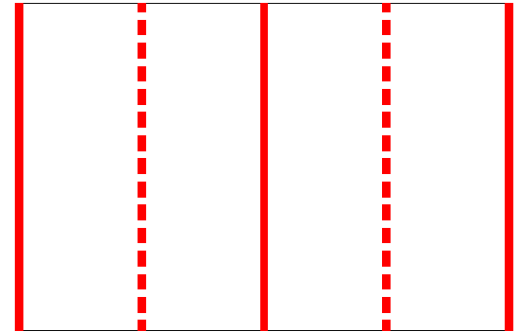
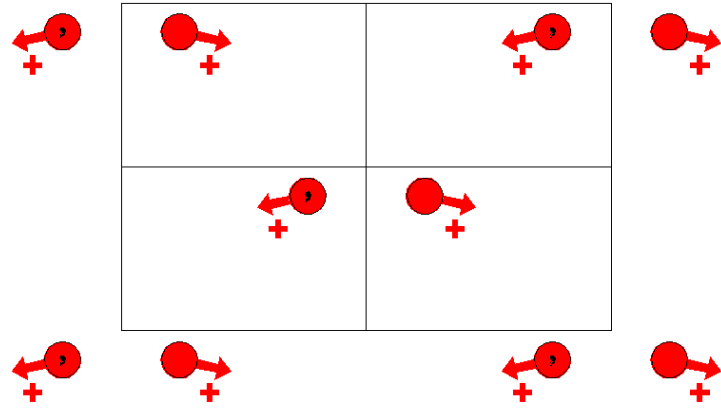
Cm'

8.3.40

m'

C1m'1

Monoclinic



Origin on mirror plane  $m'$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0) +$  set

(1) 1  
(1 | 0,0,0)

(2)  $m'$   $x,0,z$   
( $m_y$  | 0,0,0)'

For  $(1/2,1/2,0) +$  set

(1)  $t$   $(1/2,1/2,0)$   
(1 |  $1/2,1/2,0$ )

(2)  $a'$   $(1/2,0,0)$   $x,1/4,z$   
( $m_y$  |  $1/2,1/2,0$ )'

Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,0)$ ; (2).

Positions

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

$(0,0,0) +$   $(1/2,1/2,0) +$

4 b 1 (1)  $x,y,z$  [ $u,v,w$ ] (2)  $x,\bar{y},z$  [ $u,\bar{v},w$ ]

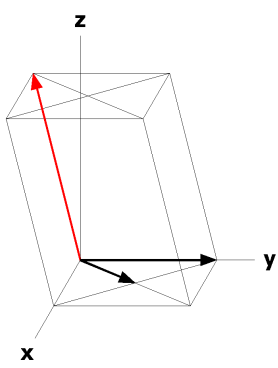
2 a  $m'$   $x,0,z$  [ $u,0,w$ ]

Symmetry of Special Projections

Along  $[0,0,1]$   $c1m'1$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
Origin at  $x,0,0$

Along  $[0,1,0]$   $p1$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
Origin at  $0,y,0$



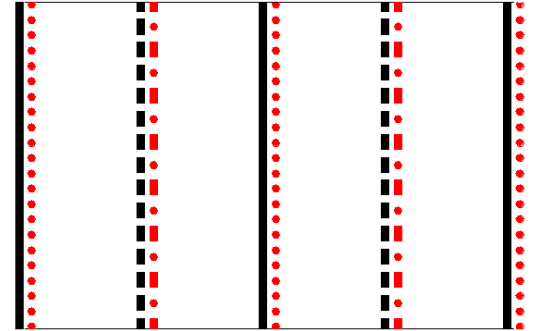
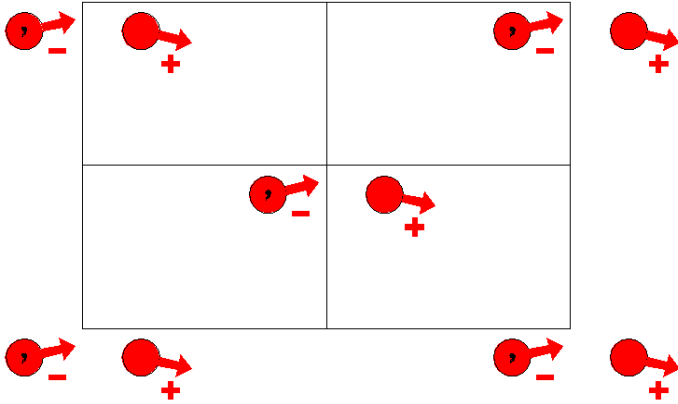
$C_{2c}m$

8.4.41

$m1'$

$C_{2c}1m1$

Monoclinic



**Origin** on mirror plane  $m$

**Asymmetric unit**  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1)  $1$   
(1 | 0,0,0)

(2)  $m$   $x,0,z$   
( $m_y$  | 0,0,0)

For (0,0,0) + set

(1)  $t$  (1/2,1/2,0)  
(1 | 1/2,1/2,0)

(2)  $a$  (1/2,0,0)  $x,1/4,z$   
( $m_y$  | 1/2,1/2,0)

For (1/2,1/2,0) + set

(1)  $t'$  (0,0,1)  
(1 | 0,0,1)'

(2)  $c'$  (0,0,1)  $x,0,z$   
( $m_y$  | 0,0,1)'

For (0,0,1)' + set

(1)  $t''$  (1/2,1/2,1)  
(1 | 1/2,1/2,1)'

(2)  $n'$  (1/2,0,1)  $x,1/4,z$   
( $m_y$  | 1/2,1/2,1)'

For (1/2,1/2,1)' + set

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; t(1/2,1/2,0); (2).

**Positions**

		Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.			
		(0,0,0) + (0,0,1)'	(1/2,1/2,0) + (1/2,1/2,1)'
8	b 1	(1) x,y,z [u,v,w]	(2) x, $\bar{y}$ ,z [ $\bar{u}$ ,v, $\bar{w}$ ]
4	a m	x,0,z [0,v,0]	

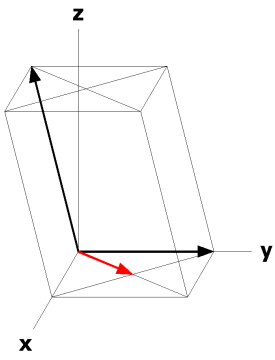
**Symmetry of Special Projections**

Along [0,0,1] c1m1  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>'1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0





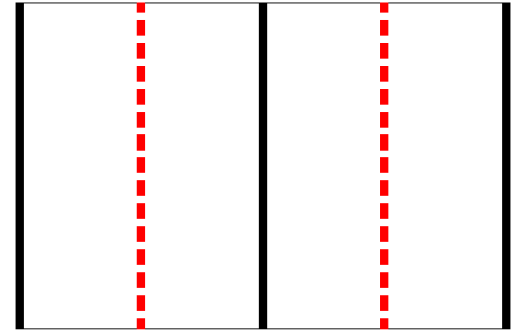
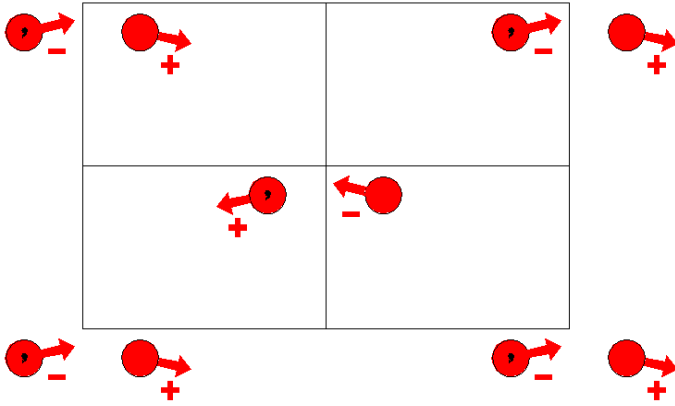
$C_{2v}$

8.5.42

$m\bar{1}'$

$C_{2v}1m1$

Monoclinic



**Origin** on mirror plane  $m$

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0) +$  set

(1)  $1$   
(1 |  $0,0,0$ )

(2)  $m$   $x,0,z$   
( $m_y$  |  $0,0,0$ )

For  $(1/2,1/2,0)'$  + set

(1)  $t'$   $(1/2,1/2,0)$   
(1 |  $1/2,1/2,0$ )'

(2)  $a'$   $(1/2,0,0)$   $x,1/4,z$   
( $m_y$  |  $1/2,1/2,0$ )'

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,0)'$ ; (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

$(0,0,0) +$   $(1/2,1/2,0)'$  +

4  $b$  1 (1)  $x,y,z$  [ $u,v,w$ ] (2)  $x,\bar{y},z$  [ $\bar{u},v,\bar{w}$ ]

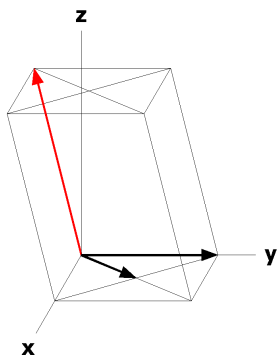
2  $a$   $m$   $x,0,z$  [ $0,v,0$ ]

**Symmetry of Special Projections**

Along  $[0,0,1]$   $c_p1m1$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a'}1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
Origin at  $x,0,0$

Along  $[0,1,0]$   $p11'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
Origin at  $0,y,0$



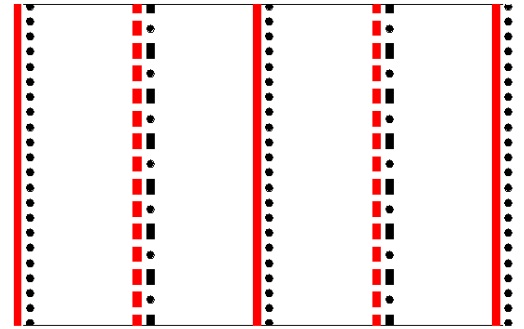
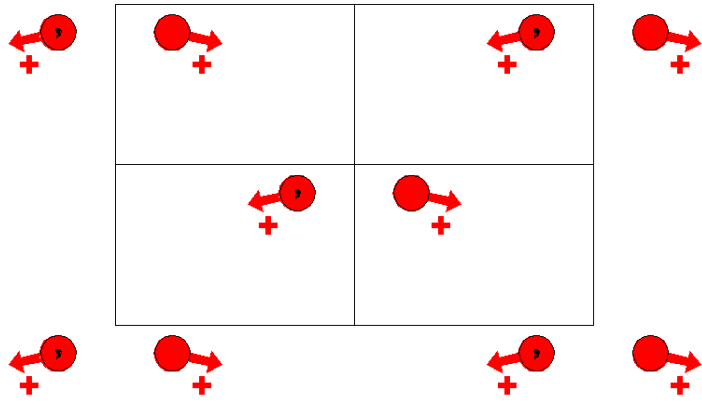
$C_{2c}m'$

8.6.43

$m1'$

$C_{2c}1m'1$

Monoclinic



**Origin** on mirror plane  $m'$

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0) + \text{set}$

(1)  $1$   
(1 | 0,0,0)

(2)  $m'$   $x,0,z$   
( $m_y$  | 0,0,0)'

For  $(1/2,1/2,0) + \text{set}$

(1)  $t$   $(1/2,1/2,0)$   
(1 |  $1/2,1/2,0$ )

(2)  $a'$   $(1/2,0,0)$   $x,1/4,z$   
( $m_y$  |  $1/2,1/2,0$ )'

For  $(0,0,1)' + \text{set}$

(1)  $t'$   $(0,0,1)$   
(1 | 0,0,1)'

(2)  $c$   $(0,0,1)$   $x,0,z$   
( $m_y$  | 0,0,1)

For  $(1/2,1/2,1)' + \text{set}$

(1)  $t'$   $(1/2,1/2,1)$   
(1 |  $1/2,1/2,1$ )'

(2)  $n$   $(1/2,0,1)$   $x,1/4,z$   
( $m_y$  |  $1/2,1/2,1$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; t(1/2,1/2,0); (2).

**Positions**

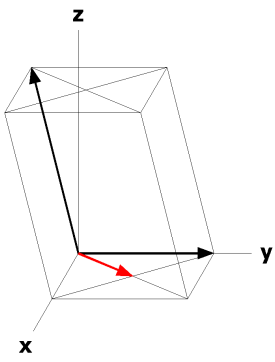
		Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.			
		(0,0,0) + (0,0,1)'	(1/2,1/2,0) + (1/2,1/2,1)'
8	b 1	(1) x,y,z [u,v,w]	(2) x, $\bar{y}$ ,z [u, $\bar{v}$ ,w]
4	a m'	x,0,z [u,0,w]	

**Symmetry of Special Projections**

Along [0,0,1] c1m11'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>'1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>'1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



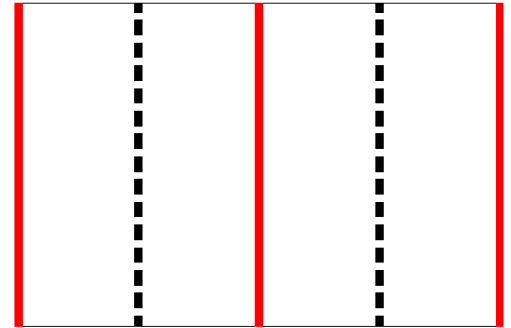
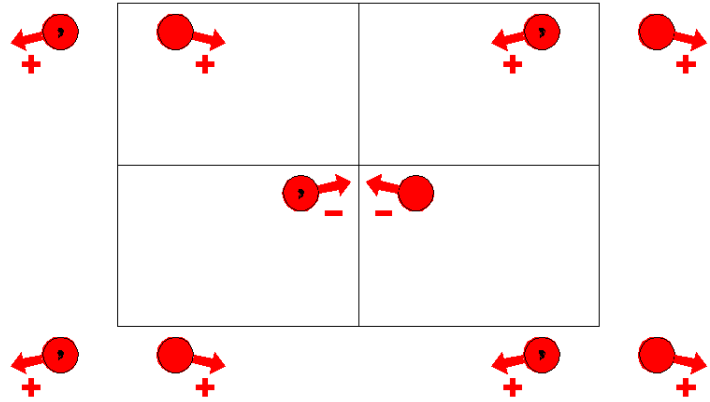
$C_p m'$

8.7.44

$m1'$

$C_p 1m'1$

Monoclinic



**Origin** on mirror plane  $m'$

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0) +$  set

- (1) 1  $(1 | 0,0,0)$
- (2)  $m'$   $x,0,z$   $(m_y | 0,0,0)'$

For  $(1/2,1/2,0)'$  + set

- (1)  $t'$   $(1/2,1/2,0)$   $(1 | 1/2,1/2,0)'$
- (2)  $a$   $(1/2,0,0)$   $x,1/4,z$   $(m_y | 1/2,1/2,0)$

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,0)'$ ; (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

$(0,0,0) +$   $(1/2,1/2,0)'$  +

4 b 1 (1)  $x,y,z [u,v,w]$  (2)  $x,\bar{y},z [u,\bar{v},w]$

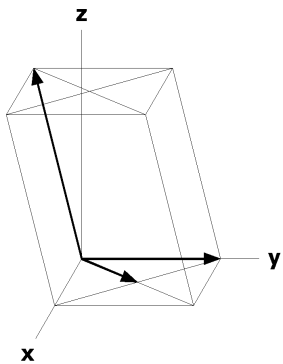
2 a  $m'$   $x,0,z [u,0,w]$

**Symmetry of Special Projections**

Along  $[0,0,1]$   $c_p 1m'1$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a'} 1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
Origin at  $x,1/4,0$

Along  $[0,1,0]$   $p_{2a'} 1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $0,y,0$



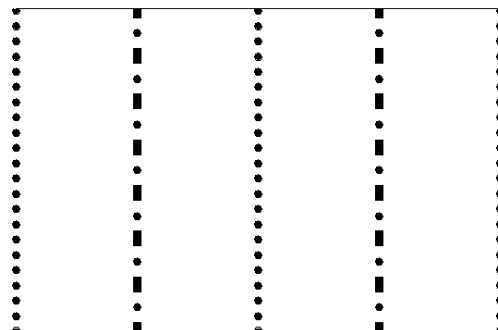
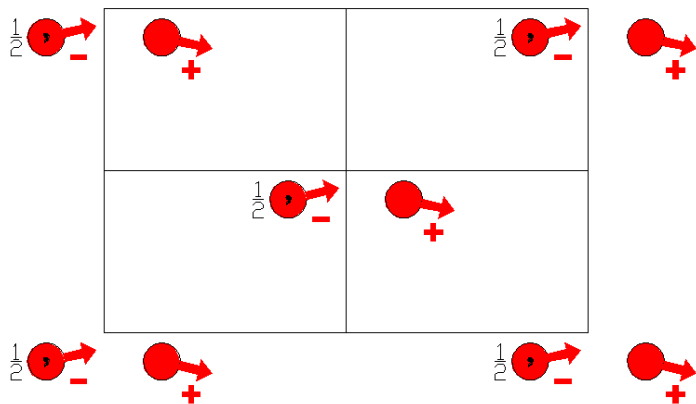
Cc

m

Monoclinic

9.1.45

C1c1



**Origin** on glide plane c

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1 | 0,0,0)

(2) c (0,0,1/2) x,0,z  
(m<sub>y</sub> | 0,0,1/2)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1 | 1/2,1/2,0)

(2) n (1/2,0,1/2) x,1/4,z  
(m<sub>y</sub> | 1/2,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

(0,0,0) + (1/2,1/2,0) +

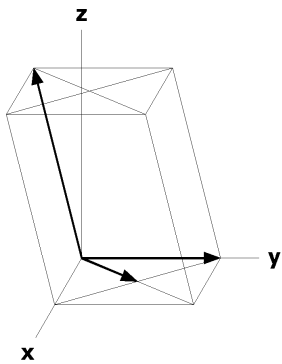
4 a 1 (1) x,y,z [u,v,w] (2) x, $\bar{y}$ ,z+1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] c1m1  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
Origin at 0,0,z

Along [1,0,0] p1g1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
Origin at x,0,0

Along [0,1,0] p<sub>2a</sub><sup>-1</sup>  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
Origin at 0,y,0



Cc1'

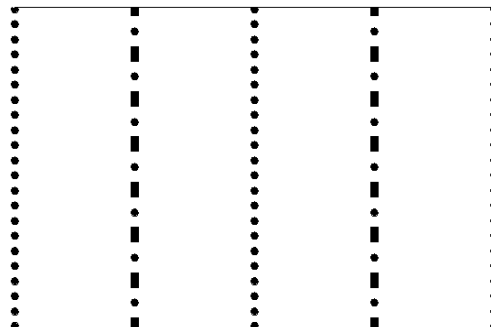
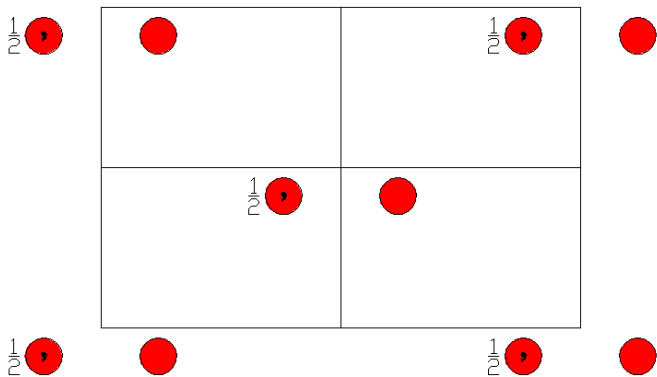
9.2.46

m1'

C1c11'

Monoclinic

1'



Origin on glide plane  $c1'$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

Symmetry Operations

(1)  $1$   
(1 | 0,0,0)

(2)  $c$  (0,0,1/2)  $x,0,z$   
( $m_y$  | 0,0,1/2)

For (0,0,0) + set

For (1/2,1/2,0) + set

(1)  $t$  (1/2,1/2,0)  
(1 | 1/2,1/2,0)

(2)  $n$  (1/2,0,1/2)  $x,1/4,z$   
( $m_y$  | 1/2,1/2,1/2)

For (0,0,0)' + set

For (1/2,1/2,0)' + set

(1)  $1'$   
(1 | 0,0,0)'

(2)  $c'$  (0,0,1/2)  $x,0,z$   
( $m_y$  | 0,0,1/2)'

(1)  $t'$  (1/2,1/2,0)  
(1 | 1/2,1/2,0)'

(2)  $n'$  (1/2,0,1/2)  $x,1/4,z$   
( $m_y$  | 1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); 1'.

**Positions**

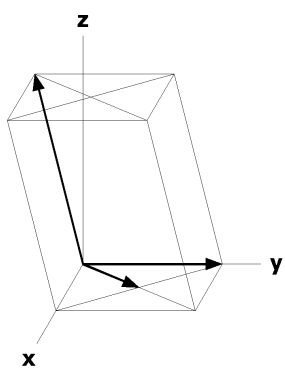
		Coordinates	
Multiplicity,			
Wyckoff letter,			
Site Symmetry.			
		(0,0,0) +	(1/2,1/2,0) +
		(0,0,0)' +	(1/2,1/2,0)' +
4	a 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y}, z+1/2$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] c1m11'  
 $\mathbf{a}^* = -\mathbf{b}^*$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p11'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



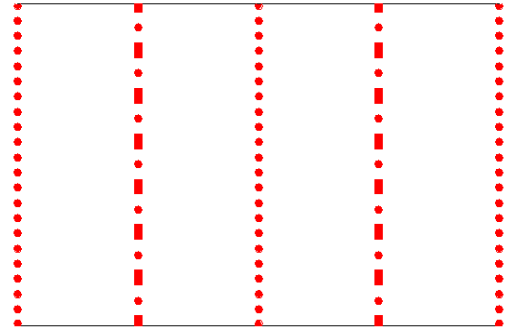
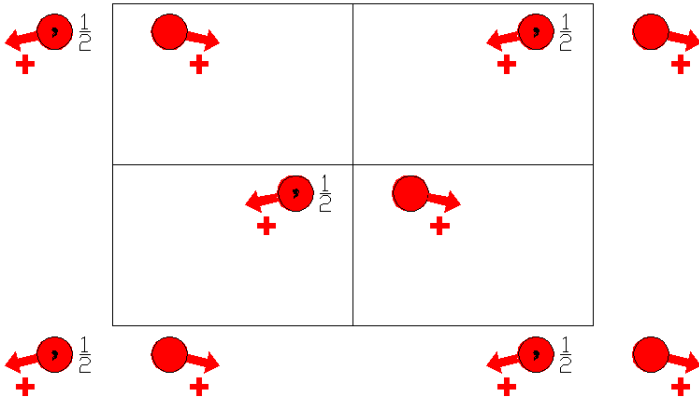
Cc'

9.3.47

m'

C1c'1

Monoclinic



**Origin** on glide plane  $c'$

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1 | 0,0,0)

(2)  $c'$  (0,0,1/2)  $x,0,z$   
( $m_y$  | 0,0,1/2)'

For (1/2,1/2,0) + set

(1)  $t$  (1/2,1/2,0)  
(1 | 1/2,1/2,0)

(2)  $n'$  (1/2,0,1/2)  $x,1/4,z$   
( $m_y$  | 1/2,1/2,1/2)'

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,0)$ ; (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

(0,0,0) + (1/2,1/2,0) +

4 a 1 (1)  $x,y,z$  [u,v,w] (2)  $x,\bar{y},z+1/2$  [ $\bar{u},\bar{v},w$ ]

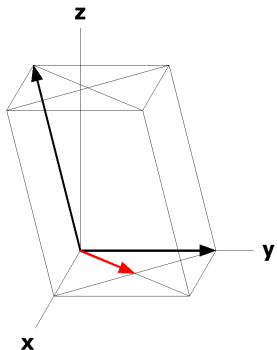
**Symmetry of Special Projections**

Along [0,0,1]  $c1m'1$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
Origin at 0,0,z

Along [1,0,0]  $p1g'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
Origin at x,0,0

Along [0,1,0]  $p1$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
Origin at 0,y,0





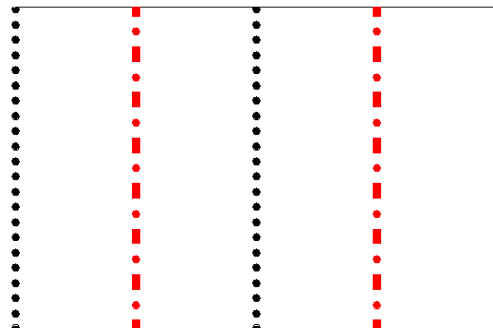
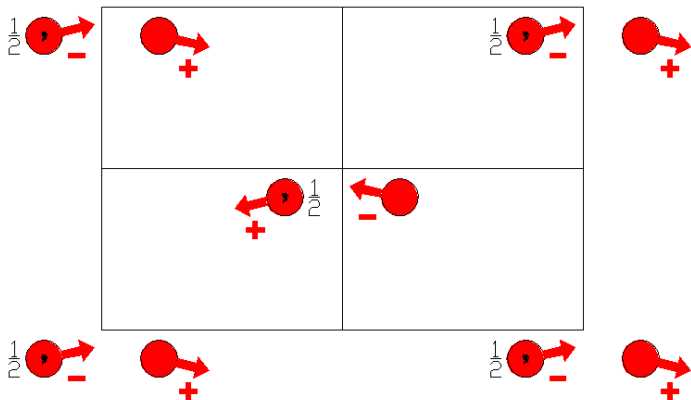
$C_{2c}$

9.4.48

$m1'$

$C_{2c}1c1$

Monoclinic



**Origin** on glide plane  $c$

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1 | 0,0,0)

(2)  $c$   $(0,0,1/2)$   $x,0,z$   
( $m_y$  |  $0,0,1/2$ )

For  $(1/2,1/2,0)'$  + set

(1)  $t'$   $(1/2,1/2,0)$   
(1 |  $1/2,1/2,0$ )'

(2)  $n'$   $(1/2,0,1/2)$   $x,1/4,z$   
( $m_y$  |  $1/2,1/2,1/2$ )'

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,0)'$ ; (2).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

$(0,0,0)$  +  $(1/2,1/2,0)'$  +

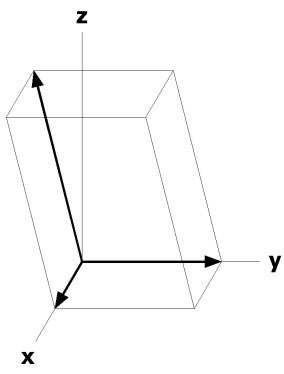
4 a 1 (1)  $x,y,z$  [ $u,v,w$ ] (2)  $x,\bar{y},z+1/2$  [ $\bar{u},v,\bar{w}$ ]

**Symmetry of Special Projections**

Along  $[0,0,1]$   $c_p 1m1$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a'} 1g1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
Origin at  $x,0,0$

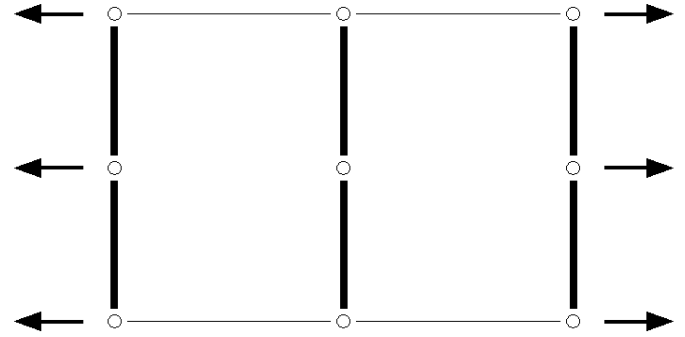
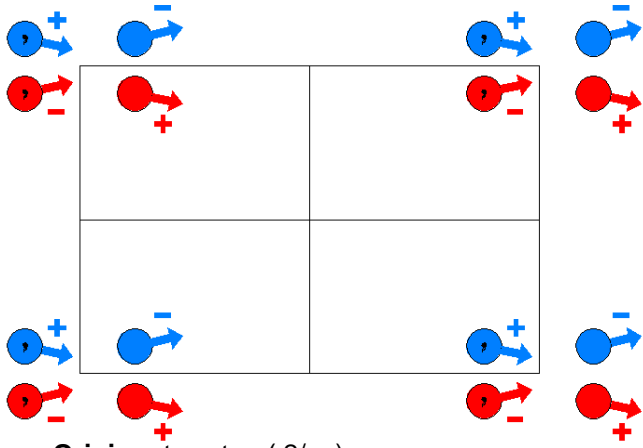
Along  $[0,1,0]$   $p_{2a'} 1$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2 + \mathbf{c}/2$   
Origin at  $0,y,0$



P2/m  
10.1.49

2/m  
P12/m1

Monoclinic



Origin at center (2/m)

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 0,y,0  
(2<sub>y</sub>|0,0,0)

(3)  $\bar{1}$  0,0,0  
( $\bar{1}$ |0,0,0)

(4) m x,0,z  
(m<sub>y</sub>|0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

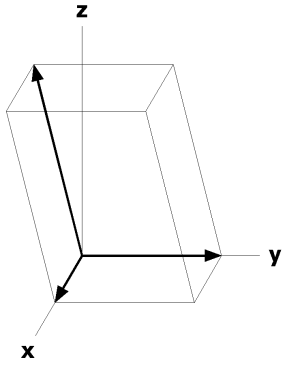
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
4	o	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(4) x, $\bar{y}$ ,z [ $\bar{u},\bar{v},\bar{w}$ ]
2	n	m	x,1/2,z [0,v,0]	$\bar{x},1/2,\bar{z}$ [0,v,0]		
2	m	m	x,0,z [0,v,0]	$\bar{x},0,\bar{z}$ [0,v,0]		
2	l	2	1/2,y,1/2 [0,v,0]	1/2, $\bar{y}$ ,1/2 [0,v,0]		
2	k	2	0,y,1/2 [0,v,0]	0, $\bar{y}$ ,1/2 [0,v,0]		
2	j	2	1/2,y,0 [0,v,0]	1/2, $\bar{y}$ ,0 [0,v,0]		
2	i	2	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0,v,0]		
1	h	2/m	1/2,1/2,1/2 [0,v,0]			
1	g	2/m	1/2,0,1/2 [0,v,0]			
1	f	2/m	0,1/2,1/2 [0,v,0]			
1	e	2/m	1/2,1/2,0 [0,v,0]			
1	d	2/m	1/2,0,0 [0,v,0]			
1	c	2/m	0,0,1/2 [0,v,0]			
1	b	2/m	0,1/2,0 [0,v,0]			
1	a	2/m	0,0,0 [0,v,0]			

**Symmetry of Special Projections**

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



P2/m1'

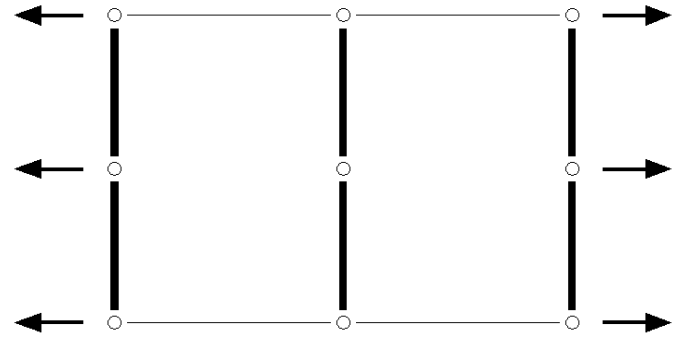
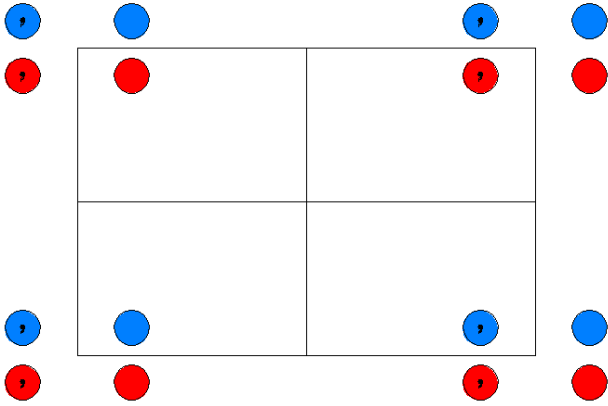
10.2.50

2/m1'

P12/m11'

Monoclinic

1'



Origin at center (2/m1')

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 0,y,0  
(2<sub>y</sub>|0,0,0)

(3)  $\bar{1}$  0,0,0  
( $\bar{1}$ |0,0,0)

(4) m x,0,z  
(m<sub>y</sub>|0,0,0)

For 1 + set

For 1' + set

(1) 1'  
(1|0,0,0)'

(2) 2' 0,y,0  
(2'<sub>y</sub>|0,0,0)'

(3)  $\bar{1}$ ' 0,0,0  
( $\bar{1}$ '|0,0,0)'

(4) m' x,0,z  
(m'<sub>y</sub>|0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

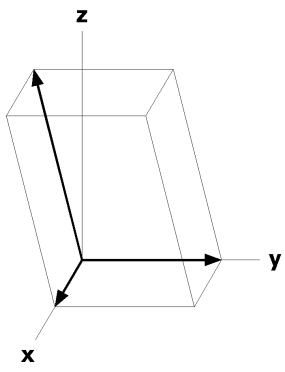
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +	1 +	1' +	1' +
4 o 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},y,\bar{z}$ [0,0,0]	(3) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(4) x, $\bar{y}$ ,z [0,0,0]
2 n m1'	x,1/2,z [0,0,0]	$\bar{x},1/2,\bar{z}$ [0,0,0]		
2 m m1'	x,0,z [0,0,0]	$\bar{x},0,\bar{z}$ [0,0,0]		
2 l 21'	1/2,y,1/2 [0,0,0]	1/2, $\bar{y}$ ,1/2 [0,0,0]		
2 k 21'	0,y,1/2 [0,0,0]	0, $\bar{y}$ ,1/2 [0,0,0]		
2 j 21'	1/2,y,0 [0,0,0]	1/2, $\bar{y}$ ,0 [0,0,0]		
2 i 21'	0,y,0 [0,0,0]	0, $\bar{y}$ ,0 [0,0,0]		
1 h 2/m1'	1/2,1/2,1/2 [0,0,0]			
1 g 2/m1'	1/2,0,1/2 [0,0,0]			
1 f 2/m1'	0,1/2,1/2 [0,0,0]			
1 e 2/m1'	1/2,1/2,0 [0,0,0]			
1 d 2/m1'	1/2,0,0 [0,0,0]			
1 c 2/m1'	0,0,1/2 [0,0,0]			
1 b 2/m1'	0,1/2,0 [0,0,0]			
1 a 2/m1'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



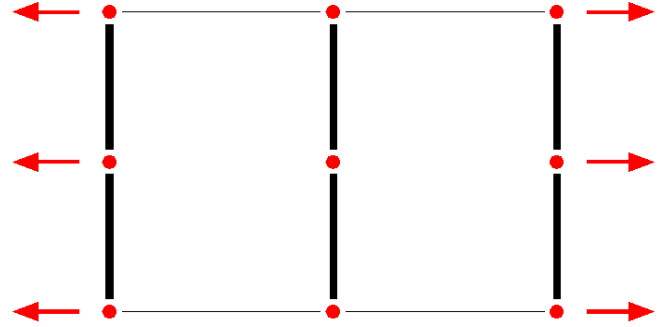
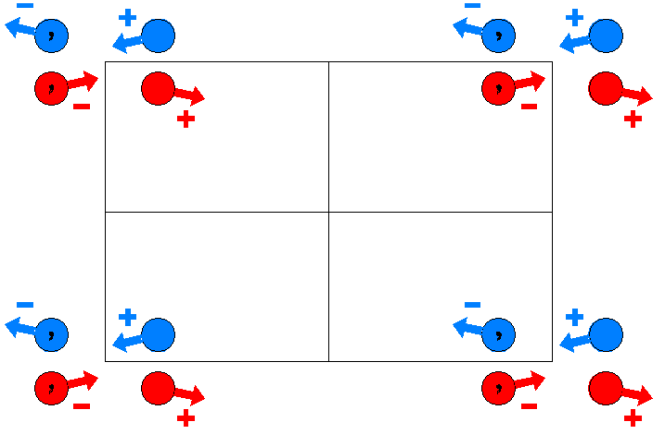
P2'/m

10.3.51

2'/m

P12'/m1

Monoclinic



Origin at center (2'/m)

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2'  $0,y,0$   
(2<sub>y</sub>|0,0,0)'

(3)  $\bar{1}$ '  $0,0,0$   
( $\bar{1}$ |0,0,0)'

(4) m  $x,0,z$   
(m<sub>y</sub>|0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

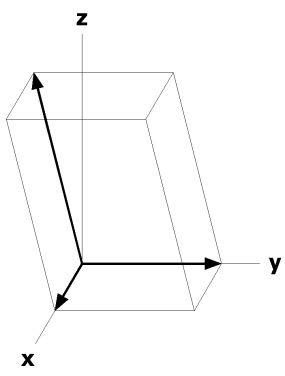
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) x, $\bar{y}$ ,z [ $\bar{u},\bar{v},\bar{w}$ ]
4 o 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) x, $\bar{y}$ ,z [ $\bar{u},\bar{v},\bar{w}$ ]
2 n m	x,1/2,z [0,v,0]	$\bar{x},1/2,\bar{z}$ [0, $\bar{v}$ ,0]		
2 m m	x,0,z [0,v,0]	$\bar{x},0,\bar{z}$ [0, $\bar{v}$ ,0]		
2 l 2'	1/2,y,1/2 [u,0,w]	1/2, $\bar{y}$ ,1/2 [ $\bar{u}$ ,0, $\bar{w}$ ]		
2 k 2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ ,1/2 [ $\bar{u}$ ,0, $\bar{w}$ ]		
2 j 2'	1/2,y,0 [u,0,w]	1/2, $\bar{y}$ ,0 [ $\bar{u}$ ,0, $\bar{w}$ ]		
2 i 2'	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [ $\bar{u}$ ,0, $\bar{w}$ ]		
1 h 2'/m	1/2,1/2,1/2 [0,0,0]			
1 g 2'/m	1/2,0,1/2 [0,0,0]			
1 f 2'/m	0,1/2,1/2 [0,0,0]			
1 e 2'/m	1/2,1/2,0 [0,0,0]			
1 d 2'/m	1/2,0,0 [0,0,0]			
1 c 2'/m	0,0,1/2 [0,0,0]			
1 b 2'/m	0,1/2,0 [0,0,0]			
1 a 2'/m	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

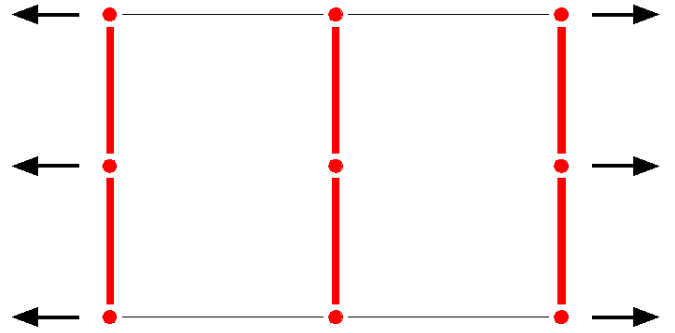
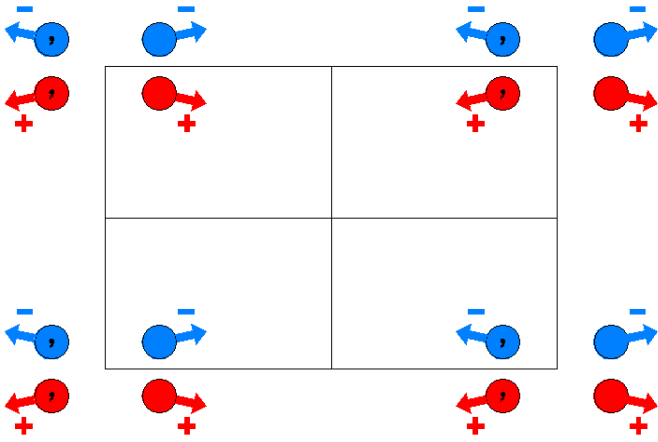
Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



P2/m'  
10.4.52

2/m'  
P12/m'1

Monoclinic



Origin at center (2/m')

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2  $0,y,0$   
( $2_y$ |0,0,0)

(3)  $\bar{1}$   $0,0,0$   
( $\bar{1}$ |0,0,0)'

(4)  $m'$   $x,0,z$   
( $m_y$ |0,0,0)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

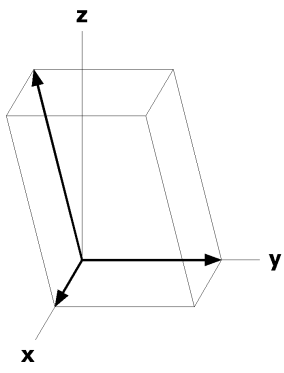
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
4	o	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) x, $\bar{y}$ ,z [u, $\bar{v}$ ,w]
2	n	m'	x,1/2,z [u,0,w]	$\bar{x},1/2,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]		
2	m	m'	x,0,z [u,0,w]	$\bar{x},0,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]		
2	l	2	1/2,y,1/2 [0,v,0]	1/2, $\bar{y}$ ,1/2 [0, $\bar{v}$ ,0]		
2	k	2	0,y,1/2 [0,v,0]	0, $\bar{y}$ ,1/2 [0, $\bar{v}$ ,0]		
2	j	2	1/2,y,0 [0,v,0]	1/2, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]		
2	i	2	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]		
1	h	2/m'	1/2,1/2,1/2 [0,0,0]			
1	g	2/m'	1/2,0,1/2 [0,0,0]			
1	f	2/m'	0,1/2,1/2 [0,0,0]			
1	e	2/m'	1/2,1/2,0 [0,0,0]			
1	d	2/m'	1/2,0,0 [0,0,0]			
1	c	2/m'	0,0,1/2 [0,0,0]			
1	b	2/m'	0,1/2,0 [0,0,0]			
1	a	2/m'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

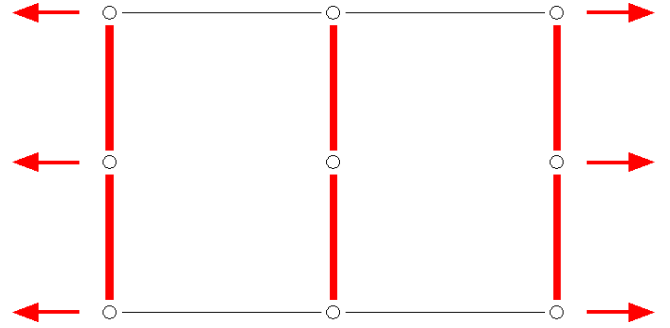
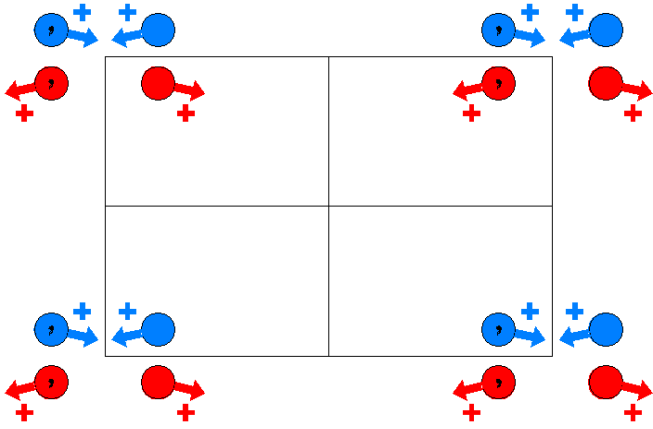
Along [0,1,0] p211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



P2'/m'  
10.5.53

2'/m'  
P12'/m'1

Monoclinic



Origin at center (2'/m')

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2' 0,y,0  
(2<sub>y</sub>|0,0,0)'

(3)  $\bar{1}$  0,0,0  
( $\bar{1}$ |0,0,0)

(4) m' x,0,z  
(m<sub>y</sub>|0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

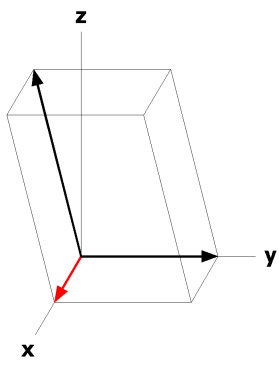
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}$ [u, $\bar{v}$ ,w]	(3) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(4) x, $\bar{y}$ ,z [u, $\bar{v}$ ,w]
4 o 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}$ [u, $\bar{v}$ ,w]	(3) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(4) x, $\bar{y}$ ,z [u, $\bar{v}$ ,w]
2 n m'	x,1/2,z [u,0,w]	$\bar{x},1/2,\bar{z}$ [u,0,w]		
2 m m'	x,0,z [u,0,w]	$\bar{x},0,\bar{z}$ [u,0,w]		
2 l 2'	1/2,y,1/2 [u,0,w]	1/2, $\bar{y}$ ,1/2 [u,0,w]		
2 k 2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ ,1/2 [u,0,w]		
2 j 2'	1/2,y,0 [u,0,w]	1/2, $\bar{y}$ ,0 [u,0,w]		
2 i 2'	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [u,0,w]		
1 h 2'/m'	1/2,1/2,1/2 [u,0,w]			
1 g 2'/m'	1/2,0,1/2 [u,0,w]			
1 f 2'/m'	0,1/2,1/2 [u,0,w]			
1 e 2'/m'	1/2,1/2,0 [u,0,w]			
1 d 2'/m'	1/2,0,0 [u,0,w]			
1 c 2'/m'	0,0,1/2 [u,0,w]			
1 b 2'/m'	0,1/2,0 [u,0,w]			
1 a 2'/m'	0,0,0 [u,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



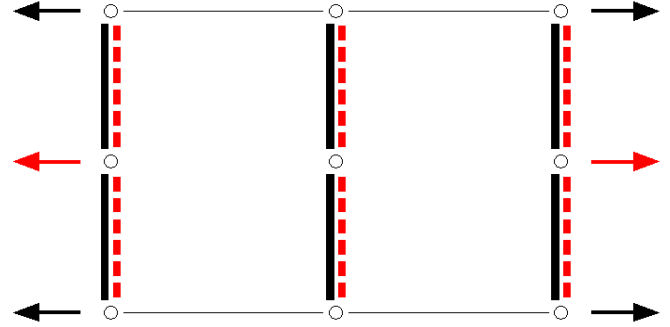
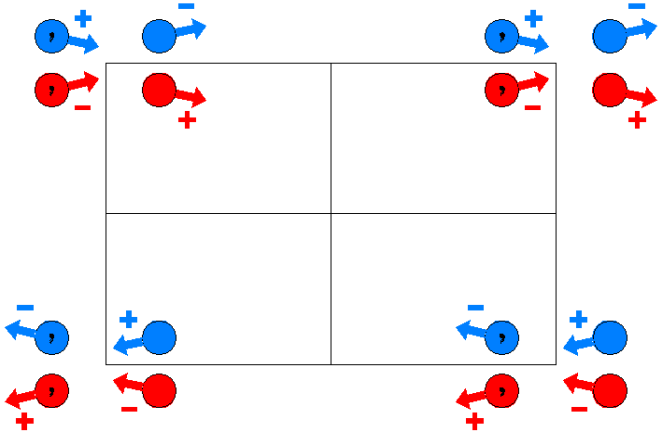
$P_{2a} 2/m$

10.6.54

$2/m1'$

$P_{2a} 12/m1$

Monoclinic



**Origin** at center ( $2/m$ )

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,y,0$   
( $2_y$ |0,0,0)

(3)  $\bar{1}$   $0,0,0$   
( $\bar{1}$ |0,0,0)

(4) m  $x,0,z$   
( $m_y$ |0,0,0)

For (0,0,0) + set

(1)  $t'$  (1,0,0)  
(1|1,0,0)'

(2)  $2'$   $1/2,y,0$   
( $2_y$ |1,0,0)'

(3)  $\bar{1}'$   $1/2,0,0$   
( $\bar{1}$ |1,0,0)'

(4)  $a'$  (1,0,0)  $x,0,z$   
( $m_y$ |1,0,0)'

**Generators selected** (1); t(1,0,0)<sup>'</sup>; t(0,1,0); t(0,0,1); (2); (3).

**Positions**

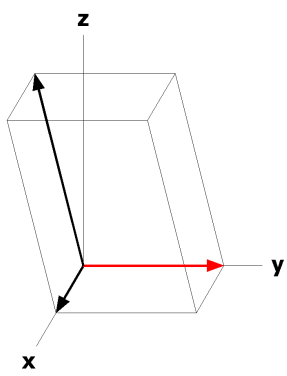
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0) <sup>'</sup> +		
8 o 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(4) x, $\bar{y}$ ,z [ $\bar{u},\bar{v},\bar{w}$ ]
4 n m	x,1/2,z [0,v,0]	$\bar{x},1/2,\bar{z}$ [0,v,0]		
4 m m	x,0,z [0,v,0]	$\bar{x},0,\bar{z}$ [0,v,0]		
4 l 2'	1/2,y,1/2 [u,0,w]	1/2, $\bar{y}$ ,1/2 [ $\bar{u},0,\bar{w}$ ]		
4 k 2	0,y,1/2 [0,v,0]	0, $\bar{y}$ ,1/2 [0,v,0]		
4 j 2'	1/2,y,0 [u,0,w]	1/2, $\bar{y}$ ,0 [ $\bar{u},0,\bar{w}$ ]		
4 i 2	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0,v,0]		
2 h 2'/m	1/2,1/2,1/2 [0,0,0]			
2 g 2'/m	1/2,0,1/2 [0,0,0]			
2 f 2/m	0,1/2,1/2 [0,v,0]			
2 e 2'/m	1/2,1/2,0 [0,0,0]			
2 d 2'/m	1/2,0,0 [0,0,0]			
2 c 2/m	0,0,1/2 [0,v,0]			
2 b 2/m	0,1/2,0 [0,v,0]			
2 a 2/m	0,0,0 [0,v,0]			

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/2,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



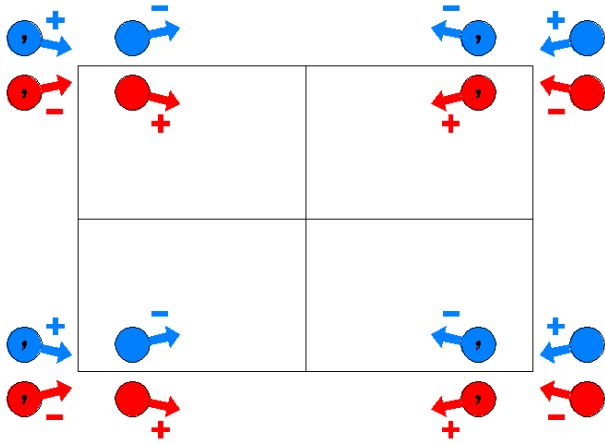
$P_{2b} 2/m$

10.7.55

$2/m1'$

$P_{2b} 12/m1$

Monoclinic



Origin at center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,y,0$   
( $2_y$ |0,0,0)

(3)  $\bar{1}$   $0,0,0$   
( $\bar{1}$ |0,0,0)

(4) m  $x,0,z$   
( $m_y$ |0,0,0)

For (0,0,0) + set

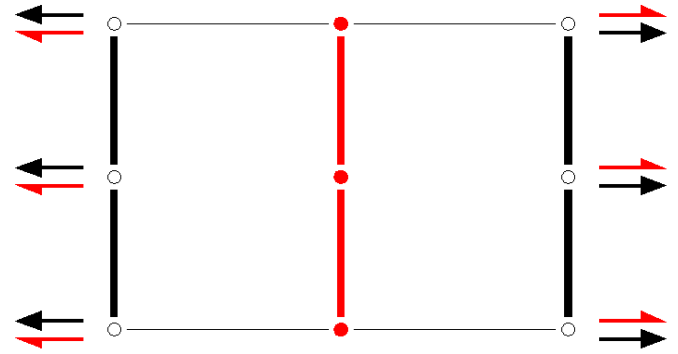
(1)  $t'$   $(0,1,0)$   
(1|0,1,0)'

(2)  $2'$   $(0,1,0) 0,y,0$   
( $2_y$ |0,1,0)'

(3)  $\bar{1}'$   $0,1/2,0$   
( $\bar{1}$ |0,1,0)'

(4)  $m'$   $x,1/2,z$   
( $m_y$ |0,1,0)'

For (0,1,0)' + set



**Generators selected** (1); t(1,0,0); t(0,1,0)'; t(0,0,1); (2); (3).

**Positions**

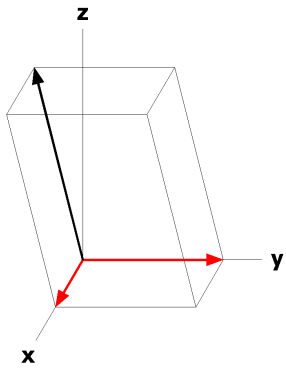
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
8 o 1	(1) x,y,z [u,v,w]	(2) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(4) x, $\bar{y}$ ,z [ $\bar{u},v,\bar{w}$ ]
4 n m'	x,1/2,z [u,0,w]	$\bar{x},1/2,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]		
4 m m	x,0,z [0,v,0]	$\bar{x},0,\bar{z}$ [0,v,0]		
4 l 2	1/2,y,1/2 [0,v,0]	1/2, $\bar{y}$ ,1/2 [0,v,0]		
4 k 2	0,y,1/2 [0,v,0]	0, $\bar{y}$ ,1/2 [0,v,0]		
4 j 2	1/2,y,0 [0,v,0]	1/2, $\bar{y}$ ,0 [0,v,0]		
4 i 2	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0,v,0]		
2 h 2/m'	1/2,1/2,1/2 [0,0,0]			
2 g 2/m	1/2,0,1/2 [0,v,0]			
2 f 2/m'	0,1/2,1/2 [0,0,0]			
2 e 2/m'	1/2,1/2,0 [0,0,0]			
2 d 2/m	1/2,0,0 [0,v,0]			
2 c 2/m	0,0,1/2 [0,v,0]			
2 b 2/m'	0,1/2,0 [0,0,0]			
2 a 2/m	0,0,0 [0,v,0]			

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,1/2,z

Along [1,0,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,1/2,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



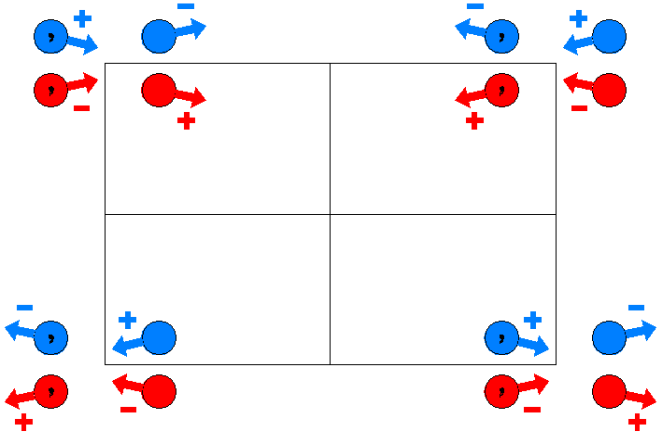
$P_C 2/m$

10.8.56

$2/m1'$

$P_C 12/m1$

Monoclinic



Origin at center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,y,0$   
( $2_y$ |0,0,0)

(3)  $\bar{1}$   $0,0,0$   
( $\bar{1}$ |0,0,0)

(4) m  $x,0,z$   
( $m_y$ |0,0,0)

For (0,0,0) + set

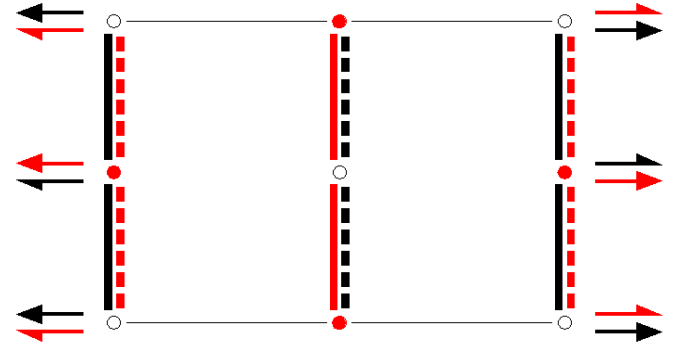
(1)  $t'$  (1,0,0)  
(1|1,0,0)'

(2)  $2'$   $1/2,y,0$   
( $2_y$ |1,0,0)'

(3)  $\bar{1}'$   $1/2,0,0$   
( $\bar{1}$ |1,0,0)'

(4)  $a'$  (1,0,0)  $x,0,z$   
( $m_y$ |1,0,0)'

For (1,0,0)' + set





**Generators selected** (1); t(1,0,0)<sup>'</sup>; t(0,1,0)<sup>'</sup>; t(0,0,1); (2); (3).

**Positions**

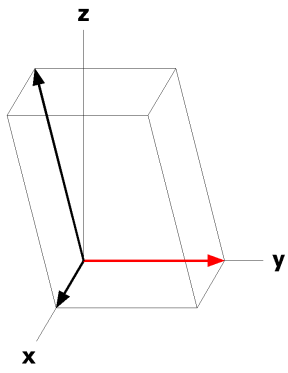
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1,0,0) <sup>'</sup> +		
8	o	1	(1) x,y,z [u,v,w]	(2) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(4) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]
4	n	m'	x,1/2,z [u,0,w]	$\bar{x},1/2,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]		
4	m	m	x,0,z [0,v,0]	$\bar{x},0,\bar{z}$ [0,v,0]		
4	l	2'	1/2,y,1/2 [u,0,w]	1/2, $\bar{y},1/2$ [ $\bar{u},0,\bar{w}$ ]		
4	k	2	0,y,1/2 [0,v,0]	0, $\bar{y},1/2$ [0,v,0]		
4	j	2'	1/2,y,0 [u,0,w]	1/2, $\bar{y},0$ [ $\bar{u},0,\bar{w}$ ]		
4	i	2	0,y,0 [0,v,0]	0, $\bar{y},0$ [0,v,0]		
2	h	2'/m'	1/2,1/2,1/2 [u,0,w]			
2	g	2'/m	1/2,0,1/2 [0,0,0]			
2	f	2/m'	0,1/2,1/2 [0,0,0]			
2	e	2'/m'	1/2,1/2,0 [u,0,w]			
2	d	2'/m	1/2,0,0 [0,0,0]			
2	c	2/m	0,0,1/2 [0,v,0]			
2	b	2/m'	0,1/2,0 [0,0,0]			
2	a	2/m	0,0,0 [0,v,0]			

**Symmetry of Special Projections**

Along [0,0,1] p<sub>c</sub>2mm  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/2,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



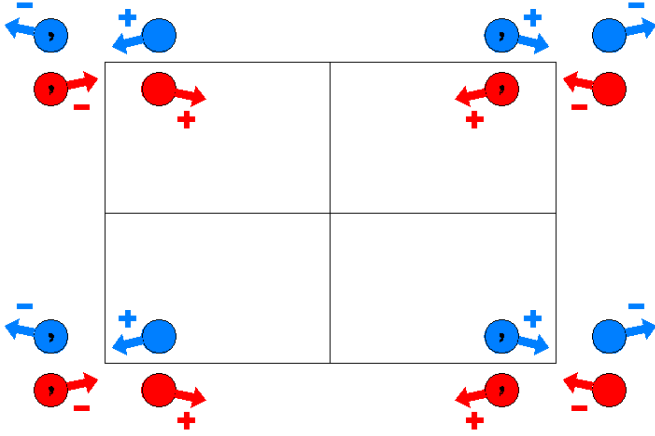
$P_{2b} 2'/m$

10.9.57

$2/m1'$

$P_{2b} 12'/m1$

Monoclinic



Origin at center ( $2'/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2)  $2'$   $0,y,0$   
( $2_y$ |0,0,0)'

(3)  $\bar{1}'$   $0,0,0$   
( $\bar{1}$ |0,0,0)'

(4)  $m$   $x,0,z$   
( $m_y$ |0,0,0)

For (0,0,0) + set

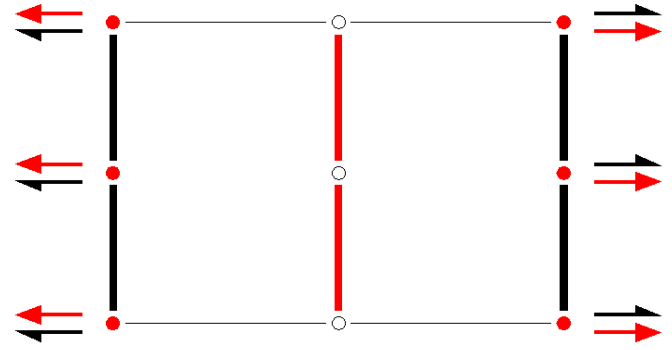
For (0,1,0)' + set

(1)  $t'$  (0,1,0)  
(1|0,1,0)'

(2) 2 (0,1,0)  $0,y,0$   
( $2_y$ |0,1,0)

(3)  $\bar{1}$   $0,1/2,0$   
( $\bar{1}$ |0,1,0)

(4)  $m'$   $x,1/2,z$   
( $m_y$ |0,1,0)'



**Generators selected** (1); t(1,0,0); t(0,1,0)'; t(0,0,1); (2); (3).

**Positions**

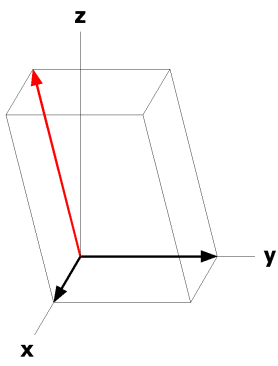
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
8 o 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}$ [u, $\bar{v}$ ,w]	(3) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) x, $\bar{y}$ ,z [ $\bar{u},v,\bar{w}$ ]
4 n m'	x,1/2,z [u,0,w]	$\bar{x},1/2,\bar{z}$ [u,0,w]		
4 m m	x,0,z [0,v,0]	$\bar{x},0,\bar{z}$ [0, $\bar{v}$ ,0]		
4 l 2'	1/2,y,1/2 [u,0,w]	1/2, $\bar{y}$ ,1/2 [ $\bar{u},0,\bar{w}$ ]		
4 k 2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ ,1/2 [ $\bar{u},0,\bar{w}$ ]		
4 j 2'	1/2,y,0 [u,0,w]	1/2, $\bar{y}$ ,0 [ $\bar{u},0,\bar{w}$ ]		
4 i 2'	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [ $\bar{u},0,\bar{w}$ ]		
2 h 2'/m'	1/2,1/2,1/2 [u,0,w]			
2 g 2'/m	1/2,0,1/2 [0,0,0]			
2 f 2'/m'	0,1/2,1/2 [u,0,w]			
2 e 2'/m'	1/2,1/2,0 [u,0,w]			
2 d 2'/m	1/2,0,0 0,0,0]			
2 c 2'/m	0,0,1/2 [0,0,0]			
2 b 2'/m'	0,1/2,0 [u,0,w]			
2 a 2'/m	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,1/2,z

Along [1,0,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,1/2,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



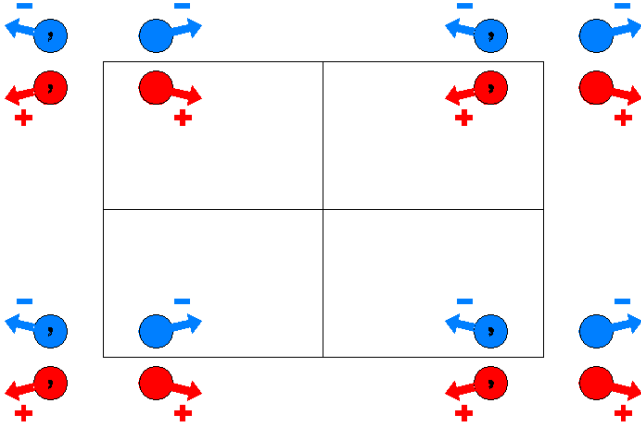
$P_{2c} 2/m'$

10.10.58

$2/m1'$

$P_{2c} 12/m'1$

Monoclinic



Origin at center ( $2/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2)  $2 \quad 0,y,0$   
( $2_y$ |0,0,0)

(3)  $\bar{1}' \quad 0,0,0$   
( $\bar{1}$ |0,0,0)'

(4)  $m' \quad x,0,z$   
( $m_y$ |0,0,0)'

For (0,0,0) + set

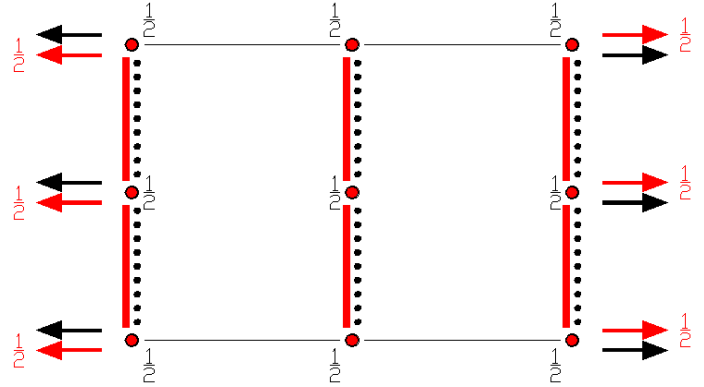
For (0,0,1)' + set

(1)  $t' \quad (0,0,1)$   
(1|0,0,1)'

(2)  $2' \quad 0,y,1/2$   
( $2_y$ |0,0,1)'

(3)  $\bar{1} \quad 0,0,1/2$   
( $\bar{1}$ |0,0,1)

(4)  $c \quad (0,0,1) \quad x,0,z$   
( $m_y$ |0,0,1)



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

**Positions**

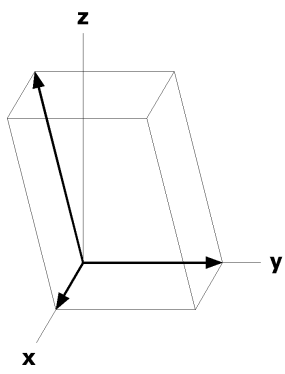
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
8 o 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) x, $\bar{y}$ ,z [u, $\bar{v}$ ,w]
4 n m'	x,1/2,z [u,0,w]	$\bar{x},1/2,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]		
4 m m'	x,0,z [u,0,w]	$\bar{x},0,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]		
4 l 2'	1/2,y,1/2 [u,0,w]	1/2, $\bar{y}$ ,1/2 [u,0,w]		
4 k 2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ ,1/2 [u,0,w]		
4 j 2	1/2,y,0 [0,v,0]	1/2, $\bar{y}$ ,0 [0,v,0]		
4 i 2	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0,v,0]		
2 h 2'/m'	1/2,1/2,1/2 [u,0,w]			
2 g 2'/m'	1/2,0,1/2 [u,0,w]			
2 f 2'/m'	0,1/2,1/2 [u,0,w]			
2 e 2/m'	1/2,1/2,0 [0,0,0]			
2 d 2/m'	1/2,0,0 [0,0,0]			
2 c 2'/m'	0,0,1/2 [u,0,w]			
2 b 2/m'	0,1/2,0 [0,0,0]			
2 a 2/m'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



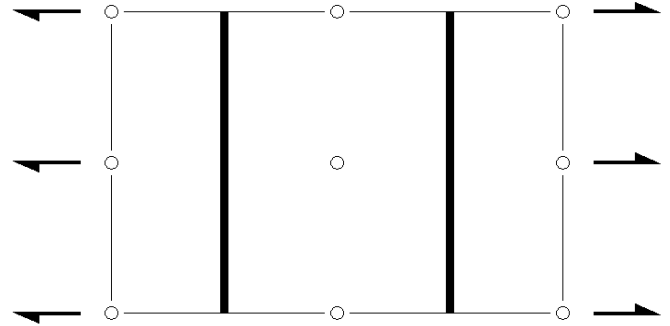
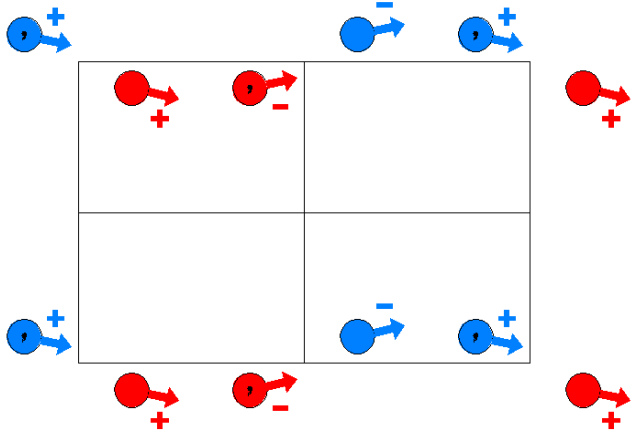
$P2_1/m$

11.1.59

$2/m$

$P12_1/m1$

Monoclinic



Origin at  $\bar{1}$  on 2,

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 (0,1/2,0) 0,y,0  
(2<sub>y</sub>|0,1/2,0)

(3)  $\bar{1}$  0,0,0  
( $\bar{1}$ |0,0,0)

(4) m x,1/4,z  
(m<sub>y</sub>|0,1/2,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

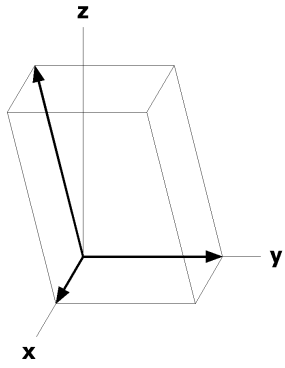
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
4	f	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, y+1/2, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(3) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(4) x, $\bar{y}+1/2, z$ [ $\bar{u}, v, \bar{w}$ ]
2	e	m	x, 1/4, z [0,v,0]	$\bar{x}, 3/4, \bar{z}$ [0,v,0]		
2	d	$\bar{1}$	1/2, 0, 1/2 [u,v,w]	1/2, 1/2, 1/2 [ $\bar{u}, v, \bar{w}$ ]		
2	c	$\bar{1}$	0, 0, 1/2 [u,v,w]	0, 1/2, 1/2 [ $\bar{u}, v, \bar{w}$ ]		
2	b	$\bar{1}$	1/2, 0, 0 [u,v,w]	1/2, 1/2, 0 [ $\bar{u}, v, \bar{w}$ ]		
2	a	$\bar{1}$	0, 0, 0 [u,v,w]	0, 1/2, 0 [ $\bar{u}, v, \bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2'mg'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



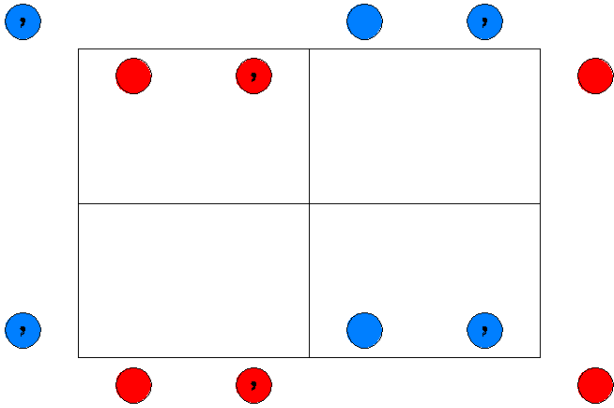
$P2_1/m1'$

11.2.60

$2/m1'$

$P12_1/m11'$

Monoclinic



Origin at  $\bar{1}1'$  on  $2_11'$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

**Symmetry Operations**

(1)  $1$   
( $1|0,0,0$ )

(2)  $2$  ( $0,1/2,0$ )  $0,y,0$   
( $2_y|0,1/2,0$ )

(3)  $\bar{1}$   $0,0,0$   
( $\bar{1}|0,0,0$ )

(4)  $m$   $x,1/4,z$   
( $m_y|0,1/2,0$ )

For  $1 + \text{set}$

(1)  $1'$   
( $1|0,0,0$ )'

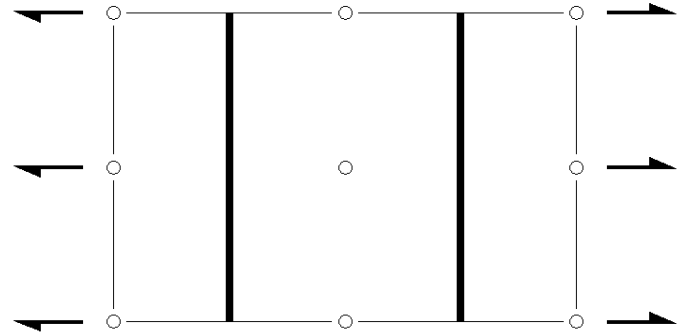
(2)  $2'$  ( $0,1/2,0$ )  $0,y,0$   
( $2_y|0,1/2,0$ )'

(3)  $\bar{1}'$   $0,0,0$   
( $\bar{1}'|0,0,0$ )'

(4)  $m'$   $x,1/4,z$   
( $m_y|0,1/2,0$ )'

For  $1' + \text{set}$

**1'**





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

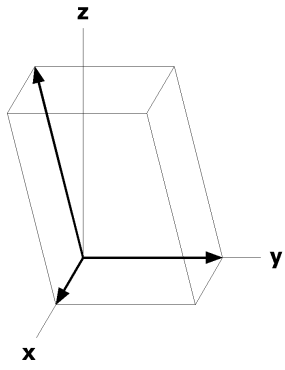
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
4 f 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, y+1/2, \bar{z}$ [0,0,0]	(3) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]	(4) x, $\bar{y}+1/2, z$ [0,0,0]
2 e m1'	x, 1/4, z [0,0,0]	$\bar{x}, 3/4, \bar{z}$ [0,0,0]		
2 d $\bar{1}1'$	1/2, 0, 1/2 [0,0,0]	1/2, 1/2, 1/2 [0,0,0]		
2 c $\bar{1}1'$	0, 0, 1/2 [0,0,0]	0, 1/2, 1/2 [0,0,0]		
2 b $\bar{1}1'$	1/2, 0, 0 [0,0,0]	1/2, 1/2, 0 [0,0,0]		
2 a $\bar{1}1'$	0, 0, 0 [0,0,0]	0, 1/2, 0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mg1'  
 $\mathbf{a}^* = -\mathbf{b} \quad \mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



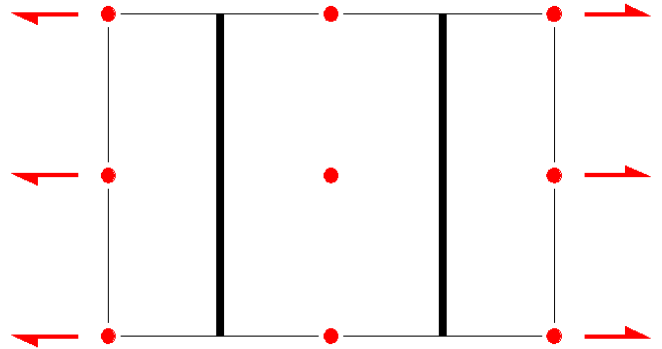
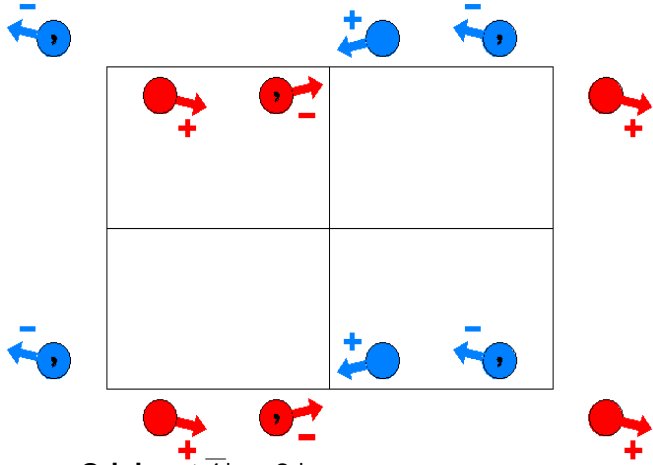
$P2_1/m$

$2'/m$

Monoclinic

11.3.61

$P12_1/m1$



Origin at  $\bar{1}'$  on  $2_1'$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

**Symmetry Operations**

(1)  $1$   
( $1|0,0,0$ )

(2)  $2'$  ( $0,1/2,0$ )  $0,y,0$   
( $2_y|0,1/2,0$ )'

(3)  $\bar{1}'$   $0,0,0$   
( $\bar{1}'|0,0,0$ )'

(4)  $m$   $x,1/4,z$   
( $m_y|0,1/2,0$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

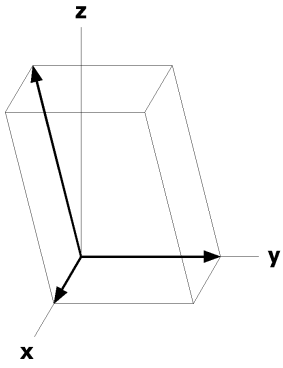
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
4	f	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, y+1/2, \bar{z}$ [u, $\bar{v}$ , w]	(3) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(4) x, $\bar{y}+1/2, z$ [ $\bar{u}, v, \bar{w}$ ]
2	e	m	x, 1/4, z [0,v,0]	$\bar{x}, 3/4, \bar{z}$ [0, $\bar{v}$ , 0]		
2	d	$\bar{1}'$	1/2, 0, 1/2 [0,0,0]	1/2, 1/2, 1/2 [0,0,0]		
2	c	$\bar{1}'$	0, 0, 1/2 [0,0,0]	0, 1/2, 1/2 [0,0,0]		
2	b	$\bar{1}'$	1/2, 0, 0 [0,0,0]	1/2, 1/2, 0 [0,0,0]		
2	a	$\bar{1}'$	0, 0, 0 [0,0,0]	0, 1/2, 0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mg  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



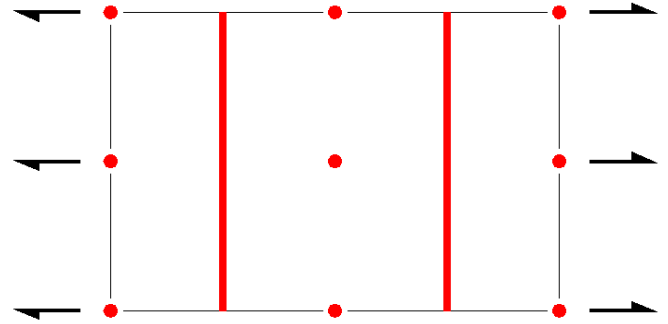
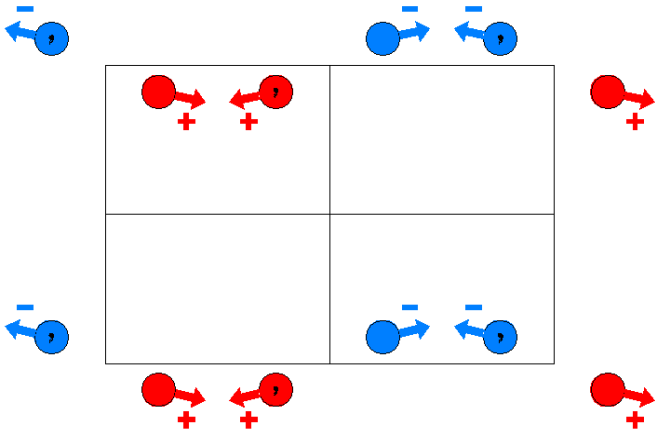
$P2_1/m'$

11.4.62

$2/m'$

$P12_1/m'1$

Monoclinic



Origin at  $\bar{1}'$  on  $2_1$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 (0,1/2,0) 0,y,0  
(2<sub>y</sub>|0,1/2,0)

(3)  $\bar{1}'$  0,0,0  
( $\bar{1}'$ |0,0,0)'

(4)  $m'$  x,1/4,z  
( $m_y$ |0,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

### Positions

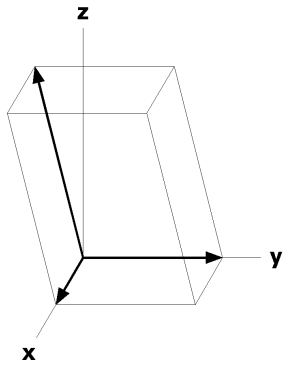
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
4	f	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, y+1/2, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(3) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(4) x, $\bar{y}+1/2, z$ [u, $\bar{v}, w$ ]
2	e	m'	x, 1/4, z [u, 0, w]	$\bar{x}, 3/4, \bar{z}$ [ $\bar{u}, 0, \bar{w}$ ]		
2	d	$\bar{1}'$	1/2, 0, 1/2 [0, 0, 0]	1/2, 1/2, 1/2 [0, 0, 0]		
2	c	$\bar{1}'$	0, 0, 1/2 [0, 0, 0]	0, 1/2, 1/2 [0, 0, 0]		
2	b	$\bar{1}'$	1/2, 0, 0 [0, 0, 0]	1/2, 1/2, 0 [0, 0, 0]		
2	a	$\bar{1}'$	0, 0, 0 [0, 0, 0]	0, 1/2, 0 [0, 0, 0]		

### Symmetry of Special Projections

Along [0,0,1] p2m'g'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



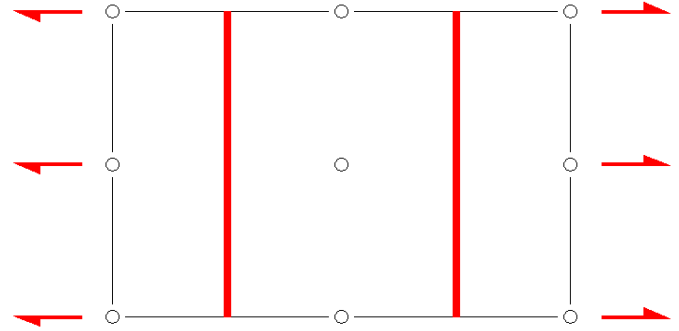
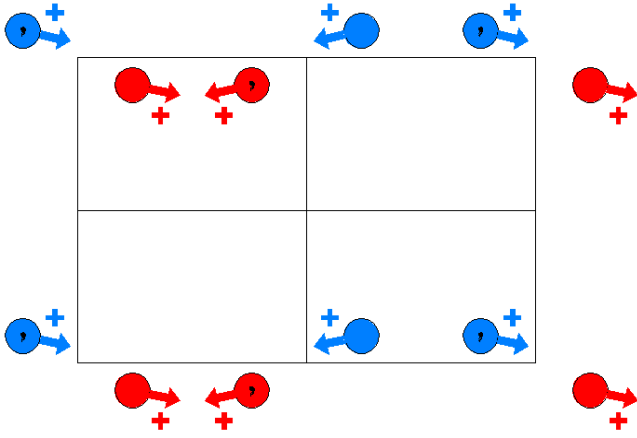
$P2_1/m'$

11.5.63

$2'/m'$

$P12_1'/m'1$

Monoclinic



Origin at  $\bar{1}$  on  $2_1'$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

**Symmetry Operations**

(1)  $1$   
( $1|0,0,0$ )

(2)  $2'$  ( $0,1/2,0$ )  $0,y,0$   
( $2_y|0,1/2,0$ )'

(3)  $\bar{1}$   $0,0,0$   
( $\bar{1}|0,0,0$ )

(4)  $m'$   $x,1/4,z$   
( $m_y|0,1/2,0$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

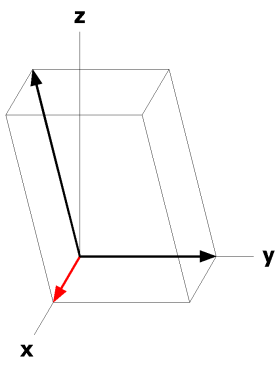
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
4	f	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, y+1/2, \bar{z}$ [u, $\bar{v}$ , w]	(3) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(4) x, $\bar{y}+1/2, z$ [u, $\bar{v}$ , w]
2	e	m'	x, 1/4, z [u,0,w]	$\bar{x}, 3/4, \bar{z}$ [u,0,w]		
2	d	$\bar{1}$	1/2,0,1/2 [u,v,w]	1/2,1/2,1/2 [u, $\bar{v}$ , w]		
2	c	$\bar{1}$	0,0,1/2 [u,v,w]	0,1/2,1/2 [u, $\bar{v}$ , w]		
2	b	$\bar{1}$	1/2,0,0 [u,v,w]	1/2,1/2,0 [u, $\bar{v}$ , w]		
2	a	$\bar{1}$	0,0,0 [u,v,w]	0,1/2,0 [u, $\bar{v}$ , w]		

**Symmetry of Special Projections**

Along [0,0,1] p2'm'g  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



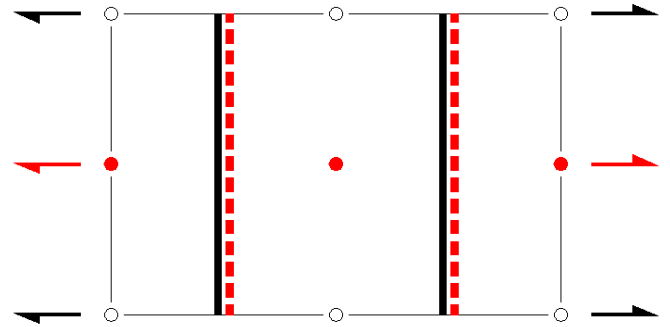
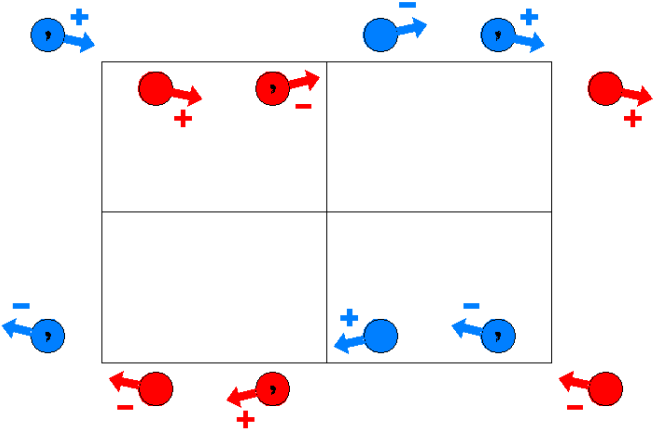
$P_{2a}2_1/m$

11.6.64

$2/m$

$P_{2a}12_1/m1$

Monoclinic



Origin at  $\bar{1}$  on  $2_1$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $(0,1/2,0)$   $0,y,0$   
( $2_y$ | $0,1/2,0$ )

(3)  $\bar{1}$   $0,0,0$   
( $\bar{1}$ | $0,0,0$ )

(4) m  $x,1/4,z$   
( $m_y$ | $0,1/2,0$ )

For  $(1,0,0)'$  + set

(1)  $t'$   $(1,0,0)$   
(1| $1,0,0$ )'

(2)  $2'$   $(0,1/2,0)$   $1/2,y,0$   
( $2_y$ | $1,1/2,0$ )'

(3)  $\bar{1}'$   $1/2,0,0$   
( $\bar{1}$ | $1,0,0$ )'

(4)  $a'$   $(1,0,0)$   $x,1/4,z$   
( $m_y$ | $1,1/2,0$ )'



**Generators selected** (1);  $t(1,0,0)'$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3).

**Positions**

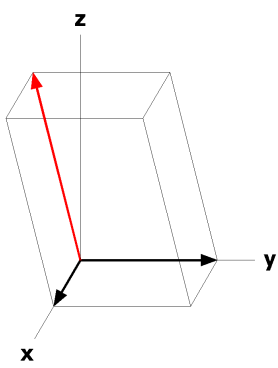
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1,0,0)' +		
8	f	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(4) $x,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]
4	e	m	$x,1/4,z$ [0,v,0]	$\bar{x},3/4,\bar{z}$ [0,v,0]		
4	d	$\bar{1}'$	$1/2,0,1/2$ [0,0,0]	$1/2,1/2,1/2$ [0,0,0]		
4	c	$\bar{1}$	$0,0,1/2$ [u,v,w]	$0,1/2,1/2$ [ $\bar{u},v,\bar{w}$ ]		
4	b	$\bar{1}'$	$1/2,0,0$ [0,0,0]	$1/2,1/2,0$ [0,0,0]		
4	a	$\bar{1}$	$0,0,0$ [u,v,w]	$0,1/2,0$ [ $\bar{u},v,\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2b}2mg$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0]  $p2mg1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0]  $p2111'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



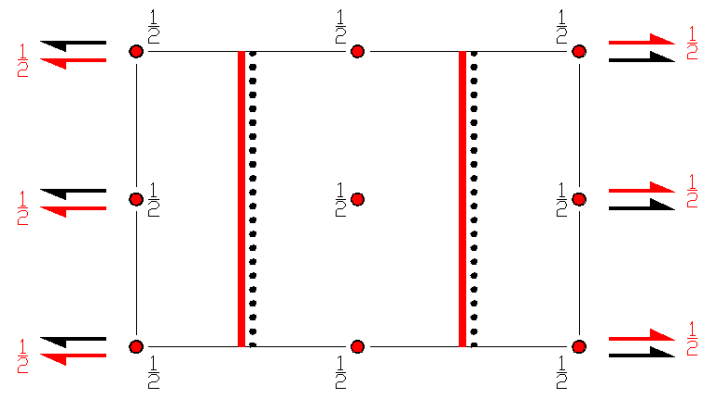
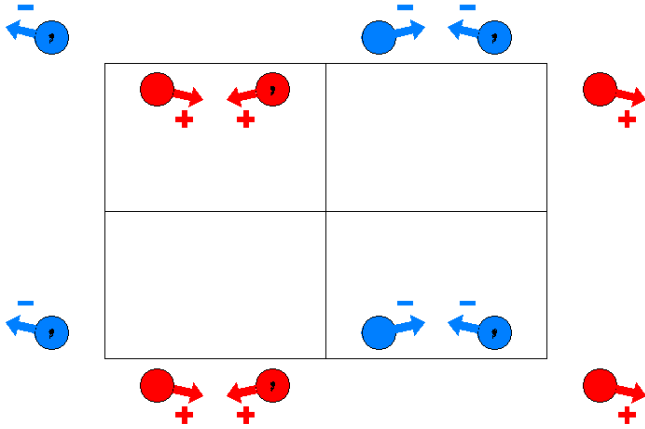
$P_{2c}2_1/m'$

11.7.65

$2/m1'$

$P_{2c}12_1/m'1$

Monoclinic



Origin at  $\bar{1}'$  on  $2_1$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0)$  + set

(1)  $1$   
 $(1|0,0,0)$

(2)  $2$   $(0,1/2,0)$   $0,y,0$   
 $(2_y|0,1/2,0)$

(3)  $\bar{1}'$   $0,0,0$   
 $(\bar{1}'|0,0,0)'$

(4)  $m'$   $x,1/4,z$   
 $(m_y|0,1/2,0)'$

For  $(0,0,1)'$  + set

(1)  $t'$   $(0,0,1)$   
 $(1|0,0,1)'$

(2)  $2'$   $(0,1/2,0)$   $0,y,1/2$   
 $(2_y|0,1/2,1)'$

(3)  $\bar{1}$   $0,0,1/2$   
 $(\bar{1}|0,0,1)$

(4)  $c$   $(0,0,1)$   $x,1/4,z$   
 $(m_y|0,1/2,1)$

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ '; (2); (3).

**Positions**

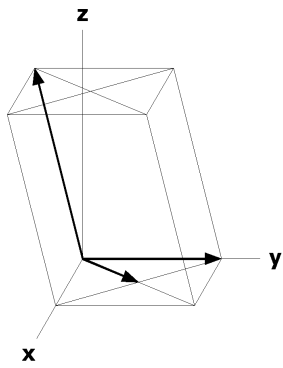
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +		(0,0,1)' +	
8	f	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) $x,\bar{y}+1/2,z$ [ $u,\bar{v},w$ ]
4	e	$m'$	$x,1/4,z$ [u,0,w]	$\bar{x},3/4,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]		
4	d	$\bar{1}$	$1/2,0,1/2$ [u,v,w]	$1/2,1/2,1/2$ [ $u,\bar{v},w$ ]		
4	c	$\bar{1}$	$0,0,1/2$ [u,v,w]	$0,1/2,1/2$ [ $u,\bar{v},w$ ]		
4	b	$\bar{1}'$	$1/2,0,0$ [0,0,0]	$1/2,1/2,0$ [0,0,0]		
4	a	$\bar{1}'$	$0,0,0$ [0,0,0]	$0,1/2,0$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p2mg1'$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b}2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a}211$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



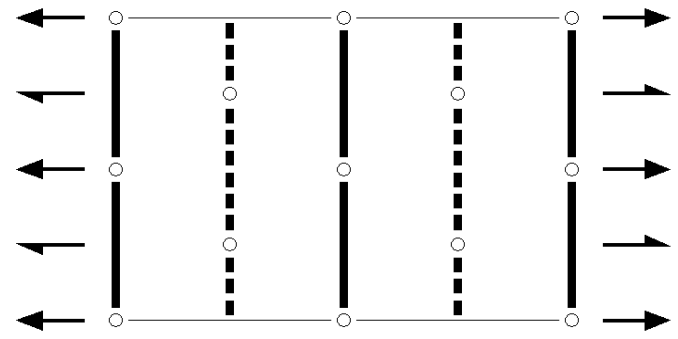
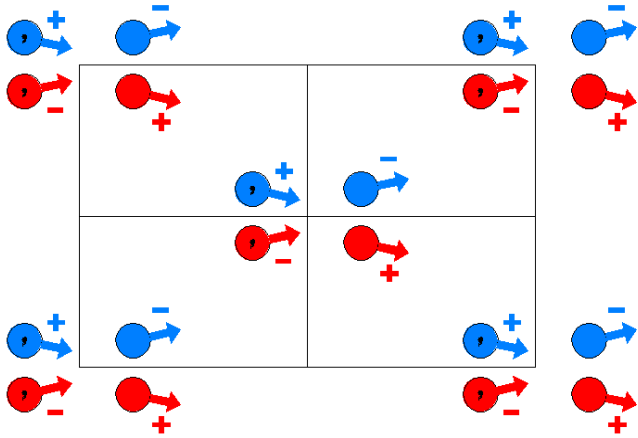
C2/m

2/m

Monoclinic

12.1.66

C12/m1



Origin at center ( 2/m )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- (1) 1  $(1|0,0,0)$
- (2) 2  $(2_y|0,0,0)$
- (3)  $\bar{1}$   $(\bar{1}|0,0,0)$
- (4) m  $(m_x|0,0,0)$

For (1/2,1/2,0) + set

- (1) t  $(1|1/2,1/2,0)$
- (2) 2  $(2_y|1/2,1/2,0)$
- (3)  $\bar{1}$   $(\bar{1}|1/2,1/2,0)$
- (4) a  $(a_x|1/2,0,0)$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

**Positions**

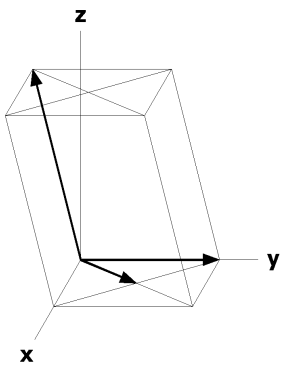
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
8 j 1	(1) x,y,z [u,v,w]	(2) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(4) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]
4 i m	x,0,z [0,v,0]	$\bar{x},0,\bar{z}$ [0,v,0]		
4 h 2	0,y,1/2 [0,v,0]	0, $\bar{y}$ ,1/2 [0,v,0]		
4 g 2	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0,v,0]		
4 f $\bar{1}$	1/4,1/4,1/2 [u,v,w]	3/4,1/4,1/2 [ $\bar{u},v,\bar{w}$ ]		
4 e $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,1/4,0 [ $\bar{u},v,\bar{w}$ ]		
2 d 2/m	0,1/2,1/2 [0,v,0]			
2 c 2/m	0,0,1/2 [0,v,0]			
2 b 2/m	0,1/2,0 [0,v,0]			
2 a 2/m	0,0,0 [0,v,0]			

**Symmetry of Special Projections**

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



C2/m1'

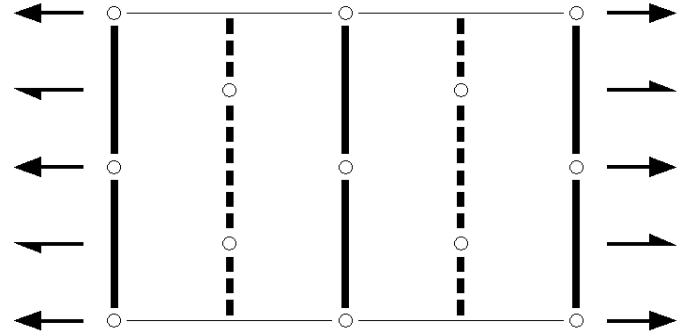
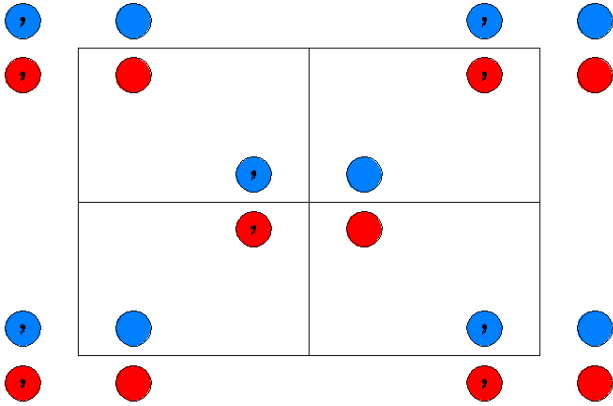
12.2.67

2/m1'

C12/m11'

Monoclinic

1'



Origin at center (2/m1')

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

- |                    |   |  |   |
|--------------------|---|--|---|
| (1) 1<br>(1 0,0,0) | (2) 2 <sub>y</sub> 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (3) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (4) m <sub>x</sub> x,0,z<br>(m <sub>x</sub>  0,0,0) |
|--------------------|---|--|---|

For (1/2,1/2,0) + set

- |                                    |   |  |  |
|------------------------------------|---|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) 2 <sub>y</sub> (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (3) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (4) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) |
|------------------------------------|---|--|--|

For (0,0,0)' + set

- |                      |  |  |  |
|----------------------|--|--|--|
| (1) 1'<br>(1 0,0,0)' | (2) 2' <sub>y</sub> 0,y,0<br>(2' <sub>y</sub>  0,0,0)' | (3) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$ ' 0,0,0)' | (4) m' <sub>x</sub> x,0,z<br>(m' <sub>x</sub>  0,0,0)' |
|----------------------|--|--|--|

For (1/2,1/2,0)' + set

- |                                      |  |  |   |
|--------------------------------------|--|--|---|
| (1) t' (1/2,1/2,0)<br>(1 1/2,1/2,0)' | (2) 2' <sub>y</sub> (0,1/2,0) 1/4,y,0<br>(2' <sub>y</sub>  1/2,1/2,0)' | (3) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$ ' 1/2,1/2,0)' | (4) a' (1/2,0,0) x,1/4,z<br>(m' <sub>y</sub>  1/2,1/2,0)' |
|--------------------------------------|--|--|---|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); 1'.

### Positions

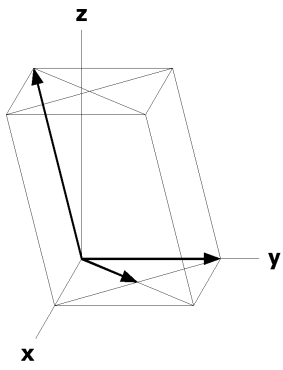
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,0)' +	(1/2,1/2,0) + (1/2,1/2,0)' +	
8 j 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(3) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(4) x, $\bar{y}$ ,z [0,0,0]
4 i m1'	x,0,z [0,0,0]	$\bar{x},0,\bar{z}$ [0,0,0]		
4 h 21'	0,y,1/2 [0,0,0]	0, $\bar{y}$ ,1/2 [0,0,0]		
4 g 21'	0,y,0 [0,0,0]	0, $\bar{y}$ ,0 [0,0,0]		
4 f $\bar{1}1'$	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 e $\bar{1}1'$	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
2 d 2/m1'	0,1/2,1/2 [0,0,0]			
2 c 2/m1'	0,0,1/2 [0,0,0]			
2 b 2/m1'	0,1/2,0 [0,0,0]			
2 a 2/m1'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

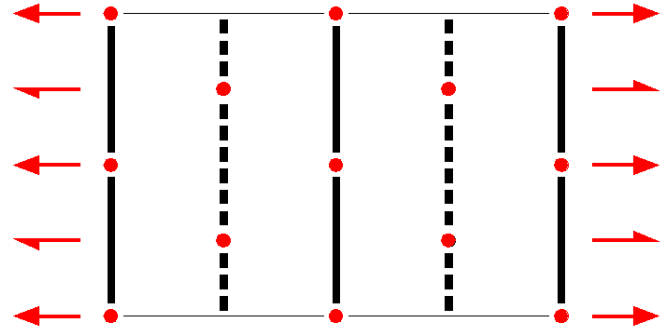
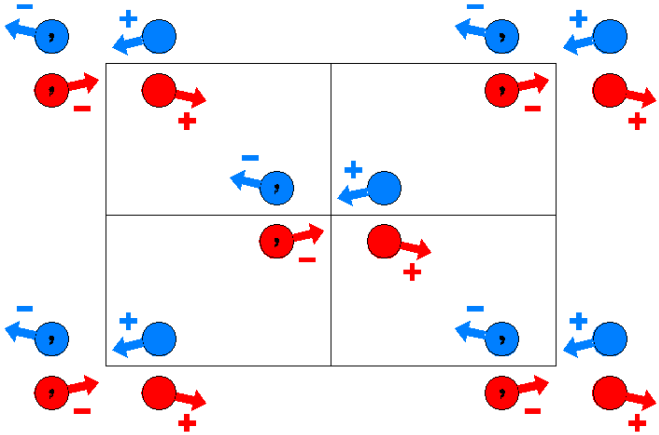
Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



C2'/m  
12.3.68

2'/m  
C12'/m1

Monoclinic



Origin at center (2'/m)

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2' 0,y,0  
(2<sub>y</sub>|0,0,0)'

(3)  $\bar{1}$ ' 0,0,0  
( $\bar{1}$ |0,0,0)'

(4) m x,0,z  
(m<sub>y</sub>|0,0,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)

(2) 2' (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)'

(3)  $\bar{1}$ ' 1/4,1/4,0  
( $\bar{1}$ |1/2,1/2,0)'

(4) a (1/2,0,0) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,0)



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

**Positions**

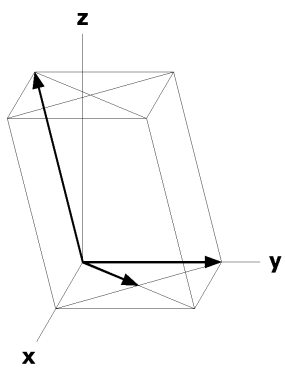
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
8 j 1	(1) x,y,z [u,v,w]	(2) $\bar{x},y,\bar{z}$ [u, $\bar{v}$ ,w]	(3) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) x, $\bar{y}$ ,z [ $\bar{u},v,\bar{w}$ ]
4 i m	x,0,z [0,v,0]	$\bar{x},0,\bar{z}$ [0, $\bar{v}$ ,0]		
4 h 2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ ,1/2 [ $\bar{u}$ ,0, $\bar{w}$ ]		
4 g 2'	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [ $\bar{u}$ ,0, $\bar{w}$ ]		
4 f $\bar{1}'$	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 e $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
2 d 2'/m	0,1/2,1/2 [0,0,0]			
2 c 2'/m	0,0,1/2 [0,0,0]			
2 b 2'/m	0,1/2,0 [0,0,0]			
2 a 2'/m	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



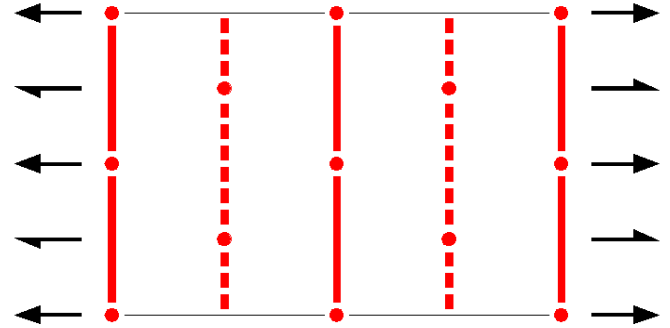
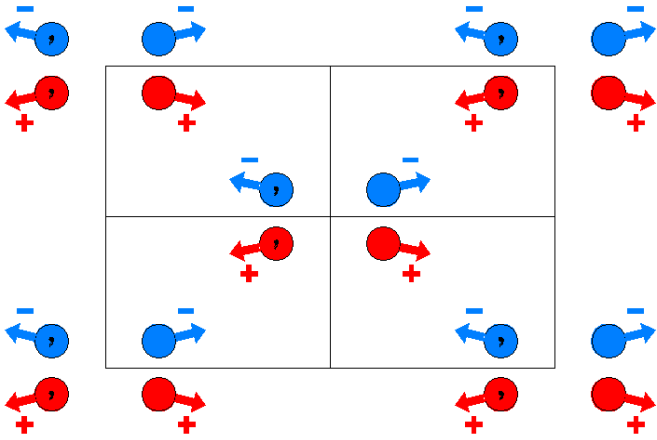
C2/m'

12.4.69

2/m'

C12/m'1

Monoclinic



Origin at center (2/m')

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2 0,y,0  
(2<sub>y</sub>|0,0,0)

(3)  $\bar{1}$ ' 0,0,0  
( $\bar{1}$ |0,0,0)'

(4) m' x,0,z  
(m<sub>y</sub>|0,0,0)'

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)

(2) 2 (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)

(3)  $\bar{1}$ ' 1/4,1/4,0  
( $\bar{1}$ |1/2,1/2,0)'

(4) a' (1/2,0,0) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

**Positions**

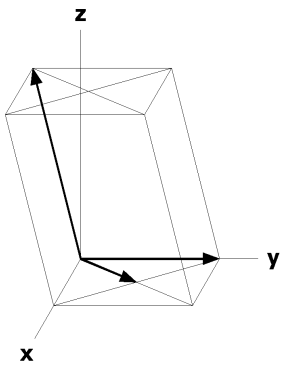
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
8 j 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) x, $\bar{y}$ ,z [u, $\bar{v}$ ,w]
4 i m'	x,0,z [u,0,w]	$\bar{x},0,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]		
4 h 2	0,y,1/2 [0,v,0]	0, $\bar{y}$ ,1/2 [0, $\bar{v}$ ,0]		
4 g 2	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]		
4 f $\bar{1}'$	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 e $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
2 d 2/m'	0,1/2,1/2 [0,0,0]			
2 c 2/m'	0,0,1/2 [0,0,0]			
2 b 2/m'	0,1/2,0 [0,0,0]			
2 a 2/m'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



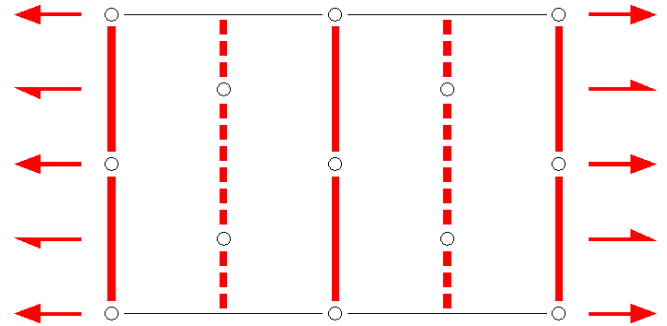
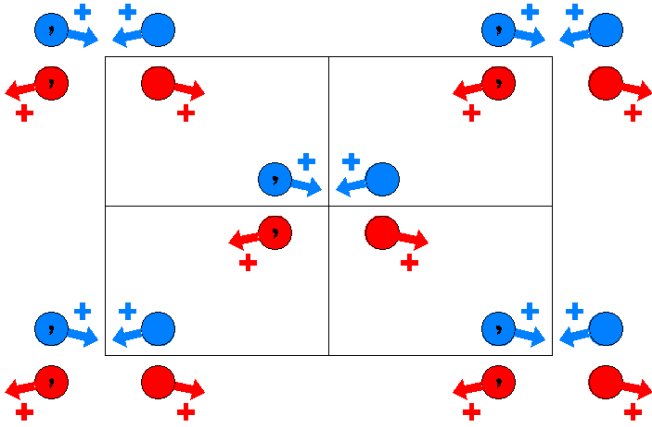
C2'/m'

12.5.70

2'/m'

C12'/m'1

Monoclinic



Origin at center (2'/m')

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2' 0,y,0  
(2<sub>y</sub>|0,0,0)'

(3)  $\bar{1}$  0,0,0  
( $\bar{1}$ |0,0,0)

(4) m' x,0,z  
(m<sub>y</sub>|0,0,0)'

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)

(2) 2' (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)'

(3)  $\bar{1}$  1/4,1/4,0  
( $\bar{1}$ |1/2,1/2,0)

(4) a' (1/2,0,0) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

**Positions**

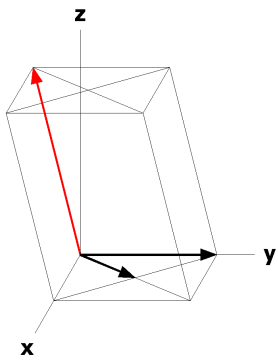
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
8 j 1	(1) x,y,z [u,v,w]	(2) $\bar{x},y,\bar{z}$ [u, $\bar{v}$ ,w]	(3) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(4) x, $\bar{y}$ ,z [u, $\bar{v}$ ,w]
4 i m'	x,0,z [u,0,w]	$\bar{x},0,\bar{z}$ [u,0,w]		
4 h 2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ ,1/2 [u,0,w]		
4 g 2'	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [u,0,w]		
4 f $\bar{1}$	1/4,1/4,1/2 [u,v,w]	3/4,1/4,1/2 [u, $\bar{v}$ ,w]		
4 e $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,1/4,0 [u, $\bar{v}$ ,w]		
2 d 2'/m'	0,1/2,1/2 [u,0,w]			
2 c 2'/m'	0,0,1/2 [u,0,w]			
2 b 2'/m'	0,1/2,0 [u,0,w]			
2 a 2'/m'	0,0,0 [u,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



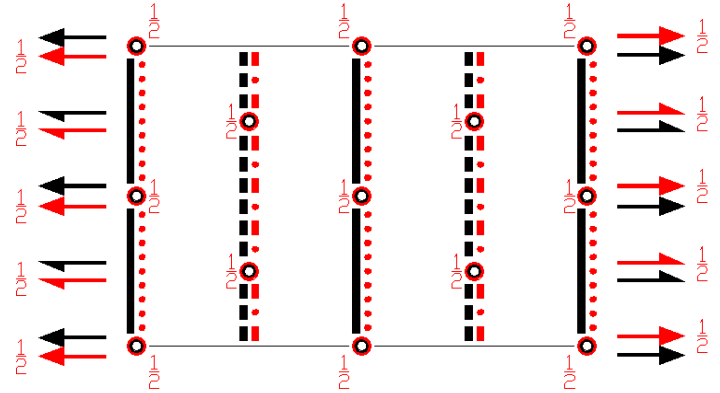
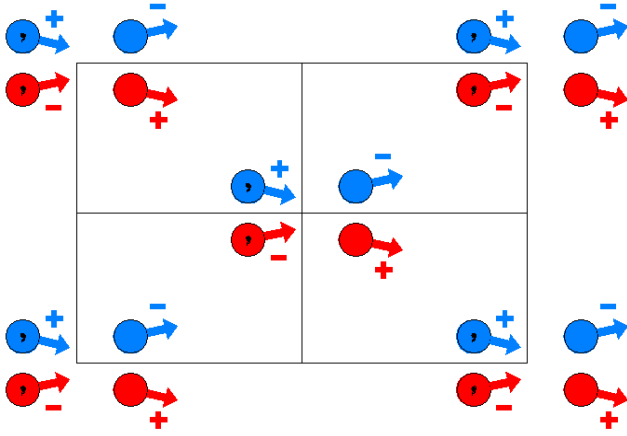
$C_{2c}2/m$

12.6.71

$2/m1'$

$C_{2c}12/m1$

Monoclinic



Origin at center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |                    |                                  |  |                                  |
|--------------------|----------------------------------|--|----------------------------------|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,y,0$<br>( $2_y$  0,0,0) | (3) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0) | (4) m $x,0,z$<br>( $m_y$  0,0,0) |
|--------------------|----------------------------------|--|----------------------------------|

For (1/2,1/2,0) + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t $(1/2,1/2,0)$<br>(1 1/2,1/2,0) | (2) 2 $(0,1/2,0) 1/4,y,0$<br>( $2_y$  1/2,1/2,0) | (3) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$  1/2,1/2,0) | (4) a $(1/2,0,0) x,1/4,z$<br>( $m_y$  1/2,1/2,0) |
|--------------------------------------|--|--|--|

For (0,0,1)' + set

- |                                |                                      |   |  |
|--------------------------------|--------------------------------------|---|--|
| (1) t' $(0,0,1)$<br>(1 0,0,1)' | (2) 2' $0,y,1/2$<br>( $2_y$  0,0,1)' | (3) $\bar{1}$ ' $0,0,1/2$<br>( $\bar{1}$  0,0,1)' | (4) c' $(0,0,1) x,0,z$<br>( $m_y$  0,0,1)' |
|--------------------------------|--------------------------------------|---|--|

For (1/2,1/2,1)' + set

- |  |  |   |  |
|--|--|---|--|
| (1) t' $(1/2,1/2,1)$<br>(1 1/2,1/2,1)' | (2) 2' $(0,1/2,0) 1/4,y,1/2$<br>( $2_y$  1/2,1/2,1)' | (3) $\bar{1}$ ' $1/4,1/4,1/2$<br>( $\bar{1}$  1/2,1/2,1)' | (4) n' $(1/2,0,1) x,1/4,z$<br>( $m_y$  1/2,1/2,1)' |
|--|--|---|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)<sup>'</sup>; t(1/2,1/2,0); (2); (3).

### Positions

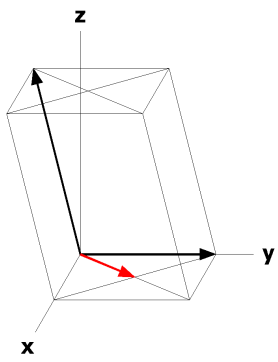
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,1) <sup>'</sup> +	(1/2,1/2,0) + (1/2,1/2,1) <sup>'</sup> +	
16 j 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(4) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]
8 i m	x,0,z [0,v,0]	$\bar{x},0,\bar{z}$ [0,v,0]		
8 h 2'	0,y,1/2 [u,0,w]	0, $\bar{y},1/2$ [ $\bar{u},0,\bar{w}$ ]		
8 g 2	0,y,0 [0,v,0]	0, $\bar{y},0$ [0,v,0]		
8 f $\bar{1}'$	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
8 e $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,1/4,0 [ $\bar{u},v,\bar{w}$ ]		
4 d 2'/m	0,1/2,1/2 [0,0,0]			
4 c 2'/m	0,0,1/2 [0,0,0]			
4 b 2/m	0,1/2,0 [0,v,0]			
4 a 2/m	0,0,0 [0,v,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



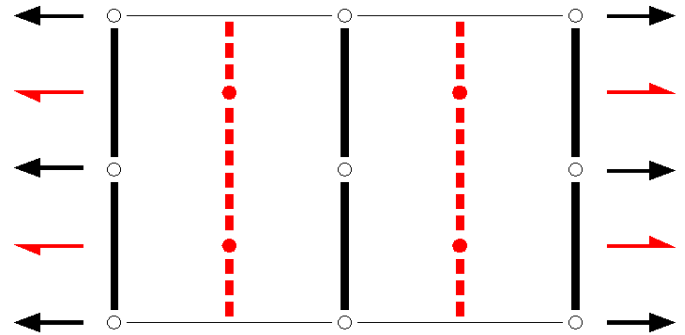
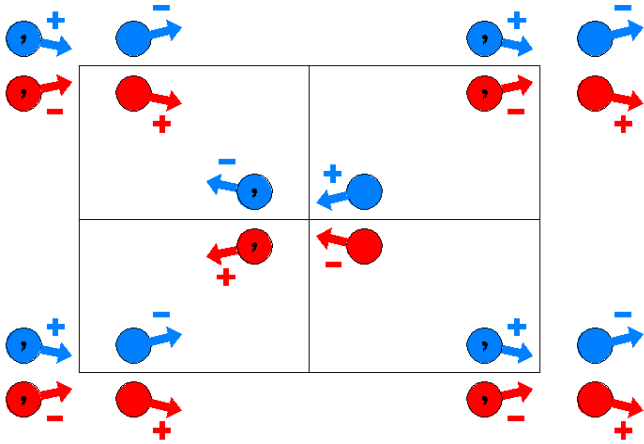
$C_p 2/m$

12.7.72

$2/m 1'$

$C_p 12/m 1$

Monoclinic



Origin at center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2)  $2$   $0,y,0$   
( $2_y$ |0,0,0)

(3)  $\bar{1}$   $0,0,0$   
( $\bar{1}$ |0,0,0)

(4)  $m$   $x,0,z$   
( $m_y$ |0,0,0)

For  $(1/2,1/2,0)'$  + set

(1)  $t'$   $(1/2,1/2,0)$   
(1| $1/2,1/2,0$ )'

(2)  $2'$   $(0,1/2,0)$   $1/4,y,0$   
( $2_y$ | $1/2,1/2,0$ )'

(3)  $\bar{1}'$   $1/4,1/4,0$   
( $\bar{1}$ | $1/2,1/2,0$ )'

(4)  $a'$   $(1/2,0,0)$   $x,1/4,z$   
( $m_y$ | $1/2,1/2,0$ )'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

**Positions**

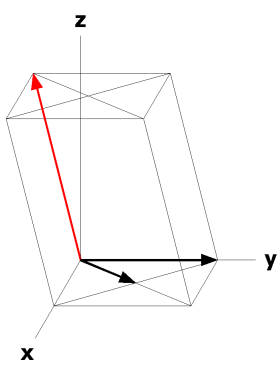
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
8 j 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(4) x, $\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]
4 i m	x,0,z [0,v,0]	$\bar{x},0,\bar{z}$ [0,v,0]		
4 h 2	0,y,1/2 [0,v,0]	0, $\bar{y},1/2$ [0,v,0]		
4 g 2	0,y,0 [0,v,0]	0, $\bar{y},0$ [0,v,0]		
4 f $\bar{1}'$	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 e $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
2 d 2/m	0,1/2,1/2 [0,v,0]			
2 c 2/m	0,0,1/2 [0,v,0]			
2 b 2/m	0,1/2,0 [0,v,0]			
2 a 2/m	0,0,0 [0,v,0]			

**Symmetry of Special Projections**

Along [0,0,1] c<sub>p</sub>2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



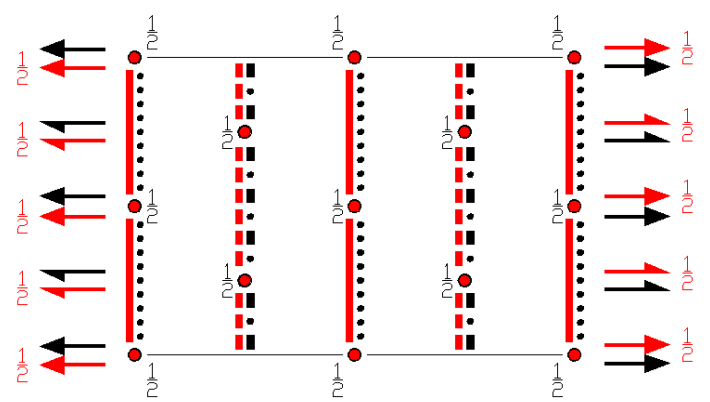
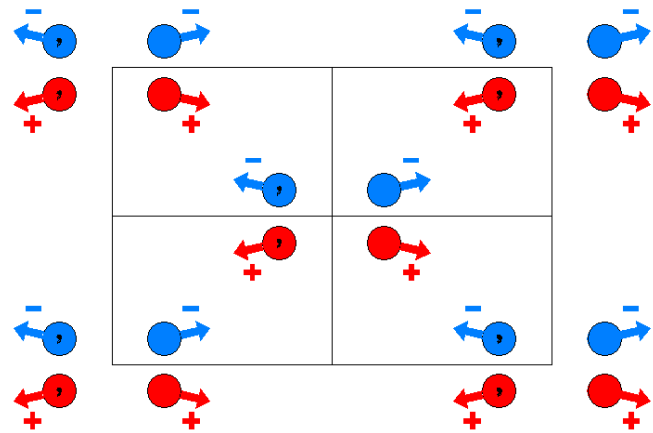
$C_{2c}2/m'$

12.8.73

$2/m1'$

$C_{2c}12/m'1$

Monoclinic



Origin at center ( $2/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |                    |                                  |  |                                      |
|--------------------|----------------------------------|--|--------------------------------------|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,y,0$<br>( $2_y$  0,0,0) | (3) $\bar{1}'$ $0,0,0$<br>( $\bar{1}$  0,0,0)' | (4) $m'$ $x,0,z$<br>( $m_y$  0,0,0)' |
|--------------------|----------------------------------|--|--------------------------------------|

For (1/2,1/2,0) + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) $t$ (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) 2 (0,1/2,0) $1/4,y,0$<br>( $2_y$  1/2,1/2,0) | (3) $\bar{1}'$ $1/4,1/4,0$<br>( $\bar{1}$  1/2,1/2,0)' | (4) $a'$ (1/2,0,0) $x,1/4,z$<br>( $m_y$  1/2,1/2,0)' |
|--------------------------------------|--|--|--|

For (0,0,1)' + set

- |                                |  |  |   |
|--------------------------------|--|--|---|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)' | (2) $2'$ $0,y,1/2$<br>( $2_y$  0,0,1)' | (3) $\bar{1}'$ $0,0,1/2$<br>( $\bar{1}$  0,0,1)' | (4) $c$ (0,0,1) $x,0,z$<br>( $m_y$  0,0,1)' |
|--------------------------------|--|--|---|

For (1/2,1/2,1)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) $t'$ (1/2,1/2,1)<br>(1 1/2,1/2,1)' | (2) $2'$ (0,1/2,0) $1/4,y,1/2$<br>( $2_y$  1/2,1/2,1)' | (3) $\bar{1}'$ $1/4,1/4,1/2$<br>( $\bar{1}$  1/2,1/2,1)' | (4) $n$ (1/2,0,1) $x,1/4,z$<br>( $m_y$  1/2,1/2,1)' |
|--|--|--|---|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; t(1/2,1/2,0); (2); (3).

### Positions

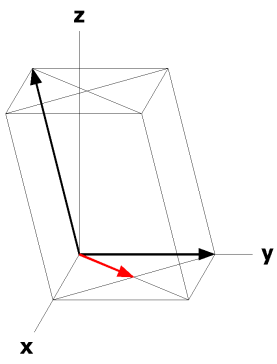
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,1)'	(1/2,1/2,0) + (1/2,1/2,1)'	
16 j 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) x, $\bar{y}$ ,z [u, $\bar{v}$ ,w]
8 i m'	x,0,z [u,0,w]	$\bar{x},0,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]		
8 h 2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ ,1/2 [u,0,w]		
8 g 2	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]		
8 f $\bar{1}$	1/4,1/4,1/2 [u,v,w]	3/4,1/4,1/2 [u, $\bar{v}$ ,w]		
8 e $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
4 d 2'/m'	0,1/2,1/2 [u,0,w]			
4 c 2'/m'	0,0,1/2 [u,0,w]			
4 b 2'/m'	0,1/2,0 [0,0,0]			
4 a 2'/m'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>-211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



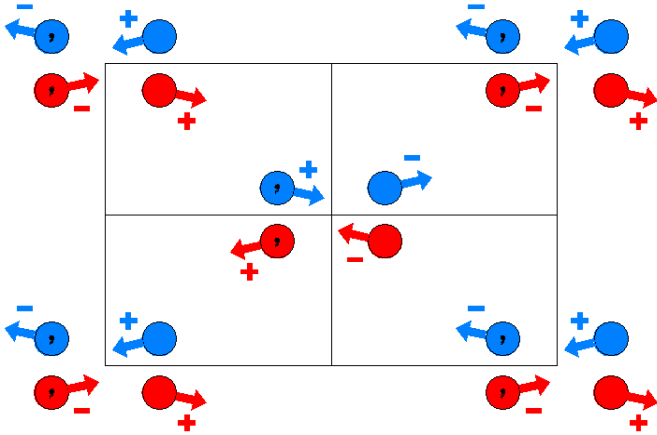
$C_p 2'/m$

12.9.74

$2/m1'$

$C_p 12'/m1$

Monoclinic



Origin at center ( $2'/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2)  $2'$  0,y,0  
( $2_y$ |0,0,0)'

(3)  $\bar{1}'$  0,0,0  
( $\bar{1}$ |0,0,0)'

(4) m x,0,z  
( $m_y$ |0,0,0)

For (0,0,0) + set

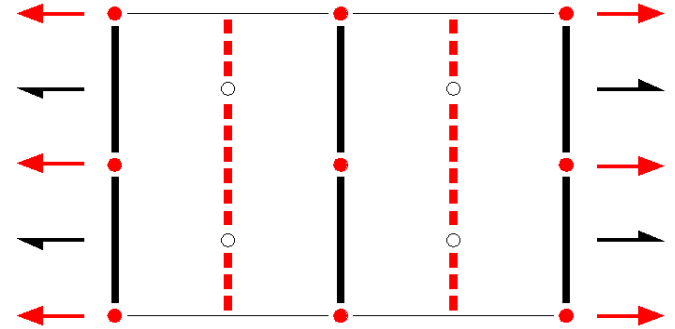
For (1/2,1/2,0)' + set

(1)  $t'$  (1/2,1/2,0)  
(1|1/2,1/2,0)'

(2) 2 (0,1/2,0) 1/4,y,0  
( $2_y$ |1/2,1/2,0)

(3)  $\bar{1}$  1/4,1/4,0  
( $\bar{1}$ |1/2,1/2,0)

(4)  $a'$  (1/2,0,0) x,1/4,z  
( $m_y$ |1/2,1/2,0)'



**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,0)'$ ; (2); (3).

### Positions

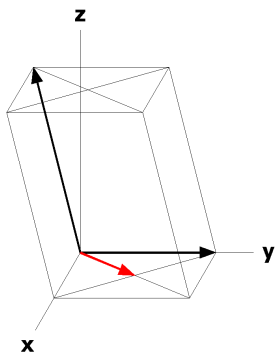
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
8 j 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},y,\bar{z} [u,\bar{v},w]$	(3) $\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$	(4) $x,\bar{y},z [\bar{u},v,\bar{w}]$
4 i m	$x,0,z [0,v,0]$	$\bar{x},0,\bar{z} [0,\bar{v},0]$		
4 h 2'	$0,y,1/2 [u,0,w]$	$0,\bar{y},1/2 [\bar{u},0,\bar{w}]$		
4 g 2'	$0,y,0 [u,0,w]$	$0,\bar{y},0 [\bar{u},0,\bar{w}]$		
4 f $\bar{1}$	$1/4,1/4,1/2 [u,v,w]$	$3/4,1/4,1/2 [u,\bar{v},w]$		
4 e $\bar{1}$	$1/4,1/4,0 [u,v,w]$	$3/4,1/4,0 [u,\bar{v},w]$		
2 d 2'/m	$0,1/2,1/2 [0,0,0]$			
2 c 2'/m	$0,0,1/2 [0,0,0]$			
2 b 2'/m	$0,1/2,0 [0,0,0]$			
2 a 2'/m	$0,0,0 [0,0,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $c_p2mm$   
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a}2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $p2111'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at  $0,y,0$



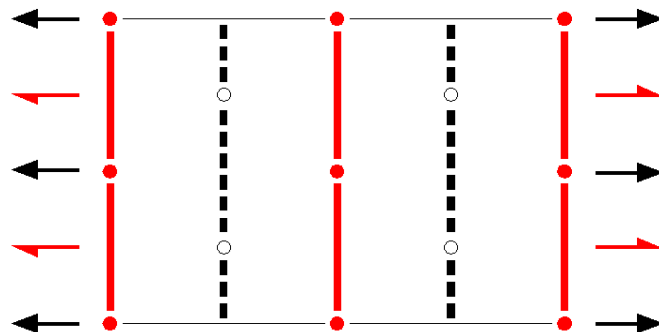
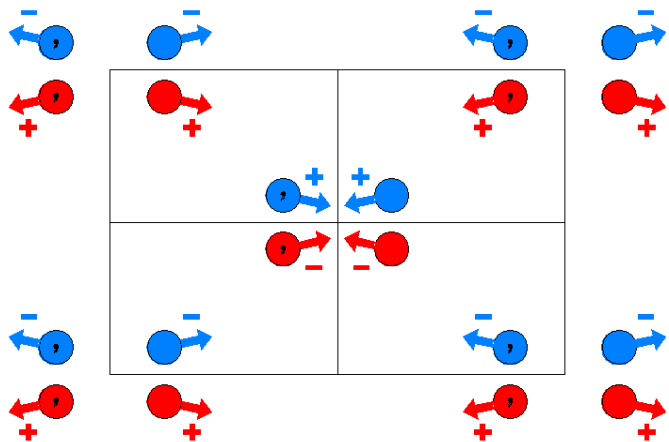
$C_p 2/m'$

12.10.75

$2/m1'$

$C_p 12/m'1$

Monoclinic



Origin at center ( $2/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2  $0,y,0$   
( $2_y$ |0,0,0)

(3)  $\bar{1}$   $0,0,0$   
( $\bar{1}$ |0,0,0)'

(4)  $m'$   $x,0,z$   
( $m_y$ |0,0,0)'

For (1/2,1/2,0)' + set

(1)  $t'$  (1/2,1/2,0)  
(1|1/2,1/2,0)'

(2)  $2'$  (0,1/2,0)  $1/4,y,0$   
( $2_y$ |1/2,1/2,0)'

(3)  $\bar{1}$   $1/4,1/4,0$   
( $\bar{1}$ |1/2,1/2,0)

(4)  $a$  (1/2,0,0)  $x,1/4,z$   
( $m_y$ |1/2,1/2,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

### Positions

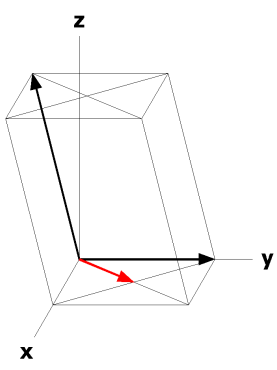
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
8 j 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) x, $\bar{y}$ ,z [u, $\bar{v}$ ,w]
4 i m'	x,0,z [u,0,w]	$\bar{x},0,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]		
4 h 2	0,y,1/2 [0,v,0]	0, $\bar{y}$ ,1/2 [0, $\bar{v}$ ,0]		
4 g 2	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]		
4 f $\bar{1}$	1/4,1/4,1/2 [u,v,w]	3/4,1/4,1/2 [ $\bar{u},\bar{v},\bar{w}$ ]		
4 e $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,1/4,0 [ $\bar{u},\bar{v},\bar{w}$ ]		
2 d 2/m'	0,1/2,1/2 [0,0,0]			
2 c 2/m'	0,0,1/2 [0,0,0]			
2 b 2/m'	0,1/2,0 [0,0,0]			
2 a 2/m'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c<sub>p</sub>2m'm'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>211  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



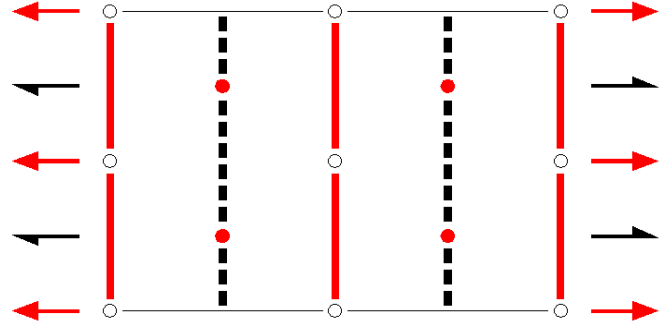
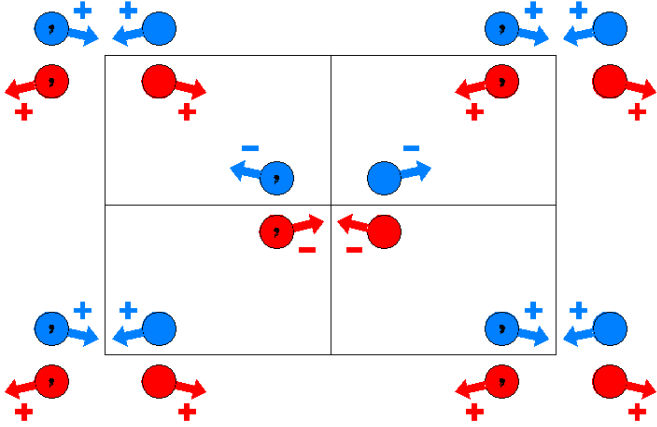
$C_p 2'/m'$

12.11.76

$2/m1'$

$C_p 12'/m'1$

Monoclinic



Origin at center ( $2'/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2)  $2'_y$  0,y,0  
( $2_y$ |0,0,0)'

(3)  $\bar{1}$  0,0,0  
( $\bar{1}$ |0,0,0)

(4)  $m'_x$  x,0,z  
( $m_x$ |0,0,0)'

For (0,0,0) + set

For (1/2,1/2,0)' + set

(1)  $t'_x$  (1/2,1/2,0)  
( $1$ |1/2,1/2,0)'

(2) 2 (0,1/2,0) 1/4,y,0  
( $2_y$ |1/2,1/2,0)

(3)  $\bar{1}'$  1/4,1/4,0  
( $\bar{1}$ |1/2,1/2,0)'

(4) a (1/2,0,0) x,1/4,z  
( $m_x$ |1/2,1/2,0)



**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,0)'$ ; (2); (3).

### Positions

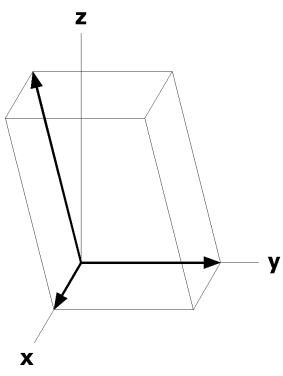
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
8 j 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},y,\bar{z} [u,\bar{v},w]$	(3) $\bar{x},\bar{y},\bar{z} [u,v,w]$	(4) $x,\bar{y},z [u,\bar{v},w]$
4 i $m'$	$x,0,z [u,0,w]$	$\bar{x},0,\bar{z} [u,0,w]$		
4 h $2'$	$0,y,1/2 [u,0,w]$	$0,\bar{y},1/2 [u,0,w]$		
4 g $2'$	$0,y,0 [u,0,w]$	$0,\bar{y},0 [u,0,w]$		
4 f $\bar{1}'$	$1/4,1/4,1/2 [0,0,0]$	$3/4,1/4,1/2 [0,0,0]$		
4 e $\bar{1}'$	$1/4,1/4,0 [0,0,0]$	$3/4,1/4,0 [0,0,0]$		
2 d $2'/m'$	$0,1/2,1/2 [u,0,w]$			
2 c $2'/m'$	$0,0,1/2 [u,0,w]$			
2 b $2'/m'$	$0,1/2,0 [u,0,w]$			
2 a $2'/m'$	$0,0,0 [u,0,w]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $c_p 2'mm'$   
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a} 2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at  $x,1/4,0$

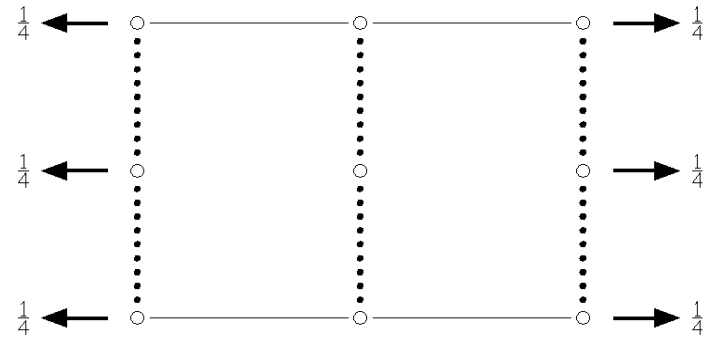
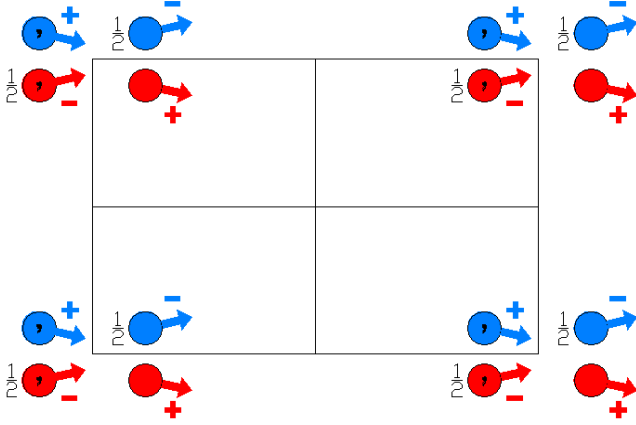
Along  $[0,1,0]$   $p_{2a} 211$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $1/4,y,0$



P2/c  
13.1.77

2/m  
P12/c1

Monoclinic



Origin at  $\bar{1}$  on glide plane c

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2  $0, y, 1/4$   
( $2_y$ |0,0,1/2)

(3)  $\bar{1}$  0,0,0  
( $\bar{1}$ |0,0,0)

(4) c  $(0,0,1/2)$  x,0,z  
( $m_y$ |0,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

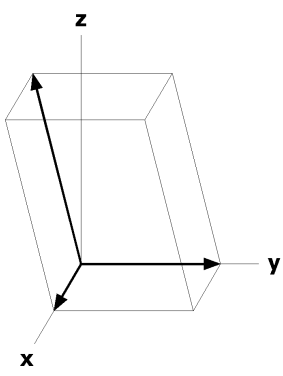
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
4	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(4) x, $\bar{y},z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]
2	f	2	1/2,y,1/4 [0,v,0]	1/2, $\bar{y},3/4$ [0,v,0]		
2	e	2	0,y,1/4 [0,v,0]	0, $\bar{y},3/4$ [0,v,0]		
2	d	$\bar{1}$	1/2,0,0 [u,v,w]	1/2,0,1/2 [ $\bar{u},\bar{v},\bar{w}$ ]		
2	c	$\bar{1}$	0,1/2,0 [u,v,w]	0,1/2,1/2 [ $\bar{u},\bar{v},\bar{w}$ ]		
2	b	$\bar{1}$	1/2,1/2,0 [u,v,w]	1/2,1/2,1/2 [ $\bar{u},\bar{v},\bar{w}$ ]		
2	a	$\bar{1}$	0,0,0 [u,v,w]	0,0,1/2 [ $\bar{u},\bar{v},\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>-211  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



P2/c1'

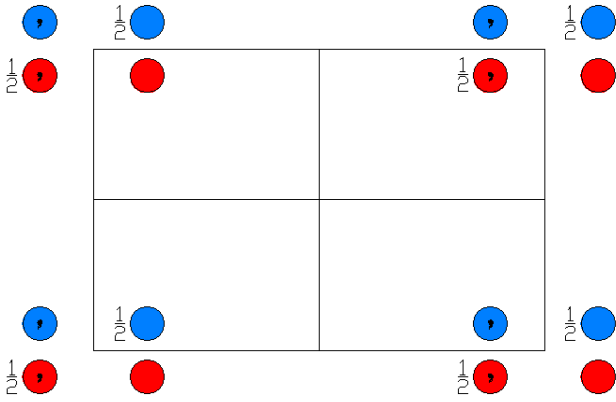
13.2.78

2/m1'

P12/c11'

Monoclinic

1'



Origin at  $\bar{1}1'$  on glide plane  $c1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/2$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2  $0,y,1/4$   
( $2_y$ |0,0,1/2)

(3)  $\bar{1}$  0,0,0  
( $\bar{1}$ |0,0,0)

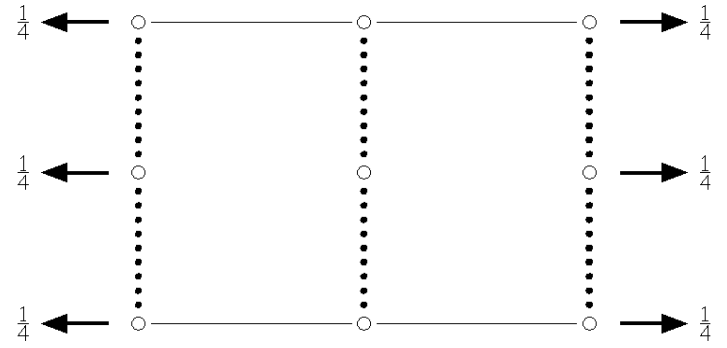
(4) c (0,0,1/2) x,0,z  
( $m_y$ |0,0,1/2)

(1) 1'  
(1|0,0,0)'

(2) 2'  $0,y,1/4$   
( $2_y$ |0,0,1/2)'

(3)  $\bar{1}'$  0,0,0  
( $\bar{1}'$ |0,0,0)'

(4) c' (0,0,1/2) x,0,z  
( $m_y$ |0,0,1/2)'



For 1 + set

For 1' + set

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

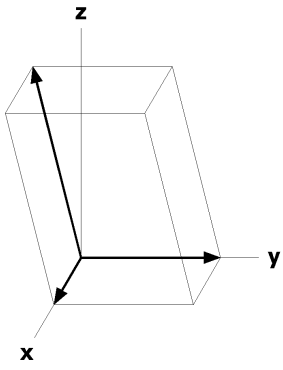
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
4 g 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},\bar{z}+1/2$ [0,0,0]	(3) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(4) x, $\bar{y}$ ,z+1/2 [0,0,0]
2 f 21'	1/2,y,1/4 [0,0,0]	1/2, $\bar{y}$ ,3/4 [0,0,0]		
2 e 21'	0,y,1/4 [0,0,0]	0, $\bar{y}$ ,3/4 [0,0,0]		
2 d $\bar{1}1'$	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2 c $\bar{1}1'$	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
2 b $\bar{1}1'$	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 0,0,0]		
2 a $\bar{1}1'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

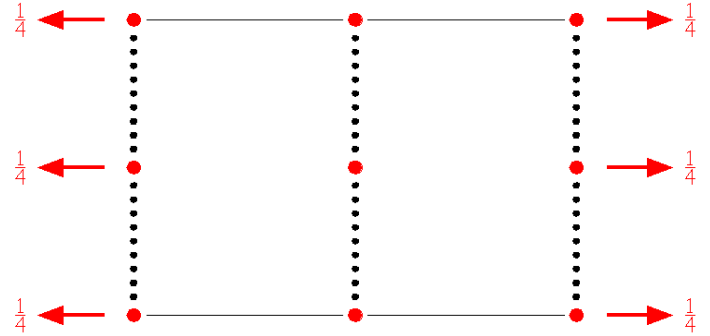
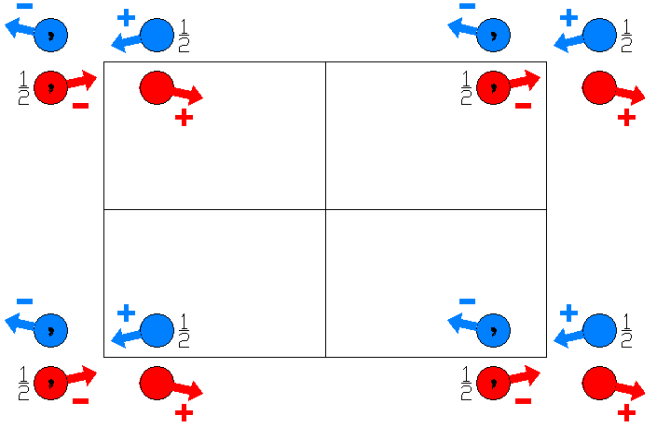
Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



P2'/c  
13.3.79

2'/m  
P12'/c1

Monoclinic



Origin at  $\bar{1}$ ' on glide plane c

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2'  $0, y, 1/4$   
(2<sub>y</sub>|0,0,1/2)'

(3)  $\bar{1}$ '  $0,0,0$   
( $\bar{1}$ |0,0,0)'

(4) c  $(0,0,1/2)$   $x,0,z$   
(m<sub>y</sub>|0,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

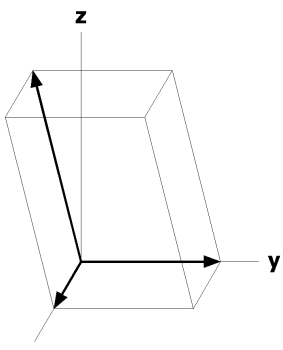
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
4	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(3) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(4) x, $\bar{y},z+1/2$ [ $\bar{u}$ ,v, $\bar{w}$ ]
2	f	2'	1/2,y,1/4 [u,0,w]	1/2, $\bar{y}$ ,3/4 [ $\bar{u}$ ,0, $\bar{w}$ ]		
2	e	2'	0,y,1/4 [u,0,w]	0, $\bar{y}$ ,3/4 [ $\bar{u}$ ,0, $\bar{w}$ ]		
2	d	$\bar{1}'$	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	c	$\bar{1}'$	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	b	$\bar{1}'$	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a	$\bar{1}'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

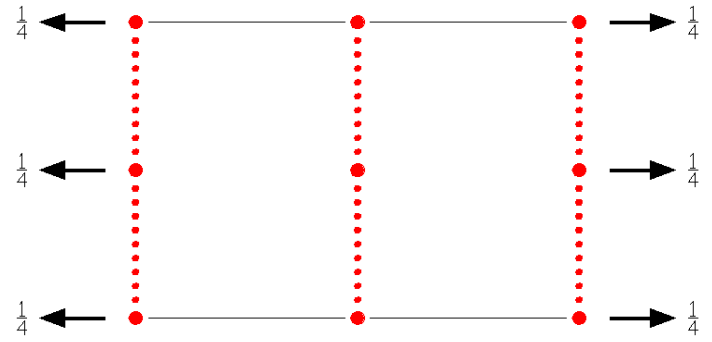
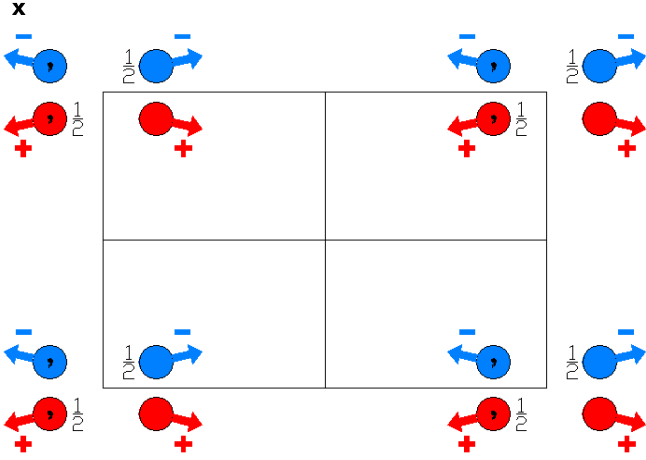
Along [0,1,0] p<sub>2a</sub>'-211  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



P2/c'  
13.4.80

2/m'  
P12/c'1

Monoclinic



Origin at  $\bar{1}$ ' on glide plane  $c'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2  $0, y, 1/4$   
( $2_y$ |0,0,1/2)

(3)  $\bar{1}$ ' 0,0,0  
( $\bar{1}$ '|0,0,0)'

(4)  $c'$  (0,0,1/2)  $x, 0, z$   
( $m_y$ |0,0,1/2)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

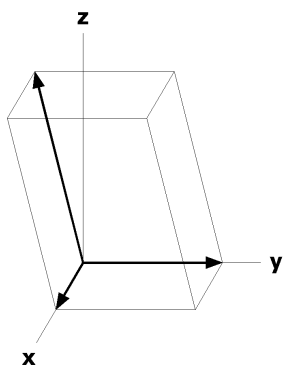
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
4	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) x, $\bar{y}$ ,z+1/2 [u, $\bar{v}$ ,w]
2	f	2	1/2,y,1/4 [0,v,0]	1/2, $\bar{y}$ ,3/4 [0, $\bar{v}$ ,0]		
2	e	2	0,y,1/4 [0,v,0]	0, $\bar{y}$ ,3/4 [0, $\bar{v}$ ,0]		
2	d	$\bar{1}'$	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	c	$\bar{1}'$	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	b	$\bar{1}'$	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a	$\bar{1}'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p211  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



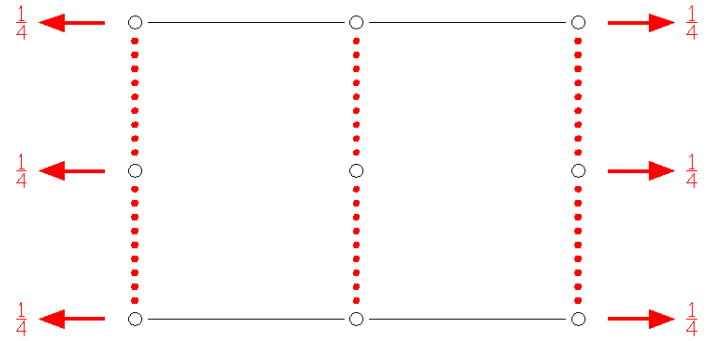
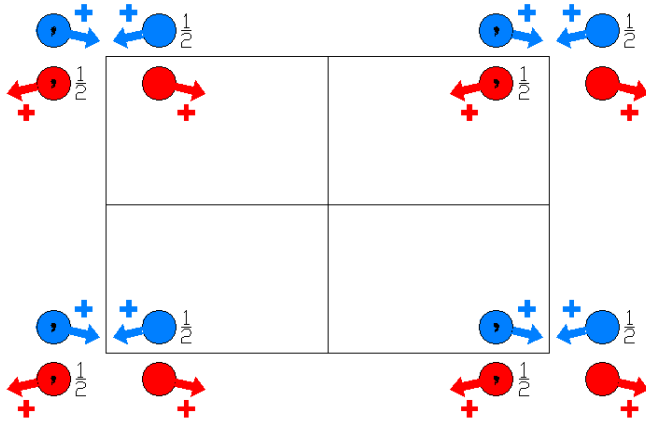
P2'/c'

13.5.81

2'/m'

P12'/c'1

Monoclinic



Origin at  $\bar{1}$  on glide plane  $c'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2'  $0, y, 1/4$   
( $2_y$ |0,0,1/2)'

(3)  $\bar{1}$   $0,0,0$   
( $\bar{1}$ |0,0,0)

(4)  $c'$   $(0,0,1/2)$   $x,0,z$   
( $m_y$ |0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

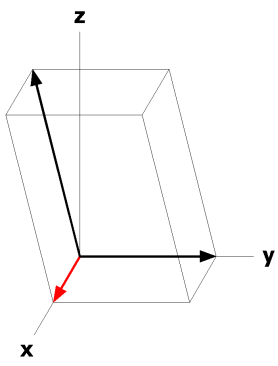
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
4	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(3) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(4) x, $\bar{y},z+1/2$ [u, $\bar{v}$ ,w]
2	f	2'	1/2,y,1/4 [u,0,w]	1/2, $\bar{y}$ ,3/4 [u,0,w]		
2	e	2'	0,y,1/4 [u,0,w]	0, $\bar{y}$ ,3/4 [u,0,w]		
2	d	$\bar{1}$	1/2,0,0 [u,v,w]	1/2,0,1/2 [u, $\bar{v}$ ,w]		
2	c	$\bar{1}$	0,1/2,0 [u,v,w]	0,1/2,1/2 [u, $\bar{v}$ ,w]		
2	b	$\bar{1}$	1/2,1/2,0 [u,v,w]	1/2,1/2,1/2 [u, $\bar{v}$ ,w]		
2	a	$\bar{1}$	0,0,0 [u,v,w]	0,0,1/2 [u, $\bar{v}$ ,w]		

**Symmetry of Special Projections**

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



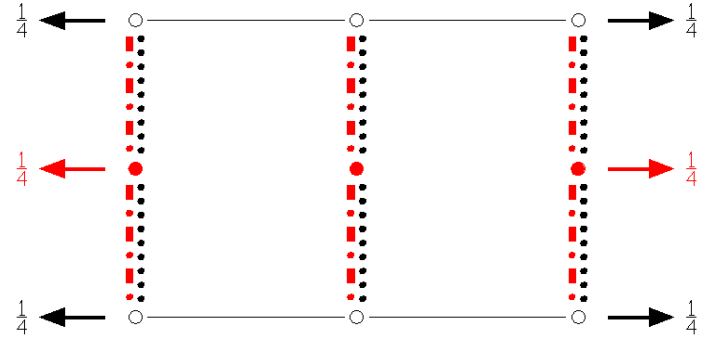
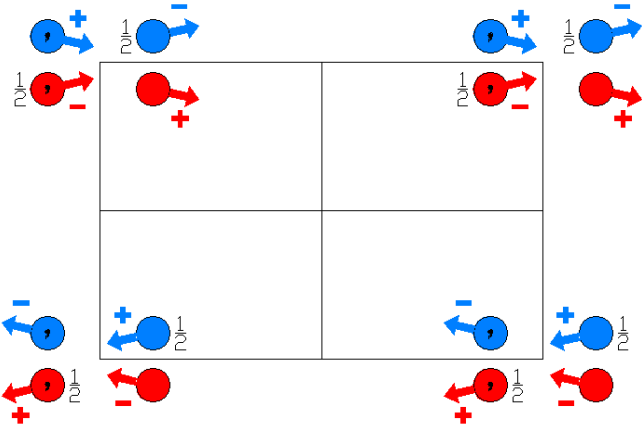
$P_{2a}2/c$

13.6.82

$2/m1'$

$P_{2a}12/c1$

Monoclinic



**Origin** at  $\bar{1}$  on glide plane c

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0, y, 1/4$   
( $2_y$ |0,0,1/2)

(3)  $\bar{1}$  0,0,0  
( $\bar{1}$ |0,0,0)

(4) c (0,0,1/2) x,0,z  
( $m_y$ |0,0,1/2)

For (0,0,0) + set

(1)  $t'$  (1,0,0)  
(1|1,0,0)'

(2)  $2'$  1/2,y,1/4  
( $2_y$ |1,0,1/2)'

(3)  $\bar{1}'$  1/2,0,0  
( $\bar{1}$ |1,0,0)'

(4)  $n'$  (1,0,1/2) x,0,z  
( $m_y$ |1,0,1/2)'

For (1,0,0)' + set

**Generators selected** (1); t(1,0,0)<sup>'</sup>; t(0,1,0); t(0,0,1); (2); (3).

**Positions**

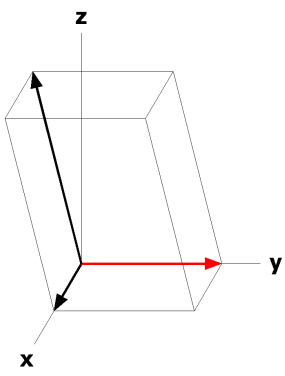
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0) <sup>'</sup> +		
8 g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(4) x, $\bar{y},z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]
4 f 2'	1/2,y,1/4 [u,0,w]	1/2, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]		
4 e 2	0,y,1/4 [0,v,0]	0, $\bar{y},3/4$ [0,v,0]		
4 d $\bar{1}'$	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 c $\bar{1}$	0,1/2,0 [u,v,w]	0,1/2,1/2 [ $\bar{u},\bar{v},\bar{w}$ ]		
4 b $\bar{1}'$	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a $\bar{1}$	0,0,0 [u,v,w]	0,0,1/2 [ $\bar{u},\bar{v},\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 1/2,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>-211  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{a} + \mathbf{c}/2$   
 Origin at 0,y,1/4



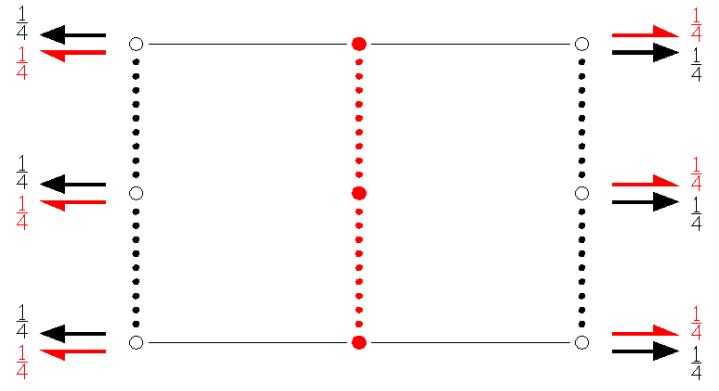
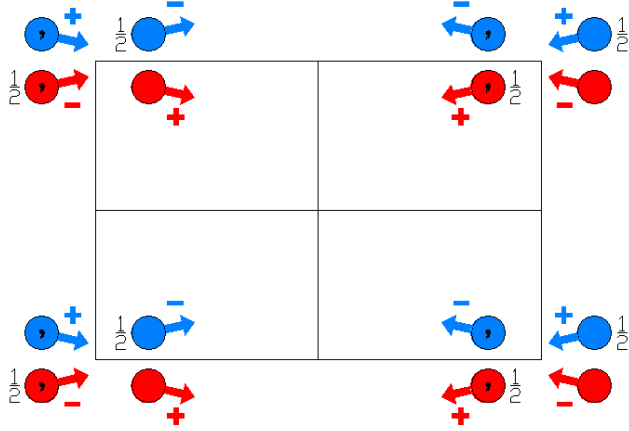
$P_{2b}2/c$

13.7.83

$2/m1'$

$P_{2b}12/c1$

Monoclinic



**Origin** at  $\bar{1}$  on glide plane c

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0, y, 1/4$   
( $2_y$ |0,0,1/2)

(3)  $\bar{1}$  0,0,0  
( $\bar{1}$ |0,0,0)

(4) c (0,0,1/2) x,0,z  
( $m_y$ |0,0,1/2)

For (0,0,0) + set

(1)  $t'$  (0,1,0)  
(1|0,1,0)'

(2)  $2'$  (0,1,0)  $0, y, 1/4$   
( $2_y$ |0,1,1/2)'

(3)  $\bar{1}'$  0,1/2,0  
( $\bar{1}$ |0,1,0)'

(4)  $c'$  (0,0,1/2) x,1/2,z  
( $m_y$ |0,1,1/2)'

For (0,1,0)' + set

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

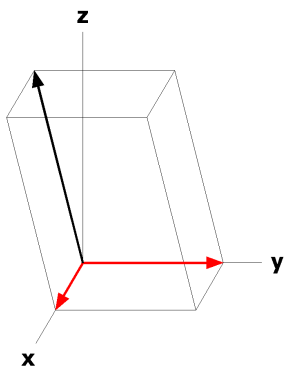
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(0,1,0) <sup>'</sup> +	
8 g 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, \bar{z} + 1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(3) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(4) x, $\bar{y}, z + 1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]
4 f 2	1/2,y,1/4 [0,v,0]	1/2, $\bar{y}, 3/4$ [0,v,0]		
4 e 2	0,y,1/4 [0,v,0]	0, $\bar{y}, 3/4$ [0,v,0]		
4 d $\bar{1}$	1/2,0,0 [u,v,w]	1/2,0,1/2 [ $\bar{u}, \bar{v}, \bar{w}$ ]		
4 c $\bar{1}'$	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 b $\bar{1}'$	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a $\bar{1}$	0,0,0 [u,v,w]	0,0,1/2 [ $\bar{u}, \bar{v}, \bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>-2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 1/2,0,z

Along [1,0,0] p<sub>2b</sub>-2mg  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,1/2,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



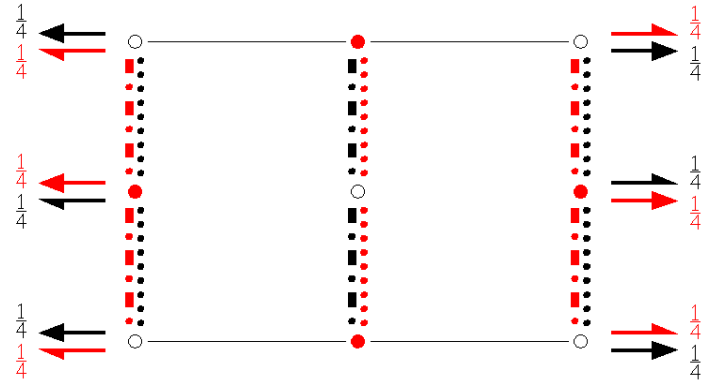
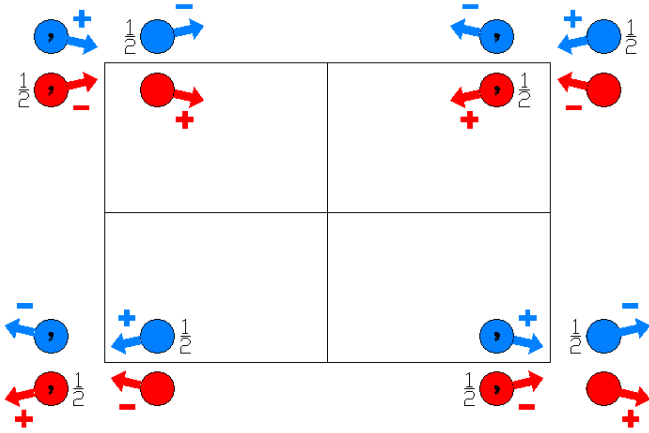
$P_c2/c$

13.8.84

$2/m1'$

$P_c12/c1$

Monoclinic



**Origin** at  $\bar{1}$  on glide plane c

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |                                |  |  |  |
|--------------------------------|--|--|--|
| (1) 1<br>(1 0,0,0)             | (2) 2 $0,y,1/4$<br>( $2_y$  0,0,1/2)     | (3) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)     | (4) c (0,0,1/2) x,0,z<br>( $m_y$  0,0,1/2)     |
| (1) $t'$ (1,0,0)<br>(1 1,0,0)' | (2) $2'$ 1/2,y,1/4<br>( $2_y$  1,0,1/2)' | (3) $\bar{1}'$ 1/2,0,0<br>( $\bar{1}$  1,0,0)' | (4) $n'$ (1,0,1/2) x,0,z<br>( $m_y$  1,0,1/2)' |



**Generators selected** (1); t(1,0,0)<sup>+</sup>; t(0,1,0)<sup>+</sup>; t(0,0,1); (2); (3).

**Positions**

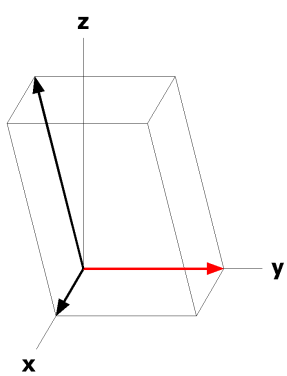
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1,0,0) <sup>+</sup> +	
8 g 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, \bar{z} + 1/2 [\bar{u}, \bar{v}, \bar{w}]$	(3) $\bar{x}, \bar{y}, \bar{z} [u, v, w]$	(4) $x, \bar{y}, z + 1/2 [\bar{u}, v, \bar{w}]$
4 f 2'	1/2, y, 1/4 [u, 0, w]	1/2, $\bar{y}$ , 3/4 [ $\bar{u}$ , 0, $\bar{w}$ ]		
4 e 2	0, y, 1/4 [0, v, 0]	0, $\bar{y}$ , 3/4 [0, v, 0]		
4 d $\bar{1}'$	1/2, 0, 0 [0, 0, 0]	1/2, 0, 1/2 [0, 0, 0]		
4 c $\bar{1}'$	0, 1/2, 0 [0, 0, 0]	0, 1/2, 1/2 [0, 0, 0]		
4 b $\bar{1}$	1/2, 1/2, 0 [u, v, w]	1/2, 1/2, 1/2 [u, $\bar{v}$ , w]		
4 a $\bar{1}$	0, 0, 0 [u, v, w]	0, 0, 1/2 [ $\bar{u}$ , v, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 1/2,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p211  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



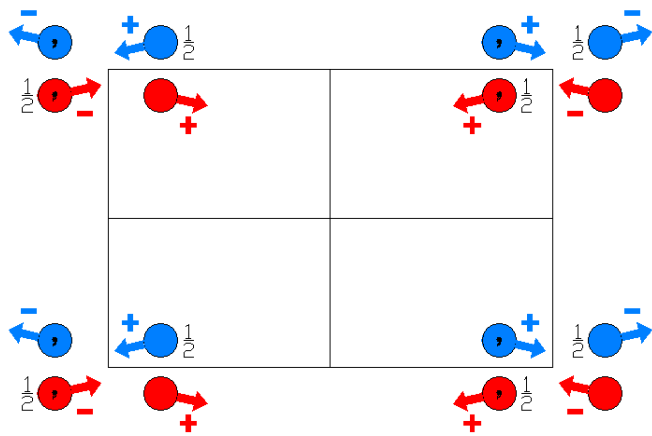
$P_{2b}2'c$

13.9.85

$2/m1'$

$P_{2b}12'c1$

Monoclinic



**Origin** at  $\bar{1}'$  on glide plane c

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2)  $2'$   $0,y,1/4$   
( $2_y$ | $0,0,1/2$ )'

(3)  $\bar{1}'$   $0,0,0$   
( $\bar{1}$ | $0,0,0$ )'

(4) c  $(0,0,1/2)$   $x,0,z$   
( $m_y$ | $0,0,1/2$ )'

For  $(0,0,0)$  + set

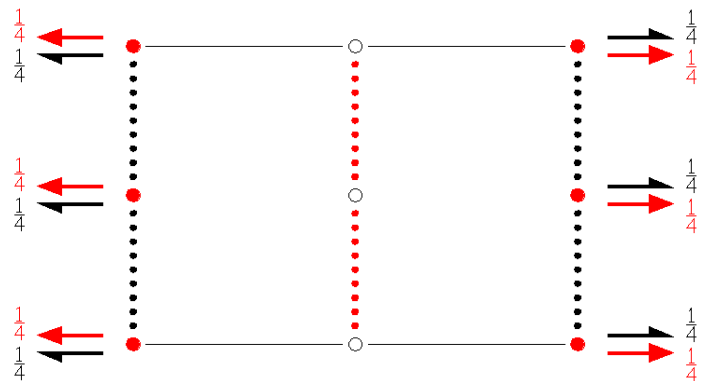
For  $(0,1,0)$  + set

(1)  $t'$   $(0,1,0)$   
(1| $0,1,0$ )'

(2)  $2$   $(0,1,0)$   $0,y,1/4$   
( $2_y$ | $0,1,1/2$ )'

(3)  $\bar{1}$   $0,1/2,0$   
( $\bar{1}$ | $0,1,0$ )'

(4)  $c'$   $(0,0,1/2)$   $x,1/2,z$   
( $m_y$ | $0,1,1/2$ )'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

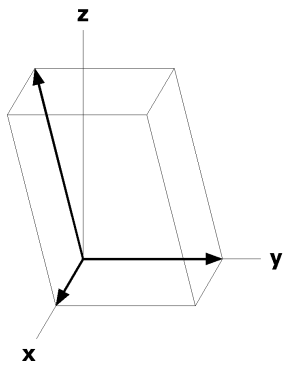
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(0,1,0)' +	
8 g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(3) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) x, $\bar{y}$ ,z+1/2 [ $\bar{u},v,\bar{w}$ ]
4 f 2'	1/2,y,1/4 [u,0,w]	1/2, $\bar{y}$ ,3/4 [ $\bar{u},0,\bar{w}$ ]		
4 e 2'	0,y,1/4 [u,0,w]	0, $\bar{y}$ ,3/4 [ $\bar{u},0,\bar{w}$ ]		
4 d $\bar{1}'$	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 c $\bar{1}$	0,1/2,0 [u,v,w]	0,1/2,1/2 [u, $\bar{v}$ ,w]		
4 b $\bar{1}$	1/2,1/2,0 [u,v,w]	1/2,1/2,1/2 [u, $\bar{v}$ ,w]		
4 a $\bar{1}'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 1/2,0,z

Along [1,0,0] p<sub>2b</sub>2mg  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,1/2,0

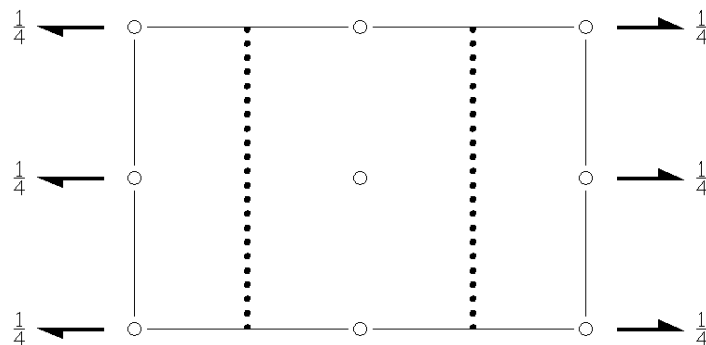
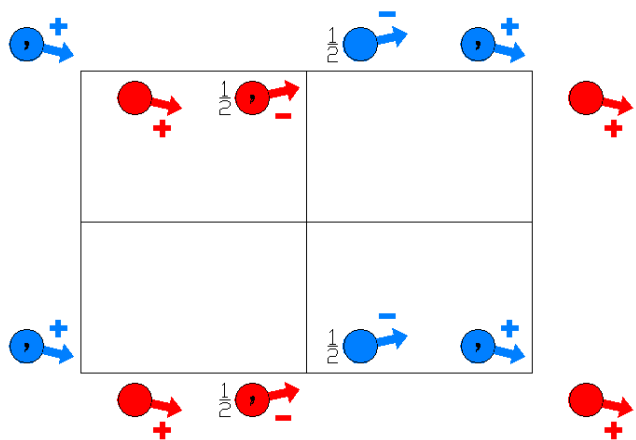
Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



$P2_1/c$   
14.1.86

$2/m$   
 $P12_1/c1$

Monoclinic



Origin at  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

Symmetry Operations

(1)  $1$   
( $1|0,0,0$ )

(2)  $2$  ( $0,1/2,0$ )  $0,y,1/4$   
( $2_y|0,1/2,1/2$ )

(3)  $\bar{1}$   $0,0,0$   
( $\bar{1}|0,0,0$ )

(4)  $c$  ( $0,0,1/2$ )  $x,1/4,z$   
( $m_y|0,1/2,1/2$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

### Positions

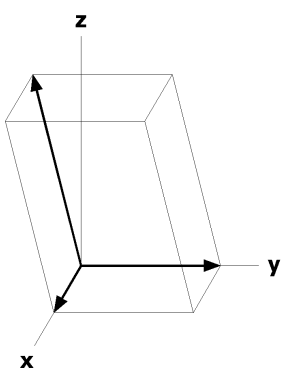
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
4	e	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(3) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(4) x, $\bar{y}+1/2, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]
2	d	$\bar{1}$	1/2,0,0 [u,v,w]	1/2,0,1/2 [ $\bar{u}, v, \bar{w}$ ]		
2	c	$\bar{1}$	0,1/2,0 [u,v,w]	0,1/2,1/2 [ $\bar{u}, v, \bar{w}$ ]		
2	b	$\bar{1}$	1/2,1/2,0 [u,v,w]	1/2,1/2,1/2 [ $\bar{u}, v, \bar{w}$ ]		
2	a	$\bar{1}$	0,0,0 [u,v,w]	0,0,1/2 [ $\bar{u}, v, \bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p2'mg'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p2'gg'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>'211  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



$P2_1/c1'$

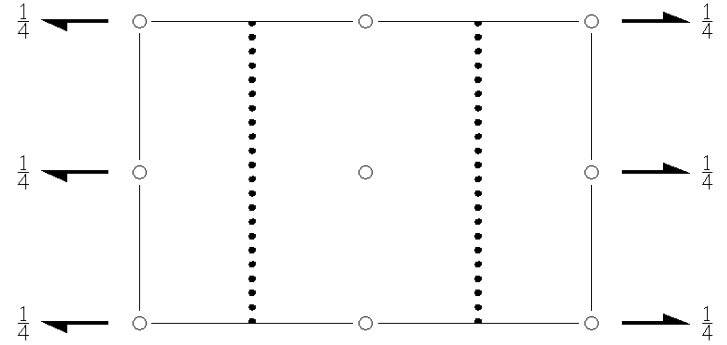
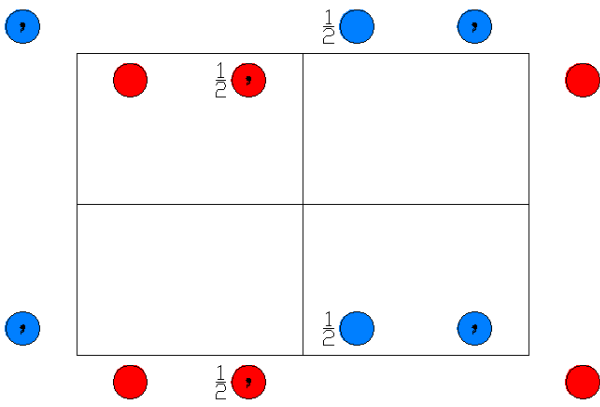
14.2.87

$2/m1'$

$P12_1/c11'$

Monoclinic

$1'$



Origin at  $\bar{1}1'$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

Symmetry Operations

For 1 + set

(1) 1  
(1|0,0,0)

(2) 2 (0,1/2,0) 0,y,1/4  
(2<sub>y</sub>|0,1/2,1/2)

(3)  $\bar{1}$  0,0,0  
( $\bar{1}$ |0,0,0)

(4) c (0,0,1/2) x,1/4,z  
(m<sub>y</sub>|0,1/2,1/2)

For 1' + set

(1) 1'  
(1|0,0,0)'

(2) 2' (0,1/2,0) 0,y,1/4  
(2<sub>y</sub>|0,1/2,1/2)'

(3)  $\bar{1}'$  0,0,0  
( $\bar{1}$ |0,0,0)'

(4) c' (0,0,1/2) x,1/4,z  
(m<sub>y</sub>|0,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

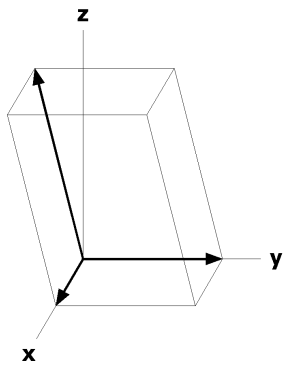
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1+	1' +	
4 e 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, y+1/2, \bar{z}+1/2$ [0,0,0]	(3) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]	(4) $x, \bar{y}+1/2, z+1/2$ [0,0,0]
2 d $\bar{1}1'$	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2 c $\bar{1}1'$	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
2 b $\bar{1}1'$	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2 a $\bar{1}1'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mg1'  
 $\mathbf{a}^* = -\mathbf{b} \quad \mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p2gg1'  
 $\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}/2 \quad \mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



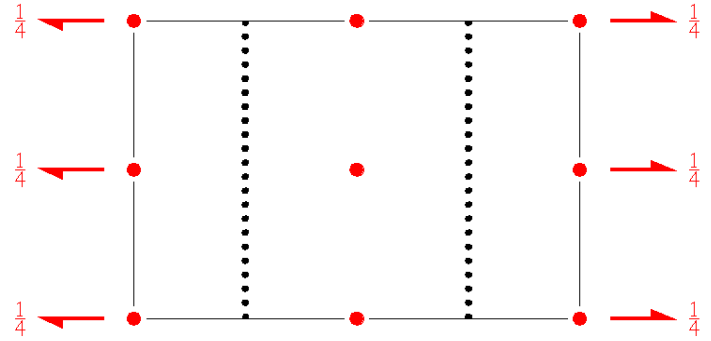
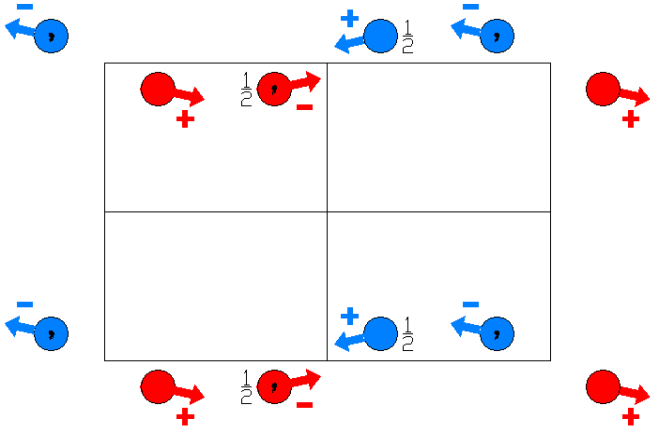
$P2_1/c$

14.3.88

$2'/m$

$P12_1/c1$

Monoclinic



Origin at  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2)  $2'$  (0,1/2,0)  $0,y,1/4$   
( $2_y$ |0,1/2,1/2)'

(3)  $\bar{1}'$  0,0,0  
( $\bar{1}$ |0,0,0)'

(4) c (0,0,1/2)  $x,1/4,z$   
( $m_y$ |0,1/2,1/2)



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

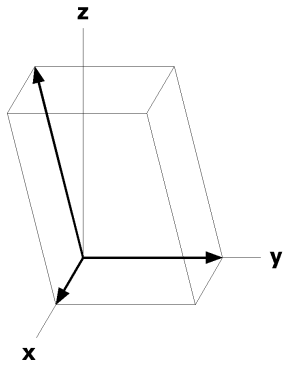
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
4	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, y+1/2, \bar{z}+1/2$ [u, $\bar{v}$ , w]	(3) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(4) x, $\bar{y}+1/2, z+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]
2	d $\bar{1}'$	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	c $\bar{1}'$	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	b $\bar{1}'$	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a $\bar{1}'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mg  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p2gg  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>.211  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



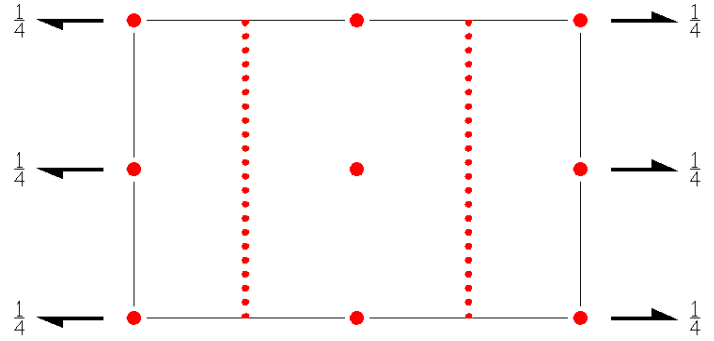
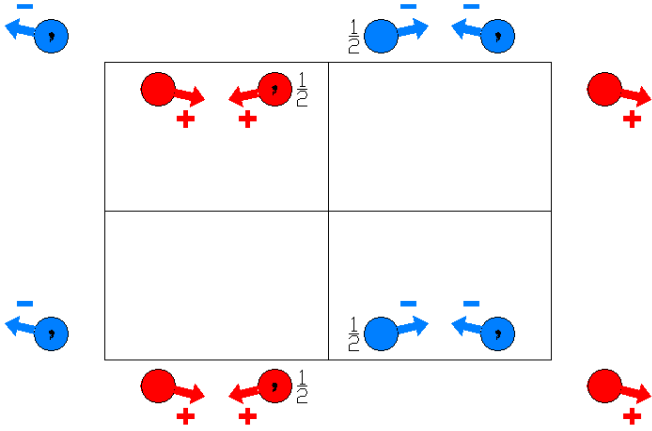
$P2_1/c'$

14.4.89

$2/m'$

$P12_1/c'1$

Monoclinic



Origin at  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 (0,1/2,0) 0,y,1/4  
(2<sub>y</sub>|0,1/2,1/2)

(3)  $\bar{1}'$  0,0,0  
( $\bar{1}$ |0,0,0)'

(4) c' (0,0,1/2) x,1/4,z  
(m<sub>y</sub>|0,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

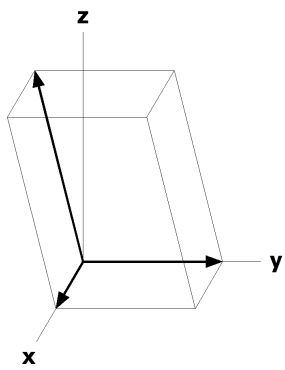
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
4	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(3) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(4) x, $\bar{y}+1/2, z+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]
2	d $\bar{1}'$	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	c $\bar{1}'$	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	b $\bar{1}'$	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a $\bar{1}'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2m'g'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p2g'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0] p211  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



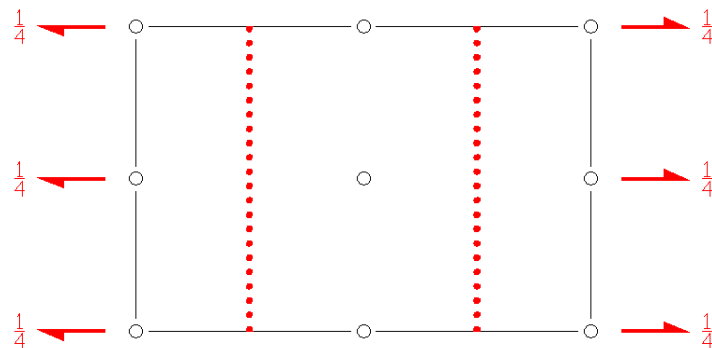
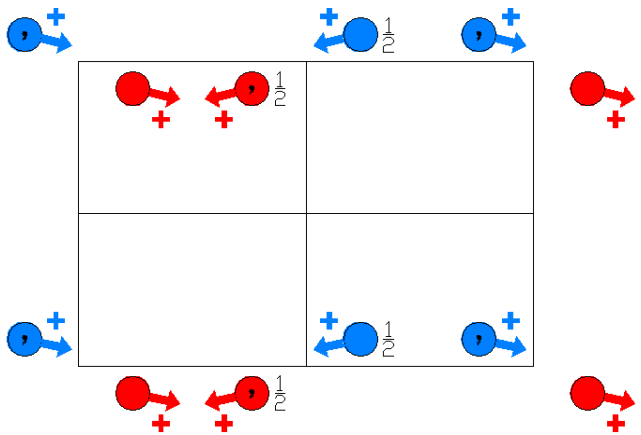
$P2_1/c'$

14.5.90

$2'/m'$

$P12_1/c'1$

Monoclinic



Origin at  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

Symmetry Operations

(1)  $1$   
( $1|0,0,0$ )

(2)  $2'$  ( $0,1/2,0$ )  $0,y,1/4$   
( $2_y|0,1/2,1/2$ )'

(3)  $\bar{1}$   $0,0,0$   
( $\bar{1}|0,0,0$ )

(4)  $c'$  ( $0,0,1/2$ )  $x,1/4,z$   
( $m_y|0,1/2,1/2$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

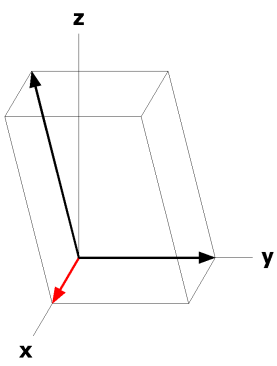
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
4	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, y+1/2, \bar{z}+1/2$ [u, $\bar{v}$ , w]	(3) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(4) x, $\bar{y}+1/2, z+1/2$ [u, $\bar{v}$ , w]
2	d $\bar{1}$	1/2,0,0 [u,v,w]	1/2,0,1/2 [u, $\bar{v}$ , w]		
2	c $\bar{1}$	0,1/2,0 [u,v,w]	0,1/2,1/2 [u, $\bar{v}$ , w]		
2	b $\bar{1}$	1/2,1/2,0 [u,v,w]	1/2,1/2,1/2 [u, $\bar{v}$ , w]		
2	a $\bar{1}$	0,0,0 [u,v,w]	0,0,1/2 [u, $\bar{v}$ , w]		

**Symmetry of Special Projections**

Along [0,0,1] p2'm'g  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'gg'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



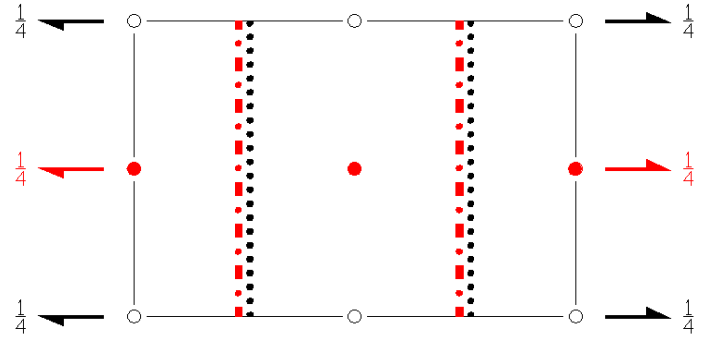
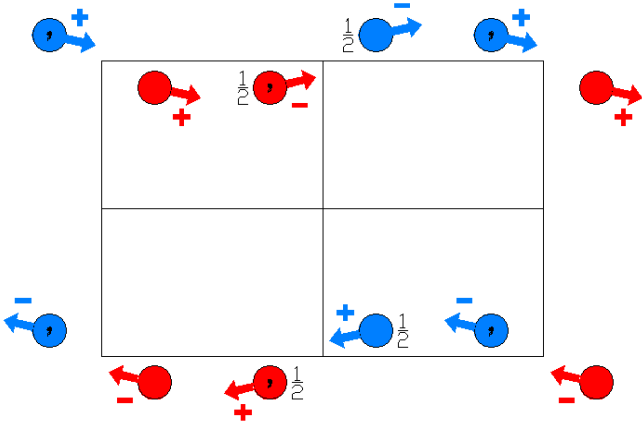
$P_{2a}2_1/c$

14.6.91

$2/m1'$

$P_{2a}12_1/c1$

Monoclinic



Origin at  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2) | (3) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (4) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2) |
|--------------------|--|--|--|

For (1,0,0)' + set

- |                              |  |   |  |
|------------------------------|--|---|--|
| (1) t' (1,0,0)<br>(1 1,0,0)' | (2) 2' (0,1/2,0) 1/2,y,1/4<br>(2 <sub>y</sub>  1,1/2,1/2)' | (3) $\bar{1}$ ' 1/2,0,0<br>( $\bar{1}$  1,0,0)' | (4) n' (1,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1,1/2,1/2)' |
|------------------------------|--|---|--|

**Generators selected** (1);  $t(1,0,0)'$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3).

**Positions**

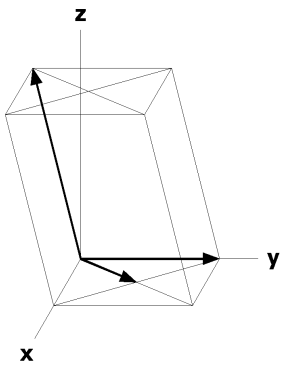
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +	(0,0,0) +	(1,0,0)' +
8 e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(3) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(4) $x, \bar{y}+1/2, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]
4 d $\bar{1}'$	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 c $\bar{1}$	0,1/2,0 [u,v,w]	0,1/2,1/2 [ $\bar{u}, v, \bar{w}$ ]		
4 b $\bar{1}'$	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a $\bar{1}$	0,0,0 [u,v,w]	0,0,1/2 [ $\bar{u}, v, \bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2b}2mg$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 1/2,0,z

Along [1,0,0]  $p2gg1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}_p$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a}211$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a} + \mathbf{c}/2$   
 Origin at 0,y,1/4



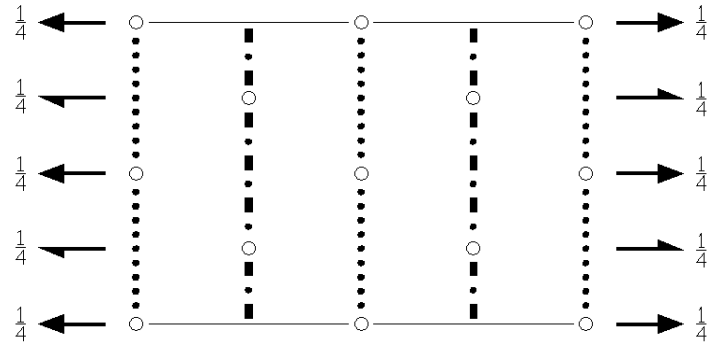
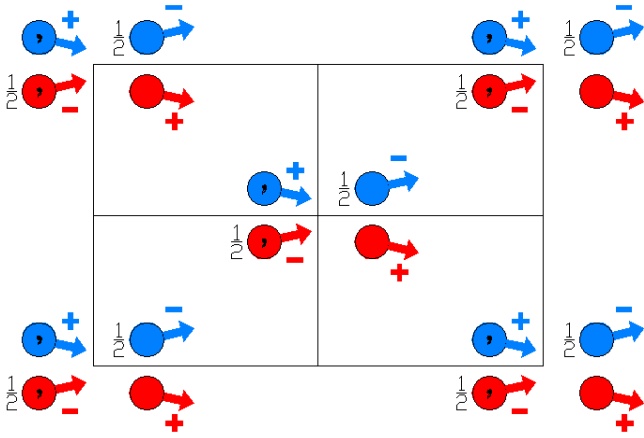
C2/c

15.1.92

2/m

C12/c1

Monoclinic



**Origin** at  $\bar{1}$  on glide plane c

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- (1) 1 (2) 2  $0, y, 1/4$  (3)  $\bar{1} 0, 0, 0$  (4) c  $(0, 0, 1/2) x, 0, z$
- (1|0,0,0) (2<sub>y</sub>|0,0,1/2) ( $\bar{1}$ |0,0,0) (m<sub>y</sub>|0,0,1/2)

For (1/2,1/2,0) + set

- (1) t  $(1/2, 1/2, 0)$  (2) 2  $(0, 1/2, 0) 1/4, y, 1/4$  (3)  $\bar{1} 1/4, 1/4, 0$  (4) n  $(1/2, 0, 1/2) x, 1/4, z$
- (1|1/2,1/2,0) (2<sub>y</sub>|1/2,1/2,1/2) ( $\bar{1}$ |1/2,1/2,0) (m<sub>y</sub>|1/2,1/2,1/2)



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t (1/2,1/2,0); (2); (3).

### Positions

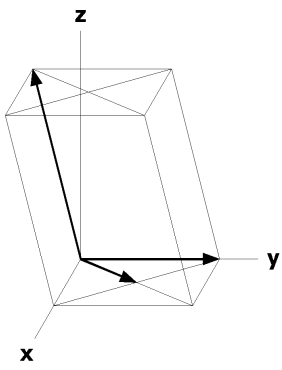
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1/2,1/2,0) +		
8	f	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, \bar{z} + 1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(3) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(4) x, $\bar{y}, z + 1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]
4	e	2	0,y,1/4 [0,v,0]	0, $\bar{y}, 3/4$ [0,v,0]		
4	d	$\bar{1}$	1/4,1/4,1/2[u,v,w]	3/4,1/4,0 [ $\bar{u}, \bar{v}, \bar{w}$ ]		
4	c	$\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,1/4,1/2 [ $\bar{u}, \bar{v}, \bar{w}$ ]		
4	b	$\bar{1}$	0,1/2,0 [u,v,w]	0,1/2,1/2 [ $\bar{u}, \bar{v}, \bar{w}$ ]		
4	a	$\bar{1}$	0,0,0 [u,v,w]	0,0,1/2 [ $\bar{u}, \bar{v}, \bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>-211  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



C2/c1'

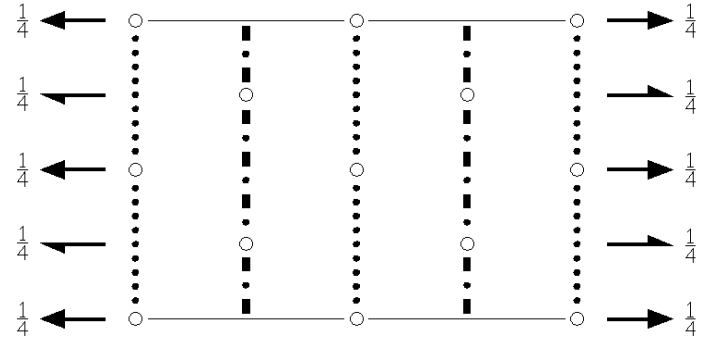
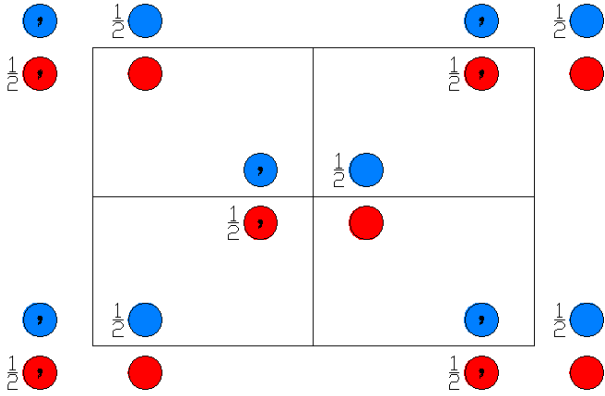
15.2.93

2/m1'

C12/c11'

Monoclinic

1'



Origin at  $\bar{1}1'$  on glide plane  $c1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |                    |                                      |  |  |
|--------------------|--------------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,y,1/4$<br>( $2_y$  0,0,1/2) | (3) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (4) c (0,0,1/2) x,0,z<br>( $m_y$  0,0,1/2) |
|--------------------|--------------------------------------|--|--|

For (1/2,1/2,0) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) 2 (0,1/2,0) 1/4,y,1/4<br>( $2_y$  1/2,1/2,1/2) | (3) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (4) n (1/2,0,1/2) x,1/4,z<br>( $m_y$  1/2,1/2,1/2) |
|------------------------------------|--|--|--|

For (0,0,0)' + set

- |                      |  |   |  |
|----------------------|--|---|--|
| (1) 1'<br>(1 0,0,0)' | (2) 2' $0,y,1/4$<br>( $2_y$  0,0,1/2)' | (3) $\bar{1}'$ 0,0,0<br>( $\bar{1}'$  0,0,0)' | (4) c' (0,0,1/2) x,0,z<br>( $m_y$  0,0,1/2)' |
|----------------------|--|---|--|

For (1/2,1/2,0)' + set

- |                                      |  |   |  |
|--------------------------------------|--|---|--|
| (1) t' (1/2,1/2,0)<br>(1 1/2,1/2,0)' | (2) 2' (0,1/2,0) 1/4,y,1/4<br>( $2_y$  1/2,1/2,1/2)' | (3) $\bar{1}'$ 1/4,1/4,0<br>( $\bar{1}'$  1/2,1/2,0)' | (4) n' (1/2,0,1/2) x,1/4,z<br>( $m_y$  1/2,1/2,1/2)' |
|--------------------------------------|--|---|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t (1/2,1/2,0); (2); (3); 1'.

### Positions

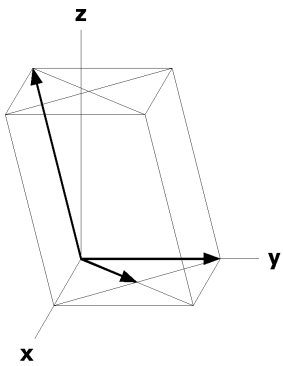
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
8 f 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},\bar{z}+1/2$ [0,0,0]	(3) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(4) x, $\bar{y}$ ,z+1/2 [0,0,0]
4 e 21'	0,y,1/4 [0,0,0]	0, $\bar{y}$ ,3/4 [0,0,0]		
4 d $\bar{1}1'$	1/4,1/4,1/2[0,0,0]	3/4,1/4,0 [0,0,0]		
4 c $\bar{1}1'$	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 b $\bar{1}1'$	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 a $\bar{1}1'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



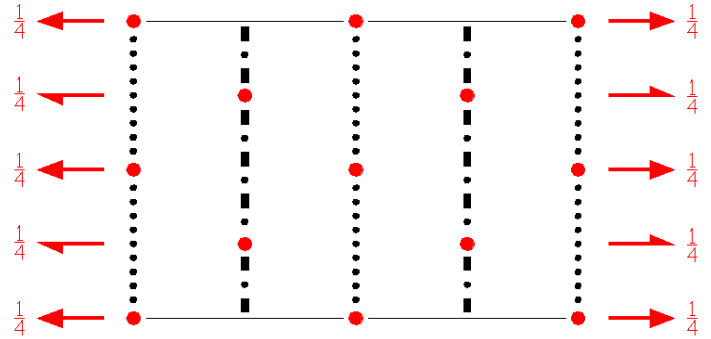
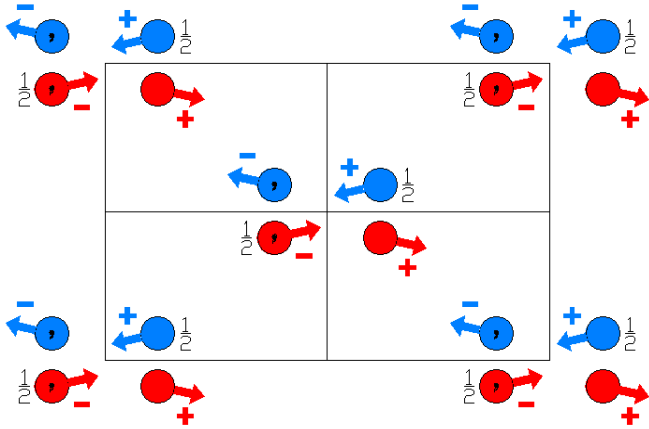
C2'/c

15.3.94

2'/m

C12'/c1

Monoclinic



**Origin** at  $\bar{1}$ ' on glide plane c

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |                    |                                      |   |                                    |
|--------------------|--------------------------------------|---|------------------------------------|
| (1) 1<br>(1 0,0,0) | (2) 2'<br>(2 <sub>y</sub>  0,0,1/2)' | (3) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)' | (4) c<br>(m <sub>y</sub>  0,0,1/2) |
|--------------------|--------------------------------------|---|------------------------------------|

For (1/2,1/2,0) + set

- |                        |  |   |  |
|------------------------|--|---|--|
| (1) t<br>(1 1/2,1/2,0) | (2) 2'<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (3) $\bar{1}$ '<br>( $\bar{1}$  1/2,1/2,0)' | (4) n<br>(m <sub>y</sub>  1/2,1/2,1/2) |
|------------------------|--|---|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t (1/2,1/2,0); (2); (3).

### Positions

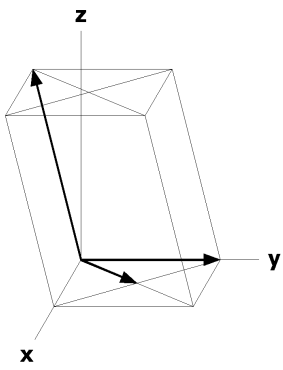
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,0) +		
8	f	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, \bar{z} + 1/2$ [u, $\bar{v}$ , w]	(3) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(4) x, $\bar{y}, z + 1/2$ [ $\bar{u}, v, \bar{w}$ ]
4	e	2'	0,y,1/4 [u,0,w]	0, $\bar{y}, 3/4$ [ $\bar{u}, 0, \bar{w}$ ]		
4	d	$\bar{1}'$	1/4,1/4,1/2[0,0,0]	3/4,1/4,0 [0,0,0]		
4	c	$\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4	b	$\bar{1}'$	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4	a	$\bar{1}'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a}211$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



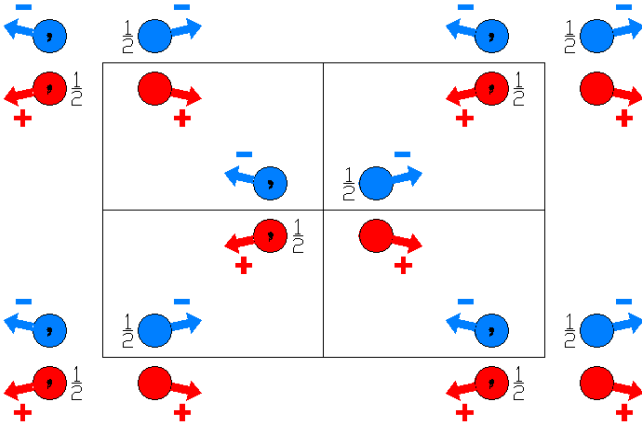
C2/c'

15.4.95

2/m'

C12/c'1

Monoclinic



Origin at  $\bar{1}$ ' on glide plane c'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

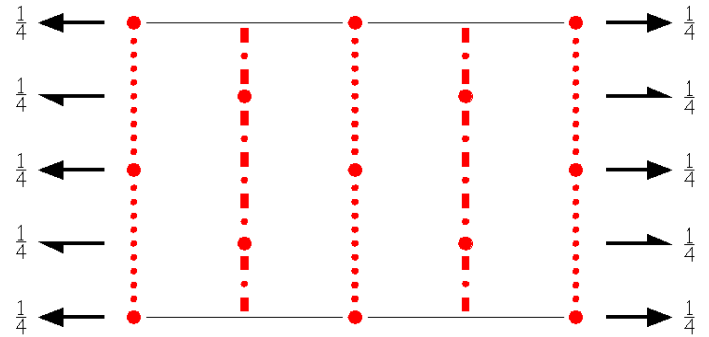
**Symmetry Operations**

For (0,0,0) + set

- |                    |  |   |  |
|--------------------|--|---|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0, y, 1/4$<br>(2 <sub>y</sub>  0,0,1/2) | (3) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (4) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' |
|--------------------|--|---|--|

For (1/2,1/2,0) + set

- |                                    |  |   |  |
|------------------------------------|--|---|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (3) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (4) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' |
|------------------------------------|--|---|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t (1/2,1/2,0); (2); (3).

### Positions

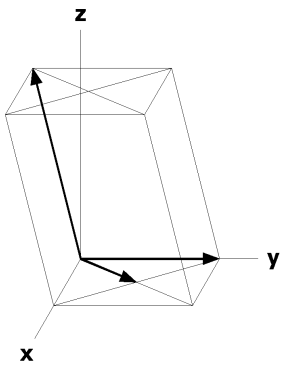
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,0) +		
8	f	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, \bar{z} + 1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(3) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(4) x, $\bar{y}, z + 1/2$ [u, $\bar{v}, w$ ]
4	e	2	0,y,1/4 [0,v,0]	0, $\bar{y}, 3/4$ [0, $\bar{v}, 0$ ]		
4	d	$\bar{1}'$	1/4,1/4,1/2[0,0,0]	3/4,1/4,0 [0,0,0]		
4	c	$\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4	b	$\bar{1}'$	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4	a	$\bar{1}'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p211  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



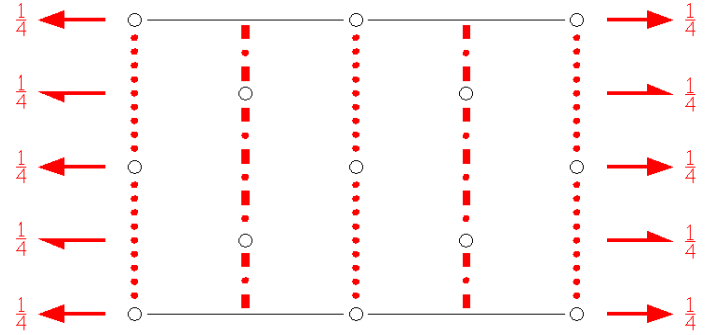
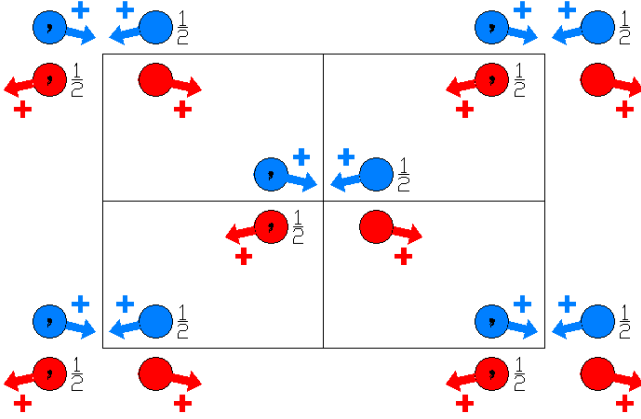
C2'/c'

15.5.96

2'/m'

C12'/c'1

Monoclinic



Origin at  $\bar{1}$  on glide plane  $c'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)' | (3) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (4) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' |
|--------------------|--|--|--|

For (1/2,1/2,0) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (3) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (4) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' |
|------------------------------------|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t (1/2,1/2,0); (2); (3).

### Positions

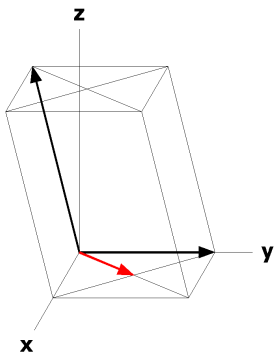
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1/2,1/2,0) +	
8 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(3) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(4) x, $\bar{y},z+1/2$ [u, $\bar{v}$ ,w]
4 e 2'	0,y,1/4 [u,0,w]	0, $\bar{y}$ ,3/4 [u,0,w]		
4 d $\bar{1}$	1/4,1/4,1/2[u,v,w]	3/4,1/4,0 [u, $\bar{v}$ ,w]		
4 c $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,1/4,1/2 [u, $\bar{v}$ ,w]		
4 b $\bar{1}$	0,1/2,0 [u,v,w]	0,1/2,1/2 [u, $\bar{v}$ ,w]		
4 a $\bar{1}$	0,0,0 [u,v,w]	0,0,1/2 [u, $\bar{v}$ ,w]		

### Symmetry of Special Projections

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



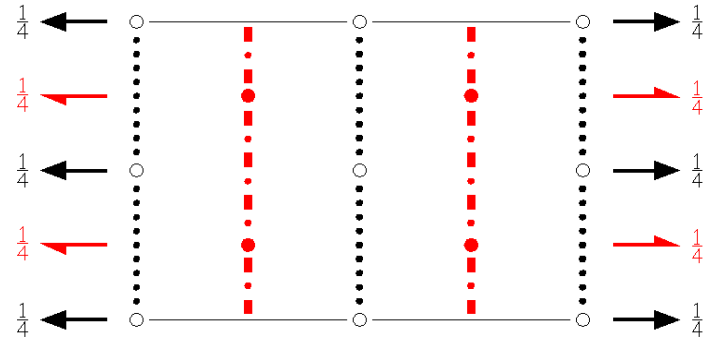
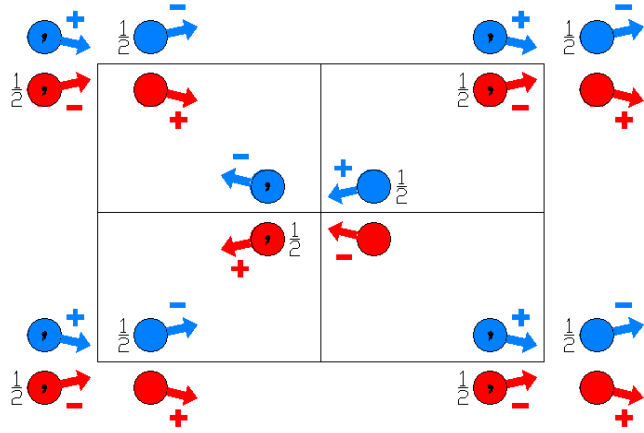
$C_p2/c$

15.6.97

$2/m1'$

$C_p12/c1$

Monoclinic



**Origin** at  $\bar{1}$  on glide plane  $c$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                      |  |  |
|--------------------|--------------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,y,1/4$<br>( $2_y$  0,0,1/2) | (3) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (4) $c$ (0,0,1/2) $x,0,z$<br>( $m_y$  0,0,1/2) |
|--------------------|--------------------------------------|--|--|

For  $(1/2,1/2,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (1/2,1/2,0)<br>(1 1/2,1/2,0)' | (2) $2'$ (0,1/2,0) $1/4,y,1/4$<br>( $2_y$  1/2,1/2,1/2)' | (3) $\bar{1}'$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (4) $n'$ (1/2,0,1/2) $x,1/4,z$<br>( $m_y$  1/2,1/2,1/2)' |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t (1/2,1/2,0)'; (2); (3).

### Positions

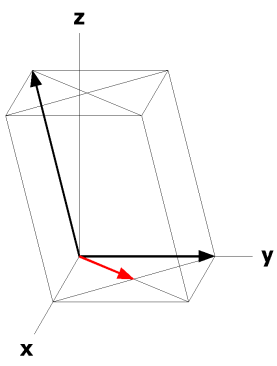
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,0)' +		
8	f	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, \bar{z} + 1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(3) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(4) x, $\bar{y}, z + 1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]
4	e	2	0,y,1/4 [0,v,0]	0, $\bar{y}, 3/4$ [0,v,0]		
4	d	$\bar{1}'$	1/4,1/4,1/2[0,0,0]	3/4,1/4,0 [0,0,0]		
4	c	$\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4	b	$\bar{1}$	0,1/2,0 [u,v,w]	0,1/2,1/2 [ $\bar{u}, \bar{v}, \bar{w}$ ]		
4	a	$\bar{1}$	0,0,0 [u,v,w]	0,0,1/2 [ $\bar{u}, \bar{v}, \bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] c<sub>p</sub>2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}_p$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>-2mg  
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,1/2,0

Along [0,1,0] p<sub>2a</sub>-211  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2 + \mathbf{c}/2$   
 Origin at 0,y,1/4



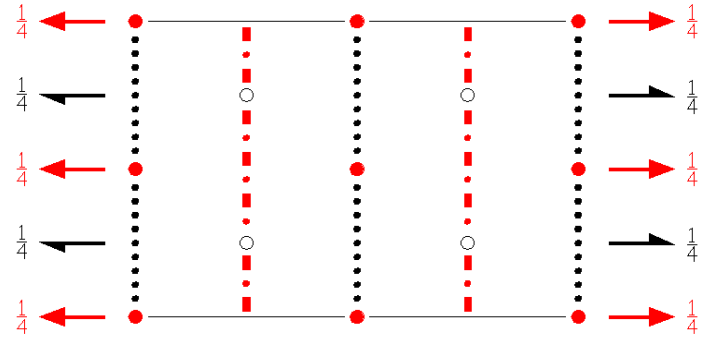
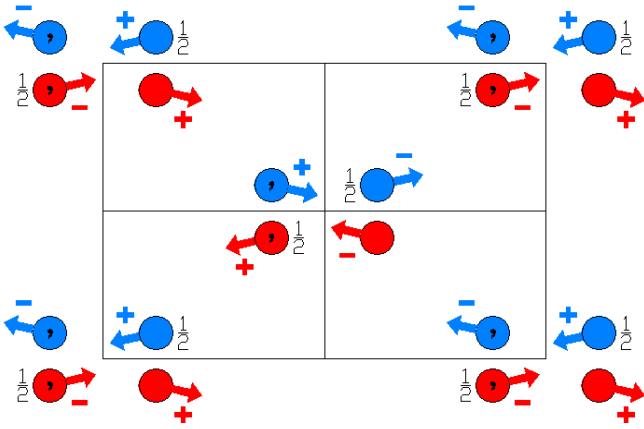
$C_p 2'/c$

15.7.98

$2/m1'$

$C_p 12/c1$

Monoclinic



**Origin** at  $\bar{1}'$  on glide plane c

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) $2'$ $0,y,1/4$<br>( $2_y$  0,0,1/2)' | (3) $\bar{1}'$ $0,0,0$<br>( $\bar{1}$  0,0,0)' | (4) c $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2) |
|--------------------|--|--|--|

For  $(1/2,1/2,0)$ ' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,0)$<br>(1 1/2,1/2,0)' | (2) 2 $(0,1/2,0)$ $1/4,y,1/4$<br>( $2_y$  1/2,1/2,1/2) | (3) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$  1/2,1/2,0) | (4) $n'$ $(1/2,0,1/2)$ $x,1/4,z$<br>( $m_y$  1/2,1/2,1/2)' |
|--|--|--|--|

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,0)'$ ; (2); (3).

**Positions**

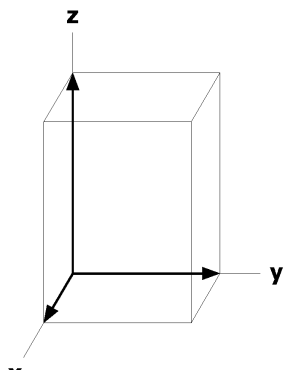
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1/2,1/2,0)' +		
8	f	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(3) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]]	(4) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]
4	e	2'	$0,y,1/4$ [u,0,w]	$0,\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]		
4	d	$\bar{1}$	$1/4,1/4,1/2$ [u,v,w]	$3/4,1/4,0$ [u, $\bar{v}$ ,w]		
4	c	$\bar{1}$	$1/4,1/4,0$ [u,v,w]	$3/4,1/4,1/2$ [u, $\bar{v}$ ,w]		
4	b	$\bar{1}'$	$0,1/2,0$ [0,0,0]	$0,1/2,1/2$ [0,0,0]		
4	a	$\bar{1}'$	$0,0,0$ [0,0,0]	$0,0,1/2$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $c_p2mm$   
 $\mathbf{a}^* = \mathbf{a}_p$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b}2mg$   
 $\mathbf{a}^* = -\mathbf{c}_p$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

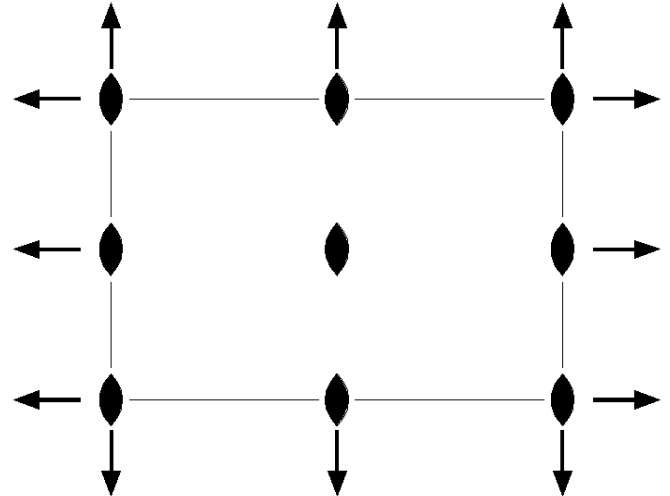
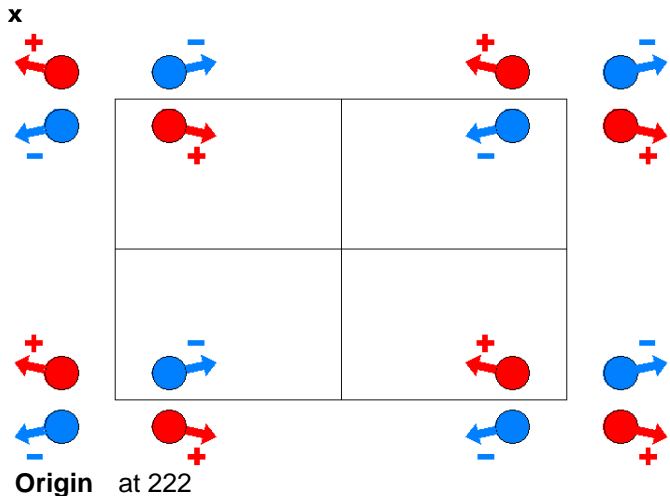
Along [0,1,0]  $p_{2a}211$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2 + \mathbf{c}/2$   
 Origin at 0,y,0



P222  
16.1.99

222  
P222

Orthorhombic



Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 2 0,y,0  
(2<sub>y</sub>|0,0,0)

(4) 2 x,0,0  
(2<sub>x</sub>|0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

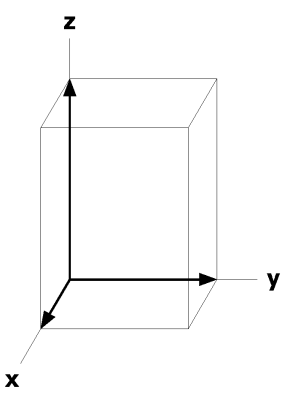
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
4	u	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
2	t	..2	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	s	..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	r	..2	1/2,0,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	q	..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	p	.2.	1/2,y,1/2 [0,v,0]	1/2, $\bar{y}$ ,1/2 [0, $\bar{v}$ ,0]		
2	o	.2.	1/2,y,0 [0,v,0]	1/2, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]		
2	n	.2.	0,y,1/2 [0,v,0]	0, $\bar{y}$ ,1/2 [0, $\bar{v}$ ,0]		
2	m	.2.	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]		
2	l	2..	x,1/2,1/2 [u,0,0]	$\bar{x}$ ,1/2,1/2 [ $\bar{u}$ ,0,0]		
2	k	2..	x,1/2,0 [u,0,0]	$\bar{x}$ ,1/2,0 [ $\bar{u}$ ,0,0]		
2	j	2..	x,0,1/2 [u,0,0]	$\bar{x}$ ,0,1/2 [ $\bar{u}$ ,0,0]		
2	i	2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0]		
1	h	222	1/2,1/2,1/2 [0,0,0]			
1	g	222	0,1/2,1/2 [0,0,0]			
1	f	222	1/2,0,1/2 [0,0,0]			
1	e	222	1/2,1/2,0 [0,0,0]			
1	d	222	0,0,1/2 [0,0,0]			
1	c	222	0,1/2,0 [0,0,0]			
1	b	222	1/2,0,0 [0,0,0]			
1	a	222	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

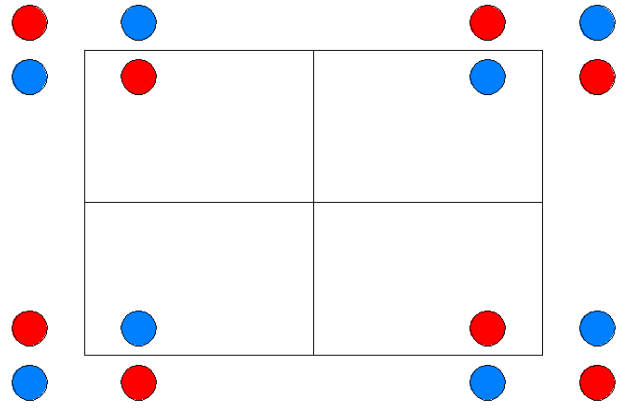
Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



P2221'  
16.2.100

2221'  
P2221'

Orthorhombic



Origin at 2221'

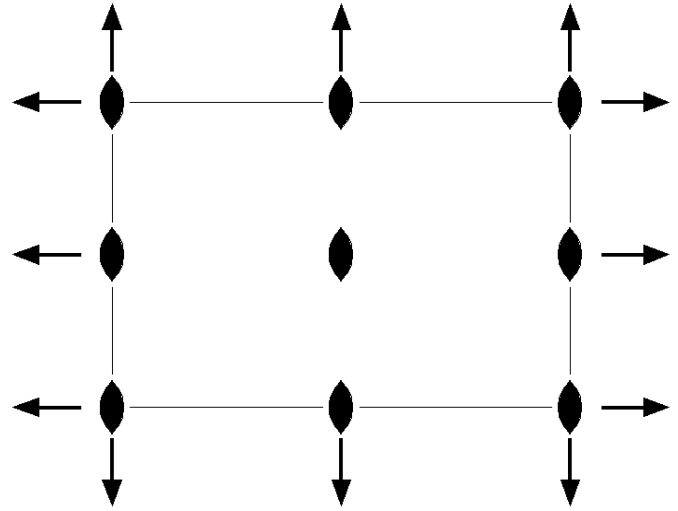
Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) |
|--------------------|--|--|--|

- |                      |  |  |  |
|----------------------|--|--|--|
| (1) 1'<br>(1 0,0,0)' | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |
|----------------------|--|--|--|

1'



For 1 + set

For 1' + set



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

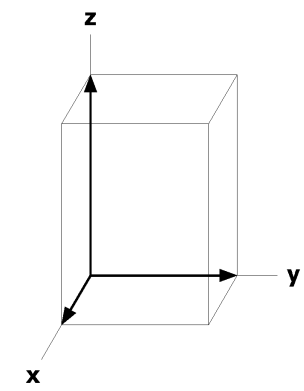
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
4	u 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{x},y,\bar{z}$ [0,0,0]	(4) x, $\bar{y},\bar{z}$ [0,0,0]
2	t ..21'	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
2	s ..21'	0,1/2,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]		
2	r ..21'	1/2,0,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
2	q ..21'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	p .2.1'	1/2,y,1/2 [0,0,0]	1/2, $\bar{y}$ ,1/2 [0,0,0]		
2	o .2.1'	1/2,y,0 [0,0,0]	1/2, $\bar{y}$ ,0 [0,0,0]		
2	n .2.1'	0,y,1/2 [0,0,0]	0, $\bar{y}$ ,1/2 [0,0,0]		
2	m .2.1'	0,y,0 [0,0,0]	0, $\bar{y}$ ,0 [0,0,0]		
2	l 2..1'	x,1/2,1/2 [0,0,0]	$\bar{x}$ ,1/2,1/2 [0,0,0]		
2	k 2..1'	x,1/2,0 [0,0,0]	$\bar{x}$ ,1/2,0 [0,0,0]		
2	j 2..1'	x,0,1/2 [0,0,0]	$\bar{x}$ ,0,1/2 [0,0,0]		
2	i 2..1'	x,0,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0]		
1	h 2221'	1/2,1/2,1/2 [0,0,0]			
1	g 2221'	0,1/2,1/2 [0,0,0]			
1	f 2221'	1/2,0,1/2 [0,0,0]			
1	e 2221'	1/2,1/2,0 [0,0,0]			
1	d 2221'	0,0,1/2 [0,0,0]			
1	c 2221'	0,1/2,0 [0,0,0]			
1	b 2221'	1/2,0,0 [0,0,0]			
1	a 2221'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

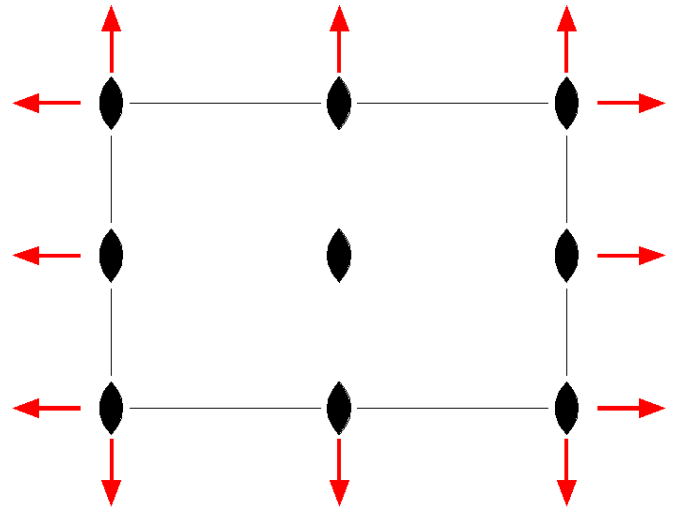
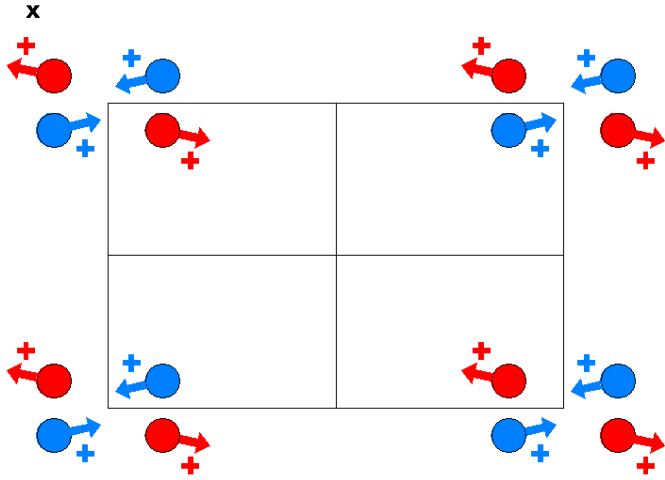
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



P2'2'2'  
16.3.101

2'2'2'  
P2'2'2'

Orthorhombic



Origin at 2'2'2'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) 2'  $0,y,0$   
( $2_y$ |0,0,0)'

(4) 2'  $x,0,0$   
( $2_x$ |0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

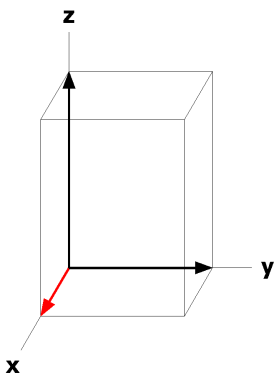
		Coordinates				
Multiplicity,	Wyckoff letter,	Site Symmetry.				
4	u	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]
2	t	..2	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
2	s	..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]		
2	r	..2	1/2,0,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]		
2	q	..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
2	p	.2'	1/2,y,1/2 [u,0,w]	1/2, $\bar{y}$ ,1/2 [ $\bar{u}$ ,0,w]		
2	o	.2'	1/2,y,0 [u,0,w]	1/2, $\bar{y}$ ,0 [ $\bar{u}$ ,0,w]		
2	n	.2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ ,1/2 [ $\bar{u}$ ,0,w]		
2	m	.2'	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [ $\bar{u}$ ,0,w]		
2	l	2'..	x,1/2,1/2 [0,v,w]	$\bar{x}$ ,1/2,1/2 [0, $\bar{v}$ ,w]		
2	k	2'..	x,1/2,0 [0,v,w]	$\bar{x}$ ,1/2,0 [0, $\bar{v}$ ,w]		
2	j	2'..	x,0,1/2 [0,v,w]	$\bar{x}$ ,0,1/2 [0, $\bar{v}$ ,w]		
2	i	2'..	x,0,0 [0,v,w]	$\bar{x}$ ,0,0 [0, $\bar{v}$ ,w]		
1	h	2'2'2	1/2,1/2,1/2 [0,0,w]			
1	g	2'2'2	0,1/2,1/2 [0,0,w]			
1	f	2'2'2	1/2,0,1/2 [0,0,w]			
1	e	2'2'2	1/2,1/2,0 [0,0,w]			
1	d	2'2'2	0,0,1/2 [0,0,w]			
1	c	2'2'2	0,1/2,0 [0,0,w]			
1	b	2'2'2	1/2,0,0 [0,0,w]			
1	a	2'2'2	0,0,0 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



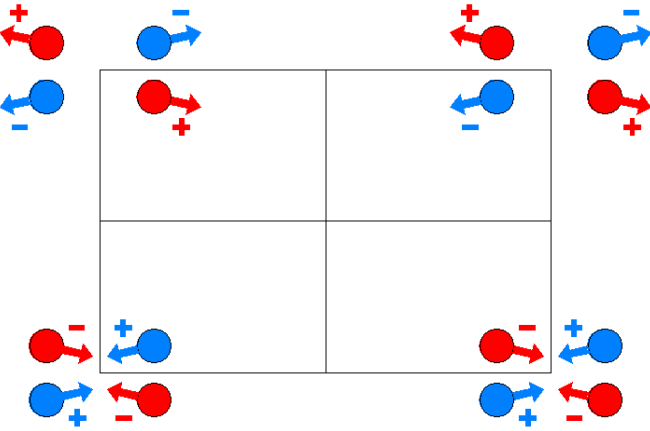
$P_{2a}222$

16.4.102

$2221'$

$P_{2a}222$

Orthorhombic



Origin at 222

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) 2  $0,y,0$   
( $2_y$ |0,0,0)

(4) 2  $x,0,0$   
( $2_x$ |0,0,0)

For (0,0,0) + set

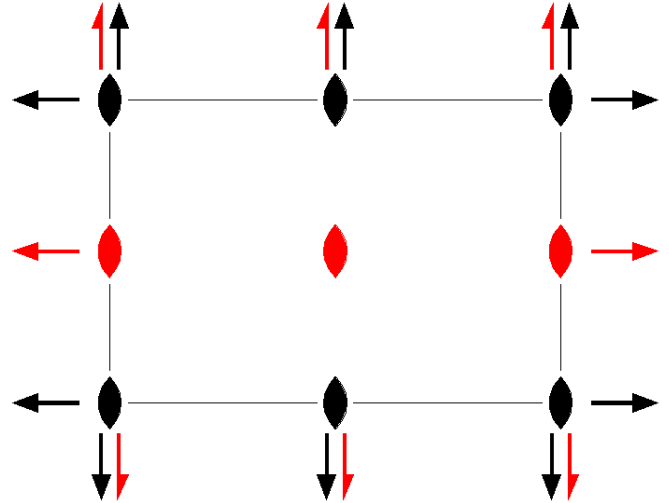
(1)  $t'(1,0,0)$   
(1|1,0,0)'

(2)  $2'(1/2,0,z)$   
( $2_z$ |1,0,0)'

(3)  $2'(1/2,y,0)$   
( $2_y$ |1,0,0)'

(4)  $2'(1,0,0) x,0,0$   
( $2_x$ |1,0,0)'

For (1,0,0)' + set



**Generators selected** (1); t(1,0,0)<sup>1</sup>; t(0,1,0); t(0,0,1); (2); (3).

### Positions

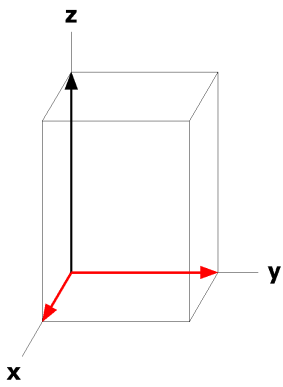
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0) <sup>1</sup> +		
8 u 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
4 t ..2'	1/2,1/2,z [u,v,0]	1/2,1/2, $\bar{z}$ [u, $\bar{v},0$ ]		
4 s ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 r ..2'	1/2,0,z [u,v,0]	1/2,0, $\bar{z}$ [u, $\bar{v},0$ ]		
4 q ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 p .2'	1/2,y,1/2 [u,0,w]	1/2, $\bar{y},1/2$ [u,0, $\bar{w}$ ]		
4 o .2'	1/2,y,0 [u,0,w]	1/2, $\bar{y},0$ [u,0, $\bar{w}$ ]		
4 n .2.	0,y,1/2 [0,v,0]	0, $\bar{y},1/2$ [0, $\bar{v},0$ ]		
4 m .2.	0,y,0 [0,v,0]	0, $\bar{y},0$ [0, $\bar{v},0$ ]		
4 l 2..	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]		
4 k 2..	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]		
4 j 2..	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]		
4 i 2..	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]		
2 h 22'2'	1/2,1/2,1/2 [u,0,0]			
2 g 222	0,1/2,1/2 [0,0,0]			
2 f 22'2'	1/2,0,1/2 [u,0,0]			
2 e 22'2'	1/2,1/2,0 [u,0,0]			
2 d 222	0,0,1/2 [0,0,0]			
2 c 222	0,1/2,0 [0,0,0]			
2 b 22'2'	1/2,0,0 [u,0,0]			
2 a 222	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



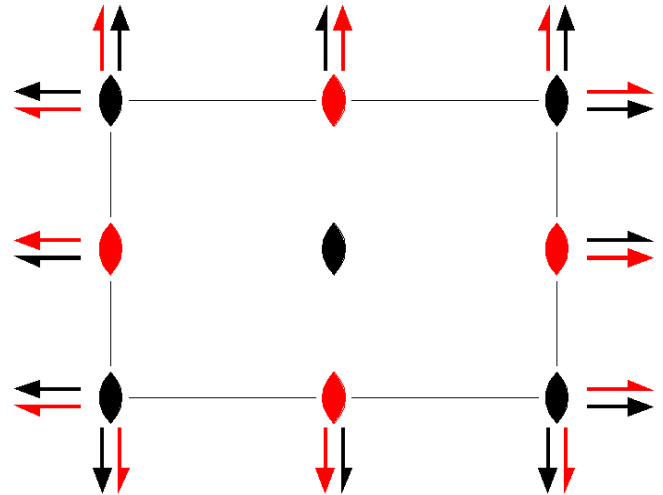
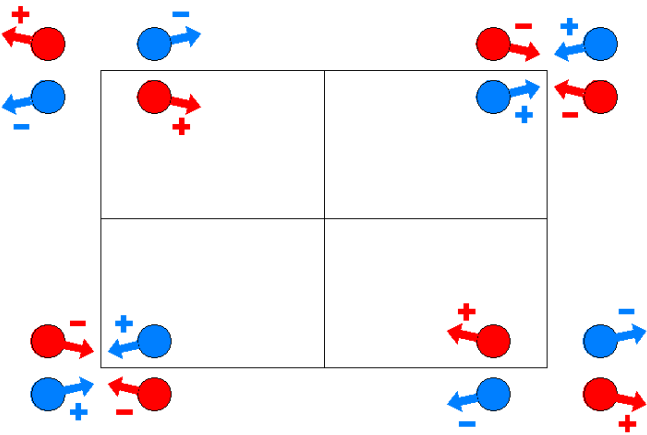
$P_C222$

16.5.103

$2221'$

$P_C222$

Orthorhombic



Origin at 222

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) 2  $0,y,0$   
( $2_y$ |0,0,0)

(4) 2  $x,0,0$   
( $2_x$ |0,0,0)

For (1,0,0)' + set

(1)  $t'(1,0,0)$   
( $1|1,0,0$ )'

(2)  $2' 1/2,0,z$   
( $2_z|1,0,0$ )'

(3)  $2' 1/2,y,0$   
( $2_y|1,0,0$ )'

(4)  $2' (1,0,0) x,0,0$   
( $2_x|1,0,0$ )'

**Generators selected** (1); t(1,0,0)<sup>1</sup>; t(0,1,0)<sup>1</sup>; t(0,0,1); (2); (3).

**Positions**

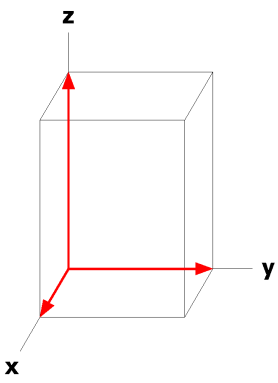
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0) <sup>1</sup> +		
8 u 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
4 t ..2	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 s ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}$ [ $\bar{u},v,0$ ]		
4 r ..2'	1/2,0,z [u,v,0]	1/2,0, $\bar{z}$ [u, $\bar{v},0$ ]		
4 q ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 p .2'	1/2,y,1/2 [u,0,w]	1/2, $\bar{y},1/2$ [u,0, $\bar{w}$ ]		
4 o .2'	1/2,y,0 [u,0,w]	1/2, $\bar{y},0$ [u,0, $\bar{w}$ ]		
4 n .2.	0,y,1/2 [0,v,0]	0, $\bar{y},1/2$ [0, $\bar{v},0$ ]		
4 m .2.	0,y,0 [0,v,0]	0, $\bar{y},0$ [0, $\bar{v},0$ ]		
4 l 2'..	x,1/2,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0,v, $\bar{w}$ ]		
4 k 2'..	x,1/2,0 [0,v,w]	$\bar{x},1/2,0$ [0,v, $\bar{w}$ ]		
4 j 2..	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]		
4 i 2..	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]		
2 h 2'2'2	1/2,1/2,1/2 [0,0,w]			
2 g 2'22'	0,1/2,1/2 [0,v,0]			
2 f 22'2'	1/2,0,1/2 [u,0,0]			
2 e 2'2'2	1/2,1/2,0 [0,0,w]			
2 d 222	0,0,1/2 [0,0,0]			
2 c 2'22'	0,1/2,0 [0,v,0]			
2 b 22'2'	1/2,0,0 [u,0,0]			
2 a 222	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

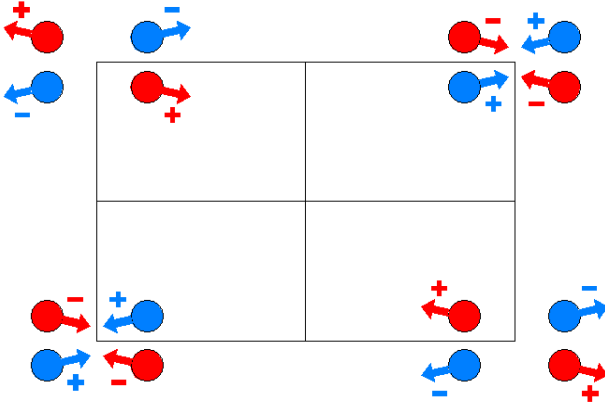
Along [0,0,1] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/2,1/2,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



$P_{F222}$   
16.6.104



Origin at 222

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) 2  $0,y,0$   
( $2_y$ |0,0,0)

(4) 2  $x,0,0$   
( $2_x$ |0,0,0)

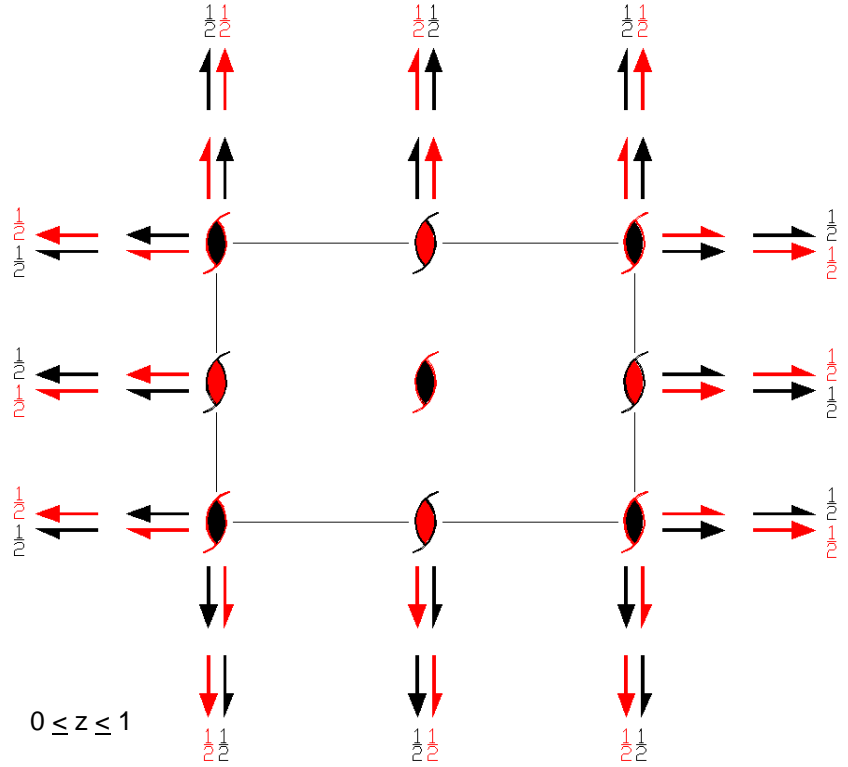
(1)  $t'(1,0,0)$   
(1|1,0,0)'

(2)  $2'(1/2,0,z)$   
( $2_z$ |1,0,0)'

(3)  $2'(1/2,y,0)$   
( $2_y$ |1,0,0)'

(4)  $2'(1,0,0) x,0,0$   
( $2_x$ |1,0,0)'

$2221'$   
 $P_{F222}$



For (0,0,0) + set

For (1,0,0)' + set

Orthorhombic



**Generators selected** (1); t(1,0,0)<sup>1</sup>; t(0,1,0)<sup>1</sup>; t(0,0,1)<sup>1</sup>; (2); (3).

**Positions**

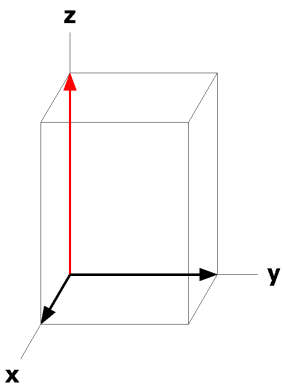
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0) <sup>1</sup> +		
8 u 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
4 t ..2	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
4 s ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}$ [ $\bar{u},v,0$ ]		
4 r ..2'	1/2,0,z [u,v,0]	1/2,0, $\bar{z}$ [u, $\bar{v},0$ ]		
4 q ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 p .2.	1/2,y,1/2 [0,v,0]	1/2, $\bar{y},1/2$ [0,v,0]		
4 o .2'	1/2,y,0 [u,0,w]	1/2, $\bar{y},0$ [u,0, $\bar{w}$ ]		
4 n .2'	0,y,1/2 [u,0,w]	0, $\bar{y},1/2$ [ $\bar{u},0,w$ ]		
4 m .2.	0,y,0 [0,v,0]	0, $\bar{y},0$ [0, $\bar{v},0$ ]		
4 l 2..	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]		
4 k 2'..	x,1/2,0 [0,v,w]	$\bar{x},1/2,0$ [0,v, $\bar{w}$ ]		
4 j 2'..	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]		
4 i 2..	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]		
2 h 222	1/2,1/2,1/2 [0,0,0]			
2 g 22'2'	0,1/2,1/2 [u,0,0]			
2 f 2'22'	1/2,0,1/2 [0,v,0]			
2 e 2'2'2	1/2,1/2,0 [0,0,w]			
2 d 2'2'2	0,0,1/2 [0,0,w]			
2 c 2'22'	0,1/2,0 [0,v,0]			
2 b 22'2'	1/2,0,0 [u,0,0]			
2 a 222	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



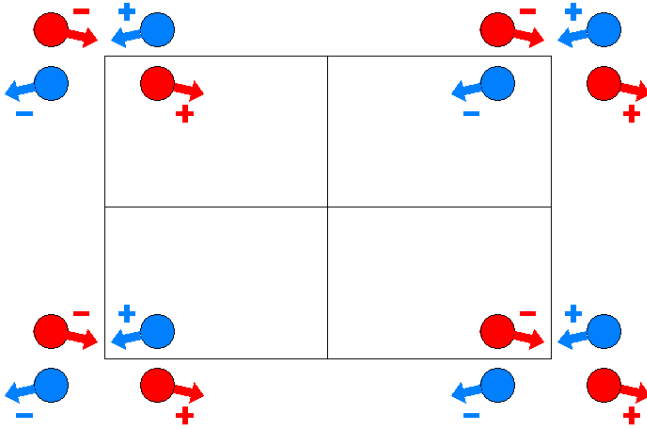
$P_{2c}22'2'$

16.7.105

$2221'$

$P_{2c}22'2'$

Orthorhombic



Origin at  $22'2'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2)  $2'_z$  0,0,z  
( $2_z$ |0,0,0)'

(3)  $2'_y$  0,y,0  
( $2_y$ |0,0,0)'

(4) 2 x,0,0  
( $2_x$ |0,0,0)

For (0,0,0) + set

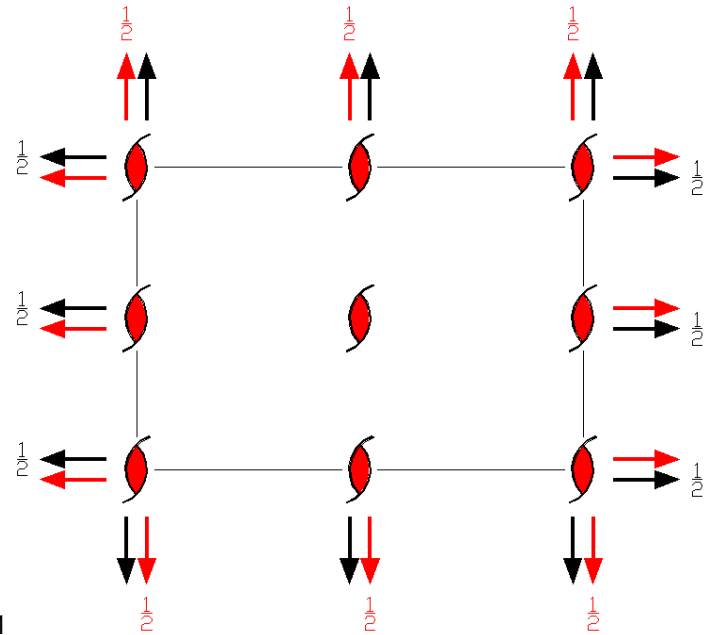
For (0,0,1)' + set

(1)  $t'_z$  (0,0,1)  
(1|0,0,1)'

(2) 2 (0,0,1) 0,0,z  
( $2_z$ |0,0,1)

(3) 2 0,y,1/2  
( $2_y$ |0,0,1)

(4)  $2'_x$  x,0,1/2  
( $2_x$ |0,0,1)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

**Positions**

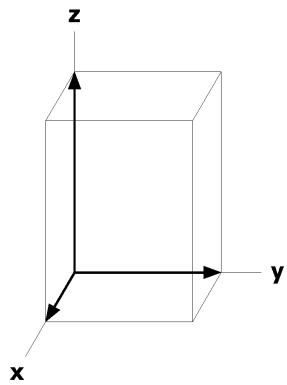
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
8 u 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
4 t ..2'	1/2,1/2,z [u,v,0]	1/2,1/2, $\bar{z}$ [u, $\bar{v}$ ,0]		
4 s ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}$ [u, $\bar{v}$ ,0]		
4 r ..2'	1/2,0,z [u,v,0]	1/2,0, $\bar{z}$ [u, $\bar{v}$ ,0]		
4 q ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [u, $\bar{v}$ ,0]		
4 p .2.	1/2,y,1/2 [0,v,0]	1/2, $\bar{y}$ ,1/2 [0,v,0]		
4 o .2'.	1/2,y,0 [u,0,w]	1/2, $\bar{y}$ ,0 [u,0, $\bar{w}$ ]		
4 n .2.	0,y,1/2 [0,v,0]	0, $\bar{y}$ ,1/2 [0,v,0]		
4 m .2'.	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [u,0, $\bar{w}$ ]		
4 l 2'..	x,1/2,1/2 [0,v,w]	$\bar{x}$ ,1/2,1/2 [0,v, $\bar{w}$ ]		
4 k 2..	x,1/2,0 [u,0,0]	$\bar{x}$ ,1/2,0 [u,0,0]		
4 j 2'..	x,0,1/2 [0,v,w]	$\bar{x}$ ,0,1/2 [0,v, $\bar{w}$ ]		
4 i 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [u,0,0]		
2 h 2'22'	1/2,1/2,1/2 [0,v,0]			
2 g 2'22'	0,1/2,1/2 [0,v,0]			
2 f 2'22'	1/2,0,1/2 [0,v,0]			
2 e 22'2'	1/2,1/2,0 [u,0,0]			
2 d 2'22'	0,0,1/2 [0,v,0]			
2 c 22'2'	0,1/2,0 [u,0,0]			
2 b 22'2'	1/2,0,0 [u,0,0]			
2 a 22'2'	0,0,0 [u,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

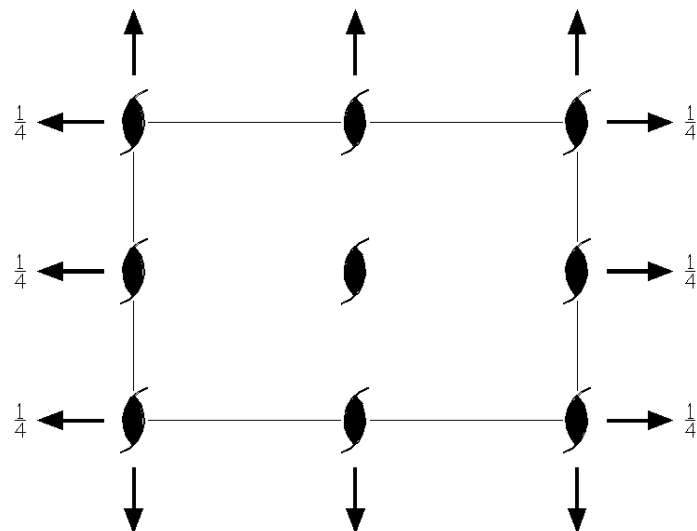
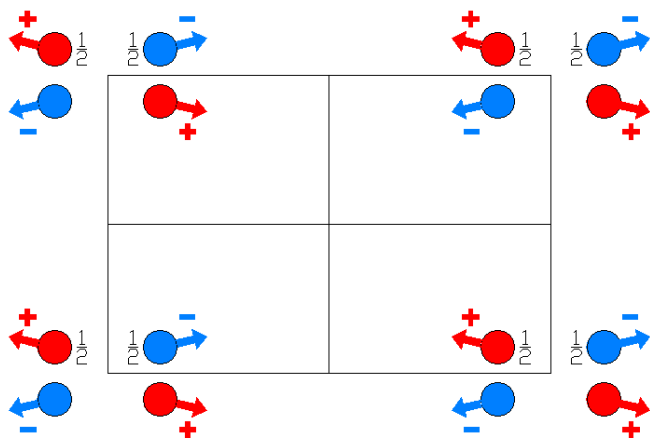
Along [0,1,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 1/2,y,0



P222<sub>1</sub>  
17.1.106

222  
P222<sub>1</sub>

Orthorhombic



Origin at 212<sub>1</sub>

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)

(3) 2 0,y,1/4  
(2<sub>y</sub>|0,0,1/2)

(4) 2 x,0,0  
(2<sub>x</sub>|0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

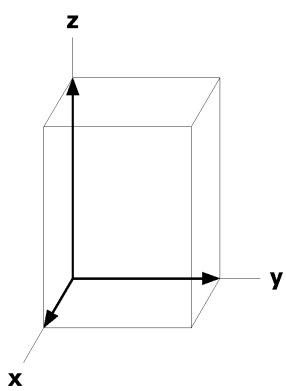
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
4	e	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
2	d	.2.	1/2,y,1/4 [0,v,0]	1/2, $\bar{y}, 3/4$ [0, $\bar{v}, 0$ ]		
2	c	.2.	0,y,1/4 [0,v,0]	0, $\bar{y}, 3/4$ [0, $\bar{v}, 0$ ]		
2	b	2..	x,1/2,0 [u,0,0]	$\bar{x}, 1/2, 1/2$ [ $\bar{u}, 0, 0$ ]		
2	a	2..	x,0,0 [u,0,0]	$\bar{x}, 0, 1/2$ [ $\bar{u}, 0, 0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



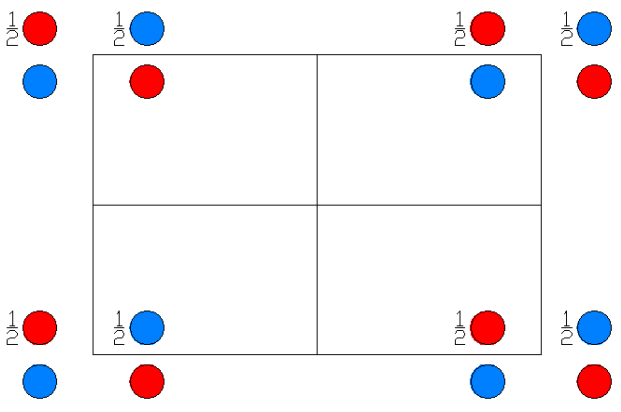
P222<sub>1</sub>'

17.2.107

2221'

P222<sub>1</sub>'

Orthorhombic



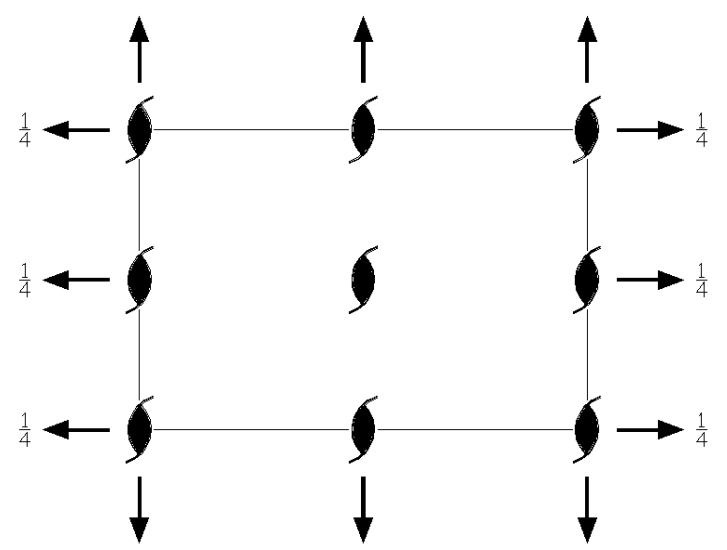
Origin at 212<sub>1</sub>'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

- |                      |  |  |  |
|----------------------|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)   | (3) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (1) 1'<br>(1 0,0,0)' | (2) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)' | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)' | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |

1'



For 1 + set

For 1' + set

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

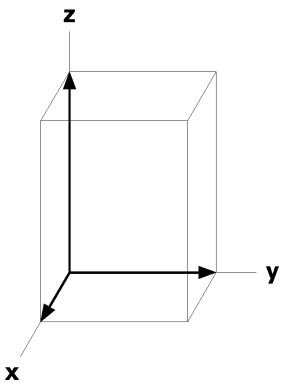
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
4 e 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y}, z+1/2$ [0,0,0]	(3) $\bar{x}, y, \bar{z}+1/2$ [0,0,0]	(4) x, $\bar{y}, \bar{z}$ [0,0,0]
2 d .2.1'	1/2,y,1/4 [0,0,0]	1/2, $\bar{y}$ , 3/4 [0,0,0]		
2 c .2.1'	0,y,1/4 [0,0,0]	0, $\bar{y}$ , 3/4 [0,0,0]		
2 b 2..1'	x,1/2,0 [0,0,0]	$\bar{x}$ , 1/2, 1/2 [0,0,0]		
2 a 2..1'	x,0,0 [0,0,0]	$\bar{x}$ , 0, 1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

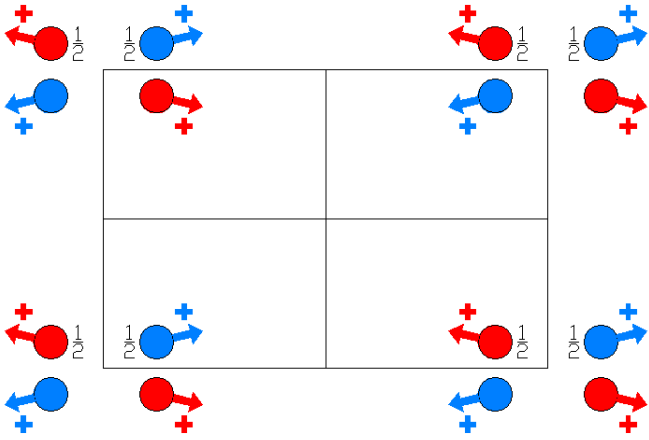
Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



P2'2'2<sub>1</sub>  
17.3.108

2'2'2  
P2'2'2<sub>1</sub>

Orthorhombic



Origin at 2'12<sub>1</sub>

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

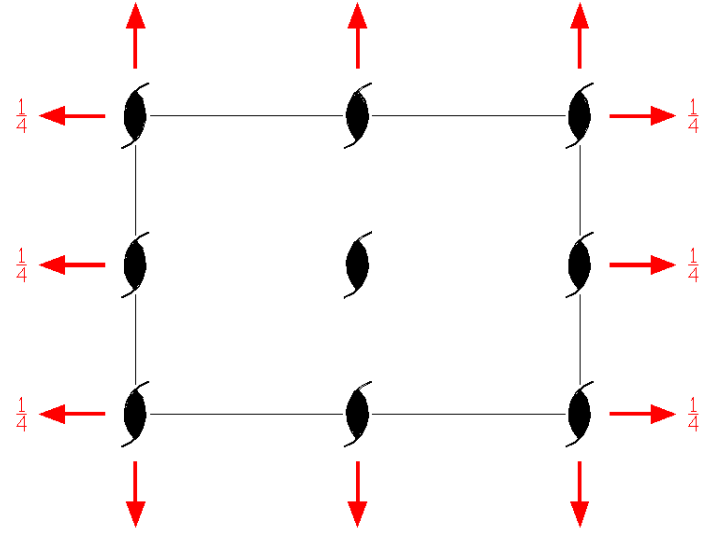
**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)

(3) 2' 0,y,1/4  
(2<sub>y</sub>|0,0,1/2)'

(4) 2' x,0,0  
(2<sub>x</sub>|0,0,0)'





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

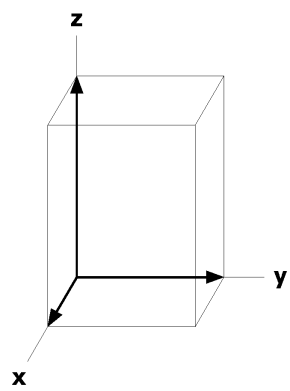
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
4	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}+1/2$ [u, $\bar{v}, w$ ]	(4) x, $\bar{y}, \bar{z}$ [ $\bar{u}, v, w$ ]
2	d .2'	1/2,y,1/4 [u,0,w]	1/2, $\bar{y}, 3/4$ [ $\bar{u}, 0, w$ ]		
2	c .2'	0,y,1/4 [u,0,w]	0, $\bar{y}, 3/4$ [ $\bar{u}, 0, w$ ]		
2	b 2'..	x,1/2,0 [0,v,w]	$\bar{x}, 1/2, 1/2$ [0, $\bar{v}, w$ ]		
2	a 2'..	x,0,0 [0,v,w]	$\bar{x}, 0, 1/2$ [0, $\bar{v}, w$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

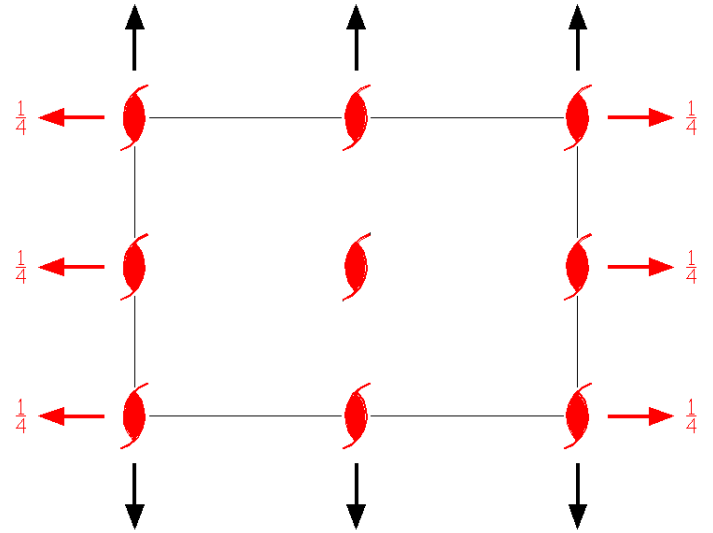
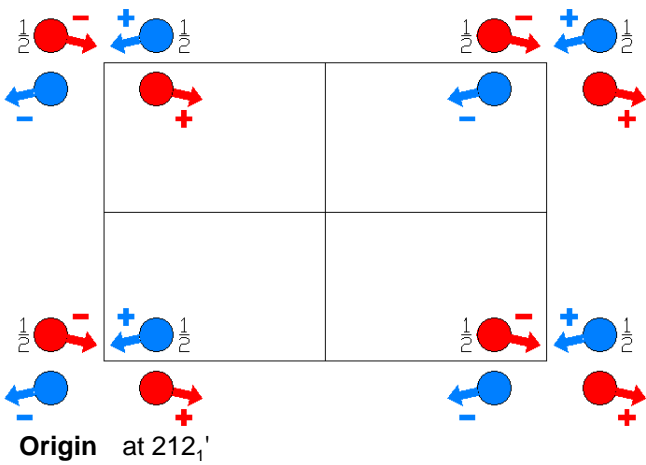
Along [0,1,0] p2'mg'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



P22'2<sub>1</sub>'  
17.4.109

22'2'  
P22'2<sub>1</sub>'

Orthorhombic



Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

- (1) 1  
(1|0,0,0)
- (2) 2' (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)'
- (3) 2' 0,y,1/4  
(2<sub>y</sub>|0,0,1/2)'
- (4) 2 x,0,0  
(2<sub>x</sub>|0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

### Positions

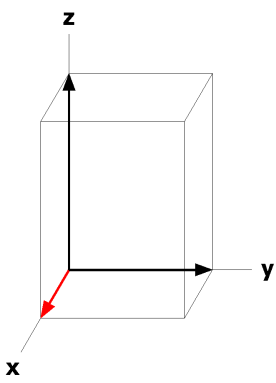
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
4	e	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
2	d	.2'	1/2,y,1/4 [u,0,w]	1/2, $\bar{y}$ ,3/4 [u,0, $\bar{w}$ ]		
2	c	.2'	0,y,1/4 [u,0,w]	0, $\bar{y}$ ,3/4 [u,0, $\bar{w}$ ]		
2	b	2..	x,1/2,0 [u,0,0]	$\bar{x}$ ,1/2,1/2 [u,0,0]		
2	a	2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,1/2 [u,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



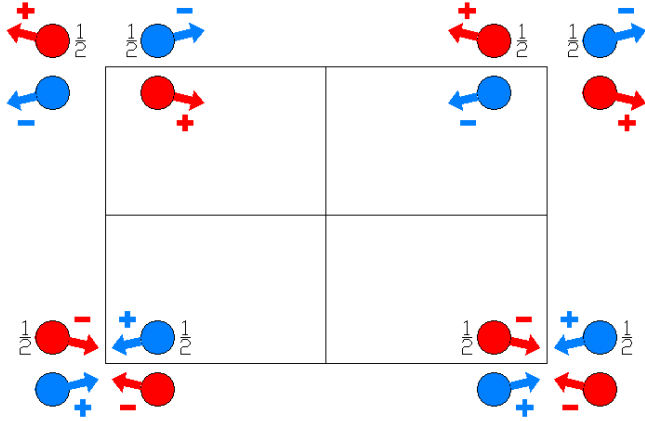
$P_{2a} 222_1$

17.5.110

$2221'$

$P_{2a} 222_1$

Orthorhombic



Origin at  $212_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)

(3) 2 0,y,1/4  
(2<sub>y</sub>|0,0,1/2)

(4) 2 x,0,0  
(2<sub>x</sub>|0,0,0)

For (0,0,0) + set

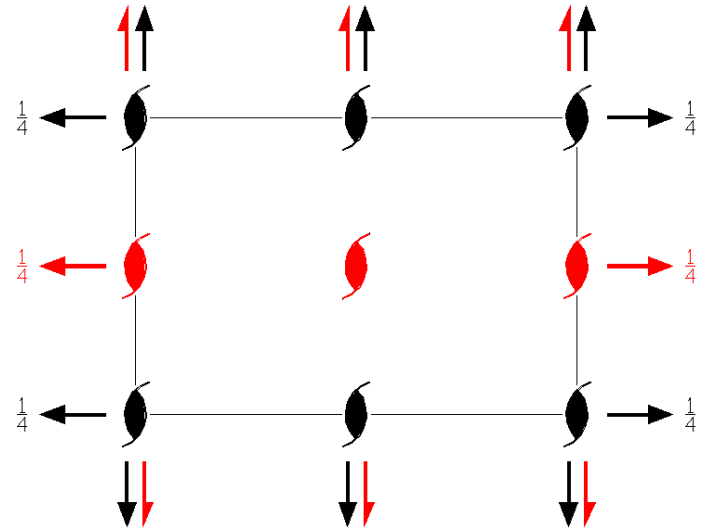
(1) t' (1,0,0)  
(1|1,0,0)'

(2) 2' (0,0,1/2) 1/2,0,z  
(2<sub>z</sub>|1,0,1/2)'

(3) 2' 1/2,y,1/4  
(2<sub>y</sub>|1,0,1/2)'

(4) 2' (1,0,0) x,0,0  
(2<sub>x</sub>|1,0,0)'

For (1,0,0)' + set



**Generators selected** (1); t(1,0,0)<sup>1</sup>; t(0,1,0); t(0,0,1); (2); (3).

### Positions

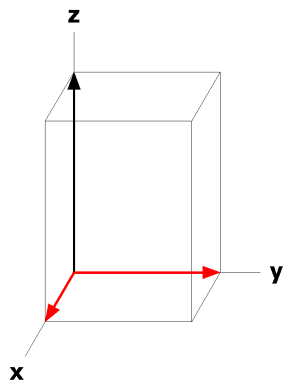
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1,0,0) <sup>1</sup> +	
8 e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
4 d .2'	1/2,y,1/4 [u,0,w]	1/2, $\bar{y}, 3/4$ [u,0, $\bar{w}$ ]		
4 c .2.	0,y,1/4 [0,v,0]	0, $\bar{y}, 3/4$ [0, $\bar{v}, 0$ ]		
4 b 2..	x,1/2,0 [u,0,0]	$\bar{x}, 1/2, 1/2$ [ $\bar{u}, 0, 0$ ]		
4 a 2..	x,0,0 [u,0,0]	$\bar{x}, 0, 1/2$ [ $\bar{u}, 0, 0$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>·2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2b</sub>·2m'g'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



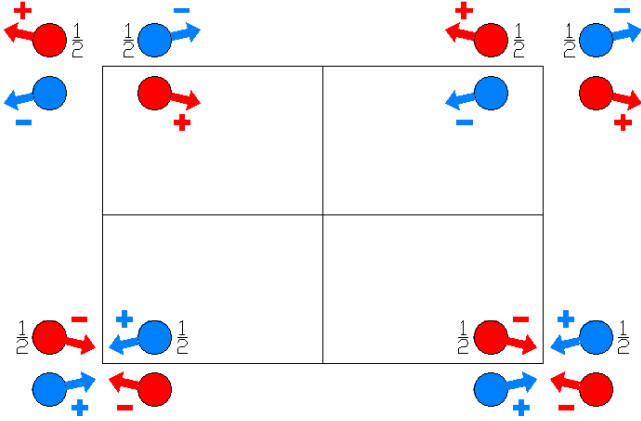
$P_C 222_1$

17.6.111

$2221'$

$P_C 222_1$

Orthorhombic



Origin at  $212_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)

(3) 2 0,y,1/4  
(2<sub>y</sub>|0,0,1/2)

(4) 2 x,0,0  
(2<sub>x</sub>|0,0,0)

For (0,0,0) + set

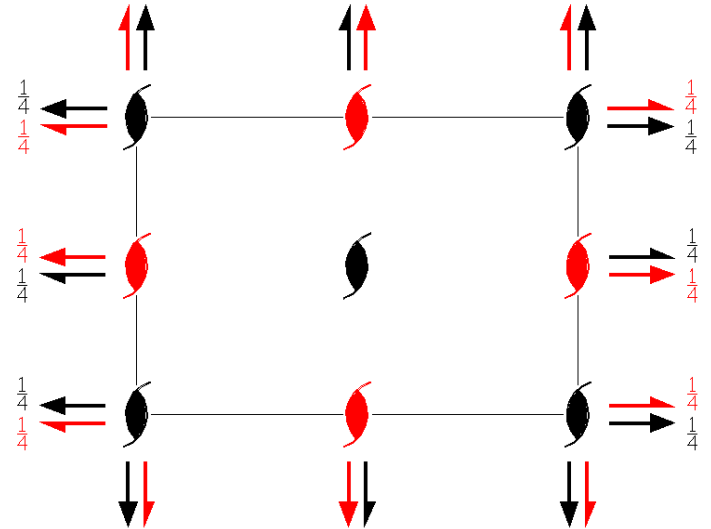
For (1,0,0)' + set

(1) t' (1,0,0)  
(1|1,0,0)'

(2) 2' (0,0,1/2) 1/2,0,z  
(2<sub>z</sub>|1,0,1/2)'

(3) 2' 1/2,y,1/4  
(2<sub>y</sub>|1,0,1/2)'

(4) 2' (1,0,0) x,0,0  
(2<sub>x</sub>|1,0,0)'



**Generators selected** (1); t(1,0,0)<sup>'</sup>; t(0,1,0)<sup>'</sup>; t(0,0,1); (2); (3).

### Positions

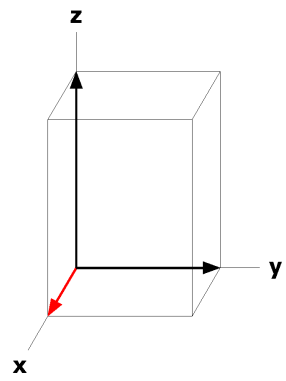
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1,0,0) <sup>'</sup> +	
8 e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) x, $\bar{y}, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]
4 d .2'	1/2,y,1/4 [u,0,w]	1/2, $\bar{y}, 3/4$ [u,0, $\bar{w}$ ]		
4 c .2.	0,y,1/4 [0,v,0]	0, $\bar{y}, 3/4$ [0, $\bar{v}, 0$ ]		
4 b 2'..	x,1/2,0 [0,v,w]	$\bar{x}, 1/2, 1/2$ [0,v, $\bar{w}$ ]		
4 a 2..	x,0,0 [u,0,0]	$\bar{x}, 0, 1/2$ [ $\bar{u}, 0, 0$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/2,1/2,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



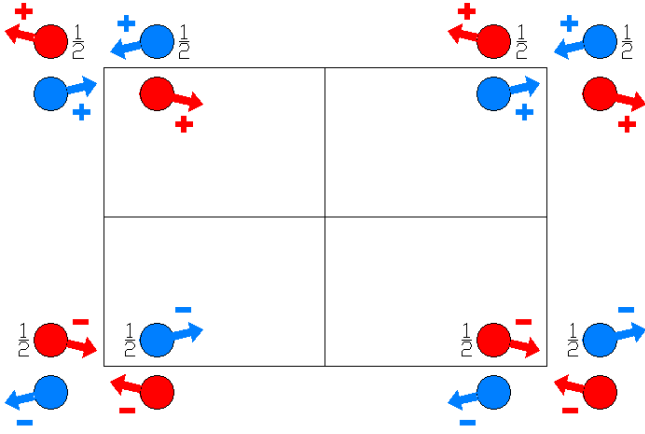
$P_{2a} 2'2'2_1$

17.7.112

2221'

$P_{2a} 2'2'2_1$

Orthorhombic

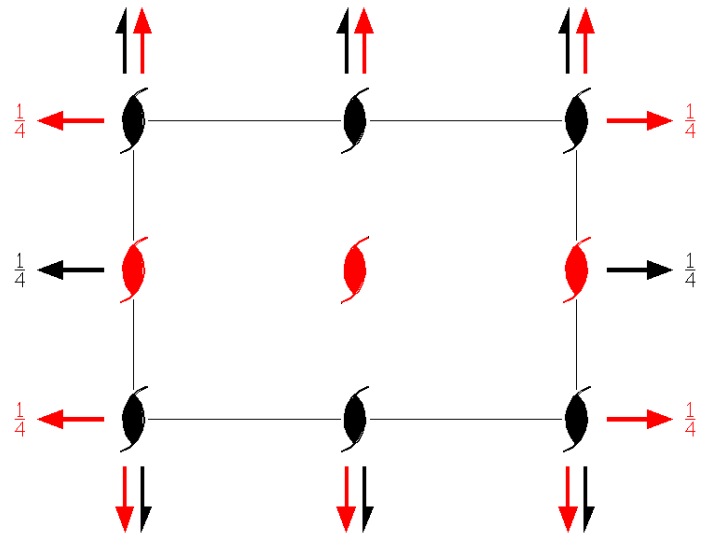


Origin at  $2'12_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

- |                              |  |  |  |
|------------------------------|--|--|--|
| For (0,0,0) + set            |  |  |  |
| (1) 1<br>(1 0,0,0)           | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)     | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)' | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'       |
| For (1,0,0)' + set           |  |  |  |
| (1) t' (1,0,0)<br>(1 1,0,0)' | (2) 2' (0,0,1/2) 1/2,0,z<br>(2 <sub>z</sub>  1,0,1/2)' | (3) 2 1/2,y,1/4<br>(2 <sub>y</sub>  1,0,1/2) | (4) 2 (1,0,0) x,0,0<br>(2 <sub>x</sub>  1,0,0) |





**Generators selected** (1); t(1,0,0)<sup>'</sup>; t(0,1,0); t(0,0,1); (2); (3).

### Positions

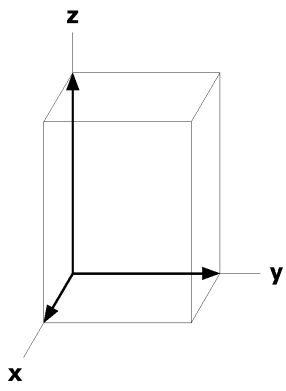
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0) <sup>'</sup> +		
8 e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
4 d .2.	1/2,y,1/4 [0,v,0]	1/2, $\bar{y}, 3/4$ [0,v,0]		
4 c .2'	0,y,1/4 [u,0,w]	0, $\bar{y}, 3/4$ [ $\bar{u}, 0, w$ ]		
4 b 2..	x,1/2,0 [u,0,0]	$\bar{x}, 1/2, 1/2$ [ $\bar{u}, 0, 0$ ]		
4 a 2..	x,0,0 [u,0,0]	$\bar{x}, 0, 1/2$ [ $\bar{u}, 0, 0$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>·2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2b</sub>·2mg'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 1/2,y,1/4



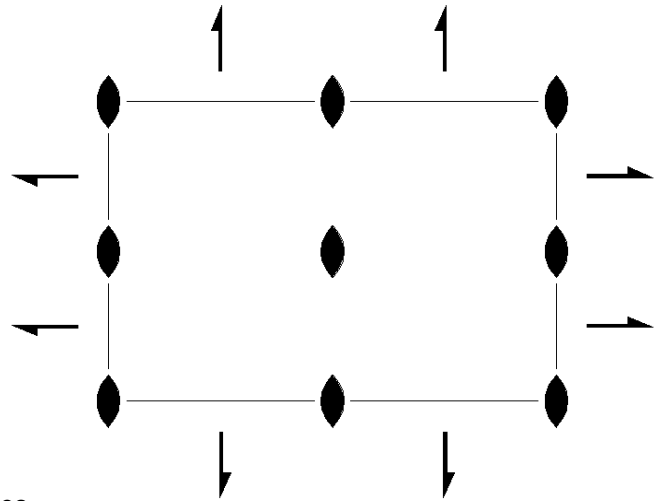
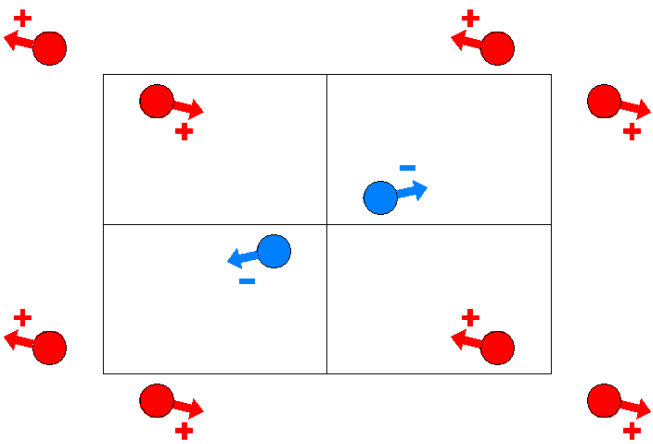
$P2_12_12$

18.1.113

222

$P2_12_12$

Orthorhombic



**Origin** at intersection of 2 with perpendicular plane containing  $2_1$  axes

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 2 (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)

(4) 2 (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

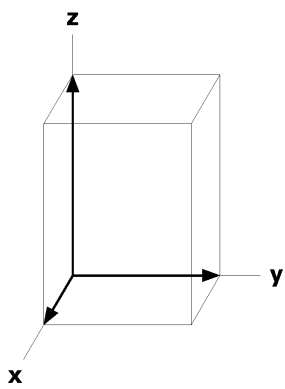
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
4	c	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
2	b	..2	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	a	..2	0,0,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2g'g'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



$P2_12_12_1'$

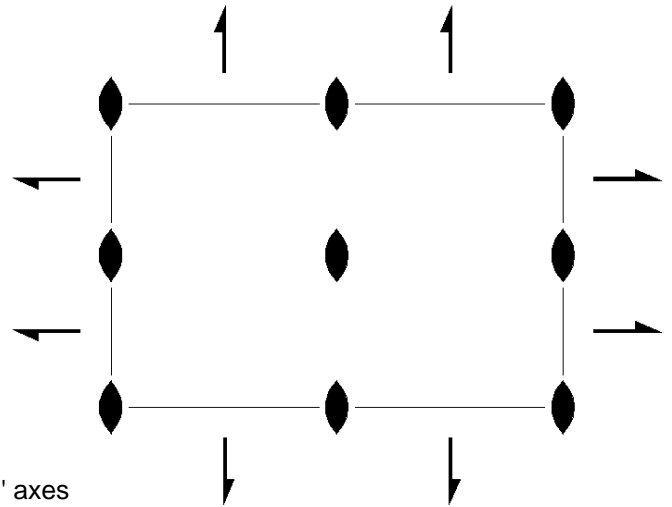
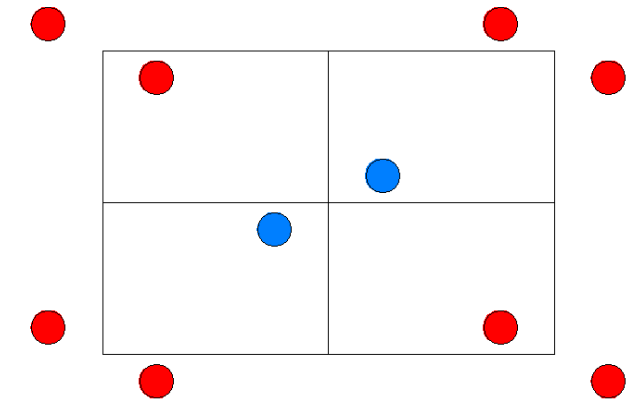
18.2.114

$2221'$

$P2_12_12_1'$

Orthorhombic

$1'$



**Origin** at intersection of  $2_1'$  with perpendicular plane containing  $2_1, 1'$  axes

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For  $1 +$  set

(1)  $1$   
( $1|0,0,0$ )

(2)  $2$   $0,0,z$   
( $2_z|0,0,0$ )

(3)  $2$   $(0,1/2,0)$   $1/4,y,0$   
( $2_y|1/2,1/2,0$ )

(4)  $2$   $(1/2,0,0)$   $x,1/4,0$   
( $2_x|1/2,1/2,0$ )

For  $1' +$  set

(1)  $1'$   
( $1|0,0,0$ )'

(2)  $2'$   $0,0,z$   
( $2_z|0,0,0$ )'

(3)  $2'$   $(0,1/2,0)$   $1/4,y,0$   
( $2_y|1/2,1/2,0$ )'

(4)  $2'$   $(1/2,0,0)$   $x,1/4,0$   
( $2_x|1/2,1/2,0$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3), 1'.

**Positions**

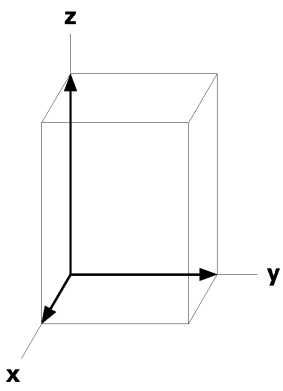
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
4 c 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [0,0,0]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [0,0,0]
2 b ..21'	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
2 a ..21'	0,0,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



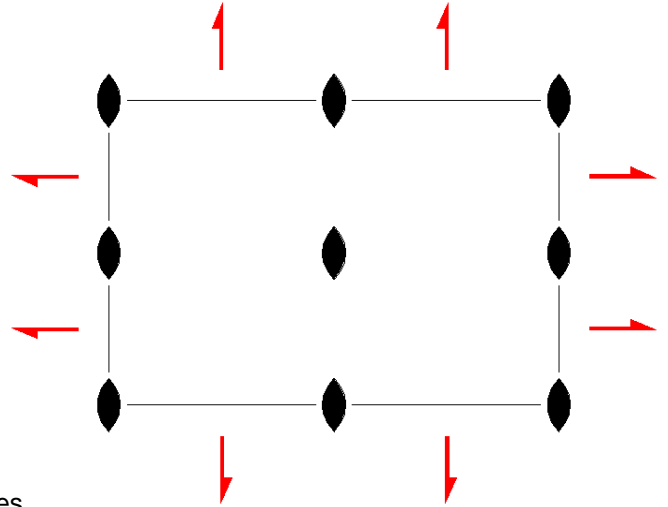
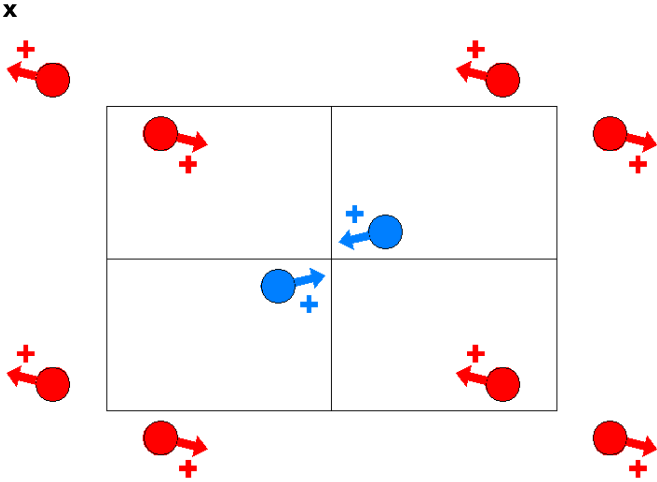
$P2_1'2_1'2$

18.3.115

$2'2'2$

$P2_1'2_1'2$

Orthorhombic



**Origin** at intersection of 2 with perpendicular plane containing  $2_1'$  axes

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 2' (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)'

(4) 2' (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

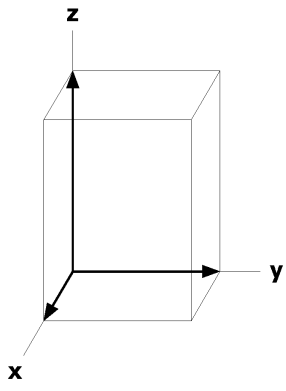
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
4	c	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $u,\bar{v},w$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]
2	b	..2	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]		
2	a	..2	0,0,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

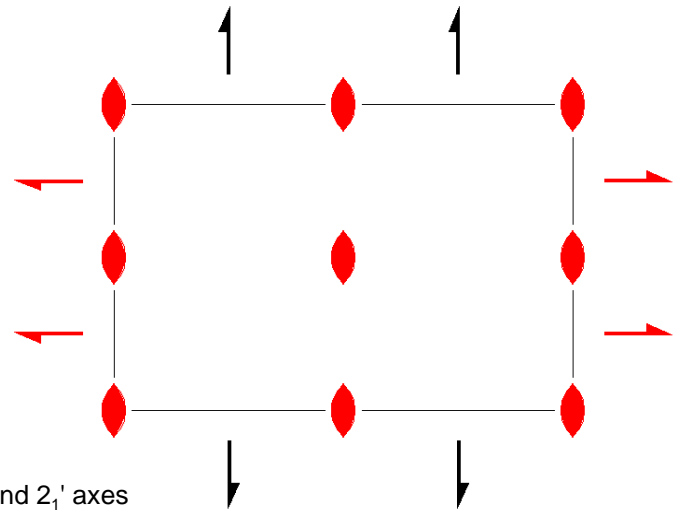
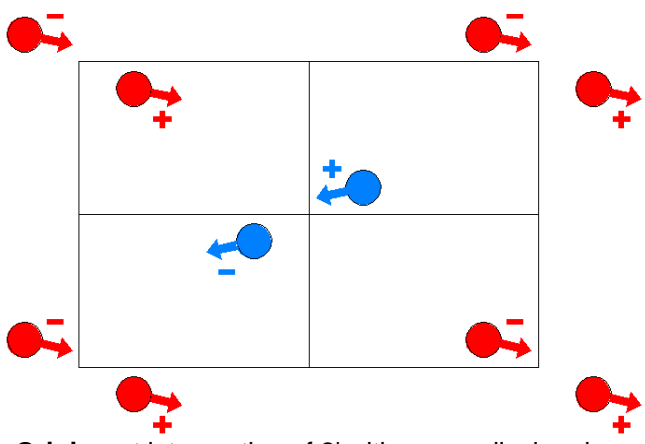
Along [0,1,0] p2'm'g  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



$P2_12_1'2'$   
18.4.116

$22'2'$   
 $P2_12_1'2'$

Orthorhombic



**Origin** at intersection of  $2'$  with perpendicular plane containing  $2_1$  and  $2_1'$  axes

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

- (1) 1  
(1|0,0,0)
- (2)  $2'$  0,0,z  
( $2_z$ |0,0,0)'
- (3)  $2'$  (0,1/2,0)  $1/4,y,0$   
( $2_y$ |1/2,1/2,0)'
- (4) 2 (1/2,0,0)  $x,1/4,0$   
( $2_x$ |1/2,1/2,0)



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

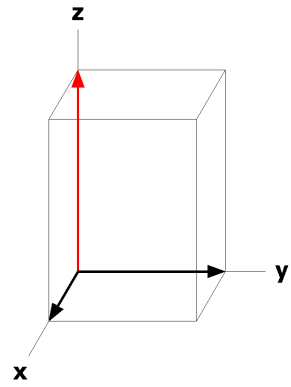
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
4	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [u, $\bar{v}$ ,w]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [u, $\bar{v},\bar{w}$ ]
2	b ..2'	0,1/2,z [u,v,0]	1/2,0, $\bar{z}$ [u, $\bar{v}$ ,0]		
2	a ..2'	0,0,z [u,v,0]	1/2,1/2, $\bar{z}$ [u, $\bar{v}$ ,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2'gg'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0] p2'mg'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



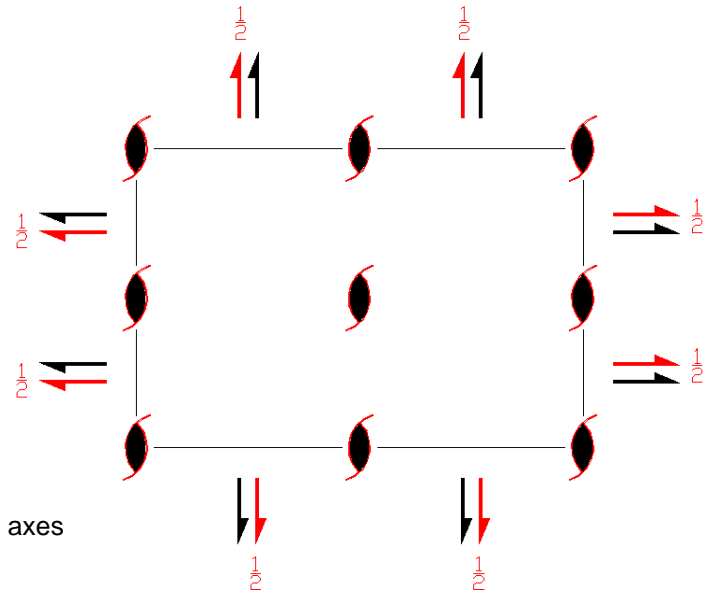
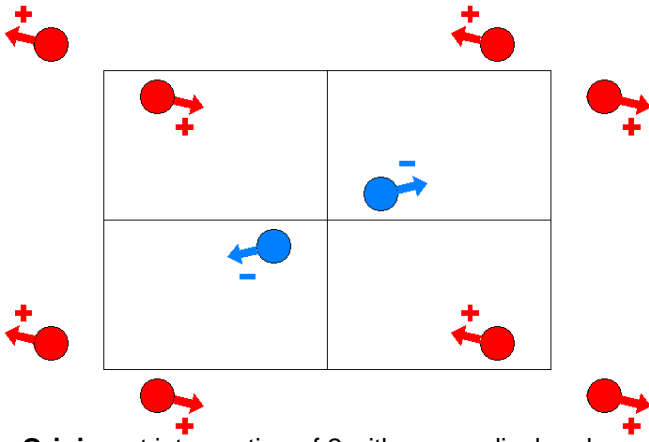
$P_{2c}2_12_12$

18.5.117

2221'

$P_{2c}2_12_12$

Orthorhombic



**Origin** at intersection of 2 with perpendicular plane containing  $2_y$  axes

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2 (0,0,z)  
(2<sub>z</sub>|0,0,0)

(3) 2 (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)

(4) 2 (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)

For (0,0,1)' + set

(1) t' (0,0,1)  
(1|0,0,1)'

(2) 2' (0,0,1) 0,0,z  
(2<sub>z</sub>|0,0,1)'

(3) 2' (0,1/2,0) 1/4,y,1/2  
(2<sub>y</sub>|1/2,1/2,1)'

(4) 2' (1/2,0,0) x,1/4,1/2  
(2<sub>x</sub>|1/2,1/2,1)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

**Positions**

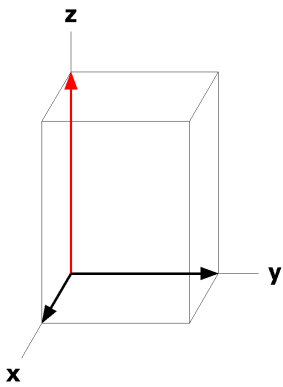
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,0,1)' +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
4	b ..2	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4	a ..2	0,0,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>·2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0] p<sub>2b</sub>·2m'g'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



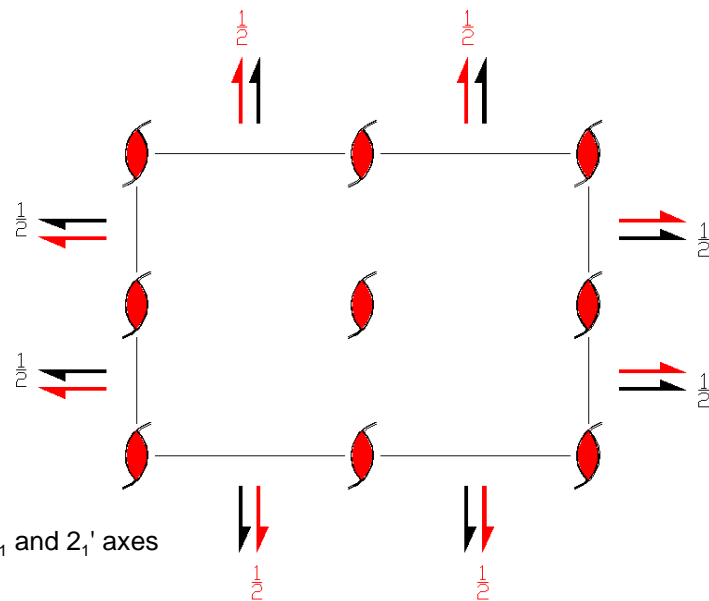
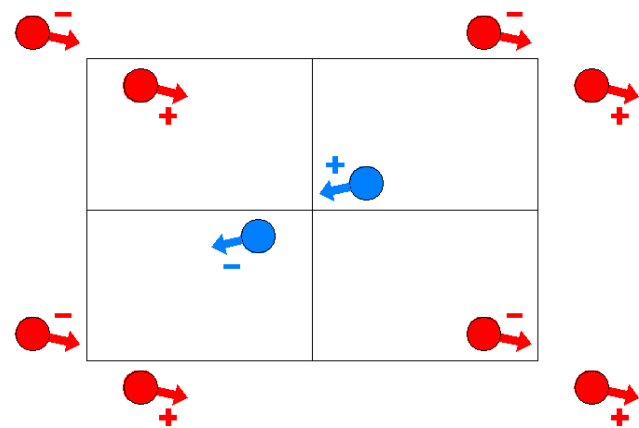
$P_{2c}2_12'_12'$

18.6.118

2221'

$P_{2c}2_12'_12'$

Orthorhombic



**Origin** at intersection of  $2'$  with perpendicular plane containing  $2_1$  and  $2'_1$  axes

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2)  $2'_1$  0,0,z  
( $2_z$ |0,0,0)'

(3)  $2'_1$  (0,1/2,0)  $1/4,y,0$   
( $2_y$ |1/2,1/2,0)'

(4)  $2$  (1/2,0,0)  $x,1/4,0$   
( $2_x$ |1/2,1/2,0)

For (0,0,1)' + set

(1)  $t'$  (0,0,1)  
(1|0,0,1)'

(2)  $2$  (0,0,1) 0,0,z  
( $2_z$ |0,0,1)

(3)  $2$  (0,1/2,0)  $1/4,y,1/2$   
( $2_y$ |1/2,1/2,1)

(4)  $2'_1$  (1/2,0,0)  $x,1/4,1/2$   
( $2_x$ |1/2,1/2,1)'

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)'$ ; (2); (3).

### Positions

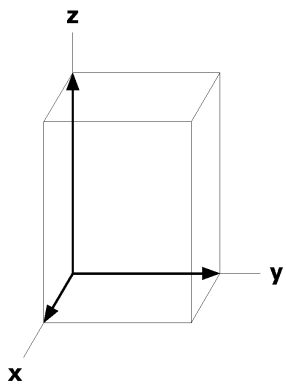
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
8 c 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [u,v,\bar{w}]$	(3) $\bar{x}+1/2,y+1/2,\bar{z} [u,\bar{v},w]$	(4) $x+1/2,\bar{y}+1/2,\bar{z} [u,\bar{v},\bar{w}]$
4 b ..2'	$0,1/2,z [u,v,0]$	$1/2,0,\bar{z} [u,\bar{v},0]$		
4 a ..2'	$0,0,z [u,v,0]$	$1/2,1/2,\bar{z} [u,\bar{v},0]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p2gg1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2b}2mg$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,1/4,0$

Along  $[0,1,0]$   $p_{2b}2mg$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $1/4,y,1/2$



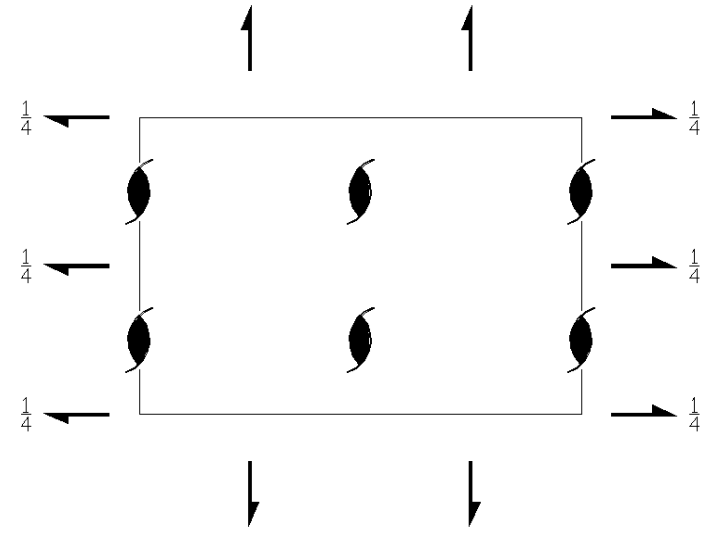
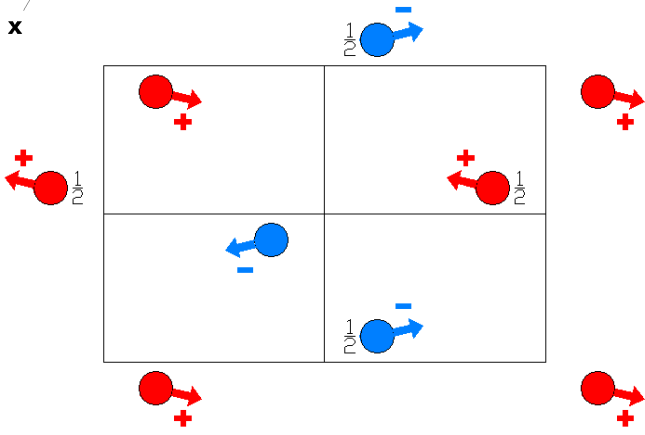
P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>

222

Orthorhombic

19.1.119

P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>



**Origin** at midpoint of three non-intersecting pairs of parallel 2<sub>1</sub> axes

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

- (1) 1  
(1|0,0,0)
- (2) 2 (0,0,1/2) 1/4,0,z  
(2<sub>z</sub>|1/2,0,1/2)
- (3) 2 (0,1/2,0) 0,y,1/4  
(2<sub>y</sub>|0,1/2,1/2)
- (4) 2 (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

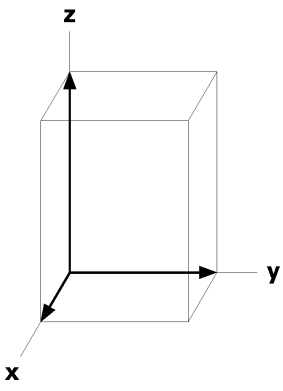
4 a 1 (1) x,y,z [u,v,w] (2)  $\bar{x}+1/2, \bar{y}, z+1/2$  [ $\bar{u}, \bar{v}, w$ ] (3)  $\bar{x}, y+1/2, \bar{z}+1/2$  [ $\bar{u}, v, \bar{w}$ ] (4)  $x+1/2, \bar{y}+1/2, \bar{z}$  [ $u, \bar{v}, \bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p2g'g'  
 $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$   
Origin at 1/4,0,z

Along [1,0,0] p2g'g'  
 $\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}$   
Origin at x,1/4,0

Along [0,1,0] p2g'g'  
 $\mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{a}$   
Origin at 0,y,1/4



$P2_12_12_11'$

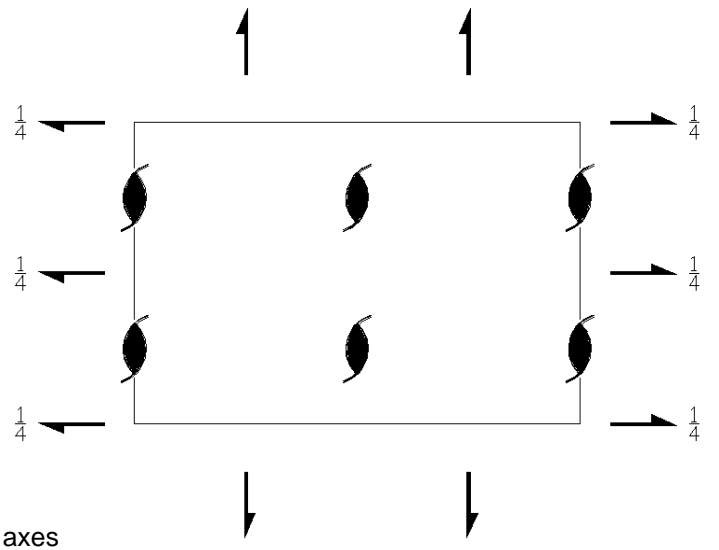
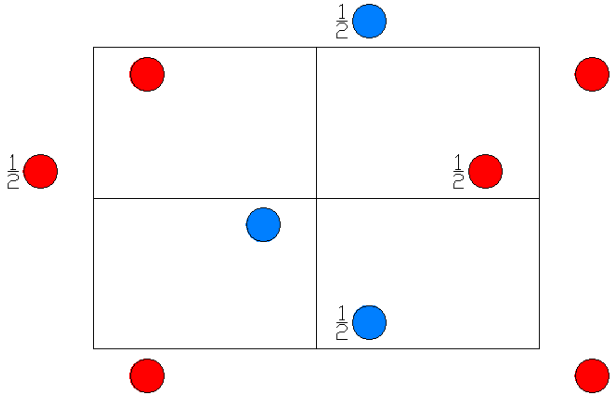
19.2.120

$2221'$

$P2_12_12_11'$

Orthorhombic

$1'$



**Origin** at midpoint of three non-intersecting pairs of parallel  $2_11'$  axes

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For 1 + set

- (1) 1  $(1|0,0,0)$
- (2) 2  $(0,0,1/2) 1/4,0,z$   $(2_z|1/2,0,1/2)$
- (3) 2  $(0,1/2,0) 0,y,1/4$   $(2_y|0,1/2,1/2)$
- (4) 2  $(1/2,0,0) x,1/4,0$   $(2_x|1/2,1/2,0)$

For 1' + set

- (1)  $1'$   $(1|0,0,0)'$
- (2)  $2'$   $(0,0,1/2) 1/4,0,z$   $(2_z|1/2,0,1/2)'$
- (3)  $2'$   $(0,1/2,0) 0,y,1/4$   $(2_y|0,1/2,1/2)'$
- (4)  $2'$   $(1/2,0,0) x,1/4,0$   $(2_x|1/2,1/2,0)'$



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

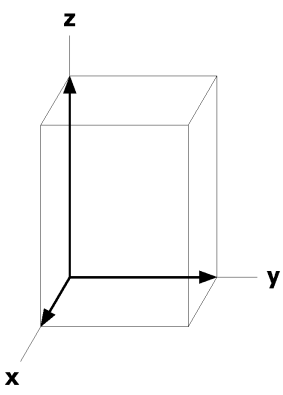
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
4 a 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [0,0,0]	(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [0,0,0]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,0,0] p2gg1'  
 $\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0] p2gg1'  
 $\mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



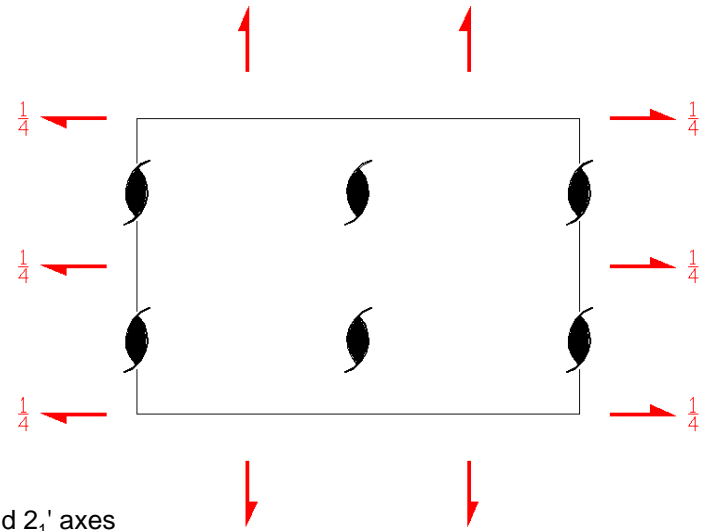
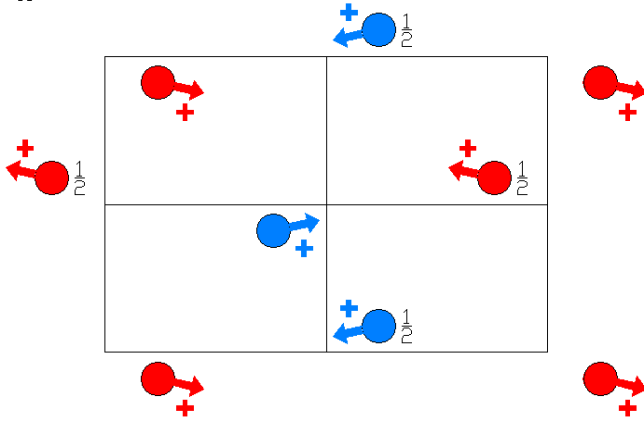
$P2_1'2_1'2_1$

19.3.121

$2'2'2$

$P2_1'2_1'2_1$

Orthorhombic



**Origin** at midpoint of three non-intersecting pairs of parallel  $2_1$  and  $2_1'$  axes

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 1/4,0,z  
(2<sub>z</sub>|1/2,0,1/2)

(3) 2' (0,1/2,0) 0,y,1/4  
(2<sub>y</sub>|0,1/2,1/2)'

(4) 2' (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

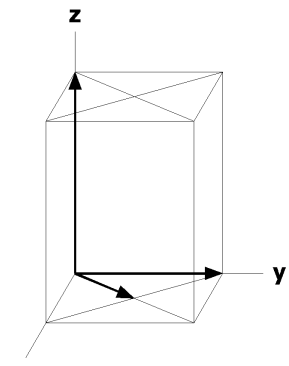
	Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.				
4 a 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [ $u, \bar{v}, w$ ]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $\bar{u}, v, w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p2gg'  
 $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,0,0] p2'gg'  
 $\mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b}$   
 Origin at x,1/4,0

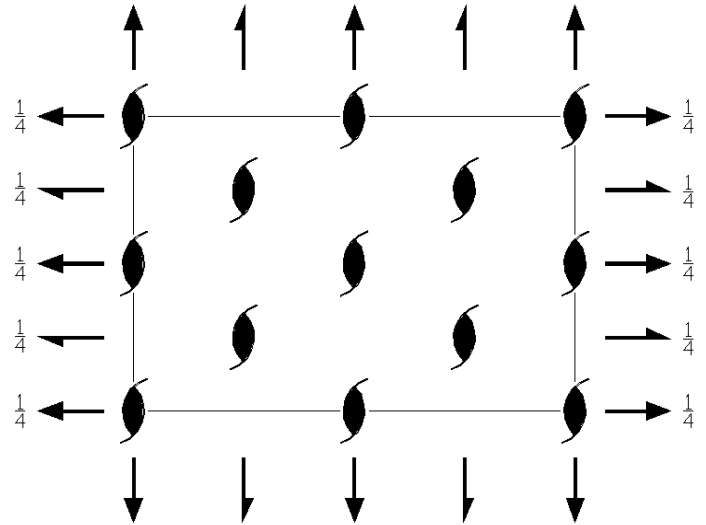
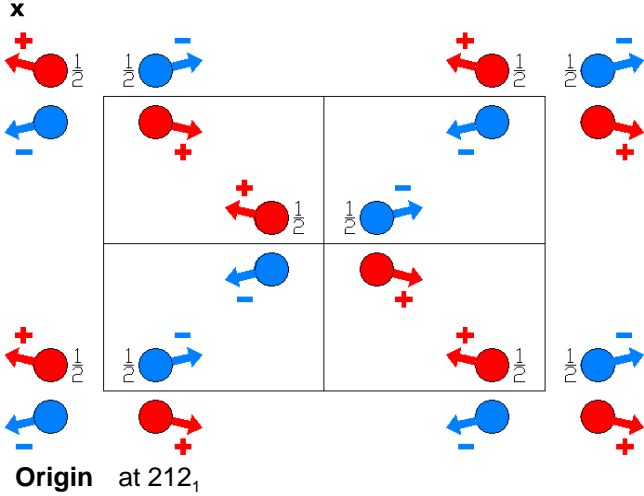
Along [0,1,0] p2'gg'  
 $\mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



C222<sub>1</sub>  
20.1.122

222  
C222<sub>1</sub>

Orthorhombic



Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- (1) 1  
(1|0,0,0)
- (2) 2 (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)
- (3) 2 0,y,1/4  
(2<sub>y</sub>|0,0,1/2)
- (4) 2 x,0,0  
(2<sub>x</sub>|0,0,0)

For (1/2,1/2,0) + set

- (1) t (1/2,1/2,0)  
(1|1/2,1/2,0)
- (2) 2 (0,0,1/2) 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,1/2)
- (3) 2 (0,1/2,0) 1/4,y,1/4  
(2<sub>y</sub>|1/2,1/2,1/2)
- (4) 2 (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

### Positions

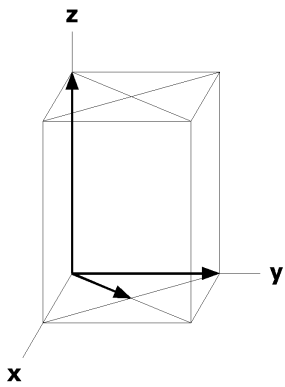
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +		(1/2,1/2,0) +	
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
4	b .2.	0,y,1/4 [0,v,0]	0, $\bar{y}$ ,3/4 [0, $\bar{v}$ ,0]		
4	a 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,1/2 [ $\bar{u}$ ,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



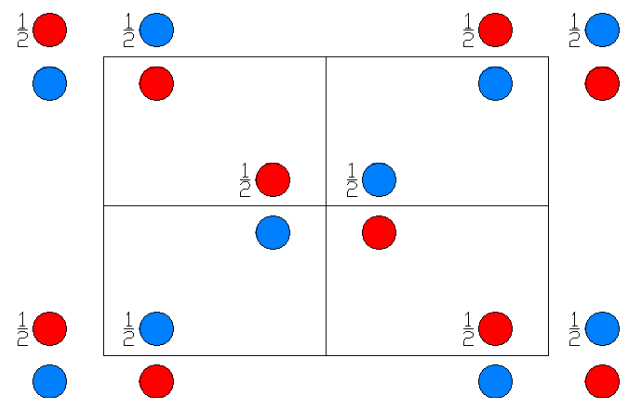
C222<sub>1</sub>'

20.2.123

2221'

C222<sub>1</sub>'

Orthorhombic



Origin at 212<sub>1</sub>'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1 (1|0,0,0) (2) 2 (0,0,1/2) 0,0,z (2<sub>z</sub>|0,0,1/2) (3) 2 0,y,1/4 (2<sub>y</sub>|0,0,1/2) (4) 2 x,0,0 (2<sub>x</sub>|0,0,0)

For (0,0,0) + set

(1) t (1/2,1/2,0) (1|1/2,1/2,0) (2) 2 (0,0,1/2) 1/4,1/4,z (2<sub>z</sub>|1/2,1/2,1/2) (3) 2 (0,1/2,0) 1/4,y,1/4 (2<sub>y</sub>|1/2,1/2,1/2) (4) 2 (1/2,0,0) x,1/4,0 (2<sub>x</sub>|1/2,1/2,0)

For (1/2,1/2,0) + set

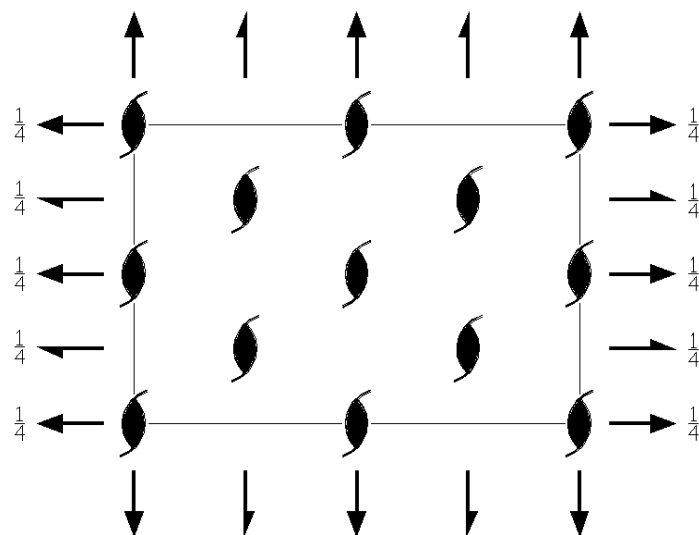
(1) 1' (1|0,0,0)' (2) 2' (0,0,1/2) 0,0,z (2<sub>z</sub>|0,0,1/2)' (3) 2' 0,y,1/4 (2<sub>y</sub>|0,0,1/2) (4) 2' x,0,0 (2<sub>x</sub>|0,0,0)'

For (0,0,0)' + set

(1) t' (1/2,1/2,0) (1|1/2,1/2,0)' (2) 2' (0,0,1/2) 1/4,1/4,z (2<sub>z</sub>|1/2,1/2,1/2)' (3) 2' (0,1/2,0) 1/4,y,1/4 (2<sub>y</sub>|1/2,1/2,1/2)' (4) 2' (1/2,0,0) x,1/4,0 (2<sub>x</sub>|1/2,1/2,0)'

For (1/2,1/2,0)' + set

1'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); 1'.

### Positions

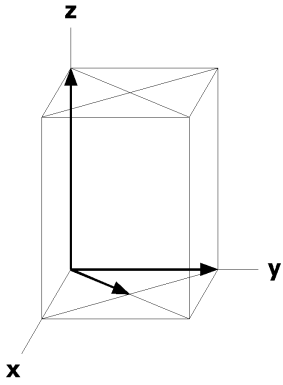
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) + (0,0,0)'	(1/2,1/2,0) + (1/2,1/2,0)'		
8	c 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y}, z+1/2$ [0,0,0]	(3) $\bar{x}, y, \bar{z}+1/2$ [0,0,0]	(4) x, $\bar{y}, \bar{z}$ [0,0,0]
4	b .2.1'	0,y,1/4 [0,0,0]	0, $\bar{y}, 3/4$ [0,0,0]		
4	a 2..1'	x,0,0 [0,0,0]	$\bar{x}, 0, 1/2$ [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

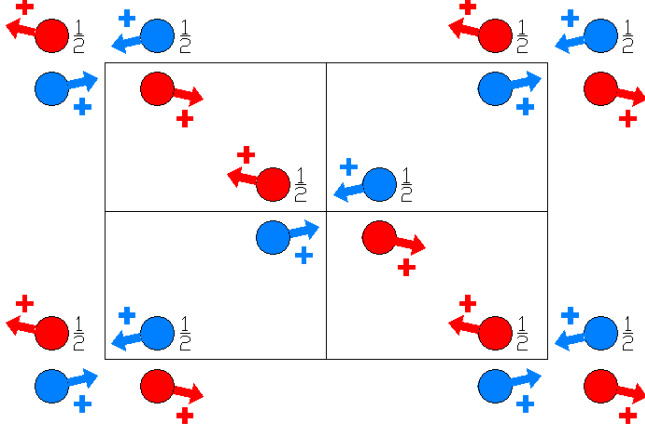
Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



C2'2'2<sub>1</sub>  
20.3.124

2'2'2  
C2'2'2<sub>1</sub>

Orthorhombic



Origin at 2'12<sub>1</sub>

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)

(3) 2' 0,y,1/4  
(2<sub>y</sub>|0,0,1/2)'

(4) 2' x,0,0  
(2<sub>x</sub>|0,0,0)'

For (0,0,0) + set

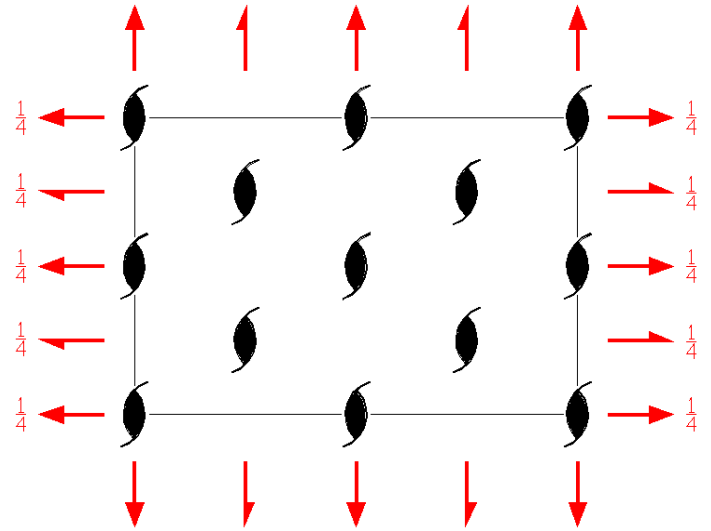
For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)

(2) 2 (0,0,1/2) 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,1/2)

(3) 2' (0,1/2,0) 1/4,y,1/4  
(2<sub>y</sub>|1/2,1/2,1/2)'

(4) 2' (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)'





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

**Positions**

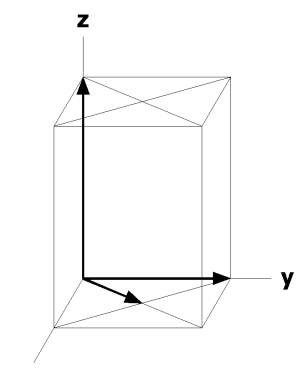
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(1/2,1/2,0) +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(4) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]
4	b .2'	0,y,1/4 [u,0,w]	0, $\bar{y}$ ,3/4 [ $\bar{u},0,w$ ]		
4	a 2'..	x,0,0 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p2'mg'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



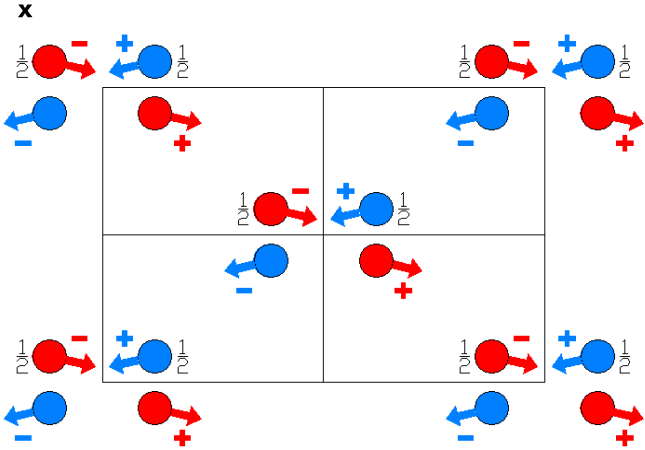
C22'2<sub>1</sub>'

20.4.125

22'2'

C22'2<sub>1</sub>'

Orthorhombic



Origin at 212<sub>1</sub>'

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2' (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)'

(3) 2' 0,y,1/4  
(2<sub>y</sub>|0,0,1/2)'

(4) 2 x,0,0  
(2<sub>x</sub>|0,0,0)

For (0,0,0) + set

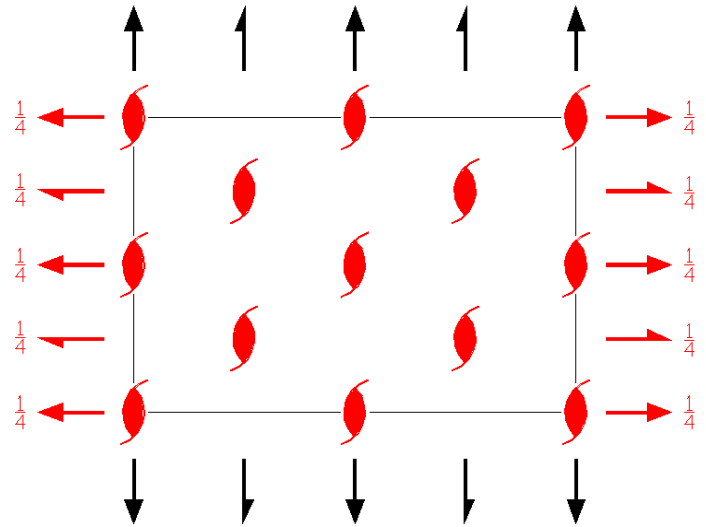
For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)

(2) 2' (0,0,1/2) 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,1/2)'

(3) 2' (0,1/2,0) 1/4,y,1/4  
(2<sub>y</sub>|1/2,1/2,1/2)'

(4) 2 (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

### Positions

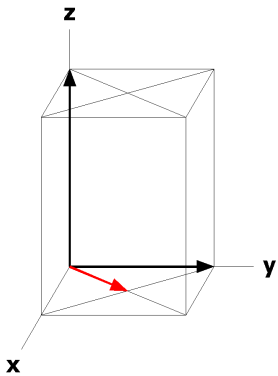
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +		(1/2,1/2,0) +	
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
4	b .2'	0,y,1/4 [u,0,w]	0, $\bar{y}$ ,3/4 [u,0, $\bar{w}$ ]		
4	a 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,1/2 [ $\bar{u}$ ,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



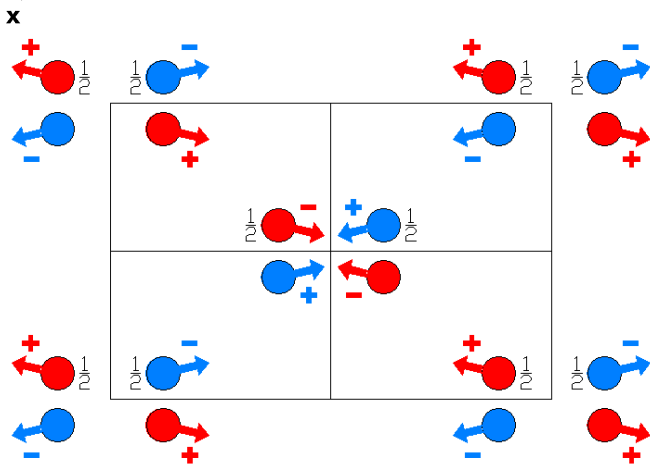
$C_{p222_1}$

20.5.126

2221'

$C_{p222_1}$

Orthorhombic



Origin at  $212_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)

(3) 2 0,y,1/4  
(2<sub>y</sub>|0,0,1/2)

(4) 2 x,0,0  
(2<sub>x</sub>|0,0,0)

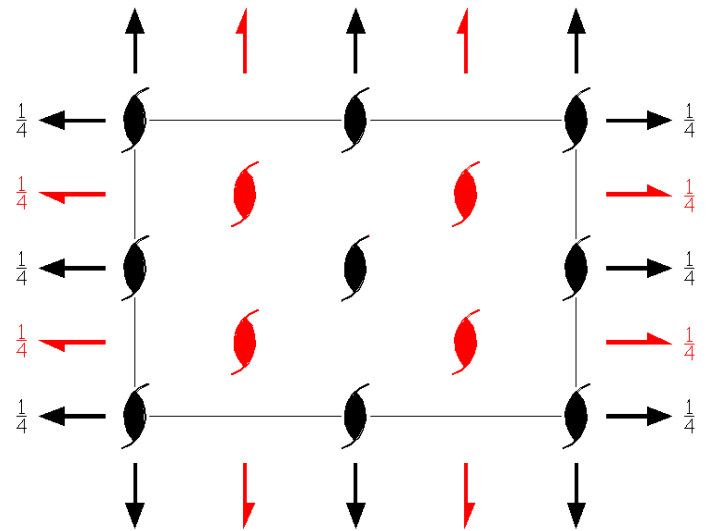
For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0)  
(1|1/2,1/2,0)'

(2) 2' (0,0,1/2) 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,1/2)'

(3) 2' (0,1/2,0) 1/4,y,1/4  
(2<sub>y</sub>|1/2,1/2,1/2)'

(4) 2' (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

### Positions

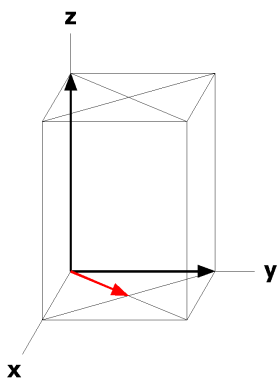
		Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.			
		(0,0,0) +	(1/2,1/2,0)' +
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ] (3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ] (4) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
4	b .2.	0,y,1/4 [0,v,0]	0, $\bar{y}$ ,3/4 [0, $\bar{v}$ ,0]
4	a 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,1/2 [ $\bar{u}$ ,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $c_p2m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b}2m'g'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2b}2m'g'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



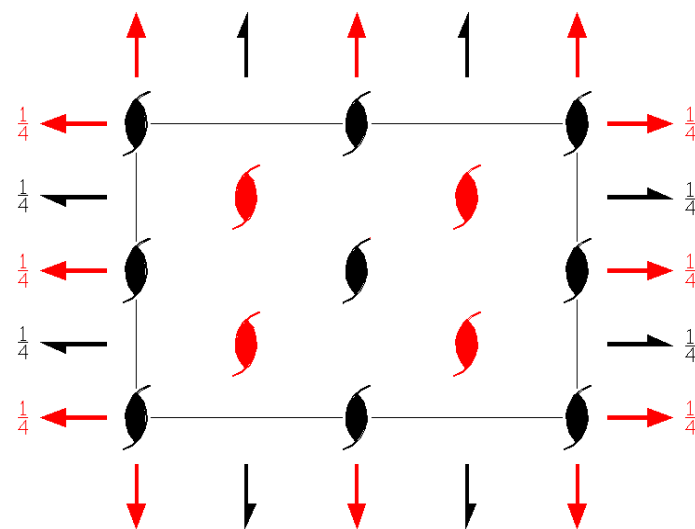
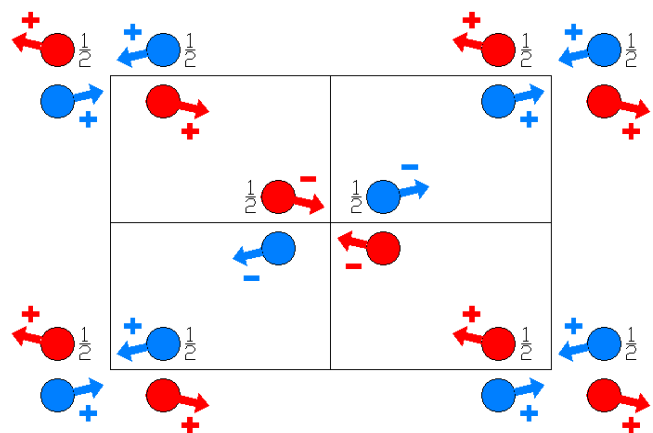
$C_p 2'2'2_1$

20.6.127

2221'

$C_p 2'2'2_1$

Orthorhombic



Origin at  $2'12_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- (1) 1  $(1|0,0,0)$
- (2) 2 (0,0,1/2)  $(2_z|0,0,1/2)$
- (3) 2'  $(2'_y|0,y,1/4)$   $(2'_y|0,0,1/2)'$
- (4) 2'  $(2'_x|x,0,0)$   $(2'_x|0,0,0)'$

For (1/2,1/2,0)' + set

- (1)  $t' (1/2,1/2,0)$   $(1|1/2,1/2,0)'$
- (2) 2' (0,0,1/2)  $(2'_z|1/4,1/4,z)$   $(2'_z|1/2,1/2,1/2)'$
- (3) 2 (0,1/2,0)  $(2_y|1/4,y,1/4)$   $(2_y|1/2,1/2,1/2)$
- (4) 2 (1/2,0,0)  $(2_x|1/2,0,0)$   $(2_x|1/2,1/2,0)$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

### Positions

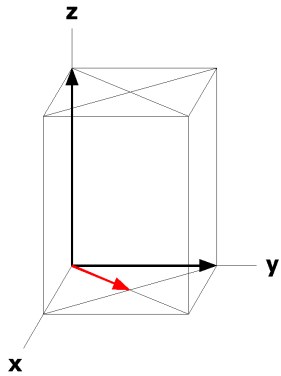
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,0)' +		
8	c	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(4) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]
4	b	.2'	0,y,1/4 [u,0,w]	0, $\bar{y}$ ,3/4 [ $\bar{u},0,w$ ]		
4	a	2'..	x,0,0 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]		

### Symmetry of Special Projections

Along [0,0,1] c<sub>p</sub>2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>·2mg  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,1/4,0

Along [0,1,0] p<sub>2b</sub>·2mg  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,1/4



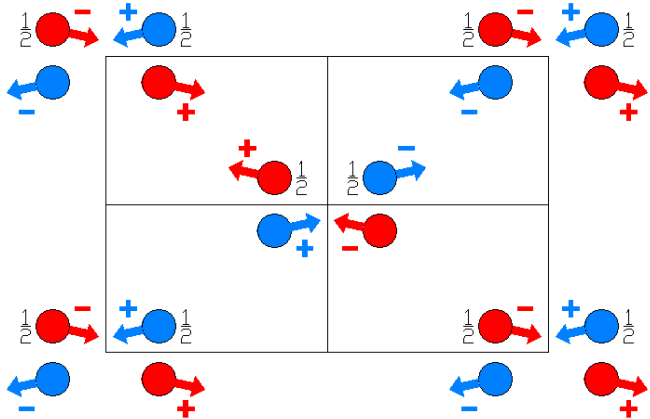
$C_{P22'2_1'}$

20.7.128

2221'

$C_{P22'2_1'}$

Orthorhombic



Origin at  $212_1'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

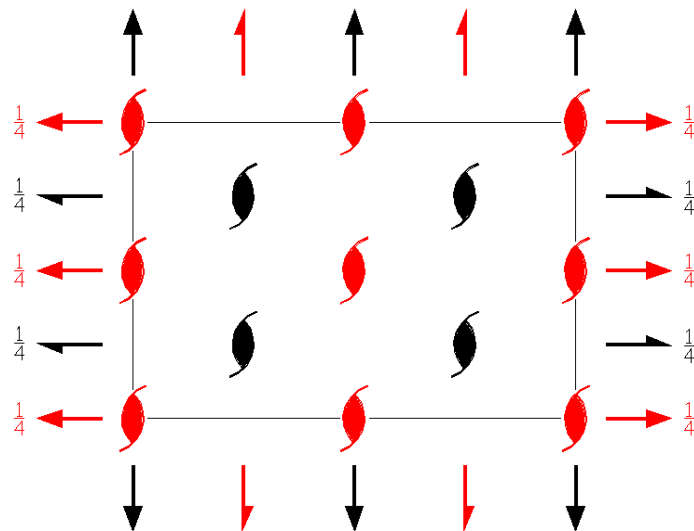
**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)' | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)' | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) |
|--------------------|--|--|--|

For (1/2,1/2,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (1/2,1/2,0)<br>(1 1/2,1/2,0)' | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
|--|--|--|--|





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

### Positions

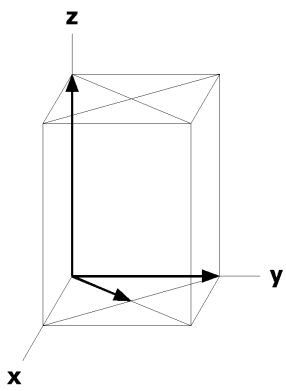
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,0)' +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
4	b .2'	0,y,1/4 [u,0,w]	0, $\bar{y}$ ,3/4 [u,0, $\bar{w}$ ]		
4	a 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,1/2 [u,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c<sub>p</sub>2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>·2mg  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

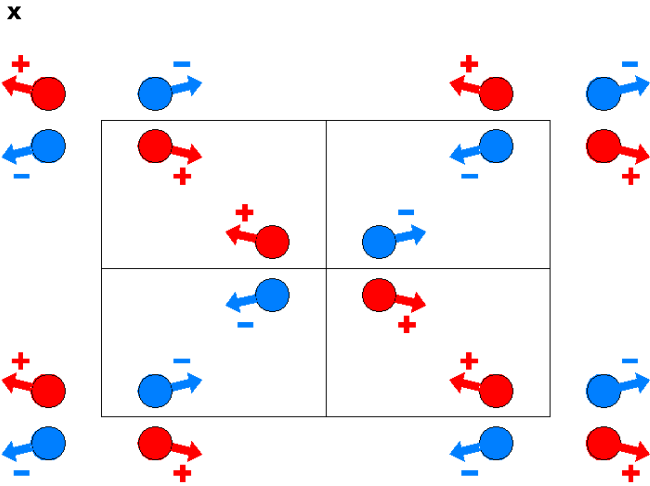
Along [0,1,0] p<sub>2b</sub>·2m'g'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,1/4



C222  
21.1.129

222  
C222

Orthorhombic



Origin at 222

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) 2  $0,y,0$   
( $2_y$ |0,0,0)

(4) 2  $x,0,0$   
( $2_x$ |0,0,0)

For (0,0,0) + set

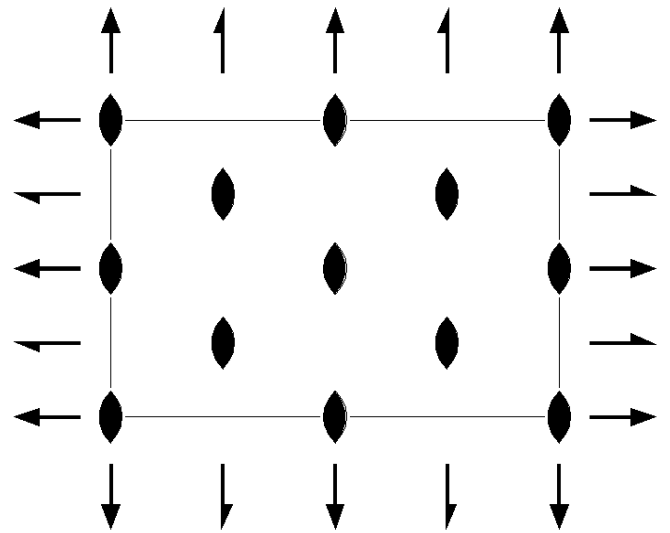
For (1/2,1/2,0) + set

(1) t  $(1/2,1/2,0)$   
(1| $1/2,1/2,0$ )

(2) 2  $1/4,1/4,z$   
( $2_z$ | $1/2,1/2,0$ )

(3) 2  $(0,1/2,0)$   $1/4,y,0$   
( $2_y$ | $1/2,1/2,0$ )

(4) 2  $(1/2,0,0)$   $x,1/4,0$   
( $2_x$ | $1/2,1/2,0$ )



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

**Positions**

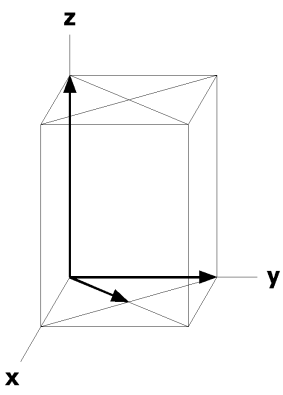
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
8 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
4 k ..2	1/4, 1/4, z [0,0,w]	3/4, 1/4, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 j ..2	0, 1/2, z [0,0,w]	0, 1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 i ..2	0, 0, z [0,0,w]	0, 0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 h ..2	0, y, 1/2 [0,v,0]	0, $\bar{y}$ , 1/2 [0, $\bar{v}$ , 0]		
4 g ..2	0, y, 0 [0,v,0]	0, $\bar{y}$ , 0 [0, $\bar{v}$ , 0]		
4 f 2..	x, 0, 1/2 [u,0,0]	$\bar{x}$ , 0, 1/2 [ $\bar{u}$ ,0,0]		
4 e 2..	x, 0, 0 [u,0,0]	$\bar{x}$ , 0, 0 [ $\bar{u}$ ,0,0]		
2 d 222	0, 0, 1/2 [0,0,0]			
2 c 222	1/2, 0, 1/2 [0,0,0]			
2 b 222	0, 1/2, 0 [0,0,0]			
2 a 222	0, 0, 0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

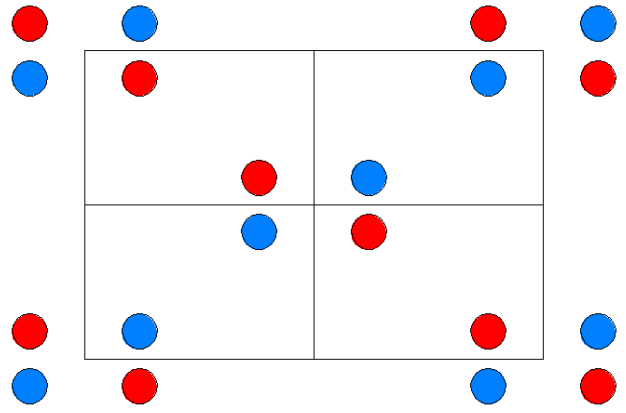
Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



C2221'  
21.2.130

2221'  
C2221'

Orthorhombic



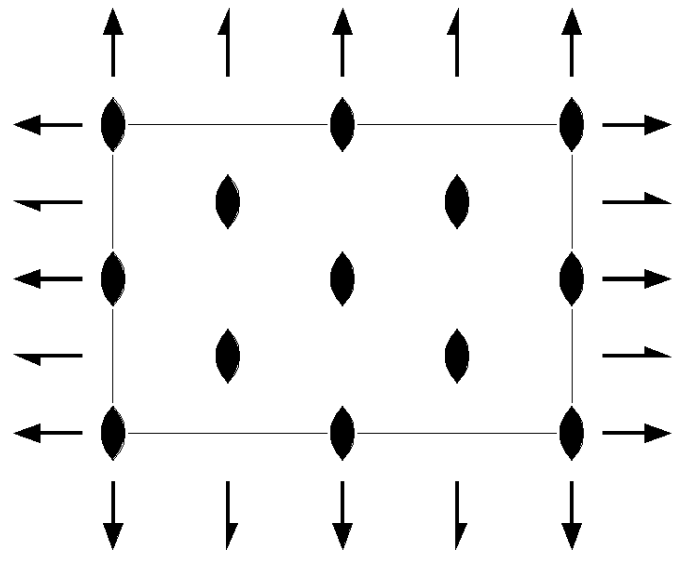
Origin at 2221'

Asymmetric unit  $0 \leq x \leq 1/4;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

- (1) 1  
(1|0,0,0)
- (2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)
- (1) t (1/2,1/2,0)  
(1|1/2,1/2,0)
- (2) 2 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,0)
- (1) 1'  
(1|0,0,0)'
- (2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'
- (1) t' (1/2,1/2,0)  
(1|1/2,1/2,0)'
- (2) 2' 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,0)'

1'



- For (0,0,0) + set
  - (3) 2 0,y,0  
(2<sub>y</sub>|0,0,0)
  - (4) 2 x,0,0  
(2<sub>x</sub>|0,0,0)
- For (1/2,1/2,0) + set
  - (3) 2 (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)
  - (4) 2 (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)
- For (0,0,0)' + set
  - (3) 2' 0,y,0  
(2<sub>y</sub>|0,0,0)'
  - (4) 2' x,0,0  
(2<sub>x</sub>|0,0,0)'
- For (1/2,1/2,0)' + set
  - (3) 2' (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)'
  - (4) 2' (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); 1'.

**Positions**

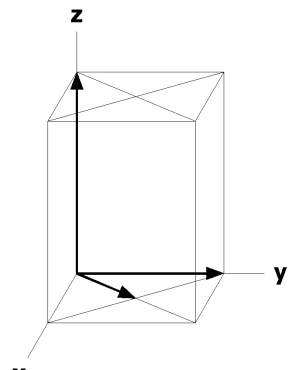
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) + (0,0,0)'	(1/2,1/2,0) + (1/2,1/2,0)'		
8 l 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y}, z$ [0,0,0]	(3) $\bar{x}, y, \bar{z}$ [0,0,0]	(4) x, $\bar{y}, \bar{z}$ [0,0,0]
4 k ..21'	1/4, 1/4, z [0,0,0]	3/4, 1/4, $\bar{z}$ [0,0,0]		
4 j ..21'	0, 1/2, z [0,0,0]	0, 1/2, $\bar{z}$ [0,0,0]		
4 i ..21'	0, 0, z [0,0,0]	0, 0, $\bar{z}$ [0,0,0]		
4 h .2.1'	0, y, 1/2 [0,0,0]	0, $\bar{y}$ , 1/2 [0,0,0]		
4 g .2.1'	0, y, 0 [0,0,0]	0, $\bar{y}$ , 0 [0,0,0]		
4 f 2..1'	x, 0, 1/2 [0,0,0]	$\bar{x}$ , 0, 1/2 [0,0,0]		
4 e 2..1'	x, 0, 0 [0,0,0]	$\bar{x}$ , 0, 0 [0,0,0]		
2 d 2221'	0, 0, 1/2 [0,0,0]			
2 c 2221'	1/2, 0, 1/2 [0,0,0]			
2 b 2221'	0, 1/2, 0 [0,0,0]			
2 a 2221'	0, 0, 0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

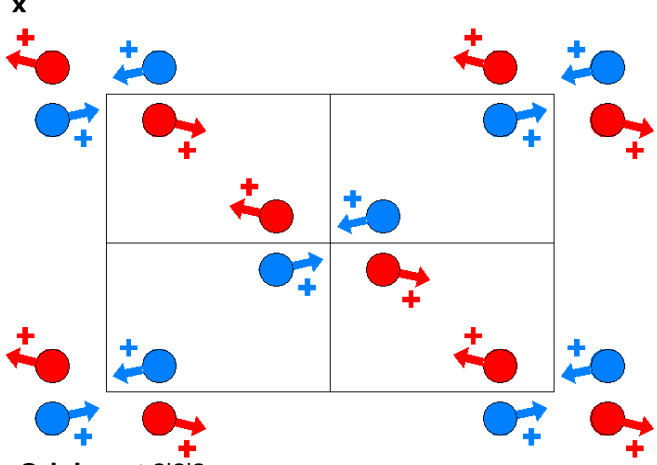
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



C2'2'2  
21.3.131

2'2'2  
C2'2'2

Orthorhombic

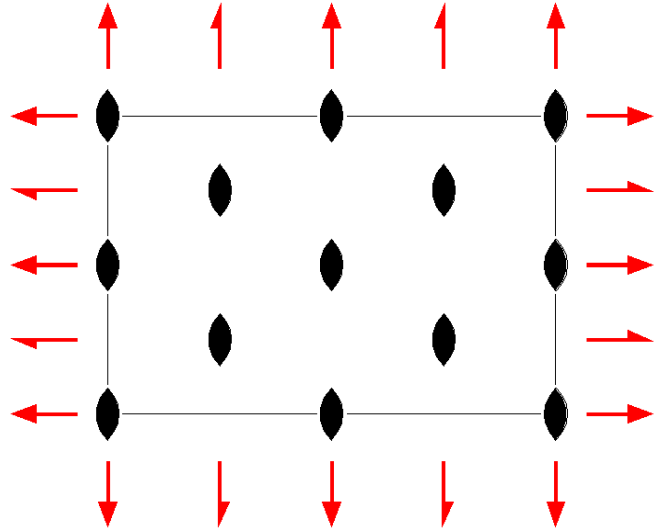


Origin at 2'2'2

Asymmetric unit  $0 \leq x \leq 1/4;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) 1<br>(1 0,0,0)                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)         | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                 | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                 |
| For (0,0,0) + set                  |  |  |  |
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0) | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| For (1/2,1/2,0) + set              |  |  |  |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

**Positions**

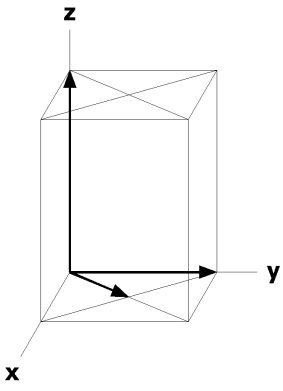
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
8 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $u, \bar{v}, w$ ]	(4) x, $\bar{y}, \bar{z}$ [ $\bar{u}, v, w$ ]
4 k ..2	1/4, 1/4, z [0,0,w]	3/4, 1/4, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 j ..2	0, 1/2, z [0,0,w]	0, 1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 i ..2	0, 0, z [0,0,w]	0, 0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 h .2'	0, y, 1/2 [u,0,w]	0, $\bar{y}$ , 1/2 [ $\bar{u}$ ,0,w]		
4 g .2'	0, y, 0 [u,0,w]	0, $\bar{y}$ , 0 [ $\bar{u}$ ,0,w]		
4 f 2'..	x, 0, 1/2 [0,v,w]	$\bar{x}$ , 0, 1/2 [0, $\bar{v}$ ,w]		
4 e 2'..	x, 0, 0 [0,v,w]	$\bar{x}$ , 0, 0 [0, $\bar{v}$ ,w]		
2 d 2'2'2	0, 0, 1/2 [0,0,w]			
2 c 2'2'2	1/2, 0, 1/2 [0,0,w]			
2 b 2'2'2	0, 1/2, 0 [0,0,w]			
2 a 2'2'2	0, 0, 0 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

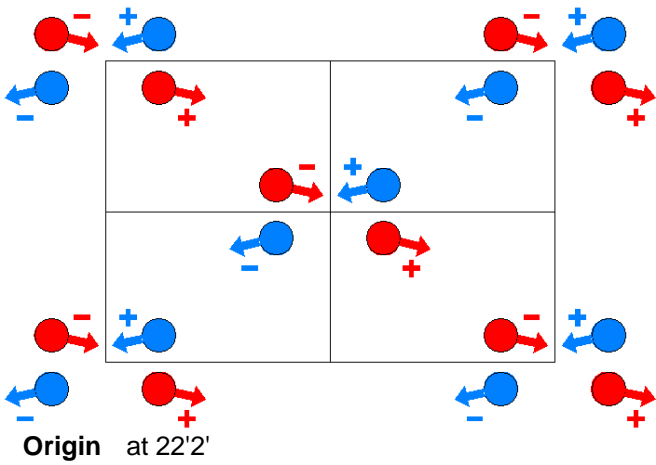
Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



C22'2'  
21.4.132

22'2'  
C22'2'

Orthorhombic



Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'

(3) 2' 0,y,0  
(2<sub>y</sub>|0,0,0)'

(4) 2 x,0,0  
(2<sub>x</sub>|0,0,0)

For (0,0,0) + set

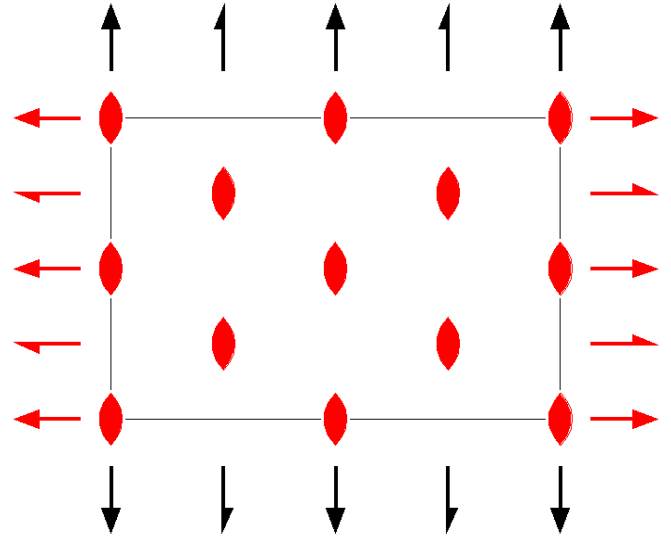
For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)

(2) 2' 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,0)'

(3) 2' (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)'

(4) 2 (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

**Positions**

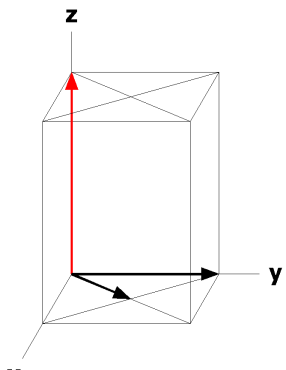
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
8 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	3) $\bar{x}, y, \bar{z}$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
4 k ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [u, $\bar{v}$ ,0]		
4 j ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}$ [u, $\bar{v}$ ,0]		
4 i ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [u, $\bar{v}$ ,0]		
4 h .2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ ,1/2 [u,0, $\bar{w}$ ]		
4 g .2'	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [u,0, $\bar{w}$ ]		
4 f 2..	x,0,1/2 [u,0,0]	$\bar{x}$ ,0,1/2 [u,0,0]		
4 e 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [u,0,0]		
2 d 22'2'	0,0,1/2 [u,0,0]			
2 c 22'2'	1/2,0,1/2 [u,0,0]			
2 b 22'2'	0,1/2,0 [u,0,0]			
2 a 22'2'	0,0,0 [u,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



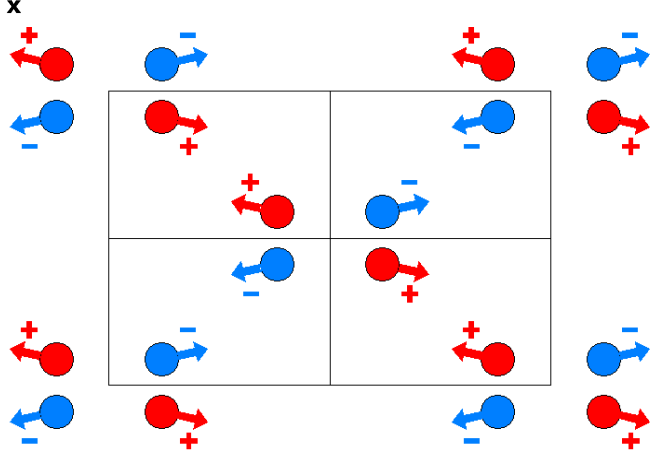
$C_{2c} 222$

21.5.133

$2221'$

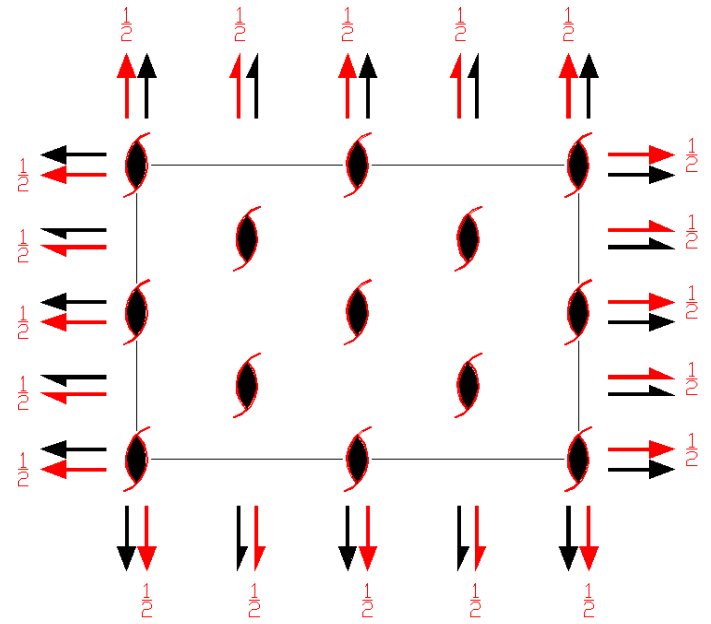
$C_{2c} 222$

Orthorhombic



Origin at 222

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1$



**Symmetry Operations**

- For (0,0,0) + set
- (1) 1  
(1|0,0,0)
  - (2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)
  - (3) 2 0,y,0  
(2<sub>y</sub>|0,0,0)
  - (4) 2 x,0,0  
(2<sub>x</sub>|0,0,0)
- For (1/2,1/2,0) + set
- (1) t (1/2,1/2,0)  
(1|1/2,1/2,0)
  - (2) 2 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,0)
  - (3) 2 (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)
  - (4) 2 (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)
- For (0,0,1)' + set
- (1) t' (0,0,1)  
(1|0,0,1)'
  - (2) 2' (0,0,1) 0,0,z  
(2<sub>z</sub>|0,0,1)'
  - (3) 2' 0,y,1/2  
(2<sub>y</sub>|0,0,1)'
  - (4) 2' x,0,1/2  
(2<sub>x</sub>|0,0,1)'
- For (1/2,1/2,1)' + set
- (1) t' (1/2,1/2,1)  
(1|1/2,1/2,1)'
  - (2) 2' (0,0,1) 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,1)'
  - (3) 2' (0,1/2,0) 1/4,y,1/2  
(2<sub>y</sub>|1/2,1/2,1)'
  - (4) 2' (1/2,0,0) x,1/4,1/2  
(2<sub>x</sub>|1/2,1/2,1)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; t(1/2,1/2,0); (2); (3).

### Positions

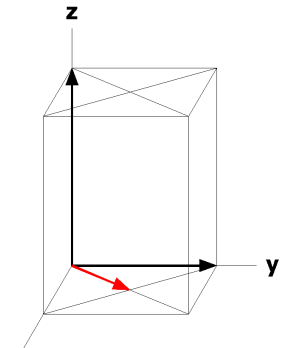
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,1)'	(1/2,1/2,0) + (1/2,1/2,1)'	
16 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x, \bar{y}, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]
8 k ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0, $\bar{w}$ ]		
8 j ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
8 i ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
8 h .2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ , 1/2 [ $\bar{u}$ ,0,w]		
8 g .2	0,y,0 [0,v,0]	0, $\bar{y}$ , 0 [0, $\bar{v}$ , 0]		
8 f 2'..	x,0,1/2 [0,v,w]	$\bar{x}$ , 0, 1/2 [0, $\bar{v}$ , w]		
8 e 2..	x,0,0 [u,0,0]	$\bar{x}$ , 0, 0 [ $\bar{u}$ , 0, 0]		
4 d 2'2'2	0,0,1/2 [0,0,w]			
4 c 2'2'2	1/2,0,1/2 [0,0,w]			
4 b 222	0,1/2,0 [0,0,0]			
4 a 222	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>.2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>.2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



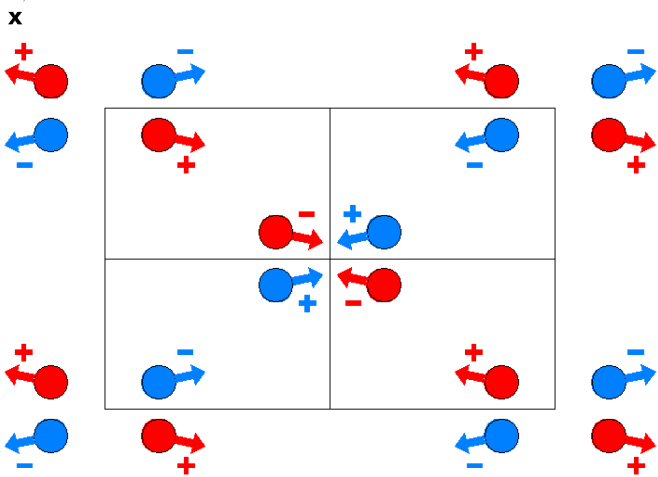
$C_{p222}$

21.6.134

$2221'$

$C_{p222}$

Orthorhombic



Origin at  $222$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) 2  $0,y,0$   
( $2_y$ |0,0,0)

(4) 2  $x,0,0$   
( $2_x$ |0,0,0)

For (0,0,0) + set

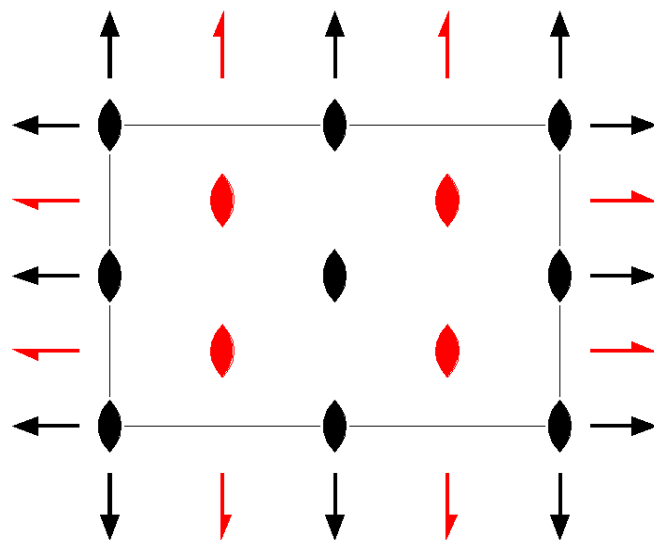
For (1/2,1/2,0)' + set

(1)  $t' (1/2,1/2,0)$   
(1|1/2,1/2,0)'

(2)  $2' 1/4,1/4,z$   
( $2_z$ |1/2,1/2,0)'

(3)  $2' (0,1/2,0) 1/4,y,0$   
( $2_y$ |1/2,1/2,0)'

(4)  $2' (1/2,0,0) x,1/4,0$   
( $2_x$ |1/2,1/2,0)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

**Positions**

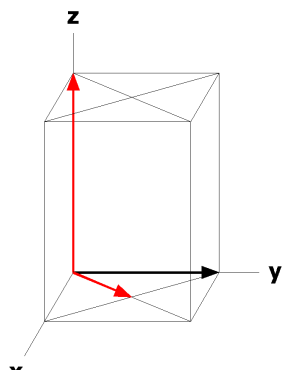
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
8 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
4 k ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [ $\bar{u}, v, 0$ ]		
4 j ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 i ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 h ..2.	0,y,1/2 [0,v,0]	0, $\bar{y}$ , 1/2 [0, $\bar{v}$ , 0]		
4 g ..2.	0,y,0 [0,v,0]	0, $\bar{y}$ , 0 [0, $\bar{v}$ , 0]		
4 f 2..	x,0,1/2 [u,0,0]	$\bar{x}$ , 0, 1/2 [ $\bar{u}$ , 0, 0]		
4 e 2..	x,0,0 [u,0,0]	$\bar{x}$ , 0, 0 [ $\bar{u}$ , 0, 0]		
2 d 222	0,0,1/2 [0,0,0]			
2 c 222	1/2,0,1/2 [0,0,0]			
2 b 222	0,1/2,0 [0,0,0]			
2 a 222	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $c_p 2m' m'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a} 2m' m'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

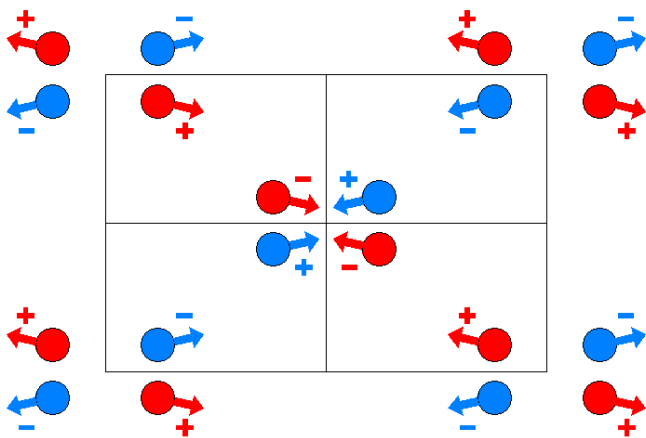
Along [0,1,0]  $p_{2a} 2m' m'$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



$C_1 222$   
21.7.135

$2221'$   
 $C_1 222$

Orthorhombic



Origin at 222

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) 2  $0,y,0$   
( $2_y$ |0,0,0)

(4) 2  $x,0,0$   
( $2_x$ |0,0,0)

For (0,0,0) + set

(1)  $t' (1/2,1/2,0)$   
(1| $1/2,1/2,0$ )'

(2)  $2' 1/4,1/4,z$   
( $2_z$ | $1/2,1/2,0$ )'

(3)  $2' (0,1/2,0) 1/4,y,0$   
( $2_y$ | $1/2,1/2,0$ )'

(4)  $2' (1/2,0,0) x,1/4,0$   
( $2_x$ | $1/2,1/2,0$ )'

For (1/2,1/2,0)' + set

(1)  $t' (0,0,1)$   
(1|0,0,1)'

(2)  $2' (0,0,1) 0,0,z$   
( $2_z$ |0,0,1)'

(3)  $2' 0,y,1/2$   
( $2_y$ |0,0,1)'

(4)  $2' x,0,1/2$   
( $2_x$ |0,0,1)'

For (0,0,1)' + set

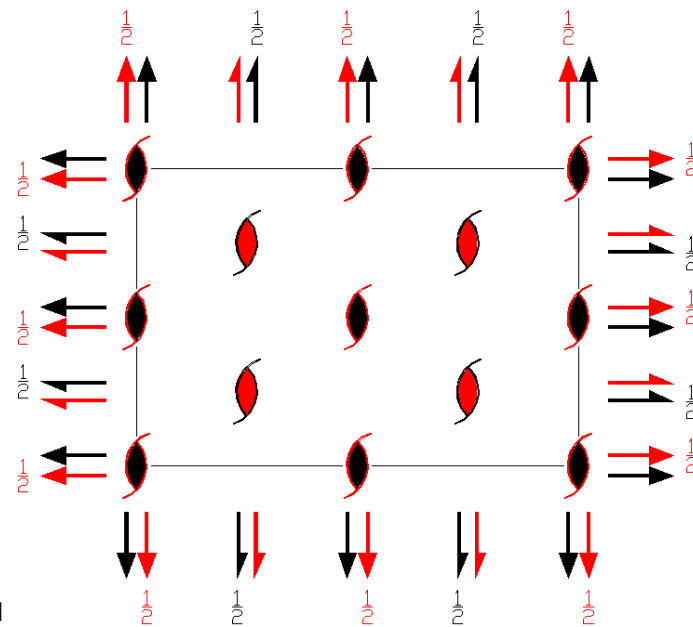
(1)  $t (1/2,1/2,1)$   
(1| $1/2,1/2,1$ )

(2) 2 (0,0,1)  $1/4,1/4,z$   
( $2_z$ | $1/2,1/2,1$ )

(3) 2 (0,1/2,0)  $1/4,y,1/2$   
( $2_y$ | $1/2,1/2,1$ )

(4) 2 (1/2,0,0)  $x,1/4,1/2$   
( $2_x$ | $1/2,1/2,1$ )

For (1/2,1/2,1) + set



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; t(1/2,1/2,0)'; (2); (3).

### Positions

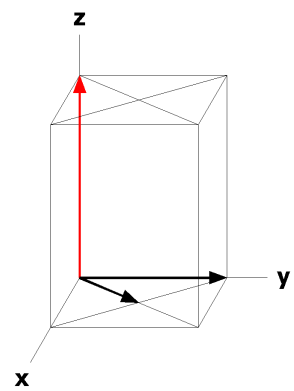
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) + (0,0,1)'	(1/2,1/2,0)' (1/2,1/2,1) +		
16 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
8 k ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [ $\bar{u}, v, 0$ ]		
8 j ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
8 i ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
8 h .2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ , 1/2 [ $\bar{u}, 0, w$ ]		
8 g .2.	0,y,0 [0,v,0]	0, $\bar{y}$ , 0 [0, $\bar{v}, 0$ ]		
8 f 2'..	x,0,1/2 [0,v,w]	$\bar{x}, 0, 1/2$ [0, $\bar{v}, w$ ]		
8 e 2..	x,0,0 [u,0,0]	$\bar{x}, 0, 0$ [ $\bar{u}, 0, 0$ ]		
4 d 2'2'2	0,0,1/2 [0,0,w]			
4 c 2'2'2	1/2,0,1/2 [0,0,w]			
4 b 222	0,1/2,0 [0,0,0]			
4 a 222	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>c</sub>2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/2

Along [0,1,0] p<sub>c</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,1/2



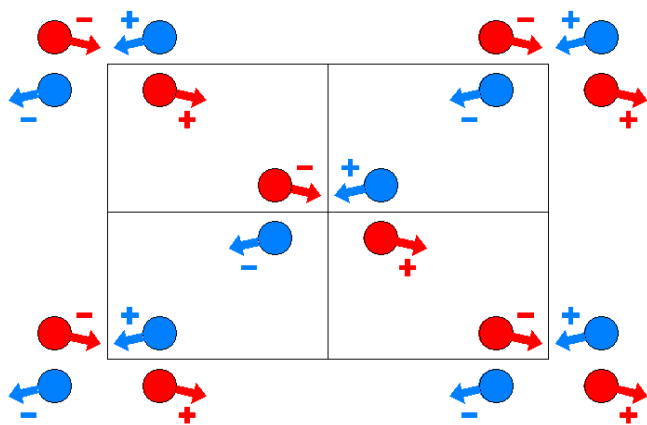
$C_{2c} 22'2'$

21.8.136

$2221'$

$C_{2c} 22'2'$

Orthorhombic



Origin at  $22'2'$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2)  $2'_z$  0,0,z  
( $2_z$ |0,0,0)'

(3)  $2'_y$  0,y,0  
( $2_y$ |0,0,0)'

(4)  $2'_x$  x,0,0  
( $2_x$ |0,0,0)

For (0,0,0) + set

(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)

(2)  $2'_z$  1/4,1/4,z  
( $2_z$ |1/2,1/2,0)'

(3)  $2'_y$  (0,1/2,0) 1/4,y,0  
( $2_y$ |1/2,1/2,0)'

(4)  $2'_x$  (1/2,0,0) x,1/4,0  
( $2_x$ |1/2,1/2,0)

For (1/2,1/2,0) + set

(1) t' (0,0,1)  
(1|0,0,1)'

(2)  $2'_z$  (0,0,1) 0,0,z  
( $2_z$ |0,0,1)

(3)  $2'_y$  0,y,1/2  
( $2_y$ |0,0,1)

(4)  $2'_x$  x,0,1/2  
( $2_x$ |0,0,1)'

For (0,0,1)' + set

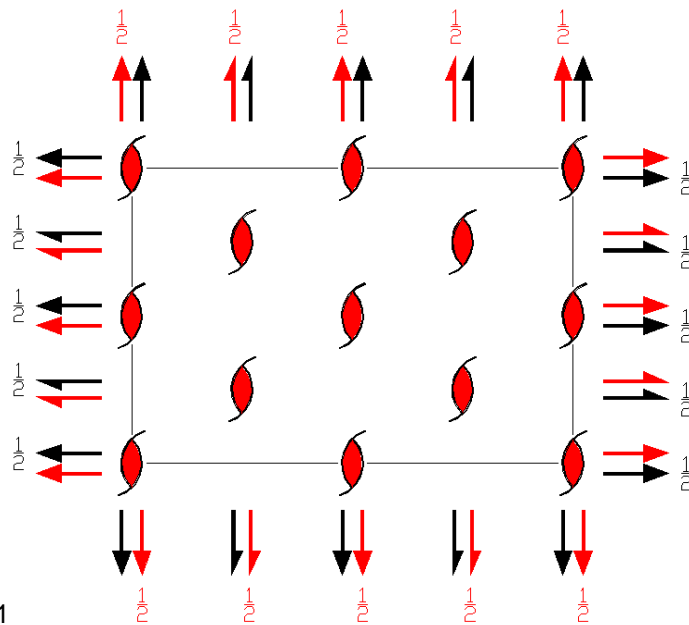
(1) t' (1/2,1/2,1)  
(1|1/2,1/2,1)'

(2)  $2'_z$  (0,0,1) 1/4,1/4,z  
( $2_z$ |1/2,1/2,1)

(3)  $2'_y$  (0,1/2,0) 1/4,y,1/2  
( $2_y$ |1/2,1/2,1)

(4)  $2'_x$  (1/2,0,0) x,1/4,1/2  
( $2_x$ |1/2,1/2,1)'

For (1/2,1/2,1)' + set





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; t(1/2,1/2,0); (2); (3).

### Positions

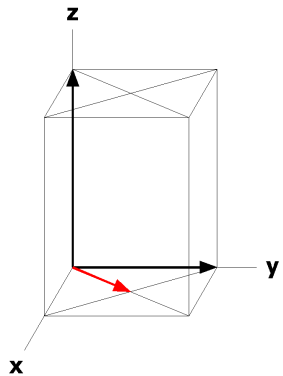
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,1)'	(1/2,1/2,0) + (1/2,1/2,1)'	
16 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}, y, \bar{z}$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
8 k ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [u, $\bar{v}$ ,0]		
8 j ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}$ [u, $\bar{v}$ ,0]		
8 i ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [u, $\bar{v}$ ,0]		
8 h .2.	0,y,1/2 [0,v,0]	0, $\bar{y}$ ,1/2 [0,v,0]		
8 g .2'	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [u,0, $\bar{w}$ ]		
8 f 2'..	x,0,1/2 [0,v,w]	$\bar{x}$ ,0,1/2 [0,v, $\bar{w}$ ]		
8 e 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [u,0,0]		
4 d 2'22'	0,0,1/2 [0,v,0]			
4 c 2'22'	1/2,0,1/2 [0,v,0]			
4 b 22'2'	0,1/2,0 [u,0,0]			
4 a 22'2'	0,0,0 [u,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>.2mm  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>.2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,0



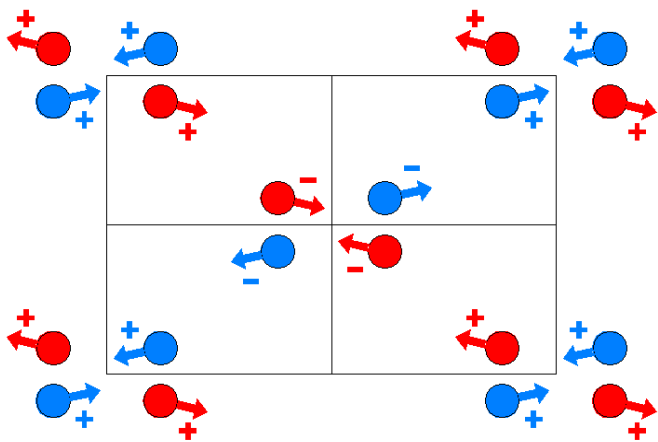
$C_p 2'2'2'$

21.9.137

2221'

$C_p 2'2'2'$

Orthorhombic



Origin at  $2'2'2'$

Asymmetric unit

$$0 \leq x \leq 1/4;$$

$$0 \leq y \leq 1/2;$$

$$0 \leq z \leq 1$$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 2' 0,y,0  
(2<sub>y</sub>|0,0,0)'

(4) 2' x,0,0  
(2<sub>x</sub>|0,0,0)'

For (0,0,0) + set

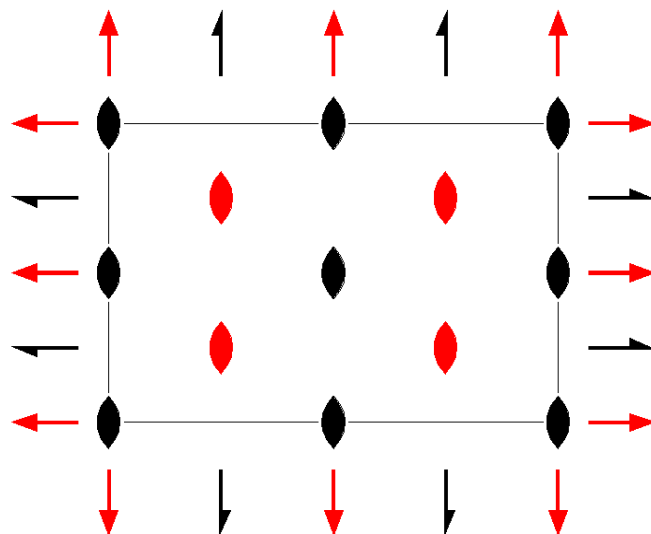
For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0)  
(1|1/2,1/2,0)'

(2) 2' 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,0)'

(3) 2 (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)

(4) 2 (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

### Positions

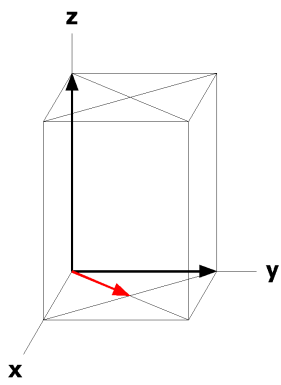
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
8 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $u, \bar{v}, w$ ]	(4) x, $\bar{y}, \bar{z}$ [ $\bar{u}, v, w$ ]
4 k ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [ $\bar{u}, v, 0$ ]		
4 j ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 i ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 h .2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ , 1/2 [ $\bar{u}, 0, w$ ]		
4 g .2'	0,y,0 [u,0,w]	0, $\bar{y}$ , 0 [ $\bar{u}, 0, w$ ]		
4 f 2'..	x,0,1/2 [0,v,w]	$\bar{x}$ , 0, 1/2 [0, $\bar{v}, w$ ]		
4 e 2'..	x,0,0 [0,v,w]	$\bar{x}$ , 0, 0 [0, $\bar{v}, w$ ]		
2 d 2'2'2	0,0,1/2 [0,0,w]			
2 c 2'2'2	1/2,0,1/2 [0,0,w]			
2 b 2'2'2	0,1/2,0 [0,0,w]			
2 a 2'2'2	0,0,0 [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] c<sub>p</sub>2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

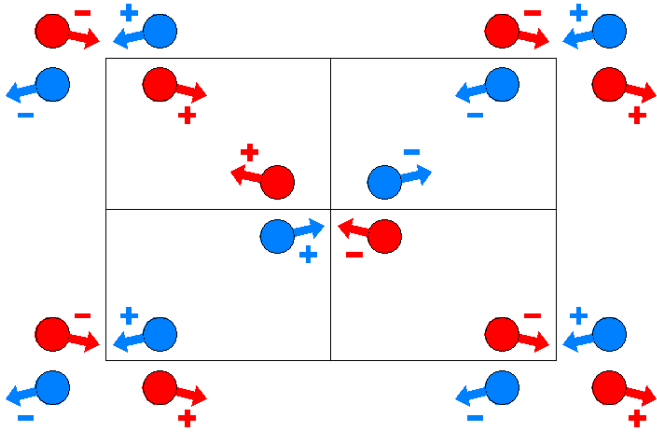
Along [0,1,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,1/4



$C_{p22'2'}$   
21.10.138

$2221'$   
 $C_{p22'2'}$

Orthorhombic



Origin at  $22'2'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2)  $2'_z$  0,0,z  
( $2_z$ |0,0,0)'

(3)  $2'_y$  0,y,0  
( $2_y$ |0,0,0)'

(4)  $2'_x$  x,0,0  
( $2_x$ |0,0,0)

For (0,0,0) + set

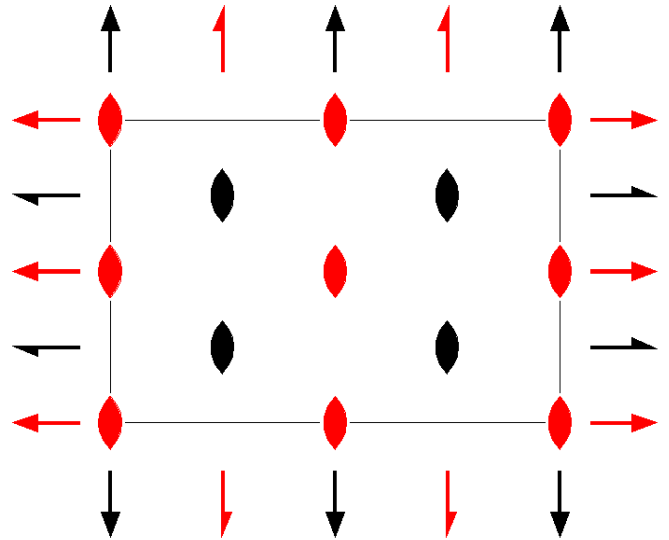
For (1/2,1/2,0)' + set

(1)  $t'$  (1/2,1/2,0)  
(1|1/2,1/2,0)'

(2)  $2'_z$  1/4,1/4,z  
( $2_z$ |1/2,1/2,0)

(3)  $2'_y$  (0,1/2,0) 1/4,y,0  
( $2_y$ |1/2,1/2,0)

(4)  $2'_x$  (1/2,0,0) x,1/4,0  
( $2_x$ |1/2,1/2,0)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

**Positions**

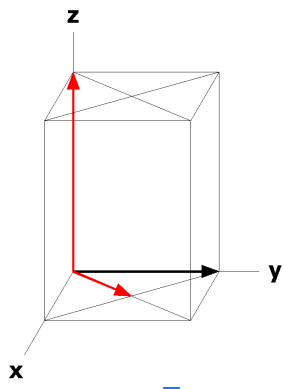
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
8 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}, y, \bar{z}$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
4 k ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0,w]		
4 j ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}$ [u, $\bar{v}$ ,0]		
4 i ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [u, $\bar{v}$ ,0]		
4 h ..2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ ,1/2 [u,0, $\bar{w}$ ]		
4 g ..2'	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [u,0, $\bar{w}$ ]		
4 f 2..	x,0,1/2 [u,0,0]	$\bar{x}$ ,0,1/2 [u,0,0]		
4 e 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [u,0,0]		
2 d 22'2'	0,0,1/2 [u,0,0]			
2 c 22'2'	1/2,0,1/2 [u,0,0]			
2 b 22'2'	0,1/2,0 [u,0,0]			
2 a 22'2'	0,0,0 [u,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] c<sub>p</sub>2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2mm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



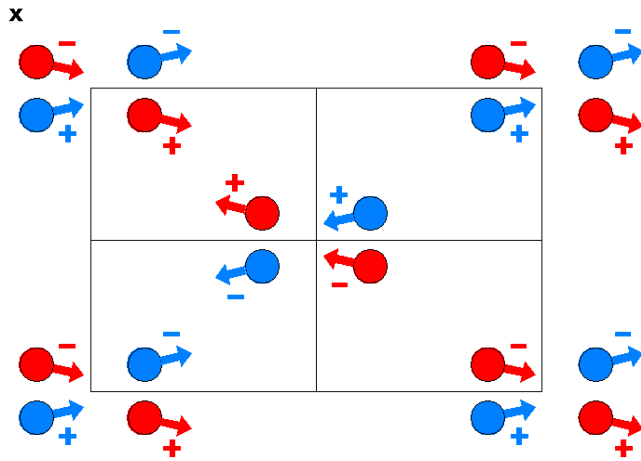
$C_1 2' 2' 2'$

21.11.139

$2221'$

$C_1 2' 2' 2'$

Orthorhombic



Origin at  $2' 2' 2'$

Asymmetric unit

$0 \leq x \leq 1/4;$

$0 \leq y \leq 1/2;$

$0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2)  $2' \ 0,0,z$   
( $2_z$ |0,0,0)'

(3)  $2 \ 0,y,0$   
( $2_y$ |0,0,0)

(4)  $2' \ x,0,0$   
( $2_x$ |0,0,0)'

For (0,0,0) + set

(1)  $t' \ (1/2,1/2,0)$   
(1|1/2,1/2,0)'

(2)  $2 \ 1/4,1/4,z$   
( $2_z$ |1/2,1/2,0)

(3)  $2' \ (0,1/2,0) \ 1/4,y,0$   
( $2_y$ |1/2,1/2,0)'

(4)  $2 \ (1/2,0,0) \ x,1/4,0$   
( $2_x$ |1/2,1/2,0)

For (1/2,1/2,0)' + set

(1)  $t' \ (0,0,1)$   
(1|0,0,1)'

(2)  $2 \ (0,0,1) \ 0,0,z$   
( $2_z$ |0,0,1)

(3)  $2' \ 0,y,1/2$   
( $2_y$ |0,0,1)'

(4)  $2 \ x,0,1/2$   
( $2_x$ |0,0,1)

For (0,0,1)' + set

(1)  $t \ (1/2,1/2,1)$   
(1|1/2,1/2,1)

(2)  $2' \ (0,0,1) \ 1/4,1/4,z$   
( $2_z$ |1/2,1/2,1)'

(3)  $2 \ (0,1/2,0) \ 1/4,y,1/2$   
( $2_y$ |1/2,1/2,1)

(4)  $2' \ (1/2,0,0) \ x,1/4,1/2$   
( $2_x$ |1/2,1/2,1)'

For (1/2,1/2,1) + set

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; t(1/2,1/2,0)'; (2); (3).

### Positions

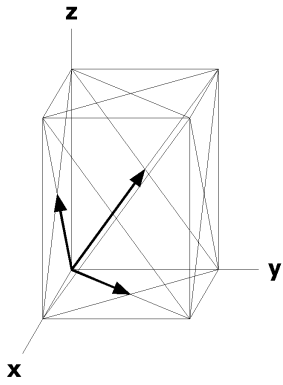
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,1)'	(1/2,1/2,0)' (1/2,1/2,1) +	
16 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) x, $\bar{y}, \bar{z}$ [ $\bar{u}, v, w$ ]
8 k ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0, $\bar{w}$ ]		
8 j ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}$ [ $\bar{u}, v, 0$ ]		
8 i ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [ $\bar{u}, v, 0$ ]		
8 h ..2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ , 1/2 [u,0, $\bar{w}$ ]		
8 g ..2	0,y,0 [0,v,0]	0, $\bar{y}$ , 0 [0,v,0]		
8 f 2..	x,0,1/2 [u,0,0]	$\bar{x}$ , 0, 1/2 [u,0,0]		
8 e 2'..	x,0,0 [0,v,w]	$\bar{x}$ , 0, 0 [0,v, $\bar{w}$ ]		
4 d 2'2'	0,0,1/2 [u,0,0]			
4 c 2'2'	1/2,0,1/2 [u,0,0]			
4 b 2'2'2'	0,1/2,0 [0,v,0]			
4 a 2'2'2'	0,0,0 [0,v,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>c</sub>2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,1/2

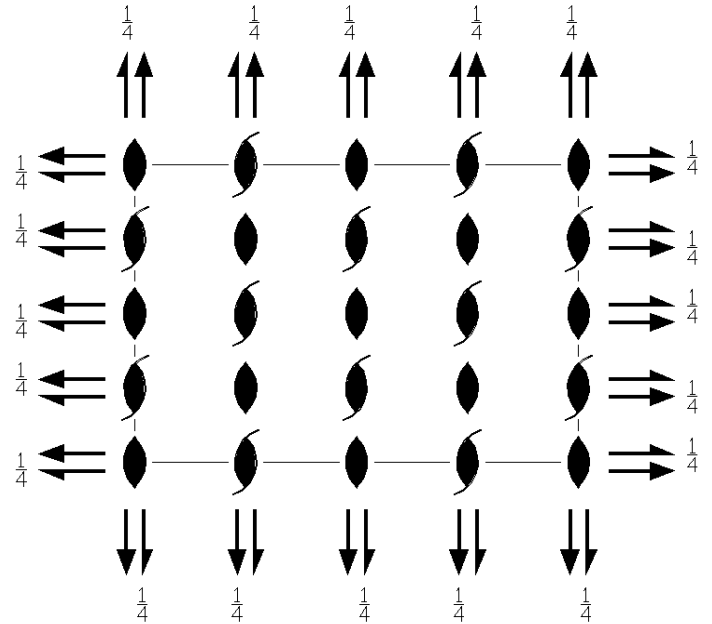
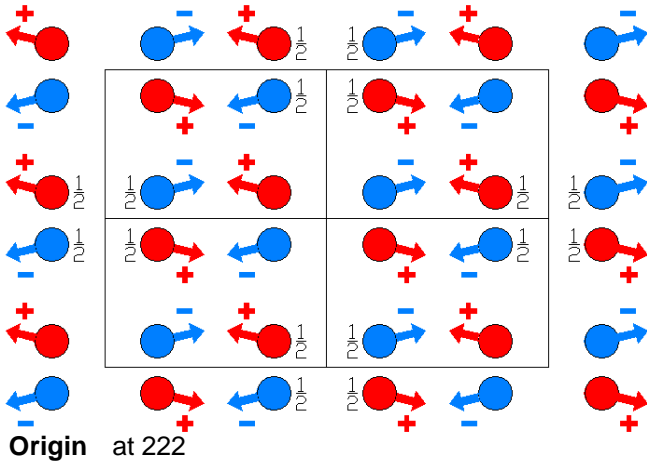
Along [0,1,0] p<sub>c</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,1/2



F222  
22.1.140

222  
F222

Orthorhombic



Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) 2  $0,y,0$   
( $2_y$ |0,0,0)

(4) 2  $x,0,0$   
( $2_x$ |0,0,0)

For (0,0,0) + set

(1) t (0,1/2,1/2)  
(1|0,1/2,1/2)

(2) 2 (0,0,1/2)  $0,1/4,z$   
( $2_z$ |0,1/2,1/2)

(3) 2 (0,1/2,0)  $0,y,1/4$   
( $2_y$ |0,1/2,1/2)

(4) 2  $x,1/4,1/4$   
( $2_x$ |0,1/2,1/2)

For (0,1/2,1/2) + set

(1) t (1/2,0,1/2)  
(1|1/2,0,1/2)

(2) 2 (0,0,1/2)  $1/4,0,z$   
( $2_z$ |1/2,0,1/2)

(3) 2  $1/4,y,1/4$   
( $2_y$ |1/2,0,1/2)

(4) 2 (1/2,0,0)  $x,0,1/4$   
( $2_x$ |1/2,0,1/2)

For (1/2,0,1/2) + set

(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)

(2) 2  $1/4,1/4,z$   
( $2_z$ |1/2,1/2,0)

(3) 2 (0,1/2,0)  $1/4,y,0$   
( $2_y$ |1/2,1/2,0)

(4) 2 (1/2,0,0)  $x,1/4,0$   
( $2_x$ |1/2,1/2,0)

For (1/2,1/2,0) + set



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

### Positions

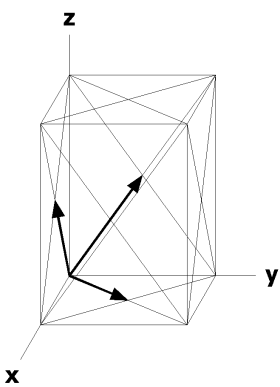
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x, \bar{y}, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]
8	j	2..	x,1/4,1/4 [u,0,0]	$\bar{x}, 3/4, 1/4$ [ $\bar{u}, 0, 0$ ]		
8	i	.2.	1/4,y,1/4 [0,v,0]	$3/4 \bar{y}, 1/4$ [ $0, \bar{v}, 0$ ]		
8	h	..2	1/4,1/4,z [0,0,w]	$3/4, 1/4, \bar{z}$ [ $0, 0, \bar{w}$ ]		
8	g	..2	0,0,z [0,0,w]	$0, 0, \bar{z}$ [ $0, 0, \bar{w}$ ]		
8	f	.2.	0,y,0 [0,v,0]	$0, \bar{y}, 0$ [ $0, \bar{v}, 0$ ]		
8	e	2..	x,0,0 [u,0,0]	$\bar{x}, 0, 0$ [ $\bar{u}, 0, 0$ ]		
4	d	222	1/4,1/4,3/4 [0,0,0]			
4	c	222	1/4,1/4,1/4 [0,0,0]			
4	b	222	0,0,1/2 [0,0,0]			
4	a	222	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

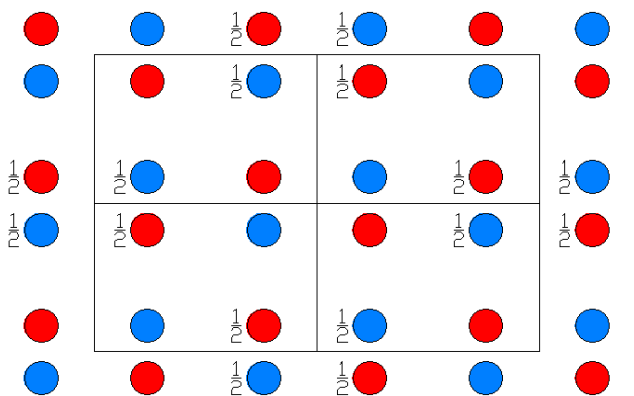
Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



F2221'  
22.2.141

2221'  
F2221'

Orthorhombic



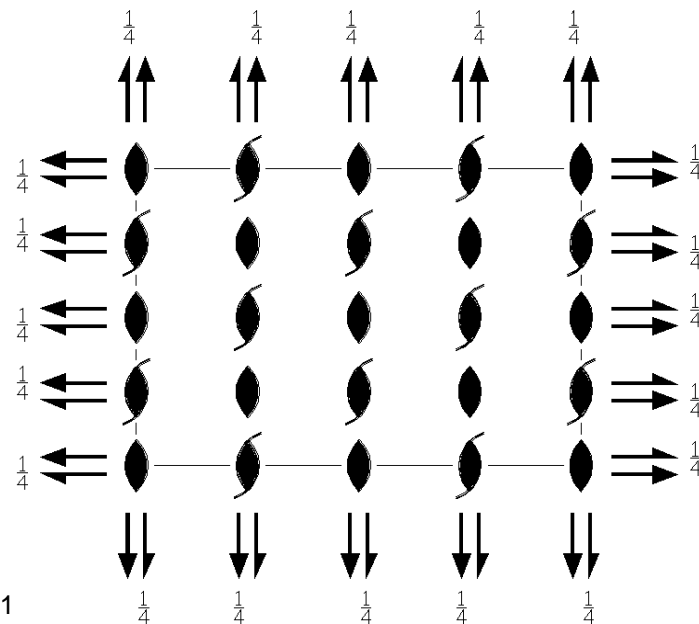
Origin at 2221'

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

Symmetry Operations

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) 1<br>(1 0,0,0)                   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                 |
| For (0,0,0) + set                    |  |  |  |
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2)   | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2 x,1/4,1/4<br>(2 <sub>x</sub>  0,1/2,1/2)         |
| For (0,1/2,1/2) + set                |  |  |  |
| (1) t (1/2,0,1/2)<br>(1 1/2,0,1/2)   | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)           | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>  1/2,0,1/2) |
| For (1/2,0,1/2) + set                |  |  |  |
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)   | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)           | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| For (1/2,1/2,0) + set                |  |  |  |
| (1) 1'<br>(1 0,0,0)'                 | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                 | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                 | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'               |
| For (0,0,0)' + set                   |  |  |  |
| (1) t' (0,1/2,1/2)<br>(1 0,1/2,1/2)' | (2) 2' (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)' | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2' x,1/4,1/4<br>(2 <sub>x</sub>  0,1/2,1/2)'       |
| For (0,1/2,1/2)' + set               |  |  |  |

1'



For (1/2,0,1/2)' + set

$$(1) t' (1/2,0,1/2) \\ (1 | 1/2,0,1/2)'$$

$$(2) 2' (0,0,1/2) \ 1/4,0,z \\ (2_z | 1/2,0,1/2)'$$

$$(3) 2' \ 1/4,y,1/4 \\ (2_y | 1/2,0,1/2)'$$

$$(4) 2' (1/2,0,0) \ x,0,1/4 \\ (2_x | 1/2,0,1/2)'$$

For (1/2,1/2,0)' + set

$$(1) t' (1/2,1/2,0) \\ (1 | 1/2,1/2,0)'$$

$$(2) 2' \ 1/4,1/4,z \\ (2_z | 1/2,1/2,0)'$$

$$(3) 2' (0,1/2,0) \ 1/4,y,0 \\ (2_y | 1/2,1/2,0)'$$

$$(4) 2' (1/2,0,0) \ x,1/4,0 \\ (2_x | 1/2,1/2,0)'$$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); 1'.

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

$$(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) + \\ (0,0,0)' + (0,1/2,1/2)' + (1/2,0,1/2)' + (1/2,1/2,0)'$$

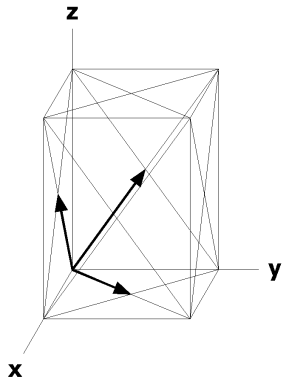
16	k	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{x},y,\bar{z}$ [0,0,0]	(4) $x,\bar{y},\bar{z}$ [0,0,0]
8	j	2..1'	x,1/4,1/4 [0,0,0]	$\bar{x},3/4,1/4$ [0,0,0]		
8	i	.2.1'	1/4,y,1/4 [0,0,0]	$3/4\bar{y},1/4$ [0,0,0]		
8	h	..21'	1/4,1/4,z [0,0,0]	$3/4,1/4,\bar{z}$ [0,0,0]		
8	g	..21'	0,0,z [0,0,0]	$0,0,\bar{z}$ [0,0,0]		
8	f	.2.1'	0,y,0 [0,0,0]	$0,\bar{y},0$ [0,0,0]		
8	e	2..1'	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
4	d	2221'	1/4,1/4,3/4 [0,0,0]			
4	c	2221'	1/4,1/4,1/4 [0,0,0]			
4	b	2221'	0,0,1/2 [0,0,0]			
4	a	2221'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2 \ \mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2 \ \mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

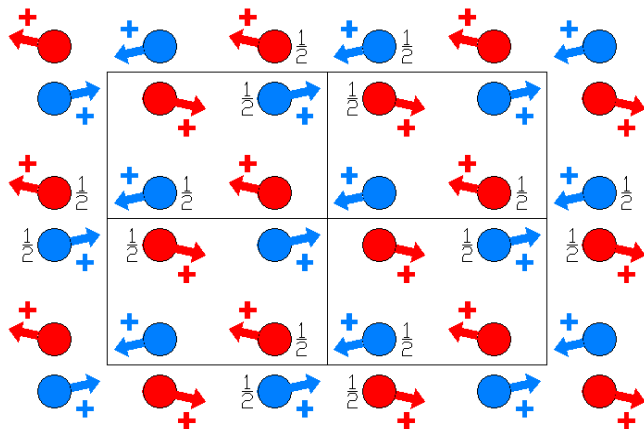
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2 \ \mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



F2'2'2  
22.3.142

2'2'2  
F2'2'2

Orthorhombic



Origin at 2'2'2

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 2' 0,y,0  
(2<sub>y</sub>|0,0,0)'

(4) 2' x,0,0  
(2<sub>x</sub>|0,0,0)'

For (0,0,0) + set

(1) t (0,1/2,1/2)  
(1|0,1/2,1/2)

(2) 2 (0,0,1/2) 0,1/4,z  
(2<sub>z</sub>|0,1/2,1/2)

(3) 2' (0,1/2,0) 0,y,1/4  
(2<sub>y</sub>|0,1/2,1/2)'

(4) 2' x,1/4,1/4  
(2<sub>x</sub>|0,1/2,1/2)'

For (0,1/2,1/2) + set

(1) t (1/2,0,1/2)  
(1|1/2,0,1/2)

(2) 2 (0,0,1/2) 1/4,0,z  
(2<sub>z</sub>|1/2,0,1/2)

(3) 2' 1/4,y,1/4  
(2<sub>y</sub>|1/2,0,1/2)'

(4) 2' (1/2,0,0) x,0,1/4  
(2<sub>x</sub>|1/2,0,1/2)'

For (1/2,0,1/2) + set

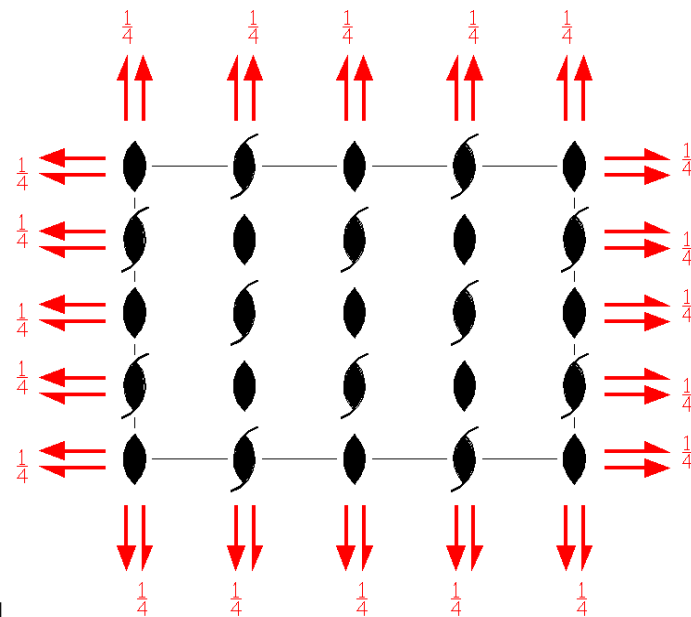
(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)

(2) 2 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,0)

(3) 2' (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)'

(4) 2' (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)'

For (1/2,1/2,0) + set



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

### Positions

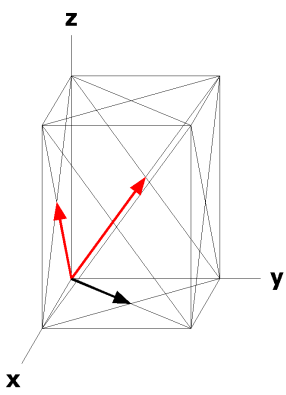
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $u, \bar{v}, w$ ]	(4) $x, \bar{y}, \bar{z}$ [ $\bar{u}, v, w$ ]
8	j	2'..	x,1/4,1/4 [0,v,w]	$\bar{x}, 3/4, 1/4$ [0, $\bar{v}, w$ ]		
8	i	.2'	1/4,y,1/4 [u,0,w]	$3/4 \bar{y}, 1/4$ [ $\bar{u}, 0, w$ ]		
8	h	..2	1/4,1/4,z [0,0,w]	$3/4, 1/4, \bar{z}$ [0,0,w]		
8	g	..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
8	f	.2'	0,y,0 [u,0,w]	0, $\bar{y}, 0$ [ $\bar{u}, 0, w$ ]		
8	e	2'..	x,0,0 [0,v,w]	$\bar{x}, 0, 0$ [0, $\bar{v}, w$ ]		
4	d	2'2'2	1/4,1/4,3/4 [0,0,w]			
4	c	2'2'2	1/4,1/4,1/4 [0,0,w]			
4	b	2'2'2	0,0,1/2 [0,0,w]			
4	a	2'2'2	0,0,0 [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



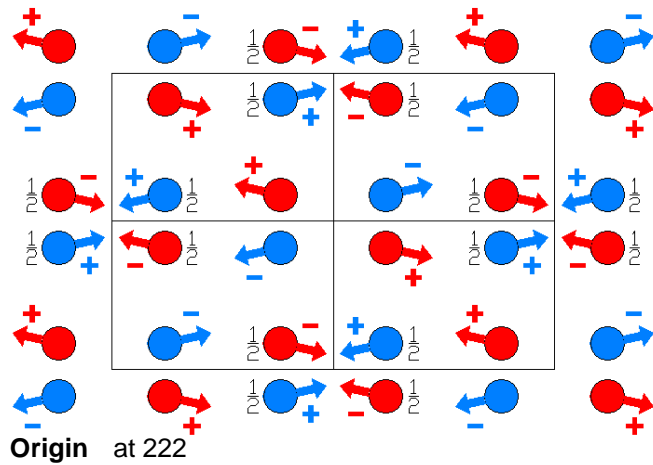
F<sub>C</sub> 222

22.4.143

2221'

F<sub>C</sub> 222

Orthorhombic



Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 2 0,y,0  
(2<sub>y</sub>|0,0,0)

(4) 2 x,0,0  
(2<sub>x</sub>|0,0,0)

For (0,0,0) + set

(1) t' (0,1/2,1/2)  
(1|0,1/2,1/2)'

(2) 2' (0,0,1/2) 0,1/4,z  
(2<sub>z</sub>|0,1/2,1/2)'

(3) 2' (0,1/2,0) 0,y,1/4  
(2<sub>y</sub>|0,1/2,1/2)'

(4) 2' x,1/4,1/4  
(2<sub>x</sub>|0,1/2,1/2)'

For (0,1/2,1/2)' + set

(1) t' (1/2,0,1/2)  
(1|1/2,0,1/2)'

(2) 2' (0,0,1/2) 1/4,0,z  
(2<sub>z</sub>|1/2,0,1/2)'

(3) 2' 1/4,y,1/4  
(2<sub>y</sub>|1/2,0,1/2)'

(4) 2' (1/2,0,0) x,0,1/4  
(2<sub>x</sub>|1/2,0,1/2)'

For (1/2,0,1/2)' + set

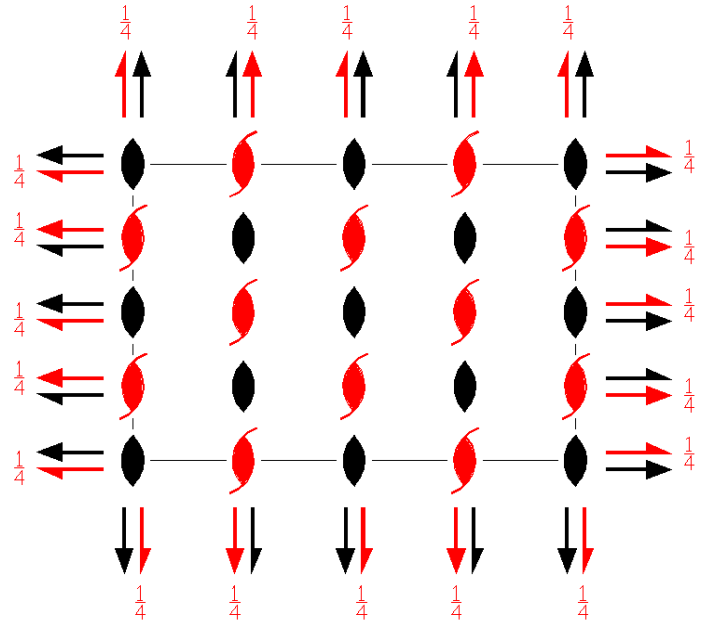
(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)

(2) 2 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,0)

(3) 2 (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)

(4) 2 (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)

For (1/2,1/2,0) + set



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2)'; t(1/2,0,1/2)'; (2); (3).

### Positions

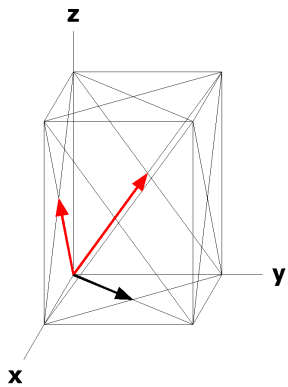
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(0,1/2,1/2)' +	(1/2,0,1/2)' +	(1/2,1/2,0) +
16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x, \bar{y}, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]
8	j	2'.	x,1/4,1/4 [0,v,w]	$\bar{x}, 3/4, 1/4$ [0, $\bar{v}, w$ ]		
8	i	.2'	1/4,y,1/4 [u,0,w]	$3/4 \bar{y}, 1/4$ [ $\bar{u}, 0, w$ ]		
8	h	..2	1/4,1/4,z [0,0,w]	$3/4, 1/4, \bar{z}$ [0,0, $\bar{w}$ ]		
8	g	..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
8	f	.2.	0,y,0 [0,v,0]	0, $\bar{y}, 0$ [0, $\bar{v}, 0$ ]		
8	e	2..	x,0,0 [u,0,0]	$\bar{x}, 0, 0$ [ $\bar{u}, 0, 0$ ]		
4	d	2'2'2	1/4,1/4,3/4 [0,0,w]			
4	c	2'2'2	1/4,1/4,1/4 [0,0,w]			
4	b	222	0,0,1/2 [0,0,0]			
4	a	222	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p<sub>c</sub> 2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] p<sub>2a</sub> 2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub> 2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



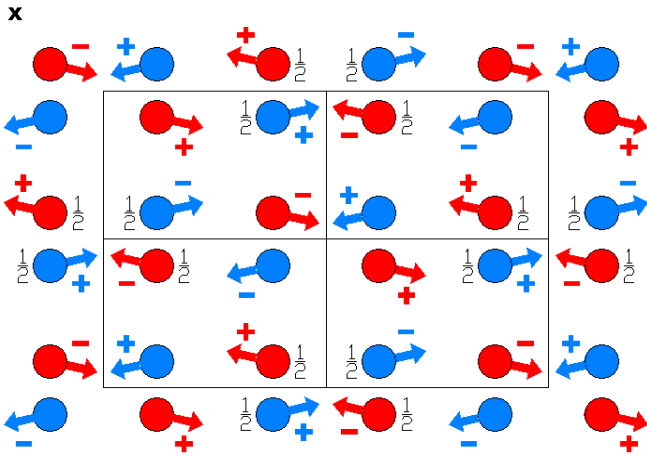
$F_C 22'2'$

22.5.144

$2221'$

$F_C 22'2'$

Orthorhombic



Origin at  $22'2'$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2)  $2'_z$  0,0,z  
( $2_z$ |0,0,0)'

(3)  $2'_y$  0,y,0  
( $2_y$ |0,0,0)'

(4)  $2'_x$  x,0,0  
( $2_x$ |0,0,0)

For (0,0,0) + set

(1)  $t'(0,1/2,1/2)$   
(1|0,1/2,1/2)'

(2)  $2'_z(0,0,1/2)$  0,1/4,z  
( $2_z$ |0,1/2,1/2)

(3)  $2'_y(0,1/2,0)$  0,y,1/4  
( $2_y$ |0,1/2,1/2)

(4)  $2'_x(x,1/4,1/4)$   
( $2_x$ |0,1/2,1/2)'

For (0,1/2,1/2)' + set

(1)  $t'(1/2,0,1/2)$   
(1|1/2,0,1/2)'

(2)  $2'_z(0,0,1/2)$  1/4,0,z  
( $2_z$ |1/2,0,1/2)

(3)  $2'_y(1/4,y,1/4)$   
( $2_y$ |1/2,0,1/2)

(4)  $2'_x(1/2,0,0)$  x,0,1/4  
( $2_x$ |1/2,0,1/2)'

For (1/2,0,1/2)' + set

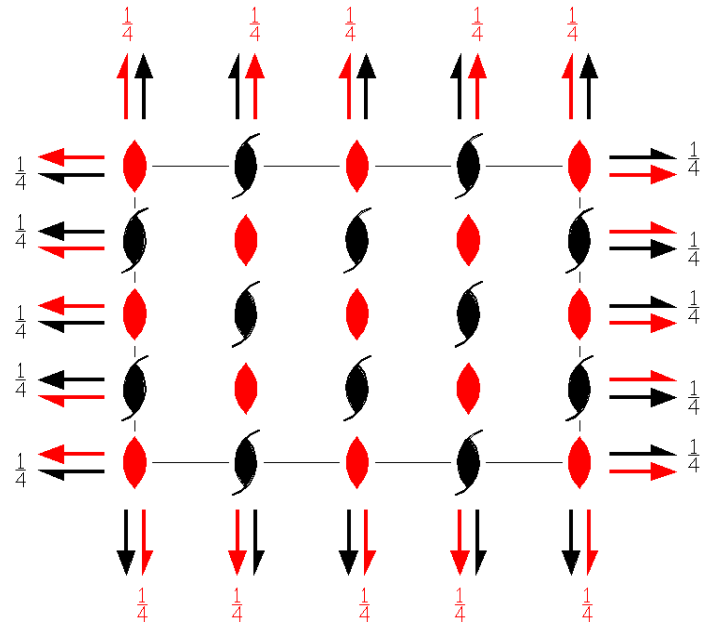
(1)  $t(1/2,1/2,0)$   
(1|1/2,1/2,0)

(2)  $2'_z(1/4,1/4,z)$   
( $2_z$ |1/2,1/2,0)'

(3)  $2'_y(0,1/2,0)$  1/4,y,0  
( $2_y$ |1/2,1/2,0)'

(4)  $2'_x(1/2,0,0)$  x,1/4,0  
( $2_x$ |1/2,1/2,0)

For (1/2,1/2,0) + set





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2)'; t(1/2,0,1/2)'; (2); (3).

### Positions

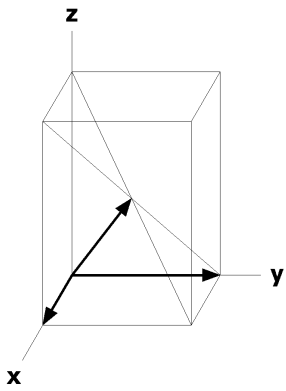
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(0,1/2,1/2)' +	(1/2,0,1/2)' +	(1/2,1/2,0) +
16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}, y, \bar{z}$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
8	j	2'..	x,1/4,1/4 [0,v,w]	$\bar{x}, 3/4, 1/4$ [0,v, $\bar{w}$ ]		
8	i	.2.	1/4,y,1/4 [0,v,0]	3/4 $\bar{y}, 1/4$ [0,v,0]		
8	h	..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [u, $\bar{v}, 0$ ]		
8	g	..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [u, $\bar{v}, 0$ ]		
8	f	.2'.	0,y,0 [u,0,w]	0, $\bar{y}, 0$ [u,0, $\bar{w}$ ]		
8	e	2..	x,0,0 [u,0,0]	$\bar{x}, 0, 0$ [u,0,0]		
4	d	2'22'	1/4,1/4,3/4 [0,v,0]			
4	c	2'22'	1/4,1/4,1/4 [0,v,0]			
4	b	22'2'	0,0,1/2 [u,0,0]			
4	a	22'2'	0,0,0 [u,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p<sub>c</sub>2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,1/4,z

Along [1,0,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

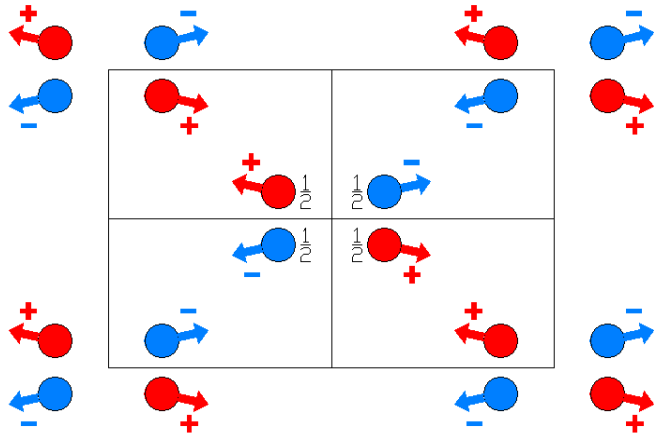
Along [0,1,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



I222  
23.1.145

222  
I222

Orthorhombic



Origin at 222

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

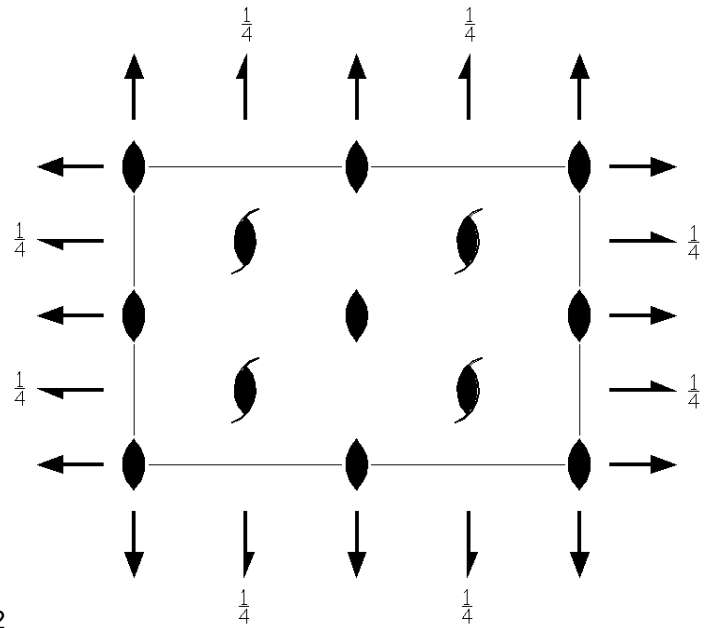
**Symmetry Operations**

For (0,0,0) + set

- (1) 1  $(1|0,0,0)$
- (2) 2  $0,0,z$   $(2_z|0,0,0)$
- (3) 2  $0,y,0$   $(2_y|0,0,0)$
- (4) 2  $x,0,0$   $(2_x|0,0,0)$

For (1/2,1/2,1/2) + set

- (1)  $t(1/2,1/2,1/2)$   $(1|1/2,1/2,1/2)$
- (2) 2  $(0,0,1/2)$   $1/4,1/4,z$   $(2_z|1/2,1/2,1/2)$
- (3) 2  $(0,1/2,0)$   $1/4,y,1/4$   $(2_y|1/2,1/2,1/2)$
- (4) 2  $(1/2,0,0)$   $x,1/4,1/4$   $(2_x|1/2,1/2,1/2)$



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

### Positions

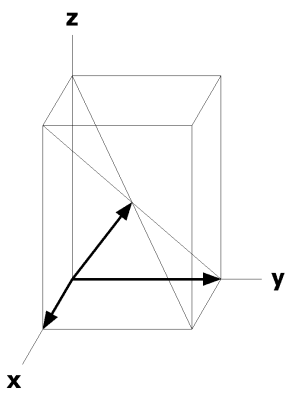
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
8 k 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
4 j ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 i ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 h .2.	1/2,y,0 [0,v,0]	1/2, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]		
4 g .2.	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]		
4 f 2..	x,0,1/2 [u,0,0]	$\bar{x}$ ,0,1/2 [ $\bar{u}$ ,0,0]		
4 e 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0]		
2 d 222	0,1/2,0 [0,0,0]			
2 c 222	0,0,1/2 [0,0,0]			
2 b 222	1/2,0,0 [0,0,0]			
2 a 222	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

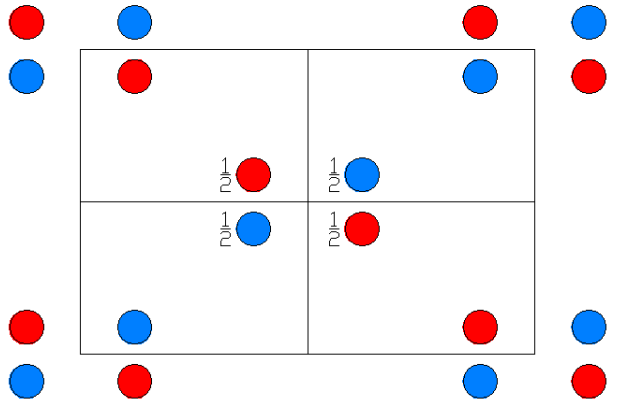
Along [0,1,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



I2221'  
23.2.146

2221'  
I2221'

Orthorhombic



Origin at 2221'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 2 0,y,0  
(2<sub>y</sub>|0,0,0)

(4) 2 x,0,0  
(2<sub>x</sub>|0,0,0)

For (0,0,0) + set

(1) t (1/2,1/2,1/2)  
(1|1/2,1/2,1/2)

(2) 2 (0,0,1/2) 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,1/2)

(3) 2 (0,1/2,0) 1/4,y,1/4  
(2<sub>y</sub>|1/2,1/2,1/2)

(4) 2 (1/2,0,0) x,1/4,1/4  
(2<sub>x</sub>|1/2,1/2,1/2)

For (1/2,1/2,1/2) + set

For (0,0,0)' + set

(1) 1'  
(1|0,0,0)'

(2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'

(3) 2' 0,y,0  
(2<sub>y</sub>|0,0,0)'

(4) 2' x,0,0  
(2<sub>x</sub>|0,0,0)'

For (1/2,1/2,1/2)' + set

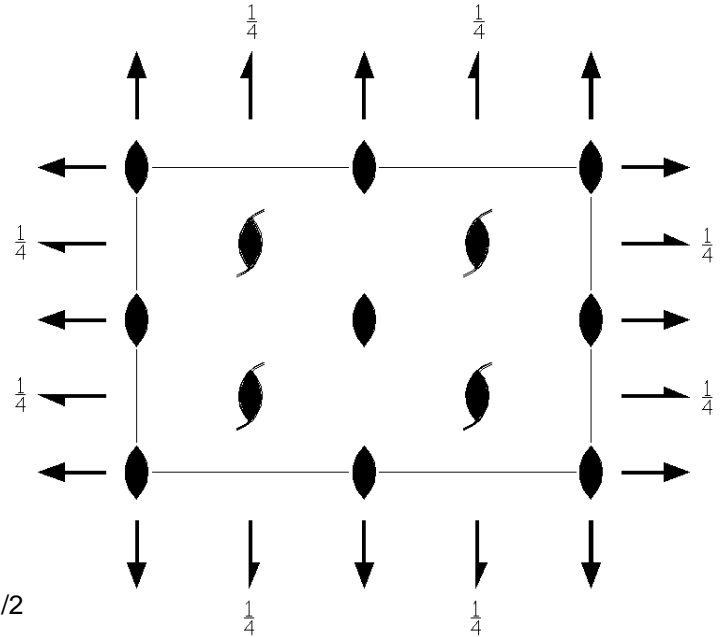
(1) t' (1/2,1/2,1/2)  
(1|1/2,1/2,1/2)'

(2) 2' (0,0,1/2) 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,1/2)'

(3) 2' (0,1/2,0) 1/4,y,1/4  
(2<sub>y</sub>|1/2,1/2,1/2)'

(4) 2' (1/2,0,0) x,1/4,1/4  
(2<sub>x</sub>|1/2,1/2,1/2)'

1'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); 1'.

### Positions

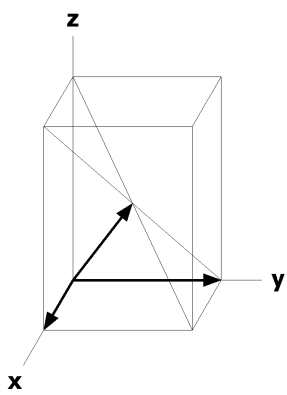
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'	(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'
8 k 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y}, z$ [0,0,0]	(3) $\bar{x}, y, \bar{z}$ [0,0,0]	(4) x, $\bar{y}, \bar{z}$ [0,0,0]
4 j ..21'	0,1/2,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]		
4 i ..21'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 h .2.1'	1/2,y,0 [0,0,0]	1/2, $\bar{y}$ ,0 [0,0,0]		
4 g .2.1'	0,y,0 [0,0,0]	0, $\bar{y}$ ,0 [0,0,0]		
4 f 2..1'	x,0,1/2 [0,0,0]	$\bar{x}$ ,0,1/2 [0,0,0]		
4 e 2..1'	x,0,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0]		
2 d 2221'	0,1/2,0 [0,0,0]			
2 c 2221'	0,0,1/2 [0,0,0]			
2 b 2221'	1/2,0,0 [0,0,0]			
2 a 2221'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

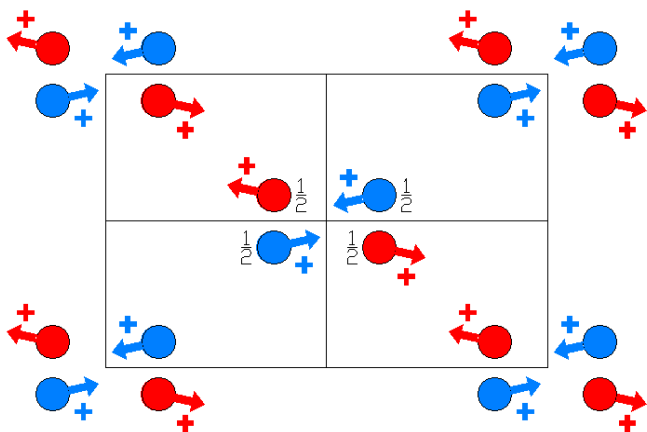
Along [0,1,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



I2'2'2  
23.3.147

2'2'2  
I2'2'2

Orthorhombic



Origin at 2'2'2

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
(2<sub>z</sub>|0,0,0)

(3) 2'  $0,y,0$   
(2<sub>y</sub>|0,0,0)'

(4) 2'  $x,0,0$   
(2<sub>x</sub>|0,0,0)'

For (0,0,0) + set

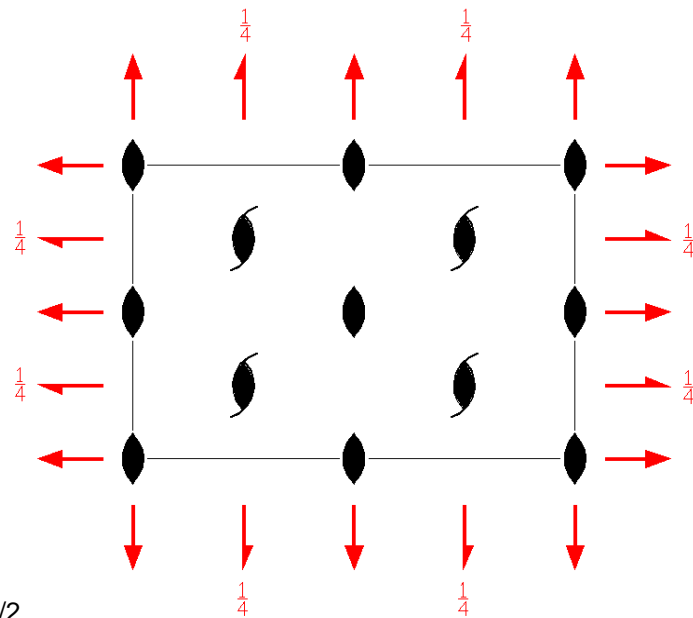
For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)  
(1|1/2,1/2,1/2)

(2) 2 (0,0,1/2)  $1/4,1/4,z$   
(2<sub>z</sub>|1/2,1/2,1/2)

(3) 2' (0,1/2,0)  $1/4,y,1/4$   
(2<sub>y</sub>|1/2,1/2,1/2)'

(4) 2' (1/2,0,0)  $x,1/4,1/4$   
(2<sub>x</sub>|1/2,1/2,1/2)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

**Positions**

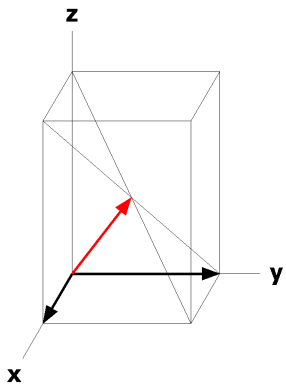
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
8 k 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $u, \bar{v}, w$ ]	(4) x, $\bar{y}, \bar{z}$ [ $\bar{u}, v, w$ ]
4 j ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]		
4 i ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
4 h .2'	1/2,y,0 [u,0,w]	1/2, $\bar{y}, 0$ [ $\bar{u}, 0, w$ ]		
4 g .2'	0,y,0 [u,0,w]	0, $\bar{y}, 0$ [ $\bar{u}, 0, w$ ]		
4 f 2'..	x,0,1/2 [0,v,w]	$\bar{x}, 0, 1/2$ [0, $\bar{v}, w$ ]		
4 e 2'..	x,0,0 [0,v,w]	$\bar{x}, 0, 0$ [0, $\bar{v}, w$ ]		
2 d 2'2'2	0,1/2,0 [0,0,w]			
2 c 2'2'2	0,0,1/2 [0,0,w]			
2 b 2'2'2	1/2,0,0 [0,0,w]			
2 a 2'2'2	0,0,0 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] c2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



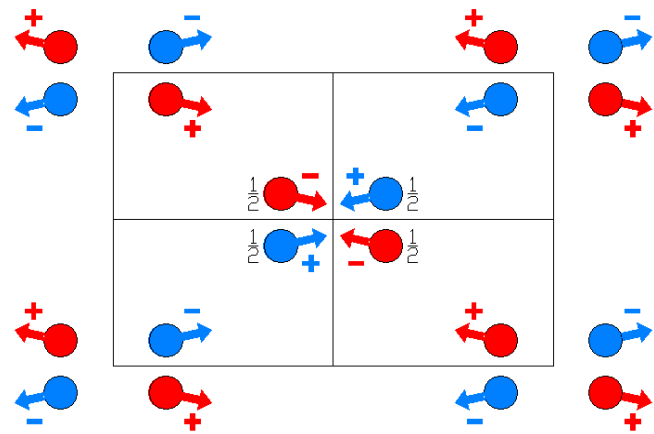
$I_p 222$

23.4.148

$2221'$

$I_p 222$

Orthorhombic



Origin at  $222$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) 2  $0,y,0$   
( $2_y$ |0,0,0)

(4) 2  $x,0,0$   
( $2_x$ |0,0,0)

For (0,0,0) + set

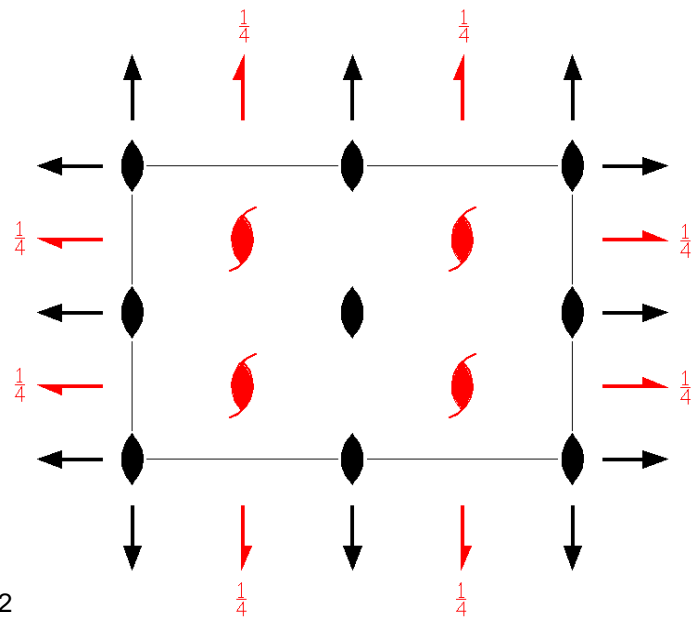
For (1/2,1/2,1/2)' + set

(1)  $t'$  (1/2,1/2,1/2)  
(1|1/2,1/2,1/2)'

(2)  $2'$  (0,0,1/2)  $1/4,1/4,z$   
( $2_z$ |1/2,1/2,1/2)'

(3)  $2'$  (0,1/2,0)  $1/4,y,1/4$   
( $2_y$ |1/2,1/2,1/2)'

(4)  $2'$  (1/2,0,0)  $x,1/4,1/4$   
( $2_x$ |1/2,1/2,1/2)'





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2)'; (2); (3).

### Positions

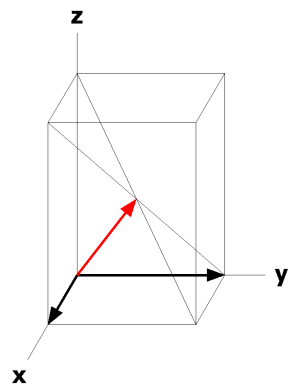
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
8 k 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
4 j ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 i ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 h .2.	1/2,y,0 [0,v,0]	1/2, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]		
4 g .2.	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]		
4 f 2..	x,0,1/2 [u,0,0]	$\bar{x}$ ,0,1/2 [ $\bar{u}$ ,0,0]		
4 e 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0]		
2 d 222	0,1/2,0 [0,0,0]			
2 c 222	0,0,1/2 [0,0,0]			
2 b 222	1/2,0,0 [0,0,0]			
2 a 222	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1]  $c_p 2m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c_p 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

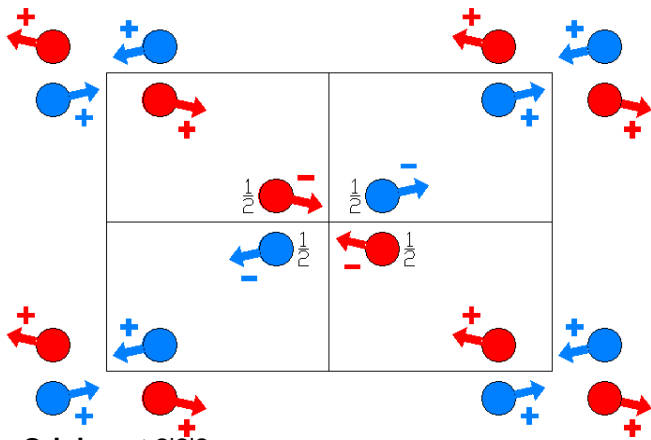
Along [0,1,0]  $c_p 2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



$I_p 2'2'2'$   
23.5.149

$2221'$   
 $I_p 2'2'2'$

Orthorhombic



Origin at  $2'2'2'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) 2'  $0,y,0$   
( $2_y$ |0,0,0)'

(4) 2'  $x,0,0$   
( $2_x$ |0,0,0)'

For (0,0,0) + set

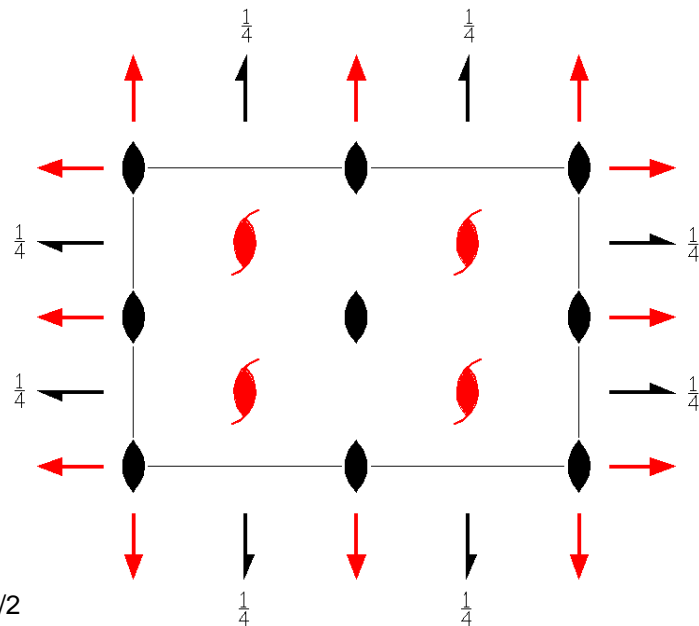
For (1/2,1/2,1/2)' + set

(1)  $t'$  (1/2,1/2,1/2)  
(1|1/2,1/2,1/2)'

(2) 2' (0,0,1/2)  $1/4,1/4,z$   
( $2_z$ |1/2,1/2,1/2)'

(3) 2 (0,1/2,0)  $1/4,y,1/4$   
( $2_y$ |1/2,1/2,1/2)

(4) 2 (1/2,0,0)  $x,1/4,1/4$   
( $2_x$ |1/2,1/2,1/2)



**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,1/2)'$ ; (2); (3).

**Positions**

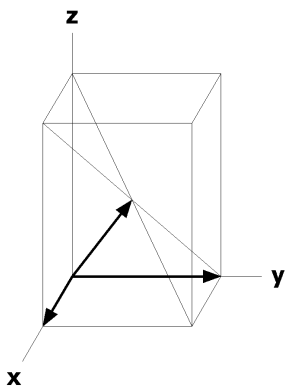
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	$(1/2,1/2,1/2)'$ +		
8 k 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(4) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]
4 j ..2	$0,1/2,z$ [0,0,w]	$0,1/2,\bar{z}$ [0,0,w]		
4 i ..2	$0,0,z$ [0,0,w]	$0,0,\bar{z}$ [0,0,w]		
4 h .2'	$1/2,y,0$ [u,0,w]	$1/2,\bar{y},0$ [ $\bar{u},0,w$ ]		
4 g .2'	$0,y,0$ [u,0,w]	$0,\bar{y},0$ [ $\bar{u},0,w$ ]		
4 f 2'..	$x,0,1/2$ [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]		
4 e 2'..	$x,0,0$ [0,v,w]	$\bar{x},0,0$ [0, $\bar{v},w$ ]		
2 d 2'2'2	$0,1/2,0$ [0,0,w]			
2 c 2'2'2	$0,0,1/2$ [0,0,w]			
2 b 2'2'2	$1/2,0,0$ [0,0,w]			
2 a 2'2'2	$0,0,0$ [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1]  $c_p 2mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c_p 2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

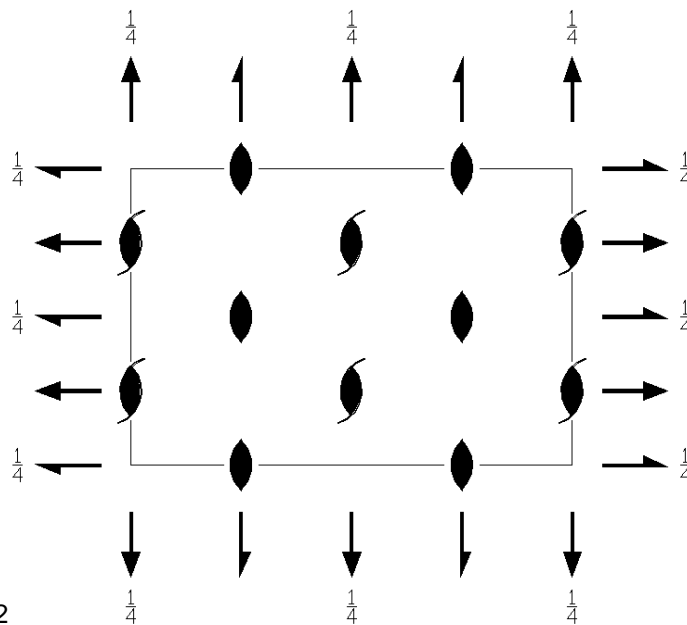
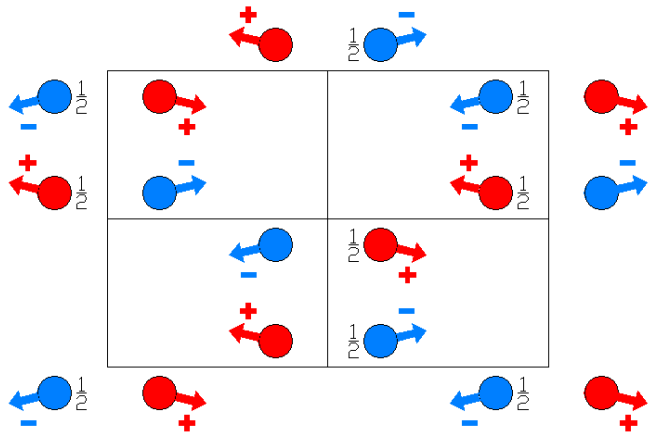
Along [0,1,0]  $c_p 2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



$I2_12_12_1$   
24.1.150

222  
 $I2_12_12_1$

Orthorhombic



**Origin** at midpoint of three non-intersecting pairs of parallel 2 axes

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
|--------------------|--|--|--|

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t$ (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2) | (2) 2 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,0) | (3) 2 1/4,y,0<br>(2 <sub>y</sub>  1/2,0,0) | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2) |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

### Positions

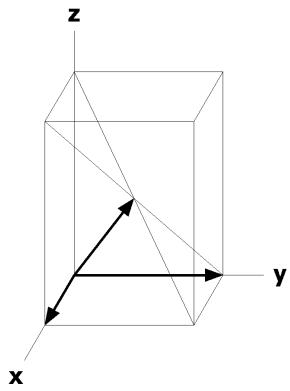
		Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(1/2,1/2,1/2) +
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ] (3) $\bar{x}, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ] (4) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]
4	c ..2	0,1/4,z [0,0,w]	0,3/4, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	b .2.	1/4,y,0 [0,v,0]	1/4, $\bar{y}, 1/2$ [0, $\bar{v}, 0$ ]
4	a 2..	x,0,1/4 [u,0,0]	$\bar{x}+1/2, 0, 3/4$ [ $\bar{u}, 0, 0$ ]

### Symmetry of Special Projections

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



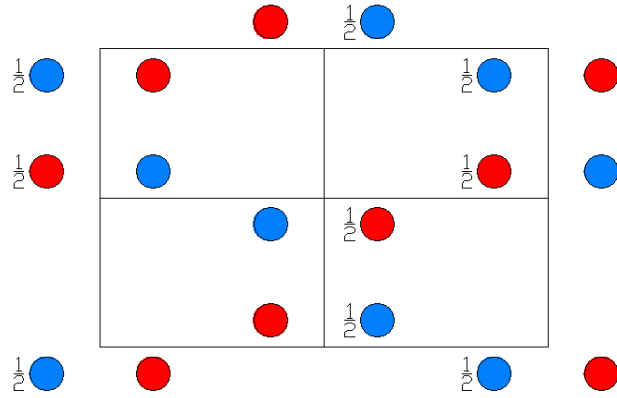
$I2_12_12_11'$

24.2.151

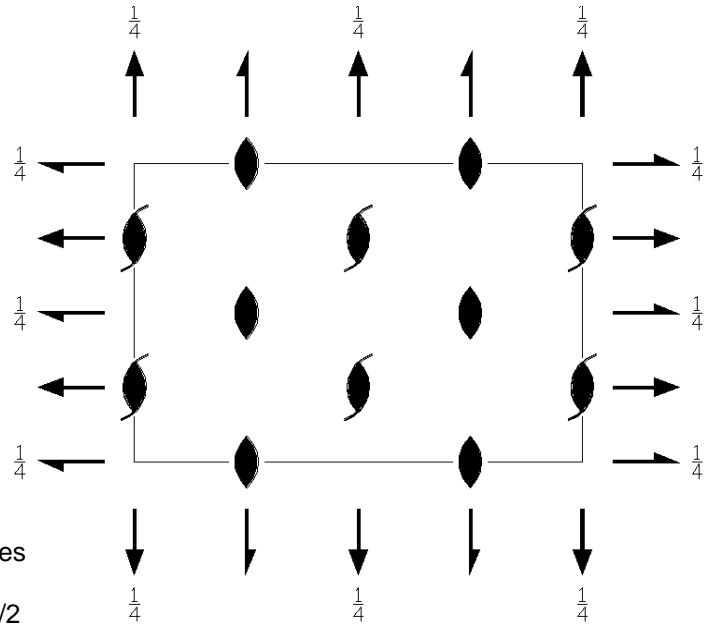
$2221'$

$I2_12_12_11'$

Orthorhombic



$1'$



**Origin** at midpoint of three non-intersecting pairs of parallel  $21'$  axes

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0) + \text{set}$

- (1)  $1$   
( $1|0,0,0$ )
- (2)  $2$   $(0,0,1/2)$   $1/4,0,z$   
( $2_z|1/2,0,1/2$ )
- (3)  $2$   $(0,1/2,0)$   $0,y,1/4$   
( $2_y|0,1/2,1/2$ )
- (4)  $2$   $(1/2,0,0)$   $x,1/4,0$   
( $2_x|1/2,1/2,0$ )

For  $(1/2,1/2,1/2) + \text{set}$

- (1)  $t$   $(1/2,1/2,1/2)$   
( $1|1/2,1/2,1/2$ )
- (2)  $2$   $0,1/4,z$   
( $2_z|0,1/2,0$ )
- (3)  $2$   $1/4,y,0$   
( $2_y|1/2,0,0$ )
- (4)  $2$   $x,0,1/4$   
( $2_x|0,0,1/2$ )

For  $(0,0,0)' + \text{set}$

- (1)  $1'$   
( $1|0,0,0$ )'
- (2)  $2'$   $(0,0,1/2)$   $1/4,0,z$   
( $2_z|1/2,0,1/2$ )'
- (3)  $2'$   $(0,1/2,0)$   $0,y,1/4$   
( $2_y|0,1/2,1/2$ )'
- (4)  $2'$   $(1/2,0,0)$   $x,1/4,0$   
( $2_x|1/2,1/2,0$ )'

For  $(1/2,1/2,1/2)' + \text{set}$

- (1)  $t'$   $(1/2,1/2,1/2)$   
( $1|1/2,1/2,1/2$ )'
- (2)  $2'$   $0,1/4,z$   
( $2_z|0,1/2,0$ )'
- (3)  $2'$   $1/4,y,0$   
( $2_y|1/2,0,0$ )'
- (4)  $2'$   $x,0,1/4$   
( $2_x|0,0,1/2$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); 1'.

### Positions

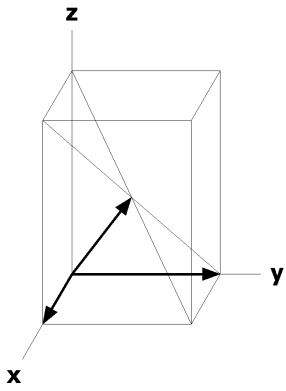
				Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.					
				(0,0,0) + (0,0,0)' +	(1/2,1/2,1/2) + (1/2,1/2,1/2)' +
8	d 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [0,0,0]	(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [0,0,0]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [0,0,0]
4	c ..21'	0,1/4,z [0,0,0]	0,3/4, $\bar{z}+1/2$ [0,0,0]		
4	b .2.1'	1/4,y,0 [0,0,0]	1/4, $\bar{y}, 1/2$ [0,0,0]		
4	a 2..1'	x,0,1/4 [0,0,0]	$\bar{x}+1/2, 0, 3/4$ [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



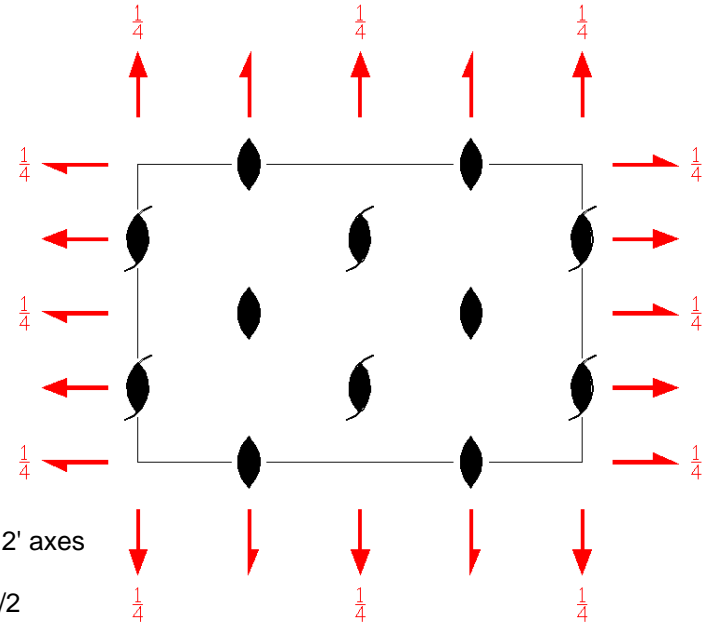
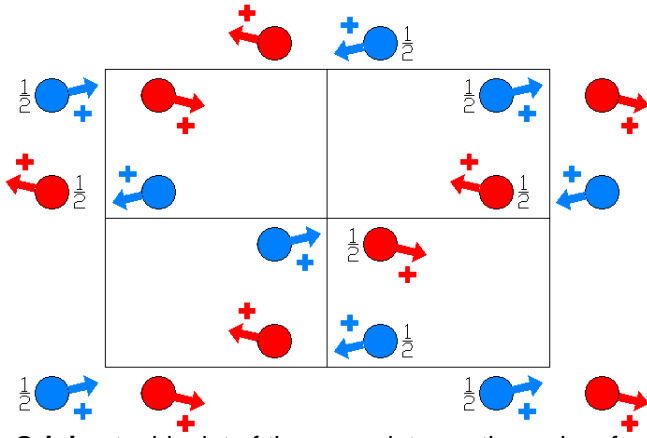
$I2_1'2_1'2_1$

24.3.152

$2'2'2$

$I2_1'2_1'2_1$

Orthorhombic



**Origin** at midpoint of three non-intersecting pairs of parallel 2 and 2' axes

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
|--------------------|--|--|--|

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2) | (2) 2 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,0) | (3) 2' 1/4,y,0<br>(2 <sub>y</sub>  1/2,0,0)' | (4) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)' |
|--|--|--|--|



**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,1/2)$ ; (2); (3).

### Positions

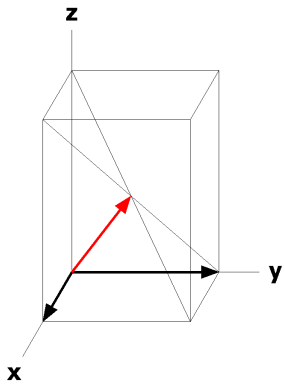
		Coordinates	
Multiplicity,	Wyckoff letter,	Site Symmetry.	
		(0,0,0) +	(1/2,1/2,1/2) +
8	d 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ] (3) $\bar{x},y+1/2,\bar{z}+1/2$ [u, $\bar{v},w$ ] (4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]
4	c ..2	$0,1/4,z$ [0,0,w]	$0,3/4,\bar{z}+1/2$ [0,0,w]
4	b .2'	$1/4,y,0$ [u,0,w]	$1/4,\bar{y},1/2$ [ $\bar{u},0,w$ ]
4	a 2'..	$x,0,1/4$ [0,v,w]	$\bar{x}+1/2,0,3/4$ [0, $\bar{v},w$ ]

### Symmetry of Special Projections

Along [0,0,1]  $c2mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $1/4,0,z$

Along [1,0,0]  $c2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $x,1/4,0$

Along [0,1,0]  $c2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at  $0,y,1/4$



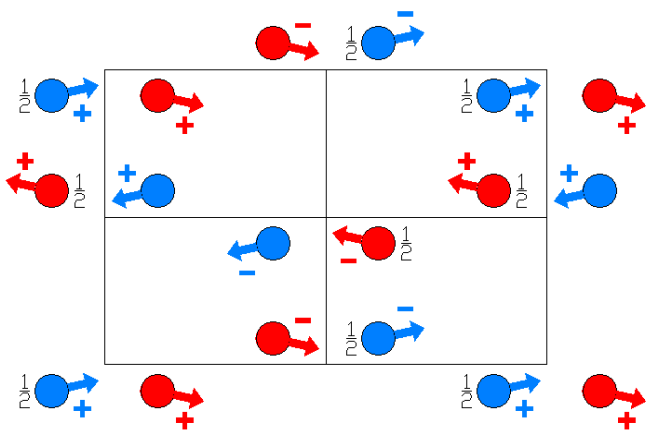
$I_p 2_1 2_1 2_1$

24.4.153

$2221'$

$I_p 2_1 2_1 2_1$

Orthorhombic



Origin at midpoint of three non-intersecting pairs of parallel  $2'$  axes

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

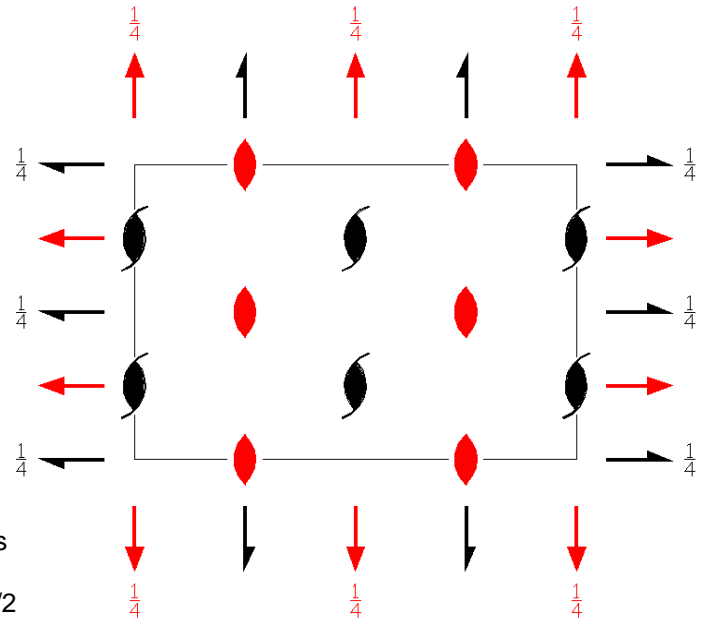
**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $(0,0,1/2)$ $1/4,0,z$<br>( $2_z$   $1/2,0,1/2$ ) | (3) 2 $(0,1/2,0)$ $0,y,1/4$<br>( $2_y$   $0,1/2,1/2$ ) | (4) 2 $(1/2,0,0)$ $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ ) |
|--------------------|--|--|--|

For  $(1/2,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,1/2)$<br>(1  $1/2,1/2,1/2$ )' | (2) $2'$ $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )' | (3) $2'$ $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )' | (4) $2'$ $x,0,1/4$<br>( $2_x$   $0,0,1/2$ )' |
|--|--|--|--|



**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,1/2)'$ ; (2); (3).

### Positions

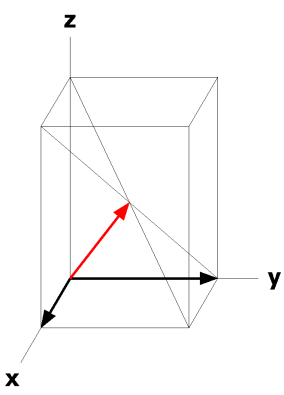
Multiplicity, Wyckoff letter, Site Symmetry.		Coordinates			
		(0,0,0) +		(1/2,1/2,1/2)' +	
8	d 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
4	c ..2'	$0,1/4,z$ [u,v,0]	$0,3/4,\bar{z}+1/2$ [ $\bar{u},v,0$ ]		
4	b .2'	$1/4,y,0$ [u,0,w]	$1/4,\bar{y},1/2$ [ $\bar{u},0,w$ ]		
4	a 2'..	$x,0,1/4$ [0,v,w]	$\bar{x}+1/2,0,3/4$ [ $0,\bar{v},w$ ]		

### Symmetry of Special Projections

Along  $[0,0,1]$   $c_p2mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $1/4,0,z$

Along  $[1,0,0]$   $c_p2mm$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,1/4,0$

Along  $[0,1,0]$   $c_p2mm$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at  $0,y,1/4$



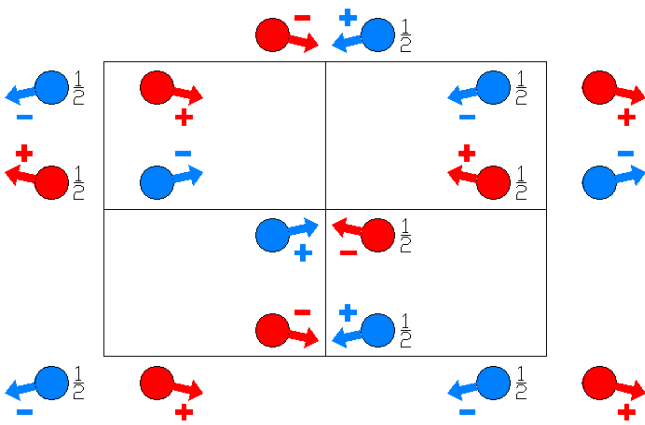
$I_p 2_1' 2_1' 2_1$

24.5.154

2221'

$I_p 2_1' 2_1' 2_1$

Orthorhombic



**Origin** at midpoint of three non-intersecting pairs of parallel 2 and 2' axes

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

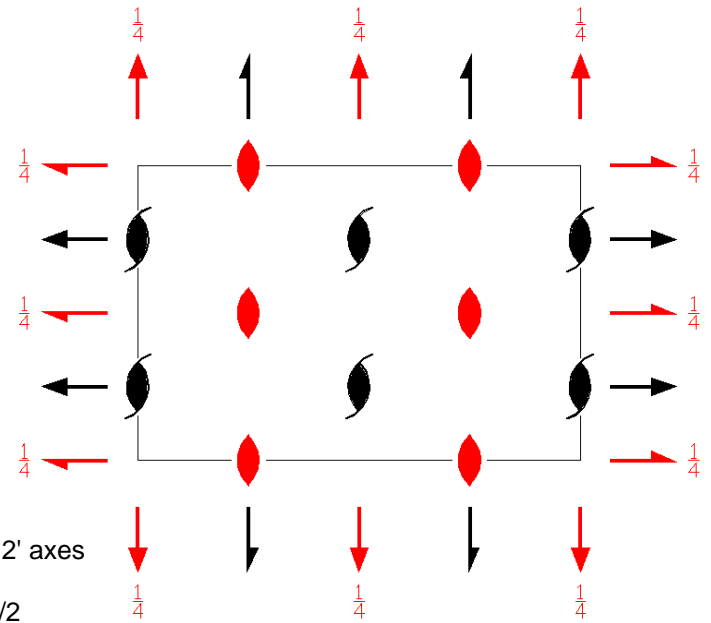
**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
|--------------------|--|--|--|

For (1/2,1/2,1/2)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)' | (2) 2' 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,0)' | (3) 2 1/4,y,0<br>(2 <sub>y</sub>  1/2,0,0) | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2) |
|--|--|--|--|



**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,1/2)'$ ; (2); (3).

### Positions

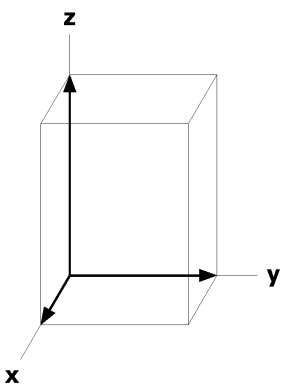
Multiplicity, Wyckoff letter, Site Symmetry.		Coordinates			
		(0,0,0) + (1/2,1/2,1/2)' +			
8	d 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]
4	c ..2'	$0,1/4,z$ [u,v,0]	$0,3/4,\bar{z}+1/2$ [ $\bar{u},v,0$ ]		
4	b .2.	$1/4,y,0$ [0,v,0]	$1/4,\bar{y},1/2$ [0, $\bar{v},0$ ]		
4	a 2..	$x,0,1/4$ [u,0,0]	$\bar{x}+1/2,0,3/4$ [ $\bar{u},0,0$ ]		

### Symmetry of Special Projections

Along  $[0,0,1]$   $c_p2mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $1/4,0,z$

Along  $[1,0,0]$   $c_p2'mm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,1/4,0$

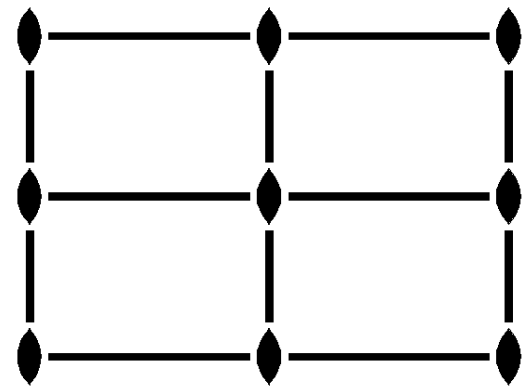
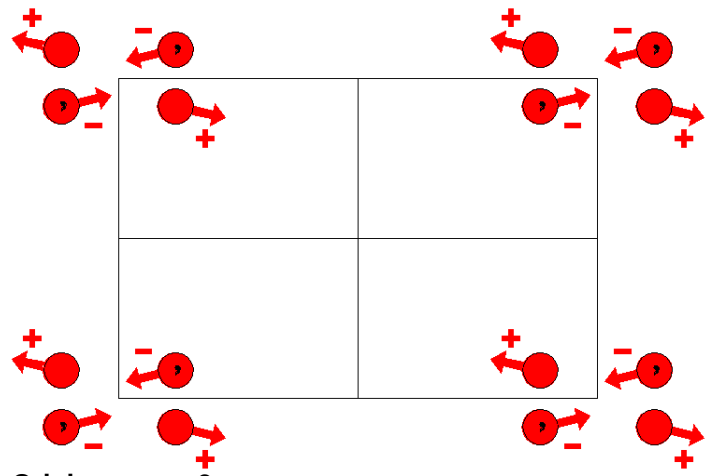
Along  $[0,1,0]$   $c_p2'mm'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $0,y,1/4$



Pmm2  
25.1.155

mm2  
Pmm2

Orthorhombic



Origin on mm2

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) m x,0,z  
(m<sub>y</sub>|0,0,0)

(4) m 0,y,z  
(m<sub>x</sub>|0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

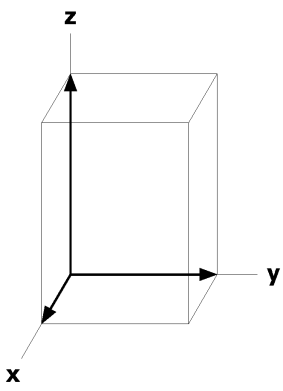
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
4	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y}$ ,z [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
2	h	m..	1/2,y,z [u,0,0]	1/2, $\bar{y}$ ,z [ $\bar{u},0,0$ ]		
2	g	m..	0,y,z [u,0,0]	0, $\bar{y}$ ,z [ $\bar{u},0,0$ ]		
2	f	.m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v},0$ ]		
2	e	.m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]		
1	d	mm2	1/2,1/2,z [0,0,0]			
1	c	mm2	1/2,0,z [0,0,0]			
1	b	mm2	0,1/2,z [0,0,0]			
1	a	mm2	0,0,z [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0

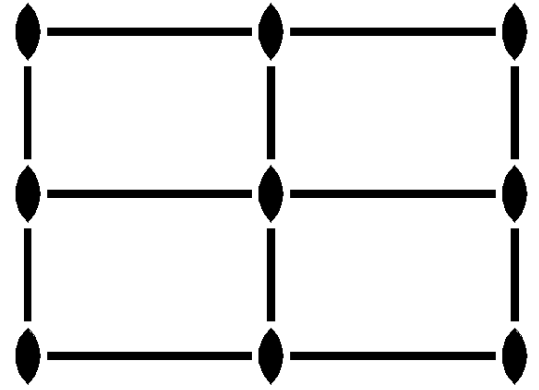
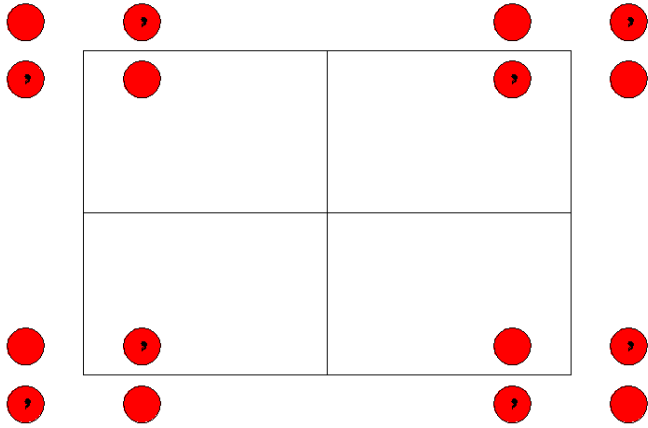


Pmm21'  
25.2.156

mm21'  
Pmm21'

Orthorhombic

1'



Origin on mm21'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For 1 + set

(1) 1  
(1|0,0,0)

(2) 2<sub>0,0,z</sub>  
(2<sub>z</sub>|0,0,0)

(3) m<sub>x,0,z</sub>  
(m<sub>y</sub>|0,0,0)

(4) m<sub>0,y,z</sub>  
(m<sub>x</sub>|0,0,0)

For 1' + set

(1) 1'  
(1|0,0,0)'

(2) 2'<sub>0,0,z</sub>  
(2<sub>z</sub>|0,0,0)'

(3) m'<sub>x,0,z</sub>  
(m<sub>y</sub>|0,0,0)'

(4) m'<sub>0,y,z</sub>  
(m<sub>x</sub>|0,0,0)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

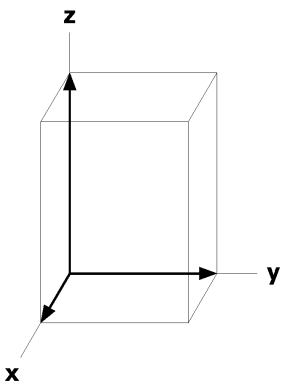
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
4 i 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) x, $\bar{y},z$ [0,0,0]	(4) $\bar{x},y,z$ [0,0,0]
2 h m..1'	1/2,y,z [0,0,0]	1/2, $\bar{y},z$ [0,0,0]		
2 g m..1'	0,y,z [0,0,0]	0, $\bar{y},z$ [0,0,0]		
2 f .m.1'	x,1/2,z [0,0,0]	$\bar{x},1/2,z$ [0,0,0]		
2 e .m.1'	x,0,z [0,0,0]	$\bar{x},0,z$ [0,0,0]		
1 d mm21'	1/2,1/2,z [0,0,0]			
1 c mm21'	1/2,0,z [0,0,0]			
1 b mm21'	0,1/2,z [0,0,0]			
1 a mm21'	0,0,z [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

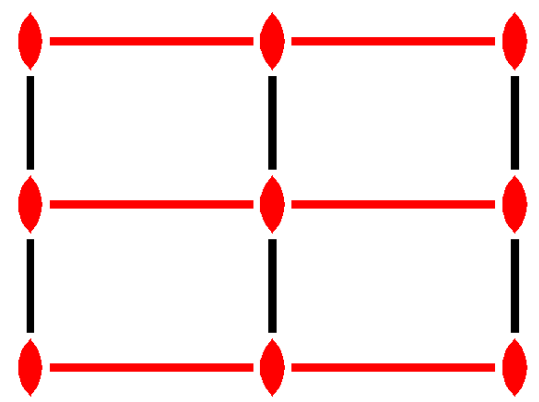
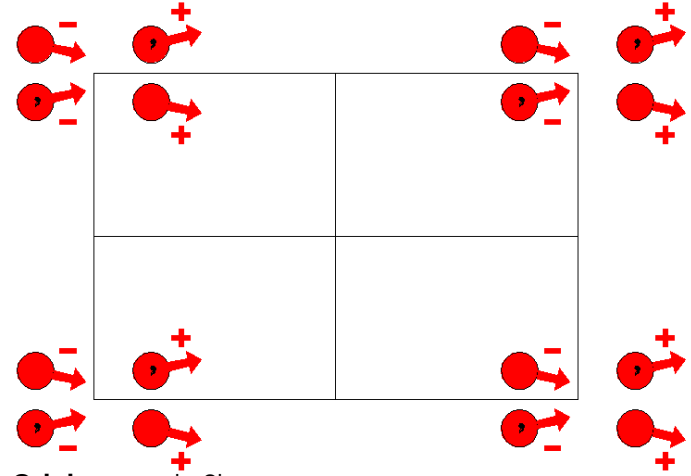
Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pm'm2'  
25.3.157

m'm2'  
Pm'm2'

Orthorhombic



Origin on m'm2'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

- (1) 1  
(1|0,0,0)
- (2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'
- (3) m x,0,z  
(m<sub>y</sub>|0,0,0)
- (4) m' 0,y,z  
(m<sub>x</sub>|0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

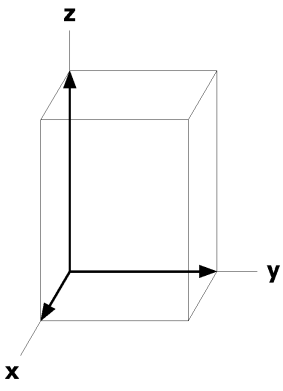
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
4 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
2 h m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0,v, $\bar{w}$ ]		
2 g m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0,v, $\bar{w}$ ]		
2 f .m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0,v,0]		
2 e .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0,v,0]		
1 d m'm2'	1/2,1/2,z [0,v,0]			
1 c m'm2'	1/2,0,z [0,v,0]			
1 b m'm2'	0,1/2,z [0,v,0]			
1 a m'm2'	0,0,z [0,v,0]			

**Symmetry of Special Projections**

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

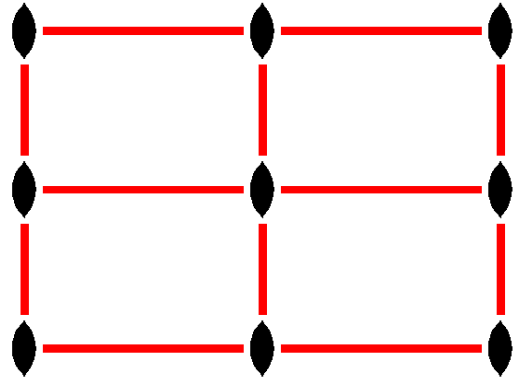
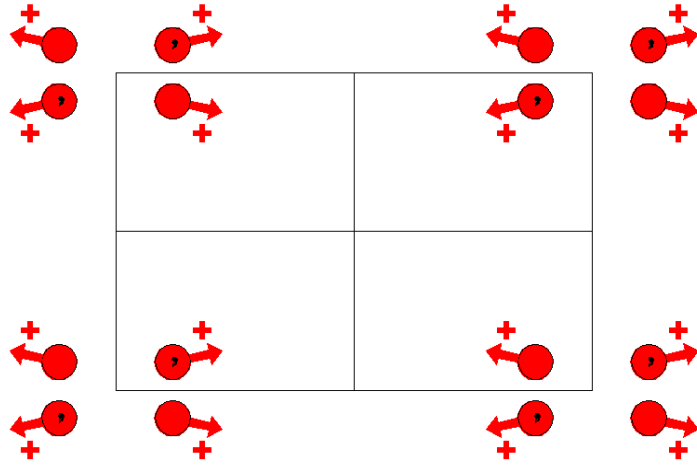
Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pm'm'2  
25.4.158

m'm'2  
Pm'm'2

Orthorhombic



Origin on m'm'2

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) m' x,0,z  
(m<sub>y</sub>|0,0,0)'

(4) m' 0,y,z  
(m<sub>x</sub>|0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

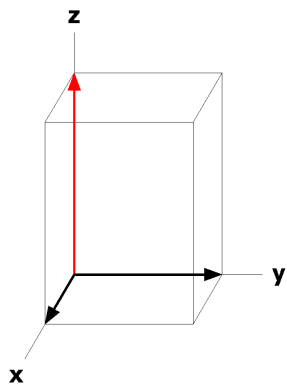
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
4	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
2	h	m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0, $\bar{v},w$ ]		
2	g	m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]		
2	f	.m'.	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ]		
2	e	.m'.	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]		
1	d	m'm'2	1/2,1/2,z [0,0,w]			
1	c	m'm'2	1/2,0,z [0,0,w]			
1	b	m'm'2	0,1/2,z [0,0,w]			
1	a	m'm'2	0,0,z [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m'1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



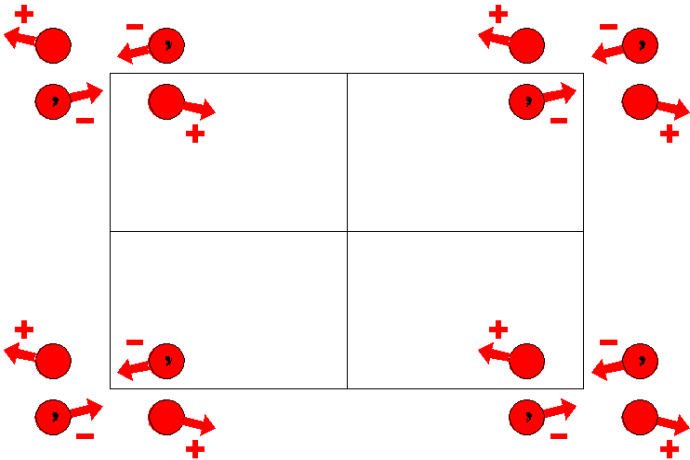
$P_{2c}mm2$

25.5.159

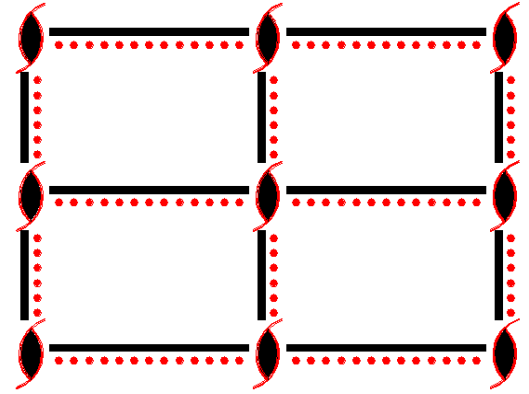
$mm21'$

$P_{2c}mm2$

Orthorhombic



Origin on  $mm2$



Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) m  $x,0,z$   
( $m_y$ |0,0,0)

(4) m  $0,y,z$   
( $m_x$ |0,0,0)

For  $(0,0,1)'$  + set

(1)  $t'$   $(0,0,1)$   
(1|0,0,1)'

(2)  $2'$   $(0,0,1)$   $0,0,z$   
( $2_z$ |0,0,1)'

(3)  $c'$   $(0,0,1)$   $x,0,z$   
( $m_y$ |0,0,1)'

(4)  $c'$   $(0,0,1)$   $0,y,z$   
( $m_x$ |0,0,1)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

**Positions**

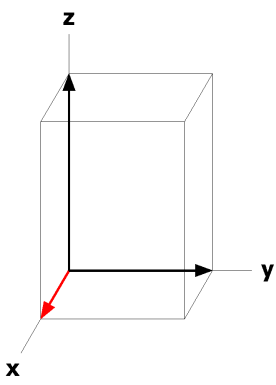
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
8 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
4 h m..	1/2,y,z [u,0,0]	1/2, $\bar{y},z$ [ $\bar{u},0,0$ ]		
4 g m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]		
4 f .m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v},0$ ]		
4 e .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]		
2 d mm2	1/2,1/2,z [0,0,0]			
2 c mm2	1/2,0,z [0,0,0]			
2 b mm2	0,1/2,z [0,0,0]			
2 a mm2	0,0,z [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



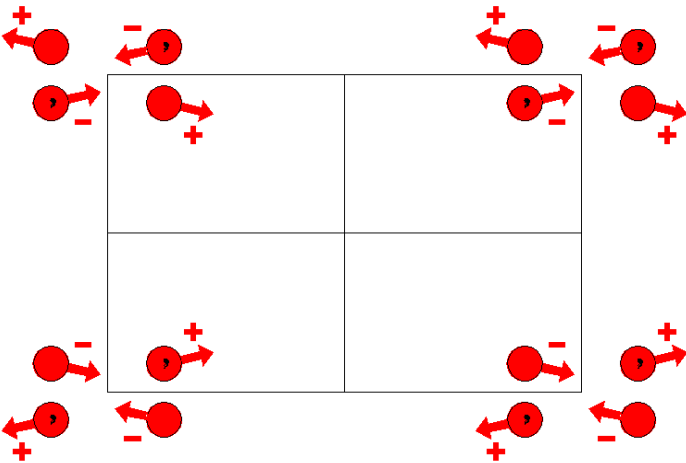
$P_{2a} mm2$

25.6.160

$mm21'$

$P_{2a} mm2$

Orthorhombic



Origin on  $mm2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

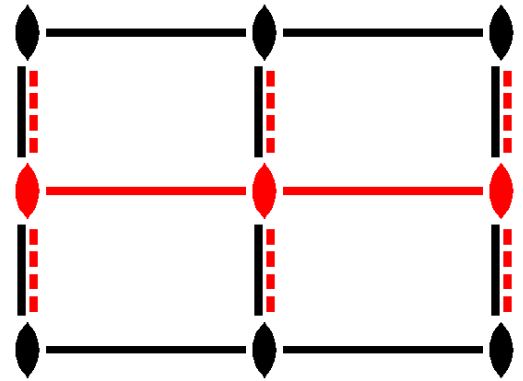
**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) m $x,0,z$<br>(m <sub>y</sub>  0,0,0) | (4) m $0,y,z$<br>(m <sub>x</sub>  0,0,0) |
|--------------------|--|--|--|

For  $(1,0,0)'$  + set

- |                                |  |  |  |
|--------------------------------|--|--|--|
| (1) t' $(1,0,0)$<br>(1 1,0,0)' | (2) 2' $1/2,0,z$<br>(2 <sub>z</sub>  1,0,0)' | (3) a' $(1,0,0) x,0,z$<br>(m <sub>y</sub>  1,0,0)' | (4) m' $1/2,y,z$<br>(m <sub>x</sub>  1,0,0)' |
|--------------------------------|--|--|--|





**Generators selected** (1); t(1,0,0)<sup>'</sup>; t(0,1,0); t(0,0,1); (2); (3).

### Positions

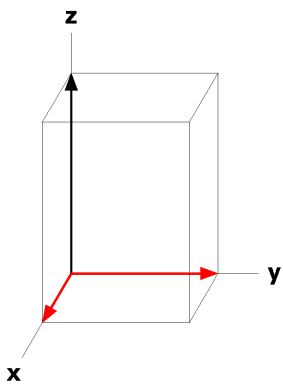
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0) <sup>'</sup> +		
8 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
4 h m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0,v, $\bar{w}$ ]		
4 g m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]		
4 f .m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v},0$ ]		
4 e .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]		
2 d m'm2'	1/2,1/2,z [0,v,0]			
2 c m'm2'	1/2,0,z [0,v,0]			
2 b mm2	0,1/2,z [0,0,0]			
2 a mm2	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



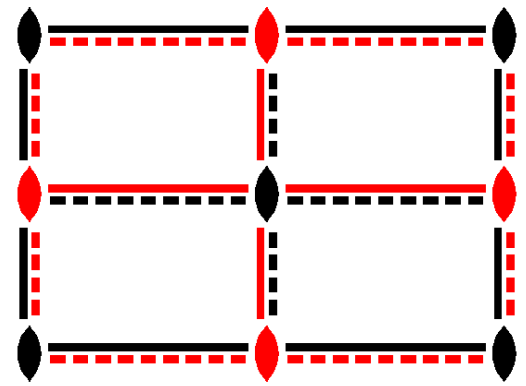
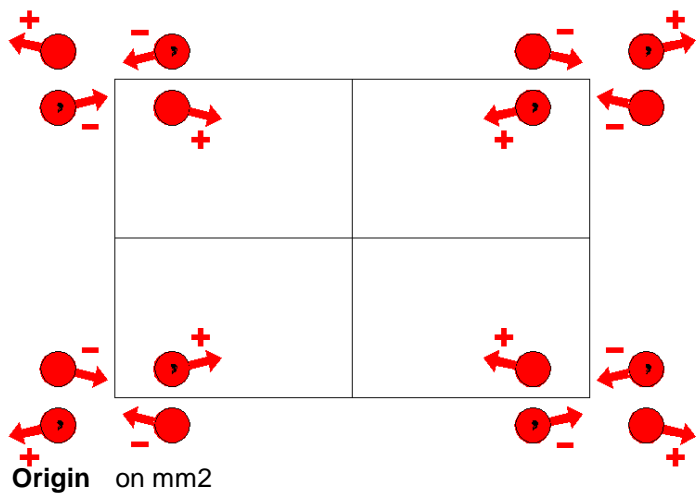
$P_C mm2$

25.7.161

$mm21'$

$P_C mm2$

Orthorhombic



**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) m  $x,0,z$   
( $m_y$ |0,0,0)

(4) m  $0,y,z$   
( $m_x$ |0,0,0)

For  $(1,0,0)'$  + set

(1)  $t' (1,0,0)$   
(1|1,0,0)'

(2)  $2' 1/2,0,z$   
( $2_z$ |1,0,0)'

(3)  $a' (1,0,0) x,0,z$   
( $m_y$ |1,0,0)'

(4)  $m' 1/2,y,z$   
( $m_x$ |1,0,0)'

**Generators selected** (1); t(1,0,0)<sup>'</sup>; t(0,1,0)<sup>'</sup>; t(0,0,1); (2); (3).

### Positions

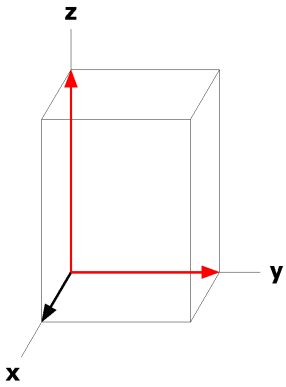
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0) <sup>'</sup> +		
8 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
4 h m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0,v, $\bar{w}$ ]		
4 g m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]		
4 f .m'.	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [u,0, $\bar{w}$ ]		
4 e .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]		
2 d m'm'2	1/2,1/2,z [0,0,w]			
2 c m'm2'	1/2,0,z [0,v,0]			
2 b mm'2'	0,1/2,z [u,0,0]			
2 a mm2	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



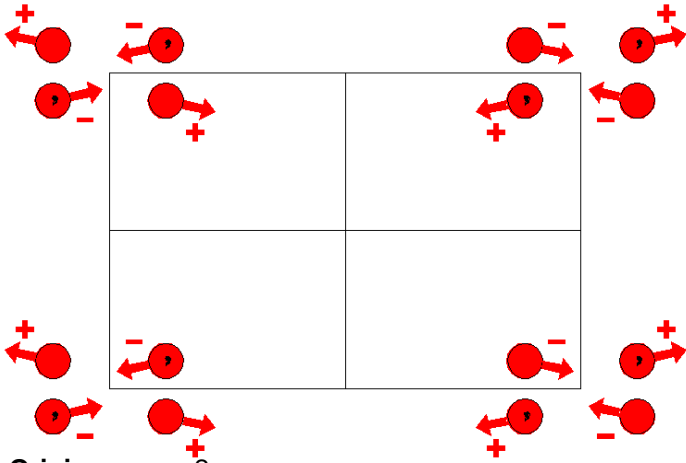
$P_A mm2$

25.8.162

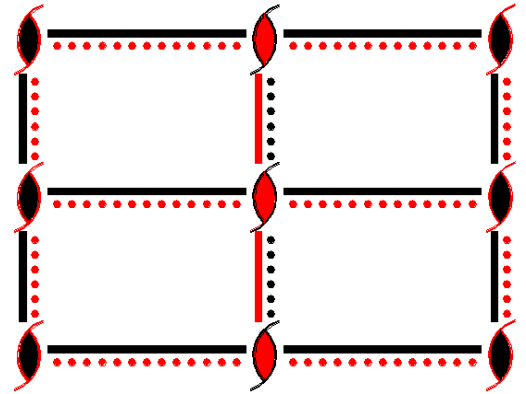
$mm2$

$P_A mm2$

Orthorhombic



Origin on  $mm2$



Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) m  $x,0,z$   
( $m_y$ |0,0,0)

(4) m  $0,y,z$   
( $m_x$ |0,0,0)

For  $(0,1,0)'$  + set

(1)  $t' (0,1,0)$   
(1|0,1,0)'

(2)  $2' 0,1/2,z$   
( $2_z$ |0,1,0)'

(3)  $m' x,1/2,z$   
( $m_y$ |0,1,0)'

(4)  $b' (0,1,0) 0,y,z$   
( $m_x$ |0,1,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

**Positions**

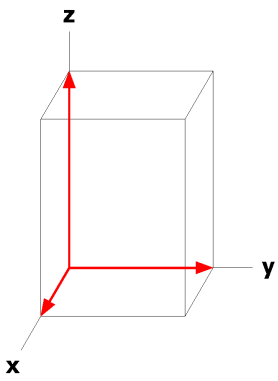
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
8 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
4 h m..	1/2,y,z [u,0,0]	1/2, $\bar{y},z$ [ $\bar{u},0,0$ ]		
4 g m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]		
4 f .m'.	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $u,0,\bar{w}$ ]		
4 e .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [ $0,\bar{v},0$ ]		
2 d mm'2'	1/2,1/2,z [u,0,0]			
2 c mm2	1/2,0,z [0,0,0]			
2 b mm'2'	0,1/2,z [u,0,0]			
2 a mm2	0,0,z [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



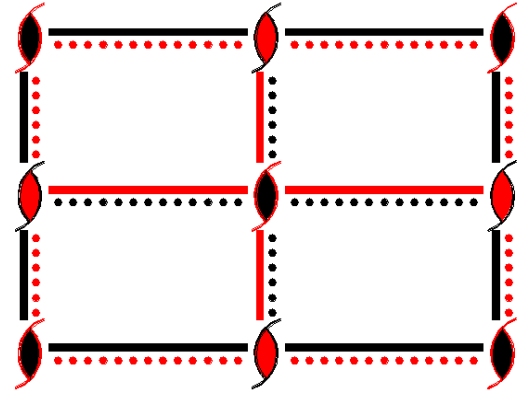
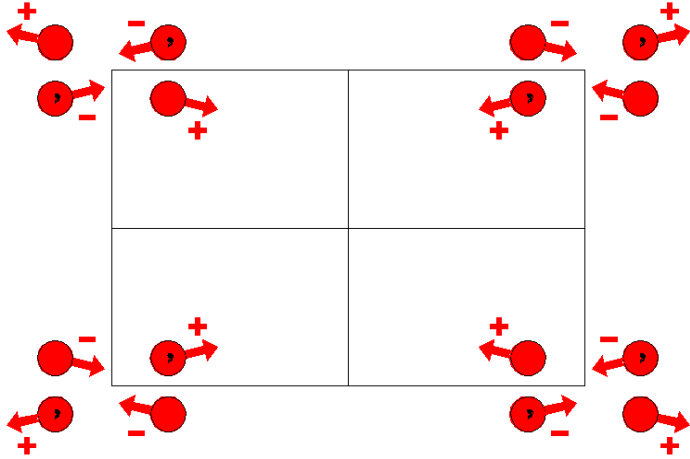
$P_Fmm2$

25.9.163

$mm21'$

$P_Fmm2$

Orthorhombic



**Origin** on  $mm2$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $m_x,0,z$   
( $m_y$ |0,0,0)

(4)  $m_0,y,z$   
( $m_x$ |0,0,0)

For  $(1,0,0)'$  + set

(1)  $t'(1,0,0)$   
(1|1,0,0)'

(2)  $2'_{1/2},0,z$   
( $2_z$ |1,0,0)'

(3)  $a'(1,0,0)$   $x,0,z$   
( $m_y$ |1,0,0)'

(4)  $m'_{1/2},y,z$   
( $m_x$ |1,0,0)'

**Generators selected** (1); t(1,0,0)<sup>'</sup>; t(0,1,0)<sup>'</sup>; t(0,0,1)<sup>'</sup>; (2); (3).

### Positions

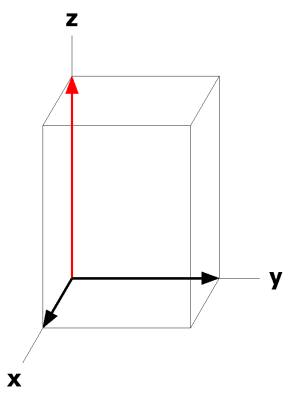
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0) <sup>'</sup> +		
8 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
4 h m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0,v, $\bar{w}$ ]		
4 g m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]		
4 f .m'.	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $u,0,\bar{w}$ ]		
4 e .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]		
2 d m'm'2	1/2,1/2,z [0,0,w]			
2 c m'm2'	1/2,0,z [0,v,0]			
2 b mm'2'	0,1/2,z [u,0,0]			
2 a mm2	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



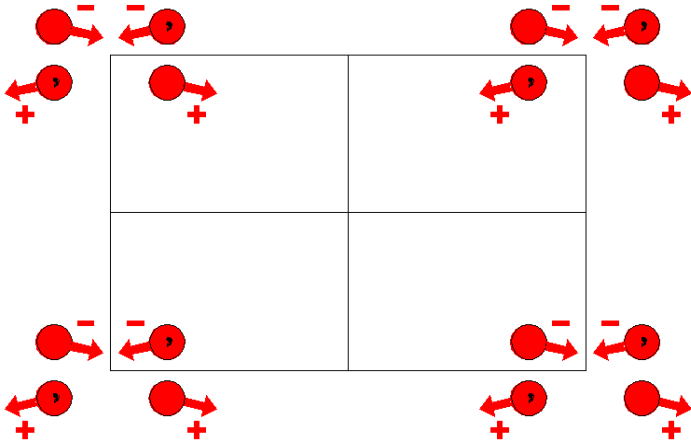
$P_{2c} mm'2'$

25.10.164

$mm21'$

$P_{2c} mm'2'$

Orthorhombic



Origin on  $mm'2'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2)  $2'_z$  0,0,z  
( $2_z$ |0,0,0)'

(3)  $m'_y$  x,0,z  
( $m_y$ |0,0,0)'

(4)  $m'_x$  0,y,z  
( $m_x$ |0,0,0)

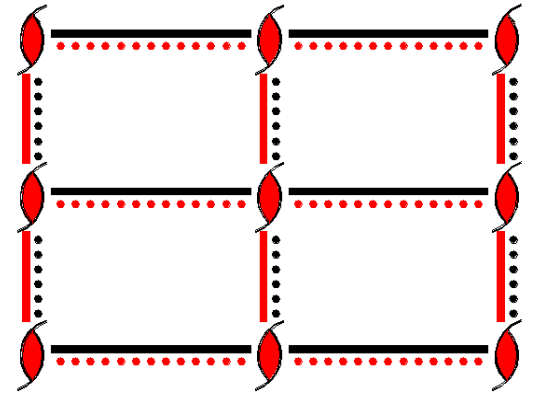
For  $(0,0,1)'$  + set

(1)  $t'_z$  (0,0,1)  
(1|0,0,1)'

(2)  $2'_z$  (0,0,1) 0,0,z  
( $2_z$ |0,0,1)

(3)  $c'_y$  (0,0,1) x,0,z  
( $m_y$ |0,0,1)

(4)  $c'_x$  (0,0,1) 0,y,z  
( $m_x$ |0,0,1)'





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

### Positions

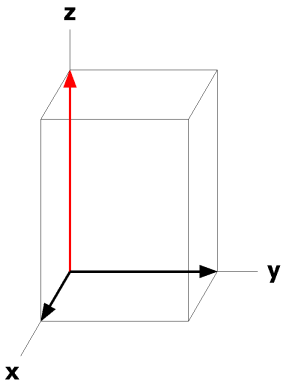
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
8 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
4 h m..	1/2,y,z [u,0,0]	1/2, $\bar{y},z$ [u,0,0]		
4 g m..	0,y,z [u,0,0]	0, $\bar{y},z$ [u,0,0]		
4 f .m'.	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [u,0, $\bar{w}$ ]		
4 e .m'.	x,0,z [u,0,w]	$\bar{x},0,z$ [u,0, $\bar{w}$ ]		
2 d mm'2'	1/2,1/2,z [u,0,0]			
2 c mm'2'	1/2,0,z [u,0,0]			
2 b mm'2'	0,1/2,z [u,0,0]			
2 a mm'2'	0,0,z [u,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2b</sub>'1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



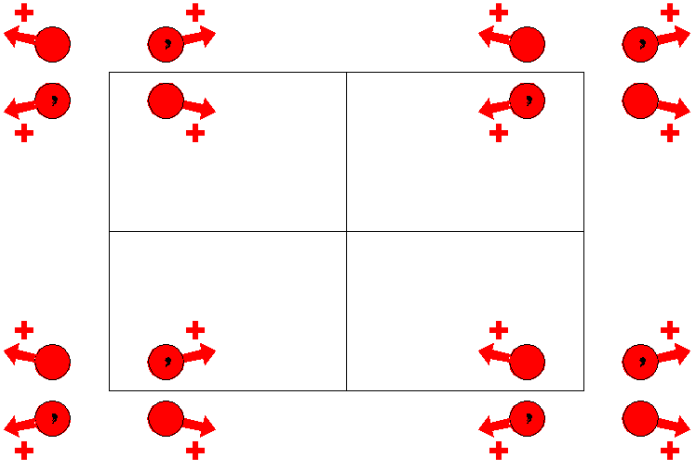
$P_{2c} m' m' 2$

25.11.165

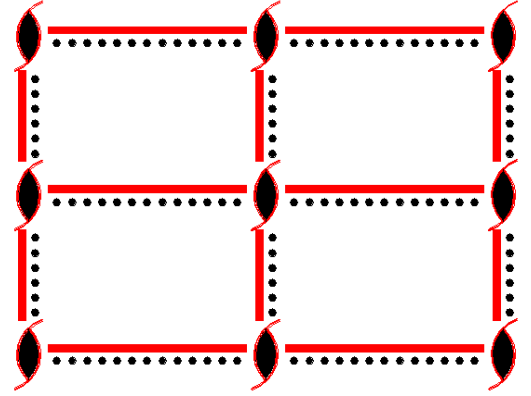
$mm21'$

$P_{2c} m' m' 2$

Orthorhombic



Origin on  $m' m' 2$



Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $m'$   $x,0,z$   
( $m_y$ |0,0,0)'

(4)  $m'$   $0,y,z$   
( $m_x$ |0,0,0)'

For  $(0,0,1)'$  + set

(1)  $t'$   $(0,0,1)$   
(1|0,0,1)'

(2)  $2'$   $(0,0,1)$   $0,0,z$   
( $2_z$ |0,0,1)'

(3)  $c$   $(0,0,1)$   $x,0,z$   
( $m_y$ |0,0,1)

(4)  $c$   $(0,0,1)$   $0,y,z$   
( $m_x$ |0,0,1)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

**Positions**

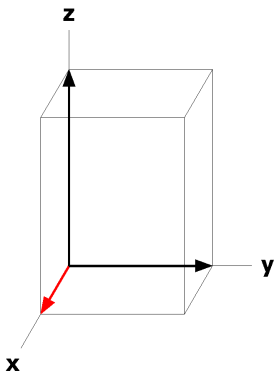
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
8 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
4 h m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0, $\bar{v},w$ ]		
4 g m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]		
4 f .m'.	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ]		
4 e .m'.	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]		
2 d m'm'2	1/2,1/2,z [0,0,w]			
2 c m'm'2	1/2,0,z [0,0,w]			
2 b m'm'2	0,1/2,z [0,0,w]			
2 a m'm'2	0,0,z [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>·1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2b</sub>·1m'1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



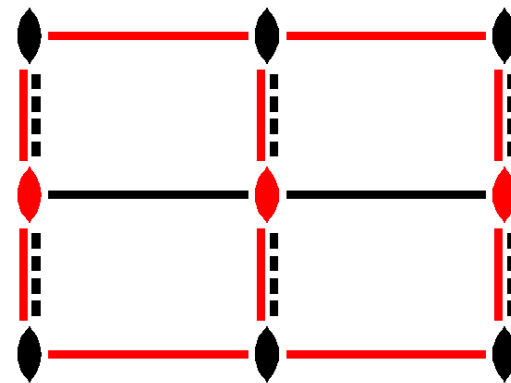
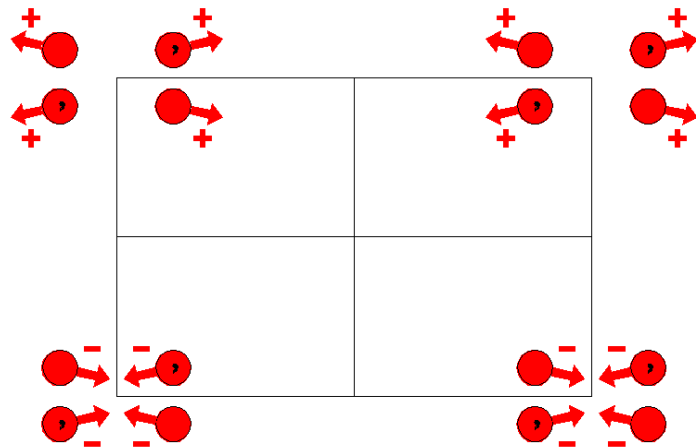
$P_{2a} m' m' 2$

25.12.166

$mm21'$

$P_{2a} m' m' 2$

Orthorhombic



Origin on  $m' m' 2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                  |                                      |                                      |
|--------------------|----------------------------------|--------------------------------------|--------------------------------------|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $m'$ $x,0,z$<br>( $m_y$  0,0,0)' | (4) $m'$ $0,y,z$<br>( $m_x$  0,0,0)' |
|--------------------|----------------------------------|--------------------------------------|--------------------------------------|

For  $(1,0,0)'$  + set

- |                                  |  |  |                                      |
|----------------------------------|--|--|--------------------------------------|
| (1) $t'$ $(1,0,0)$<br>(1 1,0,0)' | (2) $2'$ $1/2,0,z$<br>( $2_z$  1,0,0)' | (3) $a$ $(1,0,0) x,0,z$<br>( $m_y$  1,0,0) | (4) $m$ $1/2,y,z$<br>( $m_x$  1,0,0) |
|----------------------------------|--|--|--------------------------------------|

**Generators selected** (1); t(1,0,0)'; t(0,1,0); t(0,0,1); (2); (3).

**Positions**

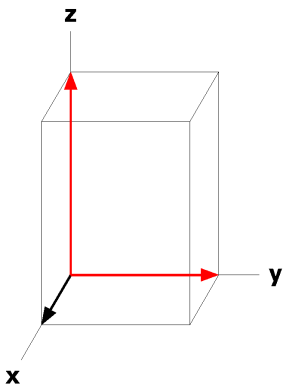
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
8 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
4 h m..	1/2,y,z [u,0,0]	1/2, $\bar{y},z$ [u,0,0]		
4 g m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]		
4 f .m'.	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ]		
4 e .m'.	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]		
2 d mm'2'	1/2,1/2,z [u,0,0]			
2 c mm'2'	1/2,0,z [u,0,0]			
2 b m'm'2	0,1/2,z [0,0,w]			
2 a m'm'2	0,0,z [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>·2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>·1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/2,y,0



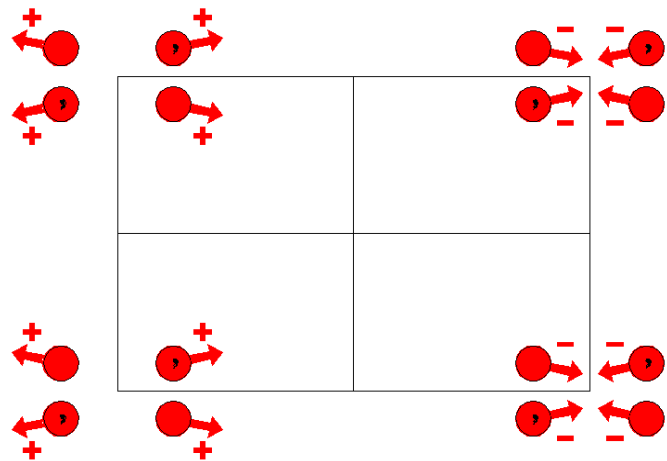
$P_A m'm'2$

25.13.167

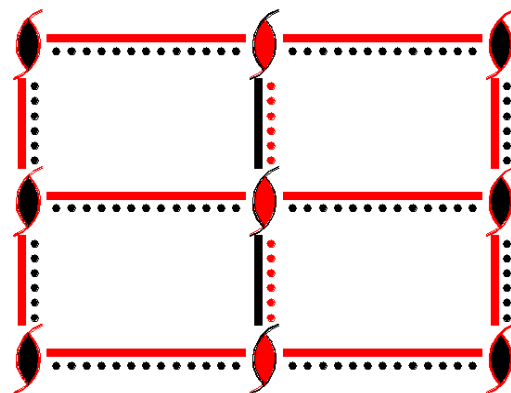
$mm21'$

$P_A m'm'2$

Orthorhombic



Origin on  $m'm'2$



Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $m'$   $x,0,z$   
( $m_y$ |0,0,0)'

(4)  $m'$   $0,y,z$   
( $m_x$ |0,0,0)'

For  $(0,1,0)'$  + set

(1)  $t'$   $(0,1,0)$   
(1|0,1,0)'

(2)  $2'$   $0,1/2,z$   
( $2_z$ |0,1,0)'

(3)  $m$   $x,1/2,z$   
( $m_y$ |0,1,0)

(4)  $b$   $(0,1,0)$   $0,y,z$   
( $m_x$ |0,1,0)

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ '; (2); (3).

### Positions

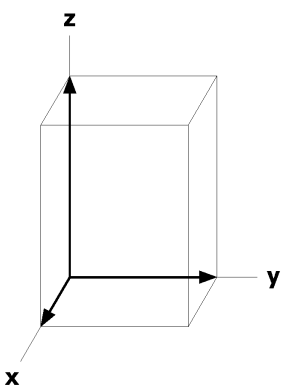
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
8 i 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $x,\bar{y},z [u,\bar{v},w]$	(4) $\bar{x},y,z [\bar{u},v,w]$
4 h $m'..$	$1/2,y,z [0,v,w]$	$1/2,\bar{y},z [0,\bar{v},w]$		
4 g $m'..$	$0,y,z [0,v,w]$	$0,\bar{y},z [0,\bar{v},w]$		
4 f $.m.$	$x,1/2,z [0,v,0]$	$\bar{x},1/2,z [0,v,0]$		
4 e $.m'$	$x,0,z [u,0,w]$	$\bar{x},0,z [\bar{u},0,w]$		
2 d $m'm2'$	$1/2,1/2,z [0,v,0]$			
2 c $m'm'2$	$1/2,0,z [0,0,w]$			
2 b $m'm2'$	$0,1/2,z [0,v,0]$			
2 a $m'm'2$	$0,0,z [0,0,w]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_c-1m1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,1/2,0$

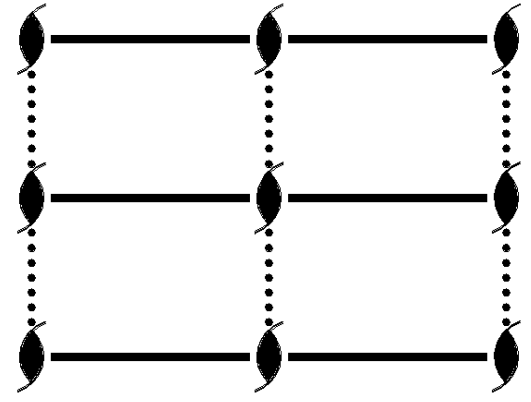
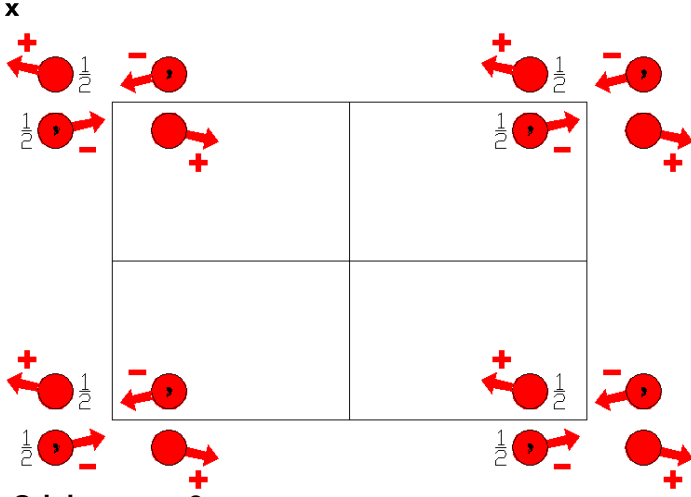
Along  $[0,1,0]$   $p1m11'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $0,y,0$



Pmc2<sub>1</sub>  
26.1.168

mm2  
Pmc2<sub>1</sub>

Orthorhombic



Origin on mc2<sub>1</sub>

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

- (1) 1 (1|0,0,0)
- (2) 2 (0,0,1/2) 0,0,z (2<sub>z</sub>|0,0,1/2)
- (3) c (0,0,1/2) x,0,z (m<sub>y</sub>|0,0,1/2)
- (4) m 0,y,z (m<sub>x</sub>|0,0,0)



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

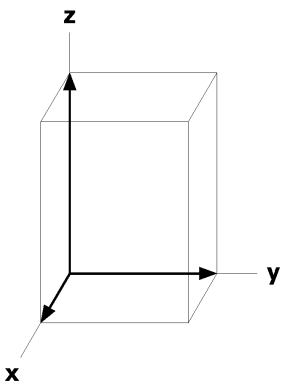
			Coordinates			
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
4	c	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
2	b	m..	1/2,y,z [u,0,0]	1/2, $\bar{y},z+1/2$ [ $\bar{u},0,0$ ]		
2	a	m..	0,y,z [u,0,0]	0, $\bar{y},z+1/2$ [ $\bar{u},0,0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2b</sub>·1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0

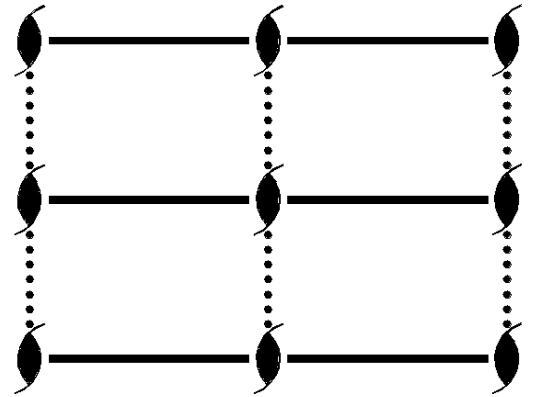
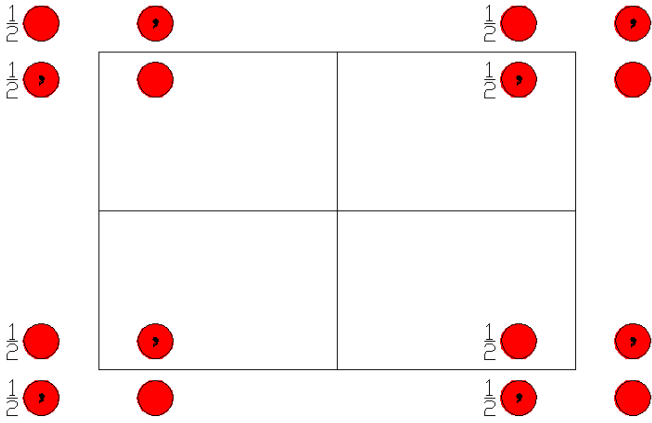


Pmc2<sub>1</sub>'  
26.2.169

mm21'  
Pmc2<sub>1</sub>'

Orthorhombic

1'



Origin on mc<sub>2</sub>,1'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For 1 + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (4) m 0,y,z<br>(m <sub>x</sub>  0,0,0) |
|--------------------|--|--|--|

For 1' + set

- |                      |  |  |  |
|----------------------|--|--|--|
| (1) 1'<br>(1 0,0,0)' | (2) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)' | (3) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (4) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |
|----------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

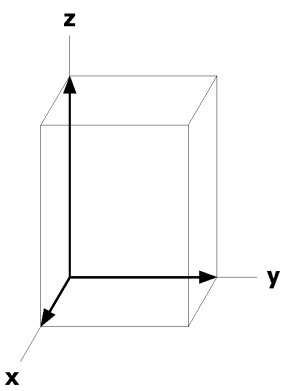
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			1 +		1' +	
4	c	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z+1/2$ [0,0,0]	(3) x, $\bar{y},z+1/2$ [0,0,0]	(4) $\bar{x},y,z$ [0,0,0]
2	b	m..1'	1/2,y,z [0,0,0]	1/2, $\bar{y},z+1/2$ [0,0,0]		
2	a	m..1'	0,y,z [0,0,0]	0, $\bar{y},z+1/2$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



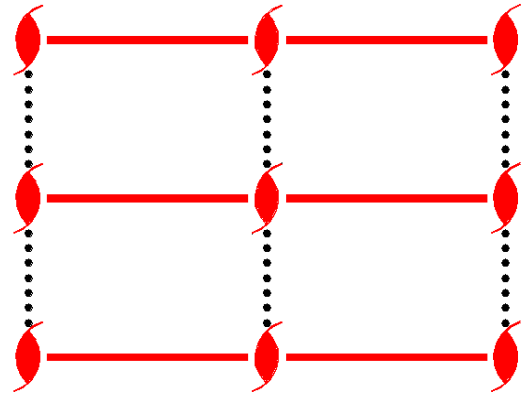
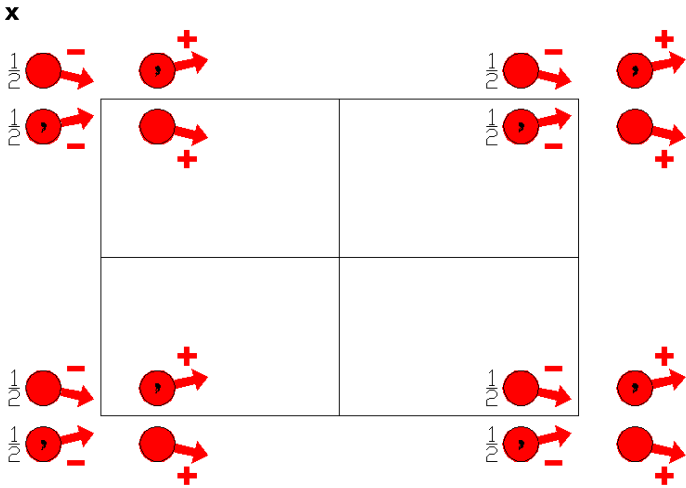
Pm'c2<sub>1</sub>'

26.3.170

m'm2'

Pm'c2<sub>1</sub>'

Orthorhombic



Origin on m'c2<sub>1</sub>'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2' (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)'

(3) c (0,0,1/2) x,0,z  
(m<sub>y</sub>|0,0,1/2)

(4) m' 0,y,z  
(m<sub>x</sub>|0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

### Positions

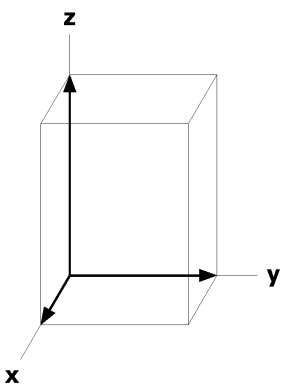
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
4	c	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
2	b	m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z+1/2$ [0,v, $\bar{w}$ ]		
2	a	m'..	0,y,z [0,v,w]	0, $\bar{y},z+1/2$ [0,v, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p1g1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

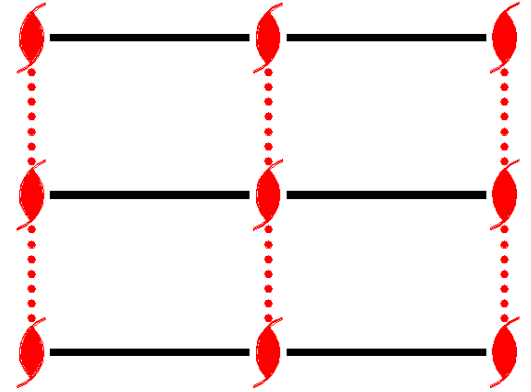
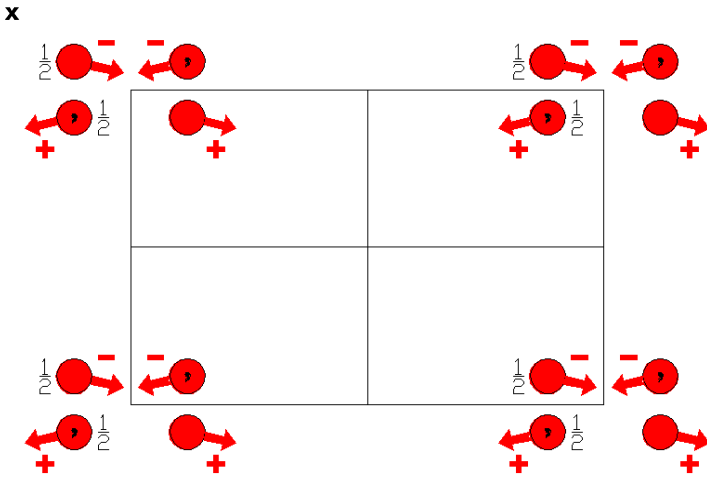
Along [0,1,0] p<sub>2b</sub>'1m'1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pmc'2<sub>1</sub>'  
26.4.171

mm'2'  
Pmc'2<sub>1</sub>'

Orthorhombic



Origin on mc'2<sub>1</sub>'

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2' (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)'

(3) c' (0,0,1/2) x,0,z  
(m<sub>y</sub>|0,0,1/2)'

(4) m 0,y,z  
(m<sub>x</sub>|0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

### Positions

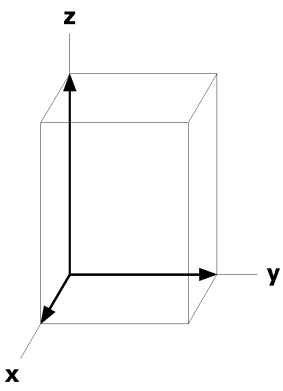
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
4	c	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
2	b	m..	1/2,y,z [u,0,0]	1/2, $\bar{y},z+1/2$ [u,0,0]		
2	a	m..	0,y,z [u,0,0]	0, $\bar{y},z+1/2$ [u,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2b</sub>'1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



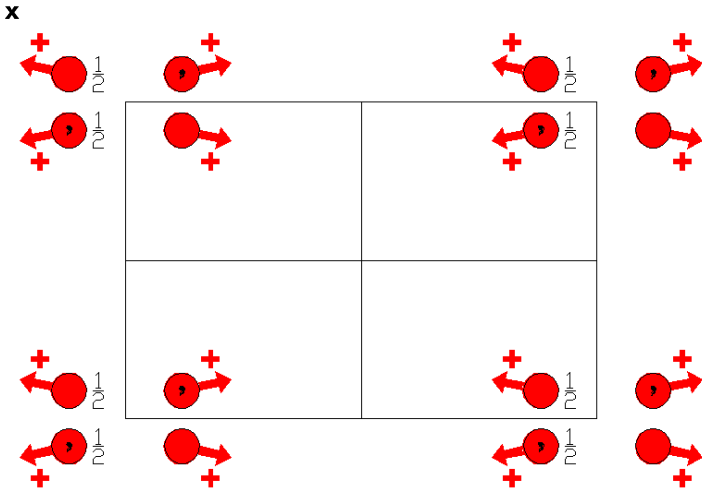
Pm'c'2<sub>1</sub>

26.5.172

m'm'2

Pm'c'2<sub>1</sub>

Orthorhombic



Origin on m'c'2<sub>1</sub>

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

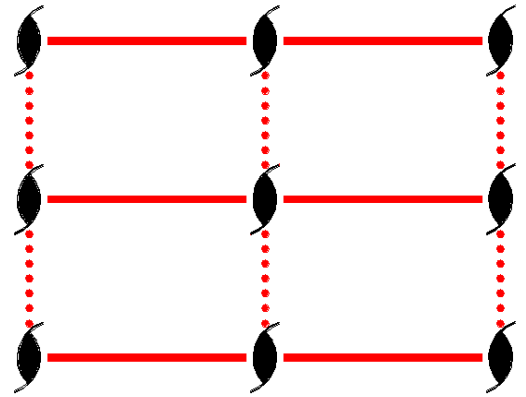
**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)

(3) c' (0,0,1/2) x,0,z  
(m<sub>y</sub>|0,0,1/2)'

(4) m' 0,y,z  
(m<sub>x</sub>|0,0,0)'





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

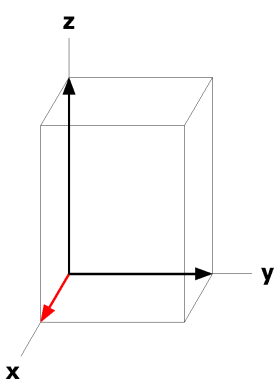
		Coordinates			
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
4	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
2	b m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z+1/2$ [0, $\bar{v},w$ ]		
2	a m'..	0,y,z [0,v,w]	0, $\bar{y},z+1/2$ [0, $\bar{v},w$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2b</sub>'1m'1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



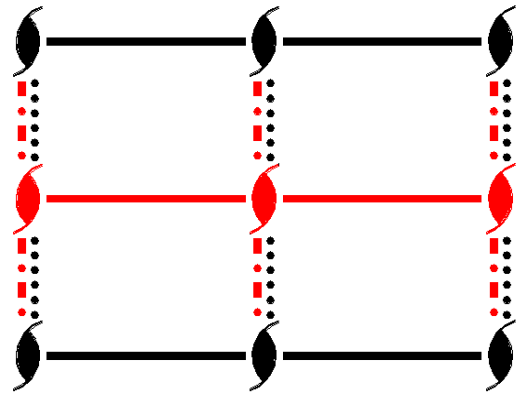
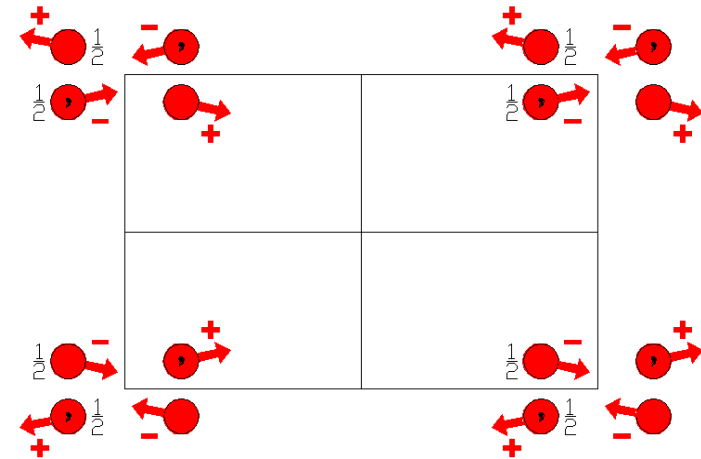
$P_{2a}mc2_1$

26.6.173

$mm21'$

$P_{2a}mc2_1$

Orthorhombic



**Origin** on  $mc2_1$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (4) m 0,y,z<br>(m <sub>x</sub>  0,0,0) |
|--------------------|--|--|--|

For (1,0,0)' + set

- |                              |  |  |  |
|------------------------------|--|--|--|
| (1) i' (1,0,0)<br>(1 1,0,0)' | (2) 2' (0,0,1/2) 1/2,0,z<br>(2 <sub>z</sub>  1,0,1/2)' | (3) n' (1,0,1/2) x,0,z<br>(m <sub>y</sub>  1,0,1/2)' | (4) m' 1/2,y,z<br>(m <sub>x</sub>  1,0,0)' |
|------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0)<sup>'</sup>; t(0,1,0); t(0,0,1); (2); (3).

### Positions

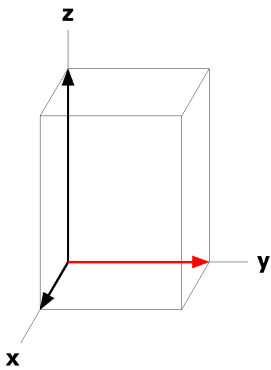
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1,0,0) <sup>'</sup> +		
8	c	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
4	b	m' <sup>..</sup>	1/2,y,z [0,v,w]	1/2, $\bar{y},z+1/2$ [0,v, $\bar{w}$ ]		
4	a	m <sup>..</sup>	0,y,z [u,0,0]	0, $\bar{y},z+1/2$ [ $\bar{u},0,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>-1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



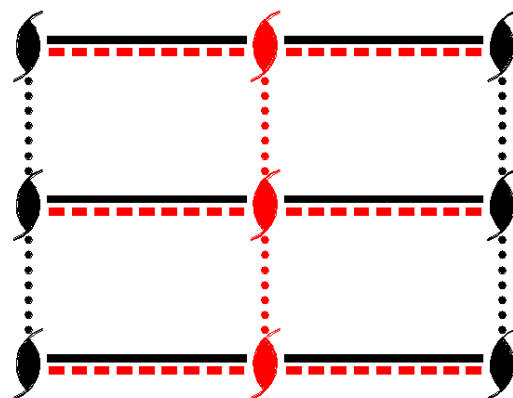
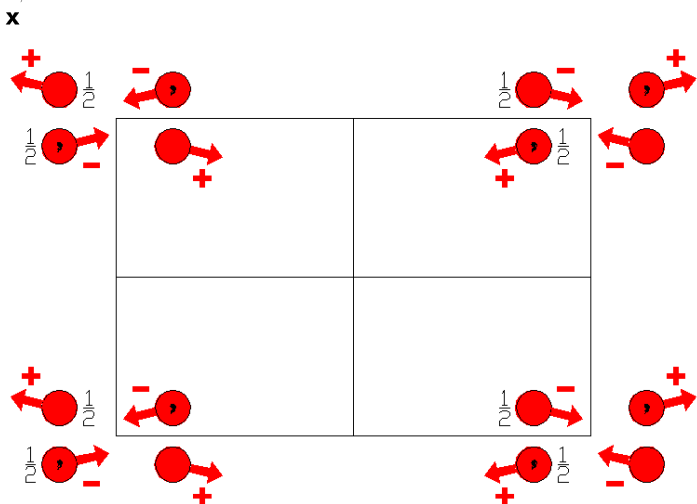
$P_{2b}mc2_1$

26.7.174

$mm21'$

$P_{2b}mc2_1$

Orthorhombic



**Origin** on  $mc2_1$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |                                      |
|--------------------|--|--|--------------------------------------|
| (1) 1<br>(1 0,0,0) | (2) 2 $(0,0,1/2)$ $0,0,z$<br>( $2_z$   $0,0,1/2$ ) | (3) c $(0,0,1/2)$ $x,0,z$<br>( $m_y$   $0,0,1/2$ ) | (4) m $0,y,z$<br>( $m_x$   $0,0,0$ ) |
|--------------------|--|--|--------------------------------------|

For  $(0,1,0)'$  + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) $t'$ $(0,1,0)$<br>(1  $0,1,0$ )' | (2) $2'$ $(0,0,1/2)$ $0,1/2,z$<br>( $2_z$   $0,1,1/2$ )' | (3) $c'$ $(0,0,1/2)$ $x,1/2,z$<br>( $m_y$   $0,1,1/2$ )' | (4) $b'$ $(0,1,0)$ $0,y,z$<br>( $m_x$   $0,1,0$ )' |
|--------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

### Positions

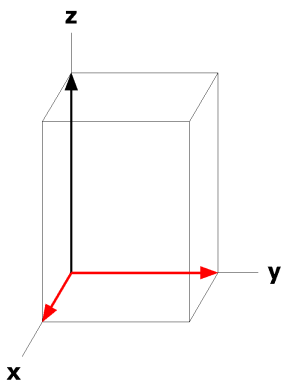
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
8	c	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
4	b	m..	1/2,y,z [u,0,0]	1/2, $\bar{y},z+1/2$ [ $\bar{u},0,0$ ]		
4	a	m..	0,y,z [u,0,0]	0, $\bar{y},z+1/2$ [ $\bar{u},0,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



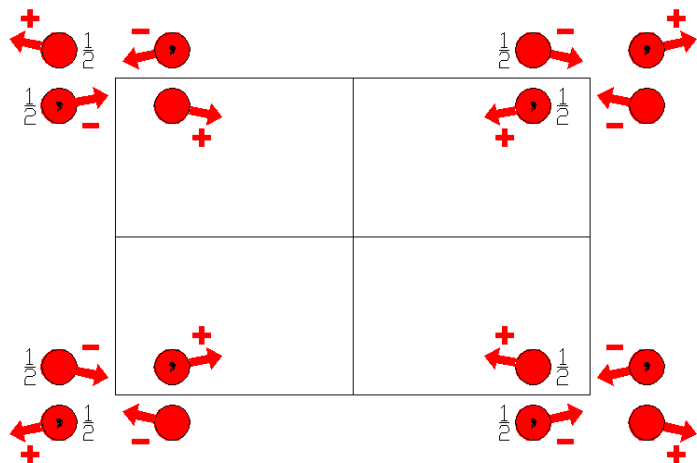
$P_C mc2_1$

26.8.175

$mm21'$

$P_C mc2_1$

Orthorhombic



Origin on  $mc2_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

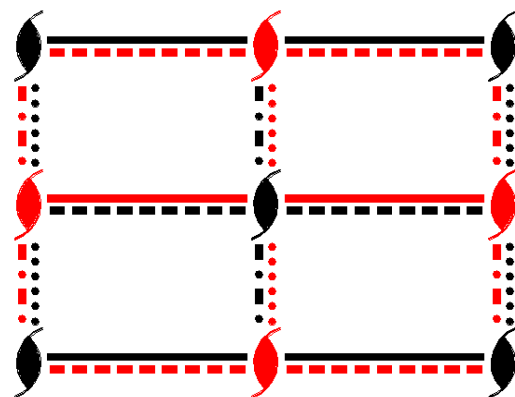
**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |                                      |
|--------------------|--|--|--------------------------------------|
| (1) 1<br>(1 0,0,0) | (2) 2 $(0,0,1/2)$ $0,0,z$<br>( $2_z$   $0,0,1/2$ ) | (3) c $(0,0,1/2)$ $x,0,z$<br>( $m_y$   $0,0,1/2$ ) | (4) m $0,y,z$<br>( $m_x$   $0,0,0$ ) |
|--------------------|--|--|--------------------------------------|

For  $(1,0,0)'$  + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) $t'$ $(1,0,0)$<br>(1  $1,0,0$ )' | (2) $2'$ $(0,0,1/2)$ $1/2,0,z$<br>( $2_z$   $1,0,1/2$ )' | (3) $n'$ $(1,0,1/2)$ $x,0,z$<br>( $m_y$   $1,0,1/2$ )' | (4) $m'$ $1/2,y,z$<br>( $m_x$   $1,0,0$ )' |
|--------------------------------------|--|--|--|



**Generators selected** (1); t(1,0,0)<sup>'</sup>; t(0,1,0)<sup>'</sup>; t(0,0,1); (2); (3).

### Positions

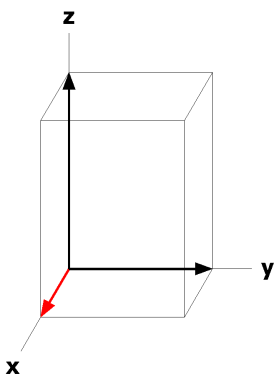
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1,0,0) <sup>'</sup> +		
8	c	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
4	b	m' <sup>..</sup>	1/2,y,z [0,v,w]	1/2, $\bar{y},z+1/2$ [0,v, $\bar{w}$ ]		
4	a	m <sup>..</sup>	0,y,z [u,0,0]	0, $\bar{y},z+1/2$ [ $\bar{u},0,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



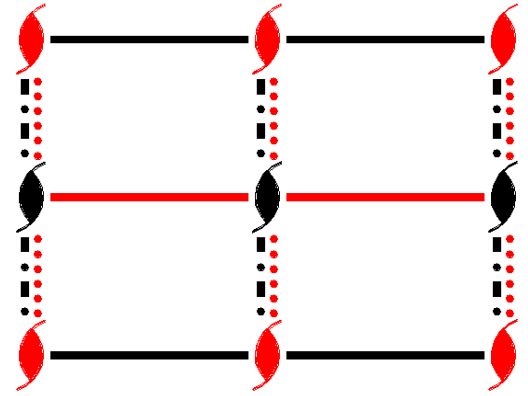
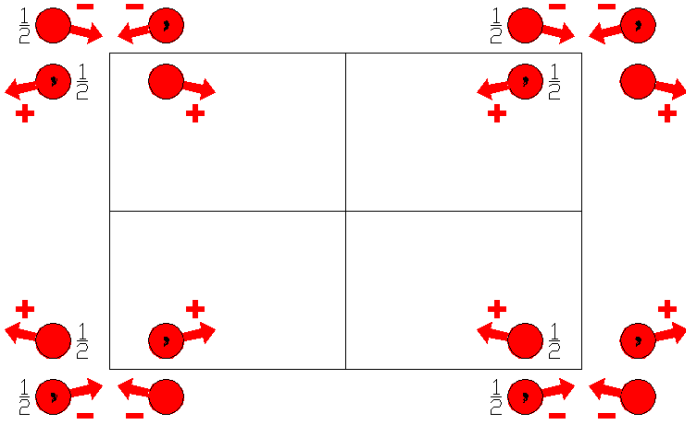
$P_{2a}mc'2_1'$

26.9.176

$mm21'$

$P_{2a}mc'2_1'$

Orthorhombic



**Origin** on  $mc'2_1'$

**Asymmetric unit**  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) $2' (0,0,1/2) \quad 0,0,z$<br>( $2_z$  0,0,1/2)' | (3) $c' (0,0,1/2) \quad x,0,z$<br>( $m_y$  0,0,1/2)' | (4) $m \quad 0,y,z$<br>( $m_x$  0,0,0) |
|--------------------|--|--|--|

For (1,0,0)' + set

- |                                |  |  |  |
|--------------------------------|--|--|--|
| (1) $t' (1,0,0)$<br>(1 1,0,0)' | (2) $2 (0,0,1/2) \quad 1/2,0,z$<br>( $2_z$  1,0,1/2) | (3) $n (1,0,1/2) \quad x,0,z$<br>( $m_y$  1,0,1/2) | (4) $m' \quad 1/2,y,z$<br>( $m_x$  1,0,0)' |
|--------------------------------|--|--|--|



**Generators selected** (1); t(1,0,0)'; t(0,1,0); t(0,0,1); (2); (3).

### Positions

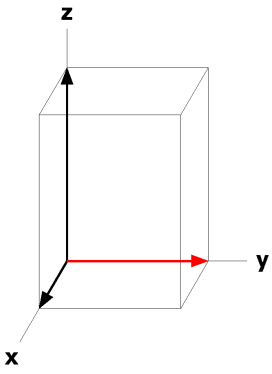
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) + (1,0,0)' +			
8	c	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
4	b	m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z+1/2$ [0, $\bar{v},w$ ]		
4	a	m..	0,y,z [u,0,0]	0, $\bar{y},z+1/2$ [u,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/2,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2b</sub>-1m1  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



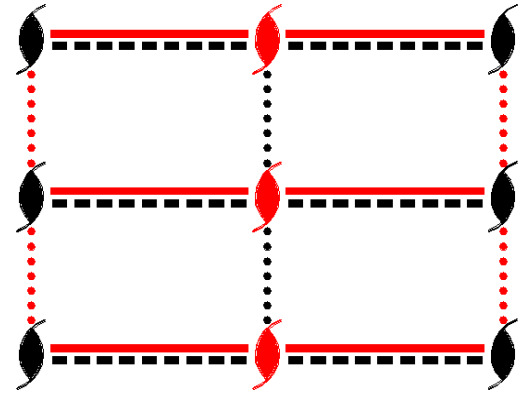
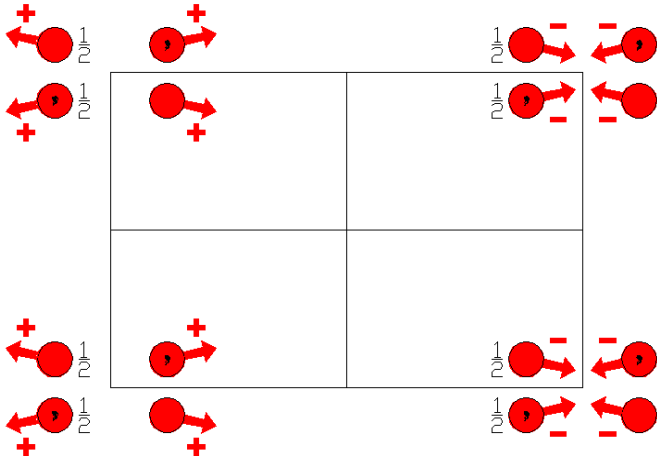
$P_{2b}m'c'2_1$

26.10.177

$mm21'$

$P_{2b}m'c'2_1$

Orthorhombic



**Origin** on  $m'c'2_1$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $(0,0,1/2)$   $0,0,z$   
( $2_z$ | $0,0,1/2$ )

(3)  $c'$   $(0,0,1/2)$   $x,0,z$   
( $m_y$ | $0,0,1/2$ )'

(4)  $m'$   $0,y,z$   
( $m_x$ | $0,0,0$ )'

For  $(0,1,0)'$  + set

(1)  $t'$   $(0,1,0)$   
(1| $0,1,0$ )'

(2)  $2'$   $(0,0,1/2)$   $0,1/2,z$   
( $2_z$ | $0,1,1/2$ )'

(3)  $c$   $(0,0,1/2)$   $x,1/2,z$   
( $m_y$ | $0,1,1/2$ )

(4)  $b$   $(0,1,0)$   $0,y,z$   
( $m_x$ | $0,1,0$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

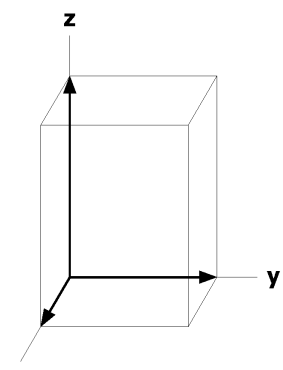
		Coordinates			
		Multiplicity, Wyckoff letter, Site Symmetry.			
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
4	b m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z+1/2$ [0, $\bar{v},w$ ]		
4	a m'..	0,y,z [0,v,w]	0, $\bar{y},z+1/2$ [0, $\bar{v},w$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>-1g1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/2,0

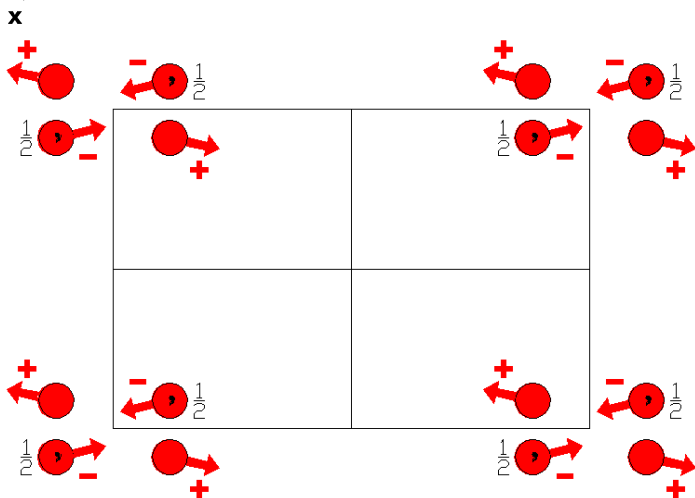
Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pcc2  
27.1.178

mm2  
Pcc2

Orthorhombic



Origin on cc2

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

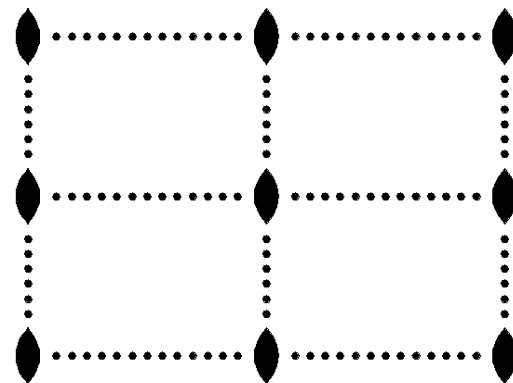
**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) c  $(0,0,1/2)$   $x,0,z$   
( $m_y$ |0,0,1/2)

(4) c  $(0,0,1/2)$   $0,y,z$   
( $m_x$ |0,0,1/2)



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

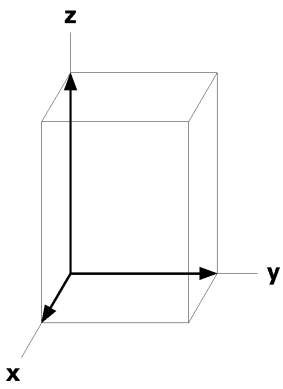
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
4	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y}$ ,z+1/2 [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z+1/2$ [u, $\bar{v},\bar{w}$ ]
2	d ..2	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]		
2	c ..2	1/2,0,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]		
2	b ..2	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]		
2	a ..2	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b} \cdot 1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2b} \cdot 1m'1$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0

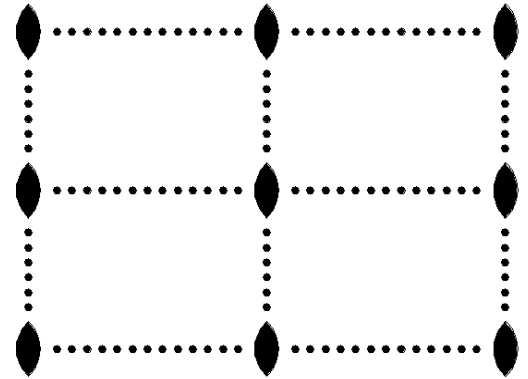
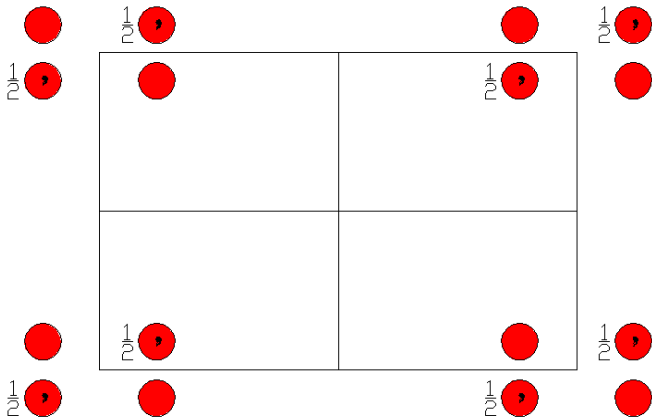


Pcc21'  
27.2.179

mm21'  
Pcc21'

Orthorhombic

1'



Origin on cc21'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For 1 + set

(1) 1  
(1|0,0,0)

(2) 2<sub>0,0,z</sub>  
(2<sub>z</sub>|0,0,0)

(3) c (0,0,1/2) x,0,z  
(m<sub>y</sub>|0,0,1/2)

(4) c (0,0,1/2) 0,y,z  
(m<sub>x</sub>|0,0,1/2)

For 1' + set

(1) 1'  
(1|0,0,0)'

(2) 2'<sub>0,0,z</sub>  
(2<sub>z</sub>|0,0,0)'

(3) c' (0,0,1/2) x,0,z  
(m<sub>y</sub>|0,0,1/2)'

(4) c' (0,0,1/2) 0,y,z  
(m<sub>x</sub>|0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

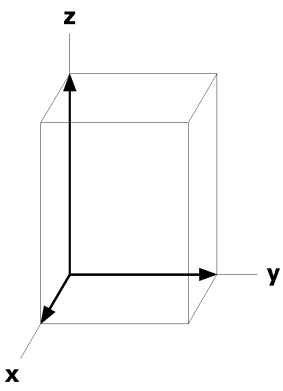
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
4	e 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $x,\bar{y},z+1/2$ [0,0,0]	(4) $\bar{x},y,z+1/2$ [0,0,0]
2	d ..21'	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]		
2	c ..21'	1/2,0,z [0,0,0]	1/2,0,z+1/2 [0,0,0]		
2	b ..21'	0,1/2,z [0,0,0]	0,1/2,z+1/2 [0,0,0]		
2	a ..21'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

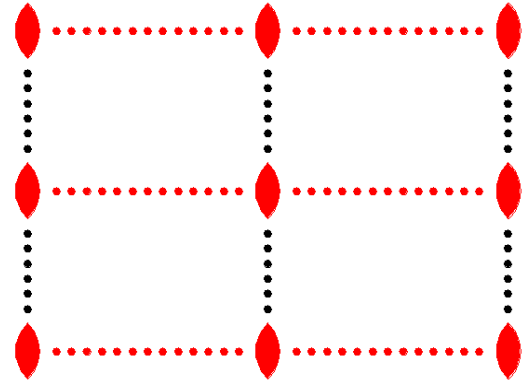
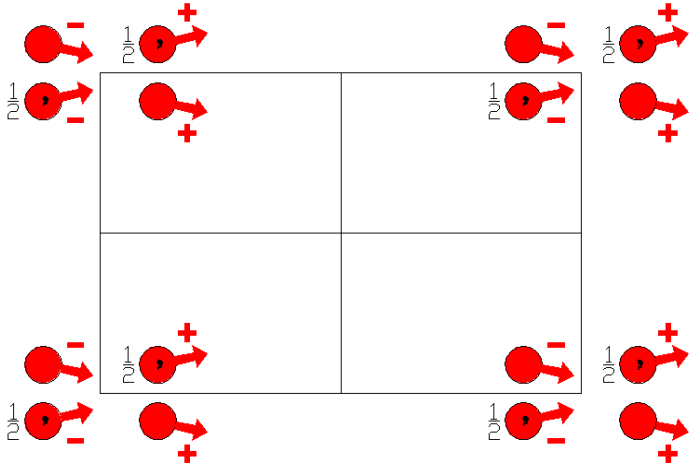
Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pc'c2'  
27.3.180

m'm2'  
Pc'c2'

Orthorhombic



Origin on c'c2'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'

(3) c (0,0,1/2) x,0,z  
(m<sub>y</sub>|0,0,1/2)

(4) c' (0,0,1/2) 0,y,z  
(m<sub>x</sub>|0,0,1/2)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

### Positions

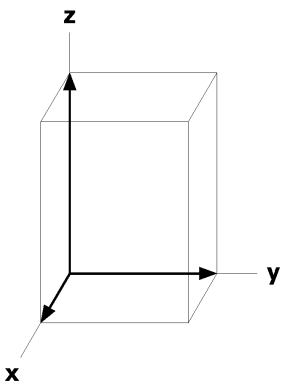
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
4	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y}$ ,z+1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) $\bar{x}$ ,y,z+1/2 [ $\bar{u}$ ,v,w]
2	d ..2'	1/2,1/2,z [u,v,0]	1/2,1/2,z+1/2 [ $\bar{u}$ ,v,0]		
2	c ..2'	1/2,0,z [u,v,0]	1/2,0,z+1/2 [ $\bar{u}$ ,v,0]		
2	b ..2'	0,1/2,z [u,v,0]	0,1/2,z+1/2 [ $\bar{u}$ ,v,0]		
2	a ..2'	0,0,z [u,v,0]	0,0,z+1/2 [ $\bar{u}$ ,v,0]		

### Symmetry of Special Projections

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

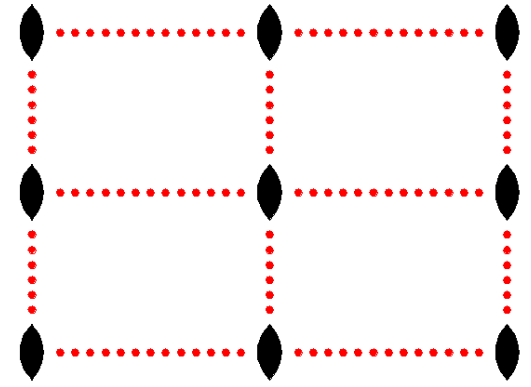
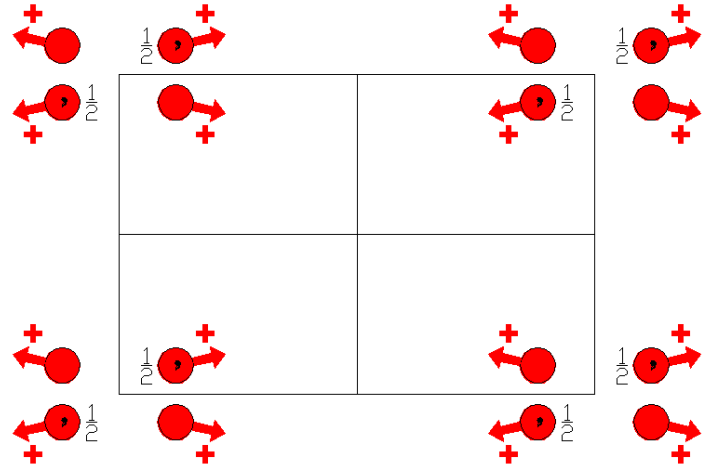
Along [0,1,0] p<sub>2b</sub>.1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pc'c'2  
27.4.181

m'm'2  
Pc'c'2

Orthorhombic



Origin on c'c'2

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

- (1) 1 (2) 2<sub>z</sub> 0,0,z (3) c' (0,0,1/2) x,0,z (4) c' (0,0,1/2) 0,y,z
- (1|0,0,0) (2<sub>z</sub>|0,0,0) (m<sub>y</sub>|0,0,1/2)' (m<sub>x</sub>|0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

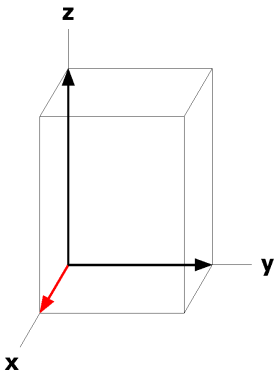
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
4	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y}$ ,z+1/2 [u, $\bar{v},w$ ]	(4) $\bar{x}$ ,y,z+1/2 [ $\bar{u},v,w$ ]
2	d ..2	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]		
2	c ..2	1/2,0,z [0,0,w]	1/2,0,z+1/2 [0,0,w]		
2	b ..2	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]		
2	a ..2	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p1m'1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



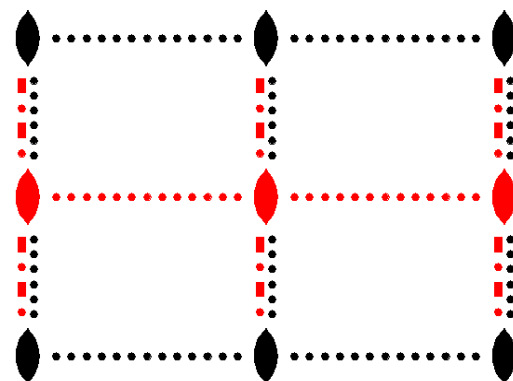
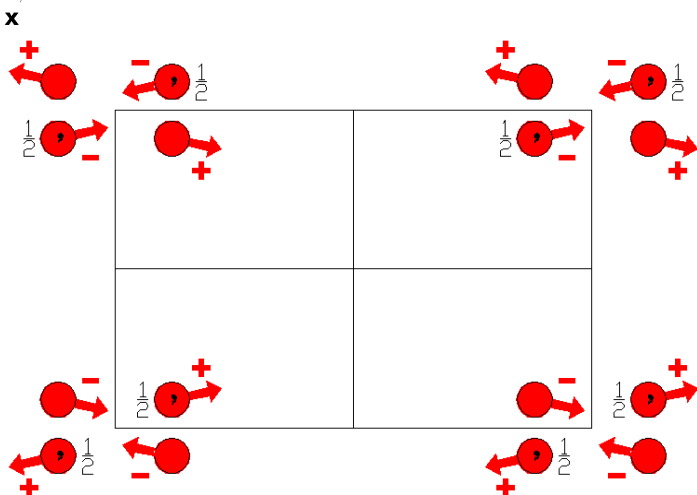
$P_{2a} cc2$

27.5.182

$mm21'$

$P_{2a} cc2$

Orthorhombic



**Origin** on  $cc2$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) c  $(0,0,1/2)$   $x,0,z$   
( $m_y$ |0,0,1/2)

(4) c  $(0,0,1/2)$   $0,y,z$   
( $m_x$ |0,0,1/2)

For  $(1,0,0)'$  + set

(1)  $t'$   $(1,0,0)$   
(1|1,0,0)'

(2)  $2'$   $1/2,0,z$   
( $2_z$ |1,0,0)'

(3)  $n'$   $(1,0,1/2)$   $x,0,z$   
( $m_y$ |1,0,1/2)'

(4)  $c'$   $(0,0,1/2)$   $1/2,y,z$   
( $m_x$ |1,0,1/2)'

**Generators selected** (1); t(1,0,0)<sup>'</sup>; t(0,1,0); t(0,0,1); (2); (3).

**Positions**

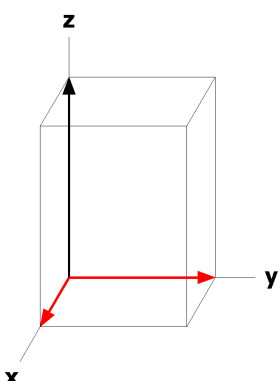
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(1,0,0) <sup>'</sup> +		
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
4	d ..2'	1/2,1/2,z [u,v,0]	1/2,1/2,z+1/2 [ $\bar{u},v,0$ ]		
4	c ..2'	1/2,0,z [u,v,0]	1/2,0,z+1/2 [ $\bar{u},v,0$ ]		
4	b ..2	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]		
4	a ..2	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>.2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>.1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 1/2,y,0



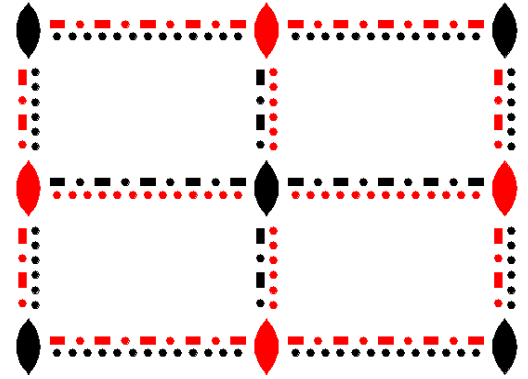
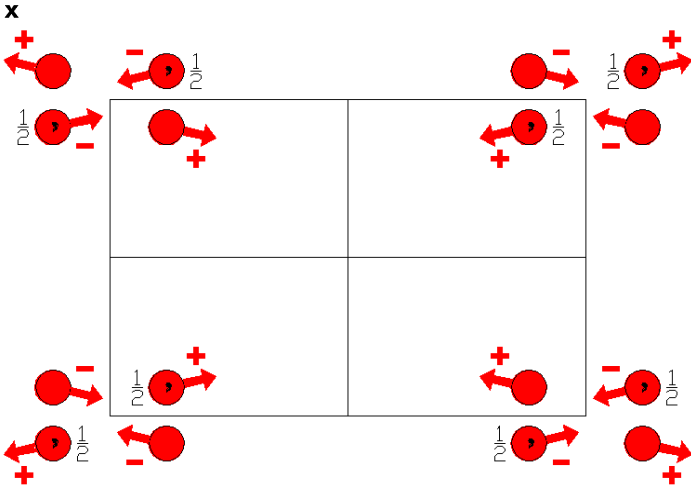
$P_C cc2$

27.6.183

$mm21'$

$P_C cc2$

Orthorhombic



Origin on  $cc2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) c  $(0,0,1/2)$   $x,0,z$   
( $m_y$ |0,0,1/2)

(4) c  $(0,0,1/2)$   $0,y,z$   
( $m_x$ |0,0,1/2)

For  $(1,0,0)'$  + set

(1)  $t'$   $(1,0,0)$   
(1|1,0,0)'

(2)  $2'$   $1/2,0,z$   
( $2_z$ |1,0,0)'

(3)  $n'$   $(1,0,1/2)$   $x,0,z$   
( $m_y$ |1,0,1/2)'

(4)  $c'$   $(0,0,1/2)$   $1/2,y,z$   
( $m_x$ |1,0,1/2)'

**Generators selected** (1); t(1,0,0)<sup>+</sup>; t(0,1,0)<sup>+</sup>; t(0,0,1); (2); (3).

### Positions

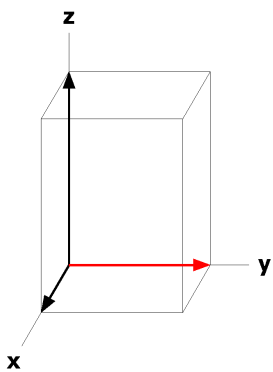
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1,0,0) <sup>+</sup> +	
8 e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
4 d ..2	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]		
4 c ..2'	1/2,0,z [u,v,0]	1/2,0,z+1/2 [ $\bar{u},v,0$ ]		
4 b ..2'	0,1/2,z [u,v,0]	0,1/2,z+1/2 [ $u,\bar{v},0$ ]		
4 a ..2	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



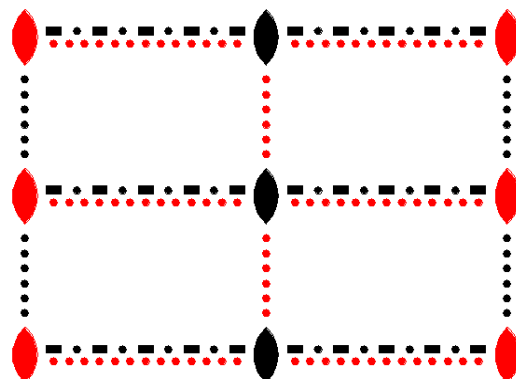
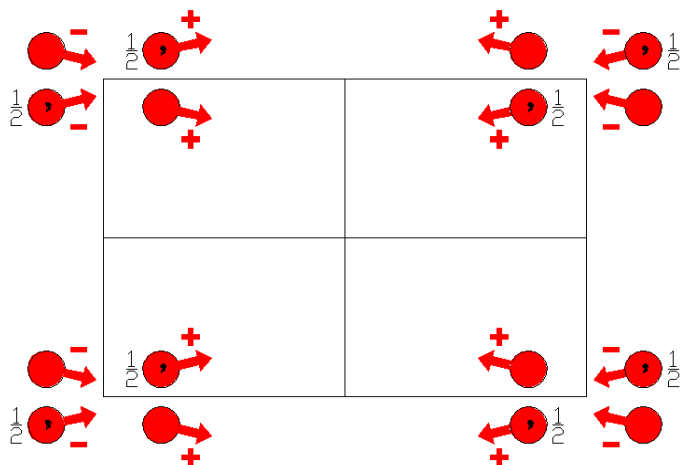
$P_{2b}c'c2'$

27.7.184

$mm21'$

$P_{2b}c'c2'$

Orthorhombic



**Origin** on  $c'c2'$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                      |  |  |
|--------------------|--------------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) $2'$ $0,0,z$<br>( $2_z$  0,0,0)' | (3) $c$ $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2) | (4) $c'$ $(0,0,1/2)$ $0,y,z$<br>( $m_x$  0,0,1/2)' |
|--------------------|--------------------------------------|--|--|

For  $(0,1,0)'$  + set

- |                                 |                                      |  |  |
|---------------------------------|--------------------------------------|--|--|
| (1) $t'$ $(0,1,0)$<br>(1 0,1,0) | (2) $2$ $0,1/2,z$<br>( $2_z$  0,1,0) | (3) $c'$ $(0,0,1/2)$ $x,1/2,z$<br>( $m_y$  0,1,1/2)' | (4) $n$ $(0,1,1/2)$ $0,y,z$<br>( $m_x$  0,1,1/2) |
|---------------------------------|--------------------------------------|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

### Positions

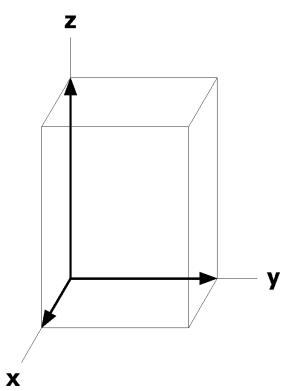
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
8 e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
4 d ..2	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]		
4 c ..2'	1/2,0,z [u,v,0]	1/2,0,z+1/2 [ $\bar{u},v,0$ ]		
4 b ..2	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]		
4 a ..2'	0,0,z [u,v,0]	0,0,z+1/2 [ $\bar{u},v,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>.2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>.1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



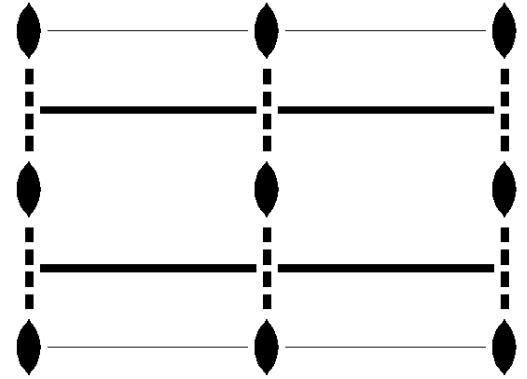
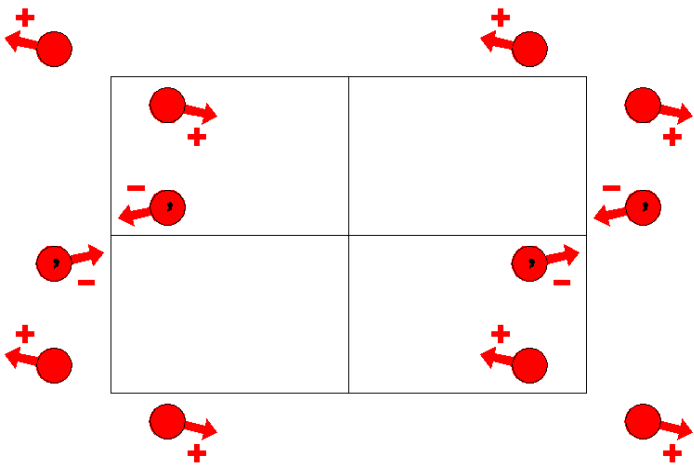
Pma2

28.1.185

mm2

Pma2

Orthorhombic



Origin on 1a2

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
(2<sub>z</sub>|0,0,0)

(3) a  $(1/2,0,0)$   $x,0,z$   
(m<sub>y</sub>|1/2,0,0)

(4) m  $1/4,y,z$   
(m<sub>x</sub>|1/2,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

### Positions

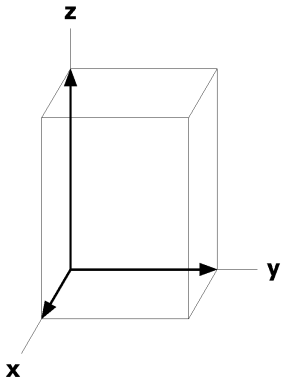
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
4	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x+1/2,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x}+1/2,y,z$ [ $u,\bar{v},\bar{w}$ ]
2	c	m..	1/4,y,z [u,0,0]	3/4, $\bar{y},z$ [ $\bar{u},0,0$ ]		
2	b	..2	0,1/2,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]		
2	a	..2	0,0,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p2mg  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a^*}1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0

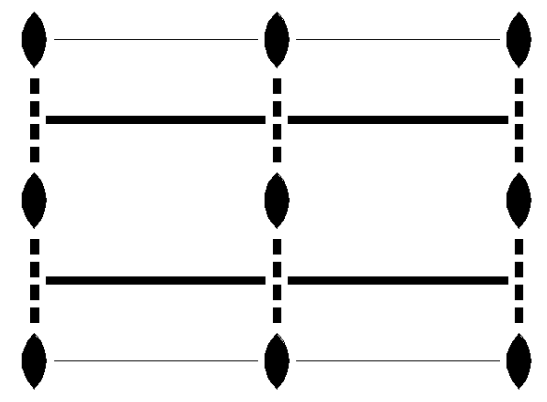
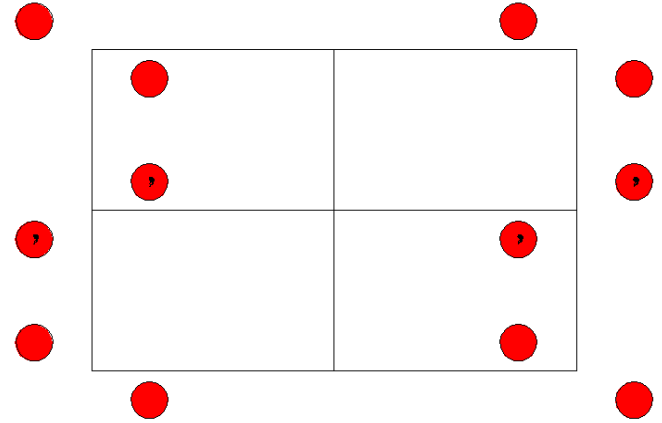


Pma21'  
28.2.186

mm21'  
Pma21'

Orthorhombic

1'



Origin on 1a21'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1$

Symmetry Operations

For 1 + set

- (1) 1  
(1|0,0,0)
- (2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)
- (3) a (1/2,0,0) x,0,z  
(m<sub>y</sub>|1/2,0,0)
- (4) m 1/4,y,z  
(m<sub>x</sub>|1/2,0,0)

For 1' + set

- (1) 1'  
(1|0,0,0)'
- (2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'
- (3) a' (1/2,0,0) x,0,z  
(m<sub>y</sub>'|1/2,0,0)'
- (4) m' 1/4,y,z  
(m<sub>x</sub>'|1/2,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

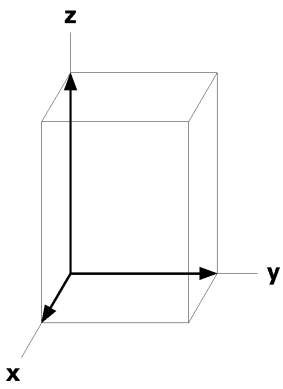
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
4 d 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $x+1/2,\bar{y},z$ [0,0,0]	(4) $\bar{x}+1/2,y,z$ [0,0,0]
2 c m..1'	1/4,y,z [0,0,0]	3/4, $\bar{y},z$ [0,0,0]		
2 b ..21'	0,1/2,z [0,0,0]	1/2,1/2,z [0,0,0]		
2 a ..21'	0,0,z [0,0,0]	1/2,0,z [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

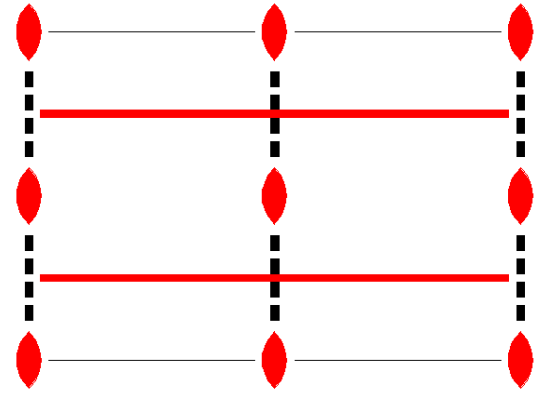
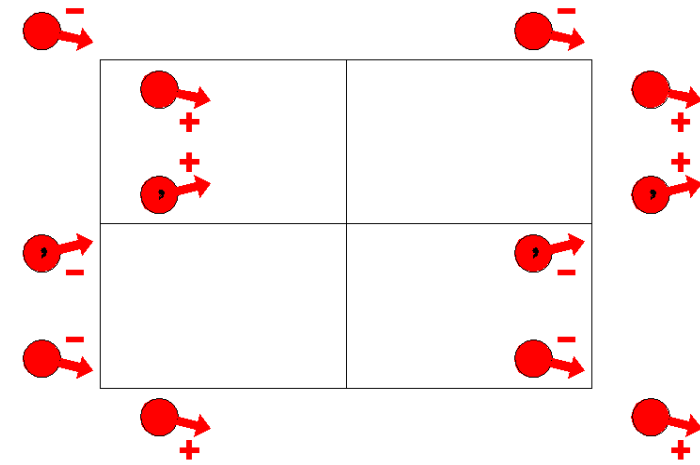
Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pm'a2'  
28.3.187

m'm2'  
Pm'a2'

Orthorhombic



Origin on 1a2'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'

(3) a (1/2,0,0) x,0,z  
(m<sub>y</sub>|1/2,0,0)

(4) m' 1/4,y,z  
(m<sub>x</sub>|1/2,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

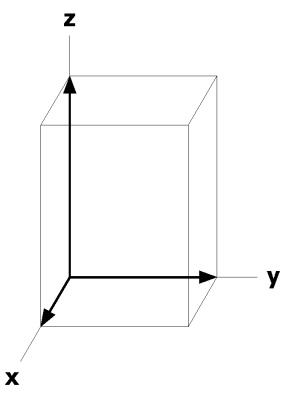
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
4	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x+1/2,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x}+1/2,y,z$ [ $\bar{u},v,w$ ]
2	c	m'..	1/4,y,z [0,v,w]	3/4, $\bar{y},z$ [0,v, $\bar{w}$ ]		
2	b	..2'	0,1/2,z [u,v,0]	1/2,1/2,z [ $\bar{u},v,0$ ]		
2	a	..2'	0,0,z [u,v,0]	1/2,0,z [ $\bar{u},v,0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2'm'g  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

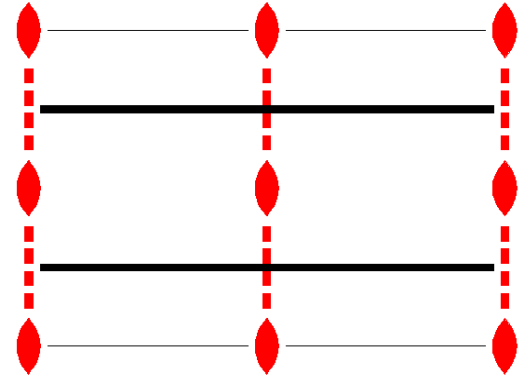
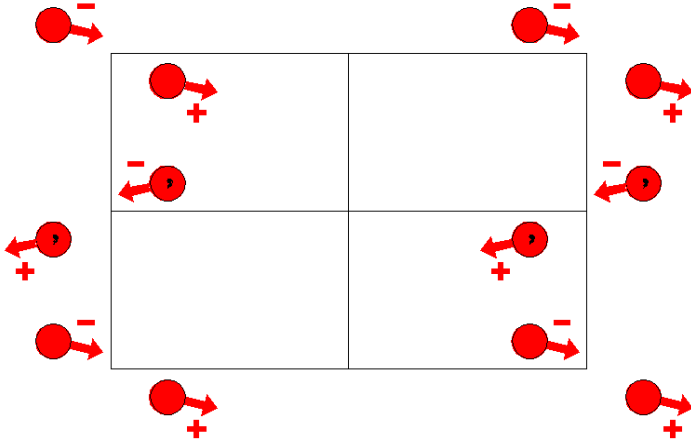
Along [0,1,0] p<sub>2a</sub>'1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pma'2'  
28.4.188

mm'2'  
Pma'2

Orthorhombic



Origin on 1a'2'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'

(3) a' (1/2,0,0) x,0,z  
(m<sub>y</sub>|1/2,0,0)'

(4) m 1/4,y,z  
(m<sub>x</sub>|1/2,0,0)



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

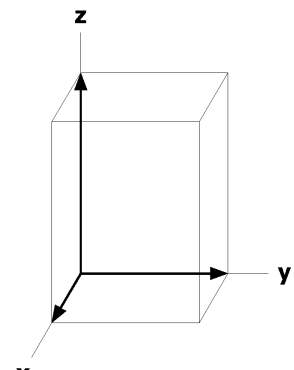
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
4	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x+1/2,\bar{y},z$ [u, $\bar{v}$ ,w]	(4) $\bar{x}+1/2,y,z$ [u, $\bar{v},\bar{w}$ ]
2	c m..	1/4,y,z [u,0,0]	3/4, $\bar{y},z$ [u,0,0]		
2	b ..2'	0,1/2,z [u,v,0]	1/2,1/2,z [u, $\bar{v}$ ,0]		
2	a ..2'	0,0,z [u,v,0]	1/2,0,z [u, $\bar{v}$ ,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2'mg'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

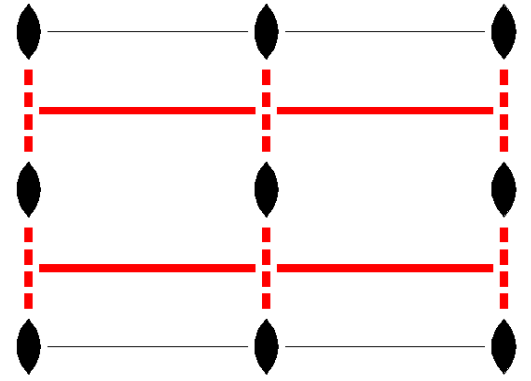
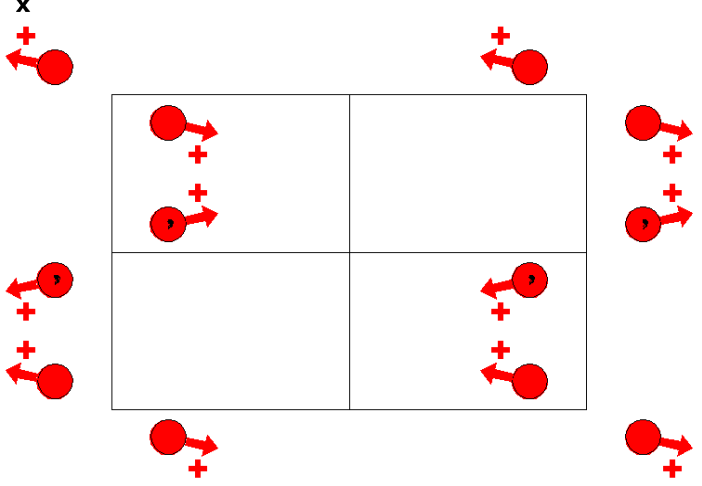
Along [0,1,0] p1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pm'a'2  
28.5.189

m'm'2  
Pm'a'2

Orthorhombic



Origin on 1a'2

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) a' (1/2,0,0) x,0,z  
(m<sub>y</sub>|1/2,0,0)'

(4) m' 1/4,y,z  
(m<sub>x</sub>|1/2,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

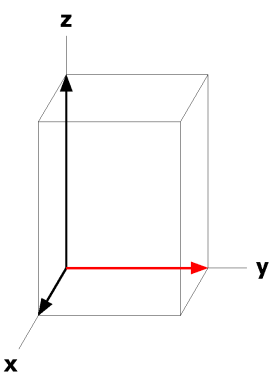
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x+1/2,\bar{y},z$ [ $u,\bar{v},w$ ]	(4) $\bar{x}+1/2,y,z$ [ $\bar{u},v,w$ ]
4 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x+1/2,\bar{y},z$ [ $u,\bar{v},w$ ]	(4) $\bar{x}+1/2,y,z$ [ $\bar{u},v,w$ ]
2 c m'..	1/4,y,z [0,v,w]	3/4, $\bar{y},z$ [0, $\bar{v},w$ ]		
2 b ..2	0,1/2,z [0,0,w]	1/2,1/2,z [0,0,w]		
2 a ..2	0,0,z [0,0,w]	1/2,0,z [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p2m'g'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m'1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



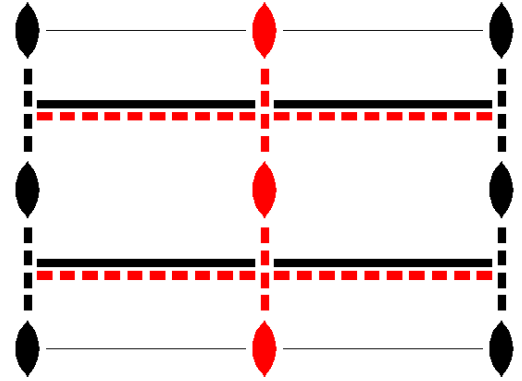
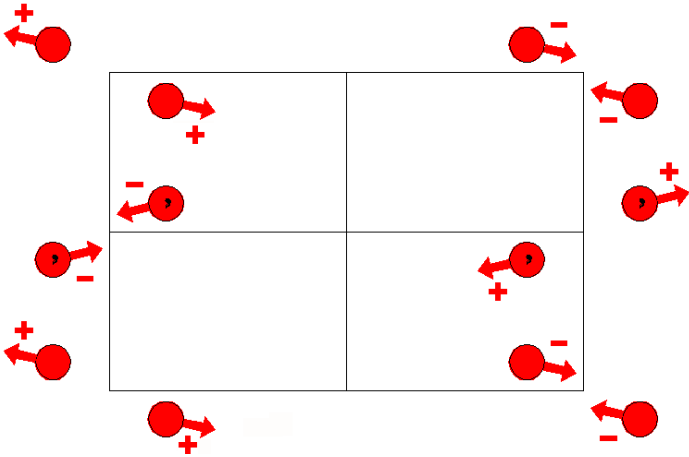
$P_{2b}ma2$

28.6.190

$mm21'$

$P_{2b}ma2$

Orthorhombic



**Origin** on  $1a_2$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) a  $(1/2,0,0)$   $x,0,z$   
( $m_y$ | $1/2,0,0$ )

(4) m  $1/4,y,z$   
( $m_x$ | $1/2,0,0$ )

For  $(0,1,0)'$  + set

(1)  $t'$   $(0,1,0)$   
(1| $0,1,0$ )'

(2)  $2'$   $0,1/2,z$   
( $2_z$ | $0,1,0$ )'

(3)  $a'$   $(1/2,0,0)$   $x,1/2,z$   
( $m_y$ | $1/2,1,0$ )'

(4)  $b'$   $(0,1,0)$   $1/4,y,z$   
( $m_x$ | $1/2,1,0$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0)'; t(0,0,1); (2); (3).

### Positions

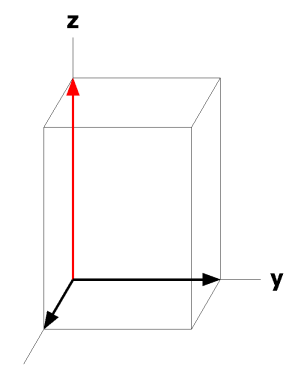
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(0,1,0)' +	
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x+1/2,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x}+1/2,y,z$ [ $u,\bar{v},\bar{w}$ ]
4 c m..	1/4,y,z [u,0,0]	3/4, $\bar{y},z$ [ $\bar{u},0,0$ ]		
4 b ..2'	0,1/2,z [u,v,0]	1/2,1/2,z [ $u,\bar{v},0$ ]		
4 a ..2	0,0,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2b</sub>-2mg  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



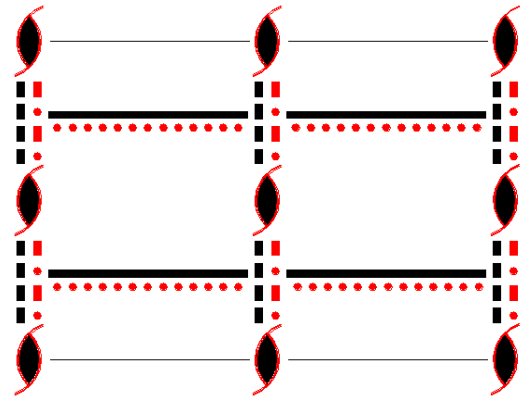
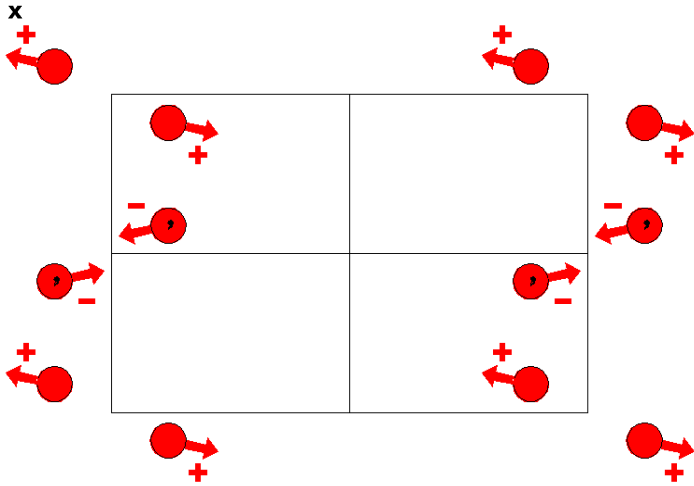
$P_{2c}ma2$

28.7.191

$mm21'$

$P_{2c}ma2$

Orthorhombic



Origin on  $1a_2$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) a  $(1/2,0,0)$   $x,0,z$   
( $m_y$ | $1/2,0,0$ )

(4) m  $1/4,y,z$   
( $m_x$ | $1/2,0,0$ )

For  $(0,0,1)'$  + set

(1)  $t'$   $(0,0,1)$   
(1|0,0,1)'

(2)  $2'$   $(0,0,1)$   $0,0,z$   
( $2_z$ |0,0,1)'

(3)  $n'$   $(1/2,0,1)$   $x,0,z$   
( $m_y$ | $1/2,0,1$ )'

(4)  $c'$   $(0,0,1)$   $1/4,y,z$   
( $m_x$ | $1/2,0,1$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

### Positions

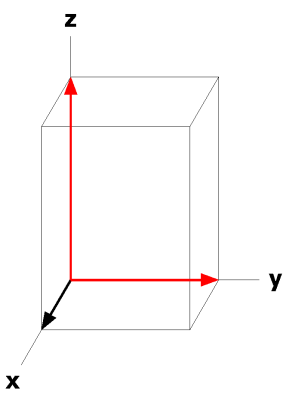
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x+1/2,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x}+1/2,y,z$ [ $u,\bar{v},\bar{w}$ ]
4 c m..	1/4,y,z [u,0,0]	3/4, $\bar{y},z$ [ $\bar{u},0,0$ ]		
4 b ..2	0,1/2,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]		
4 a ..2	0,0,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p2mg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

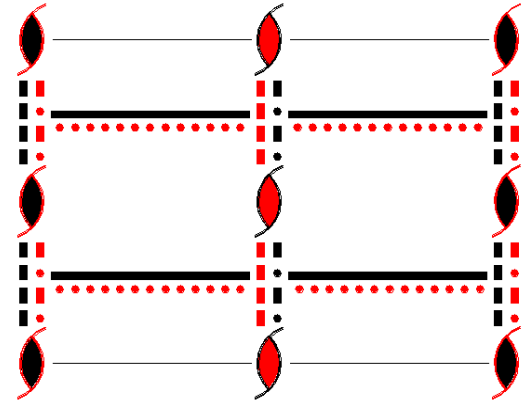
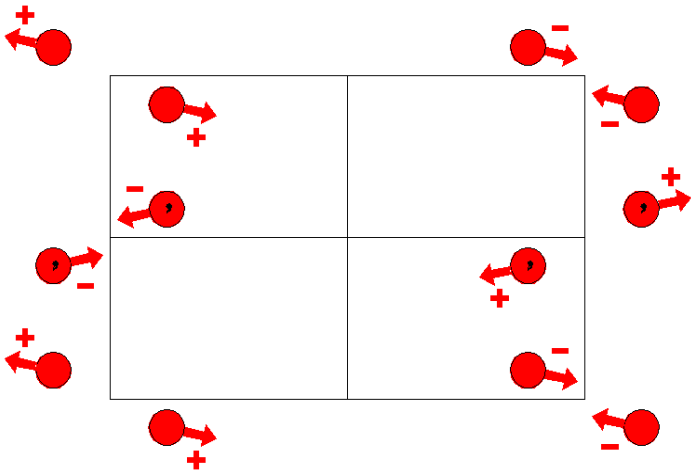
Along [0,1,0] p<sub>c</sub>-1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



$P_A ma2$   
28.8.192

$mm21'$   
 $P_A ma2$

Orthorhombic



**Origin** on  $1a2$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) a  $(1/2,0,0)$   $x,0,z$   
( $m_y$ | $1/2,0,0$ )

(4) m  $1/4,y,z$   
( $m_x$ | $1/2,0,0$ )

For  $(0,1,0)'$  + set

(1)  $t' (0,1,0)$   
(1|0,1,0)'

(2)  $2' 0,1/2,z$   
( $2_z$ |0,1,0)'

(3)  $a' (1/2,0,0)$   $x,1/2,z$   
( $m_y$ | $1/2,1,0$ )'

(4)  $b' (0,1,0)$   $1/4,y,z$   
( $m_x$ | $1/2,1,0$ )'



**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ '; (2); (3).

### Positions

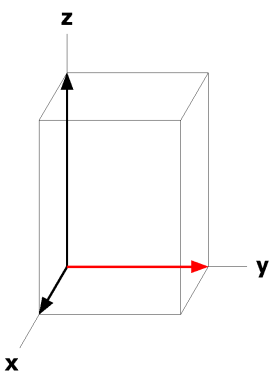
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(0,1,0)' +	
8 d 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $x+1/2,\bar{y},z [\bar{u},v,\bar{w}]$	(4) $\bar{x}+1/2,y,z [u,\bar{v},\bar{w}]$
4 c m..	$1/4,y,z [u,0,0]$	$3/4,\bar{y},z [\bar{u},0,0]$		
4 b ..2'	$0,1/2,z [u,v,0]$	$1/2,1/2,z [u,\bar{v},0]$		
4 a ..2	$0,0,z [0,0,w]$	$1/2,0,z [0,0,\bar{w}]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p2mg1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $p1m11'$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $0,y,0$



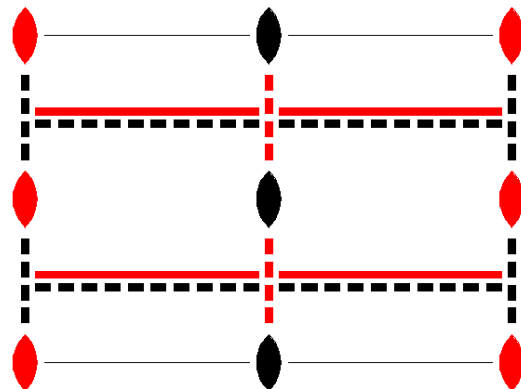
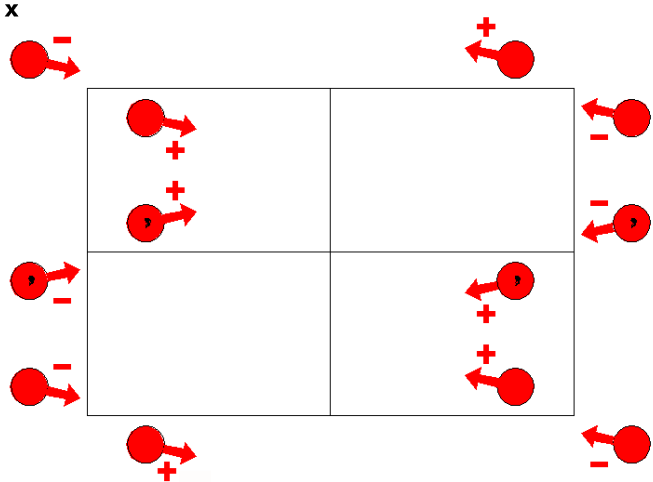
$P_{2b}m'a2'$

28.9.193

$mm21'$

$P_{2b}m'a2'$

Orthorhombic



**Origin** on  $1a2'$

**Asymmetric unit**  $0 \leq x \leq 1/4; 0 \leq y \leq 1; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2)  $2'_z$  0,0,z  
( $2_z$ |0,0,0)'

(3) a ( $1/2,0,0$ ) x,0,z  
( $m_y$ | $1/2,0,0$ )

(4)  $m'_x$   $1/4,y,z$   
( $m_x$ | $1/2,0,0$ )'

For  $(0,1,0)$ ' + set

(1)  $t'_y$  (0,1,0)  
(1|0,1,0)'

(2)  $2'_z$  0,1/2,z  
( $2_z$ |0,1,0)

(3) a' ( $1/2,0,0$ ) x,1/2,z  
( $m_y$ | $1/2,1,0$ )'

(4) b (0,1,0)  $1/4,y,z$   
( $m_x$ | $1/2,1,0$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

### Positions

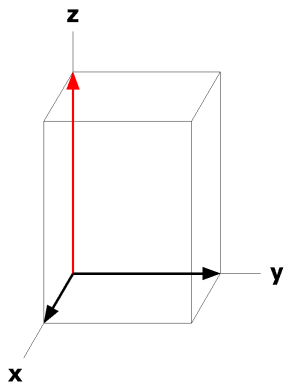
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x+1/2,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x}+1/2,y,z$ [ $\bar{u},v,w$ ]
4 c m'..	1/4,y,z [0,v,w]	3/4, $\bar{y},z$ [0,v, $\bar{w}$ ]		
4 b ..2	0,1/2,z [0,0,w]	1/2,1/2,z [0,0,w]		
4 a ..2'	0,0,z [u,v,0]	1/2,0,z [ $\bar{u},v,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2b</sub>-2m'g'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p<sub>2a</sub>-1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

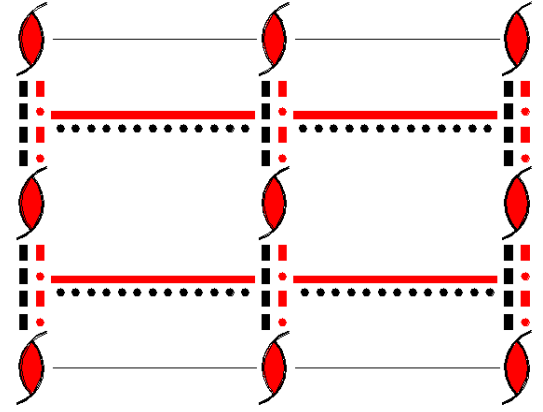
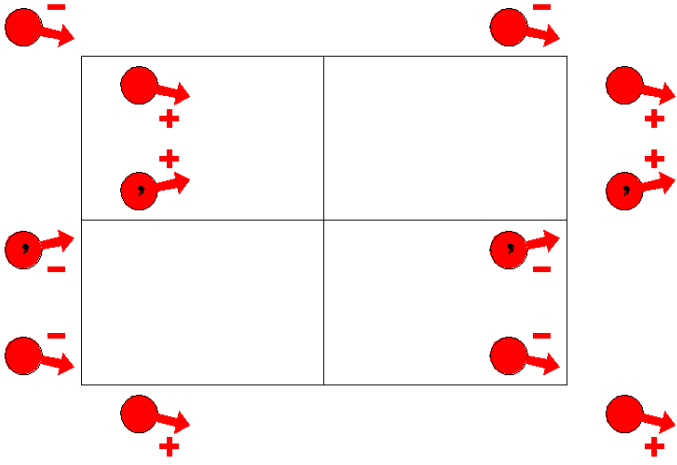
Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



$P_{2c} m'a2'$   
28.10.194

$mm21'$   
 $P_{2c} m'a2'$

Orthorhombic



**Origin** on  $1a2'$

**Asymmetric unit**  $0 \leq x \leq 1/4;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                    |  |  |
|--------------------|------------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (3) a ( $1/2,0,0$ ) x,0,z<br>( $m_y$   $1/2,0,0$ ) | (4) $m'$ $1/4,y,z$<br>( $m_x$   $1/2,0,0$ )' |
|--------------------|------------------------------------|--|--|

For  $(0,0,1)$ ' + set

- |                                |  |  |  |
|--------------------------------|--|--|--|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)' | (2) 2 (0,0,1) 0,0,z<br>( $2_z$  0,0,1) | (3) $n'$ ( $1/2,0,1$ ) x,0,z<br>( $m_y$   $1/2,0,1$ )' | (4) c (0,0,1) $1/4,y,z$<br>( $m_x$   $1/2,0,1$ ) |
|--------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x+1/2,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x}+1/2,y,z$ [ $\bar{u},v,w$ ]
4 c m'..	1/4,y,z [0,v,w]	3/4, $\bar{y},z$ [0,v, $\bar{w}$ ]		
4 b ..2'	0,1/2,z [u,v,0]	1/2,1/2,z [ $\bar{u},v,0$ ]		
4 a ..2'	0,0,z [u,v,0]	1/2,0,z [ $\bar{u},v,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] p2mg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>\*1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>c</sub>\*1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0

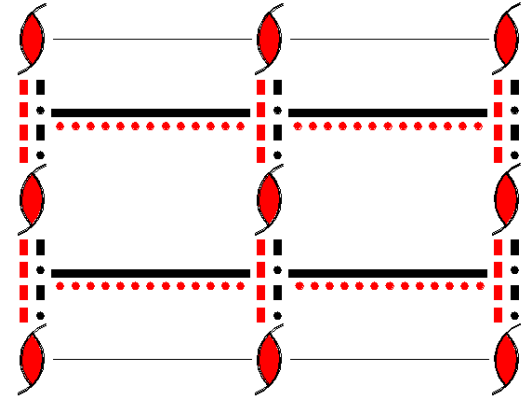
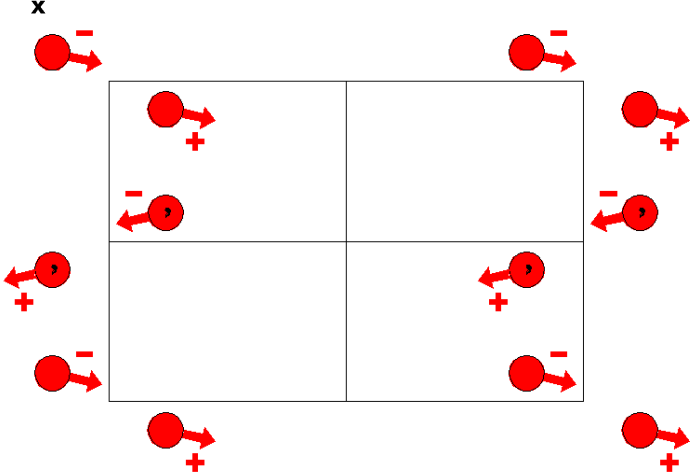
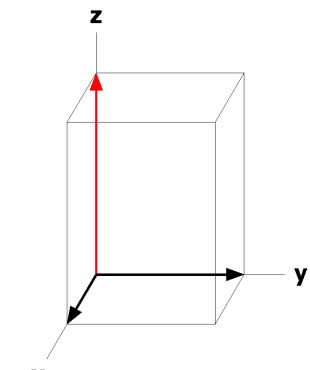
$P_{2c}ma'2'$

28.11.195

$mm21'$

$P_{2c}ma'2'$

Orthorhombic



**Origin** on  $1a'2'$

**Asymmetric unit**  $0 \leq x \leq 1/4;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2)  $2'$   $0,0,z$   
( $2_z$ | $0,0,0$ )'

(3)  $a'$   $(1/2,0,0)$   $x,0,z$   
( $m_y$ | $1/2,0,0$ )'

(4)  $m$   $1/4,y,z$   
( $m_x$ | $1/2,0,0$ )

For  $(0,0,1)'$  + set

(1)  $t'$   $(0,0,1)$   
(1| $0,0,1$ )'

(2)  $2$   $(0,0,1)$   $0,0,z$   
( $2_z$ | $0,0,1$ )

(3)  $n$   $(1/2,0,1)$   $x,0,z$   
( $m_y$ | $1/2,0,1$ )

(4)  $c'$   $(0,0,1)$   $1/4,y,z$   
( $m_x$ | $1/2,0,1$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

### Positions

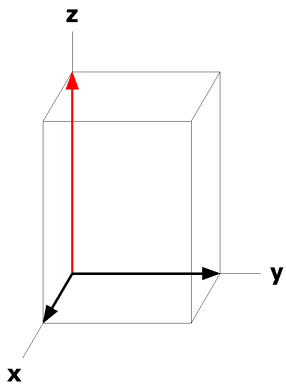
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x+1/2,\bar{y},z$ [u, $\bar{v}$ ,w]	(4) $\bar{x}+1/2,y,z$ [u, $\bar{v},\bar{w}$ ]
4 c m..	1/4,y,z [u,0,0]	3/4, $\bar{y},z$ [u,0,0]		
4 b ..2'	0,1/2,z [u,v,0]	1/2,1/2,z [u, $\bar{v}$ ,0]		
4 a ..2'	0,0,z [u,v,0]	1/2,0,z [u, $\bar{v}$ ,0]		

### Symmetry of Special Projections

Along [0,0,1] p2mg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2b</sub>1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



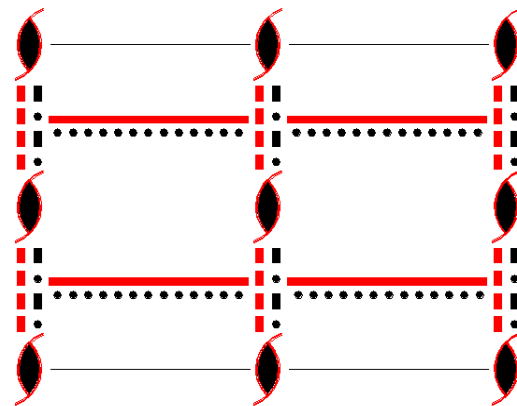
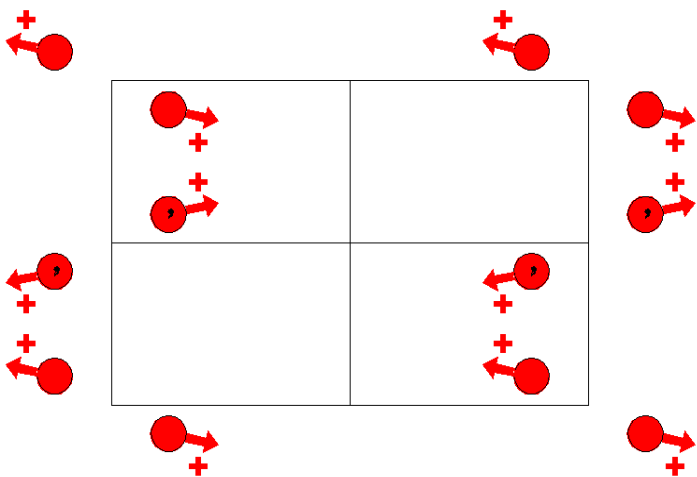
$P_{2c} m'a'2$

28.12.196

$mm21'$

$P_{2c} m'a'2$

Orthorhombic



**Origin** on  $1a'2$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $a'$   $(1/2,0,0)$   $x,0,z$   
( $m_y$ | $1/2,0,0$ )'

(4)  $m'$   $1/4,y,z$   
( $m_x$ | $1/2,0,0$ )'

For  $(0,0,1)'$  + set

(1)  $t'$   $(0,0,1)$   
(1|0,0,1)'

(2)  $2'$   $(0,0,1)$   $0,0,z$   
( $2_z$ |0,0,1)'

(3)  $n$   $(1/2,0,1)$   $x,0,z$   
( $m_y$ | $1/2,0,1$ )'

(4)  $c$   $(0,0,1)$   $1/4,y,z$   
( $m_x$ | $1/2,0,1$ )'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

### Positions

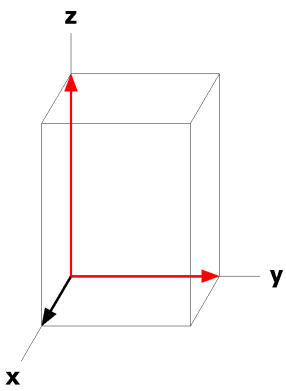
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $x+1/2, \bar{y}, z$ [ $u, \bar{v}, w$ ]	(4) $\bar{x}+1/2, y, z$ [ $\bar{u}, v, w$ ]
4 c m'..	1/4,y,z [0,v,w]	3/4, $\bar{y}, z$ [0, $\bar{v}, w$ ]		
4 b ..2	0,1/2,z [0,0,w]	1/2,1/2,z [0,0,w]		
4 a ..2	0,0,z [0,0,w]	1/2,0,z [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] p2mg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>\*1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2b</sub>\*1m'1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



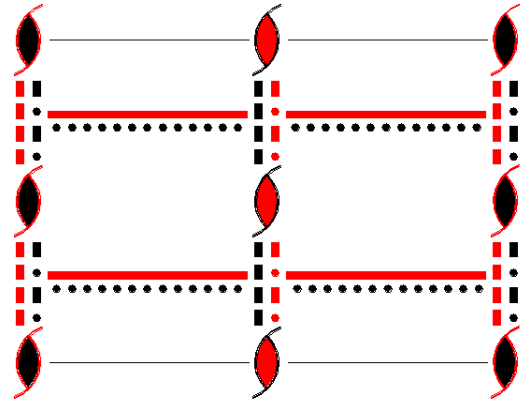
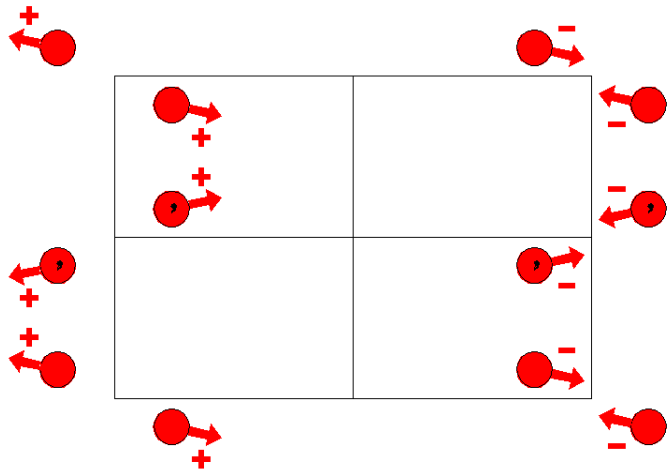
$P_A m'a'2$

28.13.197

$mm21'$

$P_A m'a'2$

Orthorhombic



**Origin** on  $1a'2$

**Asymmetric unit**  $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2)  $2 \quad 0,0,z$   
( $2_z$ |0,0,0)

(3)  $a' \quad (1/2,0,0) \quad x,0,z$   
( $m_y$ | $1/2,0,0$ )'

(4)  $m' \quad 1/4,y,z$   
( $m_x$ | $1/2,0,0$ )'

For  $(0,1,0)'$  + set

(1)  $t' \quad (0,1,0)$   
(1|0,1,0)'

(2)  $2' \quad 0,1/2,z$   
( $2_z$ |0,1,0)'

(3)  $a \quad (1/2,0,0) \quad x,1/2,z$   
( $m_y$ | $1/2,1,0$ )

(4)  $b \quad (0,1,0) \quad 1/4,y,z$   
( $m_x$ | $1/2,1,0$ )

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ '; (2); (3).

### Positions

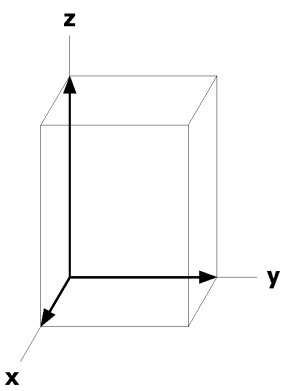
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(0,1,0)' +	
8 d 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x+1/2,\bar{y},z$ [ $u,\bar{v},w$ ]	(4) $\bar{x}+1/2,y,z$ [ $\bar{u},v,w$ ]
4 c m'..	$1/4,y,z$ [0,v,w]	$3/4,\bar{y},z$ [0, $\bar{v},w$ ]		
4 b ..2'	$0,1/2,z$ [u,v,0]	$1/2,1/2,z$ [ $\bar{u},v,0$ ]		
4 a ..2	$0,0,z$ [0,0,w]	$1/2,0,z$ [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1]  $p2mg1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_c \cdot 1m1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 1/2, 0$

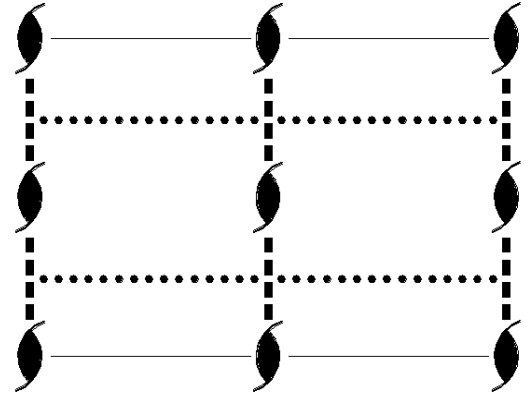
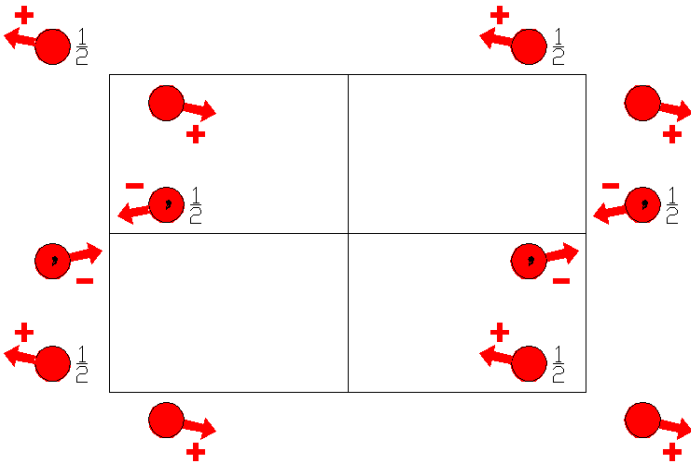
Along [0,1,0]  $p1m11'$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pca2<sub>1</sub>  
29.1.198

mm2  
Pca2<sub>1</sub>

Orthorhombic



Origin on 1a2<sub>1</sub>

Asymmetric unit  $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1$

**Symmetry Operations**

- (1) 1 (1|0,0,0)
- (2) 2 (0,0,1/2) 0,0,z (2<sub>z</sub>|0,0,1/2)
- (3) a (1/2,0,0) x,0,z (m<sub>y</sub>|1/2,0,0)
- (4) c (0,0,1/2) 1/4,y,z (m<sub>x</sub>|1/2,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

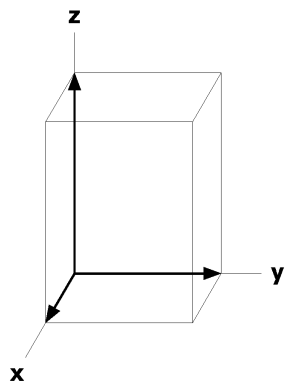
4 a 1 (1) x,y,z [u,v,w] (2)  $\bar{x},\bar{y},z+1/2$  [ $\bar{u},\bar{v},w$ ] (3)  $x+1/2,\bar{y},z$  [ $\bar{u},v,\bar{w}$ ] (4)  $\bar{x}+1/2,y,z+1/2$  [ $u,\bar{v},\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p2mg  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub><sup>\*</sup>1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,0,0

Along [0,1,0] p<sub>2a</sub><sup>\*</sup>1g1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at 1/4,y,0

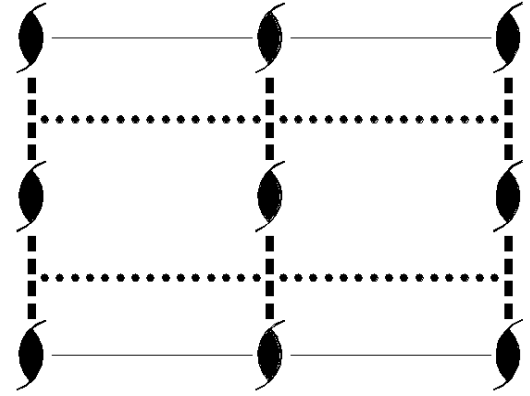
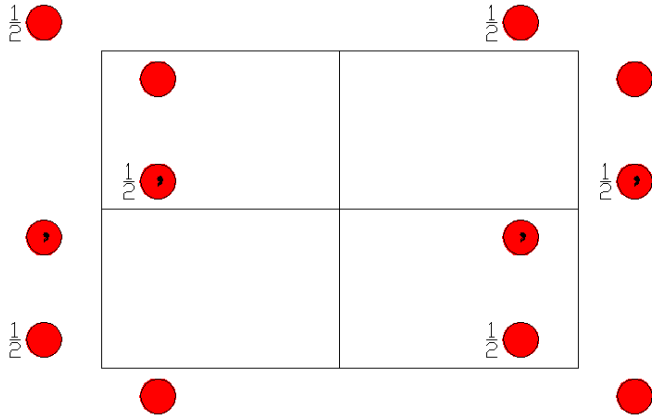


Pca2<sub>1</sub>'  
29.2.199

mm21'  
Pca2<sub>1</sub>'

Orthorhombic

1'



Origin on 1a2<sub>1</sub>'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For 1 + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) a (1/2,0,0) x,0,z<br>(m <sub>y</sub>  1/2,0,0) | (4) c (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,0,1/2) |
|--------------------|--|--|--|

For 1' + set

- |                      |  |  |  |
|----------------------|--|--|--|
| (1) 1'<br>(1 0,0,0)' | (2) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)' | (3) a' (1/2,0,0) x,0,z<br>(m <sub>y</sub>  1/2,0,0)' | (4) c' (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,0,1/2)' |
|----------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

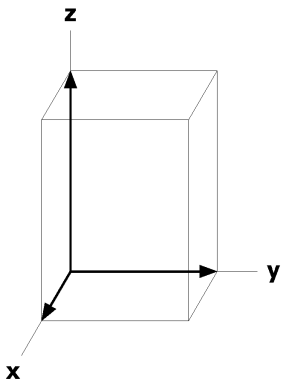
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
4 a 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z+1/2$ [0,0,0]	(3) $x+1/2,\bar{y},z$ [0,0,0]	(4) $\bar{x}+1/2,y,z+1/2$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p2mg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

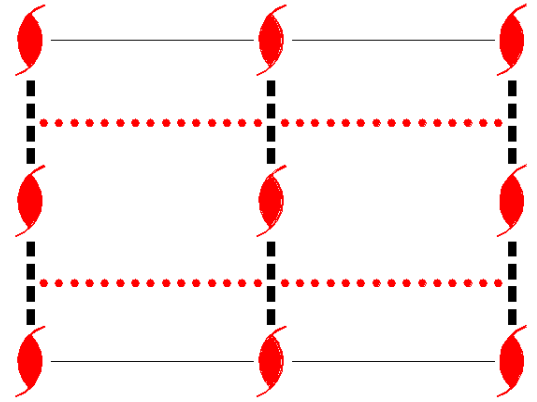
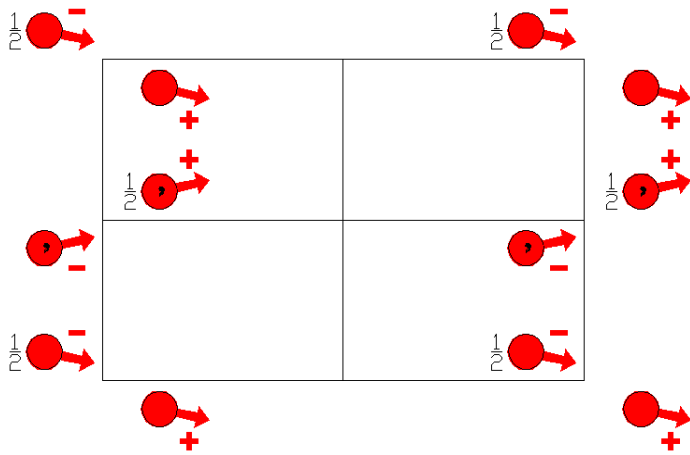
Along [0,1,0] p1g11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pc'a2<sub>1</sub>'  
29.3.200

m'm2'  
Pc'a2<sub>1</sub>'

Orthorhombic



Origin on 1a<sub>2</sub>'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2' (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)'

(3) a (1/2,0,0) x,0,z  
(m<sub>y</sub>|1/2,0,0)

(4) c' (0,0,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,0,1/2)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

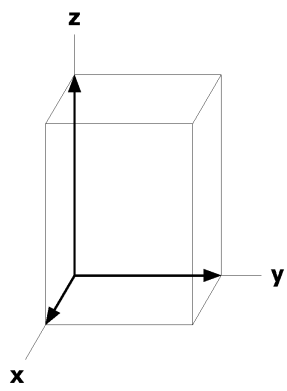
4 a 1 (1) x,y,z [u,v,w] (2)  $\bar{x}, \bar{y}, z+1/2$  [u,v, $\bar{w}$ ] (3)  $x+1/2, \bar{y}, z$  [ $\bar{u}, v, \bar{w}$ ] (4)  $\bar{x}+1/2, y, z+1/2$  [ $\bar{u}, v, w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p2m'g'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,0,0

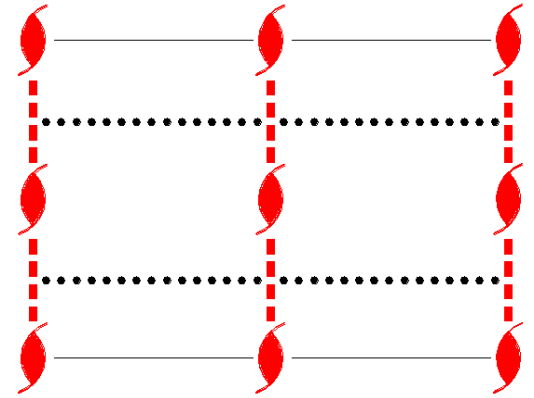
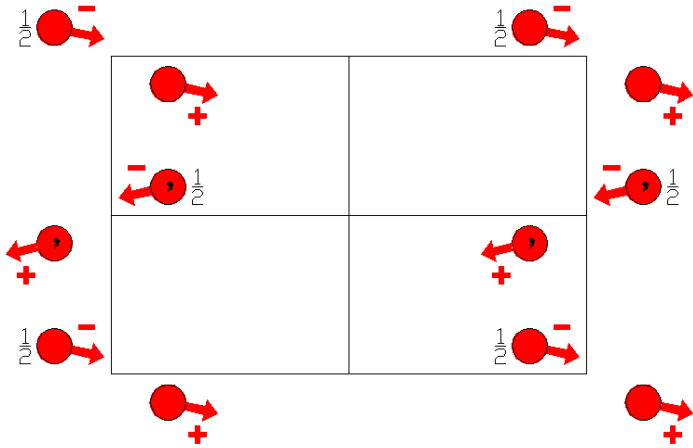
Along [0,1,0] p<sub>2a</sub>'1g1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at 0,y,0



Pca'2<sub>1</sub>'  
29.4.201

mm'2'  
Pca'2<sub>1</sub>'

Orthorhombic



Origin on 1a'2<sub>1</sub>'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2' (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)'

(3) a' (1/2,0,0) x,0,z  
(m<sub>y</sub>|1/2,0,0)'

(4) c (0,0,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

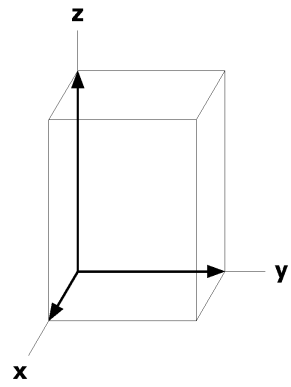
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
4	a 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $x+1/2,\bar{y},z$ [u, $\bar{v},w$ ]	(4) $\bar{x}+1/2,y,z+1/2$ [u, $\bar{v},\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p2'mg'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>'1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p1g'1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



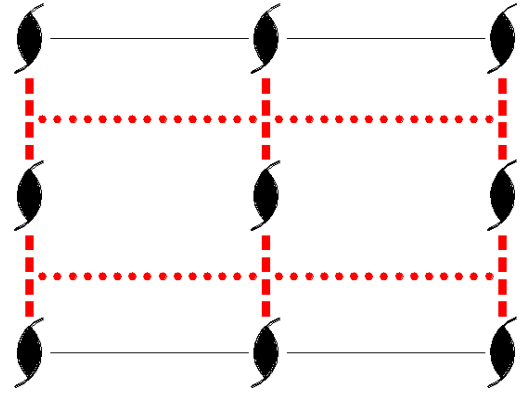
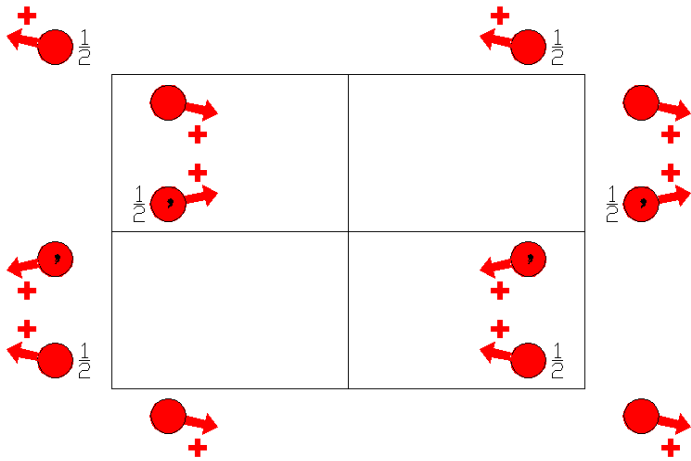
Pc'a'2<sub>1</sub>

29.5.202

m'm'2

Pc'a'2<sub>1</sub>

Orthorhombic



Origin on 1a'2<sub>1</sub>

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)

(3) a' (1/2,0,0) x,0,z  
(m<sub>y</sub>|1/2,0,0)'

(4) c' (0,0,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

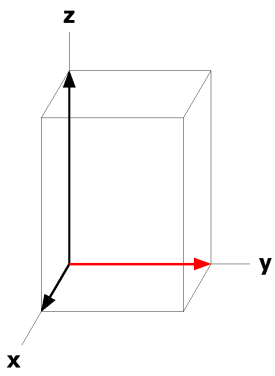
4 a 1 (1) x,y,z [u,v,w] (2)  $\bar{x},\bar{y},z+1/2$  [ $\bar{u},\bar{v},w$ ] (3)  $x+1/2,\bar{y},z$  [ $u,\bar{v},w$ ] (4)  $\bar{x}+1/2,y,z+1/2$  [ $\bar{u},v,w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p2m'g'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,0,0

Along [0,1,0] p1g'1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at 0,y,0



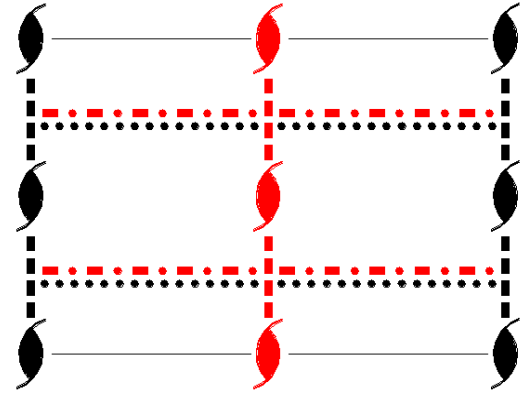
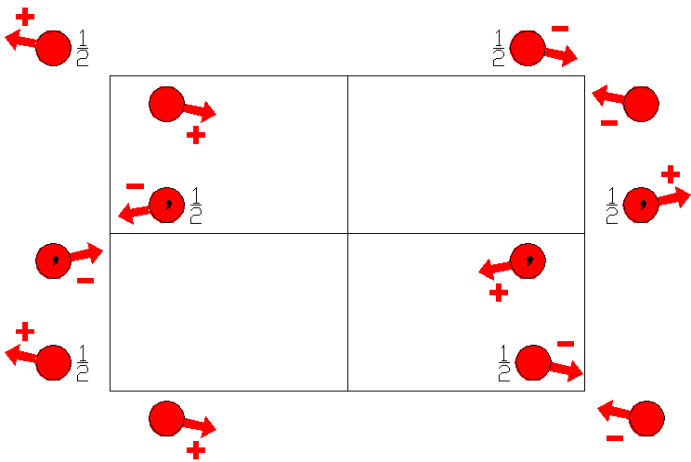
$P_{2b} ca2_1$

29.6.203

$mm21'$

$P_{2b} ca2_1$

Orthorhombic



**Origin** on  $1a_2$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $(0,0,1/2)$ $0,0,z$<br>( $2_z$   $0,0,1/2$ ) | (3) a $(1/2,0,0)$ $x,0,z$<br>( $m_y$   $1/2,0,0$ ) | (4) c $(0,0,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,0,1/2$ ) |
|--------------------|--|--|--|

For  $(0,1,0)'$  + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) $t'$ $(0,1,0)$<br>(1  $0,1,0$ )' | (2) $2'$ $(0,0,1/2)$ $0,1/2,z$<br>( $2_z$   $0,1,1/2$ )' | (3) $a'$ $(1/2,0,0)$ $x,1/2,z$<br>( $m_y$   $1/2,1,0$ )' | (4) $n'$ $(0,1,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,1,1/2$ )' |
|--------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

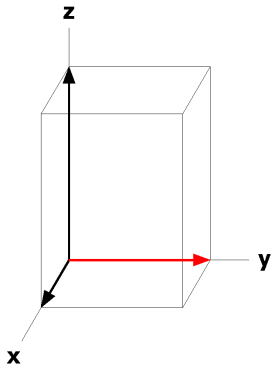
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1,0) <sup>'</sup> +		
8	a 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $x+1/2, \bar{y}, z$ [ $\bar{u}, v, \bar{w}$ ]	(4) $\bar{x}+1/2, y, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2b</sub>-2mg  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>c</sub>-1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p1g11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



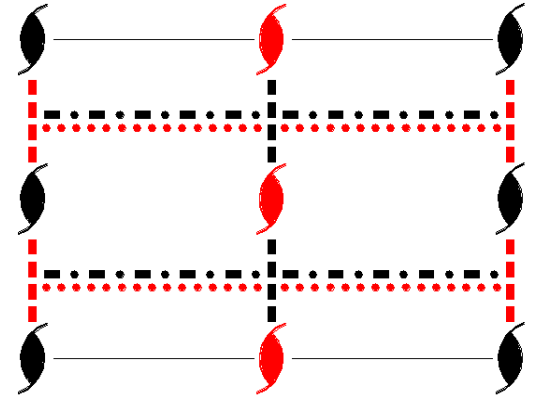
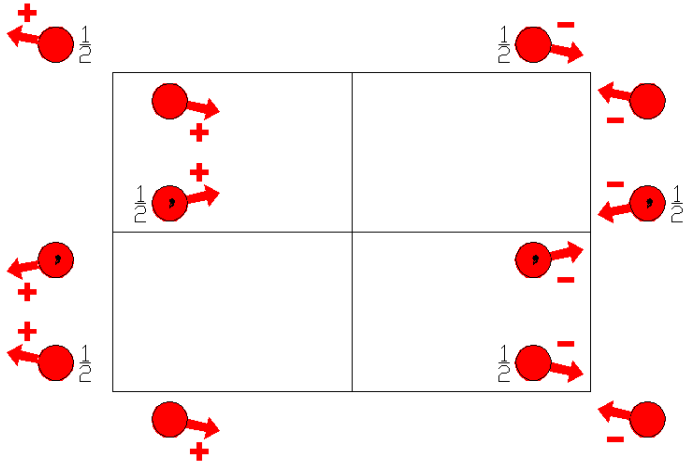
$P_{2b} c'a'2_1$

29.7.204

$mm21'$

$P_{2b} c'a'2_1$

Orthorhombic



**Origin** on  $1a'2_1$

**Asymmetric unit**  $0 \leq x \leq 1/4; 0 \leq y \leq 1; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0) +$  set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $(0,0,1/2)$ $0,0,z$<br>( $2_z$   $0,0,1/2$ ) | (3) $a'$ $(1/2,0,0)$ $x,0,z$<br>( $m_y$   $1/2,0,0$ )' | (4) $c'$ $(0,0,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,0,1/2$ )' |
|--------------------|--|--|--|

For  $(0,1,0)'$  + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) $t'$ $(0,1,0)$<br>(1  $0,1,0$ )' | (2) $2'$ $(0,0,1/2)$ $0,1/2,z$<br>( $2_z$   $0,1,1/2$ )' | (3) $a$ $(1/2,0,0)$ $x,1/2,z$<br>( $m_y$   $1/2,1,0$ ) | (4) $n$ $(0,1,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,1,1/2$ ) |
|--------------------------------------|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0)'; t(0,0,1); (2); (3).

### Positions

#### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

(0,0,0) + (0,1,0)' +

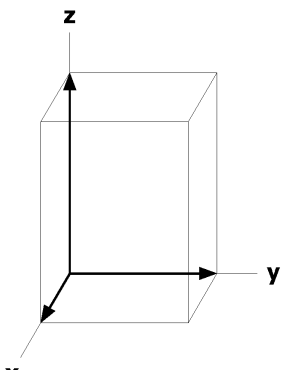
8 a 1 (1) x,y,z [u,v,w] (2)  $\bar{x}, \bar{y}, z+1/2$  [ $\bar{u}, \bar{v}, w$ ] (3)  $x+1/2, \bar{y}, z$  [u, $\bar{v}, w$ ] (4)  $\bar{x}+1/2, y, z+1/2$  [ $\bar{u}, v, w$ ]

### Symmetry of Special Projections

Along [0,0,1] p<sub>2b</sub>-2m'g'  
**a\*** = **a** **b\*** = **b**  
Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>\*1m1  
**a\*** = **b** **b\*** = **c**/2  
Origin at x,1/2,0

Along [0,1,0] p1g11'  
**a\*** = **-a**/2 **b\*** = **c**  
Origin at 0,y,0



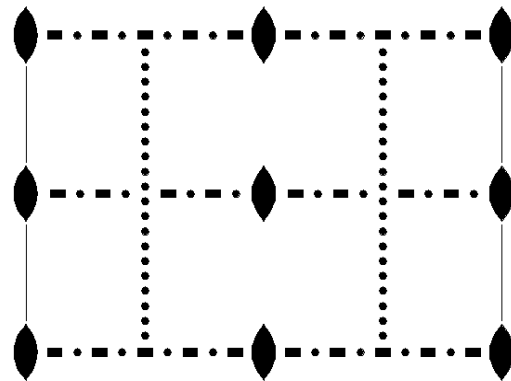
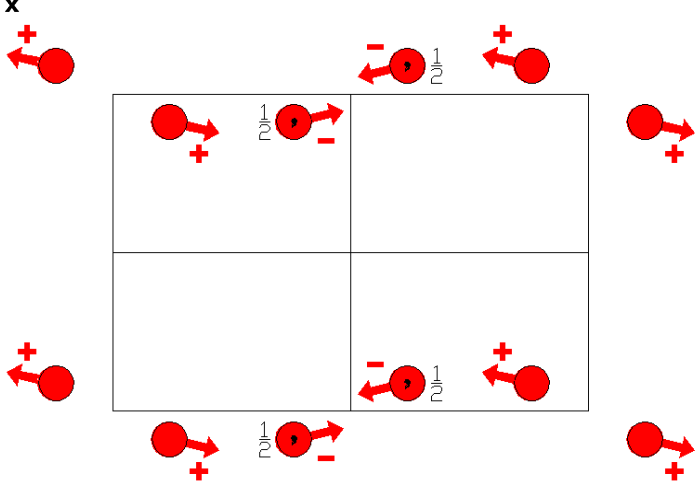
Pnc2

30.1.205

mm2

Pnc2

Orthorhombic



Origin on n12

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) c  $(0,0,1/2)$   $x,1/4,z$   
( $m_y$ |0,1/2,1/2)

(4) n  $(0,1/2,1/2)$   $0,y,z$   
( $m_x$ |0,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

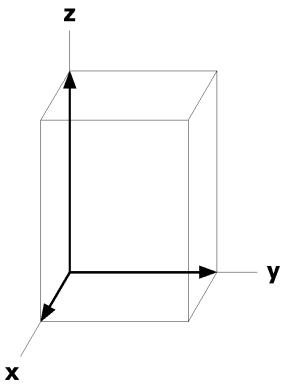
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
4	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) x, $\bar{y}+1/2, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $\bar{x}, y+1/2, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]
2	b ..2	1/2,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]		
2	a ..2	0,0,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2mg  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $p_{2b} \cdot 1m'1$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0

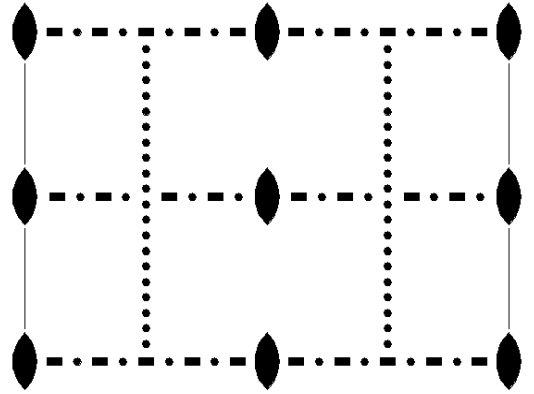
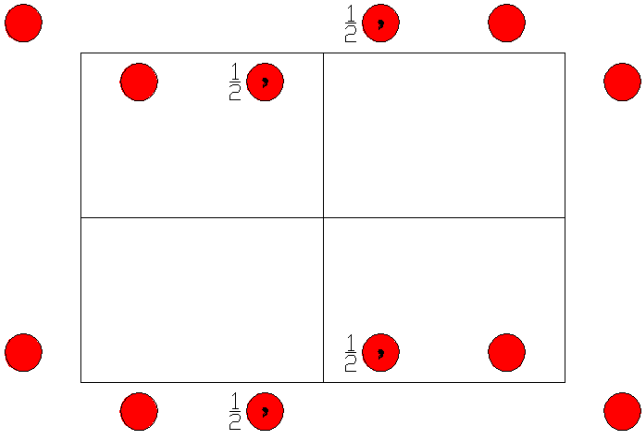


Pnc21'  
30.2.206

mm21'  
Pnc21'

Orthorhombic

1'



Origin on n121'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

For 1 + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2) | (4) n (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>  0,1/2,1/2) |
|--------------------|--|--|--|

For 1' + set

- |                      |  |  |  |
|----------------------|--|--|--|
| (1) 1'<br>(1 0,0,0)' | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (4) n' (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>  0,1/2,1/2)' |
|----------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

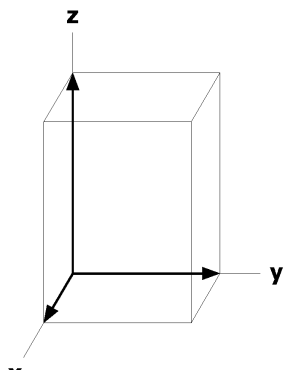
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
4 c 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y}, z$ [0,0,0]	(3) x, $\bar{y}+1/2, z+1/2$ [0,0,0]	(4) $\bar{x}, y+1/2, z+1/2$ [0,0,0]
2 b ..21'	1/2,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]		
2 a ..21'	0,0,z [0,0,0]	0,1/2,z+1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mg1'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

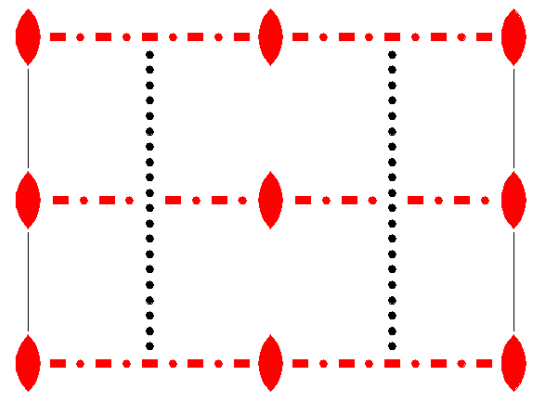
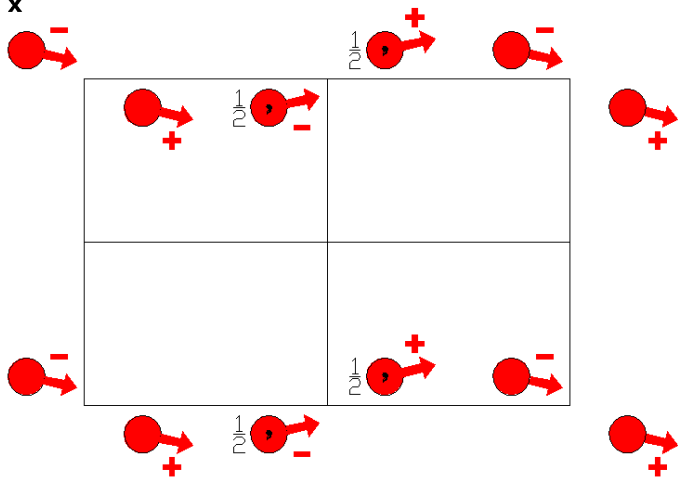
Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pn'c2'  
30.3.207

m'm2'  
Pn'c2'

Orthorhombic



Origin on n'12'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- (1) 1 (2) 2' 0,0,z (3) c (0,0,1/2) x,1/4,z (4) n' (0,1/2,1/2) 0,y,z
- (1|0,0,0) (2z|0,0,0)' (my|0,1/2,1/2) (mx|0,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

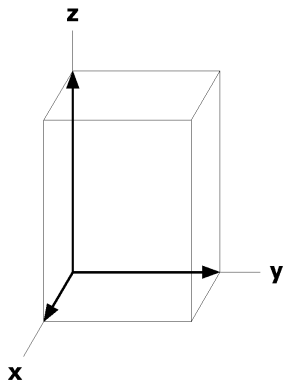
		Coordinates			
		Multiplicity, Wyckoff letter, Site Symmetry.			
4	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y}+1/2, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $\bar{x}, y+1/2, z+1/2$ [ $\bar{u}, v, w$ ]
2	b ..2'	1/2,0,z [u,v,0]	1/2,1/2,z+1/2 [ $\bar{u}, v, 0$ ]		
2	a ..2'	0,0,z [u,v,0]	0,1/2,z+1/2 [ $\bar{u}, v, 0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2'mg'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] c1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

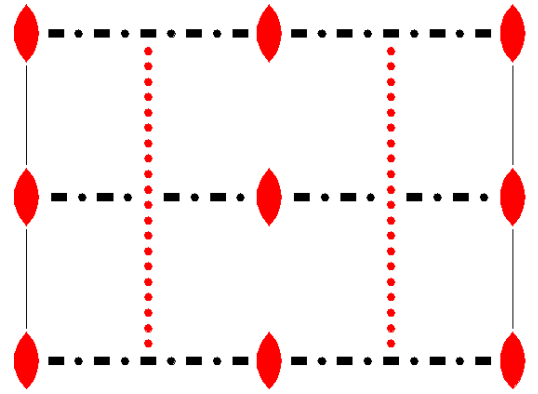
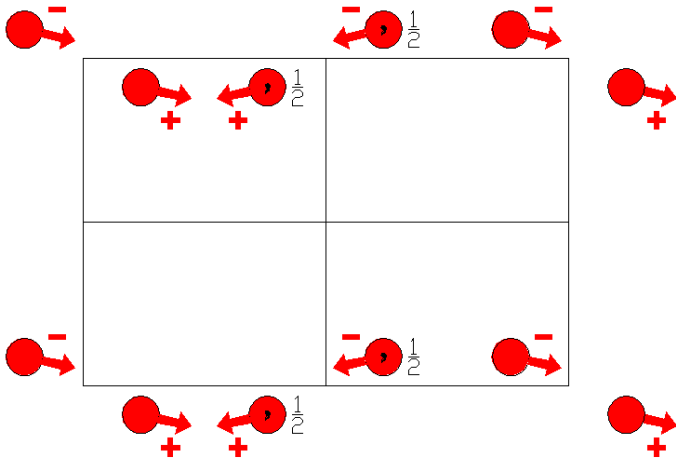
Along [0,1,0] p<sub>2b</sub>'1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pnc'2'  
30.4.208

mm'2'  
Pnc'2'

Orthorhombic



Origin on n12'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'

(3) c' (0,0,1/2) x,1/4,z  
(m<sub>y</sub>|0,1/2,1/2)'

(4) n (0,1/2,1/2) 0,y,z  
(m<sub>x</sub>|0,1/2,1/2)



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

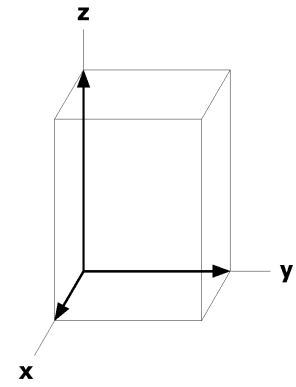
		Coordinates			
		Multiplicity, Wyckoff letter, Site Symmetry.			
4	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y}+1/2, z+1/2$ [u, $\bar{v}$ , w]	(4) $\bar{x}, y+1/2, z+1/2$ [u, $\bar{v}, \bar{w}$ ]
2	b ..2'	1/2,0,z [u,v,0]	1/2,1/2,z+1/2 [u, $\bar{v}$ ,0]		
2	a ..2'	0,0,z [u,v,0]	0,1/2,z+1/2 [u, $\bar{v}$ ,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2'm'g  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0]  $c_p$ 1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

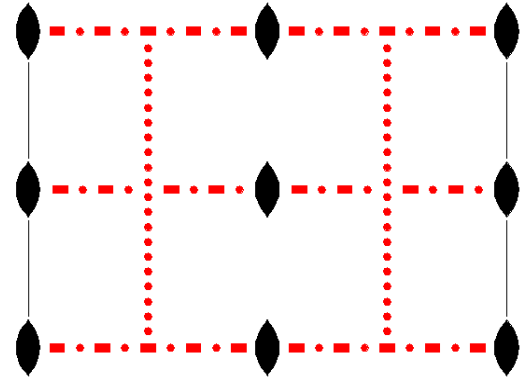
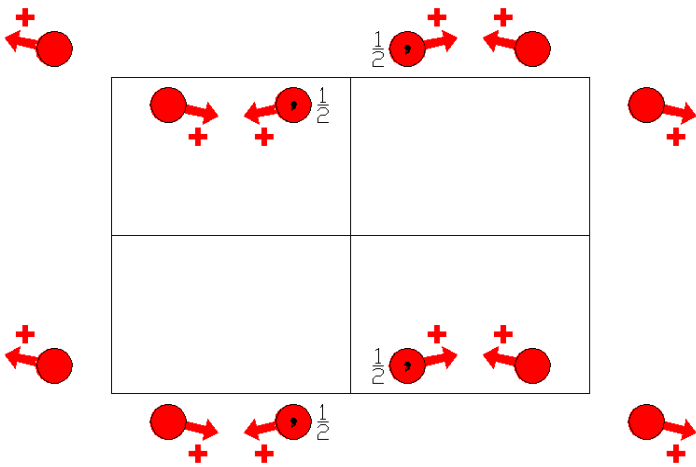
Along [0,1,0] p1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pn'c'2  
30.5.209

m'm'2  
Pn'c'2

Orthorhombic



Origin on n'12

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $c'$   $(0,0,1/2)$   $x,1/4,z$   
( $m_y$ | $0,1/2,1/2$ )'

(4)  $n'$   $(0,1/2,1/2)$   $0,y,z$   
( $m_x$ | $0,1/2,1/2$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

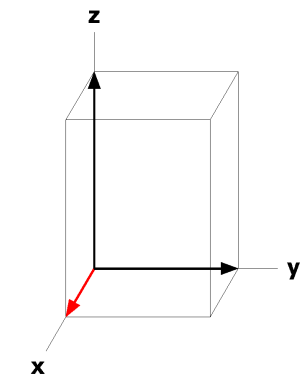
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
4	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $x, \bar{y}+1/2, z+1/2$ [ $u, \bar{v}, w$ ]	(4) $\bar{x}, y+1/2, z+1/2$ [ $\bar{u}, v, w$ ]
2	b ..2	1/2,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]		
2	a ..2	0,0,z [0,0,w]	0,1/2,z+1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p2m'g'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] c1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



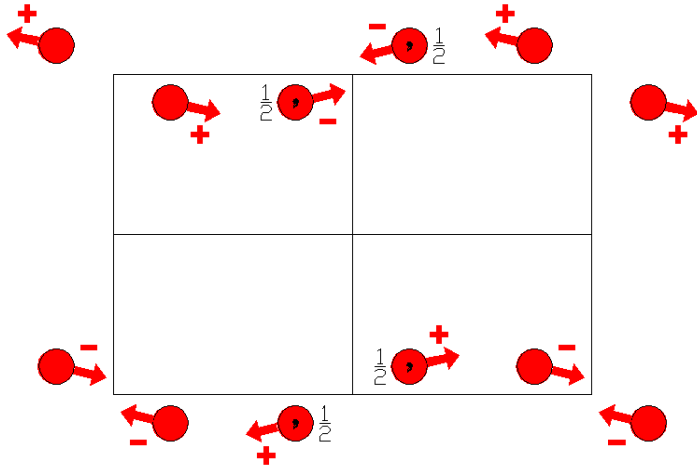
$P_{2a}nc2$

30.6.210

$mm21'$

$P_{2a}nc2$

Orthorhombic



Origin on n12

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) c  $(0,0,1/2) \ x,1/4,z$   
( $m_y$ |0,1/2,1/2)

(4) n  $(0,1/2,1/2) \ 0,y,z$   
( $m_x$ |0,1/2,1/2)

For (0,0,0) + set

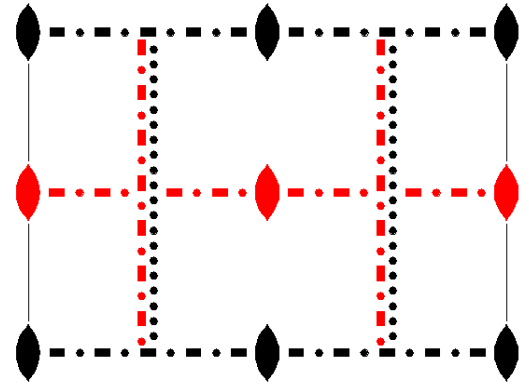
(1)  $t' (1,0,0)$   
(1|1,0,0)'

(2)  $2' \ 1/2,0,z$   
( $2_z$ |1,0,0)'

(3)  $n' (1,0,1/2) \ x,1/4,z$   
( $m_y$ |1,1/2,1/2)'

(4)  $n' (0,1/2,1/2) \ 1/2,y,z$   
( $m_x$ |1,1/2,1/2)'

For (1,0,0)' + set



**Generators selected** (1); t(1,0,0)<sup>'</sup>; t(0,1,0); t(0,0,1); (2); (3).

### Positions

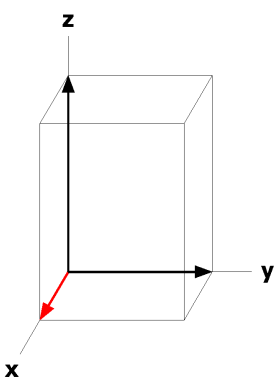
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(1,0,0) <sup>'</sup> +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) x, $\bar{y}+1/2, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $\bar{x}, y+1/2, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]
4	b ..2'	1/2,0,z [u,v,0]	1/2,1/2,z+1/2 [ $\bar{u}, v, 0$ ]		
4	a ..2	0,0,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2b</sub>·2mg  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

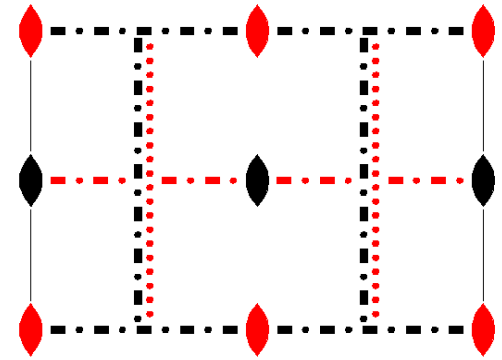
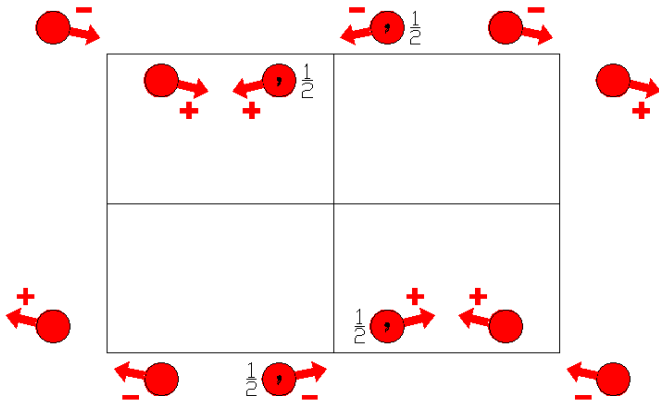
Along [0,1,0] p<sub>c</sub>·1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 1/2,y,0



$P_{2a}nc'2'$   
30.7.211

$mm21'$   
 $P_{2a}nc'2'$

Orthorhombic



**Origin** on  $n12'$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2)  $2'$  0,0,z  
( $2_z$ |0,0,0)'

(3)  $c'$  (0,0,1/2) x,1/4,z  
( $m_y$ |0,1/2,1/2)'

(4) n (0,1/2,1/2) 0,y,z  
( $m_x$ |0,1/2,1/2)

For (0,0,0) + set

For (1,0,0)' + set

(1)  $t'$  (1,0,0)  
(1|1,0,0)

(2) 2 1/2,0,z  
( $2_z$ |1,0,0)

(3) n (1,0,1/2) x,1/4,z  
( $m_y$ |1,1/2,1/2)

(4)  $n'$  (0,1/2,1/2) 1/2,y,z  
( $m_x$ |1,1/2,1/2)'

**Generators selected** (1); t(1,0,0)'; t(0,1,0); t(0,0,1); (2); (3).

**Positions**

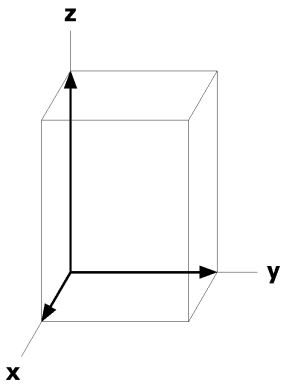
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(1,0,0)' +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y}+1/2, z+1/2$ [u, $\bar{v}$ , w]	(4) $\bar{x}, y+1/2, z+1/2$ [u, $\bar{v}, \bar{w}$ ]
4	b ..2	1/2,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]		
4	a ..2'	0,0,z [u,v,0]	0,1/2,z+1/2 [u, $\bar{v}$ , 0]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2b</sub>·2m'g'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 1/2,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

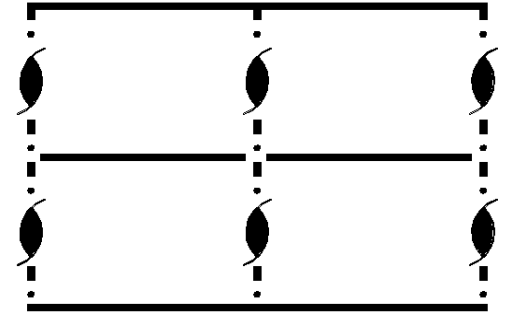
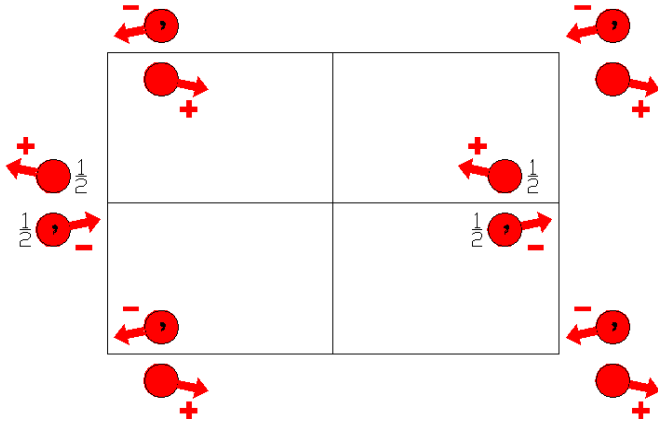
Along [0,1,0] p<sub>2a</sub>·1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pmn2<sub>1</sub>  
31.1.212

mm2  
Pmn2<sub>1</sub>

Orthorhombic



**Origin** on mn1

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 1/4,0,z  
(2<sub>z</sub>|1/2,0,1/2)

(3) n (1/2,0,1/2) x,0,z  
(m<sub>y</sub>|1/2,0,1/2)

(4) m 0,y,z  
(m<sub>x</sub>|0,0,0)



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

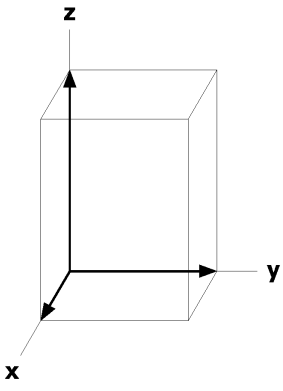
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
4	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $x+1/2, \bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $\bar{x}, y, z$ [ $u, \bar{v}, \bar{w}$ ]
2	a m..	0,y,z [u,0,0]	$1/2, \bar{y}, z+1/2$ [ $\bar{u}, 0, 0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2mg  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $c_p^*1m1$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0

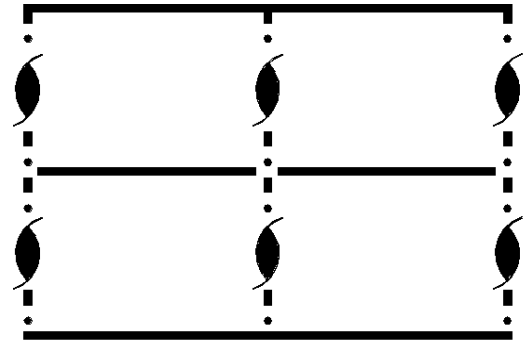
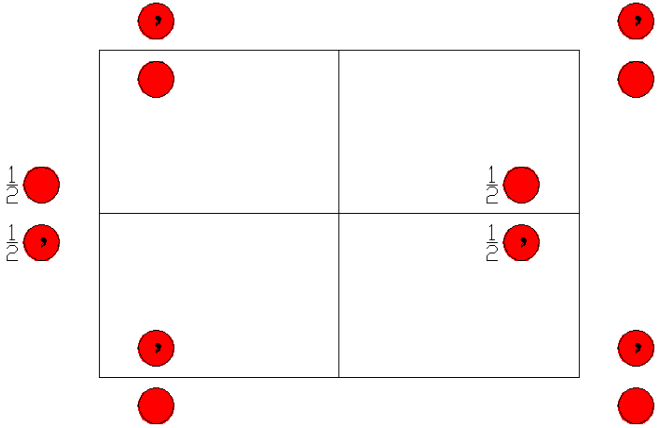


Pmn2<sub>1</sub>'  
31.2.213

mm2<sub>1</sub>'  
Pmn2<sub>1</sub>'

Orthorhombic

1'



Origin on mn11'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For 1 + set

- (1) 1  
(1|0,0,0)
- (2) 2 (0,0,1/2) 1/4,0,z  
(2<sub>z</sub>|1/2,0,1/2)
- (3) n (1/2,0,1/2) x,0,z  
(m<sub>y</sub>|1/2,0,1/2)
- (4) m 0,y,z  
(m<sub>x</sub>|0,0,0)

For 1' + set

- (1) 1'  
(1|0,0,0)'
- (2) 2' (0,0,1/2) 1/4,0,z  
(2<sub>z</sub>|1/2,0,1/2)'
- (3) n' (1/2,0,1/2) x,0,z  
(m<sub>y</sub>|1/2,0,1/2)'
- (4) m' 0,y,z  
(m<sub>x</sub>|0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

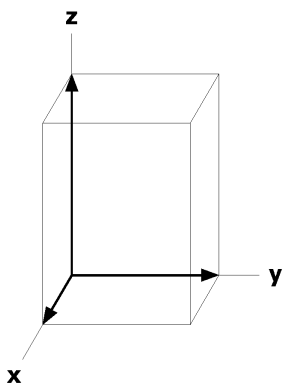
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		1 +	1' +		
4	b 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [0,0,0]	(3) $x+1/2, \bar{y}, z+1/2$ [0,0,0]	(4) $\bar{x}, y, z$ [0,0,0]
2	a m..1'	0,y,z [0,0,0]	$1/2, \bar{y}, z+1/2$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mg1'  
 $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] c1m11'  
 $\mathbf{a}^* = -\mathbf{a} \quad \mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



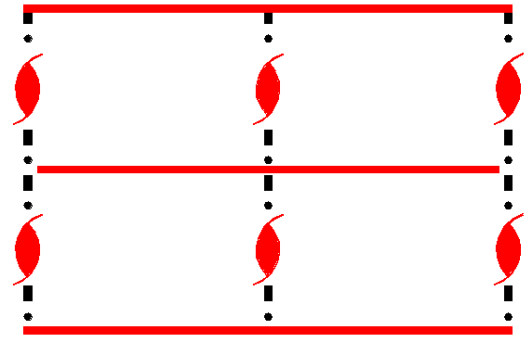
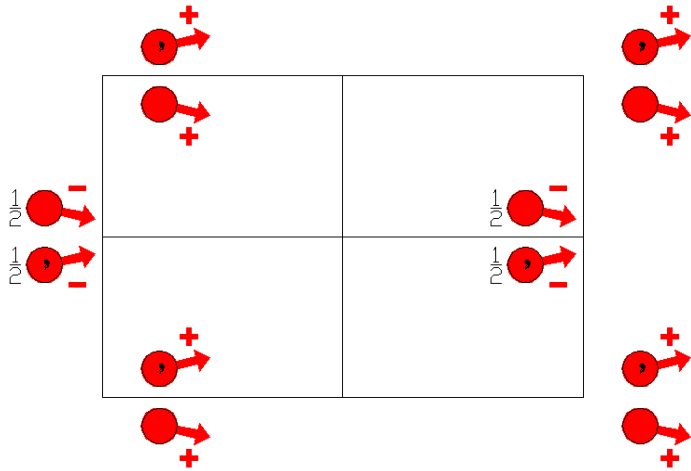
Pm'n2<sub>1</sub>'

31.3.214

m'm2'

Pm'n2<sub>1</sub>'

Orthorhombic



Origin on m'n1

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2' (0,0,1/2) 1/4,0,z  
(2<sub>z</sub>|1/2,0,1/2)'

(3) n (1/2,0,1/2) x,0,z  
(m<sub>y</sub>|1/2,0,1/2)

(4) m' 0,y,z  
(m<sub>x</sub>|0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

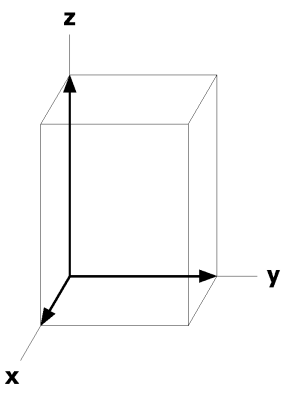
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
4	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [u,v, $\bar{w}$ ]	(3) $x+1/2, \bar{y}, z+1/2$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) $\bar{x}, y, z$ [ $\bar{u}$ ,v,w]
2	a m'..	0,y,z [0,v,w]	$1/2, \bar{y}, z+1/2$ [0,v, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2'mg'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,0,0] p1g1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

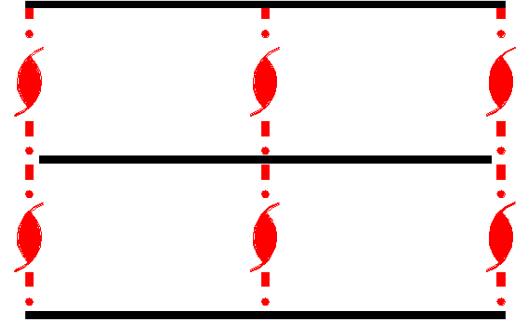
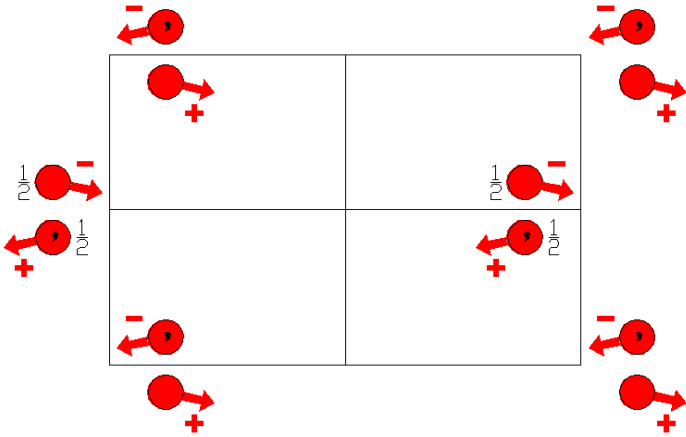
Along [0,1,0] c<sub>p</sub>\*1m'1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pmn'2<sub>1</sub>'  
31.4.215

mm'2'  
Pmn'2<sub>1</sub>'

Orthorhombic



Origin on mn'1

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2' (0,0,1/2) 1/4,0,z  
(2<sub>z</sub>|1/2,0,1/2)'

(3) n' (1/2,0,1/2) x,0,z  
(m<sub>y</sub>|1/2,0,1/2)'

(4) m 0,y,z  
(m<sub>x</sub>|0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

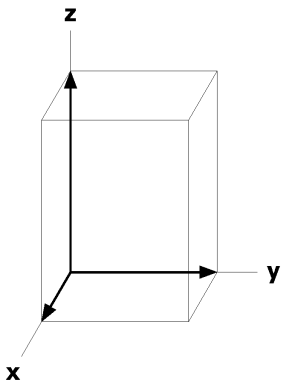
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
4	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [u,v, $\bar{w}$ ]	(3) $x+1/2, \bar{y}, z+1/2$ [u, $\bar{v}$ ,w]	(4) $\bar{x}, y, z$ [u, $\bar{v}, \bar{w}$ ]
2	a m..	0,y,z [u,0,0]	$1/2, \bar{y}, z+1/2$ [u,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2'mg'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

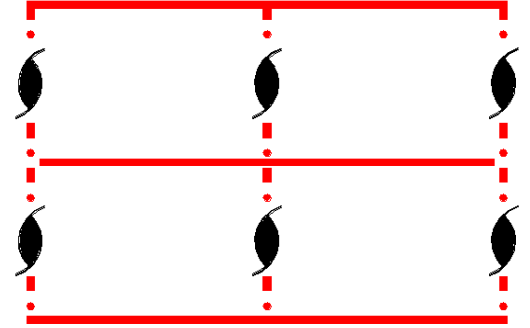
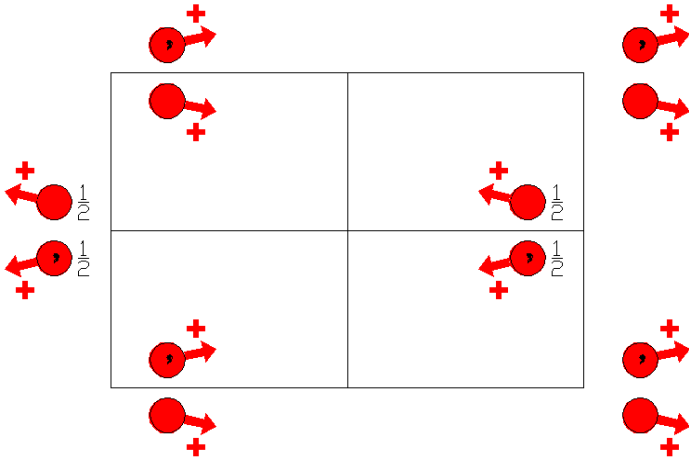
Along [0,1,0] c1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pm'n'2<sub>1</sub>  
31.5.216

m'm'2  
Pm'n'2<sub>1</sub>

Orthorhombic



Origin on m'n'1

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 1/4,0,z  
(2<sub>z</sub>|1/2,0,1/2)

(3) n' (1/2,0,1/2) x,0,z  
(m<sub>y</sub>|1/2,0,1/2)'

(4) m' 0,y,z  
(m<sub>x</sub>|0,0,0)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

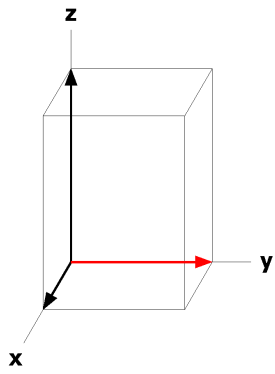
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
4	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $x+1/2, \bar{y}, z+1/2$ [u, $\bar{v}, w$ ]	(4) $\bar{x}, y, z$ [ $\bar{u}, v, w$ ]
2	a m'..	0,y,z [0,v,w]	$1/2, \bar{y}, z+1/2$ [0, $\bar{v}, w$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2m'g'  
 $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,0,0] p1g'1  
 $\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] c1m1  
 $\mathbf{a}^* = -\mathbf{a} \quad \mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



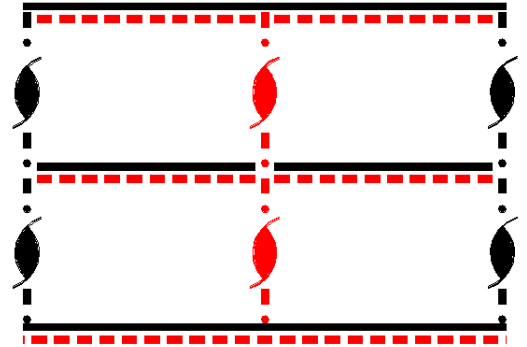
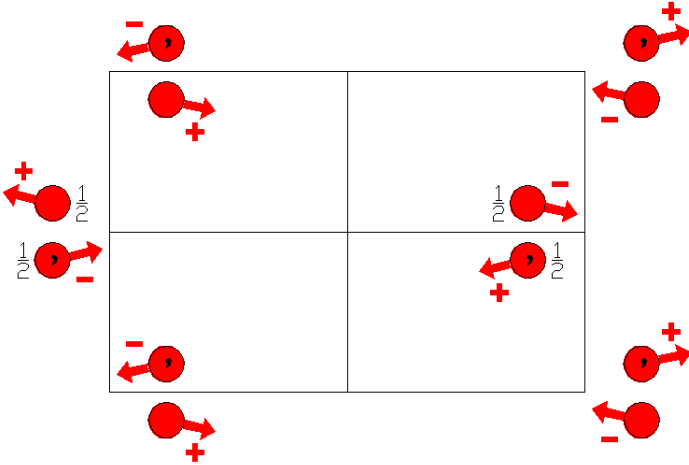
$P_{2b} mn2_1$

31.6.217

$mm21'$

$P_{2b} mn2_1$

Orthorhombic



**Origin** on  $mn1$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $(0,0,1/2) \quad 1/4,0,z$   
( $2_z$ | $1/2,0,1/2$ )

(3) n  $(1/2,0,1/2) \quad x,0,z$   
( $m_y$ | $1/2,0,1/2$ )

(4) m  $0,y,z$   
( $m_x$ | $0,0,0$ )

For  $(0,1,0)'$  + set

(1)  $t' (0,1,0)$   
(1| $0,1,0$ )'

(2)  $2' (0,0,1/2) \quad 1/4,1/2,z$   
( $2_z$ | $1/2,1,1/2$ )'

(3)  $n' (1/2,0,1/2) \quad x,1/2,z$   
( $m_y$ | $1/2,1,1/2$ )'

(4)  $b' (0,1,0) \quad 0,y,z$   
( $m_x$ | $0,1,0$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

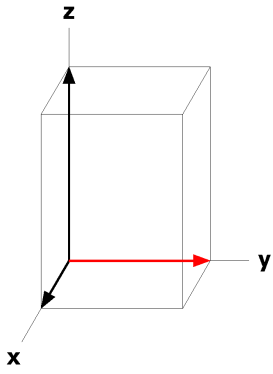
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1,0)' +		
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $x+1/2, \bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $\bar{x}, y, z$ [ $u, \bar{v}, \bar{w}$ ]
4	a m..	0,y,z [u,0,0]	$1/2, \bar{y}, z+1/2$ [ $\bar{u}, 0, 0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2b</sub>-2mg  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] c1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



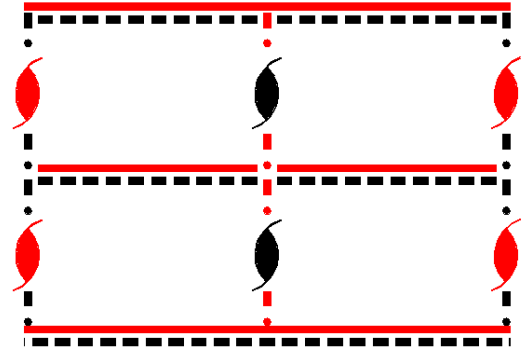
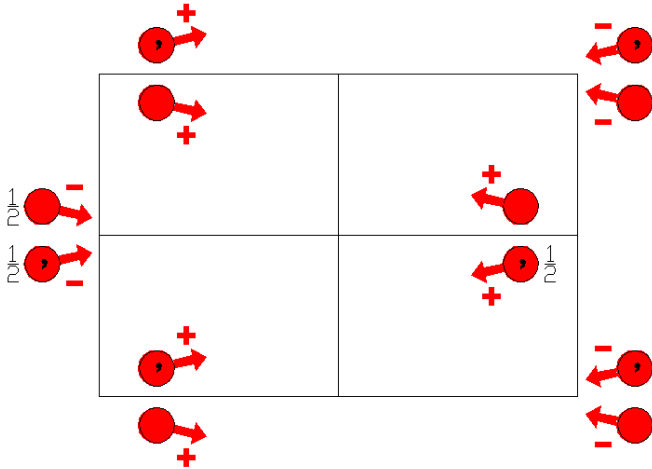
$P_{2b} m'n2_1'$

31.7.218

$mm21'$

$P_{2b} m'n2_1'$

Orthorhombic



Origin on  $m'n1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) $2'$ $(0,0,1/2)$ $1/4,0,z$<br>( $2_z$   $1/2,0,1/2$ )' | (3) $n$ $(1/2,0,1/2)$ $x,0,z$<br>( $m_y$   $1/2,0,1/2$ ) | (4) $m'$ $0,y,z$<br>( $m_x$   $0,0,0$ )' |
|--------------------|--|--|--|

For  $(0,1,0)$ ' + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) $t'$ $(0,1,0)$<br>(1  $0,1,0$ )' | (2) $2$ $(0,0,1/2)$ $1/4,1/2,z$<br>( $2_z$   $1/2,1,1/2$ ) | (3) $n'$ $(1/2,0,1/2)$ $x,1/2,z$<br>( $m_y$   $1/2,1,1/2$ )' | (4) $b$ $(0,1,0)$ $0,y,z$<br>( $m_x$   $0,1,0$ ) |
|--------------------------------------|--|--|--|

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3).

**Positions**

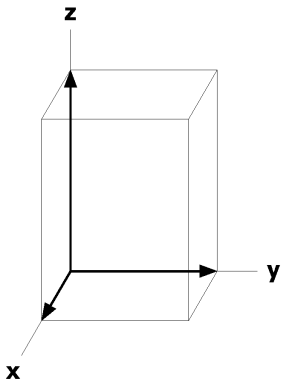
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1,0)' +		
8	b 1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $u,v, \bar{w}$ ]	(3) $x+1/2, \bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $\bar{x}, y, z$ [ $\bar{u}, v, w$ ]
4	a m'..	$0,y,z$ [ $0,v,w$ ]	$1/2, \bar{y}, z+1/2$ [ $0,v, \bar{w}$ ]		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_{2b} 2m' g'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $1/4, 1/2, z$

Along  $[1,0,0]$   $p_{2a} 1g1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 0, 0$

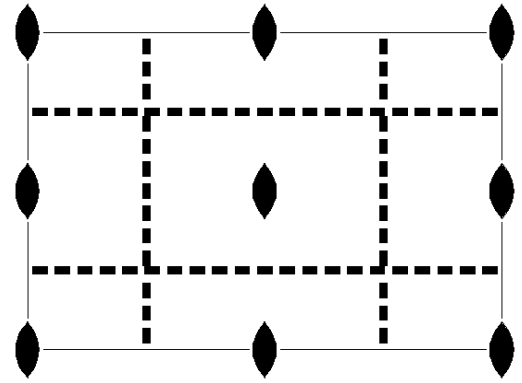
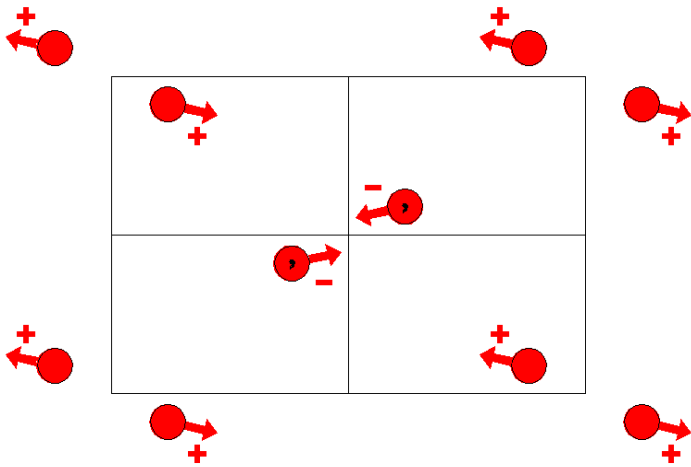
Along  $[0,1,0]$   $c1m11'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $0, y, 0$



Pba2  
32.1.219

mm2  
Pba2

Orthorhombic



Origin on 112

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) a (1/2,0,0) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,0)

(4) b (0,1/2,0) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

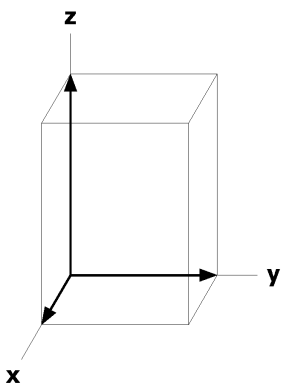
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
4	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $x+1/2, \bar{y}+1/2, z$ [ $\bar{u}, v, \bar{w}$ ]	(4) $\bar{x}+1/2, y+1/2, z$ [ $u, \bar{v}, \bar{w}$ ]
2	b ..2	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]		
2	a ..2	0,0,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a^*}1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

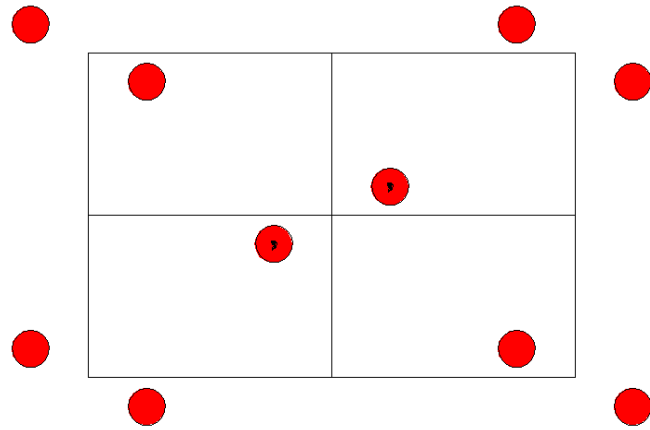
Along [0,1,0]  $p_{2a^*}1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



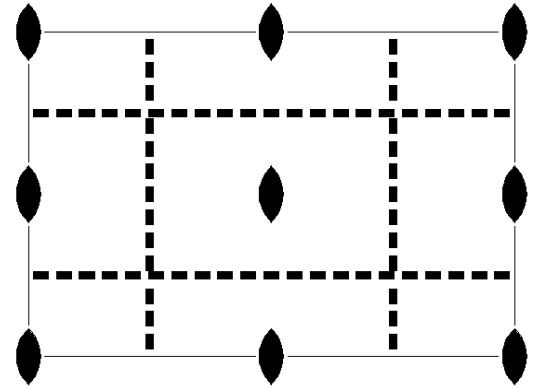
Pba21'  
32.2.220

mm21'  
Pba21'

Orthorhombic



1'



Origin on 1121'

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

For 1 + set

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) a (1/2,0,0) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,0)

(4) b (0,1/2,0) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,0)

For 1' + set

(1) 1'  
(1|0,0,0)'

(2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'

(3) a' (1/2,0,0) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,0)'

(4) b' (0,1/2,0) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,0)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

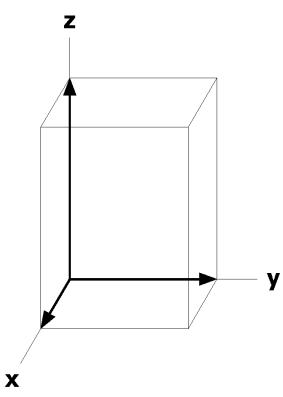
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
4 c 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y}, z$ [0,0,0]	(3) $x+1/2, \bar{y}+1/2, z$ [0,0,0]	(4) $\bar{x}+1/2, y+1/2, z$ [0,0,0]
2 b ..21'	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]		
2 a ..21'	0,0,z [0,0,0]	1/2,1/2,z [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

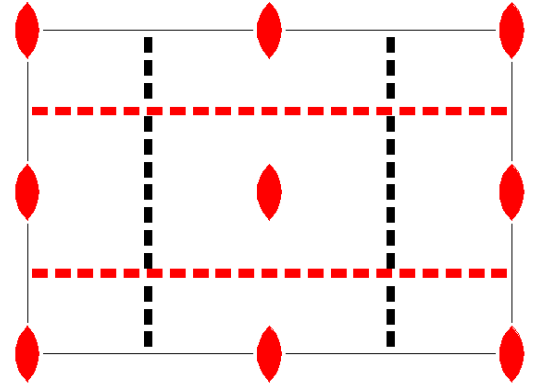
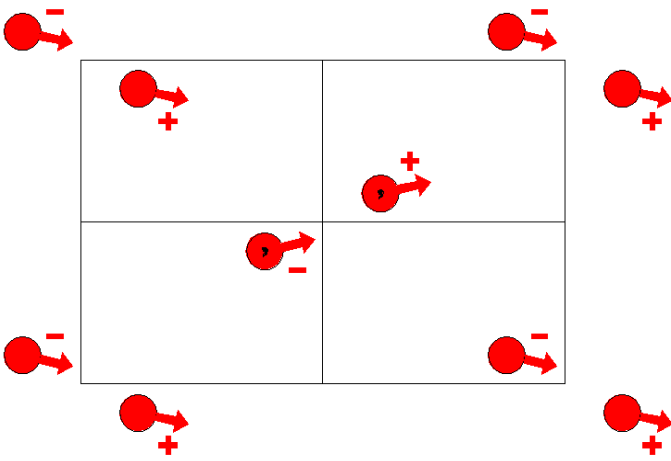
Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pb'a2'  
32.3.221

m'm2'  
Pb'a2'

Orthorhombic



Origin on 112'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'

(3) a (1/2,0,0) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,0)

(4) b' (0,1/2,0) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

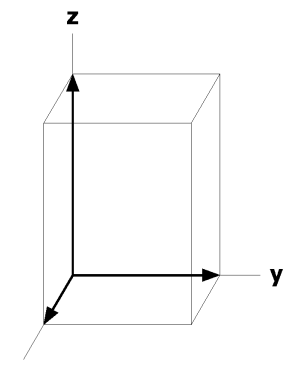
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
4	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3) $x+1/2, \bar{y}+1/2, z$ [ $\bar{u}, v, \bar{w}$ ]	(4) $\bar{x}+1/2, y+1/2, z$ [ $\bar{u}, v, w$ ]
2	b ..2'	0,1/2,z [u,v,0]	1/2,0,z [ $\bar{u}, v, 0$ ]		
2	a ..2'	0,0,z [u,v,0]	1/2,1/2,z [ $\bar{u}, v, 0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2'gg'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

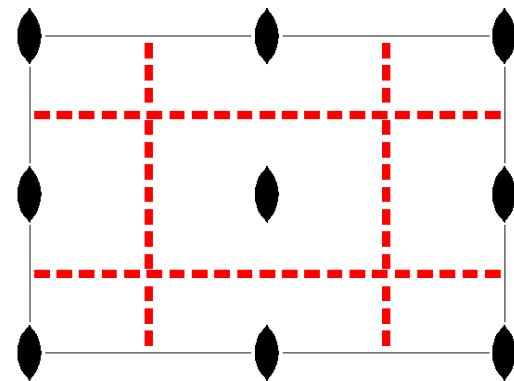
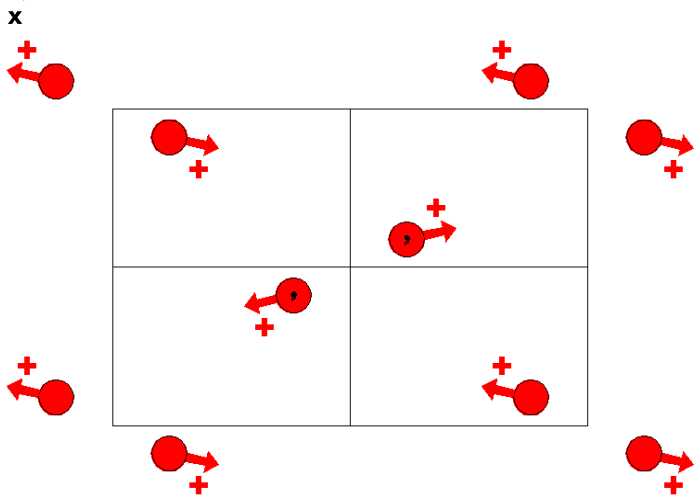
Along [0,1,0] p<sub>2a'</sub>1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pb'a'2  
32.4.222

m'm'2  
Pb'a'2

Orthorhombic



Origin on 112

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) a'  $(1/2,0,0) \ x,1/4,z$   
( $m_y$ | $1/2,1/2,0$ )'

(4) b'  $(0,1/2,0) \ 1/4,y,z$   
( $m_x$ | $1/2,1/2,0$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

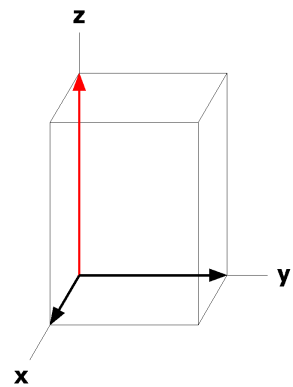
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
4	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $x+1/2, \bar{y}+1/2, z$ [ $u, \bar{v}, w$ ]	(4) $\bar{x}+1/2, y+1/2, z$ [ $\bar{u}, v, w$ ]
2	b ..2	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]		
2	a ..2	0,0,z [0,0,w]	1/2,1/2,z [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p2g'g'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>'1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



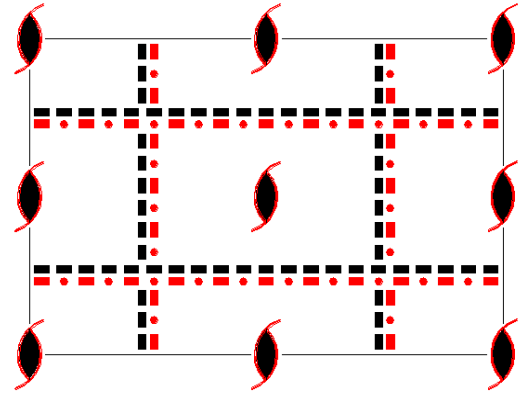
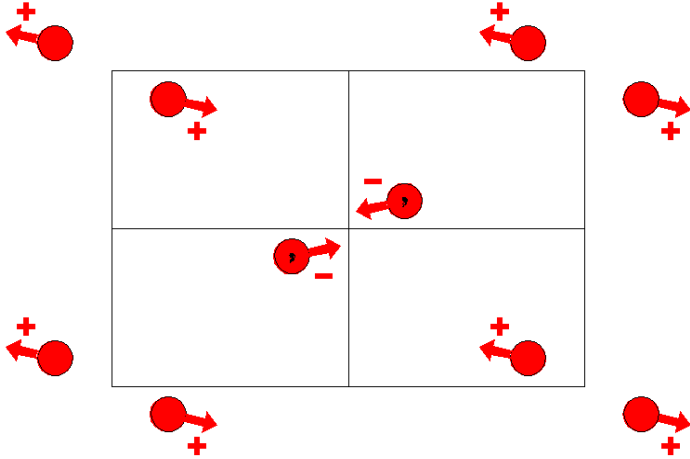
$P_{2c}, ba2$

32.5.223

$mm21'$

$P_{2c}, ba2$

Orthorhombic



Origin on 112

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) a ( $1/2,0,0$ )  $x,1/4,z$   
( $m_y$ | $1/2,1/2,0$ )

(4) b ( $0,1/2,0$ )  $1/4,y,z$   
( $m_x$ | $1/2,1/2,0$ )

For (0,0,1)' + set

(1) t' ( $0,0,1$ )  
(1| $0,0,1$ )'

(2) 2' ( $0,0,1$ )  $0,0,z$   
( $2_z$ | $0,0,1$ )'

(3) n' ( $1/2,0,1$ )  $x,1/4,z$   
( $m_y$ | $1/2,1/2,1$ )'

(4) n' ( $0,1/2,1$ )  $1/4,y,z$   
( $m_x$ | $1/2,1/2,1$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

**Positions**

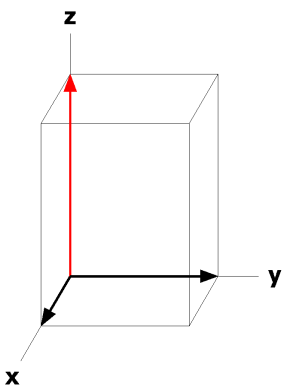
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,0,1)' +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $x+1/2, \bar{y}+1/2, z$ [ $\bar{u}, v, \bar{w}$ ]	(4) $\bar{x}+1/2, y+1/2, z$ [ $u, \bar{v}, \bar{w}$ ]
4	b ..2	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]		
4	a ..2	0,0,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>c</sub>.1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0] p<sub>c</sub>.1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



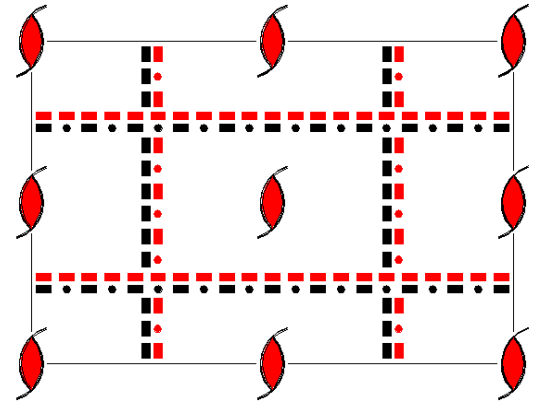
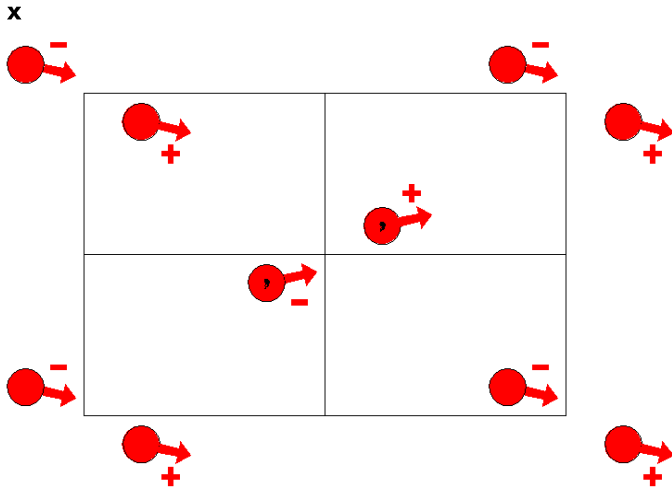
$P_{2c}, b'a2'$

32.6.224

$mm21'$

$P_{2c}, b'a2'$

Orthorhombic



Origin on  $112'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                      |  |  |
|--------------------|--------------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) $2'$ $0,0,z$<br>( $2_z$  0,0,0)' | (3) a ( $1/2,0,0$ ) $x,1/4,z$<br>( $m_y$   $1/2,1/2,0$ ) | (4) b' ( $0,1/2,0$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |
|--------------------|--------------------------------------|--|--|

For  $(0,0,1)'$  + set

- |                                  |  |  |  |
|----------------------------------|--|--|--|
| (1) t' ( $0,0,1$ )<br>(1 0,0,1)' | (2) 2 ( $0,0,1$ ) $0,0,z$<br>( $2_z$  0,0,1) | (3) n' ( $1/2,0,1$ ) $x,1/4,z$<br>( $m_y$   $1/2,1/2,1$ )' | (4) n ( $0,1/2,1$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,1$ ) |
|----------------------------------|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

**Positions**

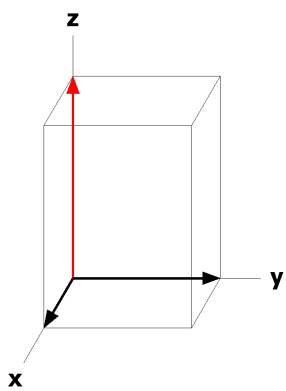
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,0,1)' +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3) $x+1/2, \bar{y}+1/2, z$ [ $\bar{u}, v, \bar{w}$ ]	(4) $\bar{x}+1/2, y+1/2, z$ [ $\bar{u}, v, w$ ]
4	b ..2'	0,1/2,z [u,v,0]	1/2,0,z [ $\bar{u}, v, 0$ ]		
4	a ..2'	0,0,z [u,v,0]	1/2,1/2,z [ $\bar{u}, v, 0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>.1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>c</sub>.1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



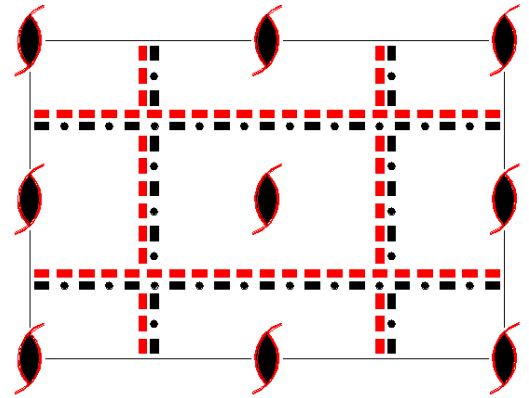
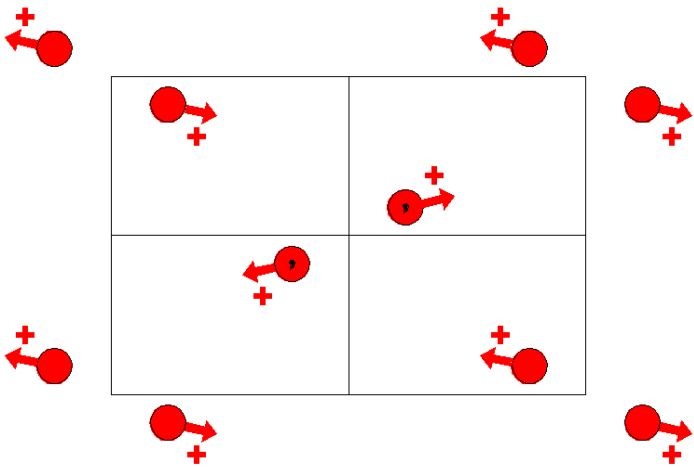
$P_{2c}, b'a'2$

32.7.225

$mm21'$

$P_{2c}, b'a'2$

Orthorhombic



Origin on 112

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) a'  $(1/2,0,0) \ x,1/4,z$   
( $m_y$ | $1/2,1/2,0$ )'

(4) b'  $(0,1/2,0) \ 1/4,y,z$   
( $m_x$ | $1/2,1/2,0$ )'

For (0,0,1)' + set

(1) t'  $(0,0,1)$   
(1|0,0,1)'

(2) 2'  $(0,0,1) \ 0,0,z$   
( $2_z$ |0,0,1)'

(3) n  $(1/2,0,1) \ x,1/4,z$   
( $m_y$ | $1/2,1/2,1$ )

(4) n  $(0,1/2,1) \ 1/4,y,z$   
( $m_x$ | $1/2,1/2,1$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

**Positions**

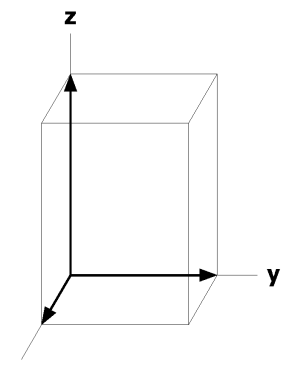
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,0,1)' +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $x+1/2, \bar{y}+1/2, z$ [ $u, \bar{v}, w$ ]	(4) $\bar{x}+1/2, y+1/2, z$ [ $\bar{u}, v, w$ ]
4	b ..2	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]		
4	a ..2	0,0,z [0,0,w]	1/2,1/2,z [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>'1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2b</sub>'1m'1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0

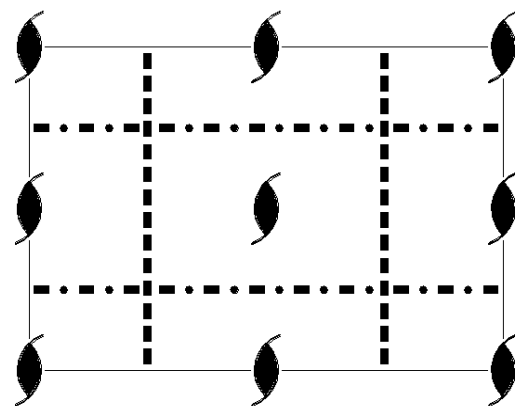
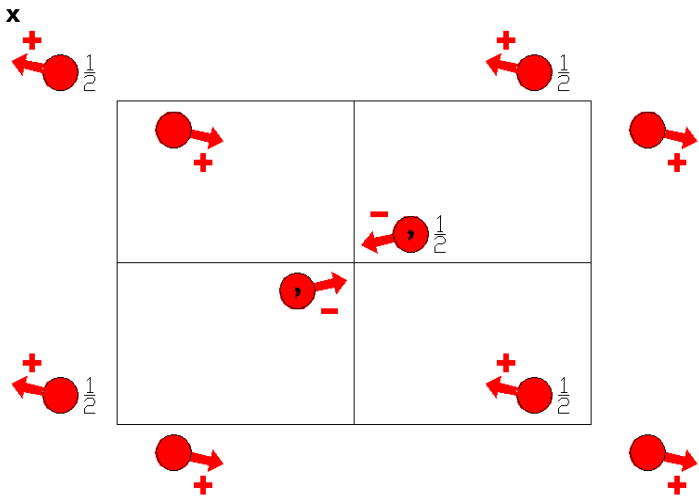


Pna2<sub>1</sub>  
33.1.226

mm2

Orthorhombic

Pna2<sub>1</sub>



Origin on 112<sub>1</sub>

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)

(3) a (1/2,0,0) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,0)

(4) n (0,1/2,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

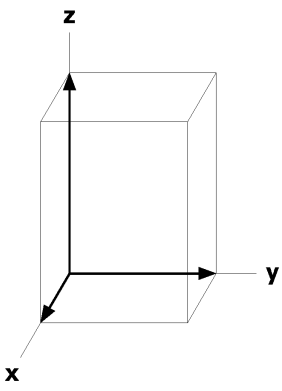
4 a 1 (1) x,y,z [u,v,w] (2)  $\bar{x}, \bar{y}, z+1/2$  [ $\bar{u}, \bar{v}, w$ ] (3)  $x+1/2, \bar{y}+1/2, z$  [ $\bar{u}, v, \bar{w}$ ] (4)  $\bar{x}+1/2, y+1/2, z+1/2$  [ $u, \bar{v}, \bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p2gg  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 1m1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x, 1/4, 0$

Along [0,1,0]  $p_{2a} \cdot 1g1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $1/4, y, 0$

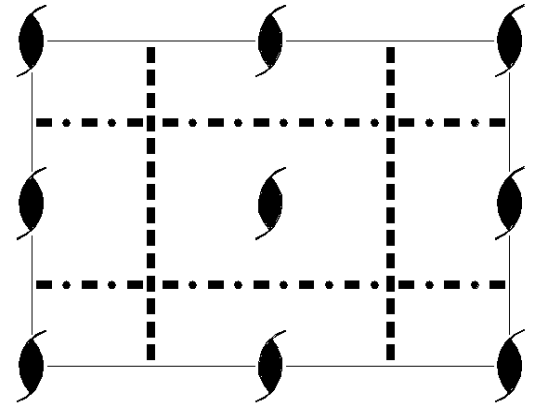
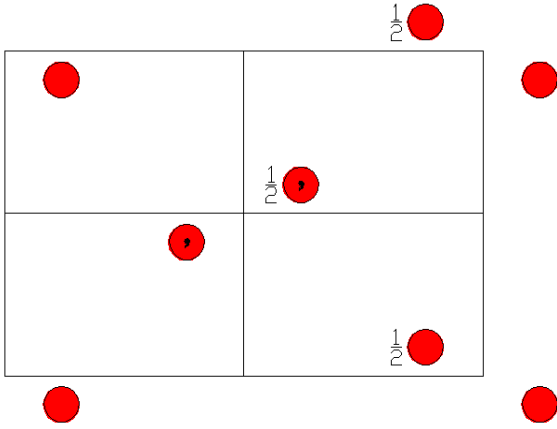


Pna2<sub>1</sub>'  
33.2.227

mm21'  
Pna2<sub>1</sub>'

Orthorhombic

1'



Origin on 112<sub>1</sub>'

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For 1 + set

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)

(3) a (1/2,0,0) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,0)

(4) n (0,1/2,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,1/2)

For 1' + set

(1) 1'  
(1|0,0,0)'

(2) 2' (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)'

(3) a' (1/2,0,0) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,0)'

(4) n' (0,1/2,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

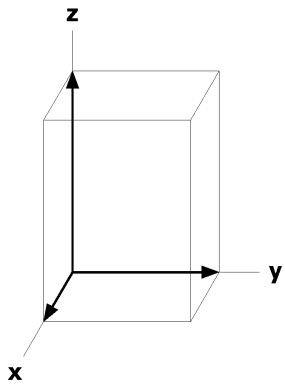
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1+	1'+	
4 a 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y}, z+1/2$ [0,0,0]	(3) $x+1/2, \bar{y}+1/2, z$ [0,0,0]	(4) $\bar{x}+1/2, y+1/2, z+1/2$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0] p1g11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



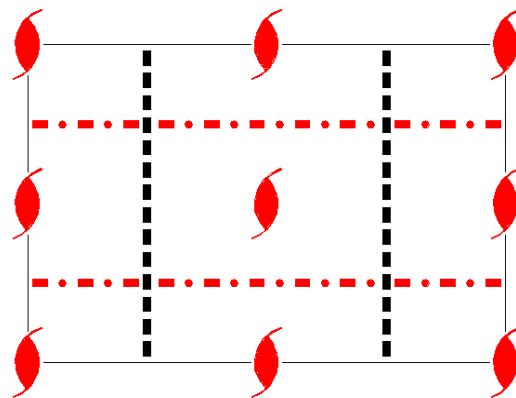
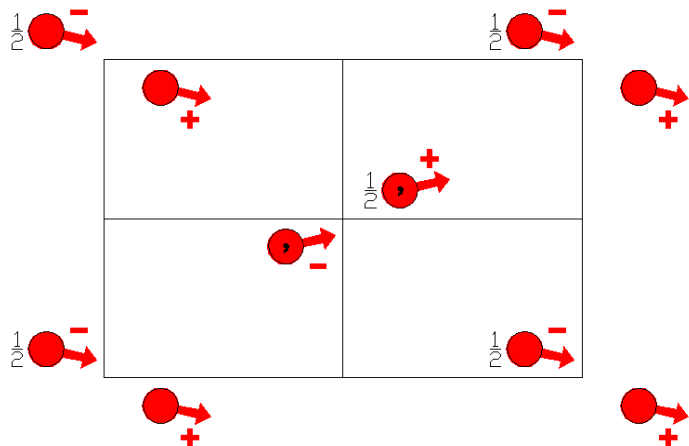
Pn'a2<sub>1</sub>'

33.3.228

m'm2'

Pn'a2<sub>1</sub>'

Orthorhombic



Origin on 112<sub>1</sub>'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2' (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)'

(3) a (1/2,0,0) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,0)

(4) n' (0,1/2,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,1/2)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

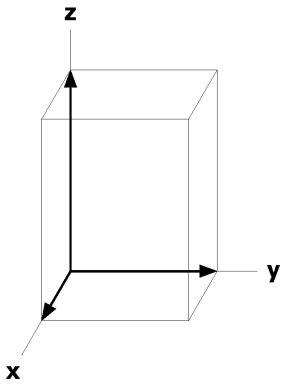
4 a 1 (1) x,y,z [u,v,w] (2)  $\bar{x}, \bar{y}, z+1/2$  [u,v, $\bar{w}$ ] (3)  $x+1/2, \bar{y}+1/2, z$  [ $\bar{u}, v, \bar{w}$ ] (4)  $\bar{x}+1/2, y+1/2, z+1/2$  [ $\bar{u}, v, w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p2'gg'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
Origin at 0,0,z

Along [1,0,0] c1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,1/4,0

Along [0,1,0] p<sub>2a</sub>'1g1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at 0,y,0



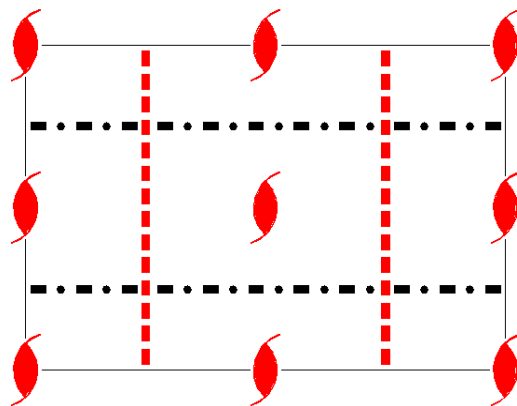
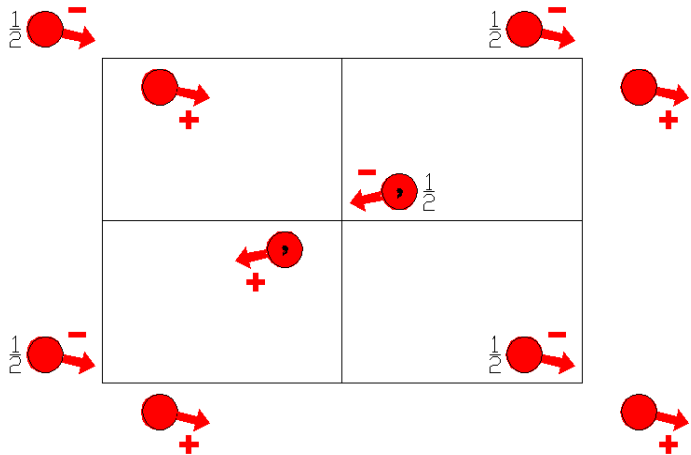
Pna'2<sub>1</sub>'

33.4.229

mm'2'

Pna'2<sub>1</sub>'

Orthorhombic



Origin on 112<sub>1</sub>'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2' (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)'

(3) a' (1/2,0,0) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,0)'

(4) n (0,1/2,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

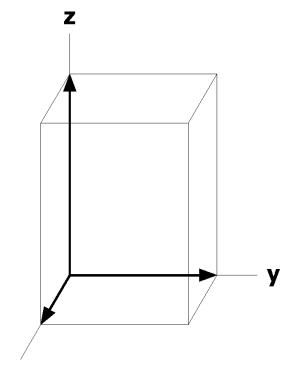
4 a 1 (1) x,y,z [u,v,w] (2)  $\bar{x}, \bar{y}, z+1/2$  [u,v, $\bar{w}$ ] (3)  $x+1/2, \bar{y}+1/2, z$  [u,  $\bar{v}$ , w] (4)  $\bar{x}+1/2, y+1/2, z+1/2$  [u,  $\bar{v}, \bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p2'gg'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] c<sub>p</sub>.1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,1/4,0

Along [0,1,0] p1g1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at 0,y,0



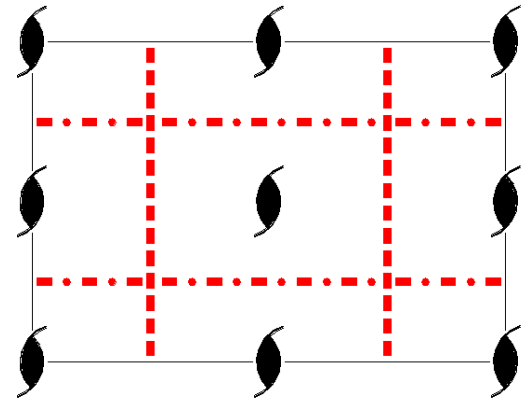
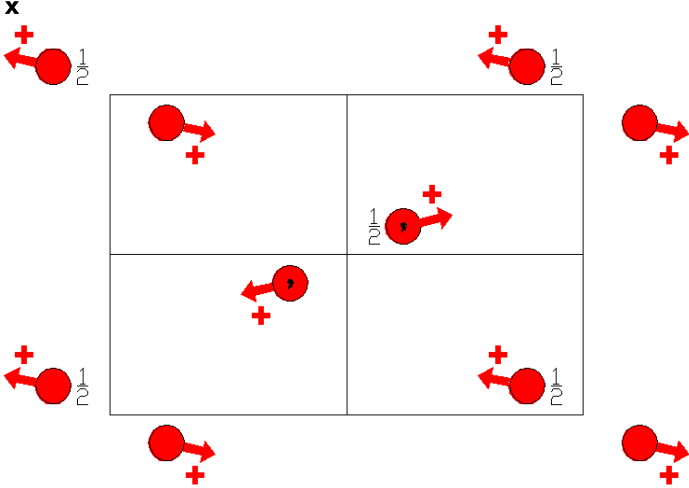
Pn'a'2<sub>1</sub>

33.5.230

m'm'2

Pn'a'2<sub>1</sub>

Orthorhombic



Origin on 112<sub>1</sub>

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)

(3) a' (1/2,0,0) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,0)'

(4) n' (0,1/2,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

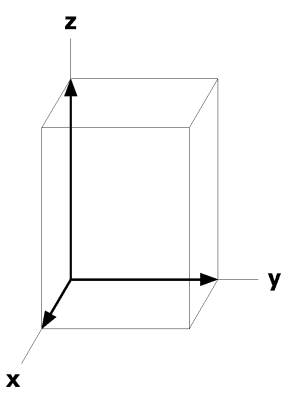
4 a 1 (1) x,y,z [u,v,w] (2)  $\bar{x}, \bar{y}, z+1/2$  [ $\bar{u}, \bar{v}, w$ ] (3)  $x+1/2, \bar{y}+1/2, z$  [ $u, \bar{v}, w$ ] (4)  $\bar{x}+1/2, y+1/2, z+1/2$  [ $\bar{u}, v, w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p2g'g'  
 $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] c1m'1  
 $\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}$   
Origin at x,1/4,0

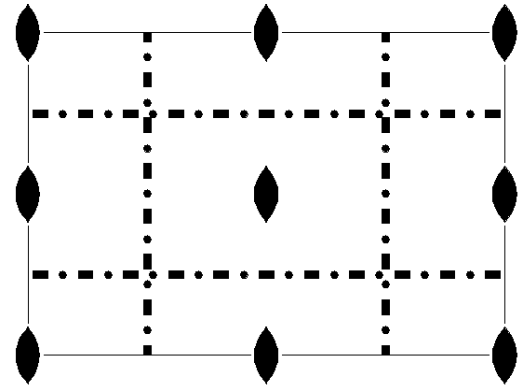
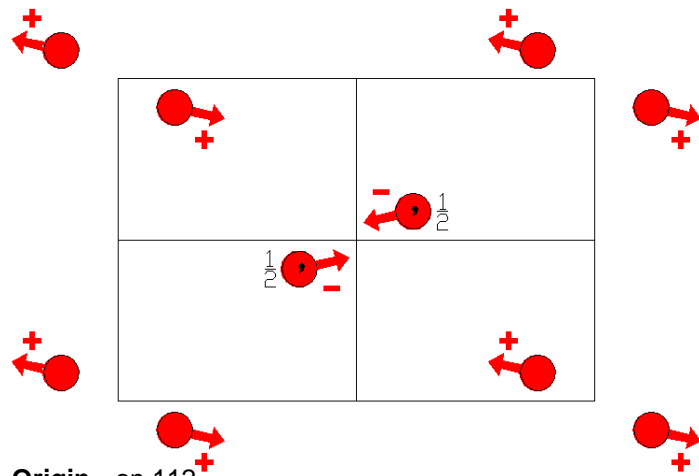
Along [0,1,0] p1g'1  
 $\mathbf{a}^* = -\mathbf{a}/2 \quad \mathbf{b}^* = \mathbf{c}$   
Origin at 0,y,0



Pnn2  
34.1.231

mm2  
Pnn2

Orthorhombic



Origin on 112

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) n ( $1/2,0,1/2$ )  $x,1/4,z$   
( $m_y$ | $1/2,1/2,1/2$ )

(4) n ( $0,1/2,1/2$ )  $1/4,y,z$   
( $m_x$ | $1/2,1/2,1/2$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

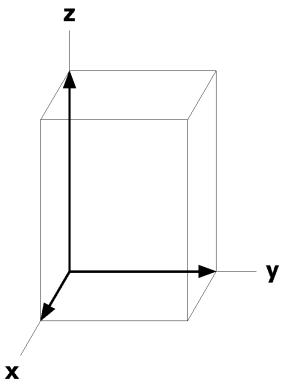
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
4	c	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x}+1/2,y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
2	b	..2	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]		
2	a	..2	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $c_p \cdot 1m'1$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0

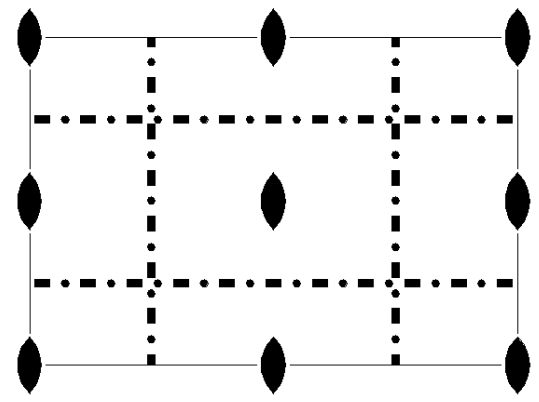
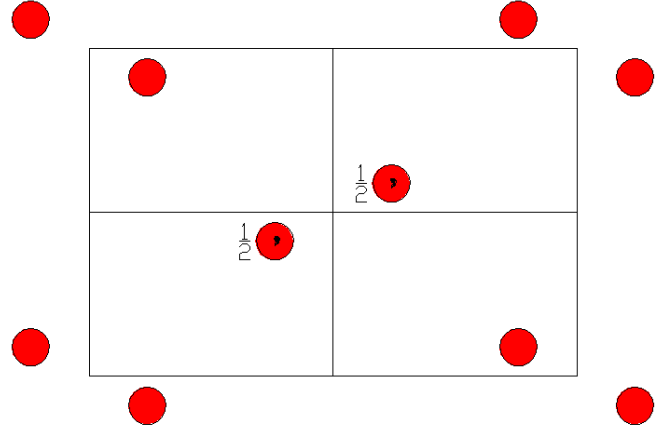


Pnn21'  
34.2.232

mm21'  
Pnn21'

Orthorhombic

1'



Origin on 1121'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

Symmetry Operations

- |                      |  |  |  |
|----------------------|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)   | (4) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)   |
| For 1 + set          |  |  |  |
| (1) 1'<br>(1 0,0,0)' | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (4) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |
| For 1' + set         |  |  |  |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

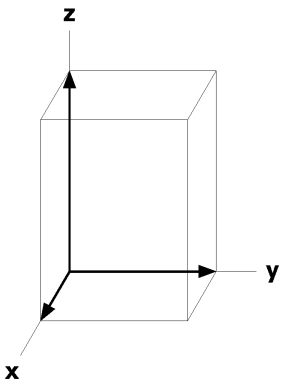
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		1+	1'+		
4	c 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $x+1/2,\bar{y}+1/2,z+1/2$ [0,0,0]	(4) $\bar{x}+1/2,y+1/2,z+1/2$ [0,0,0]
2	b ..21'	0,1/2,z [0,0,0]	1/2,0,z+1/2 [0,0,0]		
2	a ..21'	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

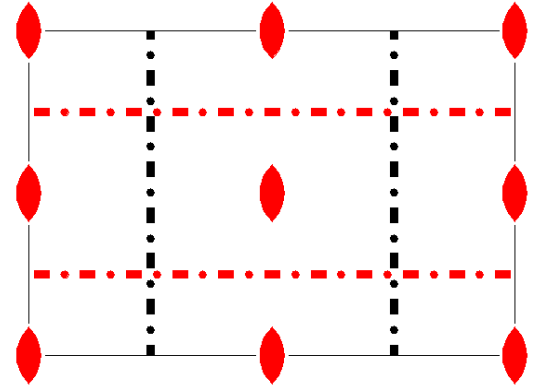
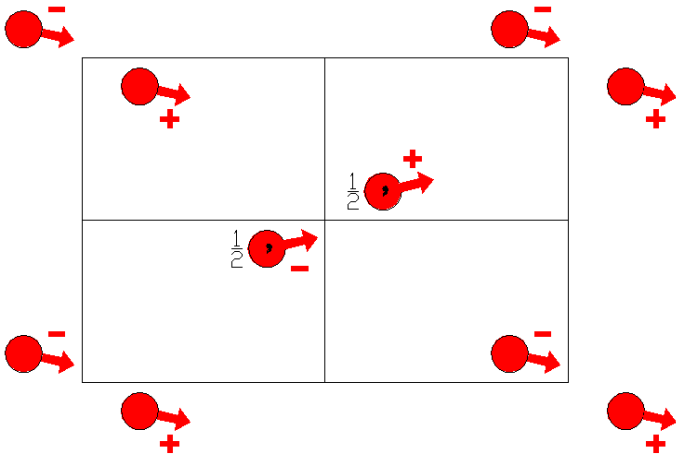
Along [0,1,0] c1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pn'n2'  
34.3.233

m'm2'  
Pn'n2'

Orthorhombic



Origin on 112'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'

(3) n (1/2,0,1/2) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,1/2)

(4) n' (0,1/2,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

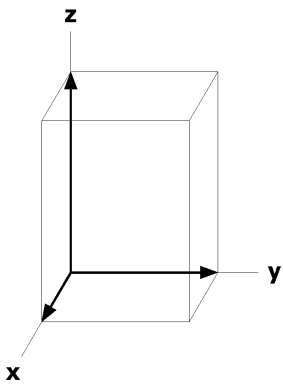
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
4	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]
2	b ..2'	0,1/2,z [u,v,0]	1/2,0,z+1/2 [ $\bar{u},v,0$ ]		
2	a ..2'	0,0,z [u,v,0]	1/2,1/2,z+1/2 [ $\bar{u},v,0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2'gg'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] c1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

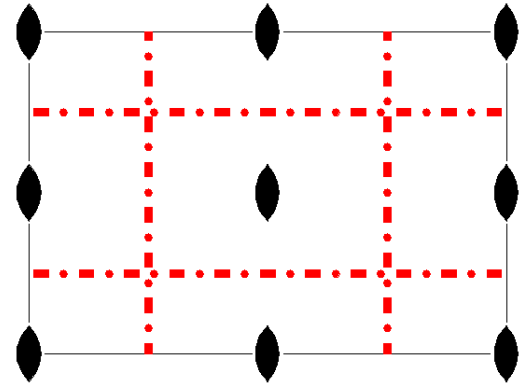
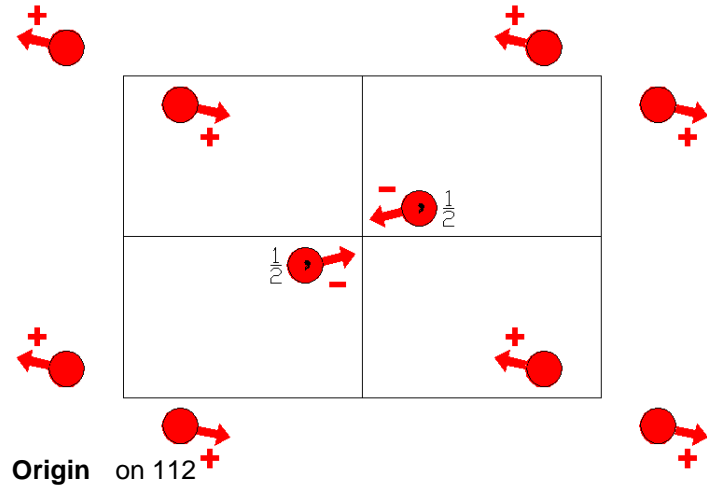
Along [0,1,0]  $c_p$ .1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pn'n'2  
34.4.234

m'm'2  
Pn'n'2

Orthorhombic



**Origin** on 112  
**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

- (1) 1  
(1|0,0,0)
- (2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)
- (3) n' (1/2,0,1/2) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,1/2)'
- (4) n' (0,1/2,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

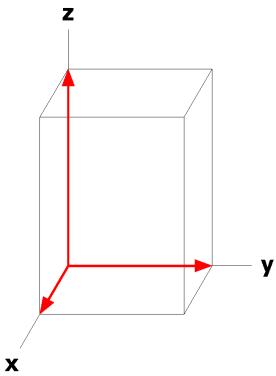
		Coordinates			
		Multiplicity, Wyckoff letter, Site Symmetry.			
4	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(4) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]
2	b ..2	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0,w]		
2	a ..2	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p2g'g'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $c1m'1$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



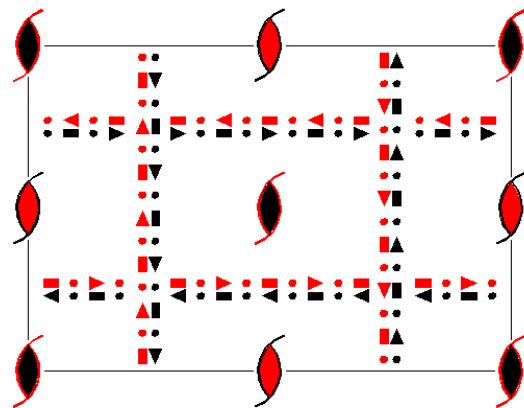
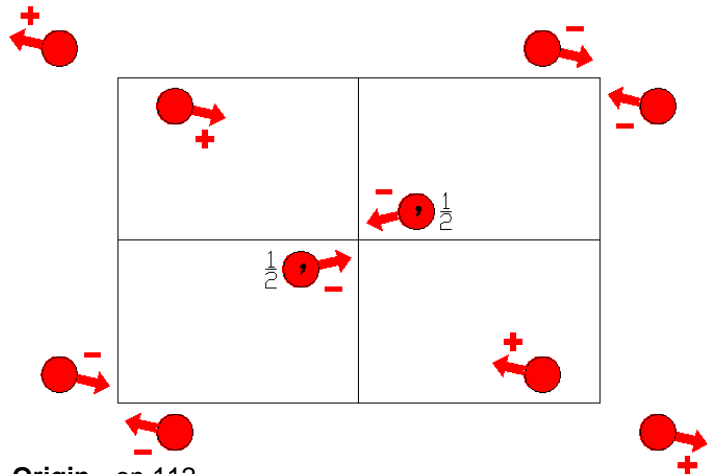
$P_F nn2$

34.5.235

$mm21'$

$P_F nn2$

Orthorhombic



Origin on 112

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |                    |                                  |  |  |
|--------------------|----------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) d ( $1/2,0,1/2$ ) $x,1/4,z$<br>( $m_y$   $1/2,1/2,1/2$ ) | (4) d ( $0,1/2,1/2$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,1/2$ ) |
|--------------------|----------------------------------|--|--|

For (1,0,0)' + set

- |                              |                                      |  |  |
|------------------------------|--------------------------------------|--|--|
| (1) t' (1,0,0)<br>(1 1,0,0)' | (2) 2' $1/2,0,z$<br>( $2_z$  1,0,0)' | (3) d' ( $3/2,0,1/2$ ) $x,1/4,z$<br>( $m_y$   $3/2,1/2,1/2$ )' | (4) d' ( $0,1/2,1/2$ ) $3/4,y,z$<br>( $m_x$   $3/2,1/2,1/2$ )' |
|------------------------------|--------------------------------------|--|--|

**Generators selected** (1);  $t(1,0,0)'$ ;  $t(0,1,0)'$ ;  $t(0,0,1)'$ ; (2); (3).

### Positions

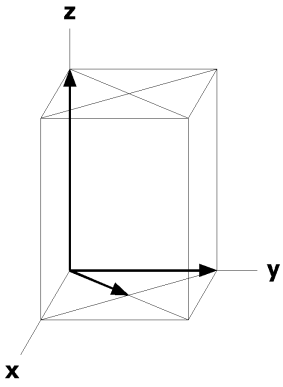
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1,0,0)'		
8	c 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $x+1/2,\bar{y}+1/2,z+1/2 [\bar{u},v,\bar{w}]$	(4) $\bar{x}+1/2,y+1/2,z+1/2 [u,\bar{v},\bar{w}]$
4	b ..2	$0,1/2,z [0,0,w]$	$1/2,0,z+1/2 [0,0,\bar{w}]$		
4	a ..2	$0,0,z [0,0,w]$	$1/2,1/2,z+1/2 [0,0,\bar{w}]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p2gg1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $c1m11'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $0,y,0$



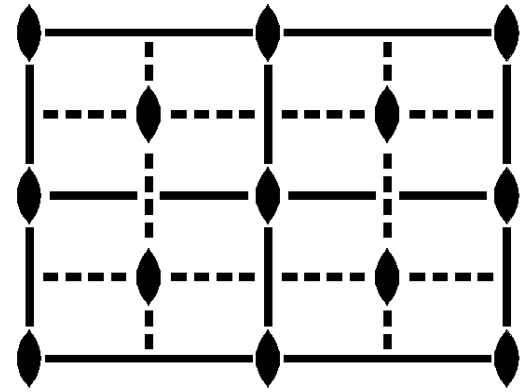
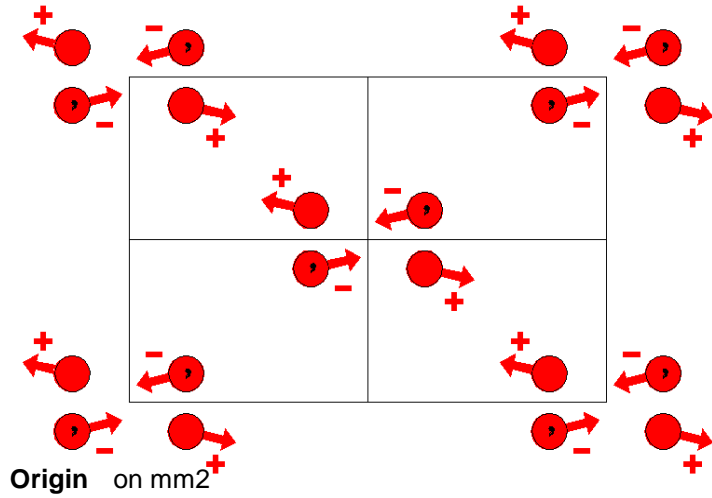
Cmm2

35.1.236

mm2

Cmm2

Orthorhombic



**Asymmetric unit**  $0 \leq x \leq 1/4;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) m x,0,z  
(m<sub>y</sub>|0,0,0)

(4) m 0,y,z  
(m<sub>x</sub>|0,0,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)

(2) 2 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,0)

(3) a (1/2,0,0) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,0)

(4) b (0,1/2,0) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,0)



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

### Positions

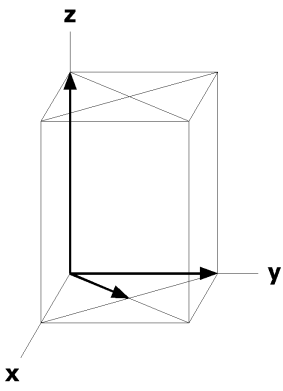
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
8 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
4 e m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]		
4 d .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]		
4 c ..2	1/4,1/4,z [0,0,w]	1/4,3/4,z [0,0, $\bar{w}$ ]		
2 b mm2	0,1/2,z [0,0,0]			
2 a mm2	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Cmm21'

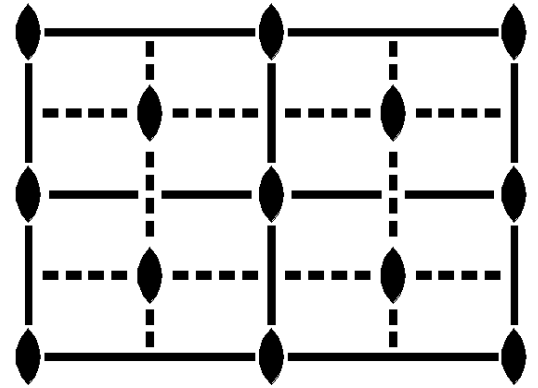
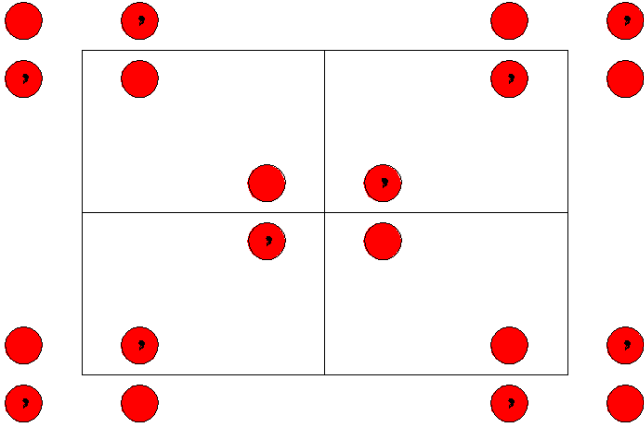
35.2.237

mm21'

Cmm21'

Orthorhombic

1'



Origin on mm21'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) m  $x,0,z$   
( $m_y$ |0,0,0)

(4) m  $0,y,z$   
( $m_x$ |0,0,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)

(2) 2  $1/4,1/4,z$   
( $2_z$ |1/2,1/2,0)

(3) a (1/2,0,0)  $x,1/4,z$   
( $m_y$ |1/2,1/2,0)

(4) b (0,1/2,0)  $1/4,y,z$   
( $m_x$ |1/2,1/2,0)

For (0,0,0)' + set

(1) 1'  
(1|0,0,0)'

(2) 2'  $0,0,z$   
( $2_z$ |0,0,0)'

(3) m'  $x,0,z$   
( $m_y$ |0,0,0)'

(4) m'  $0,y,z$   
( $m_x$ |0,0,0)'

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0)  
(1|1/2,1/2,0)'

(2) 2'  $1/4,1/4,z$   
( $2_z$ |1/2,1/2,0)'

(3) a' (1/2,0,0)  $x,1/4,z$   
( $m_y$ |1/2,1/2,0)'

(4) b' (0,1/2,0)  $1/4,y,z$   
( $m_x$ |1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); 1'.

**Positions**

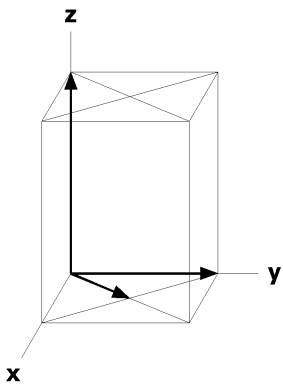
				Coordinates					
Multiplicity, Wyckoff letter, Site Symmetry.				(0,0,0) + (0,0,0)'	(1/2,1/2,0) + (1/2,1/2,0)'				
8	f 11'	(1)	x,y,z [0,0,0]	(2)	$\bar{x},\bar{y},z$ [0,0,0]	(3)	$x,\bar{y},z$ [0,0,0]	(4)	$\bar{x},y,z$ [0,0,0]
4	e m..1'		0,y,z [0,0,0]		$0,\bar{y},z$ [0,0,0]				
4	d .m.1'		x,0,z [0,0,0]		$\bar{x},0,z$ [0,0,0]				
4	c ..21'		1/4,1/4,z [0,0,0]		1/4,3/4,z [0,0,0]				
2	b mm21'		0,1/2,z [0,0,0]						
2	a mm21'		0,0,z [0,0,0]						

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



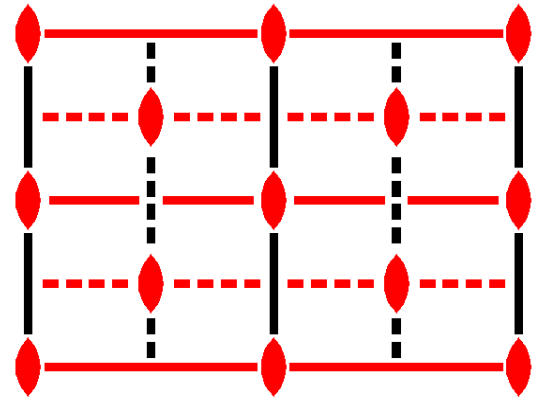
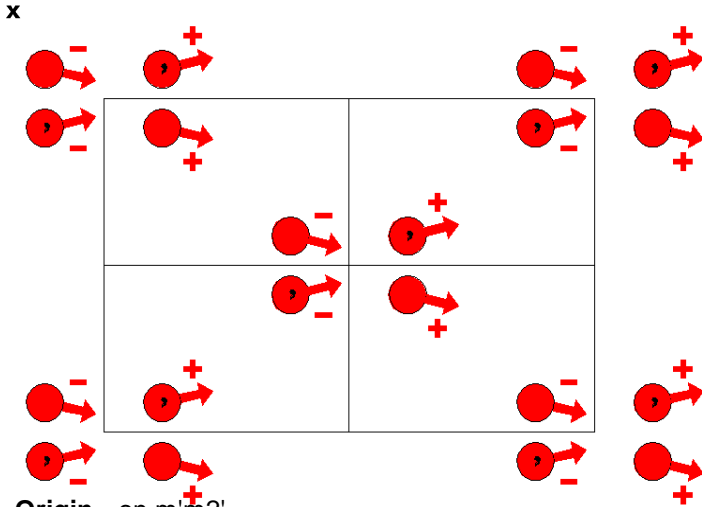
Cm'm2'

35.3.238

m'm2'

Cm'm2'

Orthorhombic



Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'

(3) m x,0,z  
(m<sub>y</sub>|0,0,0)

(4) m' 0,y,z  
(m<sub>x</sub>|0,0,0)'

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)

(2) 2' 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,0)'

(3) a (1/2,0,0) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,0)

(4) b' (0,1/2,0) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

### Positions

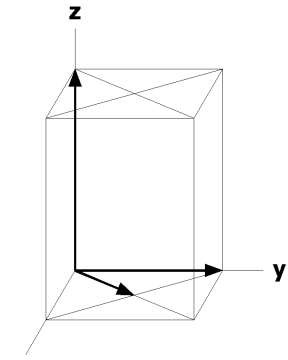
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(1/2,1/2,0) +		
8	f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y},z$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) $\bar{x},y,z$ [ $\bar{u}$ ,v,w]
4	e m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0,v, $\bar{w}$ ]		
4	d .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0,v,0]		
4	c ..2'	1/4,1/4,z [u,v,0]	1/4,3/4,z [ $\bar{u}$ ,v,0]		
2	b m'm2'	0,1/2,z [0,v,0]			
2	a m'm2'	0,0,z [0,v,0]			

### Symmetry of Special Projections

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



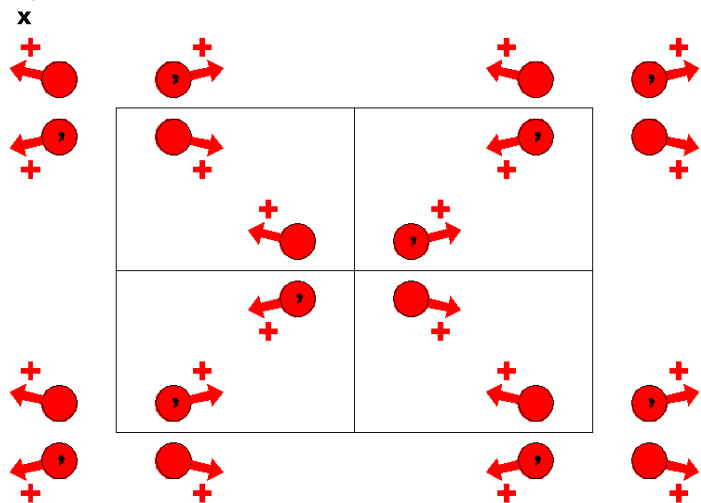
Cm'm'2

35.4.239

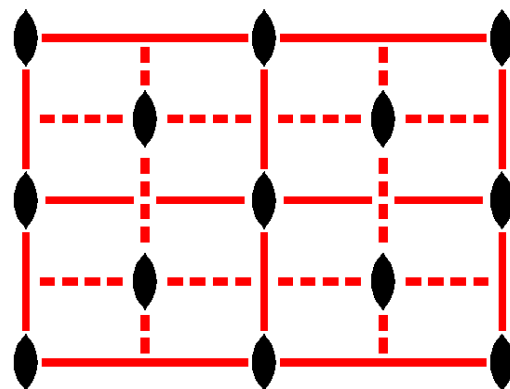
m'm'2

Cm'm'2

Orthorhombic



Origin on m'm'2



Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $m'_y$   $x,0,z$   
( $m_y$ |0,0,0)'

(4)  $m'_x$   $0,y,z$   
( $m_x$ |0,0,0)'

For (1/2,1/2,0) + set

(1)  $t$  (1/2,1/2,0)  
(1|1/2,1/2,0)

(2) 2  $1/4,1/4,z$   
( $2_z$ |1/2,1/2,0)

(3)  $a'_y$  (1/2,0,0)  $x,1/4,z$   
( $m_y$ |1/2,1/2,0)'

(4)  $b'_x$  (0,1/2,0)  $1/4,y,z$   
( $m_x$ |1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

### Positions

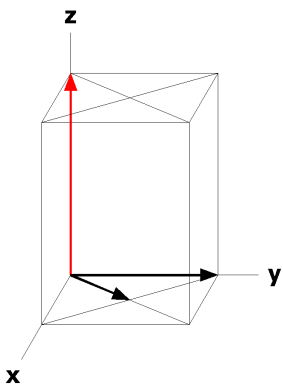
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
8 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
4 e m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]		
4 d .m'.	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]		
4 c ..2	1/4,1/4,z [0,0,w]	1/4,3/4,z [0,0,w]		
2 b m'm'2	0,1/2,z [0,0,w]			
2 a m'm'2	0,0,z [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m'1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



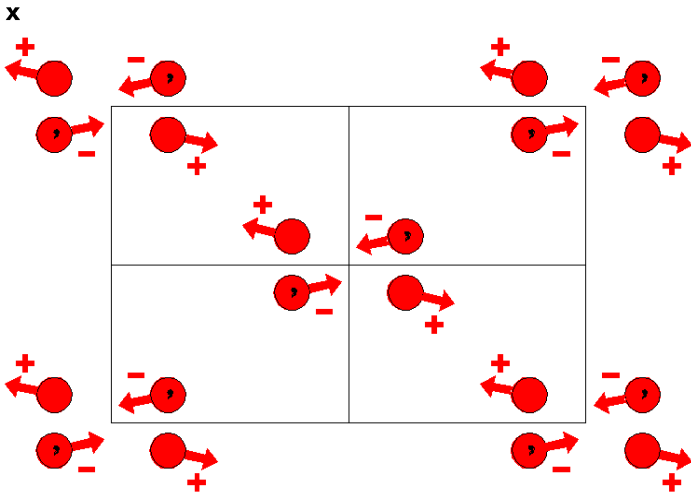
$C_{2c}mm2$

35.5.240

$mm21'$

$C_{2c}mm2$

Orthorhombic



Origin on  $mm2$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (4) m 0,y,z<br>(m <sub>x</sub>  0,0,0) |
|--------------------|--|--|--|

For (1/2,1/2,0) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0) | (3) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (4) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |
|------------------------------------|--|--|--|

For (0,0,1)' + set

- |                              |  |  |  |
|------------------------------|--|--|--|
| (1) t' (0,0,1)<br>(1 0,0,1)' | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)' | (3) c' (0,0,1) x,0,z<br>(m <sub>y</sub>  0,0,1)' | (4) c' (0,0,1) 0,y,z<br>(m <sub>x</sub>  0,0,1)' |
|------------------------------|--|--|--|

For (1/2,1/2,1)' + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t' (1/2,1/2,1)<br>(1 1/2,1/2,1)' | (2) 2' (0,0,1) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1)' | (3) n' (1/2,0,1) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1)' | (4) n' (0,1/2,1) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1)' |
|--------------------------------------|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; t(1/2,1/2,0); (2); (3).

### Positions

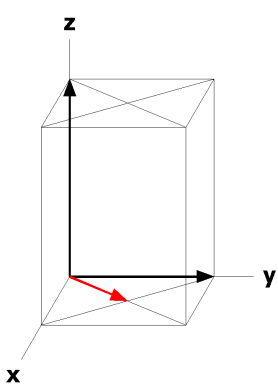
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,1)'	(1/2,1/2,0) + (1/2,1/2,1)'	
16 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 e m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]		
8 d .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]		
8 c ..2	1/4,1/4,z [0,0,w]	1/4,3/4,z [0,0, $\bar{w}$ ]		
4 b mm2	0,1/2,z [0,0,0]			
4 a mm2	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



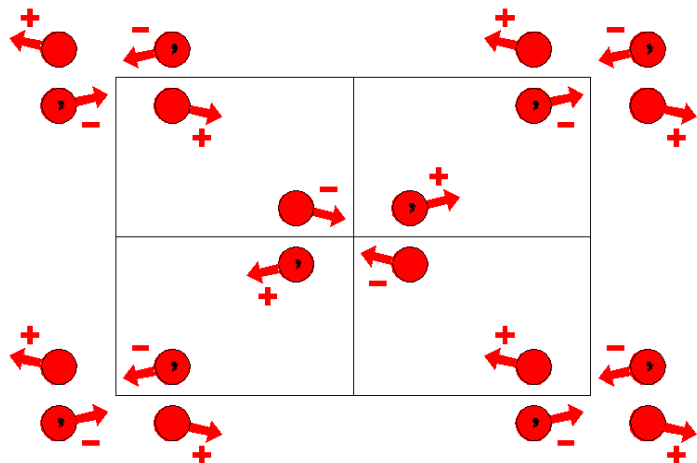
$C_p mm2$

35.6.241

$mm21'$

$C_p mm2$

Orthorhombic



Origin on  $mm2$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) m  $x,0,z$   
( $m_y$ |0,0,0)

(4) m  $0,y,z$   
( $m_x$ |0,0,0)

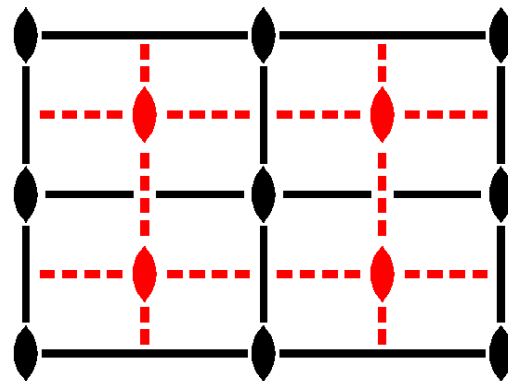
For  $(1/2,1/2,0)'$  + set

(1)  $t' (1/2,1/2,0)$   
(1| $1/2,1/2,0$ )'

(2)  $2' 1/4,1/4,z$   
( $2_z$ | $1/2,1/2,0$ )'

(3)  $a' (1/2,0,0) x,1/4,z$   
( $m_y$ | $1/2,1/2,0$ )'

(4)  $b' (0,1/2,0) 1/4,y,z$   
( $m_x$ | $1/2,1/2,0$ )'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

### Positions

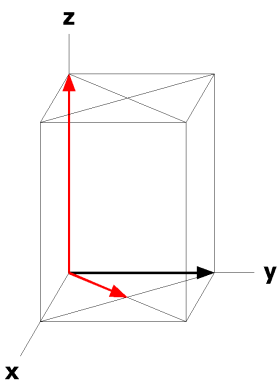
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
8 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
4 e m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]		
4 d .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]		
4 c ..2'	1/4,1/4,z [u,v,0]	1/4,3/4,z [ $\bar{u},v,0$ ]		
2 b mm2	0,1/2,z [0,0,0]			
2 a mm2	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c<sub>p</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



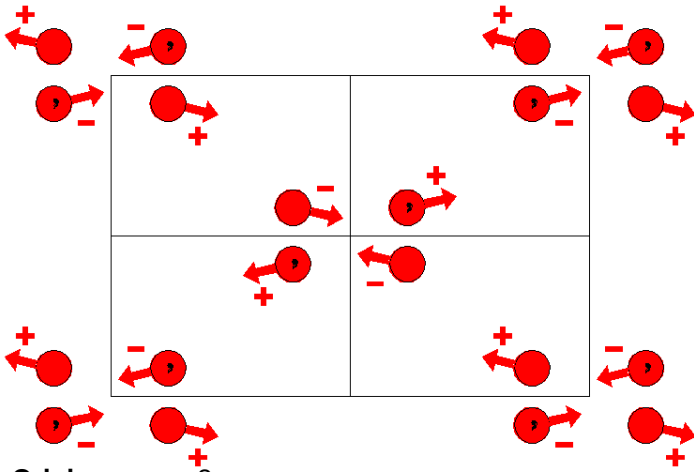
$C_1mm2$

$mm21'$

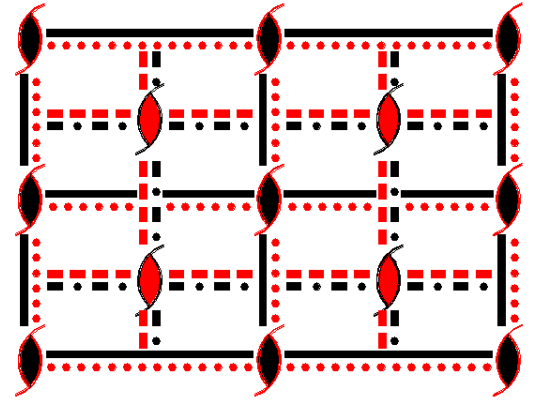
Orthorhombic

35.7.242

$C_1mm2$



Origin on  $mm2$



Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                  |                                  |                                  |
|--------------------|----------------------------------|----------------------------------|----------------------------------|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) m $x,0,z$<br>( $m_y$  0,0,0) | (4) m $0,y,z$<br>( $m_x$  0,0,0) |
|--------------------|----------------------------------|----------------------------------|----------------------------------|

For  $(1/2,1/2,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' $(1/2,1/2,0)$<br>(1  $1/2,1/2,0$ )' | (2) 2' $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,0$ )' | (3) a' $(1/2,0,0) x,1/4,z$<br>( $m_y$   $1/2,1/2,0$ )' | (4) b' $(0,1/2,0) 1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |
|--|--|--|--|

For  $(0,0,1)'$  + set

- |                                |  |  |  |
|--------------------------------|--|--|--|
| (1) t' $(0,0,1)$<br>(1 0,0,1)' | (2) 2' $(0,0,1) 0,0,z$<br>( $2_z$  0,0,1)' | (3) c' $(0,0,1) x,0,z$<br>( $m_y$  0,0,1)' | (4) c' $(0,0,1) 0,y,z$<br>( $m_x$  0,0,1)' |
|--------------------------------|--|--|--|

For  $(1/2,1/2,1)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) t $(1/2,1/2,1)$<br>(1  $1/2,1/2,1$ ) | (2) 2 $(0,0,1) 1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1$ ) | (3) n $(1/2,0,1) x,1/4,z$<br>( $m_y$   $1/2,1/2,1$ ) | (4) n $(0,1/2,1) 1/4,y,z$<br>( $m_x$   $1/2,1/2,1$ ) |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; t(1/2,1/2,0)'; (2); (3).

### Positions

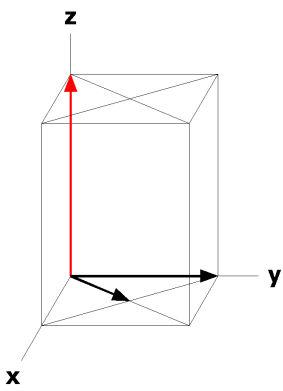
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,1)'	(1/2,1/2,0)' (1/2,1/2,1) +	
16 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 e m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]		
8 d .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]		
8 c ..2'	1/4,1/4,z [u,v,0]	1/4,3/4,z [ $\bar{u},v,0$ ]		
4 b mm2	0,1/2,z [0,0,0]			
4 a mm2	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



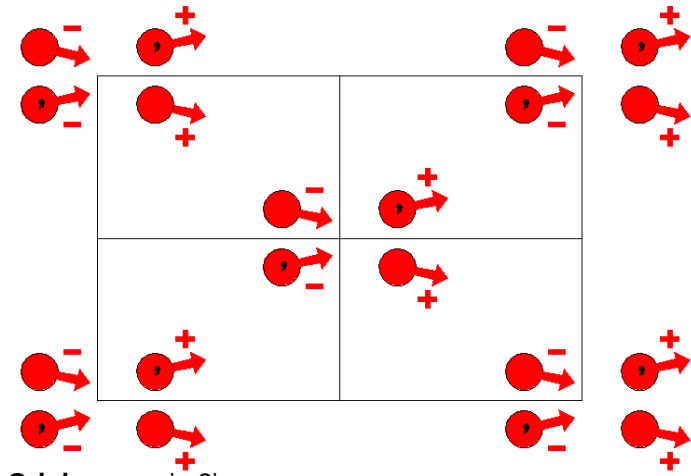
$C_{2c} m'm2'$

35.8.243

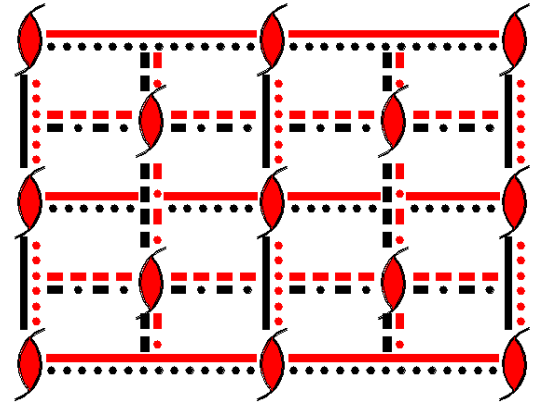
$mm21'$

$C_{2c} m'm2'$

Orthorhombic



Origin on  $m'm2'$



**Asymmetric unit**  $0 \leq x \leq 1/4;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |                    |                                      |                                    |                                       |
|--------------------|--------------------------------------|------------------------------------|---------------------------------------|
| (1) 1<br>(1 0,0,0) | (2) $2'_z$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $m_x$ x,0,z<br>( $m_y$  0,0,0) | (4) $m'_y$ 0,y,z<br>( $m'_x$  0,0,0)' |
|--------------------|--------------------------------------|------------------------------------|---------------------------------------|

For (1/2,1/2,0) + set

- |                                      |  |  |   |
|--------------------------------------|--|--|---|
| (1) $t$ (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) $2'_z$ 1/4,1/4,z<br>( $2_z$  1/2,1/2,0)' | (3) $a$ (1/2,0,0) x,1/4,z<br>( $m_y$  1/2,1/2,0) | (4) $b'_y$ (0,1/2,0) 1/4,y,z<br>( $m'_x$  1/2,1/2,0)' |
|--------------------------------------|--|--|---|

For (0,0,1)' + set

- |                                |  |  |   |
|--------------------------------|--|--|---|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)' | (2) $2$ (0,0,1) 0,0,z<br>( $2_z$  0,0,1) | (3) $c'_x$ (0,0,1) x,0,z<br>( $m_y$  0,0,1)' | (4) $c$ (0,0,1) 0,y,z<br>( $m'_x$  0,0,1) |
|--------------------------------|--|--|---|

For (1/2,1/2,1)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) $t'$ (1/2,1/2,1)<br>(1 1/2,1/2,1)' | (2) $2$ (0,0,1) 1/4,1/4,z<br>( $2_z$  1/2,1/2,1) | (3) $n'_x$ (1/2,0,1) x,1/4,z<br>( $m_y$  1/2,1/2,1)' | (4) $n$ (0,1/2,1) 1/4,y,z<br>( $m'_x$  1/2,1/2,1) |
|--|--|--|---|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; t(1/2,1/2,0); (2); (3).

### Positions

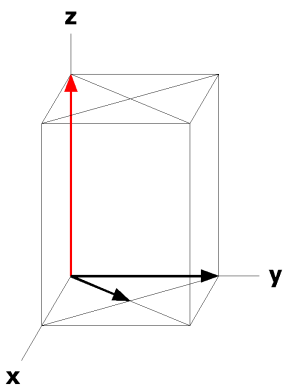
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,1)'	(1/2,1/2,0) + (1/2,1/2,1)'	
16 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y},z$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) $\bar{x},y,z$ [ $\bar{u}$ ,v,w]
8 e m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0,v, $\bar{w}$ ]		
8 d .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0,v,0]		
8 c ..2'	1/4,1/4,z [u,v,0]	1/4,3/4,z [ $\bar{u}$ ,v,0]		
4 b m'm2'	0,1/2,z [0,v,0]			
4 a m'm2'	0,0,z [0,v,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



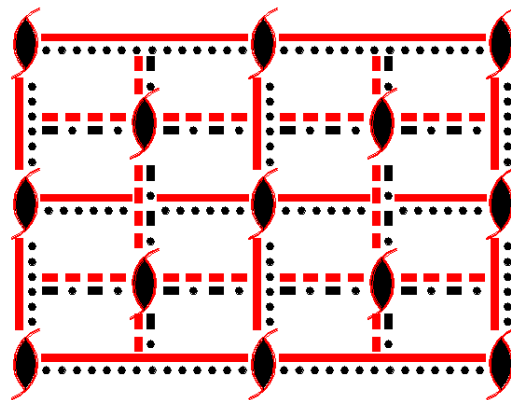
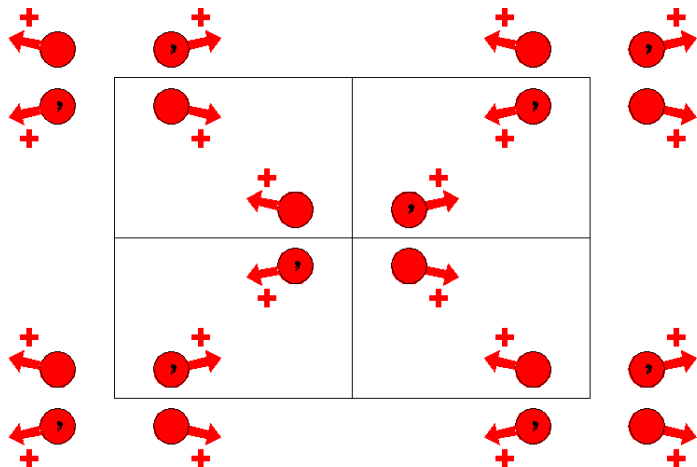
$C_{2c} m'm'2$

$mm21'$

Orthorhombic

35.9.244

$C_{2c} m'm'2$



**Origin** on  $m'm'2$

**Asymmetric unit**  $0 \leq x \leq 1/4;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                  |   |   |
|--------------------|----------------------------------|---|---|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $m'_x$ $x,0,z$<br>( $m'_y$  0,0,0)' | (4) $m'_y$ $0,y,z$<br>( $m'_x$  0,0,0)' |
|--------------------|----------------------------------|---|---|

For  $(1/2,1/2,0)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t$ $(1/2,1/2,0)$<br>(1  $1/2,1/2,0$ ) | (2) 2 $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,0$ ) | (3) $a'_x$ $(1/2,0,0)$ $x,1/4,z$<br>( $m'_y$   $1/2,1/2,0$ )' | (4) $b'_y$ $(0,1/2,0)$ $1/4,y,z$<br>( $m'_x$   $1/2,1/2,0$ )' |
|--|--|---|---|

For  $(0,0,1)$  + set

- |                                  |   |   |   |
|----------------------------------|---|---|---|
| (1) $t'$ $(0,0,1)$<br>(1 0,0,1)' | (2) $2'_z$ $(0,0,1)$ $0,0,z$<br>( $2'_z$  0,0,1)' | (3) $c'_x$ $(0,0,1)$ $x,0,z$<br>( $m'_y$  0,0,1)' | (4) $c'_y$ $(0,0,1)$ $0,y,z$<br>( $m'_x$  0,0,1)' |
|----------------------------------|---|---|---|

For  $(1/2,1/2,1)$  + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t'$ $(1/2,1/2,1)$<br>(1  $1/2,1/2,1$ )' | (2) $2'_z$ $(0,0,1)$ $1/4,1/4,z$<br>( $2'_z$   $1/2,1/2,1$ )' | (3) $n'_x$ $(1/2,0,1)$ $x,1/4,z$<br>( $m'_y$   $1/2,1/2,1$ )' | (4) $n'_y$ $(0,1/2,1)$ $1/4,y,z$<br>( $m'_x$   $1/2,1/2,1$ )' |
|--|---|---|---|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; t(1/2,1/2,0); (2); (3).

### Positions

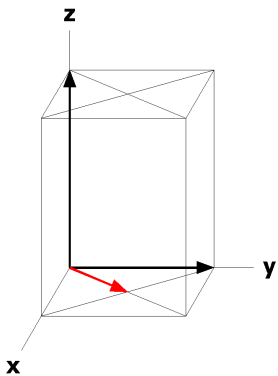
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,1)'	(1/2,1/2,0) + (1/2,1/2,1)'	
16 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 e m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]		
8 d .m'.	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]		
8 c ..2	1/4,1/4,z [0,0,w]	1/4,3/4,z [0,0,w]		
4 b m'm'2	0,1/2,z [0,0,0]			
4 a m'm'2	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>'1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2b</sub>'1m'1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



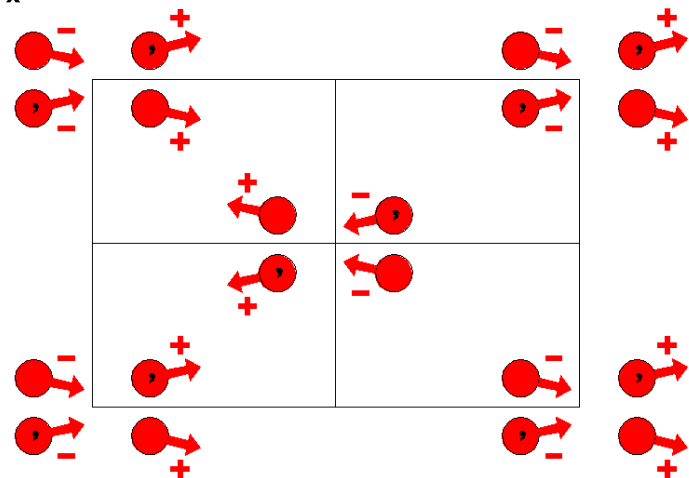
$C_p m' m 2'$

35.10.245

$mm21'$

$C_p m' m 2'$

Orthorhombic



Origin on  $m' m 2'$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2)  $2'$   $0,0,z$   
( $2_z$ |0,0,0)'

(3)  $m$   $x,0,z$   
( $m_y$ |0,0,0)

(4)  $m'$   $0,y,z$   
( $m_x$ |0,0,0)'

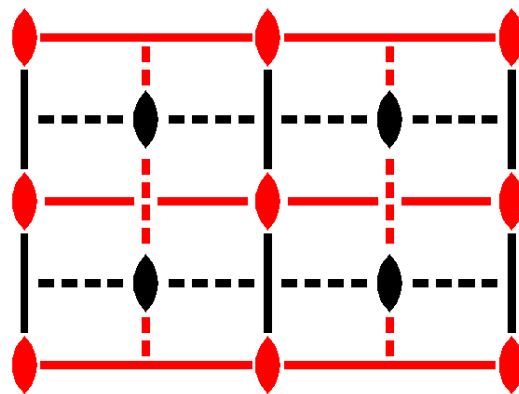
For  $(1/2,1/2,0)'$  + set

(1)  $t'$   $(1/2,1/2,0)$   
(1| $1/2,1/2,0$ )'

(2)  $2$   $1/4,1/4,z$   
( $2_z$ | $1/2,1/2,0$ )

(3)  $a'$   $(1/2,0,0) - x,1/4,z$   
( $m_y$ | $1/2,1/2,0$ )'

(4)  $b$   $(0,1/2,0) - 1/4,y,z$   
( $m_x$ | $1/2,1/2,0$ )



**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,0)'$ ; (2); (3).

### Positions

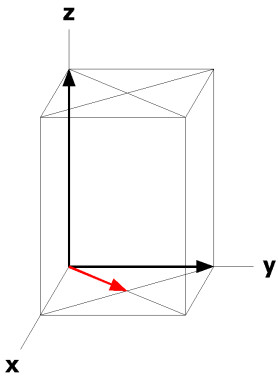
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1/2,1/2,0)' +	
8 f 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [u,v,\bar{w}]$	(3) $x,\bar{y},z [\bar{u},v,\bar{w}]$	(4) $\bar{x},y,z [\bar{u},v,w]$
4 e $m'..$	$0,y,z [0,v,w]$	$0,\bar{y},z [0,v,\bar{w}]$		
4 d $.m.$	$x,0,z [0,v,0]$	$\bar{x},0,z [0,v,0]$		
4 c $..2$	$1/4,1/4,z [0,0,w]$	$1/4,3/4,z [0,0,\bar{w}]$		
2 b $m' m 2'$	$0,1/2,z [0,v,0]$			
2 a $m' m 2'$	$0,0,z [0,v,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $c_p-2'mm'$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a}1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

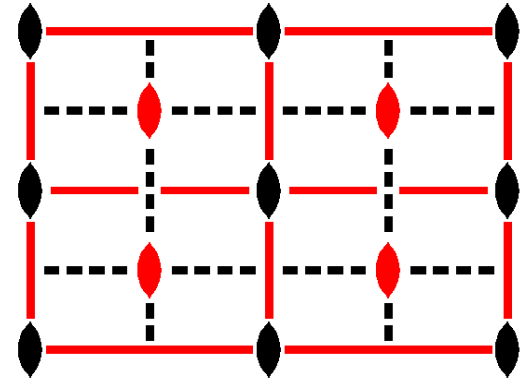
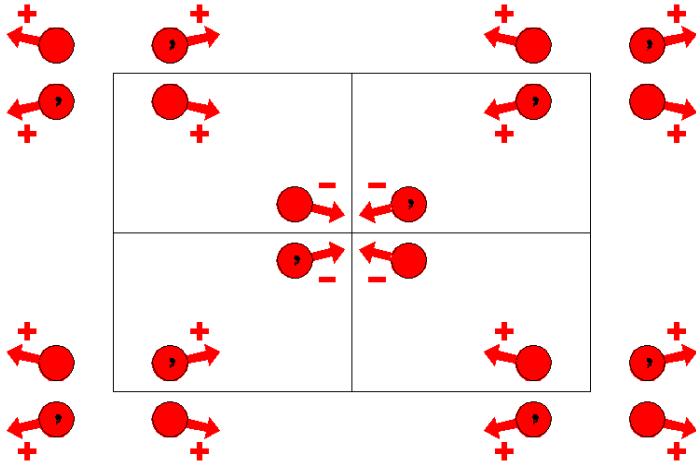
Along  $[0,1,0]$   $p1m11'$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $0,y,0$



$C_p m' m' 2$   
35.11.246

$mm21'$   
 $C_p m' m' 2$

Orthorhombic



**Origin** on  $m' m' 2$

**Asymmetric unit**  $0 \leq x \leq 1/4;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $m'$   $x,0,z$   
( $m_y$ |0,0,0)'

(4)  $m'$   $0,y,z$   
( $m_x$ |0,0,0)'

For  $(1/2,1/2,0)'$  + set

(1)  $t'$   $(1/2,1/2,0)$   
(1| $1/2,1/2,0$ )'

(2)  $2'$   $1/4,1/4,z$   
( $2_z$ | $1/2,1/2,0$ )'

(3) a  $(1/2,0,0)$   $x,1/4,z$   
( $m_y$ | $1/2,1/2,0$ )'

(4) b  $(0,1/2,0)$   $1/4,y,z$   
( $m_x$ | $1/2,1/2,0$ )'

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,0)'$ ; (2); (3).

### Positions

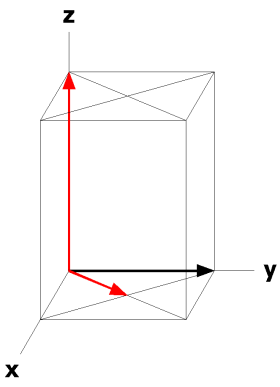
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
8 f 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $x,\bar{y},z [u,\bar{v},w]$	(4) $\bar{x},y,z [\bar{u},v,w]$
4 e $m'..$	$0,y,z [0,v,w]$	$0,\bar{y},z [0,\bar{v},w]$		
4 d $.m'$	$x,0,z [u,0,w]$	$\bar{x},0,z [\bar{u},0,w]$		
4 c $..2'$	$1/4,1/4,z [u,v,0]$	$1/4,3/4,z [u,\bar{v},0]$		
2 b $m' m' 2$	$0,1/2,z [0,0,w]$			
2 a $m' m' 2$	$0,0,z [0,0,w]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $c_p \cdot 2m' m'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a} \cdot 1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,1/4,0$

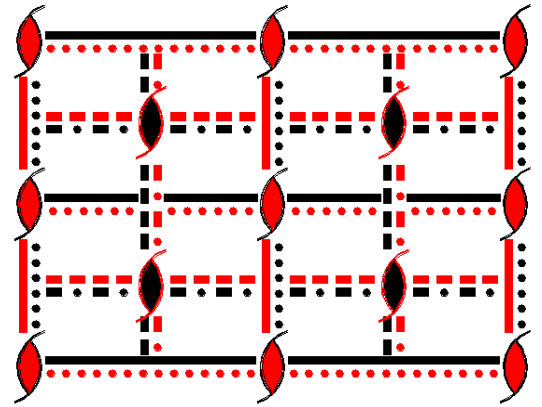
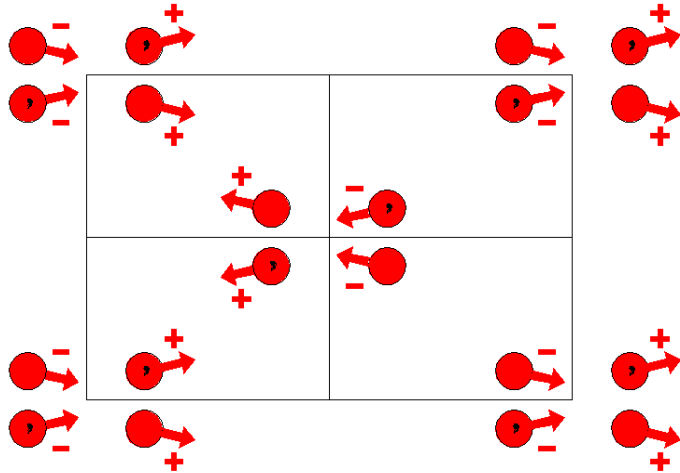
Along  $[0,1,0]$   $p_{2a} \cdot 1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $1/4,y,0$



$C_1 m' m 2'$   
35.12.247

$mm21'$   
 $C_1 m' m 2'$

Orthorhombic



**Origin** on  $m' m 2'$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                      |                                    |                                      |
|--------------------|--------------------------------------|------------------------------------|--------------------------------------|
| (1) 1<br>(1 0,0,0) | (2) $2'$ $0,0,z$<br>( $2_z$  0,0,0)' | (3) $m$ $x,0,z$<br>( $m_y$  0,0,0) | (4) $m'$ $0,y,z$<br>( $m_x$  0,0,0)' |
|--------------------|--------------------------------------|------------------------------------|--------------------------------------|

For  $(1/2,1/2,0)$ ' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,0)$<br>(1 1/2,1/2,0)' | (2) $2$ $1/4,1/4,z$<br>( $2_z$  1/2,1/2,0) | (3) $a'$ $(1/2,0,0)$ $x,1/4,z$<br>( $m_y$  1/2,1/2,0)' | (4) $b$ $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$  1/2,1/2,0) |
|--|--|--|--|

For  $(0,0,1)$ ' + set

- |                                  |  |  |  |
|----------------------------------|--|--|--|
| (1) $t'$ $(0,0,1)$<br>(1 0,0,1)' | (2) $2$ $(0,0,1)$ $0,0,z$<br>( $2_z$  0,0,1) | (3) $c'$ $(0,0,1)$ $x,0,z$<br>( $m_y$  0,0,1)' | (4) $c$ $(0,0,1)$ $0,y,z$<br>( $m_x$  0,0,1) |
|----------------------------------|--|--|--|

For  $(1/2,1/2,1)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t$ $(1/2,1/2,1)$<br>(1 1/2,1/2,1) | (2) $2'$ $(0,0,1)$ $1/4,1/4,z$<br>( $2_z$  1/2,1/2,1)' | (3) $n$ $(1/2,0,1)$ $x,1/4,z$<br>( $m_y$  1/2,1/2,1) | (4) $n'$ $(0,1/2,1)$ $1/4,y,z$<br>( $m_x$  1/2,1/2,1)' |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; t(1/2,1/2,0)'; (2); (3).

### Positions

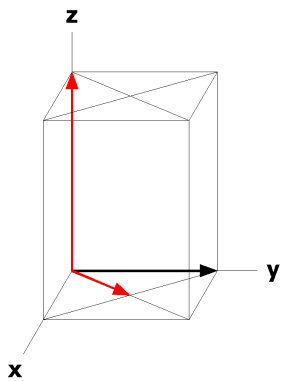
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,1)'	(1/2,1/2,0)' (1/2,1/2,1) +	
16 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 e m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]		
8 d .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0,v,0]		
8 c ..2	1/4,1/4,z [0,0,w]	1/4,3/4,z [0,0, $\bar{w}$ ]		
4 b m'm2'	0,1/2,z [0,v,0]			
4 a m'm2'	0,0,z [0,v,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>c</sub>1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

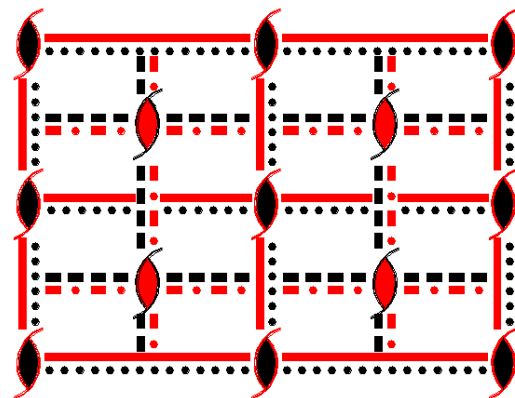
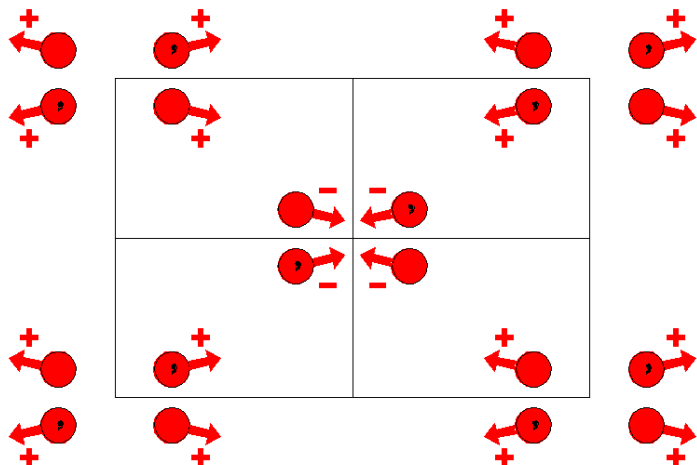
Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



$C_1 m' m' 2$   
35.13.248

$mm21'$   
 $C_1 m' m' 2$

Orthorhombic



**Origin** on  $m' m' 2$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) m' $x,0,z$<br>(m <sub>y</sub>  0,0,0)' | (4) m' $0,y,z$<br>(m <sub>x</sub>  0,0,0)' |
|--------------------|--|--|--|

For  $(1/2,1/2,0)$ ' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' $(1/2,1/2,0)$<br>(1 1/2,1/2,0)' | (2) 2' $1/4,1/4,z$<br>(2 <sub>z</sub>  1/2,1/2,0)' | (3) a $(1/2,0,0)$ $x,1/4,z$<br>(m <sub>y</sub>  1/2,1/2,0) | (4) b $(0,1/2,0)$ $1/4,y,z$<br>(m <sub>x</sub>  1/2,1/2,0) |
|--|--|--|--|

For  $(0,0,1)$ ' + set

- |                                |  |  |  |
|--------------------------------|--|--|--|
| (1) t' $(0,0,1)$<br>(1 0,0,1)' | (2) 2' $(0,0,1)$ $0,0,z$<br>(2 <sub>z</sub>  0,0,1)' | (3) c $(0,0,1)$ $x,0,z$<br>(m <sub>y</sub>  0,0,1) | (4) c $(0,0,1)$ $0,y,z$<br>(m <sub>x</sub>  0,0,1) |
|--------------------------------|--|--|--|

For  $(1/2,1/2,1)$  + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t $(1/2,1/2,1)$<br>(1 1/2,1/2,1) | (2) 2 $(0,0,1)$ $1/4,1/4,z$<br>(2 <sub>z</sub>  1/2,1/2,1) | (3) n' $(1/2,0,1)$ $x,1/4,z$<br>(m <sub>y</sub>  1/2,1/2,1)' | (4) n' $(0,1/2,1)$ $1/4,y,z$<br>(m <sub>x</sub>  1/2,1/2,1)' |
|--------------------------------------|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; t(1/2,1/2,0)'; (2); (3).

### Positions

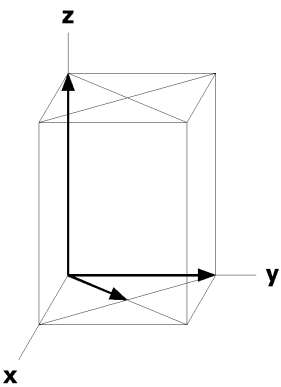
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,1)'	(1/2,1/2,0)' (1/2,1/2,1) +	
16 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 e m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]		
8 d .m'.	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]		
8 c ..2'	1/4,1/4,z [u,v,0]	1/4,3/4,z [u, $\bar{v},0$ ]		
4 b m'm'2	0,1/2,z [0,0,w]			
4 a m'm'2	0,0,z [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>c</sub>1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

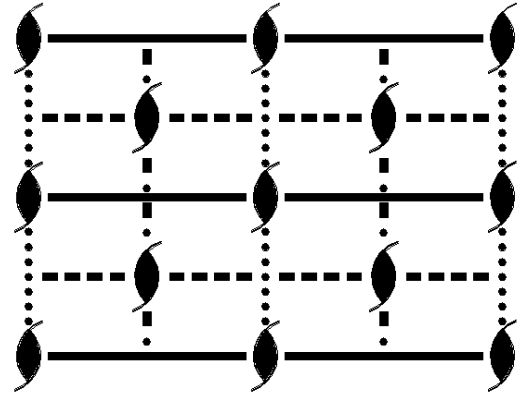
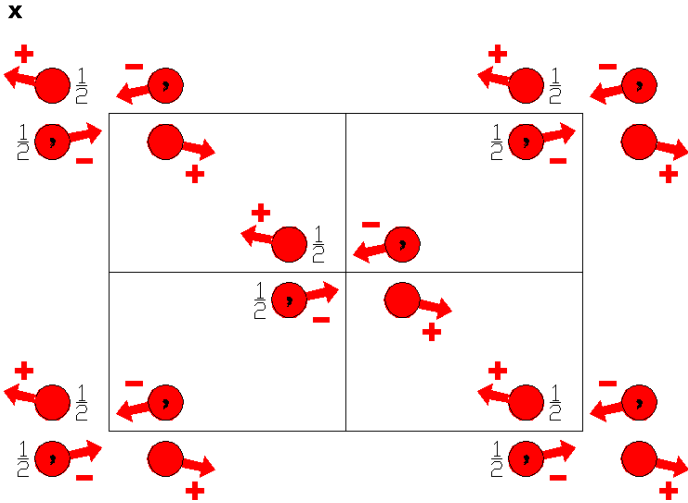
Along [0,1,0] p<sub>c</sub>1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



Cmc2<sub>1</sub>  
36.1.249

mm2  
Cmc2<sub>1</sub>

Orthorhombic



**Origin** on mc2<sub>1</sub>

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (4) m 0,y,z<br>(m <sub>x</sub>  0,0,0) |
|--------------------|--|--|--|

For (1/2,1/2,0) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (4) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |
|------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

### Positions

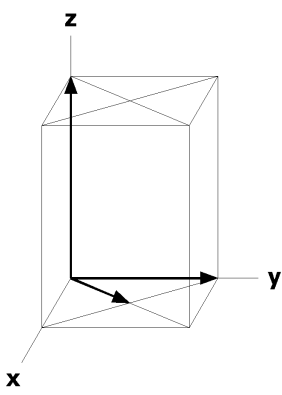
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,0) +		
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
4	a m..	0,y,z [u,0,0]	0, $\bar{y},z+1/2$ [ $\bar{u},0,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $p_{2b}1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Cmc2<sub>1</sub>'

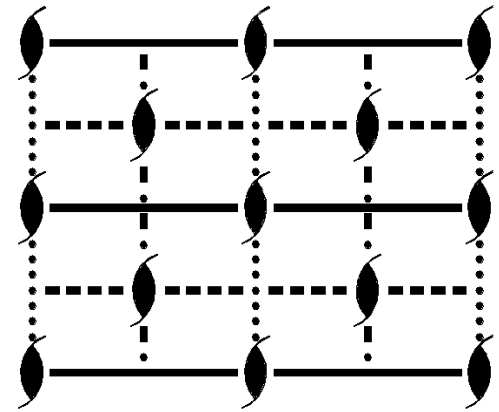
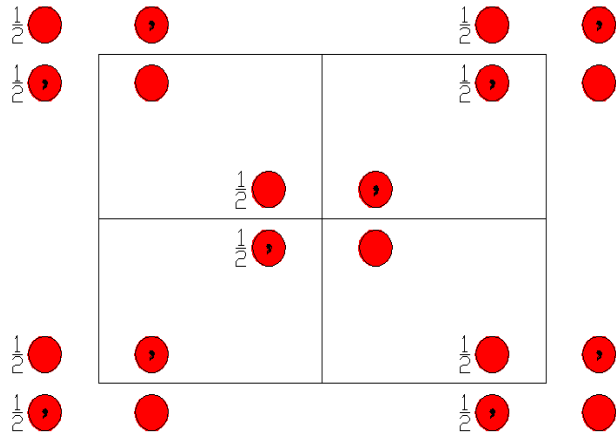
36.2.250

mm21'

Cmc2<sub>1</sub>'

Orthorhombic

1'



Origin on mc2<sub>1</sub>'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- (1) 1 (1|0,0,0)
- (2) 2 (0,0,1/2) 0,0,z (2<sub>z</sub>|0,0,1/2)
- (3) c (0,0,1/2) x,0,z (m<sub>y</sub>|0,0,1/2)
- (4) m 0,y,z (m<sub>x</sub>|0,0,0)

For (1/2,1/2,0) + set

- (1) t (1/2,1/2,0) (1|1/2,1/2,0)
- (2) 2 (0,0,1/2) 1/4,1/4,z (2<sub>z</sub>|1/2,1/2,1/2)
- (3) n (1/2,0,1/2) x,1/4,z (m<sub>y</sub>|1/2,1/2,1/2)
- (4) b (0,1/2,0) 1/4,y,z (m<sub>x</sub>|1/2,1/2,0)

For (0,0,0)' + set

- (1) 1' (1|0,0,0)'
- (2) 2' (0,0,1/2) 0,0,z (2<sub>z</sub>|0,0,1/2)'
- (3) c' (0,0,1/2) x,0,z (m<sub>y</sub>|0,0,1/2)'
- (4) m' 0,y,z (m<sub>x</sub>|0,0,0)'

For (1/2,1/2,0)' + set

- (1) t' (1/2,1/2,0) (1|1/2,1/2,0)'
- (2) 2' (0,0,1/2) 1/4,1/4,z (2<sub>z</sub>|1/2,1/2,1/2)'
- (3) n' (1/2,0,1/2) x,1/4,z (m<sub>y</sub>|1/2,1/2,1/2)'
- (4) b' (0,1/2,0) 1/4,y,z (m<sub>x</sub>|1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); 1'.

### Positions

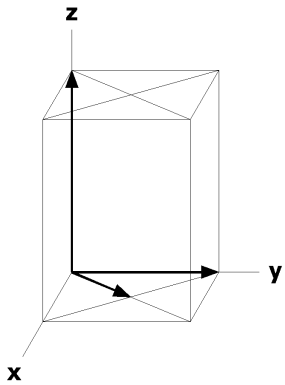
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) + (0,0,0)' +		(1/2,1/2,0) + (1/2,1/2,0)' +	
8	b 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y}, z+1/2$ [0,0,0]	(3) $x, \bar{y}, z+1/2$ [0,0,0]	(4) $\bar{x}, y, z$ [0,0,0]
4	a m..1'	0,y,z [0,0,0]	0, $\bar{y}$ ,z+1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



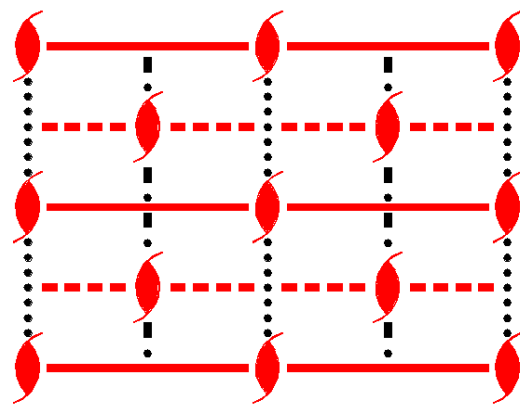
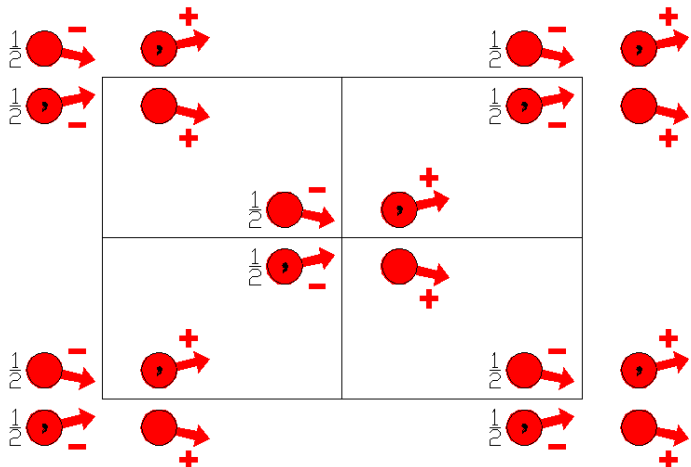
$Cm'c2_1'$

36.3.251

$m'm2'$

$Cm'c2_1'$

Orthorhombic



**Origin** on  $m'c2_1'$

**Asymmetric unit**  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2)  $2'$  (0,0,1/2) 0,0,z  
( $2_z$ |0,0,1/2)'

(3) c (0,0,1/2) x,0,z  
( $m_y$ |0,0,1/2)

(4)  $m'$  0,y,z  
( $m_x$ |0,0,0)'

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)

(2)  $2'$  (0,0,1/2) 1/4,1/4,z  
( $2_z$ |1/2,1/2,1/2)'

(3) n (1/2,0,1/2) x,1/4,z  
( $m_y$ |1/2,1/2,1/2)

(4)  $b'$  (0,1/2,0) 1/4,y,z  
( $m_x$ |1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

### Positions

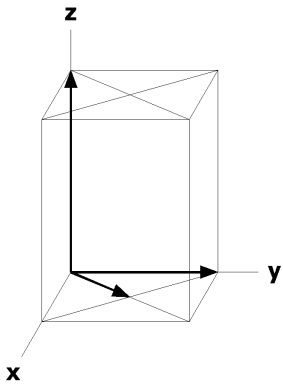
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,0) +		
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $x,\bar{y},z+1/2$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) $\bar{x},y,z$ [ $\bar{u}$ ,v,w]
4	a m'..	0,y,z [0,v,w]	0, $\bar{y},z+1/2$ [0,v, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p1g1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2b</sub>1m'1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



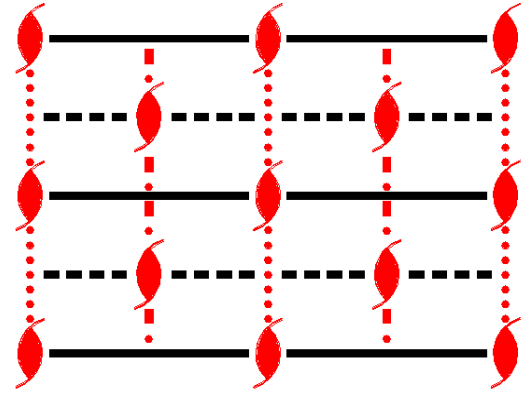
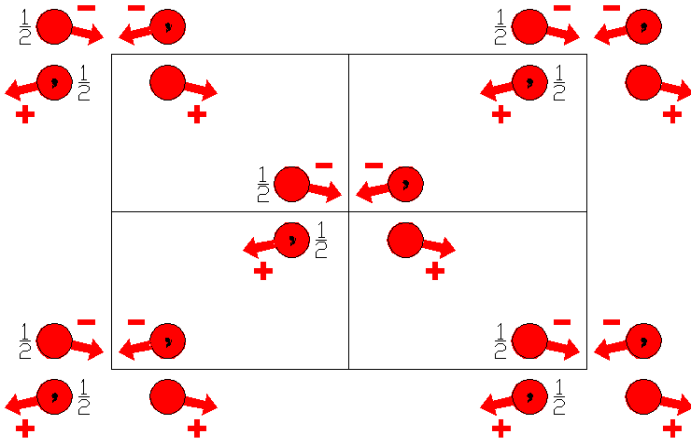
Cmc'2<sub>1</sub>'

36.4.252

mm'2'

Cmc'2<sub>1</sub>'

Orthorhombic



**Origin** on mc'2<sub>1</sub>'

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)' | (3) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (4) m 0,y,z<br>(m <sub>x</sub>  0,0,0) |
|--------------------|--|--|--|

For (1/2,1/2,0) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (4) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |
|------------------------------------|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

**Positions**

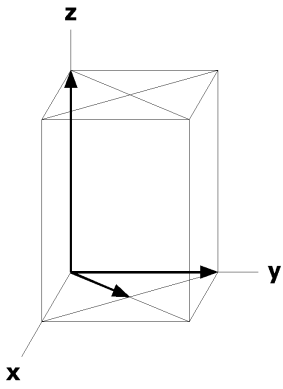
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +		(1/2,1/2,0) +	
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $x,\bar{y},z+1/2$ [u, $\bar{v}$ ,w]	(4) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
4	a m..	0,y,z [u,0,0]	0, $\bar{y},z+1/2$ [u,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



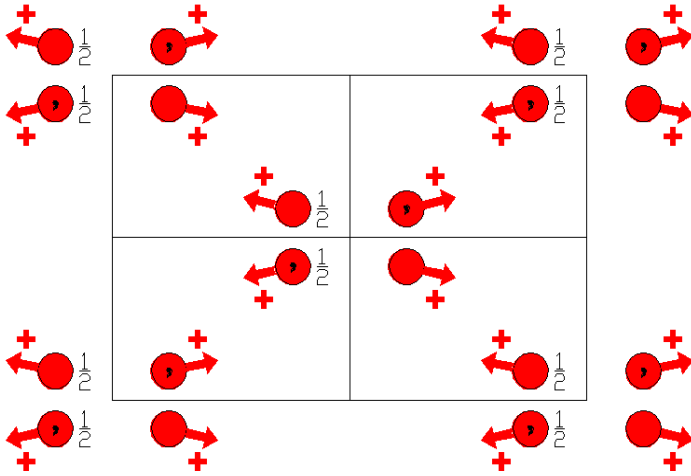
Cm'c'2<sub>1</sub>

36.5.253

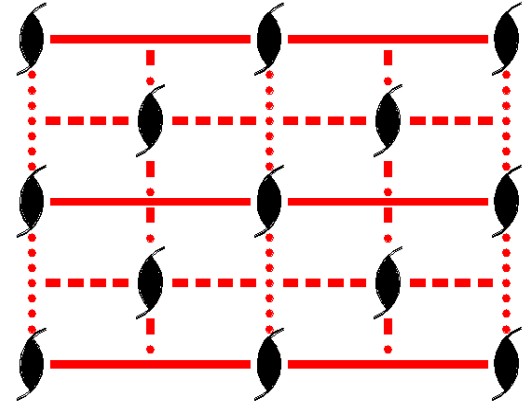
m'm'2

Cm'c'2<sub>1</sub>

Orthorhombic



Origin on m'c'2<sub>1</sub>



Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)

(3) c' (0,0,1/2) x,0,z  
(m<sub>y</sub>|0,0,1/2)'

(4) m' 0,y,z  
(m<sub>x</sub>|0,0,0)'

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)

(2) 2 (0,0,1/2) 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,1/2)

(3) n' (1/2,0,1/2) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,1/2)'

(4) b' (0,1/2,0) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

### Positions

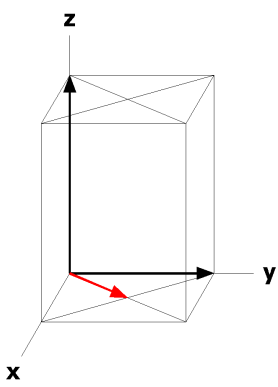
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +		(1/2,1/2,0) +	
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
4	a m'..	0,y,z [0,v,w]	0, $\bar{y},z+1/2$ [0, $\bar{v},w$ ]		

### Symmetry of Special Projections

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m'1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



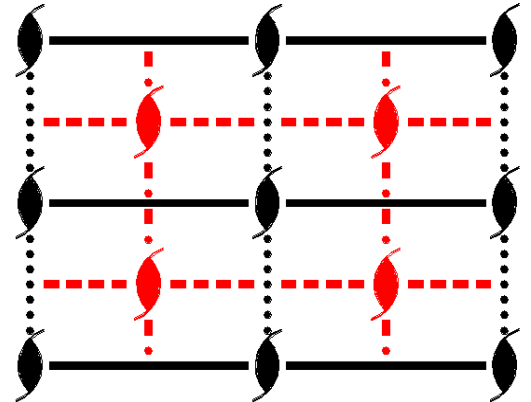
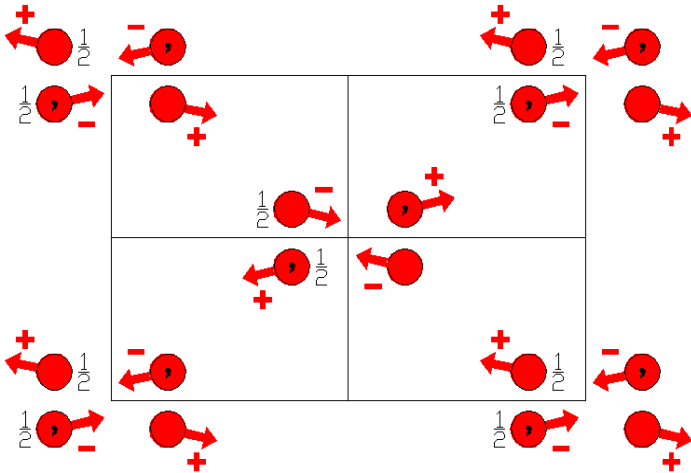
$C_pmc2_1$

36.6.254

$mm21'$

$C_pmc2_1$

Orthorhombic



**Origin** on  $mc2_1$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |                                      |
|--------------------|--|--|--------------------------------------|
| (1) 1<br>(1 0,0,0) | (2) 2 $(0,0,1/2)$ $0,0,z$<br>( $2_z$   $0,0,1/2$ ) | (3) c $(0,0,1/2)$ $x,0,z$<br>( $m_y$   $0,0,1/2$ ) | (4) m $0,y,z$<br>( $m_x$   $0,0,0$ ) |
|--------------------|--|--|--------------------------------------|

For  $(1/2,1/2,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,0)$<br>(1  $1/2,1/2,0$ )' | (2) $2'$ $(0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1/2$ )' | (3) $n'$ $(1/2,0,1/2)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,1/2$ )' | (4) $b'$ $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

### Positions

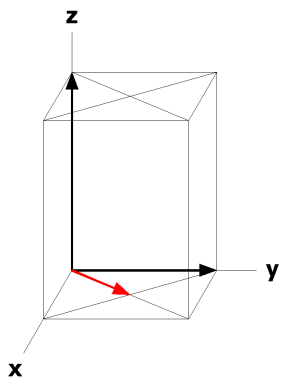
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +		(1/2,1/2,0)' +	
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
4	a m..	0,y,z [u,0,0]	0, $\bar{y},z+1/2$ [ $\bar{u},0,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] c<sub>p</sub>2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>c</sub>\*1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



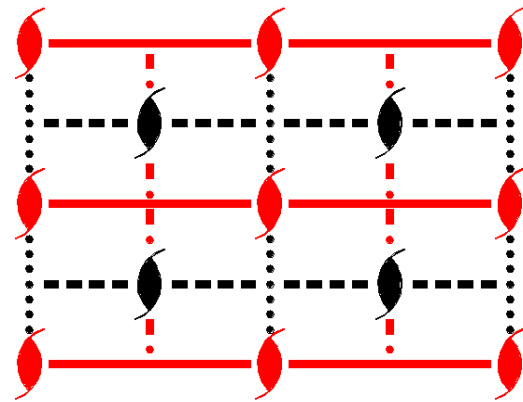
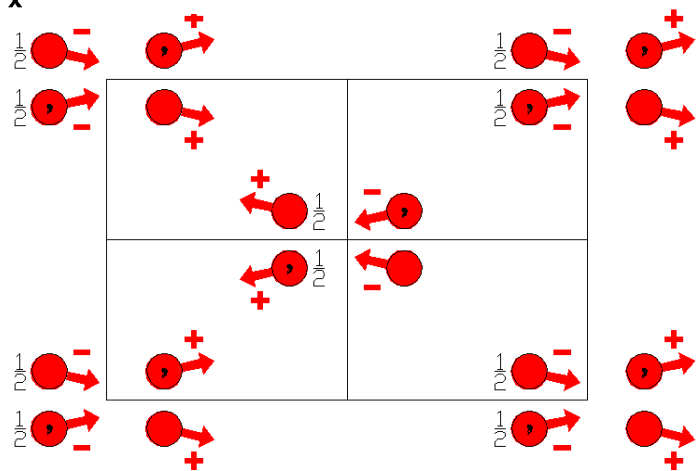
$C_{2v}m'c_2'$

36.7.255

$mm21'$

$C_{2v}m'c_2'$

Orthorhombic



**Origin** on  $m'c_2'$

**Asymmetric unit**  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |                                    |
|--------------------|--|--|------------------------------------|
| (1) 1<br>(1 0,0,0) | (2) $2' (0,0,1/2)$ $0,0,z$<br>( $2_z$  0,0,1/2)' | (3) $c (0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2) | (4) $m' 0,y,z$<br>( $m_x$  0,0,0)' |
|--------------------|--|--|------------------------------------|

For  $(1/2,1/2,0)$ ' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t' (1/2,1/2,0)$<br>(1 1/2,1/2,0)' | (2) $2 (0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2) | (3) $n' (1/2,0,1/2)$ $x,1/4,z$<br>( $m_y$  1/2,1/2,1/2)' | (4) $b (0,1/2,0)$ $1/4,y,z$<br>( $m_x$  1/2,1/2,0) |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

### Positions

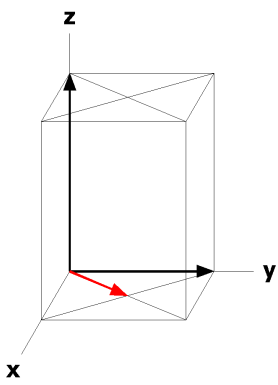
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,0)' +		
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $x,\bar{y},z+1/2$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) $\bar{x},y,z$ [ $\bar{u}$ ,v,w]
4	a m'..	0,y,z [0,v,w]	0, $\bar{y},z+1/2$ [0,v, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] c<sub>p</sub>'2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'1g1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>c</sub>'1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 1/4,y,0



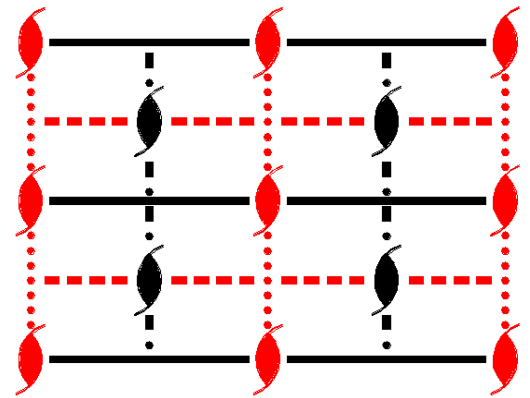
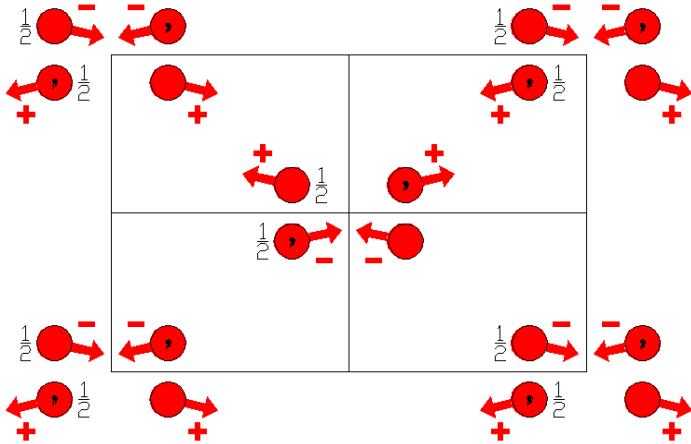
$C_p mc'2_1'$

36.8.256

$mm21'$

$C_p mc'2_1'$

Orthorhombic



**Origin** on  $mc'2_1'$

**Asymmetric unit**  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) $2'$ $(0,0,1/2)$ $0,0,z$<br>( $2_z$   $0,0,1/2$ )' | (3) $c'$ $(0,0,1/2)$ $x,0,z$<br>( $m_y$   $0,0,1/2$ )' | (4) $m$ $0,y,z$<br>( $m_x$   $0,0,0$ ) |
|--------------------|--|--|--|

For  $(1/2,1/2,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,0)$<br>(1  $1/2,1/2,0$ )' | (2) $2$ $(0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1/2$ ) | (3) $n$ $(1/2,0,1/2)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,1/2$ ) | (4) $b'$ $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |
|--|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

### Positions

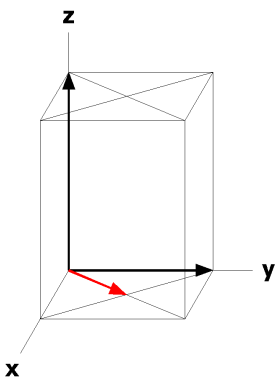
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +		(1/2,1/2,0)' +	
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $x,\bar{y},z+1/2$ [u, $\bar{v}$ ,w]	(4) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
4	a m..	0,y,z [u,0,0]	0, $\bar{y}$ ,z+1/2 [u,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c<sub>p</sub>'2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>'1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



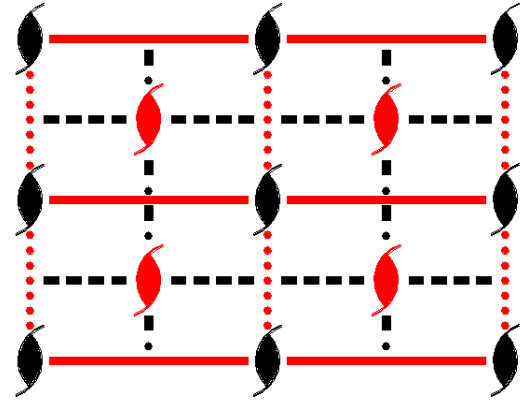
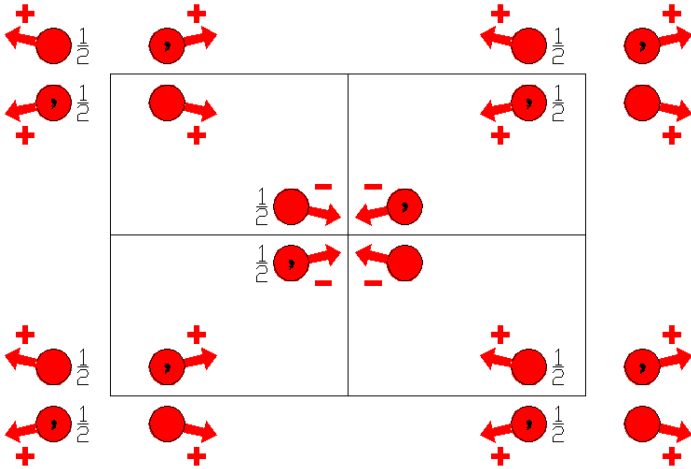
$C_p m' c' 2_1$

36.9.257

$mm21'$

$C_p m' c' 2_1$

Orthorhombic



**Origin** on  $m' c' 2_1$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $(0,0,1/2)$ $0,0,z$<br>( $2_z$   $0,0,1/2$ ) | (3) $c'$ $(0,0,1/2)$ $x,0,z$<br>( $m_y$   $0,0,1/2$ )' | (4) $m'$ $0,y,z$<br>( $m_x$   $0,0,0$ )' |
|--------------------|--|--|--|

For  $(1/2,1/2,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,0)$<br>(1  $1/2,1/2,0$ )' | (2) $2'$ $(0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1/2$ )' | (3) $n$ $(1/2,0,1/2)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,1/2$ ) | (4) $b$ $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ ) |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

### Positions

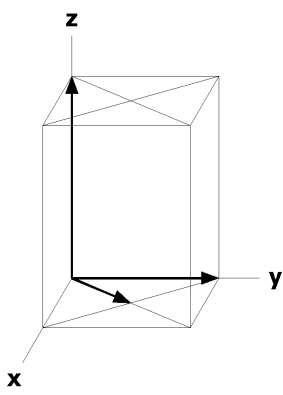
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +		(1/2,1/2,0)' +	
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
4	a m'..	0,y,z [0,v,w]	0, $\bar{y},z+1/2$ [0, $\bar{v},w$ ]		

### Symmetry of Special Projections

Along [0,0,1] c<sub>p</sub>2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>1g1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

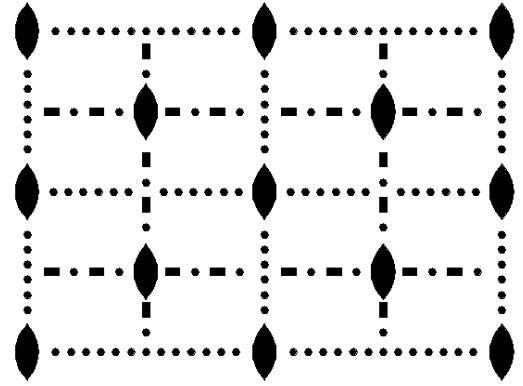
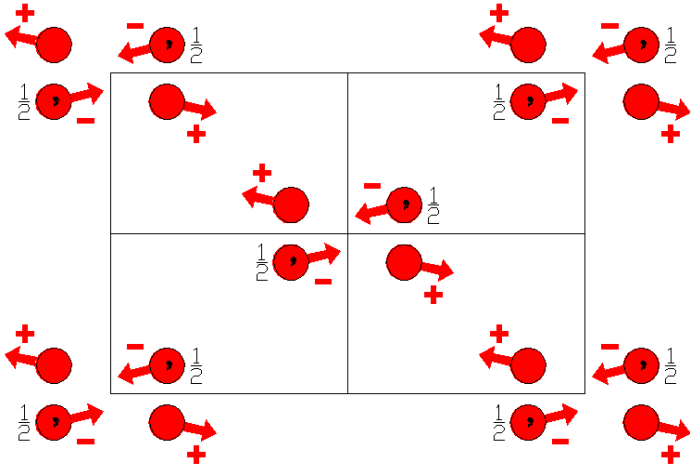
Along [0,1,0] p<sub>2a</sub>1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 1/4,y,0



Ccc2  
37.1.258

mm2  
Ccc2

Orthorhombic



Origin on cc2

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
(2<sub>z</sub>|0,0,0)

(3) c (0,0,1/2)  $x,0,z$   
(m<sub>y</sub>|0,0,1/2)

(4) c (0,0,1/2)  $0,y,z$   
(m<sub>x</sub>|0,0,1/2)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1|1/2,1/2,0)

(2) 2  $1/4,1/4,z$   
(2<sub>z</sub>|1/2,1/2,0)

(3) n (1/2,0,1/2)  $x,1/4,z$   
(m<sub>y</sub>|1/2,1/2,1/2)

(4) n (0,1/2,1/2)  $1/4,y,z$   
(m<sub>x</sub>|1/2,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

### Positions

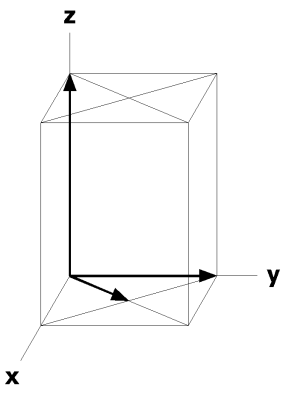
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y}$ ,z+1/2 [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
4 c ..2	1/4,1/4,z [0,0,w]	1/4,3/4,z+1/2 [0,0, $\bar{w}$ ]		
4 b ..2	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]		
4 a ..2	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b^*}1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2b^*}1m'1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0

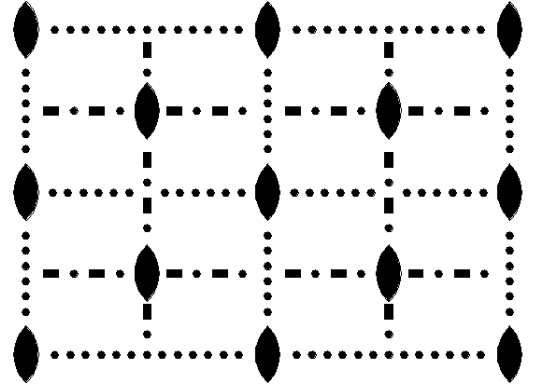
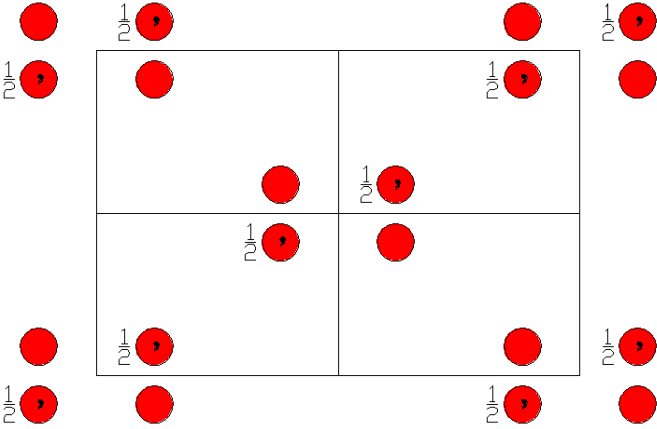


Ccc21'  
37.2.259

mm21'  
Ccc21'

Orthorhombic

1'



Origin on cc21'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (4) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) |
|--------------------|--|--|--|

For (1/2,1/2,0) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0) | (3) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (4) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) |
|------------------------------------|--|--|--|

For (0,0,0)' + set

- |                      |  |  |  |
|----------------------|--|--|--|
| (1) 1'<br>(1 0,0,0)' | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (4) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |
|----------------------|--|--|--|

For (1/2,1/2,0)' + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t' (1/2,1/2,0)<br>(1 1/2,1/2,0)' | (2) 2' 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)' | (3) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (4) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |
|--------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); 1'.

### Positions

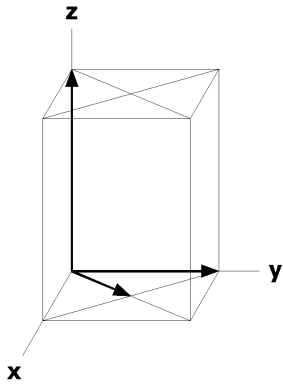
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) + (0,0,0)' +	(1/2,1/2,0) + (1/2,1/2,0)' +		
8	d 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $x,\bar{y},z+1/2$ [0,0,0]	(4) $\bar{x},y,z+1/2$ [0,0,0]
4	c ..21'	1/4,1/4,z [0,0,0]	1/4,3/4,z+1/2 [0,0,0]		
4	b ..21'	0,1/2,z [0,0,0]	0,1/2,z+1/2 [0,0,0]		
4	a ..21'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

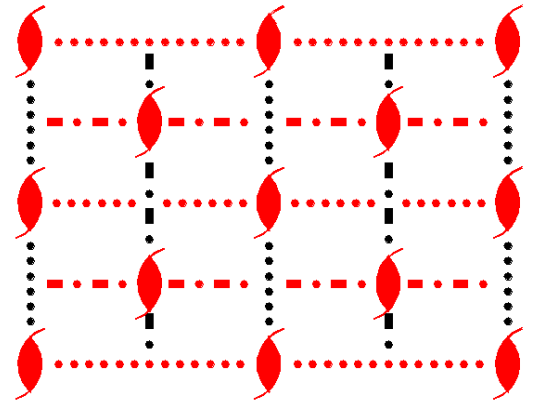
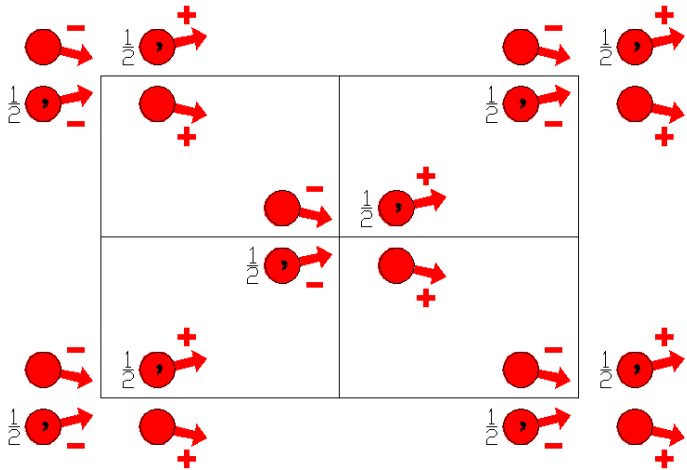
Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Cc'c2'  
37.3.260

m'm2'  
Cc'c2'

Orthorhombic



**Origin** on c'c2'

**Asymmetric unit**  $0 \leq x \leq 1/4;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (4) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |
|--------------------|--|--|--|

For (1/2,1/2,0) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) 2' 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)' | (3) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (4) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |
|------------------------------------|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

### Positions

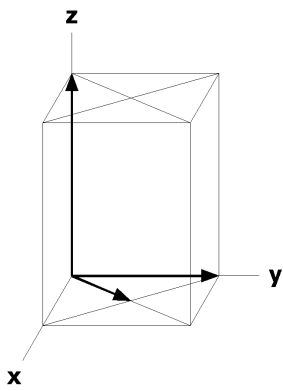
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1/2,1/2,0) +	
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y}$ ,z+1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) $\bar{x}$ ,y,z+1/2 [ $\bar{u}$ ,v,w]
4 c ..2'	1/4,1/4,z [u,v,0]	1/4,3/4,z+1/2 [ $\bar{u}$ ,v,0]		
4 b ..2'	0,1/2,z [u,v,0]	0,1/2,z+1/2 [ $\bar{u}$ ,v,0]		
4 a ..2'	0,0,z [u,v,0]	0,0,z+1/2 [ $\bar{u}$ ,v,0]		

### Symmetry of Special Projections

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

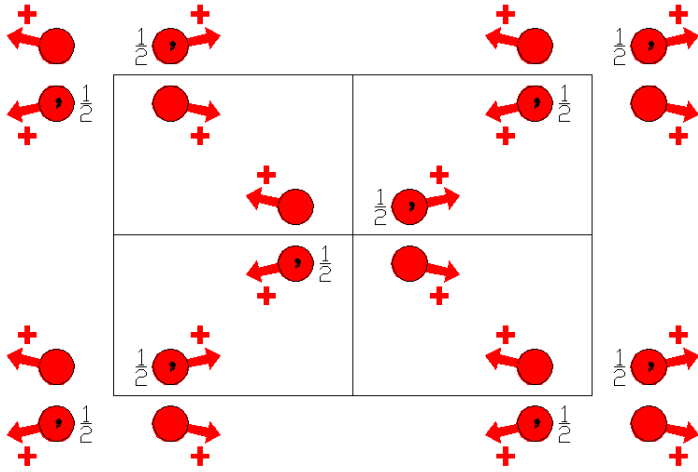
Along [0,1,0] p<sub>2b</sub>'1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Cc'c'2  
37.4.261

m'm'2  
Cc'c'2

Orthorhombic



Origin on c'c'2

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

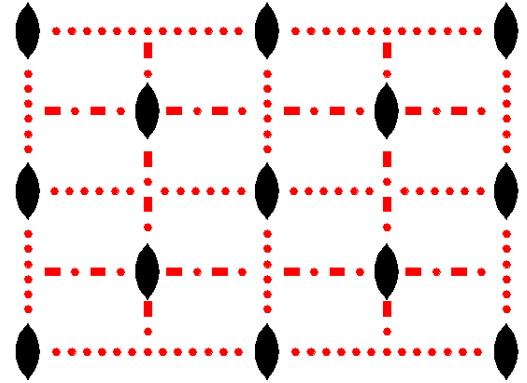
**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (4) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |
|--------------------|--|--|--|

For (1/2,1/2,0) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0) | (3) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (4) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |
|------------------------------------|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

### Positions

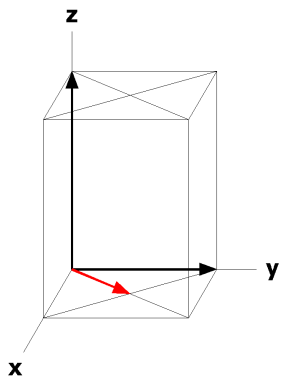
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1/2,1/2,0) +	
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(4) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
4 c ..2	1/4,1/4,z [0,0,w]	1/4,3/4,z+1/2 [0,0,w]		
4 b ..2	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]		
4 a ..2	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

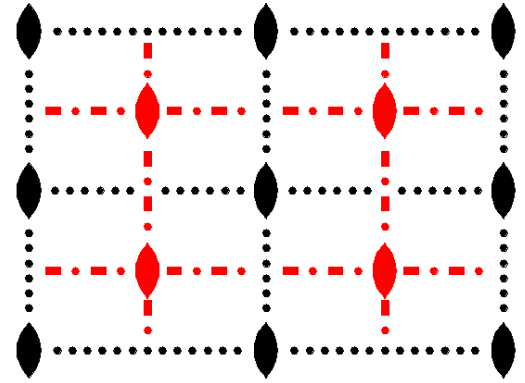
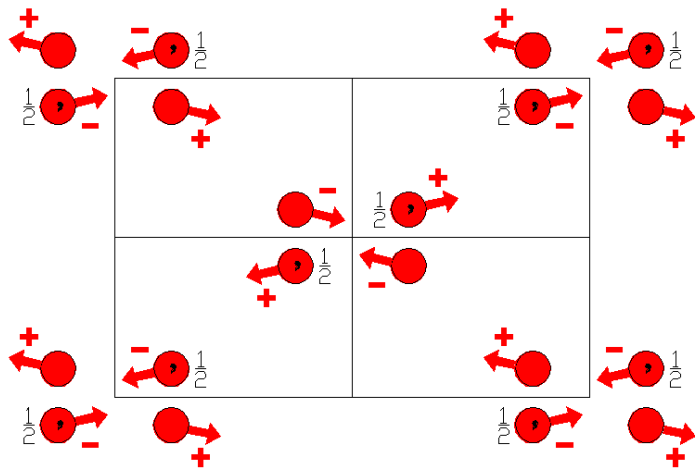
Along [0,1,0] p1m'1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$C_{pcc2}$   
37.5.262

$mm21'$   
 $C_{pcc2}$

Orthorhombic



**Origin** on  $cc2$

**Asymmetric unit**  $0 \leq x \leq 1/4;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                  |  |  |
|--------------------|----------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) c $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2) | (4) c $(0,0,1/2)$ $0,y,z$<br>( $m_x$  0,0,1/2) |
|--------------------|----------------------------------|--|--|

For  $(1/2,1/2,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,0)$<br>(1  $1/2,1/2,0$ )' | (2) $2'$ $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,0$ )' | (3) $n'$ $(1/2,0,1/2)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,1/2$ )' | (4) $n'$ $(0,1/2,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,1/2$ )' |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)<sup>'</sup>; (2); (3).

### Positions

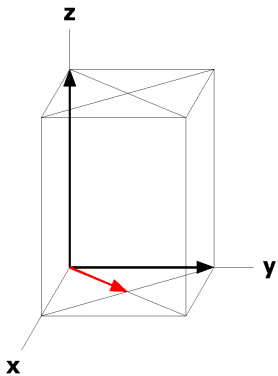
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,0) <sup>'</sup> +		
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
4	c ..2'	1/4,1/4,z [u,v,0]	1/4,3/4,z+1/2 [ $\bar{u},v,0$ ]		
4	b ..2	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]		
4	a ..2	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] c<sub>p</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>c</sub>-1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,0

Along [0,1,0] p<sub>c</sub>-1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 1/4,y,0



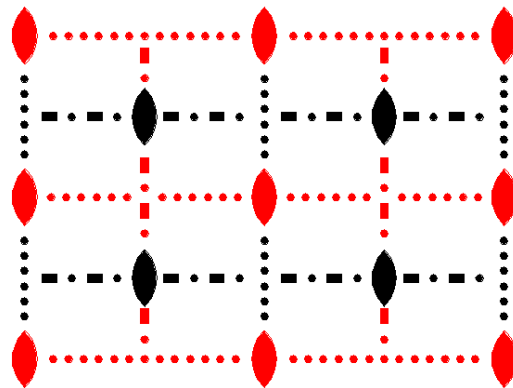
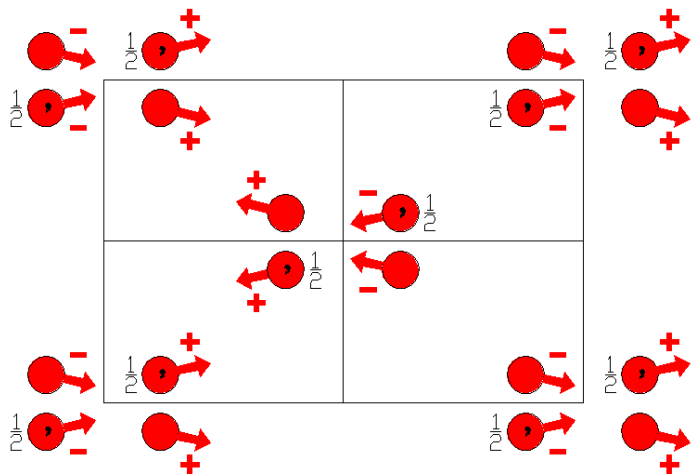
$C_{2v}$

37.6.263

$mm2$

$C_{2v}$

Orthorhombic



**Origin** on  $c_2'$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2)  $2'$  0,0,z  
( $2_z$ |0,0,0)'

(3) c (0,0,1/2) x,0,z  
( $m_y$ |0,0,1/2)

(4)  $c'$  (0,0,1/2) 0,y,z  
( $m_x$ |0,0,1/2)'

For  $(1/2,1/2,0)$ ' + set

(1)  $t'$  (1/2,1/2,0)  
(1|1/2,1/2,0)'

(2) 2 1/4,1/4,z  
( $2_z$ |1/2,1/2,0)

(3)  $n'$  (1/2,0,1/2) x,1/4,z  
( $m_y$ |1/2,1/2,1/2)'

(4) n (0,1/2,1/2) 1/4,y,z  
( $m_x$ |1/2,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

### Positions

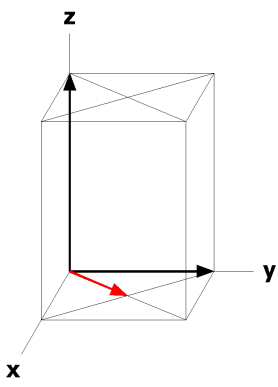
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
4 c ..2	1/4,1/4,z [0,0,w]	1/4,3/4,z+1/2 [0,0, $\bar{w}$ ]		
4 b ..2'	0,1/2,z [u,v,0]	0,1/2,z+1/2 [ $\bar{u},v,0$ ]		
4 a ..2'	0,0,z [u,v,0]	0,0,z+1/2 [ $\bar{u},v,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] c<sub>p</sub>-2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a\*</sub>1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

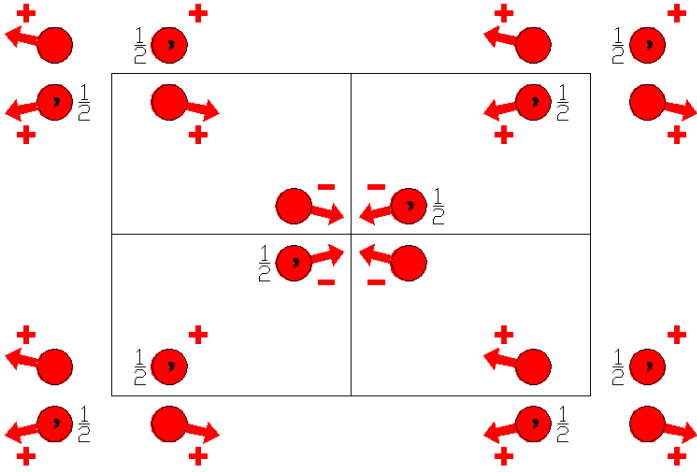
Along [0,1,0] p<sub>2a\*</sub>1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$C_p c' c' 2$   
37.7.264

$mm21'$   
 $C_p c' c' 2$

Orthorhombic



Origin on  $c' c' 2$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
(2<sub>z</sub>|0,0,0)

(3) c'  $(0,0,1/2)$   $x,0,z$   
(m<sub>y</sub>|0,0,1/2)'

(4) c'  $(0,0,1/2)$   $0,y,z$   
(m<sub>x</sub>|0,0,1/2)'

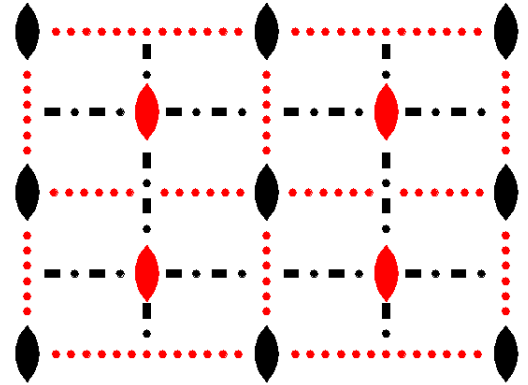
For  $(1/2,1/2,0)$ ' + set

(1) t'  $(1/2,1/2,0)$   
(1|1/2,1/2,0)'

(2) 2'  $1/4,1/4,z$   
(2<sub>z</sub>|1/2,1/2,0)'

(3) n  $(1/2,0,1/2)$   $x,1/4,z$   
(m<sub>y</sub>|1/2,1/2,1/2)

(4) n  $(0,1/2,1/2)$   $1/4,y,z$   
(m<sub>x</sub>|1/2,1/2,1/2)





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

### Positions

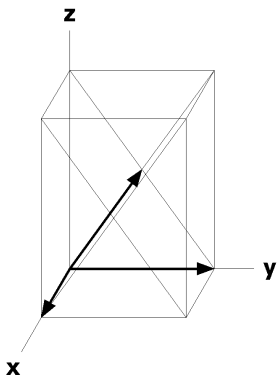
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,0)' +		
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(4) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
4	c ..2'	1/4,1/4,z [u,v,0]	1/4,3/4,z+1/2 [ $u,\bar{v},0$ ]		
4	b ..2	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]		
4	a ..2	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] c<sub>p</sub>-2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>\*-1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>\*-1m'1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



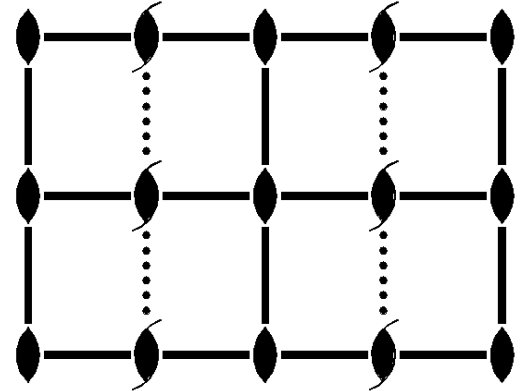
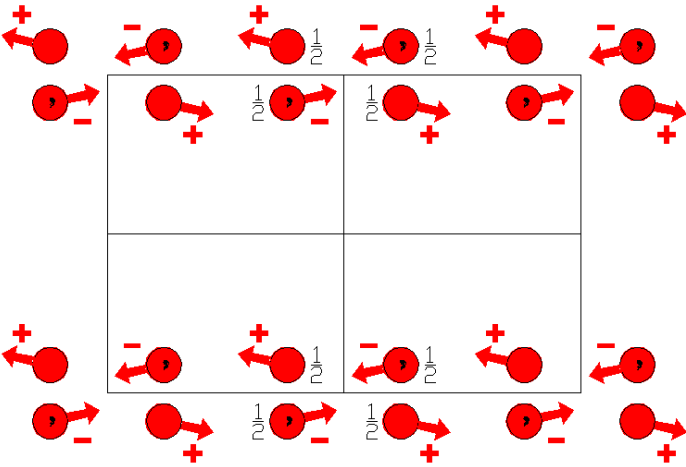
Amm2

38.1.265

mm2

Amm2

Orthorhombic



Origin on mm2

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) m x,0,z  
(m<sub>y</sub>|0,0,0)

(4) m 0,y,z  
(m<sub>x</sub>|0,0,0)

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)  
(1|0,1/2,1/2)

(2) 2 (0,0,1/2) 0,1/4,z  
(2<sub>z</sub>|0,1/2,1/2)

(3) c (0,0,1/2) x,1/4,z  
(m<sub>y</sub>|0,1/2,1/2)

(4) n (0,1/2,1/2) 0,y,z  
(m<sub>x</sub>|0,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

### Positions

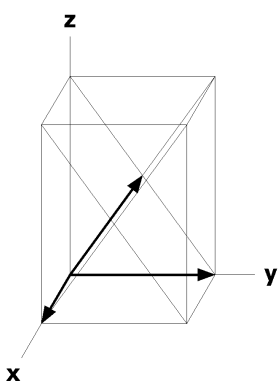
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2) +		
8 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
4 e m..	1/2,y,z [u,0,0]	1/2, $\bar{y},z$ [ $\bar{u},0,0$ ]		
4 d m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]		
4 c .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]		
2 b mm2	1/2,0,z [0,0,0]			
2 a mm2	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Amm21'

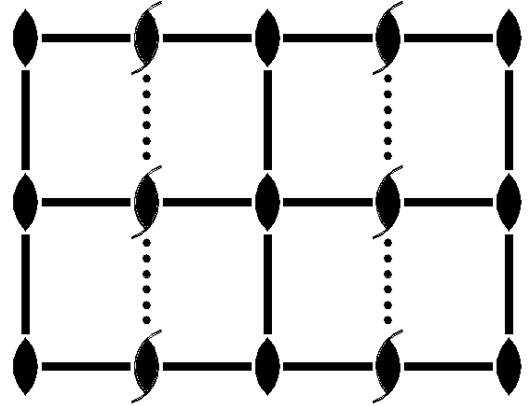
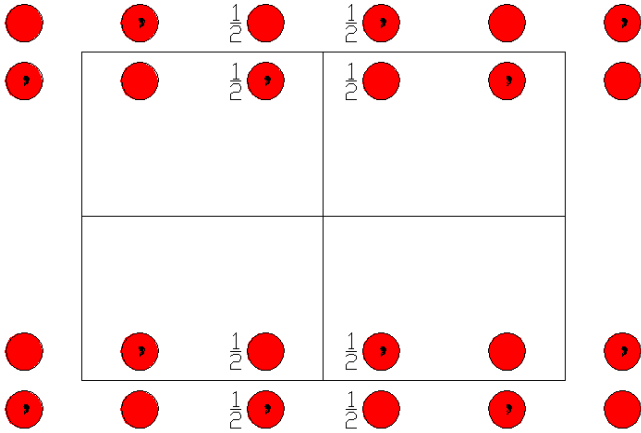
38.2.266

mm21'

Amm21'

Orthorhombic

1'



Origin on mm21'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (4) m 0,y,z<br>(m <sub>x</sub>  0,0,0) |
|--------------------|--|--|--|

For (0,1/2,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2) | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2) | (3) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2) | (4) n (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>  0,1/2,1/2) |
|------------------------------------|--|--|--|

For (0,0,0)' + set

- |                      |  |  |  |
|----------------------|--|--|--|
| (1) 1'<br>(1 0,0,0)' | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (4) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |
|----------------------|--|--|--|

For (0,1/2,1/2)' + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t' (0,1/2,1/2)<br>(1 0,1/2,1/2)' | (2) 2' (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)' | (3) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (4) n' (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>  0,1/2,1/2)' |
|--------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3); 1'.

### Positions

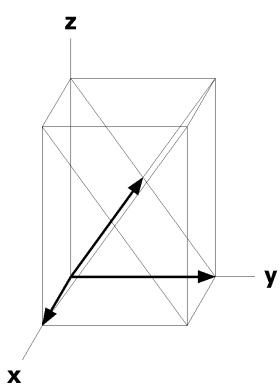
				Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.				(0,0,0) + (0,0,0)' +	(0,1/2,1/2) + (0,1/2,1/2)' +
8	f 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) x, $\bar{y},z$ [0,0,0]	(4) $\bar{x},y,z$ [0,0,0]
4	e m..1'	1/2,y,z [0,0,0]	1/2, $\bar{y},z$ [0,0,0]		
4	d m..1'	0,y,z [0,0,0]	0, $\bar{y},z$ [0,0,0]		
4	c .m.1'	x,0,z [0,0,0]	$\bar{x},0,z$ [0,0,0]		
2	b mm21'	1/2,0,z [0,0,0]			
2	a mm21'	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



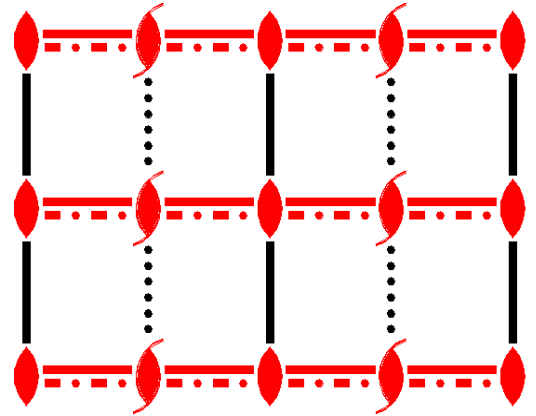
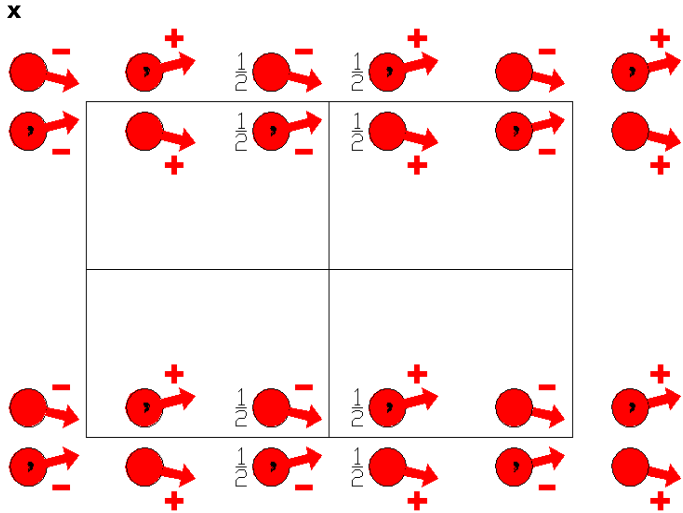
Am'm2'

38.3.267

m'm2'

Am'm2'

Orthorhombic



Origin on m'm2'

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'

(3) m x,0,z  
(m<sub>y</sub>|0,0,0)

(4) m' 0,y,z  
(m<sub>x</sub>|0,0,0)'

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)  
(1|0,1/2,1/2)

(2) 2' (0,0,1/2) 0,1/4,z  
(2<sub>z</sub>|0,1/2,1/2)'

(3) c (0,0,1/2) x,1/4,z  
(m<sub>y</sub>|0,1/2,1/2)

(4) n' (0,1/2,1/2) 0,y,z  
(m<sub>x</sub>|0,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

### Positions

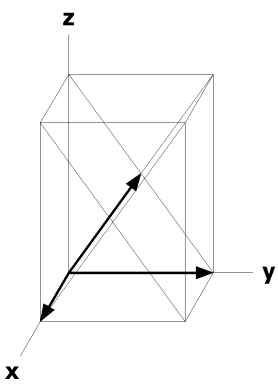
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2) +		
8 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y},z$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) $\bar{x},y,z$ [ $\bar{u}$ ,v,w]
4 e m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0,v, $\bar{w}$ ]		
4 d m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0,v, $\bar{w}$ ]		
4 c .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0,v,0]		
2 b m'm2'	1/2,0,z [0,v,0]			
2 a m'm2'	0,0,z [0,v,0]			

### Symmetry of Special Projections

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] c1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



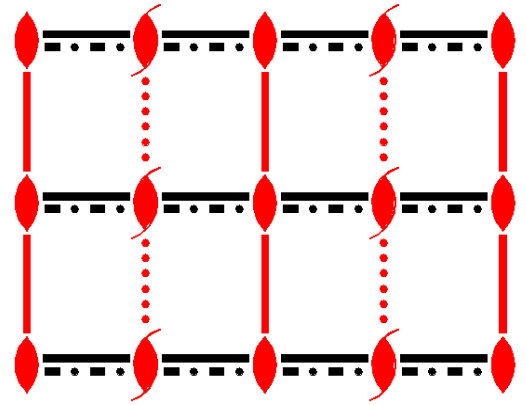
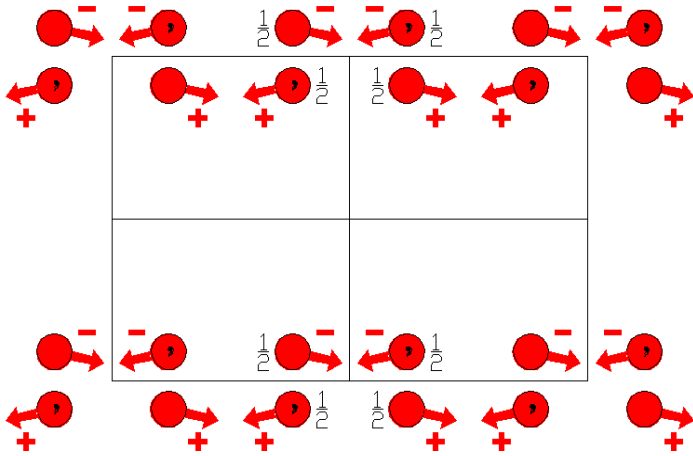
Amm'2'

38.4.268

mm'2'

Amm'2'

Orthorhombic



Origin on mm'2'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'

(3) m' x,0,z  
(m<sub>y</sub>|0,0,0)'

(4) m 0,y,z  
(m<sub>x</sub>|0,0,0)

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)  
(1|0,1/2,1/2)

(2) 2' (0,0,1/2) 0,1/4,z  
(2<sub>z</sub>|0,1/2,1/2)'

(3) c' (0,0,1/2) x,1/4,z  
(m<sub>y</sub>|0,1/2,1/2)'

(4) n (0,1/2,1/2) 0,y,z  
(m<sub>x</sub>|0,1/2,1/2)



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

### Positions

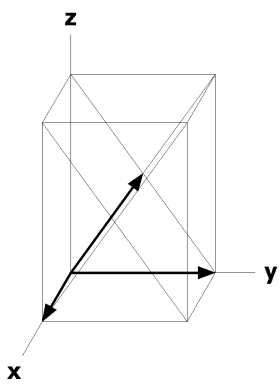
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2) +		
8 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
4 e m..	1/2,y,z [u,0,0]	1/2, $\bar{y},z$ [u,0,0]		
4 d m..	0,y,z [u,0,0]	0, $\bar{y},z$ [u,0,0]		
4 c .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [u,0, $\bar{w}$ ]		
2 b mm'2'	1/2,0,z [u,0,0]			
2 a mm'2'	0,0,z [u,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



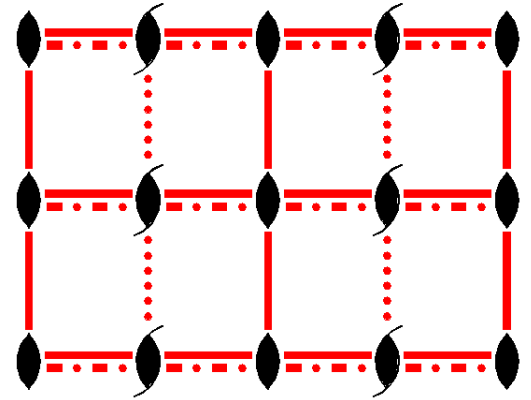
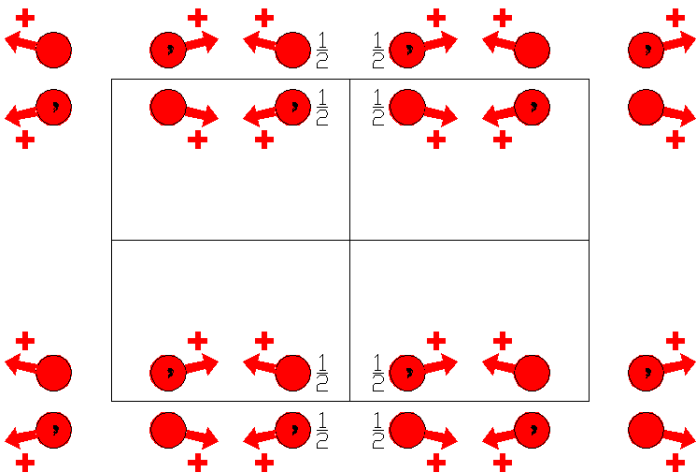
Am'm'2

38.5.269

m'm'2

Am'm'2

Orthorhombic



Origin on m'm'2

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) m' x,0,z  
(m<sub>y</sub>|0,0,0)'

(4) m' 0,y,z  
(m<sub>x</sub>|0,0,0)'

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)  
(1|0,1/2,1/2)

(2) 2 (0,0,1/2) 0,1/4,z  
(2<sub>z</sub>|0,1/2,1/2)

(3) c' (0,0,1/2) x,1/4,z  
(m<sub>y</sub>|0,1/2,1/2)'

(4) n' (0,1/2,1/2) 0,y,z  
(m<sub>x</sub>|0,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

### Positions

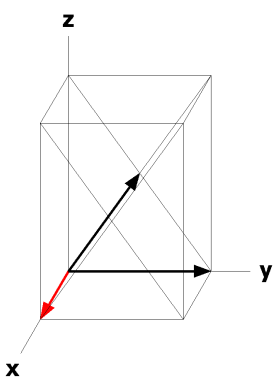
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2) +		
8 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
4 e m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0, $\bar{v},w$ ]		
4 d m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]		
4 c .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]		
2 b m'm'2	1/2,0,z [0,0,w]			
2 a m'm'2	0,0,z [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m'1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



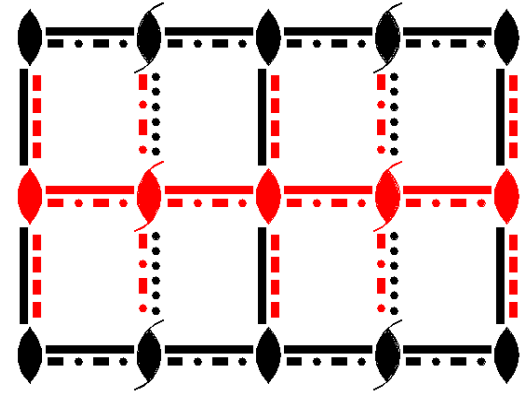
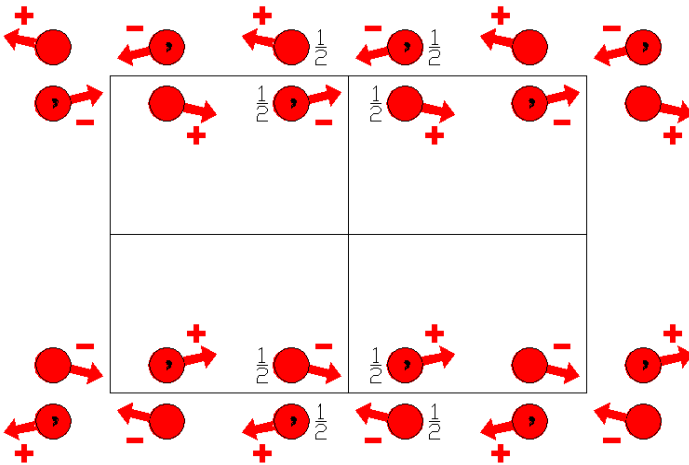
$A_{2a} mm2$

38.6.270

$mm21'$

$A_{2a} mm2$

Orthorhombic



**Origin** on  $mm2$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                  |                                  |                                  |
|--------------------|----------------------------------|----------------------------------|----------------------------------|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $m_x,0,z$<br>( $m_y$  0,0,0) | (4) $m_y,0,z$<br>( $m_x$  0,0,0) |
|--------------------|----------------------------------|----------------------------------|----------------------------------|

For  $(0,1/2,1/2)$  + set

- |                                     |  |   |   |
|-------------------------------------|--|---|---|
| (1) $t(0,1/2,1/2)$<br>(1 0,1/2,1/2) | (2) 2 $(0,0,1/2) 0,1/4,z$<br>( $2_z$  0,1/2,1/2) | (3) $c(0,0,1/2) x,1/4,z$<br>( $m_y$  0,1/2,1/2) | (4) $n(0,1/2,1/2) 0,y,z$<br>( $m_x$  0,1/2,1/2) |
|-------------------------------------|--|---|---|

For  $(1,0,0)'$  + set

- |                               |                                      |   |                                      |
|-------------------------------|--------------------------------------|---|--------------------------------------|
| (1) $t'(1,0,0)$<br>(1 1,0,0)' | (2) $2' 1/2,0,z$<br>( $2_z$  1,0,0)' | (3) $a'(1,0,0) x,0,z$<br>( $m_y$  1,0,0)' | (4) $m' 1/2,y,z$<br>( $m_x$  1,0,0)' |
|-------------------------------|--------------------------------------|---|--------------------------------------|

For  $(1,1/2,1/2)'$  + set

- |                                       |   |   |   |
|---------------------------------------|---|---|---|
| (1) $t'(1,1/2,1/2)$<br>(1 1,1/2,1/2)' | (2) $2'(0,0,1/2) 1/2,1/4,z$<br>( $2_z$  1,1/2,1/2)' | (3) $n'(1,0,1/2) x,1/4,z$<br>( $m_y$  1,1/2,1/2)' | (4) $n'(0,1/2,1/2) 1/2,y,z$<br>( $m_x$  1,1/2,1/2)' |
|---------------------------------------|---|---|---|

**Generators selected** (1); t(1,0,0)'; t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

### Positions

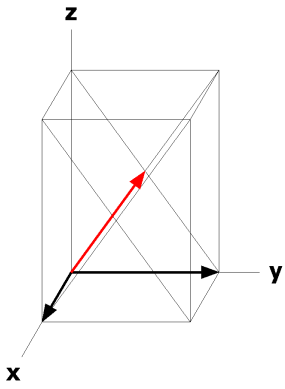
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (1,0,0)'	(0,1/2,1/2) + (1,1/2,1/2)'	
16 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $x, \bar{y}, z$ [ $\bar{u}, v, \bar{w}$ ]	(4) $\bar{x}, y, z$ [ $u, \bar{v}, \bar{w}$ ]
8 e m'..	1/2,y,z [0,v,w]	1/2, $\bar{y}, z$ [0,v, $\bar{w}$ ]		
8 d m..	0,y,z [u,0,0]	0, $\bar{y}, z$ [ $\bar{u}, 0, 0$ ]		
8 c .m.	x,0,z [0,v,0]	$\bar{x}, 0, z$ [0, $\bar{v}, 0$ ]		
4 b m'm2'	1/2,0,z [0,v,0]			
4 a mm2	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



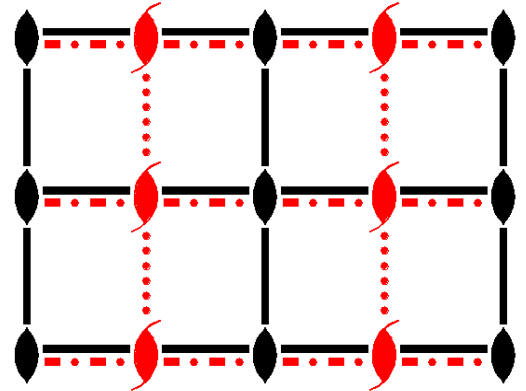
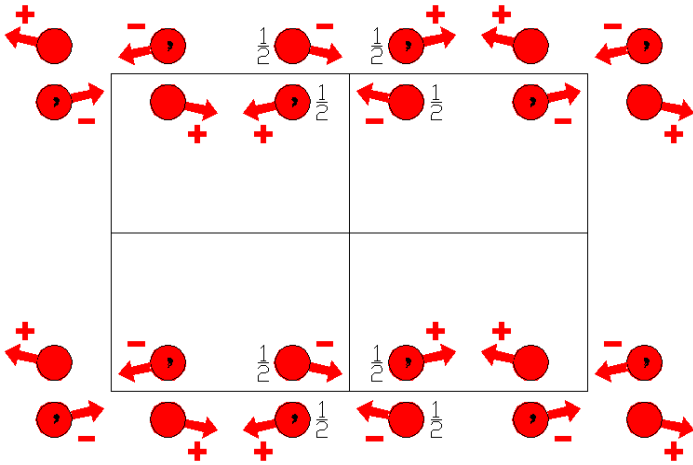
$A_p mm2$

38.7.271

$mm21'$

$A_p mm2$

Orthorhombic



**Origin** on  $mm2$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) m  $x,0,z$   
( $m_y$ |0,0,0)

(4) m  $0,y,z$   
( $m_x$ |0,0,0)

For  $(0,1/2,1/2)'$  + set

(1)  $t' (0,1/2,1/2)$   
(1| $0,1/2,1/2$ )'

(2)  $2' (0,0,1/2) \ 0,1/4,z$   
( $2_z$ | $0,1/2,1/2$ )'

(3)  $c' (0,0,1/2) \ x,1/4,z$   
( $m_y$ | $0,1/2,1/2$ )'

(4)  $n' (0,1/2,1/2) \ 0,y,z$   
( $m_x$ | $0,1/2,1/2$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2)'; (2); (3).

### Positions

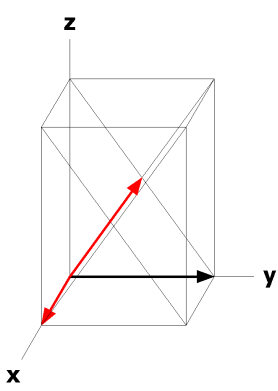
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2)' +		
8 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y}$ ,z [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
4 e m..	1/2,y,z [u,0,0]	1/2, $\bar{y}$ ,z [ $\bar{u},0,0$ ]		
4 d m..	0,y,z [u,0,0]	0, $\bar{y}$ ,z [ $\bar{u},0,0$ ]		
4 c .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]		
2 b mm2	1/2,0,z [0,0,0]			
2 a mm2	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



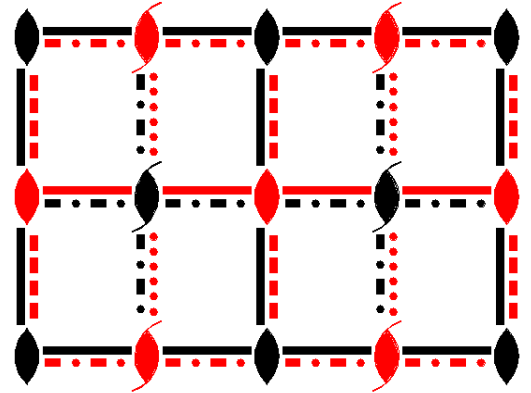
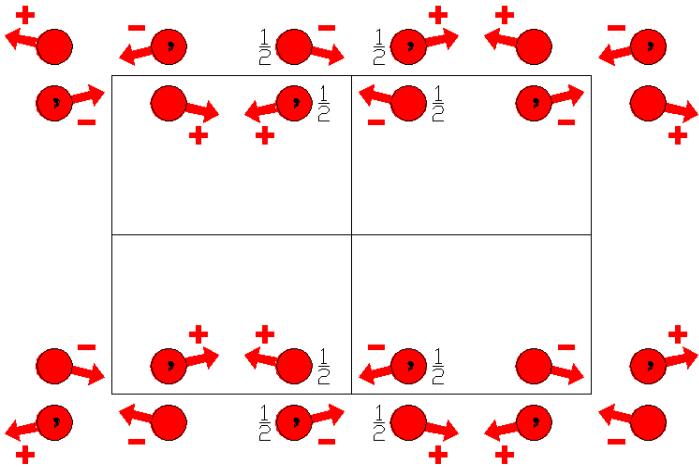
$A_1mm2$

38.8.272

$mm21'$

$A_1mm2$

Orthorhombic



Origin on  $mm2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) m $x,0,z$<br>(m <sub>y</sub>  0,0,0) | (4) m $0,y,z$<br>(m <sub>x</sub>  0,0,0) |
|--------------------|--|--|--|

For  $(0,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' $(0,1/2,1/2)$<br>(1 0,1/2,1/2)' | (2) 2' $(0,0,1/2) 0,1/4,z$<br>(2 <sub>z</sub>  0,1/2,1/2)' | (3) c' $(0,0,1/2) x,1/4,z$<br>(m <sub>y</sub>  0,1/2,1/2)' | (4) n' $(0,1/2,1/2) 0,y,z$<br>(m <sub>x</sub>  0,1/2,1/2)' |
|--|--|--|--|

For  $(1,0,0)'$  + set

- |                                |  |  |  |
|--------------------------------|--|--|--|
| (1) t' $(1,0,0)$<br>(1 1,0,0)' | (2) 2' $1/2,0,z$<br>(2 <sub>z</sub>  1,0,0)' | (3) a' $(1,0,0) x,0,z$<br>(m <sub>y</sub>  1,0,0)' | (4) m' $1/2,y,z$<br>(m <sub>x</sub>  1,0,0)' |
|--------------------------------|--|--|--|

For  $(1,1/2,1/2)$  + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t $(1,1/2,1/2)$<br>(1 1,1/2,1/2) | (2) 2 $(0,0,1/2) 1/2,1/4,z$<br>(2 <sub>z</sub>  1,1/2,1/2) | (3) n $(1,0,1/2) x,1/4,z$<br>(m <sub>y</sub>  1,1/2,1/2) | (4) n $(0,1/2,1/2) 1/2,y,z$<br>(m <sub>x</sub>  1,1/2,1/2) |
|--------------------------------------|--|--|--|



**Generators selected** (1); t(1,0,0)'; t(0,1,0); t(0,0,1); t(0,1/2,1/2)'; (2); (3).

### Positions

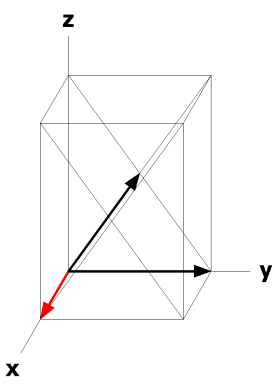
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (1,0,0)'	(0,1/2,1/2)' (1,1/2,1/2) +	
16 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 e m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0,v, $\bar{w}$ ]		
8 d m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]		
8 c .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]		
4 b m'm2'	1/2,0,z [0,v,0]			
4 a mm2	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



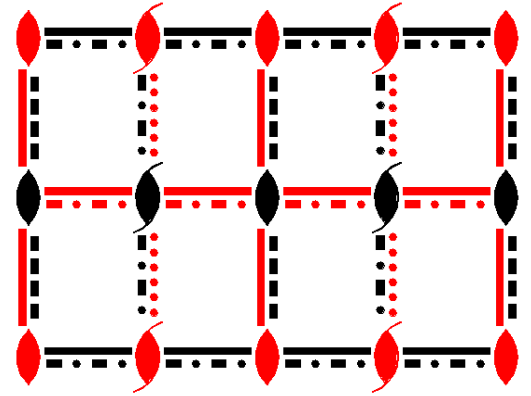
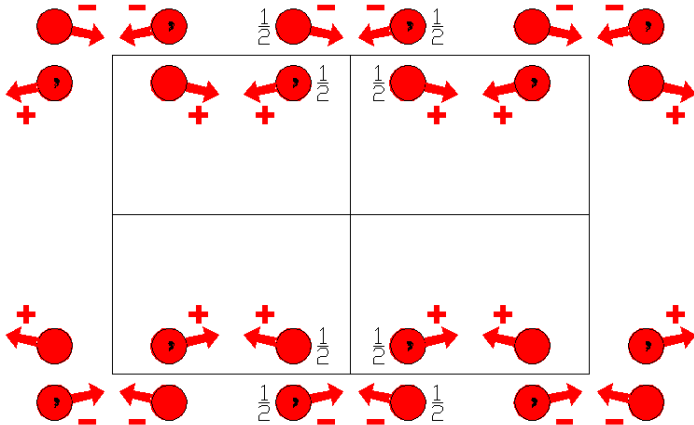
$A_{2a} mm'2'$

38.9.273

$mm21'$

$A_{2a} mm'2'$

Orthorhombic



Origin on  $mm'2'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For  $(0,0,0)$  + set

- |                      |                                      |                                      |                                    |
|----------------------|--------------------------------------|--------------------------------------|------------------------------------|
| (1) $1$<br>(1 0,0,0) | (2) $2'$ $0,0,z$<br>( $2_z$  0,0,0)' | (3) $m'$ $x,0,z$<br>( $m_y$  0,0,0)' | (4) $m$ $0,y,z$<br>( $m_x$  0,0,0) |
|----------------------|--------------------------------------|--------------------------------------|------------------------------------|

For  $(0,1/2,1/2)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t$ $(0,1/2,1/2)$<br>(1 0,1/2,1/2) | (2) $2'$ $(0,0,1/2) 0,1/4,z$<br>( $2_z$  0,1/2,1/2)' | (3) $c'$ $(0,0,1/2) x,1/4,z$<br>( $m_y$  0,1/2,1/2)' | (4) $n$ $(0,1/2,1/2) 0,y,z$<br>( $m_x$  0,1/2,1/2) |
|--|--|--|--|

For  $(1,0,0)$  + set

- |                                  |                                      |  |  |
|----------------------------------|--------------------------------------|--|--|
| (1) $t'$ $(1,0,0)$<br>(1 1,0,0)' | (2) $2$ $1/2,0,z$<br>( $2_z$  1,0,0) | (3) $a$ $(1,0,0) x,0,z$<br>( $m_y$  1,0,0) | (4) $m'$ $1/2,y,z$<br>( $m_x$  1,0,0)' |
|----------------------------------|--------------------------------------|--|--|

For  $(1,1/2,1/2)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1,1/2,1/2)$<br>(1 1,1/2,1/2)' | (2) $2$ $(0,0,1/2) 1/2,1/4,z$<br>( $2_z$  1,1/2,1/2) | (3) $n$ $(1,0,1/2) x,1/4,z$<br>( $m_y$  1,1/2,1/2) | (4) $n'$ $(0,1/2,1/2) 1/2,y,z$<br>( $m_x$  1,1/2,1/2)' |
|--|--|--|--|

**Generators selected** (1);  $t(1,0,0)'$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0,1/2,1/2)$ ; (2); (3).

### Positions

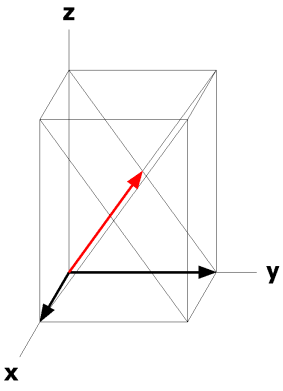
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		$(0,0,0) +$ $(1,0,0)'$ +	$(0,1/2,1/2) +$ $(1,1/2,1/2)'$ +	
16 f 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [u,v,\bar{w}]$	(3) $x,\bar{y},z [u,\bar{v},w]$	(4) $\bar{x},y,z [u,\bar{v},\bar{w}]$
8 e $m'..$	$1/2,y,z [0,v,w]$	$1/2,\bar{y},z [0,\bar{v},w]$		
8 d $m..$	$0,y,z [u,0,0]$	$0,\bar{y},z [u,0,0]$		
8 c $.m'$	$x,0,z [u,0,w]$	$\bar{x},0,z [u,0,\bar{w}]$		
4 b $m'm'2$	$1/2,0,z [0,0,w]$			
4 a $mm'2'$	$0,0,z [u,0,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $p2m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $1/2,0,z$

Along  $[1,0,0]$   $c1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

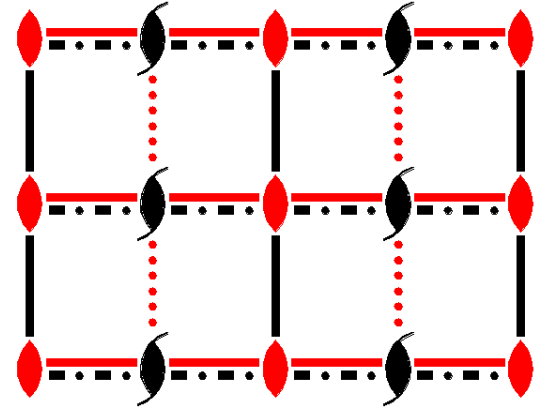
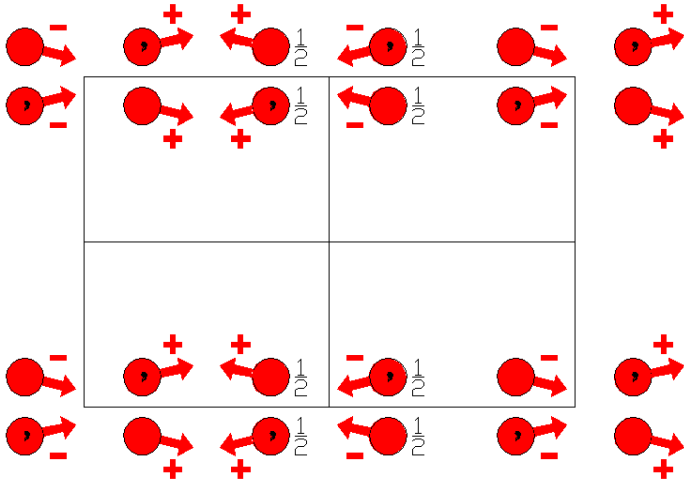
Along  $[0,1,0]$   $p_{2a}1m1$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $0,y,0$



$A_p m'm2'$   
38.10.274

$mm21'$   
 $A_p m'm2'$

Orthorhombic



Origin on  $m'm2'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                      |                                    |                                      |
|--------------------|--------------------------------------|------------------------------------|--------------------------------------|
| (1) 1<br>(1 0,0,0) | (2) $2'_z$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $m_x$ x,0,z<br>( $m_x$  0,0,0) | (4) $m'_y$ 0,y,z<br>( $m_x$  0,0,0)' |
|--------------------|--------------------------------------|------------------------------------|--------------------------------------|

For  $(0,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (0,1/2,1/2)<br>(1 0,1/2,1/2)' | (2) $2$ (0,0,1/2) 0,1/4,z<br>( $2_z$  0,1/2,1/2) | (3) $c'_x$ (0,0,1/2) x,1/4,z<br>( $m_y$  0,1/2,1/2)' | (4) $n$ (0,1/2,1/2) 0,y,z<br>( $m_x$  0,1/2,1/2) |
|--|--|--|--|

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0,1/2,1/2)'$ ; (2); (3).

### Positions

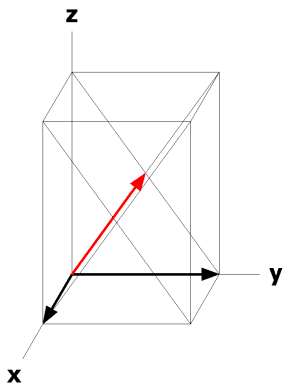
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2)' +		
8 f 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [u,v,\bar{w}]$	(3) $x,\bar{y},z [\bar{u},v,\bar{w}]$	(4) $\bar{x},y,z [\bar{u},v,w]$
4 e $m'..$	$1/2,y,z [0,v,w]$	$1/2,\bar{y},z [0,v,\bar{w}]$		
4 d $m'..$	$0,y,z [0,v,w]$	$0,\bar{y},z [0,v,\bar{w}]$		
4 c $.m.$	$x,0,z [0,v,0]$	$\bar{x},0,z [0,v,0]$		
2 b $m' m 2'$	$1/2,0,z [0,v,0]$			
2 a $m' m 2'$	$0,0,z [0,v,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $p_{2a} \cdot 2m' m'$   
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c_p \cdot 1m1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

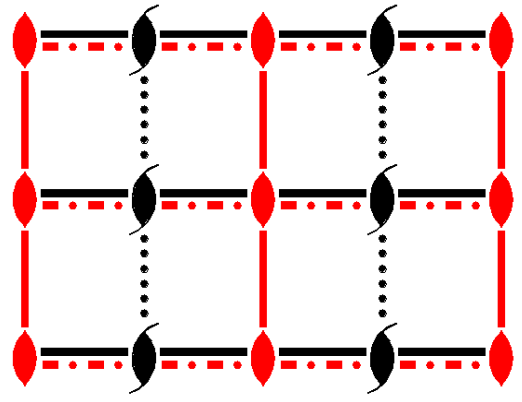
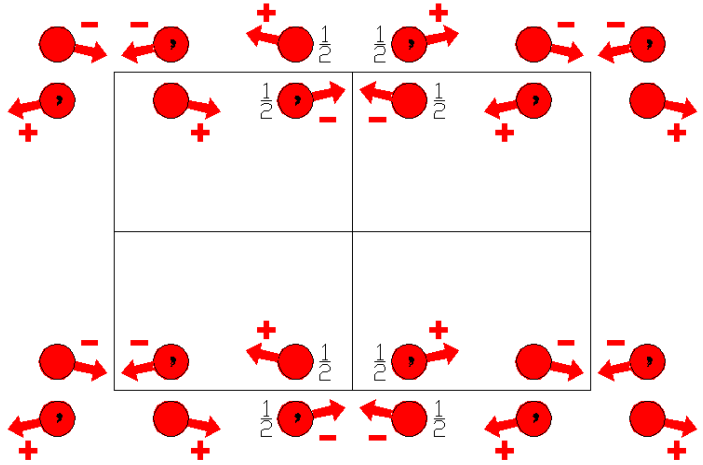
Along  $[0,1,0]$   $p1m11'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $0,y,0$



$A_p mm'2'$   
38.11.275

$mm21'$   
 $A_p mm'2'$

Orthorhombic



**Origin** on  $mm'2'$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2)  $2'_z$  0,0,z  
( $2_z$ |0,0,0)'

(3)  $m'_x$  x,0,z  
( $m_y$ |0,0,0)'

(4)  $m'_y$  0,y,z  
( $m_x$ |0,0,0)

For  $(0,1/2,1/2)'$  + set

(1)  $t'_z$  (0,1/2,1/2)  
(1|0,1/2,1/2)'

(2)  $2'_z$  (0,0,1/2) 0,1/4,z  
( $2_z$ |0,1/2,1/2)

(3)  $c$  (0,0,1/2) x,1/4,z  
( $m_y$ |0,1/2,1/2)

(4)  $n'_z$  (0,1/2,1/2) 0,y,z  
( $m_x$ |0,1/2,1/2)'

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0,1/2,1/2)'$ ; (2); (3).

### Positions

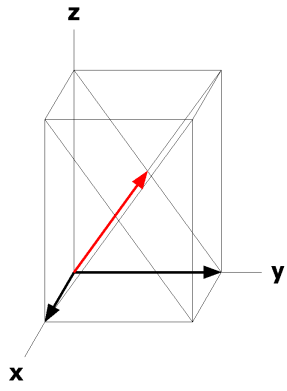
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2)' +		
8 f 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [u,v,\bar{w}]$	(3) $x,\bar{y},z [u,\bar{v},w]$	(4) $\bar{x},y,z [u,\bar{v},\bar{w}]$
4 e m..	$1/2,y,z [u,0,0]$	$1/2,\bar{y},z [u,0,0]$		
4 d m..	$0,y,z [u,0,0]$	$0,\bar{y},z [u,0,0]$		
4 c .m'	$x,0,z [u,0,w]$	$\bar{x},0,z [u,0,\bar{w}]$		
2 b $mm'2'$	$1/2,0,z [u,0,0]$			
2 a $mm'2'$	$0,0,z [u,0,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $p_{2a}2mm$   
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at  $0,1/4,z$

Along  $[1,0,0]$   $c1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $p_{2b}1m1$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $0,y,0$



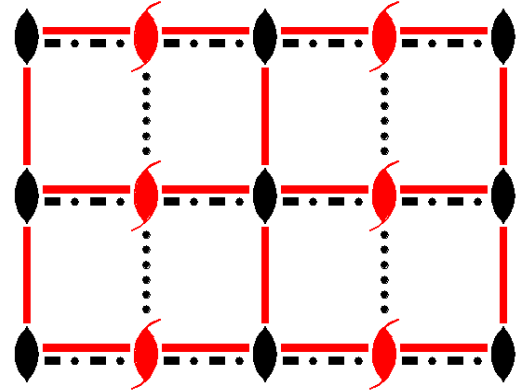
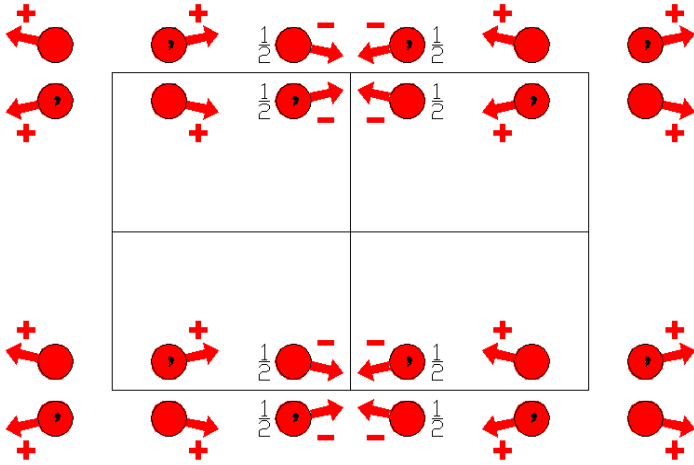
$A_p m'm'2$

38.12.276

$mm21'$

$A_p m'm'2$

Orthorhombic



Origin on  $m'm'2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
(2<sub>z</sub>|0,0,0)

(3)  $m'_x$   $x,0,z$   
( $m'_y$ |0,0,0)'

(4)  $m'_y$   $0,y,z$   
( $m'_x$ |0,0,0)'

For  $(0,1/2,1/2)'$  + set

(1)  $t'$   $(0,1/2,1/2)$   
(1|0,1/2,1/2)'

(2) 2'  $(0,0,1/2)$   $0,1/4,z$   
(2<sub>z</sub>|0,1/2,1/2)'

(3)  $c$   $(0,0,1/2)$   $x,1/4,z$   
( $m'_y$ |0,1/2,1/2)

(4)  $n$   $(0,1/2,1/2)$   $0,y,z$   
( $m'_x$ |0,1/2,1/2)



**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0,1/2,1/2)'$ ; (2); (3).

### Positions

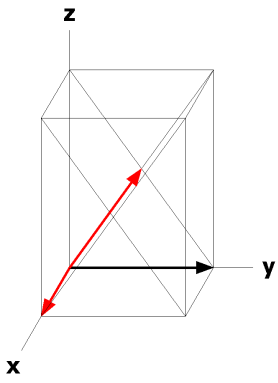
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(0,1/2,1/2)' +	
8 f 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $x,\bar{y},z [u,\bar{v},w]$	(4) $\bar{x},y,z [\bar{u},v,w]$
4 e $m'..$	$1/2,y,z [0,v,w]$	$1/2,\bar{y},z [0,\bar{v},w]$		
4 d $m'..$	$0,y,z [0,v,w]$	$0,\bar{y},z [0,\bar{v},w]$		
4 c $.m'$	$x,0,z [u,0,w]$	$\bar{x},0,z [\bar{u},0,w]$		
2 b $m' m' 2$	$1/2,0,z [0,0,w]$			
2 a $m' m' 2$	$0,0,z [0,0,w]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $p_{2a} \cdot 2m' m'$   
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c_p \cdot 1m' 1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $p_{2b} \cdot 1m' 1$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $0,y,0$



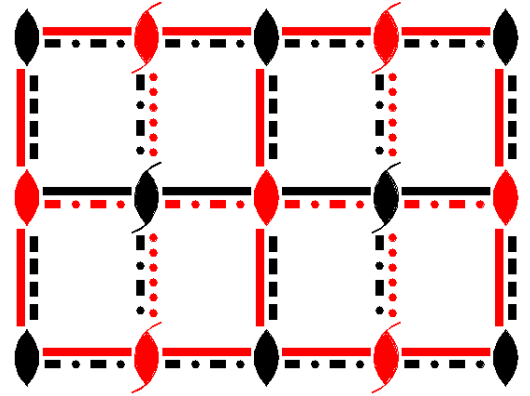
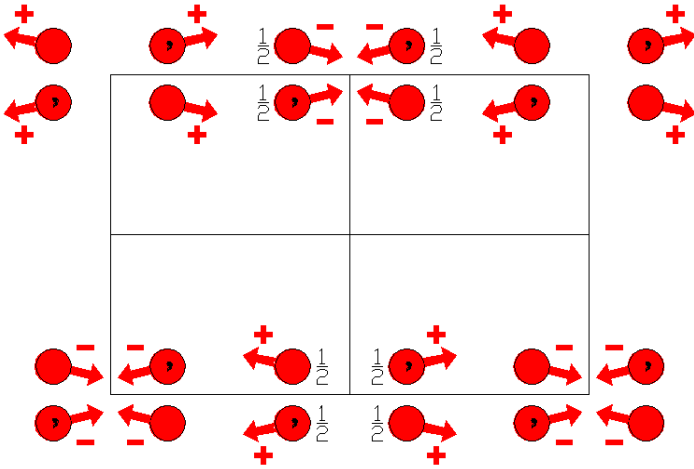
$A_1 m' m' 2$

38.13.277

$mm21'$

$A_1 m' m' 2$

Orthorhombic



**Origin** on  $m' m' 2$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |                                      |                                      |
|--------------------|--|--------------------------------------|--------------------------------------|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) $m'$ $x,0,z$<br>( $m_y$  0,0,0)' | (4) $m'$ $0,y,z$<br>( $m_x$  0,0,0)' |
|--------------------|--|--------------------------------------|--------------------------------------|

For  $(0,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(0,1/2,1/2)$<br>(1 0,1/2,1/2)' | (2) 2' $(0,0,1/2) 0,1/4,z$<br>(2 <sub>z</sub>  0,1/2,1/2)' | (3) $c$ $(0,0,1/2) x,1/4,z$<br>( $m_y$  0,1/2,1/2) | (4) $n$ $(0,1/2,1/2) 0,y,z$<br>( $m_x$  0,1/2,1/2) |
|--|--|--|--|

For  $(1,0,0)'$  + set

- |                                  |  |  |                                      |
|----------------------------------|--|--|--------------------------------------|
| (1) $t'$ $(1,0,0)$<br>(1 1,0,0)' | (2) 2' $1/2,0,z$<br>(2 <sub>z</sub>  1,0,0)' | (3) $a$ $(1,0,0) x,0,z$<br>( $m_y$  1,0,0) | (4) $m$ $1/2,y,z$<br>( $m_x$  1,0,0) |
|----------------------------------|--|--|--------------------------------------|

For  $(1,1/2,1/2)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t$ $(1,1/2,1/2)$<br>(1 1,1/2,1/2) | (2) 2 $(0,0,1/2) 1/2,1/4,z$<br>(2 <sub>z</sub>  1,1/2,1/2) | (3) $n'$ $(1,0,1/2) x,1/4,z$<br>( $m_y$  1,1/2,1/2)' | (4) $n'$ $(0,1/2,1/2) 1/2,y,z$<br>( $m_x$  1,1/2,1/2)' |
|--|--|--|--|

**Generators selected** (1); t(1,0,0)'; t(0,1,0); t(0,0,1); t(0,1/2,1/2)'; (2); (3).

### Positions

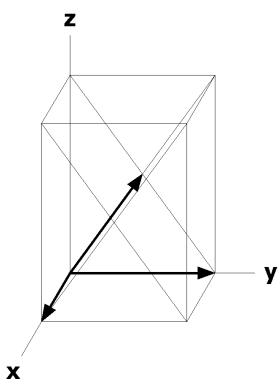
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (1,0,0)'	(0,1/2,1/2)' (1,1/2,1/2) +	
16 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 e m..	1/2,y,z [u,0,0]	1/2, $\bar{y},z$ [u,0,0]		
8 d m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]		
8 c .m'.	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]		
4 b mm'2'	1/2,0,z [u,0,0]			
4 a m'm'2	0,0,z [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/2,1/4,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

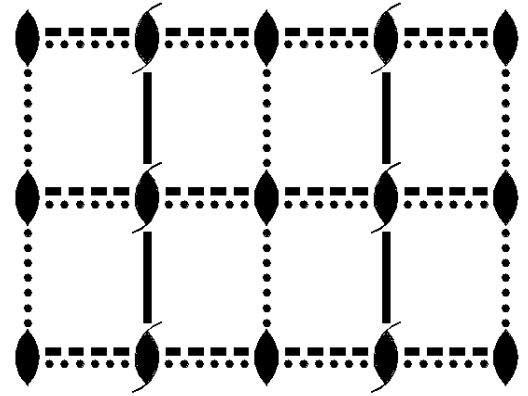
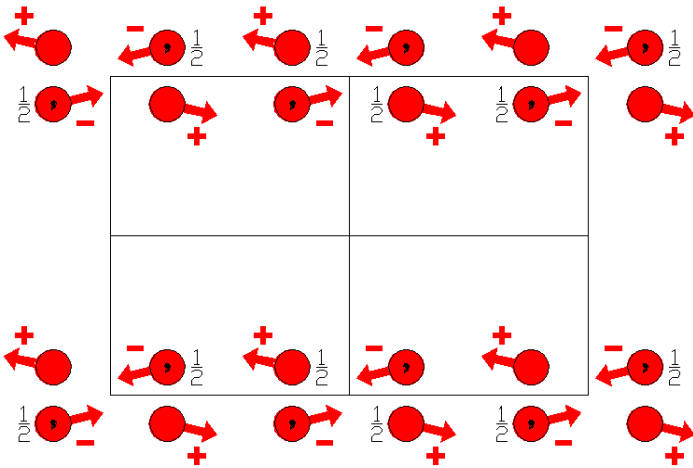
Along [0,1,0] p<sub>c</sub>-1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 1/2,y,0



Abm2  
39.1.278

mm2  
Abm2

Orthorhombic



Origin on bc2

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) m x,1/4,z<br>(m <sub>y</sub>  0,1/2,0) | (4) b (0,1/2,0) 0,y,z<br>(m <sub>x</sub>  0,1/2,0) |
|--------------------|--|--|--|

For (0,1/2,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2) | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2) | (3) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (4) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) |
|------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

### Positions

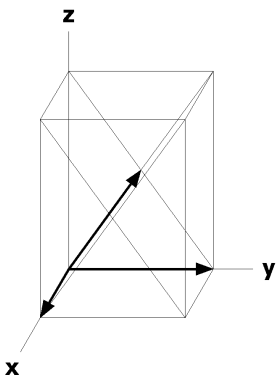
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2) +		
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]
4 c .m.	x,1/4,z [0,v,0]	$\bar{x},3/4,z$ [0, $\bar{v}$ ,0]		
4 b ..2	1/2,0,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]		
4 a ..2	0,0,z [0,0,w]	0,1/2,z [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a^*}1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Abm21'

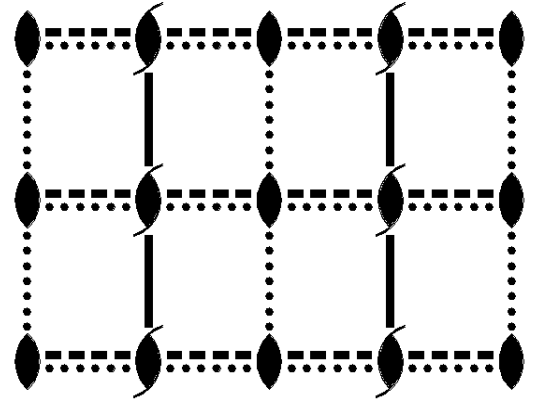
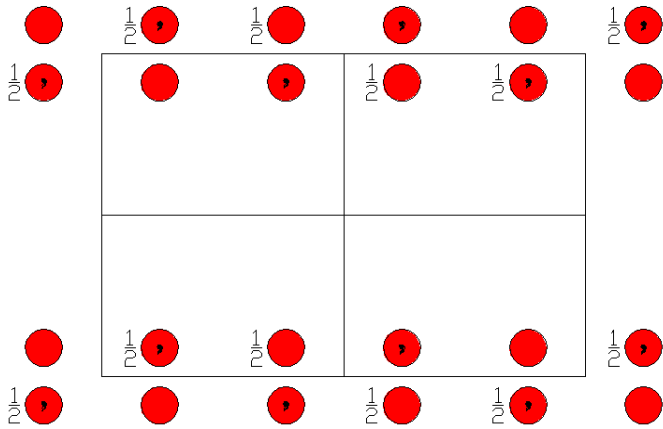
mm21'

Orthorhombic

39.2.279

Abm21'

1'



Origin on bc21'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) m x,1/4,z<br>(m <sub>y</sub>  0,1/2,0) | (4) b (0,1/2,0) 0,y,z<br>(m <sub>x</sub>  0,1/2,0) |
|--------------------|--|--|--|

For (0,1/2,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2) | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2) | (3) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (4) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) |
|------------------------------------|--|--|--|

For (0,0,0)' + set

- |                      |  |  |  |
|----------------------|--|--|--|
| (1) 1'<br>(1 0,0,0)' | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) m' x,1/4,z<br>(m <sub>y</sub>  0,1/2,0)' | (4) b' (0,1/2,0) 0,y,z<br>(m <sub>x</sub>  0,1/2,0)' |
|----------------------|--|--|--|

For (0,1/2,1/2)' + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t' (0,1/2,1/2)<br>(1 0,1/2,1/2)' | (2) 2' (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)' | (3) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (4) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |
|--------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3); 1'.

### Positions

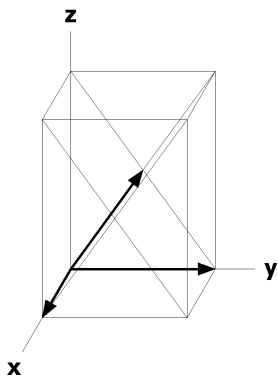
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) + (0,0,0)' +	(0,1/2,1/2) + (0,1/2,1/2)' +		
8	d 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) x, $\bar{y}+1/2,z$ [0,0,0]	(4) $\bar{x},y+1/2,z$ [0,0,0]
4	c .m.1'	x,1/4,z [0,0,0]	$\bar{x},3/4,z$ [0,0,0]		
4	b ..21'	1/2,0,z [0,0,0]	1/2,1/2,z [0,0,0]		
4	a ..21'	0,0,z [0,0,0]	0,1/2,z [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



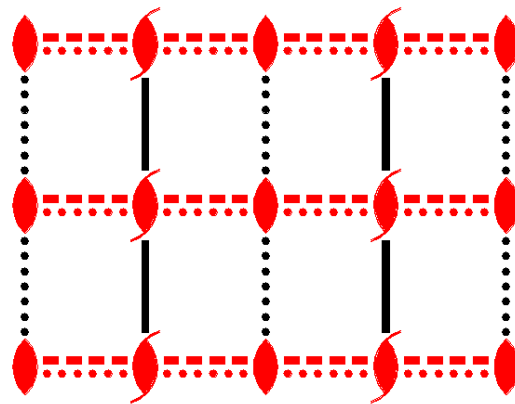
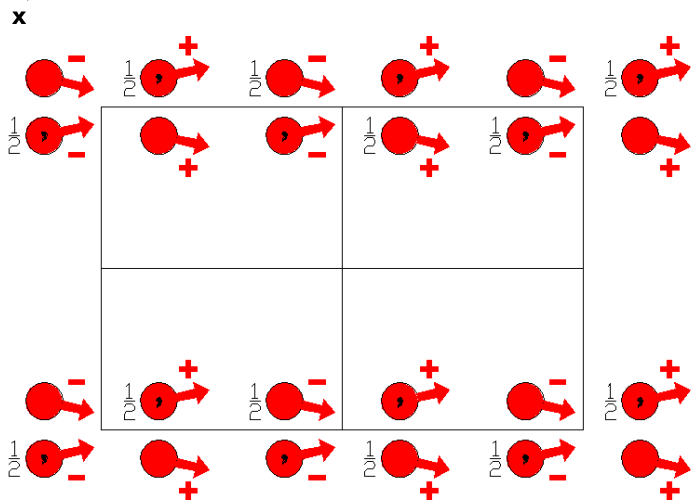
Ab'm2'

39.3.280

m'm2'

Ab'm2'

Orthorhombic



Origin on b'c2'

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

- (1) 1  
(1|0,0,0)
- (2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'
- (3) m x,1/4,z  
(m<sub>y</sub>|0,1/2,0)
- (4) b' (0,1/2,0) 0,y,z  
(m<sub>x</sub>|0,1/2,0)'

For (0,1/2,1/2) + set

- (1) t (0,1/2,1/2)  
(1|0,1/2,1/2)
- (2) 2' (0,0,1/2) 0,1/4,z  
(2<sub>z</sub>|0,1/2,1/2)'
- (3) c (0,0,1/2) x,0,z  
(m<sub>y</sub>|0,0,1/2)
- (4) c' (0,0,1/2) 0,y,z  
(m<sub>x</sub>|0,0,1/2)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

**Positions**

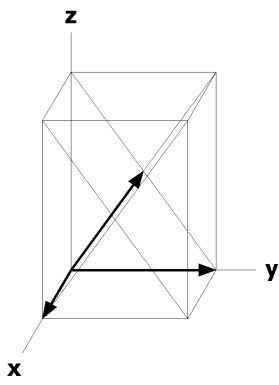
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2) +		
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y+1/2,z$ [ $\bar{u},v,w$ ]
4	c .m.	x,1/4,z [0,v,0]	$\bar{x},3/4,z$ [0,v,0]		
4	b ..2'	1/2,0,z [u,v,0]	1/2,1/2,z [ $\bar{u},v,0$ ]		
4	a ..2'	0,0,z [u,v,0]	0,1/2,z [ $\bar{u},v,0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

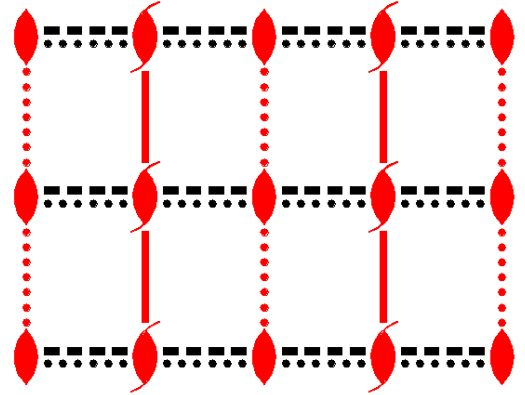
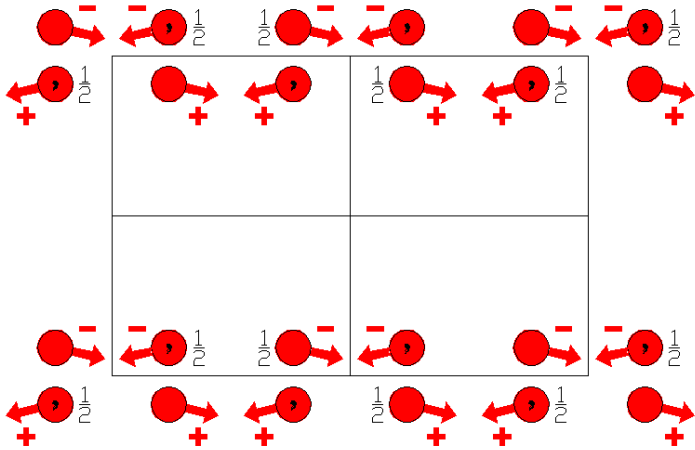
Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Abm'2'  
39.4.281

mm'2'  
Abm'2'

Orthorhombic



Origin on bc'2'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) m' x,1/4,z<br>(m <sub>y</sub>  0,1/2,0)' | (4) b (0,1/2,0) 0,y,z<br>(m <sub>x</sub>  0,1/2,0) |
|--------------------|--|--|--|

For (0,1/2,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2) | (2) 2' (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)' | (3) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (4) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) |
|------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

### Positions

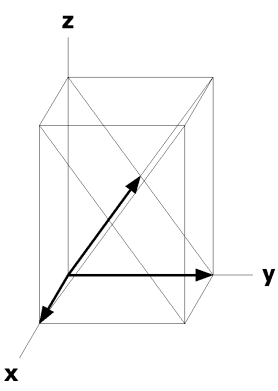
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2) +		
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x,\bar{y}+1/2,z$ [u, $\bar{v}$ ,w]	(4) $\bar{x},y+1/2,z$ [u, $\bar{v},\bar{w}$ ]
4 c .m'	x,1/4,z [u,0,w]	$\bar{x},3/4,z$ [u,0, $\bar{w}$ ]		
4 b ..2'	1/2,0,z [u,v,0]	1/2,1/2,z [u, $\bar{v}$ ,0]		
4 a ..2'	0,0,z [u,v,0]	0,1/2,z [u, $\bar{v}$ ,0]		

### Symmetry of Special Projections

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a\*</sub>1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



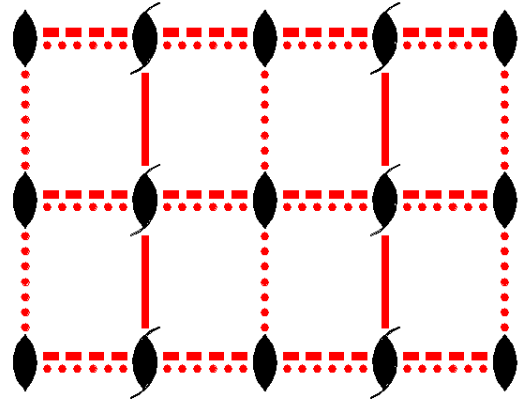
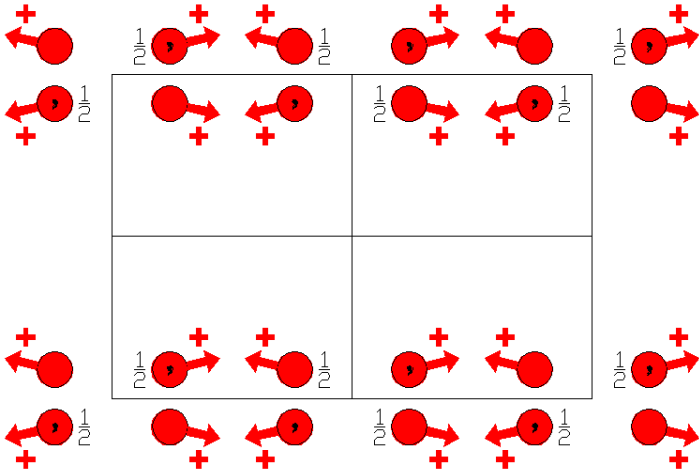
Ab'm'2

m'm'2

Orthorhombic

39.5.282

Ab'm'2



Origin on b'c'2

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

- (1) 1  
(1|0,0,0)
- (2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)
- (3) m' x,1/4,z  
(m<sub>y</sub>|0,1/2,0)'
- (4) b' (0,1/2,0) 0,y,z  
(m<sub>x</sub>|0,1/2,0)'

For (0,1/2,1/2) + set

- (1) t (0,1/2,1/2)  
(1|0,1/2,1/2)
- (2) 2 (0,0,1/2) 0,1/4,z  
(2<sub>z</sub>|0,1/2,1/2)
- (3) c' (0,0,1/2) x,0,z  
(m<sub>y</sub>|0,0,1/2)'
- (4) c' (0,0,1/2) 0,y,z  
(m<sub>x</sub>|0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

**Positions**

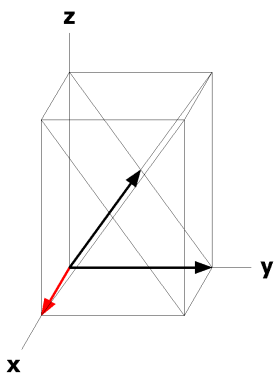
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2) +		
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x,\bar{y}+1/2,z$ [ $u,\bar{v},w$ ]	(4) $\bar{x},y+1/2,z$ [ $\bar{u},v,w$ ]
4 c .m'	x,1/4,z [u,0,w]	$\bar{x},3/4,z$ [ $\bar{u},0,w$ ]		
4 b ..2	1/2,0,z [0,0,w]	1/2,1/2,z [0,0,w]		
4 a ..2	0,0,z [0,0,w]	0,1/2,z [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p1m'1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



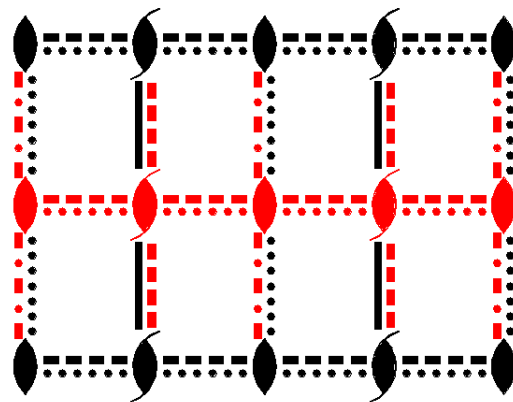
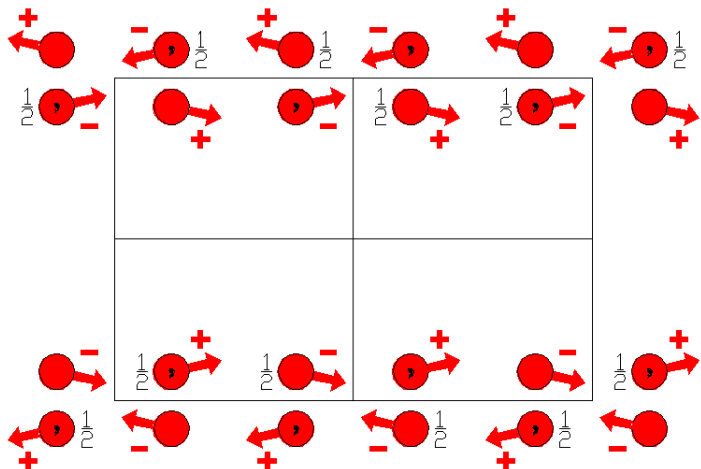
$A_{2a}bm2$

$mm21'$

Orthorhombic

39.6.283

$A_{2a}bm2$



Origin on  $bc2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) m $x,1/4,z$<br>(m <sub>y</sub>  0,1/2,0) | (4) b $(0,1/2,0) 0,y,z$<br>(m <sub>x</sub>  0,1/2,0) |
|--------------------|--|--|--|

For  $(0,1/2,1/2)$  + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t $(0,1/2,1/2)$<br>(1 0,1/2,1/2) | (2) 2 $(0,0,1/2) 0,1/4,z$<br>(2 <sub>z</sub>  0,1/2,1/2) | (3) c $(0,0,1/2) x,0,z$<br>(m <sub>y</sub>  0,0,1/2) | (4) c $(0,0,1/2) 0,y,z$<br>(m <sub>x</sub>  0,0,1/2) |
|--------------------------------------|--|--|--|

For  $(1,0,0)'$  + set

- |                                |  |  |  |
|--------------------------------|--|--|--|
| (1) t' $(1,0,0)$<br>(1 1,0,0)' | (2) 2' $1/2,0,z$<br>(2 <sub>z</sub>  1,0,0)' | (3) a' $(1,0,0) x,1/4,z$<br>(m <sub>y</sub>  1,1/2,0)' | (4) b' $(0,1/2,0) 1/2,y,z$<br>(m <sub>x</sub>  1,1/2,0)' |
|--------------------------------|--|--|--|

For  $(1,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' $(1,1/2,1/2)$<br>(1 1,1/2,1/2)' | (2) 2' $(0,0,1/2) 1/2,1/4,z$<br>(2 <sub>z</sub>  1,1/2,1/2)' | (3) n' $(1,0,1/2) x,0,z$<br>(m <sub>y</sub>  1,0,1/2)' | (4) c' $(0,0,1/2) 1/2,y,z$<br>(m <sub>x</sub>  1,0,1/2)' |
|--|--|--|--|

**Generators selected** (1); t(1,0,0)<sup>'</sup>; t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

### Positions

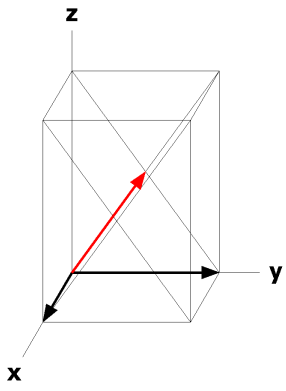
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) + (1,0,0) <sup>'</sup> +	(0,1/2,1/2) + (1,1/2,1/2) <sup>'</sup> +		
16	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y+1/2,z$ [u, $\bar{v},\bar{w}$ ]
8	c .m.	x,1/4,z [0,v,0]	$\bar{x},3/4,z$ [0, $\bar{v},0$ ]		
8	b ..2'	1/2,0,z [u,v,0]	1/2,1/2,z [ $\bar{u},v,0$ ]		
8	a ..2	0,0,z [0,0,w]	0,1/2,z [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>.2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



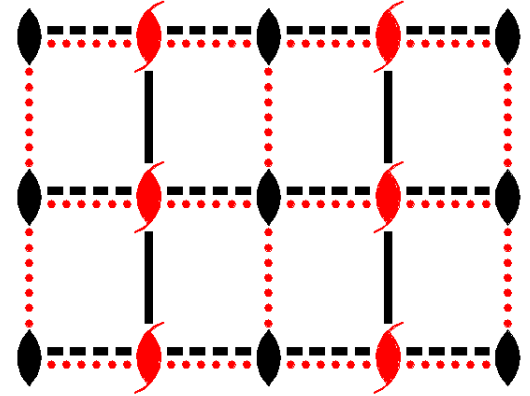
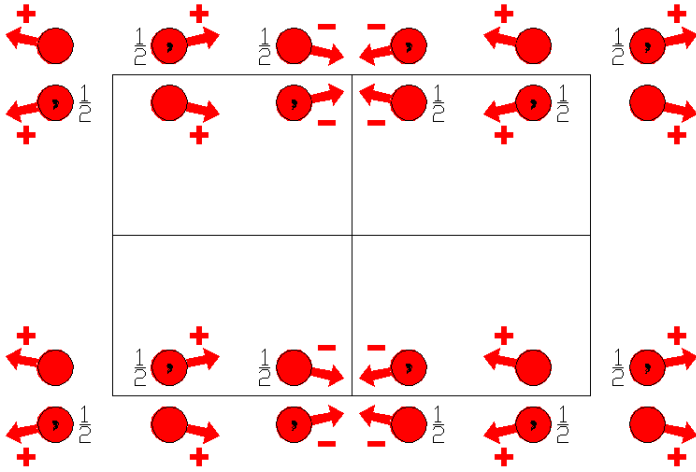
$A_pbm2$

39.7.284

$mm21'$

$A_pbm2$

Orthorhombic



Origin on  $bc'2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) m $x,1/4,z$<br>(m <sub>y</sub>  0,1/2,0) | (4) b $(0,1/2,0) 0,y,z$<br>(m <sub>x</sub>  0,1/2,0) |
|--------------------|--|--|--|

For  $(0,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' $(0,1/2,1/2)$<br>(1 0,1/2,1/2)' | (2) 2' $(0,0,1/2) 0,1/4,z$<br>(2 <sub>z</sub>  0,1/2,1/2)' | (3) c' $(0,0,1/2) x,0,z$<br>(m <sub>y</sub>  0,0,1/2)' | (4) c' $(0,0,1/2) 0,y,z$<br>(m <sub>x</sub>  0,0,1/2)' |
|--|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2)'; (2); (3).

### Positions

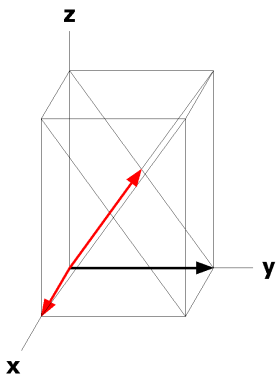
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2)' +		
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]
4	c .m.	x,1/4,z [0,v,0]	$\bar{x},3/4,z$ [0, $\bar{v}$ ,0]		
4	b ..2	1/2,0,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]		
4	a ..2	0,0,z [0,0,w]	0,1/2,z [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1]  $p_{2a^*}2mm$   
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a^*}1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,0

Along [0,1,0]  $p1m11'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



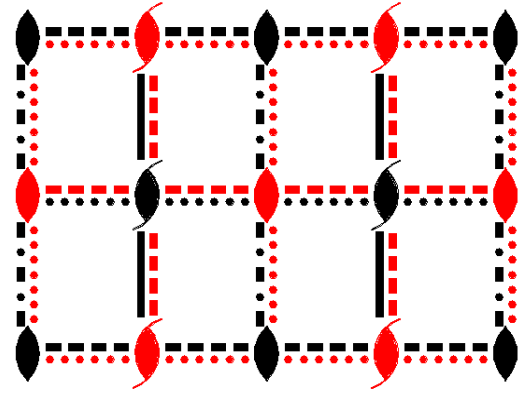
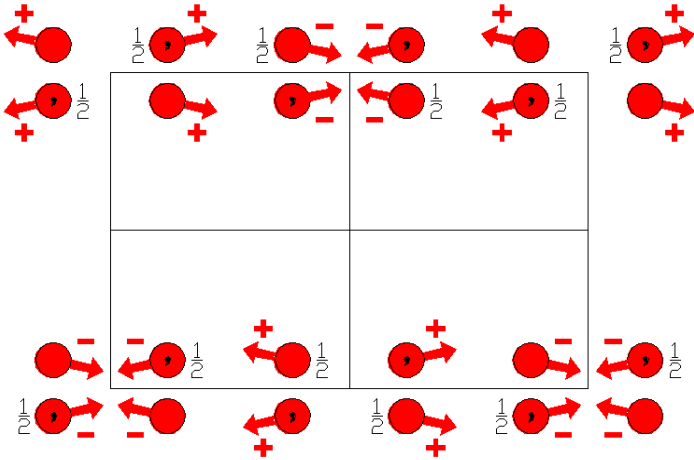
$A_1bm2$

39.8.285

$mm21'$

$A_1bm2$

Orthorhombic



**Origin** on  $bc'2$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) m $x,1/4,z$<br>(m <sub>y</sub>  0,1/2,0) | (4) b $(0,1/2,0) 0,y,z$<br>(m <sub>x</sub>  0,1/2,0) |
|--------------------|--|--|--|

For  $(0,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' $(0,1/2,1/2)$<br>(1 0,1/2,1/2)' | (2) 2' $(0,0,1/2) 0,1/4,z$<br>(2 <sub>z</sub>  0,1/2,1/2)' | (3) c' $(0,0,1/2) x,0,z$<br>(m <sub>y</sub>  0,0,1/2)' | (4) c' $(0,0,1/2) 0,y,z$<br>(m <sub>x</sub>  0,0,1/2)' |
|--|--|--|--|

For  $(1,0,0)'$  + set

- |                                |  |  |  |
|--------------------------------|--|--|--|
| (1) t' $(1,0,0)$<br>(1 1,0,0)' | (2) 2' $1/2,0,z$<br>(2 <sub>z</sub>  1,0,0)' | (3) a' $(1,0,0) x,1/4,z$<br>(m <sub>y</sub>  1,1/2,0)' | (4) b' $(0,1/2,0) 1/2,y,z$<br>(m <sub>x</sub>  1,1/2,0)' |
|--------------------------------|--|--|--|

For  $(1,1/2,1/2)$  + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t $(1,1/2,1/2)$<br>(1 1,1/2,1/2) | (2) 2 $(0,0,1/2) 1/2,1/4,z$<br>(2 <sub>z</sub>  1,1/2,1/2) | (3) n $(1,0,1/2) x,0,z$<br>(m <sub>y</sub>  1,0,1/2) | (4) c $(0,0,1/2) 1/2,y,z$<br>(m <sub>x</sub>  1,0,1/2) |
|--------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0)<sup>'</sup>; t(0,1,0); t(0,0,1); t(0,1/2,1/2)<sup>'</sup>; (2); (3).

### Positions

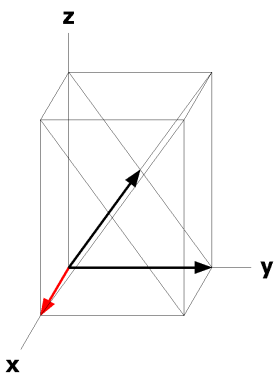
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) + (1,0,0) <sup>'</sup> +	(0,1/2,1/2) <sup>'</sup> + (1,1/2,1/2) +		
16	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y+1/2,z$ [u, $\bar{v},\bar{w}$ ]
8	c .m.	x,1/4,z [0,v,0]	$\bar{x},3/4,z$ [0, $\bar{v},0$ ]		
8	b ..2'	1/2,0,z [u,v,0]	1/2,1/2,z [ $\bar{u},v,0$ ]		
8	a ..2	0,0,z [0,0,w]	0,1/2,z [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>c</sub>2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/2,1/4,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



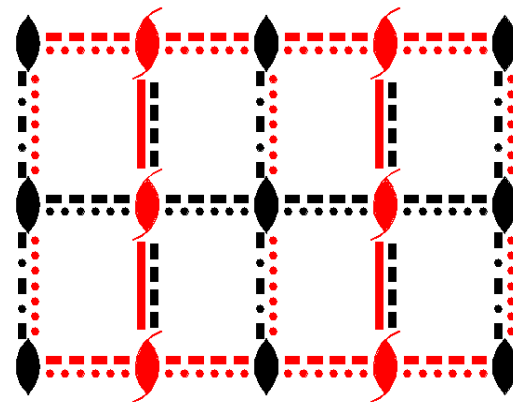
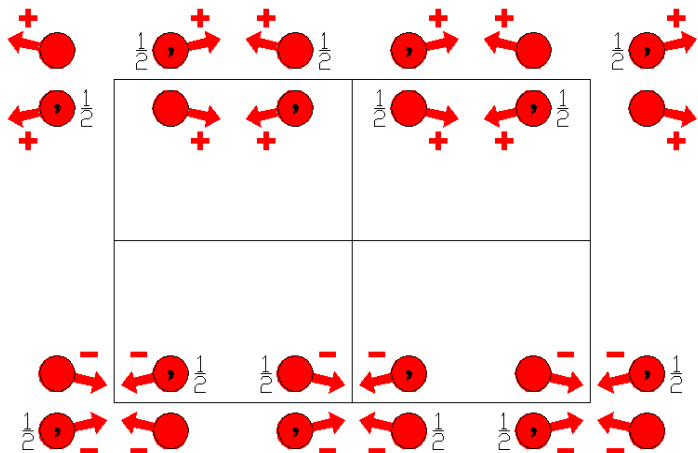
$A_{2a} b'm'2$

$mm21'$

Orthorhombic

39.9.286

$A_{2a} b'm'2$



**Origin** on  $b'c'2$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) m' $x,1/4,z$<br>(m <sub>y</sub>  0,1/2,0)' | (4) b' $(0,1/2,0)$ $0,y,z$<br>(m <sub>x</sub>  0,1/2,0)' |
|--------------------|--|--|--|

For  $(0,1/2,1/2)$  + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t $(0,1/2,1/2)$<br>(1 0,1/2,1/2) | (2) 2 $(0,0,1/2)$ $0,1/4,z$<br>(2 <sub>z</sub>  0,1/2,1/2) | (3) c' $(0,0,1/2)$ $x,0,z$<br>(m <sub>y</sub>  0,0,1/2)' | (4) c' $(0,0,1/2)$ $0,y,z$<br>(m <sub>x</sub>  0,0,1/2)' |
|--------------------------------------|--|--|--|

For  $(1,0,0)$ ' + set

- |                                |  |  |  |
|--------------------------------|--|--|--|
| (1) t' $(1,0,0)$<br>(1 1,0,0)' | (2) 2' $1/2,0,z$<br>(2 <sub>z</sub>  1,0,0)' | (3) a $(1,0,0)$ $x,1/4,z$<br>(m <sub>y</sub>  1,1/2,0) | (4) b $(0,1/2,0)$ $1/2,y,z$<br>(m <sub>x</sub>  1,1/2,0) |
|--------------------------------|--|--|--|

For  $(1,1/2,1/2)$ ' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' $(1,1/2,1/2)$<br>(1 1,1/2,1/2)' | (2) 2' $(0,0,1/2)$ $1/2,1/4,z$<br>(2 <sub>z</sub>  1,1/2,1/2)' | (3) n $(1,0,1/2)$ $x,0,z$<br>(m <sub>y</sub>  1,0,1/2) | (4) c $(0,0,1/2)$ $1/2,y,z$<br>(m <sub>x</sub>  1,0,1/2) |
|--|--|--|--|

**Generators selected** (1);  $t(1,0,0)'$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0,1/2,1/2)$ ; (2); (3).

### Positions

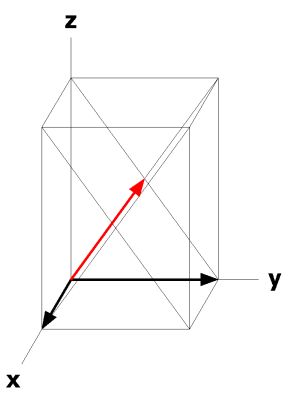
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		$(0,0,0) +$ $(1,0,0)'$ +	$(0,1/2,1/2) +$ $(1,1/2,1/2)'$ +	
16 d 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $x,\bar{y}+1/2,z [u,\bar{v},w]$	(4) $\bar{x},y+1/2,z [\bar{u},v,w]$
8 c $..m'$	$x,1/4,z [u,0,w]$	$\bar{x},3/4,z [\bar{u},0,w]$		
8 b $..2'$	$1/2,0,z [u,v,0]$	$1/2,1/2,z [u,\bar{v},0]$		
8 a $..2$	$0,0,z [0,0,w]$	$0,1/2,z [0,0,w]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p2m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,0,0$

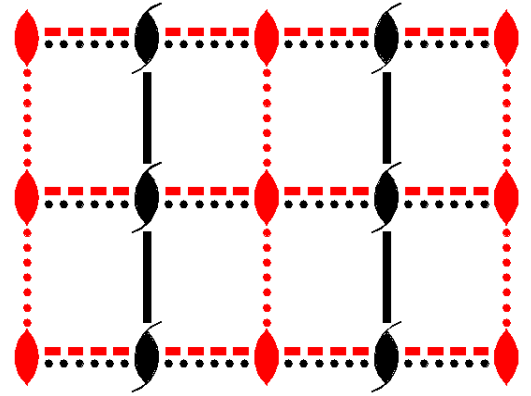
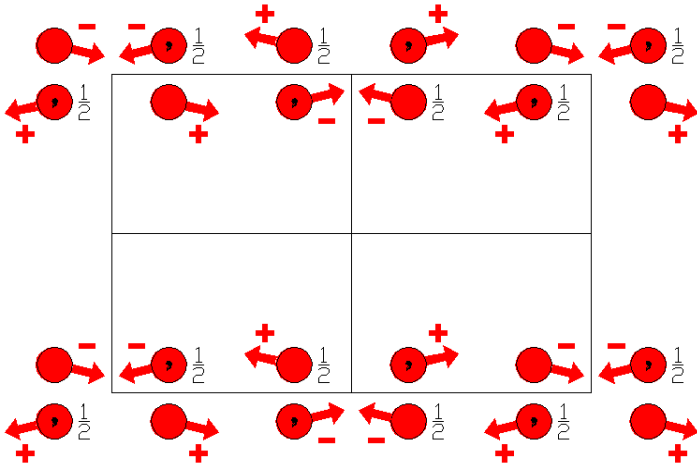
Along  $[0,1,0]$   $p_{2a}1m1$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $1/2,y,0$



$A_p b' m 2'$   
39.10.287

$mm2 1'$   
 $A_p b' m 2'$

Orthorhombic



**Origin** on  $b'c'2'$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                      |  |  |
|--------------------|--------------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) $2'$ $0,0,z$<br>( $2_z$  0,0,0)' | (3) $m$ $x,1/4,z$<br>( $m_y$  0,1/2,0) | (4) $b'$ $(0,1/2,0)$ $0,y,z$<br>( $m_x$  0,1/2,0)' |
|--------------------|--------------------------------------|--|--|

For  $(0,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(0,1/2,1/2)$<br>(1 0,1/2,1/2)' | (2) $2$ $(0,0,1/2)$ $0,1/4,z$<br>( $2_z$  0,1/2,1/2) | (3) $c'$ $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2)' | (4) $c$ $(0,0,1/2)$ $0,y,z$<br>( $m_x$  0,0,1/2) |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2)'; (2); (3).

### Positions

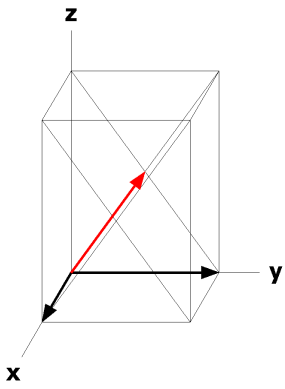
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2)' +		
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y+1/2,z$ [ $\bar{u},v,w$ ]
4 c .m.	x,1/4,z [0,v,0]	$\bar{x},3/4,z$ [0,v,0]		
4 b ..2'	1/2,0,z [u,v,0]	1/2,1/2,z [ $\bar{u},v,0$ ]		
4 a ..2'	0,0,z [u,v,0]	0,1/2,z [ $\bar{u},v,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>\*2mm  
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,1/4,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

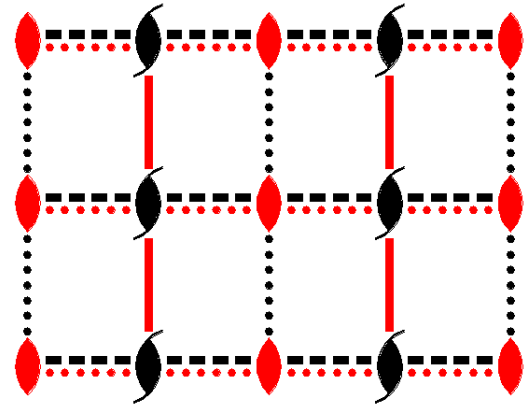
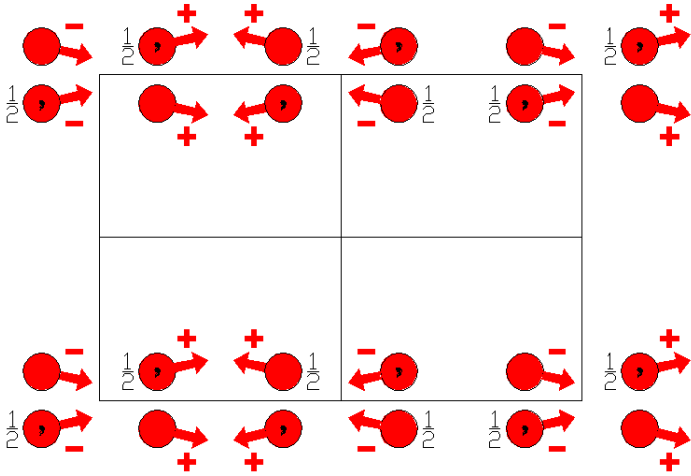
Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$A_pbm'2'$   
39.11.288

$mm21'$   
 $A_pbm'2'$

Orthorhombic



Origin on  $bc2'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                      |  |  |
|--------------------|--------------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) $2'$ $0,0,z$<br>( $2_z$  0,0,0)' | (3) $m'$ $x,1/4,z$<br>( $m_y$  0,1/2,0)' | (4) $b$ $(0,1/2,0)$ $0,y,z$<br>( $m_x$  0,1/2,0) |
|--------------------|--------------------------------------|--|--|

For  $(0,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(0,1/2,1/2)$<br>(1 0,1/2,1/2)' | (2) $2$ $(0,0,1/2)$ $0,1/4,z$<br>( $2_z$  0,1/2,1/2) | (3) $c$ $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2) | (4) $c'$ $(0,0,1/2)$ $0,y,z$<br>( $m_x$  0,0,1/2)' |
|--|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2)'; (2); (3).

### Positions

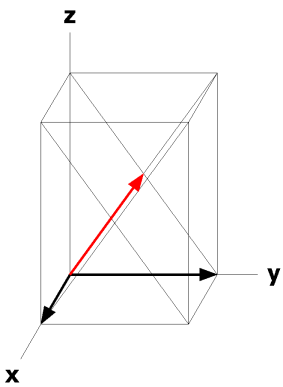
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(0,1/2,1/2)' +	
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x,\bar{y}+1/2,z$ [u, $\bar{v}$ ,w]	(4) $\bar{x},y+1/2,z$ [u, $\bar{v},\bar{w}$ ]
4 c .m'	x,1/4,z [u,0,w]	$\bar{x},3/4,z$ [u,0, $\bar{w}$ ]		
4 b ..2'	1/2,0,z [u,v,0]	1/2,1/2,z [u, $\bar{v}$ ,0]		
4 a ..2'	0,0,z [u,v,0]	0,1/2,z [u, $\bar{v}$ ,0]		

### Symmetry of Special Projections

Along [0,0,1]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,1/4,z

Along [1,0,0]  $p_{2a}1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2b}1m1$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$A_p b' m' 2$

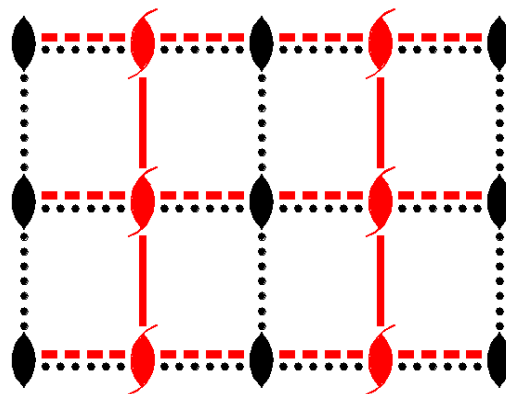
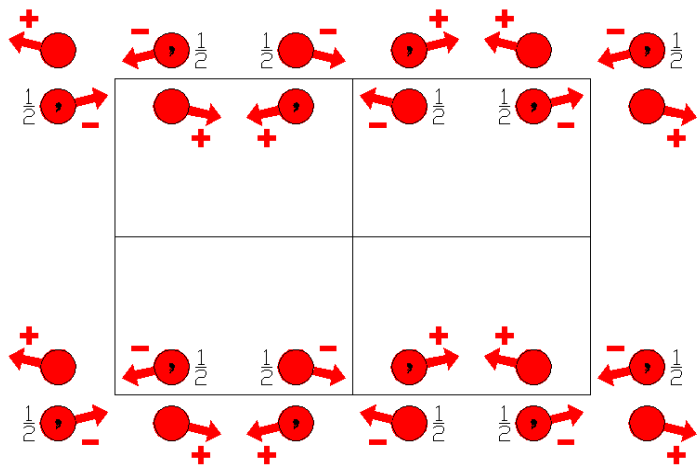
39.12.289

$mm21'$

$A_p b' m' 2$

Orthorhombic

x



Origin on  $b'c2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
(2<sub>z</sub>|0,0,0)

(3)  $m'$   $x,1/4,z$   
( $m_y$ |0,1/2,0)'

(4)  $b'$   $(0,1/2,0)$   $0,y,z$   
( $m_x$ |0,1/2,0)'

For  $(0,1/2,1/2)'$  + set

(1)  $t'$   $(0,1/2,1/2)$   
(1|0,1/2,1/2)'

(2) 2'  $(0,0,1/2)$   $0,1/4,z$   
(2<sub>z</sub>|0,1/2,1/2)'

(3)  $c$   $(0,0,1/2)$   $x,0,z$   
( $m_y$ |0,0,1/2)

(4)  $c$   $(0,0,1/2)$   $0,y,z$   
( $m_x$ |0,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2)'; (2); (3).

### Positions

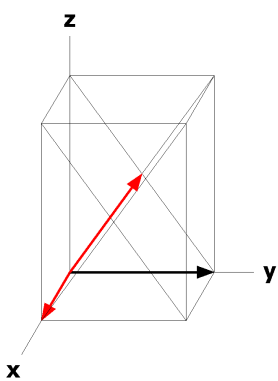
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2)' +		
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x,\bar{y}+1/2,z$ [ $u,\bar{v},w$ ]	(4) $\bar{x},y+1/2,z$ [ $\bar{u},v,w$ ]
4 c .m'	x,1/4,z [u,0,w]	$\bar{x},3/4,z$ [ $\bar{u},0,w$ ]		
4 b ..2	1/2,0,z [0,0,w]	1/2,1/2,z [0,0,w]		
4 a ..2	0,0,z [0,0,w]	0,1/2,z [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2b</sub>1m'1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



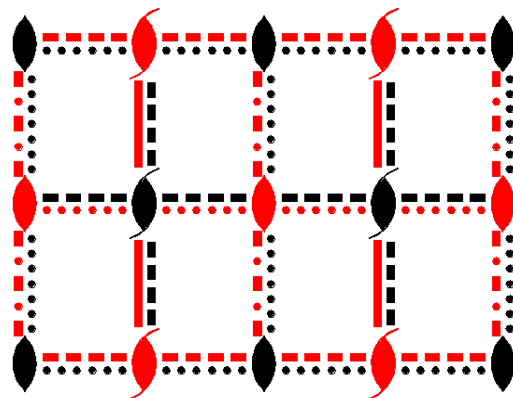
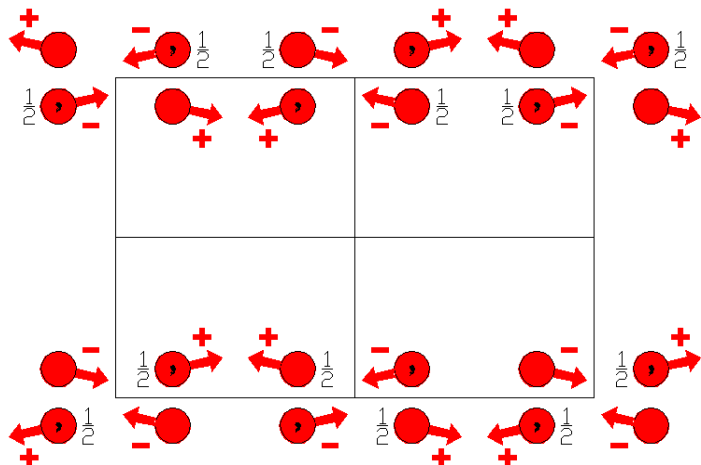
$A_1 b' m' 2$

$mm2 1'$

Orthorhombic

39.13.290

$A_1 b' m' 2$



**Origin** on  $b'c2$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0) +$  set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) m' $x,1/4,z$<br>(m <sub>y</sub>  0,1/2,0)' | (4) b' $(0,1/2,0) 0,y,z$<br>(m <sub>x</sub>  0,1/2,0)' |
|--------------------|--|--|--|

For  $(0,1/2,1/2) +$  set

- |  |  |  |  |
|--|--|--|--|
| (1) t' $(0,1/2,1/2)$<br>(1 0,1/2,1/2)' | (2) 2' $(0,0,1/2) 0,1/4,z$<br>(2 <sub>z</sub>  0,1/2,1/2)' | (3) c $(0,0,1/2) x,0,z$<br>(m <sub>y</sub>  0,0,1/2) | (4) c $(0,0,1/2) 0,y,z$<br>(m <sub>x</sub>  0,0,1/2) |
|--|--|--|--|

For  $(1,0,0) +$  set

- |                                |  |  |  |
|--------------------------------|--|--|--|
| (1) t' $(1,0,0)$<br>(1 1,0,0)' | (2) 2' $1/2,0,z$<br>(2 <sub>z</sub>  1,0,0)' | (3) a $(1,0,0) x,1/4,z$<br>(m <sub>y</sub>  1,1/2,0) | (4) b $(0,1/2,0) 1/2,y,z$<br>(m <sub>x</sub>  1,1/2,0) |
|--------------------------------|--|--|--|

For  $(1,1/2,1/2) +$  set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t $(1,1/2,1/2)$<br>(1 1,1/2,1/2) | (2) 2 $(0,0,1/2) 1/2,1/4,z$<br>(2 <sub>z</sub>  1,1/2,1/2) | (3) n' $(1,0,1/2) x,0,z$<br>(m <sub>y</sub>  1,0,1/2)' | (4) c' $(0,0,1/2) 1/2,y,z$<br>(m <sub>x</sub>  1,0,1/2)' |
|--------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0)'; t(0,1,0); t(0,0,1); t(0,1/2,1/2)'; (2); (3).

### Positions

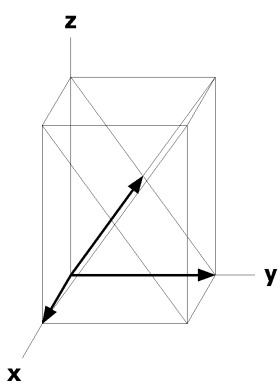
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (1,0,0)'	(0,1/2,1/2)' (1,1/2,1/2) +	
16 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $x,\bar{y}+1/2,z [u,\bar{v},w]$	(4) $\bar{x},y+1/2,z [\bar{u},v,w]$
8 c .m'	x,1/4,z [u,0,w]	$\bar{x},3/4,z [\bar{u},0,w]$		
8 b ..2'	1/2,0,z [u,v,0]	1/2,1/2,z [u, $\bar{v}$ ,0]		
8 a ..2	0,0,z [0,0,w]	0,1/2,z [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

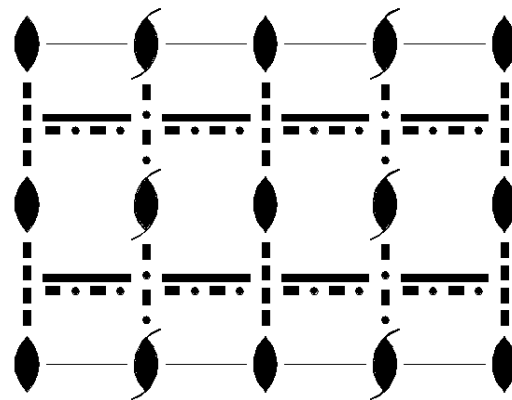
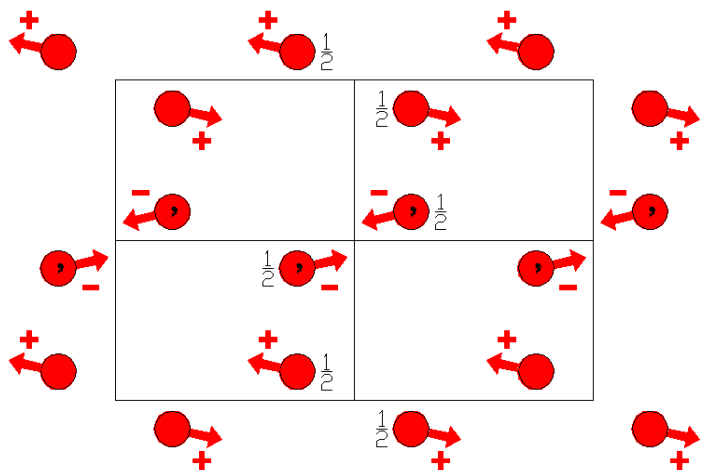
Along [0,1,0] p<sub>c</sub>-1m1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 1/2,y,0



Ama2  
40.1.291

mm2  
Ama2

Orthorhombic



**Origin** on 1a2

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) a ( $1/2,0,0$ )  $x,0,z$   
( $m_y$ | $1/2,0,0$ )

(4) m  $1/4,y,z$   
( $m_x$ | $1/2,0,0$ )

For (0,1/2,1/2) + set

(1) t ( $0,1/2,1/2$ )  
(1| $0,1/2,1/2$ )

(2) 2 ( $0,0,1/2$ )  $0,1/4,z$   
( $2_z$ | $0,1/2,1/2$ )

(3) n ( $1/2,0,1/2$ )  $x,1/4,z$   
( $m_y$ | $1/2,1/2,1/2$ )

(4) n ( $0,1/2,1/2$ )  $1/4,y,z$   
( $m_x$ | $1/2,1/2,1/2$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

### Positions

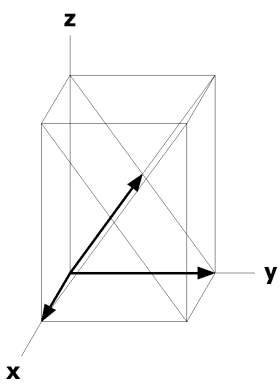
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2) +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $x+1/2,\bar{y},z [\bar{u},v,\bar{w}]$	(4) $\bar{x}+1/2,y,z [u,\bar{v},\bar{w}]$
4	b m..	1/4,y,z [u,0,0]	3/4, $\bar{y},z [\bar{u},0,0]$		
4	a ..2	0,0,z [0,0,w]	1/2,0,z [0,0, $\bar{w}]$		

### Symmetry of Special Projections

Along [0,0,1] p2mg  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>·1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 1/4,y,0



Ama21'

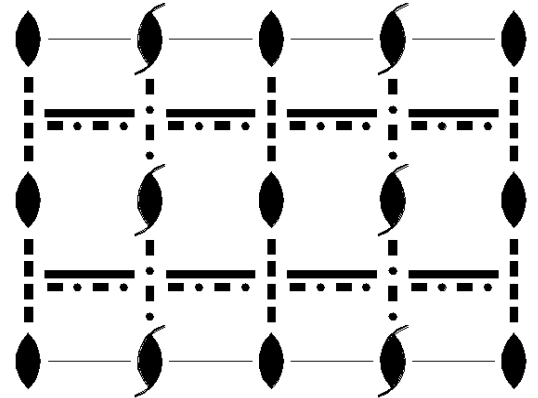
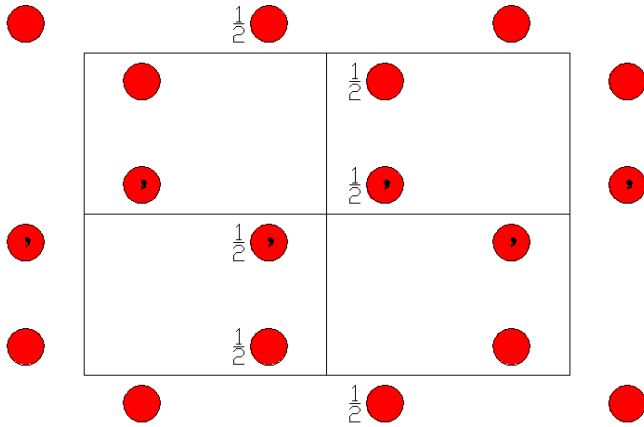
40.2.292

mm21'

Ama21'

Orthorhombic

1'



Origin on 1a21'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) a (1/2,0,0) x,0,z<br>(m <sub>y</sub>  1/2,0,0) | (4) m 1/4,y,z<br>(m <sub>x</sub>  1/2,0,0) |
|--------------------|--|--|--|

For (0,1/2,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2) | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2) | (3) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (4) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) |
|------------------------------------|--|--|--|

For (0,0,0)' + set

- |                      |  |  |  |
|----------------------|--|--|--|
| (1) 1'<br>(1 0,0,0)' | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) a' (1/2,0,0) x,0,z<br>(m <sub>y</sub>  1/2,0,0)' | (4) m' 1/4,y,z<br>(m <sub>x</sub>  1/2,0,0)' |
|----------------------|--|--|--|

For (0,1/2,1/2)' + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t' (0,1/2,1/2)<br>(1 0,1/2,1/2)' | (2) 2' (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)' | (3) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (4) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |
|--------------------------------------|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3); 1'.

### Positions

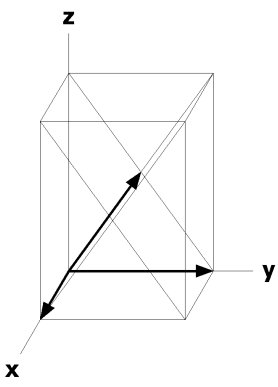
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) + (0,0,0)' +	(0,1/2,1/2) + (0,1/2,1/2)' +		
8	c 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y}, z$ [0,0,0]	(3) $x+1/2, \bar{y}, z$ [0,0,0]	(4) $\bar{x}+1/2, y, z$ [0,0,0]
4	b m..1'	1/4,y,z [0,0,0]	3/4, $\bar{y}$ ,z [0,0,0]		
4	a ..21'	0,0,z [0,0,0]	1/2,0,z [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p2mg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

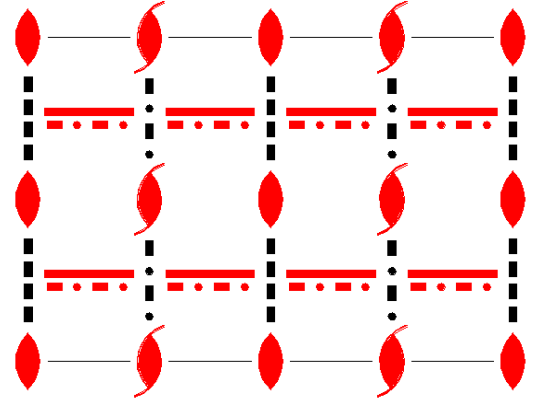
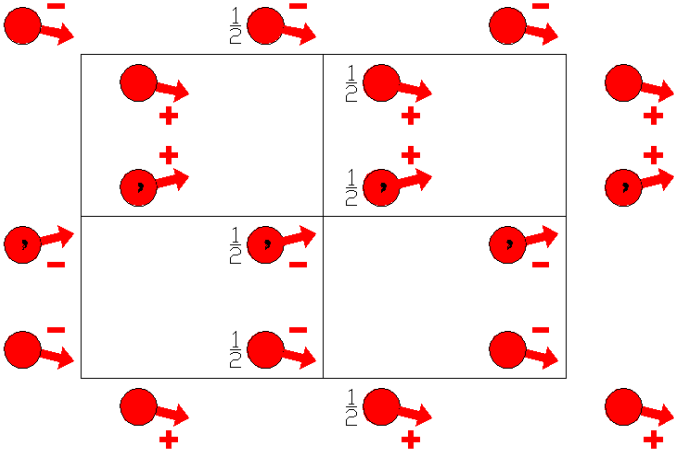
Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Am'a2'  
40.3.293

m'm2'  
Am'a2'

Orthorhombic



Origin on 1a2'

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'

(3) a (1/2,0,0) x,0,z  
(m<sub>y</sub>|1/2,0,0)

(4) m' 1/4,y,z  
(m<sub>x</sub>|1/2,0,0)'

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)  
(1|0,1/2,1/2)

(2) 2' (0,0,1/2) 0,1/4,z  
(2<sub>z</sub>|0,1/2,1/2)'

(3) n (1/2,0,1/2) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,1/2)

(4) n' (0,1/2,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

### Positions

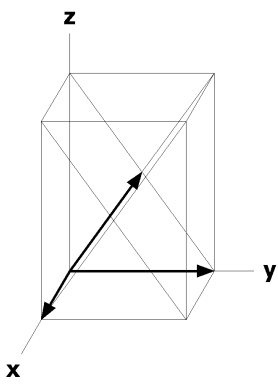
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2) +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x+1/2,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x}+1/2,y,z$ [ $\bar{u},v,w$ ]
4	b m'..	1/4,y,z [0,v,w]	3/4, $\bar{y},z$ [0,v, $\bar{w}$ ]		
4	a ..2'	0,0,z [u,v,0]	1/2,0,z [ $\bar{u},v,0$ ]		

### Symmetry of Special Projections

Along [0,0,1]  $p2'm'g$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $c1m1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a} \cdot 1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



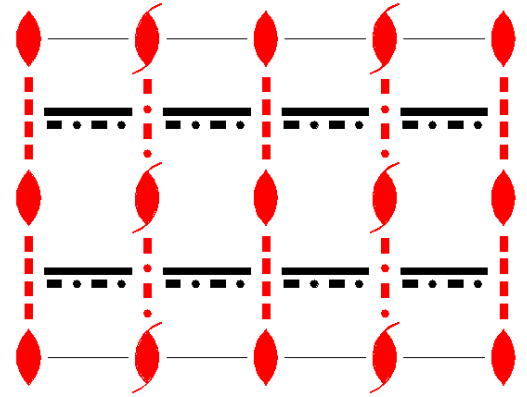
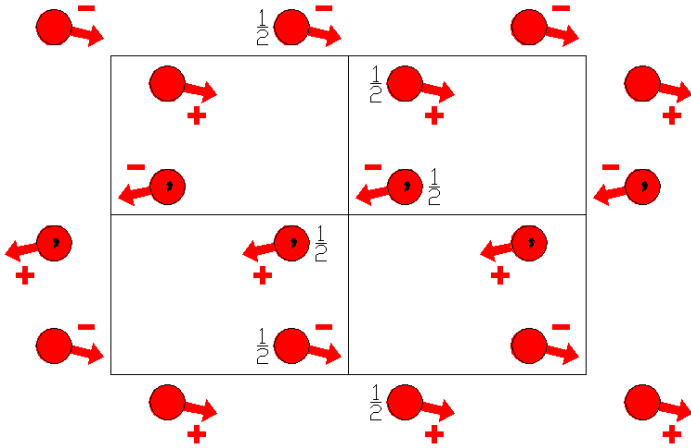
Ama'2'

40.4.294

mm'2'

Ama'2'

Orthorhombic



Origin on 1a'2'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'

(3) a' (1/2,0,0) x,0,z  
(m<sub>y</sub>|1/2,0,0)'

(4) m 1/4,y,z  
(m<sub>x</sub>|1/2,0,0)

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)  
(1|0,1/2,1/2)

(2) 2' (0,0,1/2) 0,1/4,z  
(2<sub>z</sub>|0,1/2,1/2)'

(3) n' (1/2,0,1/2) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,1/2)'

(4) n (0,1/2,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

### Positions

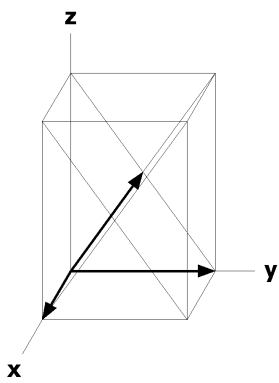
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2) +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x+1/2,\bar{y},z$ [u, $\bar{v}$ ,w]	(4) $\bar{x}+1/2,y,z$ [u, $\bar{v},\bar{w}$ ]
4	b m..	1/4,y,z [u,0,0]	3/4, $\bar{y},z$ [u,0,0]		
4	a ..2'	0,0,z [u,v,0]	1/2,0,z [u, $\bar{v}$ ,0]		

### Symmetry of Special Projections

Along [0,0,1] p2'mg'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



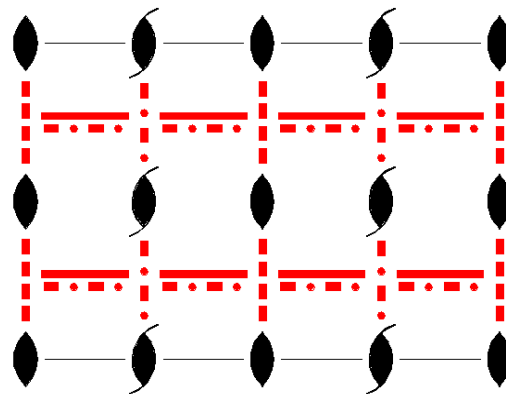
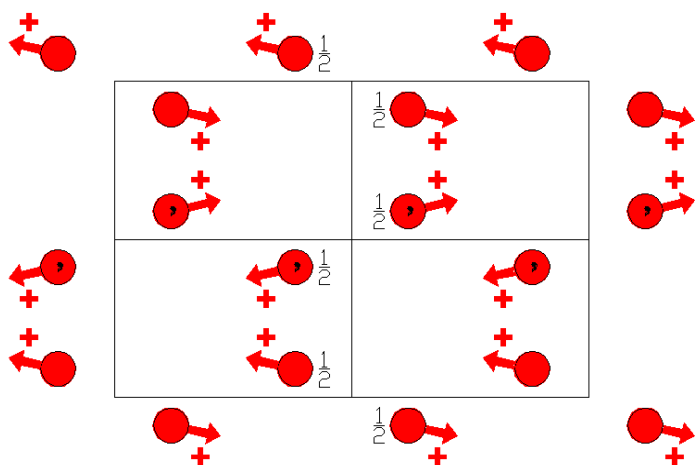
Am'a'2

40.5.295

m'm'2

Am'a'2

Orthorhombic



Origin on 1a'2

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) a' (1/2,0,0) x,0,z  
(m<sub>y</sub>|1/2,0,0)'

(4) m' 1/4,y,z  
(m<sub>x</sub>|1/2,0,0)'

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)  
(1|0,1/2,1/2)

(2) 2 (0,0,1/2) 0,1/4,z  
(2<sub>z</sub>|0,1/2,1/2)

(3) n' (1/2,0,1/2) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,1/2)'

(4) n' (0,1/2,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

### Positions

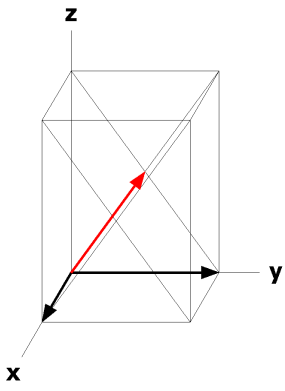
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2) +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $x+1/2, \bar{y}, z$ [ $u, \bar{v}, w$ ]	(4) $\bar{x}+1/2, y, z$ [ $\bar{u}, v, w$ ]
4	b m'..	1/4,y,z [0,v,w]	3/4, $\bar{y}, z$ [0, $\bar{v}, w$ ]		
4	a ..2	0,0,z [0,0,w]	1/2,0,z [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] p2m'g'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p1m'1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



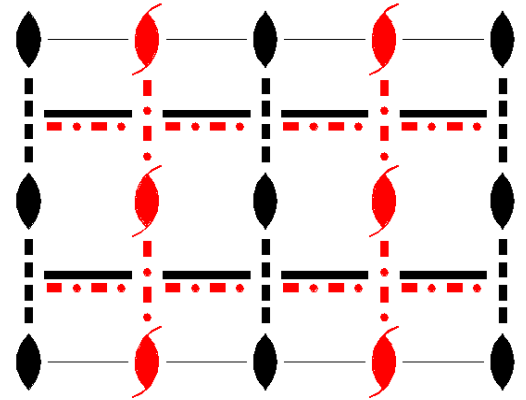
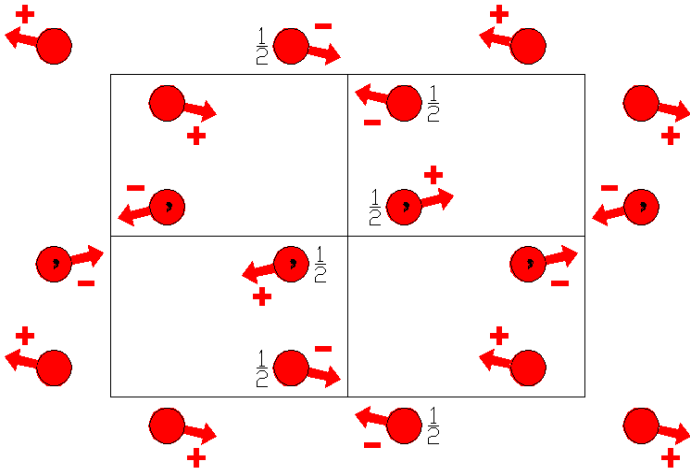
$A_p ma2$

40.6.296

$mm21'$

$A_p ma2$

Orthorhombic



Origin on  $1a2$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) a  $(1/2,0,0)$   $x,0,z$   
( $m_y$ | $1/2,0,0$ )

(4) m  $1/4,y,z$   
( $m_x$ | $1/2,0,0$ )

For  $(0,1/2,1/2)'$  + set

(1)  $t' (0,1/2,1/2)$   
(1| $0,1/2,1/2$ )'

(2)  $2' (0,0,1/2)$   $0,1/4,z$   
( $2_z$ | $0,1/2,1/2$ )'

(3)  $n' (1/2,0,1/2)$   $x,1/4,z$   
( $m_y$ | $1/2,1/2,1/2$ )'

(4)  $n' (0,1/2,1/2)$   $1/4,y,z$   
( $m_x$ | $1/2,1/2,1/2$ )'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2)'; (2); (3).

### Positions

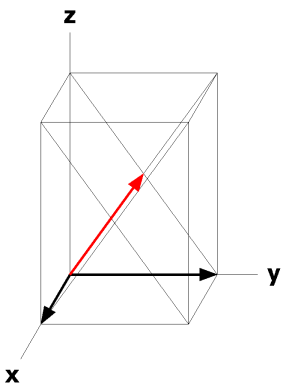
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2)' +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $x+1/2,\bar{y},z [\bar{u},v,\bar{w}]$	(4) $\bar{x}+1/2,y,z [u,\bar{v},\bar{w}]$
4	b m..	1/4,y,z [u,0,0]	3/4, $\bar{y},z [\bar{u},0,0]$		
4	a ..2	0,0,z [0,0,w]	1/2,0,z [0,0, $\bar{w}]$		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2b</sub>·2mg  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>c</sub>·1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 1/4,y,0



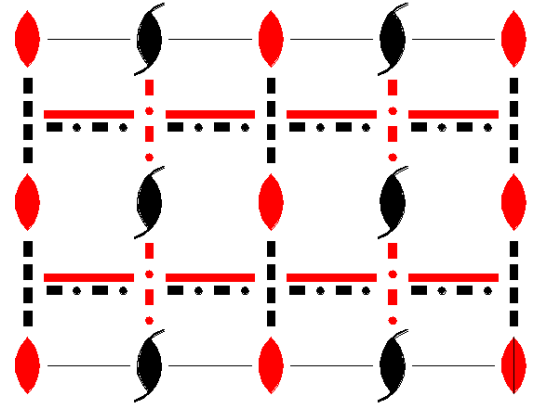
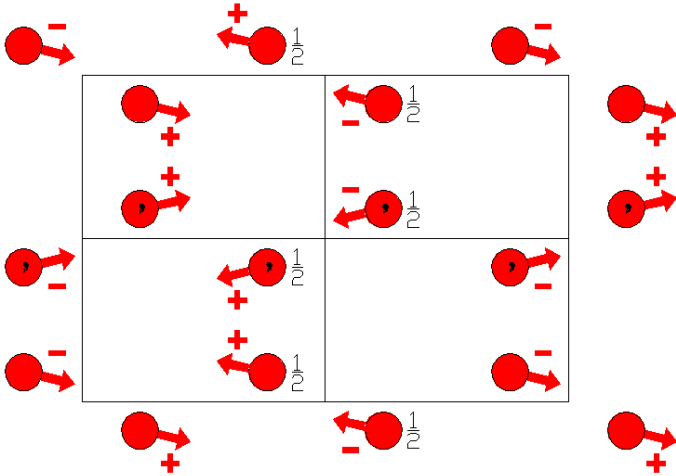
$A_p m'a2'$

40.7.297

$mm21'$

$A_p m'a2'$

Orthorhombic



**Origin** on  $1a2'$

**Asymmetric unit**  $0 \leq x \leq 1/4;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2)  $2'$   $0,0,z$   
( $2_z$ |0,0,0)'

(3) a  $(1/2,0,0)$   $x,0,z$   
( $m_y$ | $1/2,0,0$ )

(4)  $m'$   $1/4,y,z$   
( $m_x$ | $1/2,0,0$ )'

For  $(0,1/2,1/2)'$  + set

(1)  $t'$   $(0,1/2,1/2)$   
(1| $0,1/2,1/2$ )'

(2) 2  $(0,0,1/2)$   $0,1/4,z$   
( $2_z$ | $0,1/2,1/2$ )

(3)  $n'$   $(1/2,0,1/2)$   $x,1/4,z$   
( $m_y$ | $1/2,1/2,1/2$ )'

(4) n  $(0,1/2,1/2)$   $1/4,y,z$   
( $m_x$ | $1/2,1/2,1/2$ )

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0,1/2,1/2)'$ ; (2); (3).

### Positions

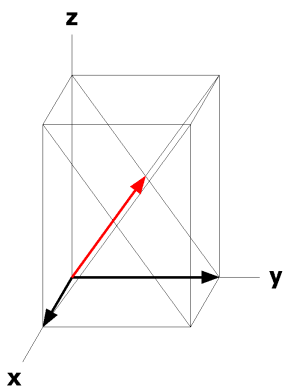
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(0,1/2,1/2)' +		
8	c 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [u,v,\bar{w}]$	(3) $x+1/2,\bar{y},z [\bar{u},v,\bar{w}]$	(4) $\bar{x}+1/2,y,z [\bar{u},v,w]$
4	b $m'..$	$1/4,y,z [0,v,w]$	$3/4,\bar{y},z [0,v,\bar{w}]$		
4	a $..2'$	$0,0,z [u,v,0]$	$1/2,0,z [\bar{u},v,0]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p_{2b} \cdot 2m'g'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $0,1/4,z$

Along  $[1,0,0]$   $c_p \cdot 1m1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $p_c \cdot 1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $1/4,y,0$



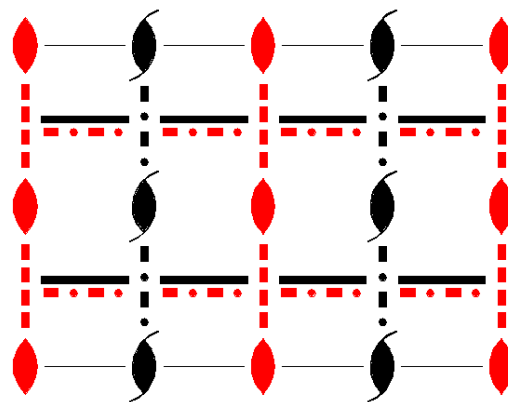
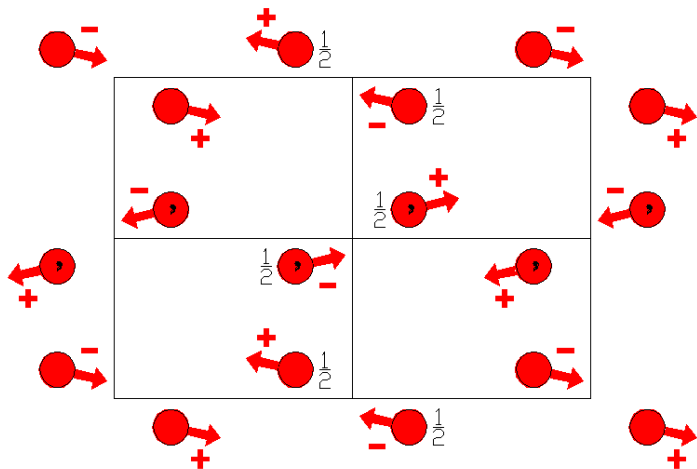
$A_p ma'2'$

40.8.298

$mm21'$

$A_p ma'2'$

Orthorhombic



**Origin** on  $1a'2'$

**Asymmetric unit**  $0 \leq x \leq 1/4;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2)  $2'$   $0,0,z$   
( $2_z$ |0,0,0)'

(3)  $a'$   $(1/2,0,0)$   $x,0,z$   
( $m_y$ | $1/2,0,0$ )'

(4)  $m$   $1/4,y,z$   
( $m_x$ | $1/2,0,0$ )

For  $(0,1/2,1/2)'$  + set

(1)  $t'$   $(0,1/2,1/2)$   
(1| $0,1/2,1/2$ )'

(2)  $2$   $(0,0,1/2)$   $0,1/4,z$   
( $2_z$ | $0,1/2,1/2$ )

(3)  $n$   $(1/2,0,1/2)$   $x,1/4,z$   
( $m_y$ | $1/2,1/2,1/2$ )

(4)  $n'$   $(0,1/2,1/2)$   $1/4,y,z$   
( $m_x$ | $1/2,1/2,1/2$ )'

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0,1/2,1/2)'$ ; (2); (3).

### Positions

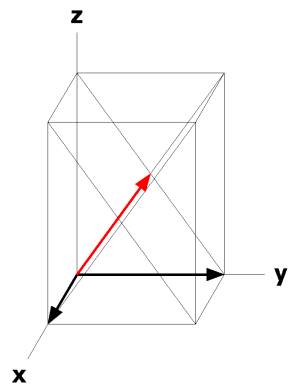
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(0,1/2,1/2)' +		
8	c 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [u,v,\bar{w}]$	(3) $x+1/2,\bar{y},z [u,\bar{v},w]$	(4) $\bar{x}+1/2,y,z [u,\bar{v},\bar{w}]$
4	b m..	$1/4,y,z [u,0,0]$	$3/4,\bar{y},z [u,0,0]$		
4	a ..2'	$0,0,z [u,v,0]$	$1/2,0,z [u,\bar{v},0]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p_{2b}\cdot 2mg$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $0,1/2,z$

Along  $[1,0,0]$   $c1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $p_{2b}\cdot 1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $0,y,0$



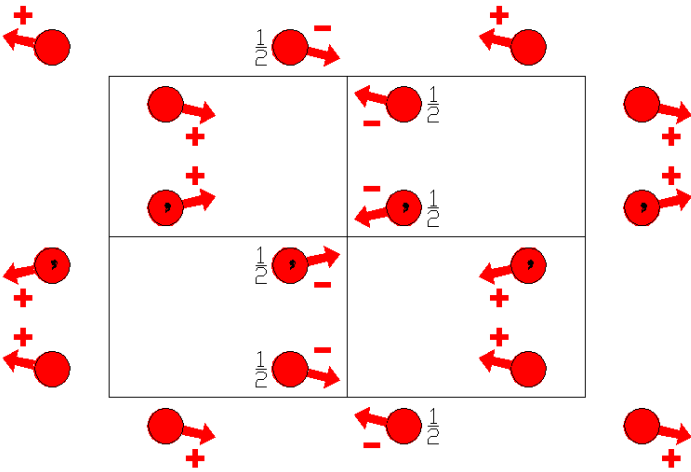
$A_p m'a'2$

40.9.299

$mm21'$

$A_p m'a'2$

Orthorhombic



Origin on  $1a'2$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0) +$  set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $a' (1/2,0,0)$   $x,0,z$   
( $m_y$ | $1/2,0,0$ )'

(4)  $m' 1/4,y,z$   
( $m_x$ | $1/2,0,0$ )'

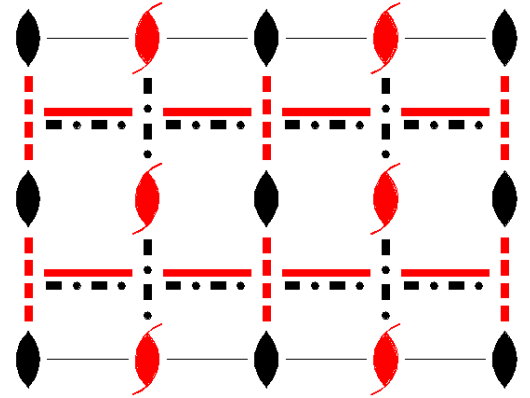
For  $(0,1/2,1/2) +$  set

(1)  $t' (0,1/2,1/2)$   
(1| $0,1/2,1/2$ )'

(2)  $2' (0,0,1/2)$   $0,1/4,z$   
( $2_z$ | $0,1/2,1/2$ )'

(3)  $n (1/2,0,1/2)$   $x,1/4,z$   
( $m_y$ | $1/2,1/2,1/2$ )'

(4)  $n (0,1/2,1/2)$   $1/4,y,z$   
( $m_x$ | $1/2,1/2,1/2$ )'



**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0,1/2,1/2)'$ ; (2); (3).

### Positions

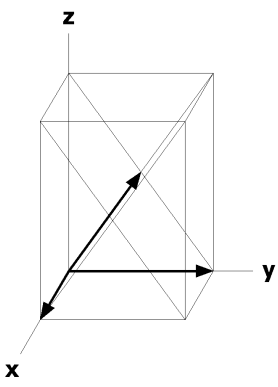
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(0,1/2,1/2)' +		
8	c 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $x+1/2,\bar{y},z [u,\bar{v},w]$	(4) $\bar{x}+1/2,y,z [\bar{u},v,w]$
4	b $m'..$	$1/4,y,z [0,v,w]$	$3/4,\bar{y},z [0,\bar{v},w]$		
4	a $..2$	$0,0,z [0,0,w]$	$1/2,0,z [0,0,w]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p_{2b} \cdot 2m'g'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c_p \cdot 1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

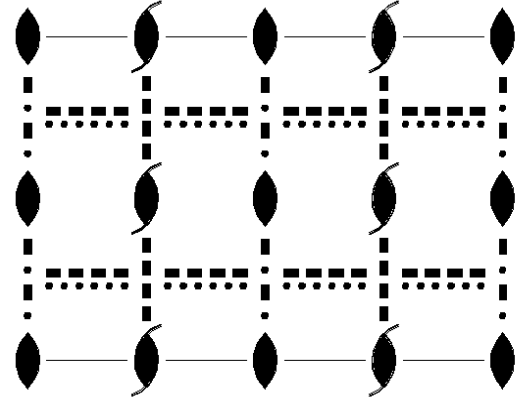
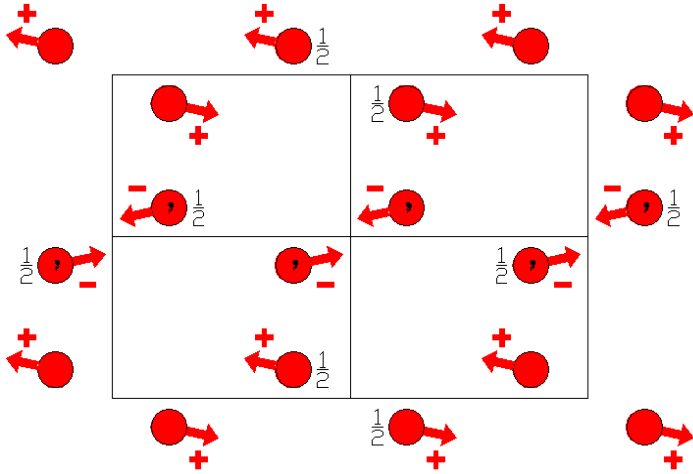
Along  $[0,1,0]$   $p_{2b} \cdot 1m'1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $0,y,0$



Aba2  
41.1.300

mm2  
Aba2

Orthorhombic



Origin on 1n2

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |                    |                                  |  |  |
|--------------------|----------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) a $(1/2,0,0)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,0$ ) | (4) b $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ ) |
|--------------------|----------------------------------|--|--|

For (0,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t $(0,1/2,1/2)$<br>(1  $0,1/2,1/2$ ) | (2) 2 $(0,0,1/2)$ $0,1/4,z$<br>( $2_z$   $0,1/2,1/2$ ) | (3) n $(1/2,0,1/2)$ $x,0,z$<br>( $m_y$   $1/2,0,1/2$ ) | (4) c $(0,0,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,0,1/2$ ) |
|--|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

**Positions**

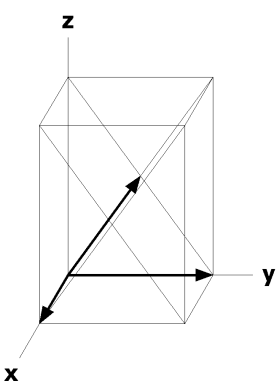
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +		(0,1/2,1/2) +	
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x}+1/2,y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]
4	a ..2	0,0,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p2mg$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a}1m'1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0

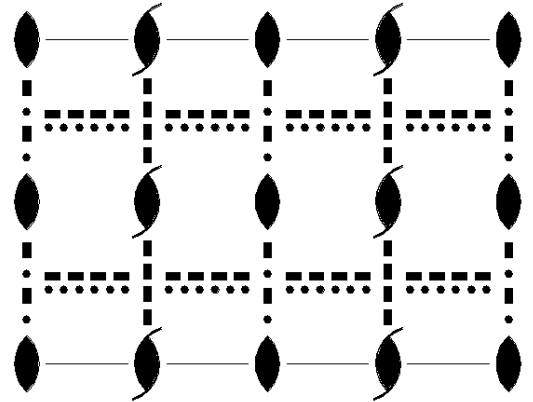
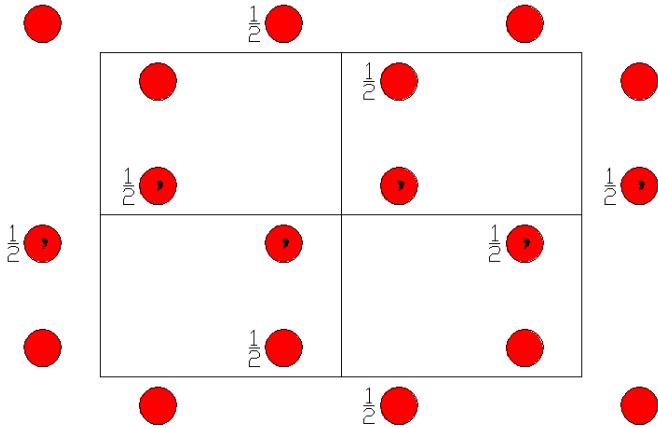


Aba21'  
41.2.301

mm21'  
Aba21'

Orthorhombic

1'



Origin on 1n21'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (4) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |
|--------------------|--|--|--|

For (0,1/2,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2) | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2) | (3) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2) | (4) c (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,0,1/2) |
|------------------------------------|--|--|--|

For (0,0,0)' + set

- |                      |  |  |  |
|----------------------|--|--|--|
| (1) 1'<br>(1 0,0,0)' | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (4) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |
|----------------------|--|--|--|

For (0,1/2,1/2) + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t' (0,1/2,1/2)<br>(1 0,1/2,1/2)' | (2) 2' (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)' | (3) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2)' | (4) c' (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,0,1/2)' |
|--------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3); 1'.

### Positions

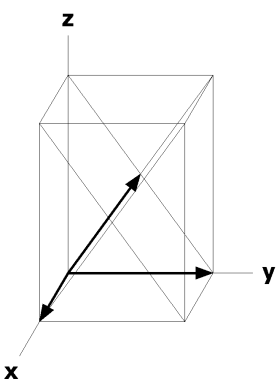
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) + (0,0,0)' +	(0,1/2,1/2) + (0,1/2,1/2)' +		
8	b 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y}, z$ [0,0,0]	(3) $x+1/2, \bar{y}+1/2, z$ [0,0,0]	(4) $\bar{x}+1/2, y+1/2, z$ [0,0,0]
4	a ..21'	0,0,z [0,0,0]	1/2,1/2,z [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p2mg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

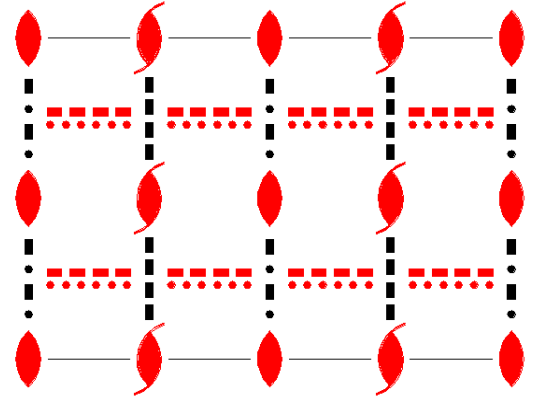
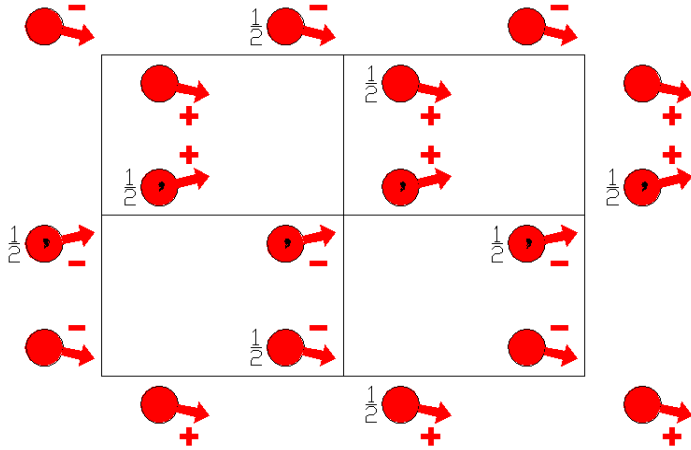
Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Ab'a2'  
41.3.302

m'm2'  
Ab'a2'

Orthorhombic



Origin on 1n2'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (4) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |
|--------------------|--|--|--|

For (0,1/2,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2) | (2) 2' (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)' | (3) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2) | (4) c' (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,0,1/2)' |
|------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

**Positions**

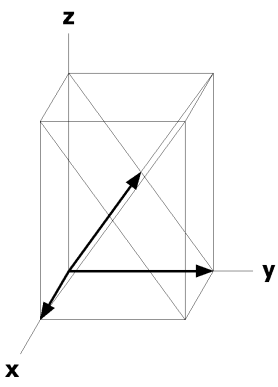
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2) +		
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]
4	a ..2'	0,0,z [u,v,0]	1/2,1/2,z [ $\bar{u},v,0$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p2'm'g$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $p1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

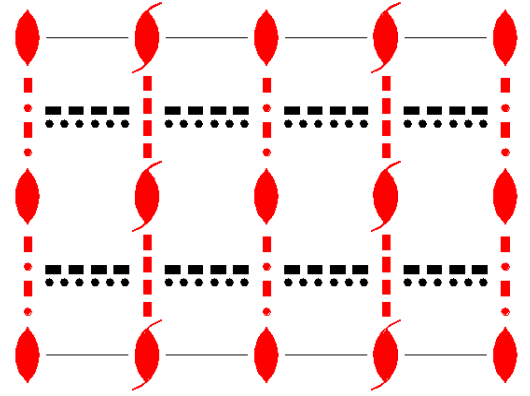
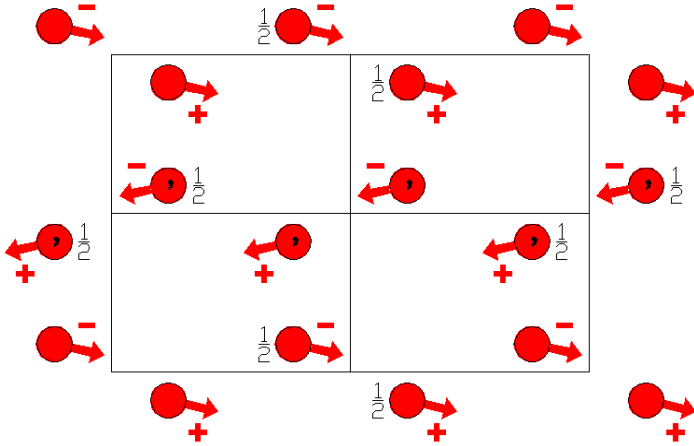
Along [0,1,0]  $p_{2a}1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Aba'2'  
41.4.303

mm'2'  
Aba'2'

Orthorhombic



Origin on 1n'2'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'

(3) a' (1/2,0,0) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,0)'

(4) b (0,1/2,0) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,0)

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)  
(1|0,1/2,1/2)

(2) 2' (0,0,1/2) 0,1/4,z  
(2<sub>z</sub>|0,1/2,1/2)'

(3) n' (1/2,0,1/2) x,0,z (4)  
(m<sub>y</sub>|1/2,0,1/2)'

c (0,0,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

**Positions**

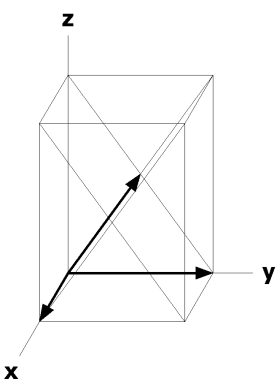
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2) +		
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x+1/2,\bar{y}+1/2,z$ [u, $\bar{v}$ ,w]	(4) $\bar{x}+1/2,y+1/2,z$ [u, $\bar{v},\bar{w}$ ]
4	a ..2'	0,0,z [u,v,0]	1/2,1/2,z [u, $\bar{v}$ ,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p2'mg'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a'}1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

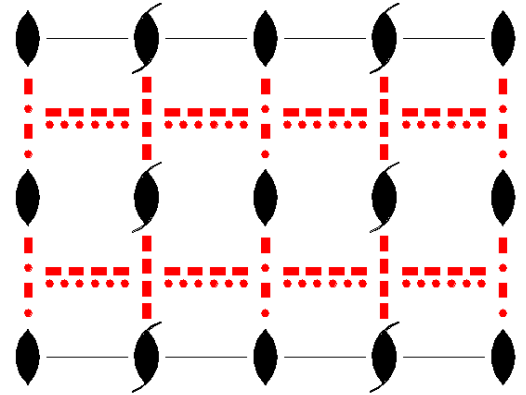
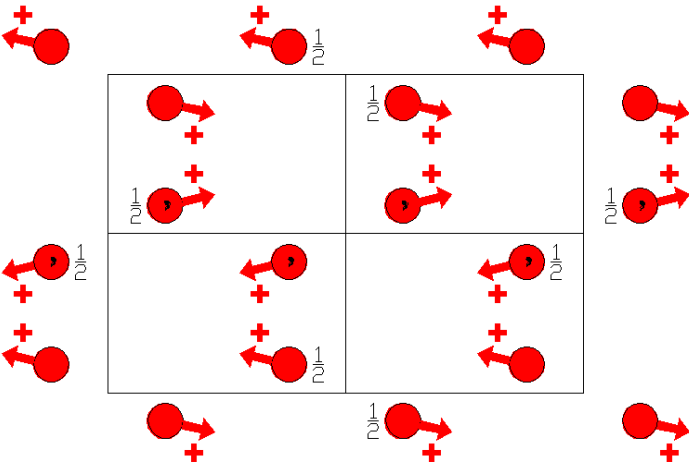
Along [0,1,0]  $p1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Ab'a'2  
41.5.304

m'm'2  
Ab'a'2

Orthorhombic



Origin on 1n'2

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (4) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |
|--------------------|--|--|--|

For (0,1/2,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2) | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2) | (3) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2)' | (4) c' (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,0,1/2)' |
|------------------------------------|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

**Positions**

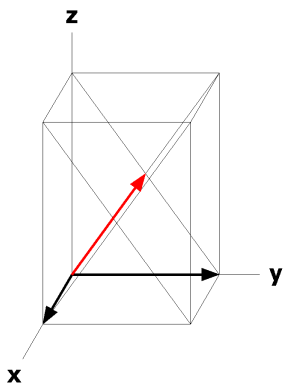
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2) +		
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x+1/2,\bar{y}+1/2,z$ [ $u,\bar{v},w$ ]	(4) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]
4	a ..2	0,0,z [0,0,w]	1/2,1/2,z [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1]  $p2m'g'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

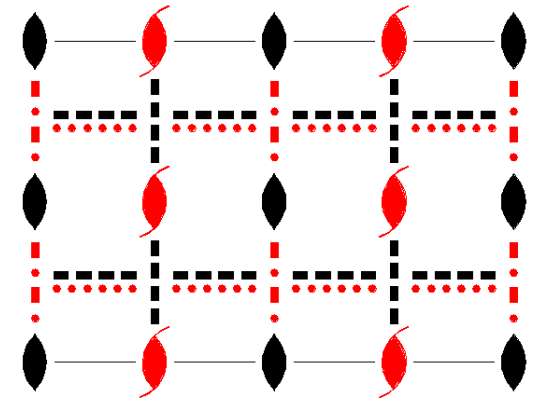
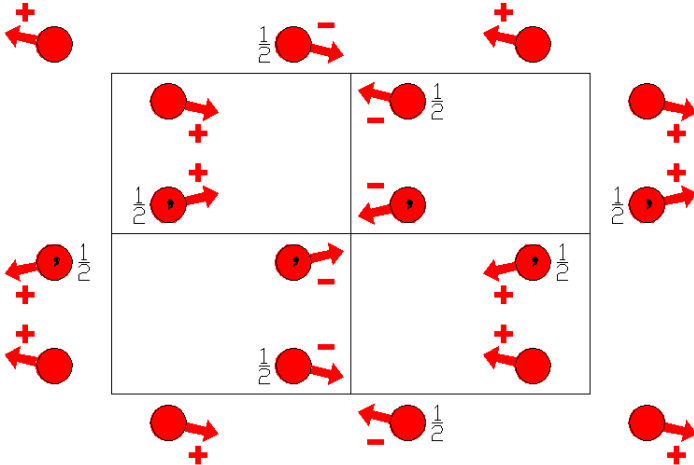
Along [0,1,0]  $p1m'1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$A_pba2$   
41.6.305

$mm21'$   
 $A_pba2$

Orthorhombic



**Origin** on  $1n'2$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                  |  |  |
|--------------------|----------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) a $(1/2,0,0)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,0$ ) | (4) b $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ ) |
|--------------------|----------------------------------|--|--|

For  $(0,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' $(0,1/2,1/2)$<br>(1  $0,1/2,1/2$ )' | (2) 2' $(0,0,1/2)$ $0,1/4,z$<br>( $2_z$   $0,1/2,1/2$ )' | (3) n' $(1/2,0,1/2)$ $x,0,z$<br>( $m_y$   $1/2,0,1/2$ )' | (4) c' $(0,0,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,0,1/2$ )' |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); (2); (3).

**Positions**

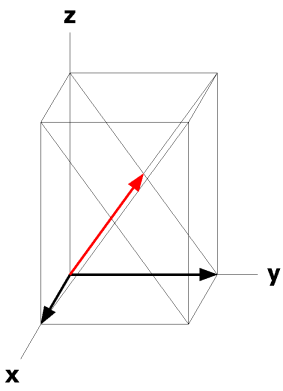
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(0,1/2,1/2)' +		
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x}+1/2,y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]
4	a ..2	0,0,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2b}2m'g'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_c1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



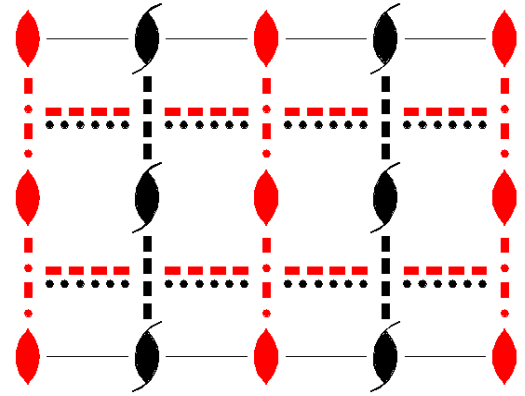
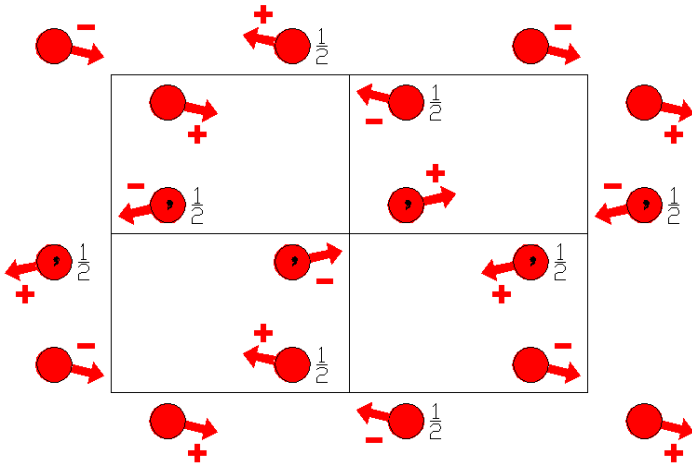
$A_p b' a_2'$

41.7.306

$mm21'$

$A_p b' a_2'$

Orthorhombic



**Origin** on  $1n'2'$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                      |  |  |
|--------------------|--------------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) $2'$ $0,0,z$<br>( $2_z$  0,0,0)' | (3) a $(1/2,0,0)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,0$ ) | (4) b' $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |
|--------------------|--------------------------------------|--|--|

For  $(0,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' $(0,1/2,1/2)$<br>(1  $0,1/2,1/2$ )' | (2) 2 $(0,0,1/2)$ $0,1/4,z$<br>( $2_z$   $0,1/2,1/2$ ) | (3) n' $(1/2,0,1/2)$ $x,0,z$<br>( $m_y$   $1/2,0,1/2$ )' | (4) c $(0,0,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,0,1/2$ ) |
|--|--|--|--|

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(0,1/2,1/2)$ ; (2); (3).

### Positions

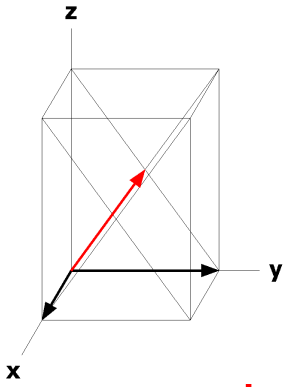
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(0,1/2,1/2)' +		
8	b 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]
4	a ..2'	0,0,z [u,v,0]	1/2,1/2,z [ $\bar{u},v,0$ ]		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p_{2b}2mg$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $0,1/4,z$

Along  $[1,0,0]$   $p_{2b}1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $p_c1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $0,y,0$



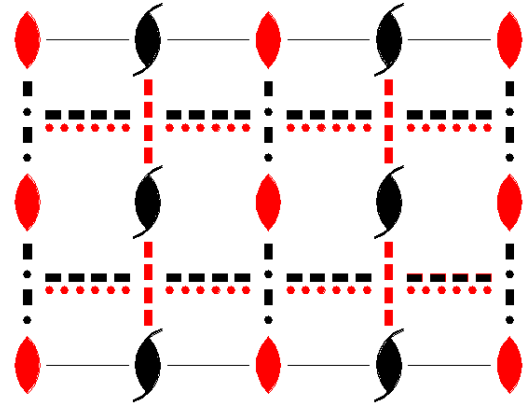
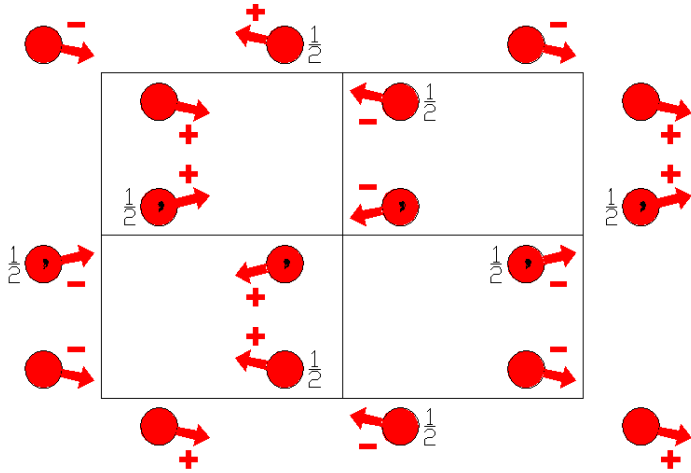
$A_pba'2'$

41.8.307

$mm21'$

$A_pba'2'$

Orthorhombic



**Origin** on  $1n2'$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                    |  |  |
|--------------------|------------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $a'$ (1/2,0,0) x,1/4,z<br>( $m_y$  1/2,1/2,0)' | (4) $b$ (0,1/2,0) 1/4,y,z<br>( $m_x$  1/2,1/2,0) |
|--------------------|------------------------------------|--|--|

For  $(0,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (0,1/2,1/2)<br>(1 0,1/2,1/2)' | (2) 2 (0,0,1/2) 0,1/4,z<br>( $2_z$  0,1/2,1/2) | (3) $n$ (1/2,0,1/2) x,0,z<br>( $m_y$  1/2,0,1/2) | (4) $c'$ (0,0,1/2) 1/4,y,z<br>( $m_x$  1/2,0,1/2)' |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); (2); (3).

**Positions**

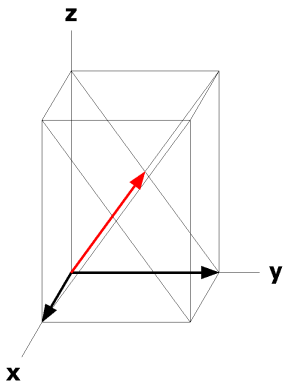
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2)' +		
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x+1/2,\bar{y}+1/2,z$ [u, $\bar{v}$ ,w]	(4) $\bar{x}+1/2,y+1/2,z$ [u, $\bar{v},\bar{w}$ ]
4	a ..2'	0,0,z [u,v,0]	1/2,1/2,z [u, $\bar{v}$ ,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2b} \cdot 2m'g'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,1/4,z

Along [1,0,0]  $p_{2a} \cdot 1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2b} \cdot 1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



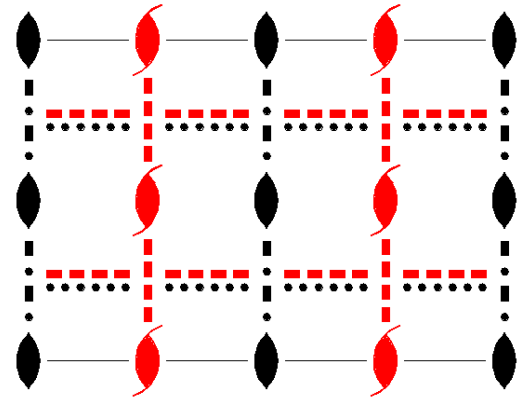
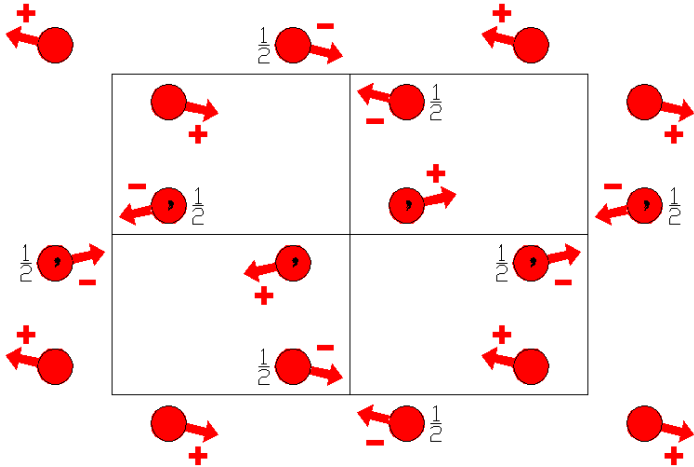
$A_p b' a' 2$

41.9.308

$mm21'$

$A_p b' a' 2$

Orthorhombic



Origin on  $1n2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $a'$   $(1/2,0,0)$   $x,1/4,z$   
( $m_y$ | $1/2,1/2,0$ )'

(4)  $b'$   $(0,1/2,0)$   $1/4,y,z$   
( $m_x$ | $1/2,1/2,0$ )'

For  $(0,1/2,1/2)'$  + set

(1)  $t'$   $(0,1/2,1/2)$   
(1| $0,1/2,1/2$ )'

(2)  $2'$   $(0,0,1/2)$   $0,1/4,z$   
( $2_z$ | $0,1/2,1/2$ )'

(3)  $n$   $(1/2,0,1/2)$   $x,0,z$   
( $m_y$ | $1/2,0,1/2$ )'

(4)  $c$   $(0,0,1/2)$   $1/4,y,z$   
( $m_x$ | $1/2,0,1/2$ )'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); (2); (3).

### Positions

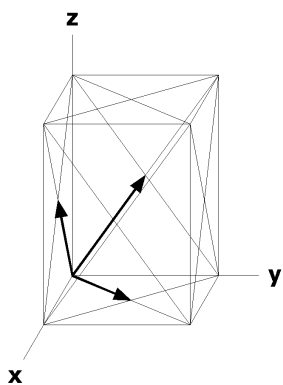
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2)' +		
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x+1/2,\bar{y}+1/2,z$ [ $u,\bar{v},w$ ]	(4) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]
4	a ..2	0,0,z [0,0,w]	1/2,1/2,z [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1]  $p_{2b} \cdot 2mg$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b} \cdot 1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

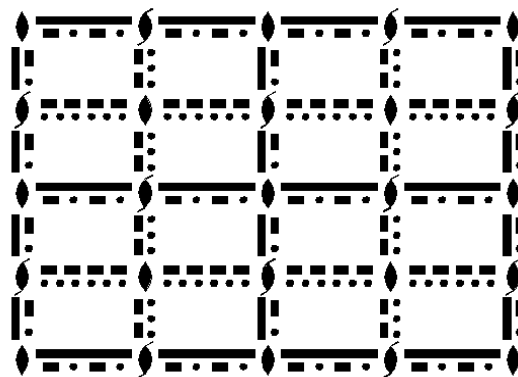
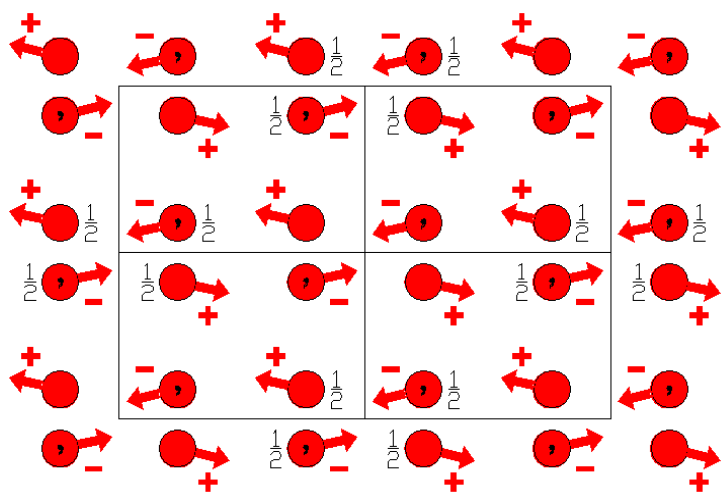
Along [0,1,0]  $p_{2b} \cdot 1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Fmm2  
42.1.309

mm2  
Fmm2

Orthorhombic



Origin on mm2

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) m $x,0,z$<br>(m <sub>y</sub>  0,0,0) | (4) m $0,y,z$<br>(m <sub>x</sub>  0,0,0) |
|--------------------|--|--|--|

For (0,1/2,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2) | (2) 2 (0,0,1/2) $0,1/4,z$<br>(2 <sub>z</sub>  0,1/2,1/2) | (3) c (0,0,1/2) $x,1/4,z$<br>(m <sub>y</sub>  0,1/2,1/2) | (4) n (0,1/2,1/2) $0,y,z$<br>(m <sub>x</sub>  0,1/2,1/2) |
|------------------------------------|--|--|--|

For (1/2,0,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,0,1/2)<br>(1 1/2,0,1/2) | (2) 2 (0,0,1/2) $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) n (1/2,0,1/2) $x,0,z$<br>(m <sub>y</sub>  1/2,0,1/2) | (4) c (0,0,1/2) $1/4,y,z$<br>(m <sub>x</sub>  1/2,0,1/2) |
|------------------------------------|--|--|--|

For (1/2,1/2,0) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) 2 $1/4,1/4,z$<br>(2 <sub>z</sub>  1/2,1/2,0) | (3) a (1/2,0,0) $x,1/4,z$<br>(m <sub>y</sub>  1/2,1/2,0) | (4) b (0,1/2,0) $1/4,y,z$<br>(m <sub>x</sub>  1/2,1/2,0) |
|------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

### Positions

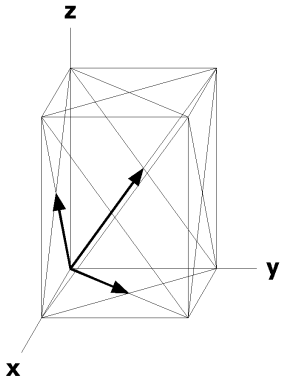
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
16	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
8	d .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]		
8	c m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]		
8	b ..2	1/4,1/4,z [0,0,w]	1/4,3/4,z [0,0, $\bar{w}$ ]		
4	a mm2	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Fmm21'

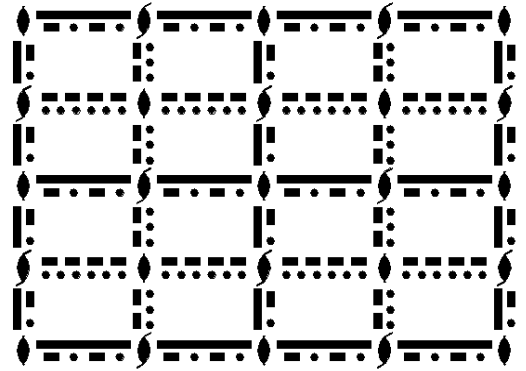
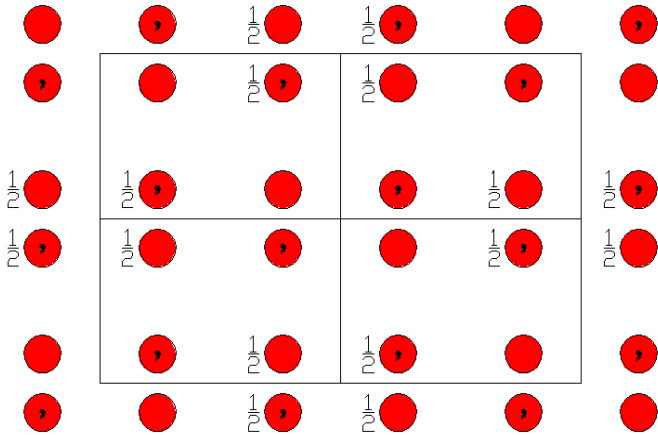
42.2.310

mm21'

Fmm21'

Orthorhombic

1'



Origin on mm21'

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

- (1) 1 (2) 2 0,0,z (3) m x,0,z (4) m 0,y,z
- (1|0,0,0) (2<sub>z</sub>|0,0,0) (m<sub>y</sub>|0,0,0) (m<sub>x</sub>|0,0,0)

For (0,1/2,1/2) + set

- (1) t (0,1/2,1/2) (2) 2 (0,0,1/2) 0,1/4,z (3) c (0,0,1/2) x,1/4,z (4) n (0,1/2,1/2) 0,y,z
- (1|0,1/2,1/2) (2<sub>z</sub>|0,1/2,1/2) (m<sub>y</sub>|0,1/2,1/2) (m<sub>x</sub>|0,1/2,1/2)

For (1/2,0,1/2) + set

- (1) t (1/2,0,1/2) (2) 2 (0,0,1/2) 1/4,0,z (3) n (1/2,0,1/2) x,0,z (4) c (0,0,1/2) 1/4,y,z
- (1|1/2,0,1/2) (2<sub>z</sub>|1/2,0,1/2) (m<sub>y</sub>|1/2,0,1/2) (m<sub>x</sub>|1/2,0,1/2)

For (1/2,1/2,0) + set

- (1) t (1/2,1/2,0) (2) 2 1/4,1/4,z (3) a (1/2,0,0) x,1/4,z (4) b (0,1/2,0) 1/4,y,z
- (1|1/2,1/2,0) (2<sub>z</sub>|1/2,1/2,0) (m<sub>y</sub>|1/2,1/2,0) (m<sub>x</sub>|1/2,1/2,0)

For (0,0,0)' + set

- (1) 1' (2) 2' 0,0,z (3) m' x,0,z (4) m' 0,y,z
- (1|0,0,0)' (2<sub>z</sub>'|0,0,0)' (m<sub>y</sub>'|0,0,0)' (m<sub>x</sub>'|0,0,0)'

For (0,1/2,1/2)' + set

- (1) t' (0,1/2,1/2) (2) 2' (0,0,1/2) 0,1/4,z (3) c' (0,0,1/2) x,1/4,z (4) n' (0,1/2,1/2) 0,y,z
- (1|0,1/2,1/2)' (2<sub>z</sub>'|0,1/2,1/2)' (m<sub>y</sub>'|0,1/2,1/2)' (m<sub>x</sub>'|0,1/2,1/2)'

For (1/2,0,1/2)' + set

$$(1) t' (1/2,0,1/2) \\ (1 | 1/2,0,1/2)'$$

$$(2) 2' (0,0,1/2) \quad 1/4,0,z \\ (2_z | 1/2,0,1/2)'$$

$$(3) n' (1/2,0,1/2) \quad x,0,z \\ (m_y | 1/2,0,1/2)'$$

$$(4) c' (0,0,1/2) \quad 1/4,y,z \\ (m_x | 1/2,0,1/2)'$$

For (1/2,1/2,0)' + set

$$(1) t' (1/2,1/2,0) \\ (1 | 1/2,1/2,0)'$$

$$(2) 2' \quad 1/4,1/4,z \\ (2_z | 1/2,1/2,0)'$$

$$(3) a' (1/2,0,0) \quad x,1/4,z \\ (m_y | 1/2,1/2,0)'$$

$$(4) b' (0,1/2,0) \quad 1/4,y,z \\ (m_x | 1/2,1/2,0)'$$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); 1'.

### Positions

#### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

$$(0,0,0) + \quad (0,1/2,1/2) + \quad (1/2,0,1/2) + \quad (1/2,1/2,0) + \\ (0,0,0)' + \quad (0,1/2,1/2)' + \quad (1/2,0,1/2)' + \quad (1/2,1/2,0)'$$

$$16 \quad e \quad 11' \quad (1) \quad x,y,z [0,0,0] \quad (2) \quad \bar{x},\bar{y},z [0,0,0] \quad (3) \quad x,\bar{y},z [0,0,0] \quad (4) \quad \bar{x},y,z [0,0,0]$$

$$8 \quad d \quad .m.1' \quad x,0,z [0,0,0] \quad \bar{x},0,z [0,0,0]$$

$$8 \quad c \quad m..1' \quad 0,y,z [0,0,0] \quad 0,\bar{y},z [0,0,0]$$

$$8 \quad b \quad ..21' \quad 1/4,1/4,z [0,0,0] \quad 1/4,3/4,z [0,0,0]$$

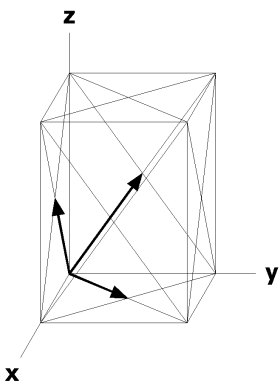
$$4 \quad a \quad mm21' \quad 0,0,z [0,0,0]$$

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $a^* = a/2 \quad b^* = b/2$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $a^* = b/2 \quad b^* = c/2$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $a^* = -a/2 \quad b^* = c/2$   
 Origin at 0,y,0



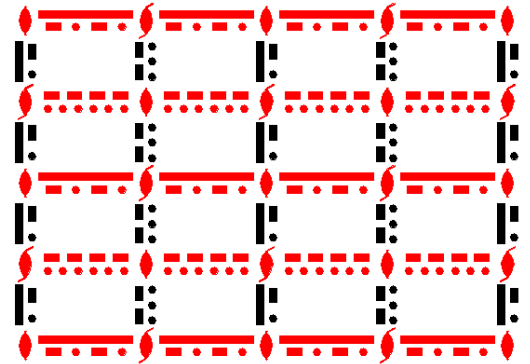
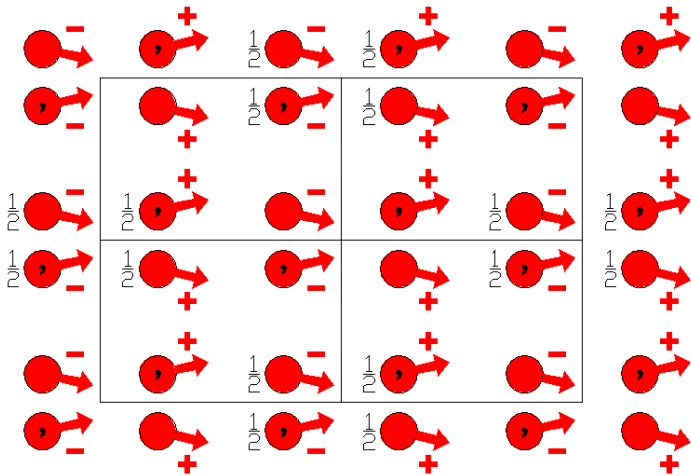
Fm'm2'

42.3.311

m'm2'

Fm'm2'

Orthorhombic



Origin on m'm2'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (4) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |
|--------------------|--|--|--|

For (0,1/2,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2) | (2) 2' (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)' | (3) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2) | (4) n' (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>  0,1/2,1/2)' |
|------------------------------------|--|--|--|

For (1/2,0,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,0,1/2)<br>(1 1/2,0,1/2) | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2) | (4) c' (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,0,1/2)' |
|------------------------------------|--|--|--|

For (1/2,1/2,0) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) 2' 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)' | (3) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (4) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |
|------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

### Positions

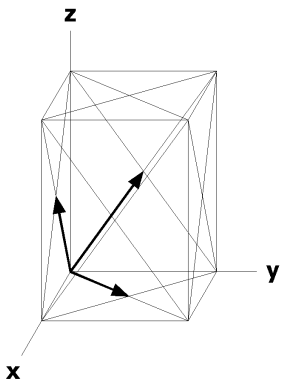
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
16	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8	d .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0,v,0]		
8	c m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0,v, $\bar{w}$ ]		
8	b ..2'	1/4,1/4,z [u,v,0]	1/4,3/4,z [ $\bar{u},v,0$ ]		
4	a m'm2'	0,0,z [0,v,0]			

### Symmetry of Special Projections

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



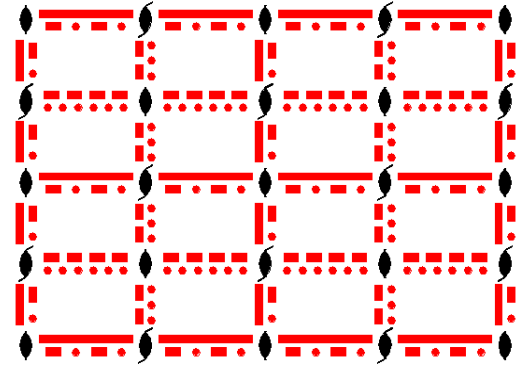
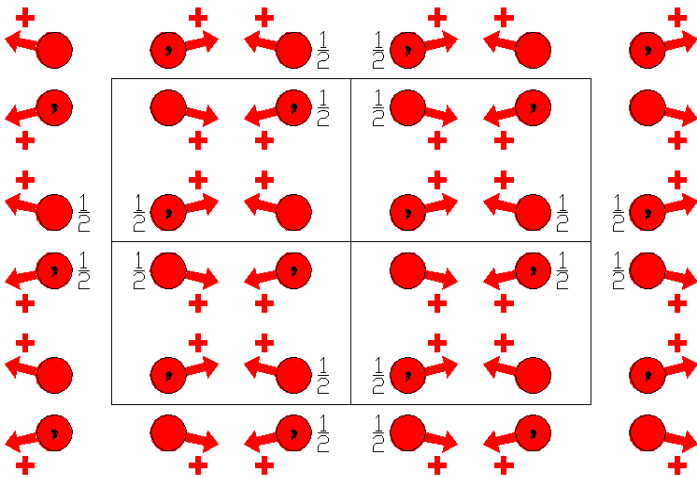
Fm'm'2

42.4.312

m'm'2

Fm'm'2

Orthorhombic



Origin on m'm'2

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (4) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |
|--------------------|--|--|--|

For (0,1/2,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2) | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2) | (3) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (4) n' (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>  0,1/2,1/2)' |
|------------------------------------|--|--|--|

For (1/2,0,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,0,1/2)<br>(1 1/2,0,1/2) | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2)' | (4) c' (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,0,1/2)' |
|------------------------------------|--|--|--|

For (1/2,1/2,0) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0) | (3) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (4) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |
|------------------------------------|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

### Positions

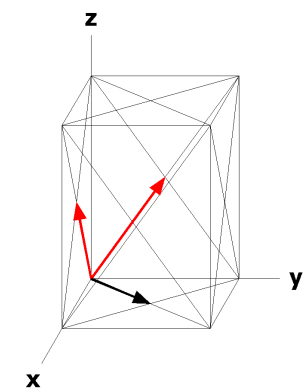
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
16 e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) x, $\bar{y},z [u,\bar{v},w]$	(4) $\bar{x},y,z [\bar{u},v,w]$
8 d .m'	x,0,z [u,0,w]	$\bar{x},0,z [\bar{u},0,w]$		
8 c m'..	0,y,z [0,v,w]	0, $\bar{y},z [0,\bar{v},w]$		
8 b ..2	1/4,1/4,z [0,0,w]	1/4,3/4,z [0,0,w]		
4 a m'm'2	0,0,z [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p1m'1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



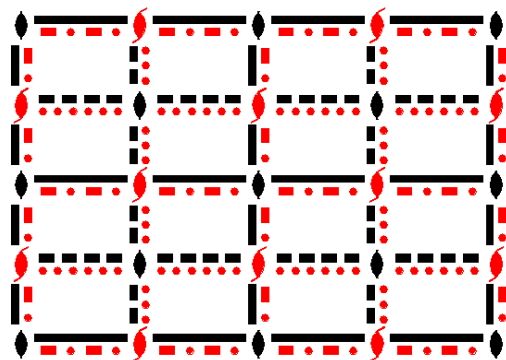
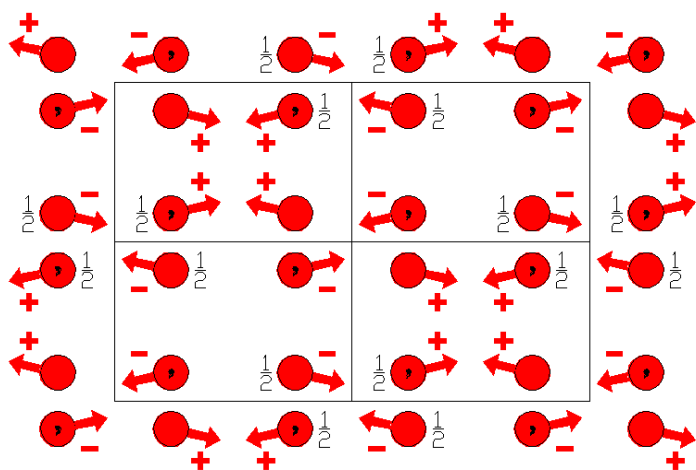
$F_C mm2$

42.5.313

$mm21'$

$F_C mm2$

Orthorhombic



**Origin** on  $mm2$

**Asymmetric unit**  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) m $x,0,z$<br>(m <sub>y</sub>  0,0,0) | (4) m $0,y,z$<br>(m <sub>x</sub>  0,0,0) |
|--------------------|--|--|--|

For  $(0,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' $(0,1/2,1/2)$<br>(1 0,1/2,1/2)' | (2) 2' $(0,0,1/2) 0,1/4,z$<br>(2 <sub>z</sub>  0,1/2,1/2)' | (3) c' $(0,0,1/2) x,1/4,z$<br>(m <sub>y</sub>  0,1/2,1/2)' | (4) n' $(0,1/2,1/2) 0,y,z$<br>(m <sub>x</sub>  0,1/2,1/2)' |
|--|--|--|--|

For  $(1/2,0,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' $(1/2,0,1/2)$<br>(1 1/2,0,1/2)' | (2) 2' $(0,0,1/2) 1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) n' $(1/2,0,1/2) x,0,z$<br>(m <sub>y</sub>  1/2,0,1/2)' | (4) c' $(0,0,1/2) 1/4,y,z$<br>(m <sub>x</sub>  1/2,0,1/2)' |
|--|--|--|--|

For  $(1/2,1/2,0)$  + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t $(1/2,1/2,0)$<br>(1 1/2,1/2,0) | (2) 2 $1/4,1/4,z$<br>(2 <sub>z</sub>  1/2,1/2,0) | (3) a $(1/2,0,0) x,1/4,z$<br>(m <sub>y</sub>  1/2,1/2,0) | (4) b $(0,1/2,0) 1/4,y,z$<br>(m <sub>x</sub>  1/2,1/2,0) |
|--------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); t'(1/2,0,1/2); (2); (3).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

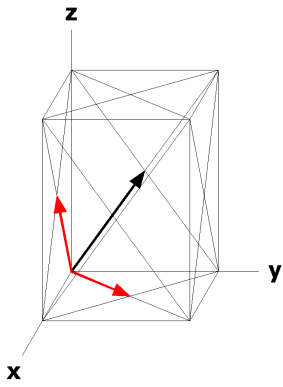
		(0,0,0) +	(0,1/2,1/2)' +	(1/2,0,1/2)' +	(1/2,1/2,0) +
16	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
8	d .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]		
8	c m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]		
8	b ..2	1/4,1/4,z [0,0,w]	1/4,3/4,z [0,0, $\bar{w}$ ]		
4	a mm2	0,0,z [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $p_c2mm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0]  $p1m11'$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



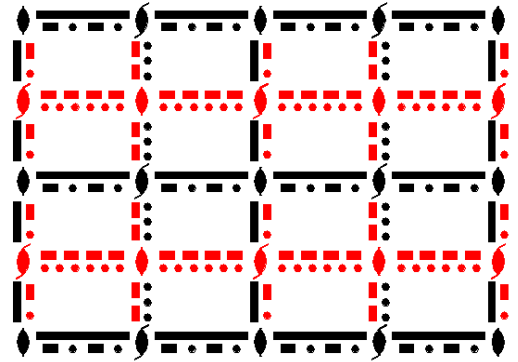
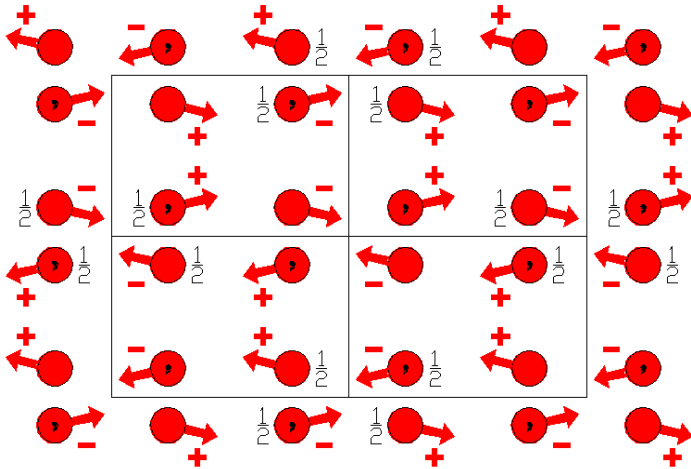
$F_A$  mm2

42.6.314

mm21'

$F_A$  mm2

Orthorhombic



**Origin** on mm2

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |                    |                                  |                                  |                                  |
|--------------------|----------------------------------|----------------------------------|----------------------------------|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) m $x,0,z$<br>( $m_y$  0,0,0) | (4) m $0,y,z$<br>( $m_x$  0,0,0) |
|--------------------|----------------------------------|----------------------------------|----------------------------------|

For (0,1/2,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2) | (2) 2 (0,0,1/2) $0,1/4,z$<br>( $2_z$  0,1/2,1/2) | (3) c (0,0,1/2) $x,1/4,z$<br>( $m_y$  0,1/2,1/2) | (4) n (0,1/2,1/2) $0,y,z$<br>( $m_x$  0,1/2,1/2) |
|------------------------------------|--|--|--|

For (1/2,0,1/2)' + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t' (1/2,0,1/2)<br>(1 1/2,0,1/2)' | (2) 2' (0,0,1/2) $1/4,0,z$<br>( $2_z$  1/2,0,1/2)' | (3) n' (1/2,0,1/2) $x,0,z$<br>( $m_y$  1/2,0,1/2)' | (4) c' (0,0,1/2) $1/4,y,z$<br>( $m_x$  1/2,0,1/2)' |
|--------------------------------------|--|--|--|

For (1/2,1/2,0)' + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t' (1/2,1/2,0)<br>(1 1/2,1/2,0)' | (2) 2' $1/4,1/4,z$<br>( $2_z$  1/2,1/2,0)' | (3) a' (1/2,0,0) $x,1/4,z$<br>( $m_y$  1/2,1/2,0)' | (4) b' (0,1/2,0) $1/4,y,z$<br>( $m_x$  1/2,1/2,0)' |
|--------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t'(1/2,0,1/2); (2); (3).

### Positions

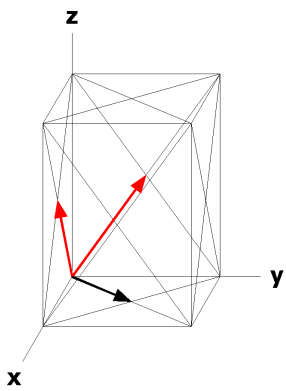
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2)' +	(1/2,1/2,0)' +
16 e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 d .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]		
8 c m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]		
8 b ..2	1/4,1/4,z [0,0,w]	1/4,3/4,z [0,0, $\bar{w}$ ]		
4 a mm2	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1]  $p_{2a}2mm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0]  $p1m11'$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



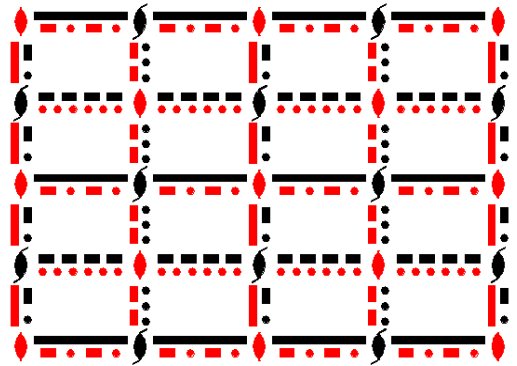
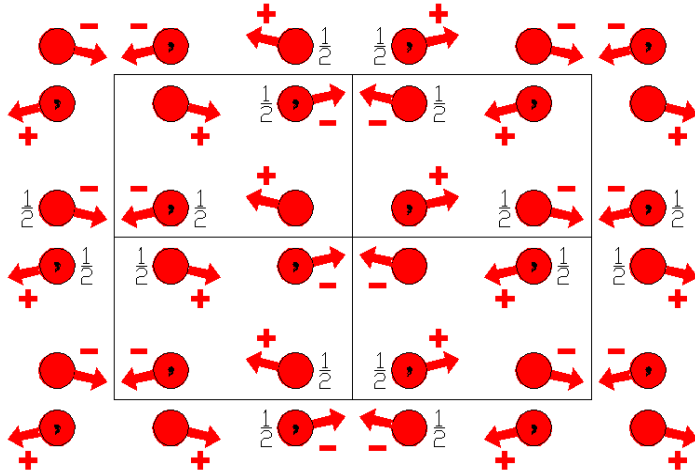
$F_cmm'2'$

42.7.315

$mm21'$

$F_cmm'2'$

Orthorhombic



Origin on  $mm'2'$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |                    |                                    |                                    |                                  |
|--------------------|------------------------------------|------------------------------------|----------------------------------|
| (1) 1<br>(1 0,0,0) | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $m'$ x,0,z<br>( $m_y$  0,0,0)' | (4) $m$ 0,y,z<br>( $m_x$  0,0,0) |
|--------------------|------------------------------------|------------------------------------|----------------------------------|

For (0,1/2,1/2)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (0,1/2,1/2)<br>(1 0,1/2,1/2)' | (2) $2$ (0,0,1/2) 0,1/4,z<br>( $2_z$  0,1/2,1/2) | (3) $c$ (0,0,1/2) x,1/4,z<br>( $m_y$  0,1/2,1/2) | (4) $n'$ (0,1/2,1/2) 0,y,z<br>( $m_x$  0,1/2,1/2)' |
|--|--|--|--|

For (1/2,0,1/2)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (1/2,0,1/2)<br>(1 1/2,0,1/2)' | (2) $2$ (0,0,1/2) 1/4,0,z<br>( $2_z$  1/2,0,1/2) | (3) $n$ (1/2,0,1/2) x,0,z<br>( $m_y$  1/2,0,1/2) | (4) $c'$ (0,0,1/2) 1/4,y,z<br>( $m_x$  1/2,0,1/2)' |
|--|--|--|--|

For (1/2,1/2,0) + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) $t$ (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) $2'$ 1/4,1/4,z<br>( $2_z$  1/2,1/2,0)' | (3) $a'$ (1/2,0,0) x,1/4,z<br>( $m_y$  1/2,1/2,0)' | (4) $b$ (0,1/2,0) 1/4,y,z<br>( $m_x$  1/2,1/2,0) |
|--------------------------------------|--|--|--|

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(0,1/2,1/2)$ ;  $t'(1/2,0,1/2)$ ; (2); (3).

**Positions**

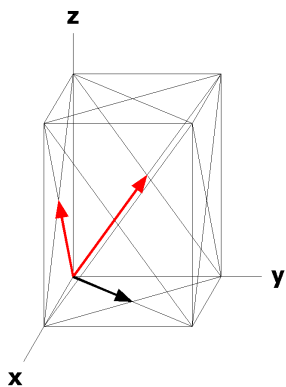
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2)' +	(1/2,0,1/2)' +	(1/2,1/2,0) +
16	e 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [u,v,\bar{w}]$	(3) $x,\bar{y},z [u,\bar{v},w]$	(4) $\bar{x},y,z [u,\bar{v},\bar{w}]$
8	d .m'	$x,0,z [u,0,w]$	$\bar{x},0,z [u,0,\bar{w}]$		
8	c m..	$0,y,z [u,0,0]$	$0,\bar{y},z [u,0,0]$		
8	b ..2'	$1/4,1/4,z [u,v,0]$	$1/4,3/4,z [u,\bar{v},0]$		
4	a mm'2'	$0,0,z [u,0,0]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_c 2mm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $0,1/4,z$

Along  $[1,0,0]$   $p_{1m} 11'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $p_{2b} 1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $0,y,0$



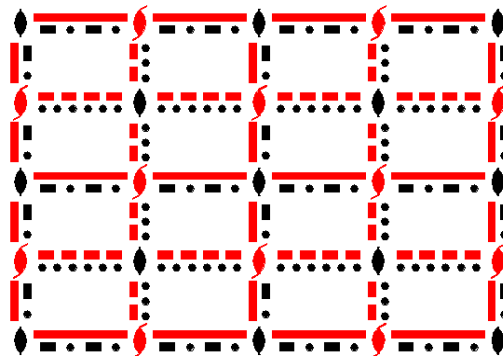
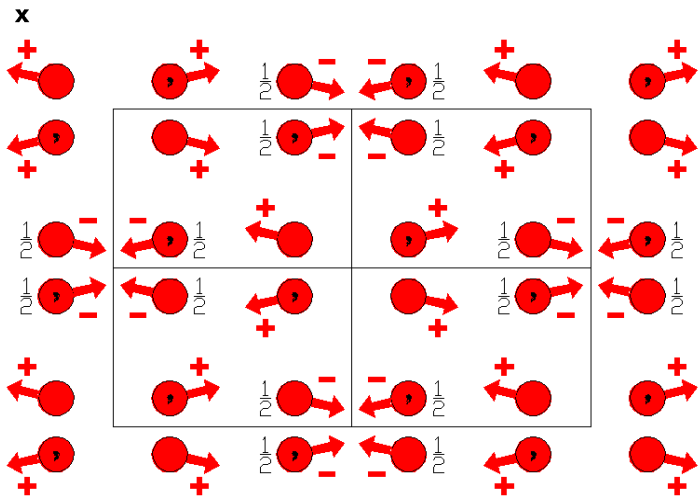
$F_c m' m' 2$

$mm21'$

Orthorhombic

42.8.316

$F_c m' m' 2$



**Origin** on  $m' m' 2$

**Asymmetric unit**  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |                                      |                                      |
|--------------------|--|--------------------------------------|--------------------------------------|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) $m'$ $x,0,z$<br>( $m_y$  0,0,0)' | (4) $m'$ $0,y,z$<br>( $m_x$  0,0,0)' |
|--------------------|--|--------------------------------------|--------------------------------------|

For  $(0,1/2,1/2)$ ' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(0,1/2,1/2)$<br>(1 0,1/2,1/2)' | (2) 2' $(0,0,1/2)$ $0,1/4,z$<br>(2 <sub>z</sub>  0,1/2,1/2)' | (3) $c$ $(0,0,1/2)$ $x,1/4,z$<br>( $m_y$  0,1/2,1/2) | (4) $n$ $(0,1/2,1/2)$ $0,y,z$<br>( $m_x$  0,1/2,1/2) |
|--|--|--|--|

For  $(1/2,0,1/2)$ ' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,0,1/2)$<br>(1 1/2,0,1/2)' | (2) 2' $(0,0,1/2)$ $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) $n$ $(1/2,0,1/2)$ $x,0,z$<br>( $m_y$  1/2,0,1/2) | (4) $c$ $(0,0,1/2)$ $1/4,y,z$<br>( $m_x$  1/2,0,1/2) |
|--|--|--|--|

For  $(1/2,1/2,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t$ $(1/2,1/2,0)$<br>(1 1/2,1/2,0) | (2) 2 $1/4,1/4,z$<br>(2 <sub>z</sub>  1/2,1/2,0) | (3) $a'$ $(1/2,0,0)$ $x,1/4,z$<br>( $m_y$  1/2,1/2,0)' | (4) $b'$ $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$  1/2,1/2,0)' |
|--|--|--|--|



**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(0,1/2,1/2)$ ;  $t'(1/2,0,1/2)$ ; (2); (3).

**Positions**

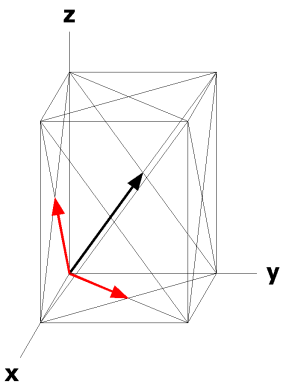
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2)' +	(1/2,0,1/2)' +	(1/2,1/2,0) +
16	e 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $x,\bar{y},z [u,\bar{v},w]$	(4) $\bar{x},y,z [\bar{u},v,w]$
8	d .m'	$x,0,z [u,0,w]$	$\bar{x},0,z [\bar{u},0,w]$		
8	c m'..	$0,y,z [0,v,w]$	$0,\bar{y},z [0,\bar{v},w]$		
8	b ..2	$1/4,1/4,z [0,0,w]$	$1/4,3/4,z [0,0,w]$		
4	a m'm'2	$0,0,z [0,0,w]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_c 2mm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $1/4,1/4,z$

Along  $[1,0,0]$   $p_{2b} 1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $p_{2b} 1m'1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $0,y,0$



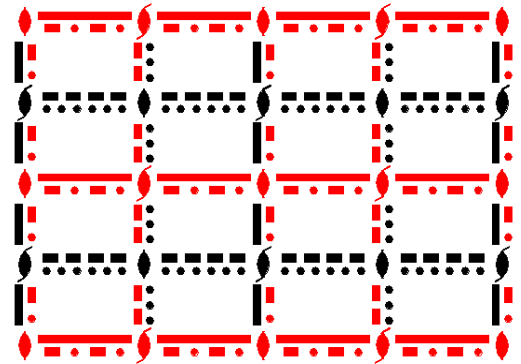
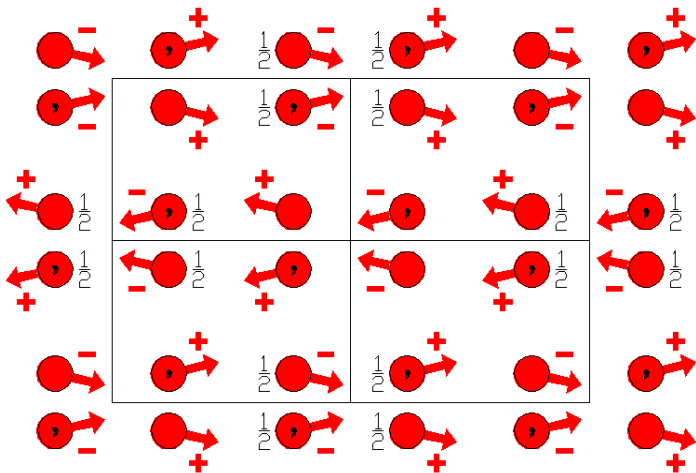
$F_A m' m 2'$

$mm21'$

Orthorhombic

42.9.317

$F_A m' m 2'$



Origin on  $m' m 2'$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                      |                                    |                                      |
|--------------------|--------------------------------------|------------------------------------|--------------------------------------|
| (1) 1<br>(1 0,0,0) | (2) $2' (0,0,z)$<br>( $2_z$  0,0,0)' | (3) $m (x,0,z)$<br>( $m_y$  0,0,0) | (4) $m' (0,y,z)$<br>( $m_x$  0,0,0)' |
|--------------------|--------------------------------------|------------------------------------|--------------------------------------|

For  $(0,1/2,1/2)$  + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) $t (0,1/2,1/2)$<br>(1 0,1/2,1/2) | (2) $2' (0,0,1/2)$ $0,1/4,z$<br>( $2_z$  0,1/2,1/2)' | (3) $c (0,0,1/2)$ $x,1/4,z$<br>( $m_y$  0,1/2,1/2) | (4) $n' (0,1/2,1/2)$ $0,y,z$<br>( $m_x$  0,1/2,1/2)' |
|--------------------------------------|--|--|--|

For  $(1/2,0,1/2)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t' (1/2,0,1/2)$<br>(1 1/2,0,1/2)' | (2) $2 (0,0,1/2)$ $1/4,0,z$<br>( $2_z$  1/2,0,1/2) | (3) $n' (1/2,0,1/2)$ $x,0,z$<br>( $m_y$  1/2,0,1/2)' | (4) $c (0,0,1/2)$ $1/4,y,z$<br>( $m_x$  1/2,0,1/2) |
|--|--|--|--|

For  $(1/2,1/2,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t' (1/2,1/2,0)$<br>(1 1/2,1/2,0)' | (2) $2 (1/4,1/4,z)$<br>( $2_z$  1/2,1/2,0) | (3) $a' (1/2,0,0)$ $x,1/4,z$<br>( $m_y$  1/2,1/2,0)' | (4) $b (0,1/2,0)$ $1/4,y,z$<br>( $m_x$  1/2,1/2,0) |
|--|--|--|--|

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0,1/2,1/2)$ ;  $t'(1/2,0,1/2)$ ; (2); (3).

**Positions**

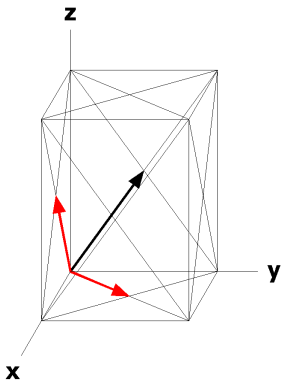
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2)' +	(1/2,1/2,0)' +
16	e 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x,\bar{y},z$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) $\bar{x},y,z$ [ $\bar{u}$ ,v,w]
8	d .m.	$x,0,z$ [0,v,0]	$\bar{x},0,z$ [0,v,0]		
8	c m'..	$0,y,z$ [0,v,w]	$0,\bar{y},z$ [0,v, $\bar{w}$ ]		
8	b ..2'	$1/4,1/4,z$ [u,v,0]	$1/4,3/4,z$ [ $\bar{u}$ ,v,0]		
4	a m'm2'	$0,0,z$ [0,v,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2a} 2mm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,1/4,z

Along [1,0,0]  $p_c 1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0]  $p1m11'$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



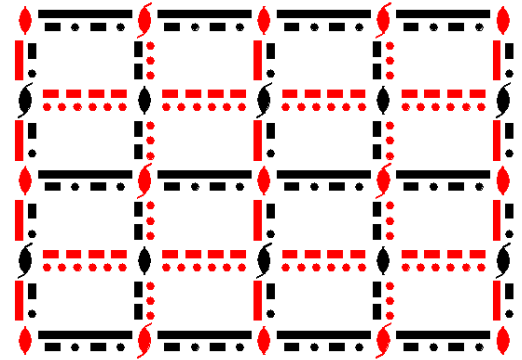
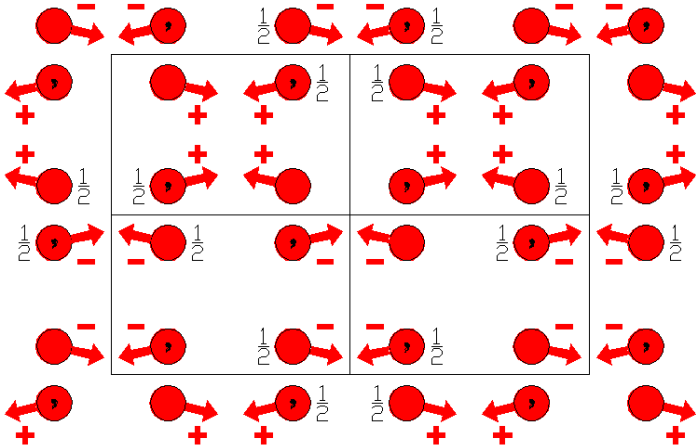
$F_A mm'2'$

42.10.318

$mm21'$

$F_A mm'2'$

Orthorhombic



**Origin** on  $mm'2'$

**Asymmetric unit**  $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                      |                                      |                                    |
|--------------------|--------------------------------------|--------------------------------------|------------------------------------|
| (1) 1<br>(1 0,0,0) | (2) $2'$ $0,0,z$<br>( $2_z$  0,0,0)' | (3) $m'$ $x,0,z$<br>( $m_y$  0,0,0)' | (4) $m$ $0,y,z$<br>( $m_x$  0,0,0) |
|--------------------|--------------------------------------|--------------------------------------|------------------------------------|

For  $(0,1/2,1/2)$  + set

- |  |  |  |                                   |
|--|--|--|-----------------------------------|
| (1) $t$ $(0,1/2,1/2)$<br>(1 0,1/2,1/2) | (2) $2'$ $(0,0,1/2) \quad 0,1/4,z$<br>( $2_z$  0,1/2,1/2)' | (3) $c'$ $(0,0,1/2) \quad x,1/4,z$<br>( $m_y$  0,1/2,1/2)' | (4) $n$ $(0,1/2,1/2) \quad 0,y,z$ |
|--|--|--|-----------------------------------|

For  $(1/2,0,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,0,1/2)$<br>(1 1/2,0,1/2)' | (2) $2$ $(0,0,1/2) \quad 1/4,0,z$<br>( $2_z$  1/2,0,1/2) | (3) $n$ $(1/2,0,1/2) \quad x,0,z$<br>( $m_y$  1/2,0,1/2) | (4) $c'$ $(0,0,1/2) \quad 1/4,y,z$<br>( $m_x$  1/2,0,1/2)' |
|--|--|--|--|

For  $(1/2,1/2,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,0)$<br>(1 1/2,1/2,0)' | (2) $2$ $1/4,1/4,z$<br>( $2_z$  1/2,1/2,0) | (3) $a$ $(1/2,0,0) \quad x,1/4,z$<br>( $m_y$  1/2,1/2,0) | (4) $b'$ $(0,1/2,0) \quad 1/4,y,z$<br>( $m_x$  1/2,1/2,0)' |
|--|--|--|--|

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0,1/2,1/2)$ ;  $t'(1/2,0,1/2)$ ; (2); (3).

### Positions

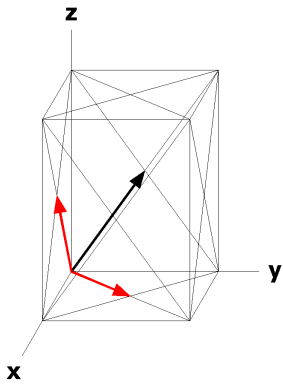
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2)' +	(1/2,1/2,0)' +
16 e 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [u,v,\bar{w}]$	(3) $x,\bar{y},z [u,\bar{v},w]$	(4) $\bar{x},y,z [u,\bar{v},\bar{w}]$
8 d .m'	$x,0,z [u,0,w]$	$\bar{x},0,z [u,0,\bar{w}]$		
8 c m..	$0,y,z [u,0,0]$	$0,\bar{y},z [u,0,0]$		
8 b ..2'	$1/4,1/4,z [u,v,0]$	$1/4,3/4,z [u,\bar{v},0]$		
4 a mm'2'	$0,0,z [u,0,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $p_{2a}2m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $1/4,0,z$

Along  $[1,0,0]$   $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $p_{2a}1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $0,y,0$



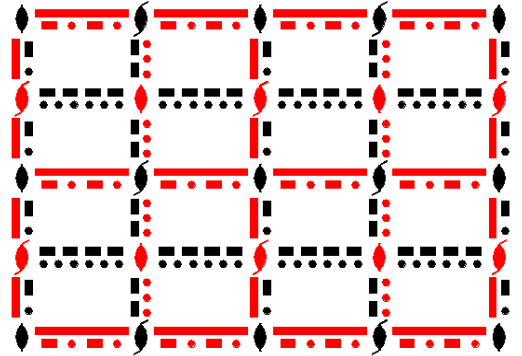
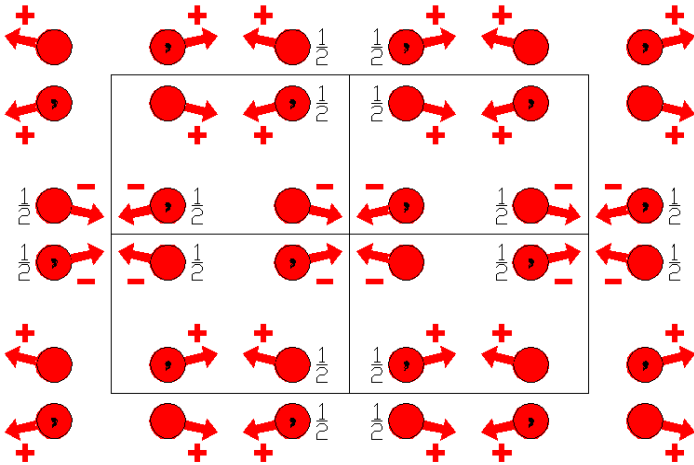
$F_A m' m' 2$

$mm21'$

Orthorhombic

42.11.319

$F_A m' m' 2$



**Origin** on  $m' m' 2$

**Asymmetric unit**  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- (1) 1  
(1 | 0,0,0)
- (2) 2  $0,0,z$   
(2<sub>z</sub> | 0,0,0)
- (3) m'  $x,0,z$   
(m<sub>y</sub> | 0,0,0)'
- (4) m'  $0,y,z$   
(m<sub>x</sub> | 0,0,0)'

For  $(0,1/2,1/2)$  + set

- (1) t  $(0,1/2,1/2)$   
(1 | 0,1/2,1/2)
- (2) 2  $(0,0,1/2) 0,1/4,z$   
(2<sub>z</sub> | 0,1/2,1/2)
- (3) c'  $(0,0,1/2) x,1/4,z$   
(m<sub>y</sub> | 0,1/2,1/2)'
- (4) n'  $(0,1/2,1/2) 0,y,z$   
(m<sub>x</sub> | 0,1/2,1/2)'

For  $(1/2,0,1/2)$ ' + set

- (1) t'  $(1/2,0,1/2)$   
(1 | 1/2,0,1/2)'
- (2) 2'  $(0,0,1/2) 1/4,0,z$   
(2<sub>z</sub> | 1/2,0,1/2)'
- (3) n  $(1/2,0,1/2) x,0,z$   
(m<sub>y</sub> | 1/2,0,1/2)
- (4) c  $(0,0,1/2) 1/4,y,z$   
(m<sub>x</sub> | 1/2,0,1/2)

For  $(1/2,1/2,0)$ ' + set

- (1) t'  $(1/2,1/2,0)$   
(1 | 1/2,1/2,0)'
- (2) 2'  $1/4,1/4,z$   
(2<sub>z</sub> | 1/2,1/2,0)'
- (3) a  $(1/2,0,0) x,1/4,z$   
(m<sub>y</sub> | 1/2,1/2,0)
- (4) b  $(0,1/2,0) 1/4,y,z$   
(m<sub>x</sub> | 1/2,1/2,0)

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0,1/2,1/2)$ ;  $t'(1/2,0,1/2)$ ; (2); (3).

**Positions**

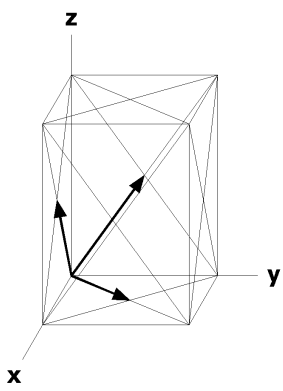
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2)' +	(1/2,1/2,0)' +
16	e 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $x,\bar{y},z [u,\bar{v},w]$	(4) $\bar{x},y,z [\bar{u},v,w]$
8	d .m'	$x,0,z [u,0,w]$	$\bar{x},0,z [\bar{u},0,w]$		
8	c m'..	$0,y,z [0,v,w]$	$0,\bar{y},z [0,\bar{v},w]$		
8	b ..2	$1/4,1/4,z [0,0,w]$	$1/4,3/4,z [0,0,w]$		
4	a m'm'2	$0,0,z [0,0,w]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_{2a} 2m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_c 1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,1/4,0$

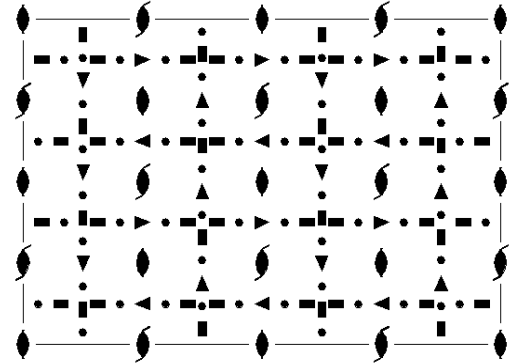
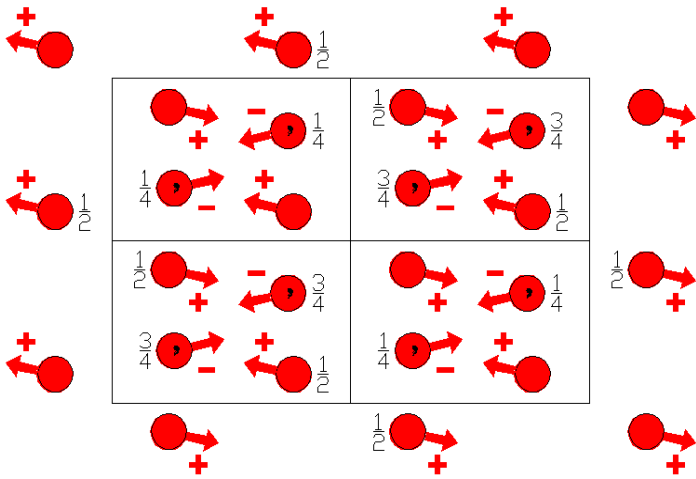
Along  $[0,1,0]$   $p_{2a} 1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $1/4,y,0$



Fdd2  
43.1.320

mm2  
Fdd2

Orthorhombic



Origin on 112

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) d $(1/4,0,1/4)$ $x,1/8,z$<br>(m <sub>y</sub>  1/4,1/4,1/4) | (4) d $(0,1/4,1/4)$ $1/8,y,z$<br>(m <sub>x</sub>  1/4,1/4,1/4) |
|--------------------|--|--|--|

For (0,1/2,1/2) + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t $(0,1/2,1/2)$<br>(1 0,1/2,1/2) | (2) 2 $(0,0,1/2)$ $0,1/4,z$<br>(2 <sub>z</sub>  0,1/2,1/2) | (3) d $(1/4,0,3/4)$ $x,3/8,z$<br>(m <sub>y</sub>  1/4,3/4,3/4) | (4) d $(0,3/4,3/4)$ $1/8,y,z$<br>(m <sub>x</sub>  1/4,3/4,3/4) |
|--------------------------------------|--|--|--|

For (1/2,0,1/2) + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t $(1/2,0,1/2)$<br>(1 1/2,0,1/2) | (2) 2 $(0,0,1/2)$ $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) d $(3/4,0,3/4)$ $x,1/8,z$<br>(m <sub>y</sub>  3/4,1/4,3/4) | (4) d $(0,1/4,3/4)$ $3/8,y,z$<br>(m <sub>x</sub>  3/4,1/4,3/4) |
|--------------------------------------|--|--|--|

For (1/2,1/2,0) + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) t $(1/2,1/2,0)$<br>(1 1/2,1/2,0) | (2) 2 $1/4,1/4,z$<br>(2 <sub>z</sub>  1/2,1/2,0) | (3) d $(3/4,0,1/4)$ $x,3/8,z$<br>(m <sub>y</sub>  3/4,3/4,1/4) | (4) d $(0,3/4,1/4)$ $3/8,y,z$<br>(m <sub>x</sub>  3/4,3/4,1/4) |
|--------------------------------------|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

### Positions

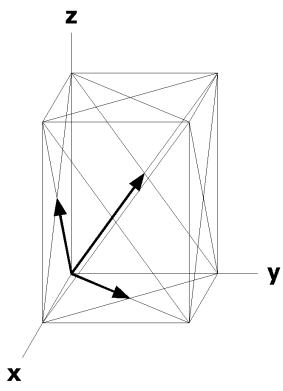
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
16	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $x+1/4, \bar{y}+1/4, z+1/4$ [ $\bar{u}, v, \bar{w}$ ]	(4) $\bar{x}+1/4, y+1/4, z+1/4$ [ $u, \bar{v}, \bar{w}$ ]
8	a ..2	0,0,z [0,0,w]	1/4,1/4,z+1/4 [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p2gg  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $c_p 1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0]  $c_p 1m'1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0

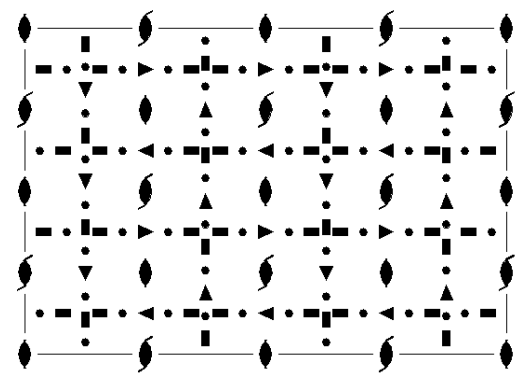
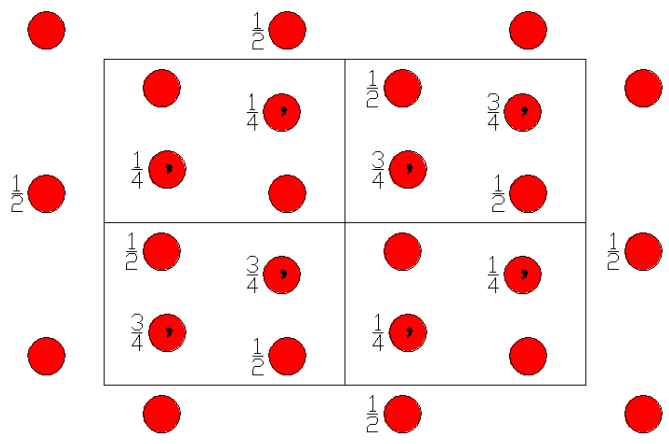


Fdd21'  
43.2.321

mm21'  
Fdd21'

Orthorhombic

1'



Origin on 112'

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

- (1) 1 (1|0,0,0)
- (2) 2<sub>z</sub> 0,0,z (2<sub>z</sub>|0,0,0)
- (3) d (1/4,0,1/4) x,1/8,z (m<sub>y</sub>|1/4,1/4,1/4)
- (4) d (0,1/4,1/4) 1/8,y,z (m<sub>x</sub>|1/4,1/4,1/4)

For (0,1/2,1/2) + set

- (1) t (0,1/2,1/2) (1|0,1/2,1/2)
- (2) 2 (0,0,1/2) 0,1/4,z (2<sub>z</sub>|0,1/2,1/2)
- (3) d (1/4,0,3/4) x,3/8,z (m<sub>y</sub>|1/4,3/4,3/4)
- (4) d (0,3/4,3/4) 1/8,y,z (m<sub>x</sub>|1/4,3/4,3/4)

For (1/2,0,1/2) + set

- (1) t (1/2,0,1/2) (1|1/2,0,1/2)
- (2) 2 (0,0,1/2) 1/4,0,z (2<sub>z</sub>|1/2,0,1/2)
- (3) d (3/4,0,3/4) x,1/8,z (m<sub>y</sub>|3/4,1/4,3/4)
- (4) d (0,1/4,3/4) 3/8,y,z (m<sub>x</sub>|3/4,1/4,3/4)

For (1/2,1/2,0) + set

- (1) t (1/2,1/2,0) (1|1/2,1/2,0)
- (2) 2 1/4,1/4,z (2<sub>z</sub>|1/2,1/2,0)
- (3) d (3/4,0,1/4) x,3/8,z (m<sub>y</sub>|3/4,3/4,1/4)
- (4) d (0,3/4,1/4) 3/8,y,z (m<sub>x</sub>|3/4,3/4,1/4)

For (0,0,0)' + set

- (1) 1' (1|0,0,0)'
- (2) 2' 0,0,z (2<sub>z</sub>|0,0,0)'
- (3) d' (1/4,0,1/4) x,1/8,z (m<sub>y</sub>|1/4,1/4,1/4)'
- (4) d' (0,1/4,1/4) 1/8,y,z (m<sub>x</sub>|1/4,1/4,1/4)'

For (0,1/2,1/2)' + set

- (1) t' (0,1/2,1/2) (1|0,1/2,1/2)'
- (2) 2' (0,0,1/2) 0,1/4,z (2<sub>z</sub>|0,1/2,1/2)'
- (3) d' (1/4,0,3/4) x,3/8,z (m<sub>y</sub>|1/4,3/4,3/4)'
- (4) d' (0,3/4,3/4) 1/8,y,z (m<sub>x</sub>|1/4,3/4,3/4)'

For (1/2,0,1/2)' + set

(1) t' (1/2,0,1/2)  
(1 | 1/2,0,1/2)'(2) 2' (0,0,1/2) 1/4,0,z  
(2<sub>z</sub> | 1/2,0,1/2)'(3) d' (3/4,0,3/4) x,1/8,z  
(m<sub>y</sub> | 3/4,1/4,3/4)'(4) d' (0,1/4,3/4) 3/8,y,z  
(m<sub>x</sub> | 3/4,1/4,3/4)'

For (1/2,1/2,0)' + set

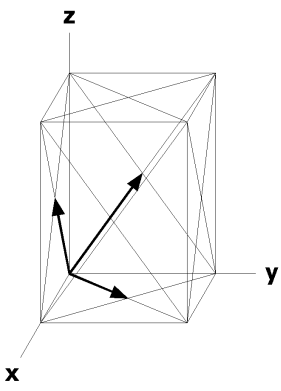
(1) t' (1/2,1/2,0)  
(1 | 1/2,1/2,0)'(2) 2' 1/4,1/4,z  
(2<sub>z</sub> | 1/2,1/2,0)'(3) d' (3/4,0/1,4) x,3/8,z  
(m<sub>y</sub> | 3/4,3/4,1/4)'(4) d' (0,3/4,1/4) 3/8,y,z  
(m<sub>x</sub> | 3/4,3/4,1/4)'**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); 1'.**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +  
(0,0,0)' + (0,1/2,1/2)' + (1/2,0,1/2)' + (1/2,1/2,0)'16 b 11' (1) x,y,z [0,0,0] (2)  $\bar{x},\bar{y},z$  [0,0,0] (3)  $x+1/4,\bar{y}+1/4,z+1/4$  [0,0,0] (4)  $\bar{x}+1/4,y+1/4,z+1/4$  [0,0,0]

8 a ..21' 0,0,z [0,0,0] 1/4,1/4,z+1/4 [0,0,0]

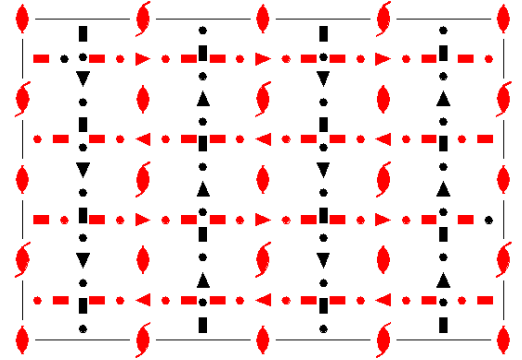
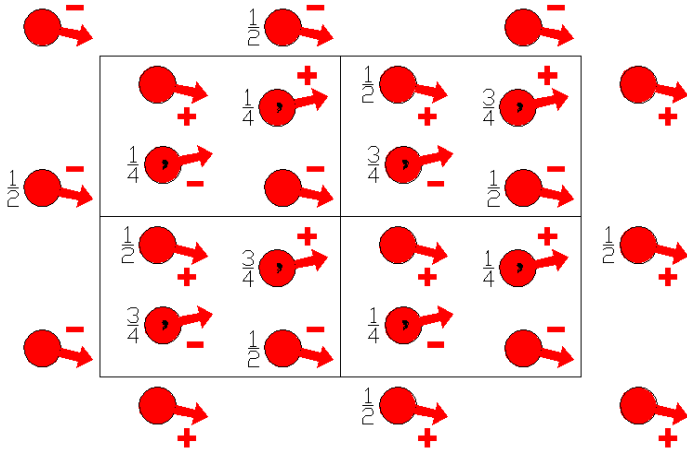
**Symmetry of Special Projections**Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at 0,0,zAlong [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,0,0Along [0,1,0] c1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at 0,y,0



Fd'd2'  
43.3.322

m'm2'  
Fd'd2'

Orthorhombic



Origin on 112'

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) d (1/4,0,1/4) x,1/8,z<br>(m <sub>y</sub>  1/4,1/4,1/4) | (4) d' (0,1/4,1/4) 1/8,y,z<br>(m <sub>x</sub>  1/4,1/4,1/4)' |
|--------------------|--|--|--|

For (0,1/2,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2) | (2) 2' (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)' | (3) d (1/4,0,3/4) x,3/8,z<br>(m <sub>y</sub>  1/4,3/4,3/4) | (4) d' (0,3/4,3/4) 1/8,y,z<br>(m <sub>x</sub>  1/4,3/4,3/4)' |
|------------------------------------|--|--|--|

For (1/2,0,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,0,1/2)<br>(1 1/2,0,1/2) | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) d (3/4,0,3/4) x,1/8,z<br>(m <sub>y</sub>  3/4,1/4,3/4) | (4) d' (0,1/4,3/4) 3/8,y,z<br>(m <sub>x</sub>  3/4,1/4,3/4)' |
|------------------------------------|--|--|--|

For (1/2,1/2,0) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) 2' 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)' | (3) d (3/4,0,1/4) x,3/8,z<br>(m <sub>y</sub>  3/4,3/4,1/4) | (4) d' (0,3/4,1/4) 3/8,y,z<br>(m <sub>x</sub>  3/4,3/4,1/4)' |
|------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

### Positions

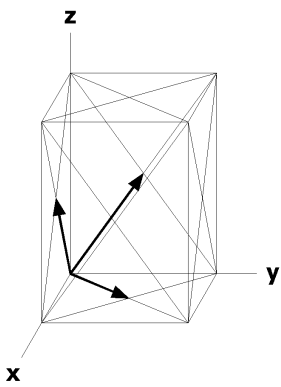
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
16	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3) $x+1/4, \bar{y}+1/4, z+1/4$ [ $\bar{u}, v, \bar{w}$ ]	(4) $\bar{x}+1/4, y+1/4, z+1/4$ [ $\bar{u}, v, w$ ]
8	a ..2'	0,0,z [u,v,0]	1/4,1/4,z+1/4 [ $\bar{u}, v, 0$ ]		

### Symmetry of Special Projections

Along [0,0,1] p2'gg'  
 $\mathbf{a}^* = -\mathbf{b}^*/2$   $\mathbf{b}^* = \mathbf{a}^*/2$   
 Origin at 0,0,z

Along [1,0,0] c1m1  
 $\mathbf{a}^* = \mathbf{b}^*/2$   $\mathbf{b}^* = \mathbf{c}^*/2$   
 Origin at x,0,0

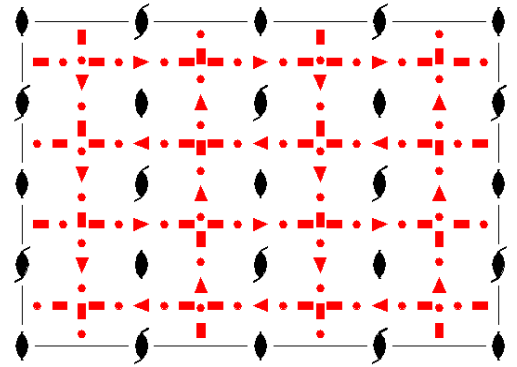
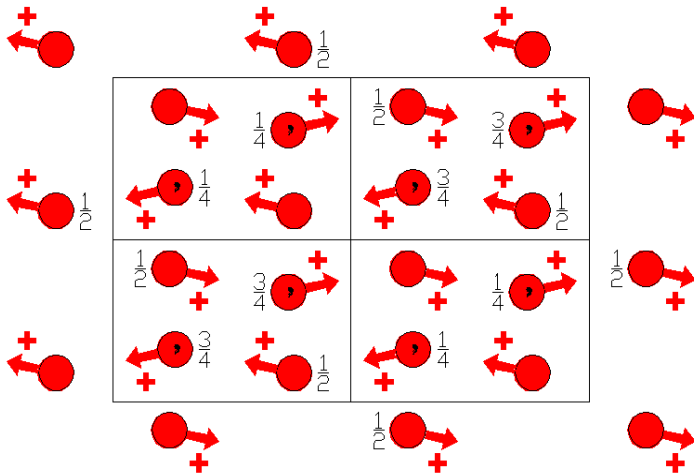
Along [0,1,0]  $c_{2'}1m1$   
 $\mathbf{a}^* = -\mathbf{a}^*/2$   $\mathbf{b}^* = \mathbf{c}^*/2$   
 Origin at 0,y,0



Fd'd'2  
43.4.323

m'm'2  
Fd'd'2

Orthorhombic



Origin on 112

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

### Symmetry Operations

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) d' (1/4,0,1/4) x,1/8,z<br>(m <sub>y</sub>  1/4,1/4,1/4)' | (4) d' (0,1/4,1/4) 1/8,y,z<br>(m <sub>x</sub>  1/4,1/4,1/4)' |
|--------------------|--|--|--|

For (0,1/2,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2) | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2) | (3) d' (1/4,0,3/4) x,3/8,z<br>(m <sub>y</sub>  1/4,3/4,3/4)' | (4) d' (0,3/4,3/4) 1/8,y,z<br>(m <sub>x</sub>  1/4,3/4,3/4)' |
|------------------------------------|--|--|--|

For (1/2,0,1/2) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,0,1/2)<br>(1 1/2,0,1/2) | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) d' (3/4,0,3/4) x,1/8,z<br>(m <sub>y</sub>  3/4,1/4,3/4)' | (4) d' (0,1/4,3/4) 3/8,y,z<br>(m <sub>x</sub>  3/4,1/4,3/4)' |
|------------------------------------|--|--|--|

For (1/2,1/2,0) + set

- |                                    |  |  |  |
|------------------------------------|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0) | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0) | (3) d' (3/4,0,1/4) x,3/8,z<br>(m <sub>y</sub>  3/4,3/4,1/4)' | (4) d' (0,3/4,1/4) 3/8,y,z<br>(m <sub>x</sub>  3/4,3/4,1/4)' |
|------------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

### Positions

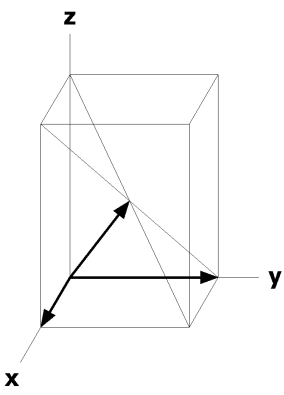
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
16	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $x+1/4, \bar{y}+1/4, z+1/4$ [ $u, \bar{v}, w$ ]	(4) $\bar{x}+1/4, y+1/4, z+1/4$ [ $\bar{u}, v, w$ ]
8	a ..2	0,0,z [0,0,w]	1/4,1/4,z+1/4 [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] p2g'g'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

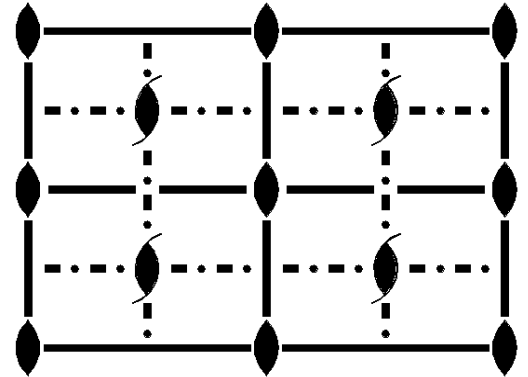
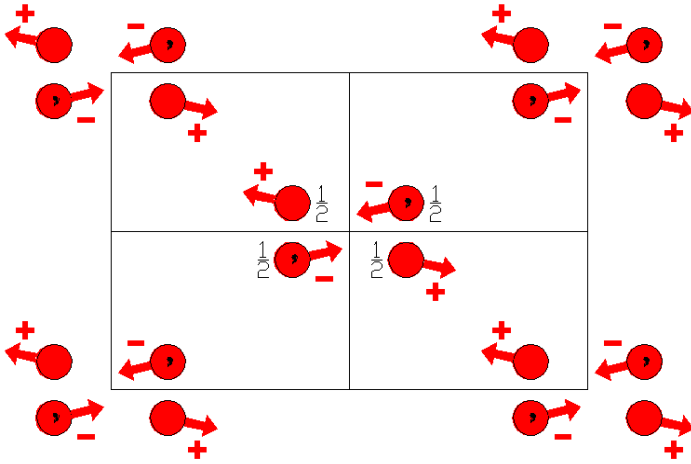
Along [0,1,0] c1m'1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Imm2  
44.1.324

mm2  
Imm2

Orthorhombic



Origin on mm2

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) m x,0,z  
(m<sub>y</sub>|0,0,0)

(4) m 0,y,z  
(m<sub>x</sub>|0,0,0)

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)  
(1|1/2,1/2,1/2)

(2) 2 (0,0,1/2) 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,1/2)

(3) n (1/2,0,1/2) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,1/2)

(4) n (0,1/2,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,1/2)



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

### Positions

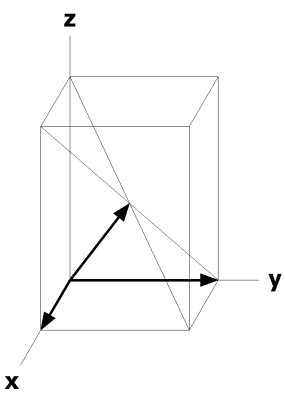
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(1/2,1/2,1/2) +		
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
4	d m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]		
4	c .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]		
2	b mm2	0,1/2,z [0,0,0]			
2	a mm2	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] c1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Imm21'

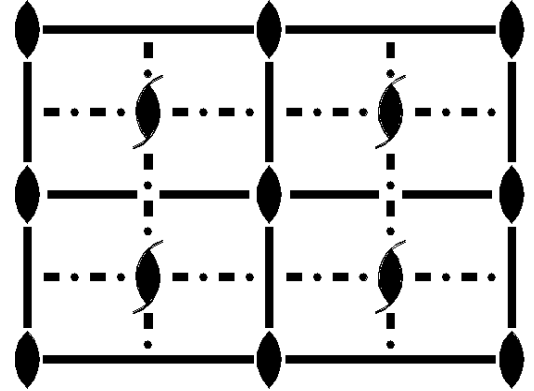
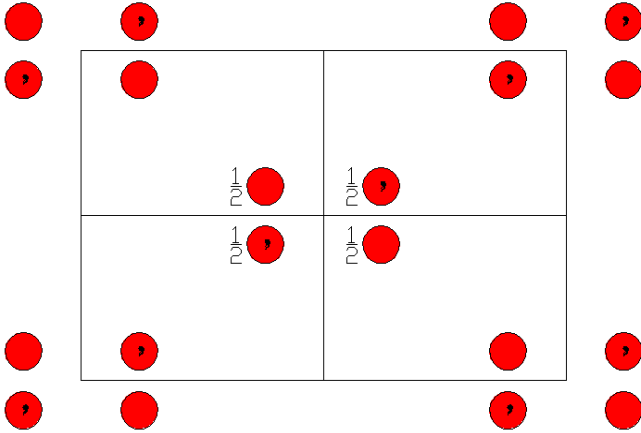
44.2.325

mm21'

Imm21'

Orthorhombic

1'



Origin on mm21'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) m x,0,z  
(m<sub>y</sub>|0,0,0)

(4) m 0,y,z  
(m<sub>x</sub>|0,0,0)

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)  
(1|1/2,1/2,1/2)

(2) 2 (0,0,1/2) 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,1/2)

(3) n (1/2,0,1/2) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,1/2)

(4) n (0,1/2,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,1/2)

For (0,0,0)' + set

(1) 1'  
(1|0,0,0)'

(2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'

(3) m' x,0,z  
(m<sub>y</sub>|0,0,0)'

(4) m' 0,y,z  
(m<sub>x</sub>|0,0,0)'

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2)  
(1|1/2,1/2,1/2)'

(2) 2' (0,0,1/2) 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,1/2)'

(3) n' (1/2,0,1/2) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,1/2)'

(4) n' (0,1/2,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); 1'.

### Positions

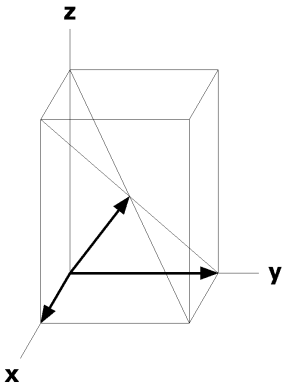
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'		
8	e 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) x, $\bar{y},z$ [0,0,0]	(4) $\bar{x},y,z$ [0,0,0]
4	d m..1'	0,y,z [0,0,0]	0, $\bar{y},z$ [0,0,0]		
4	c .m.1'	x,0,z [0,0,0]	$\bar{x},0,z$ [0,0,0]		
2	b mm21'	0,1/2,z [0,0,0]			
2	a mm21'	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

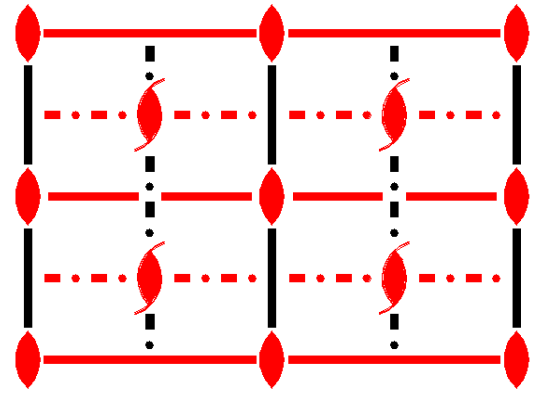
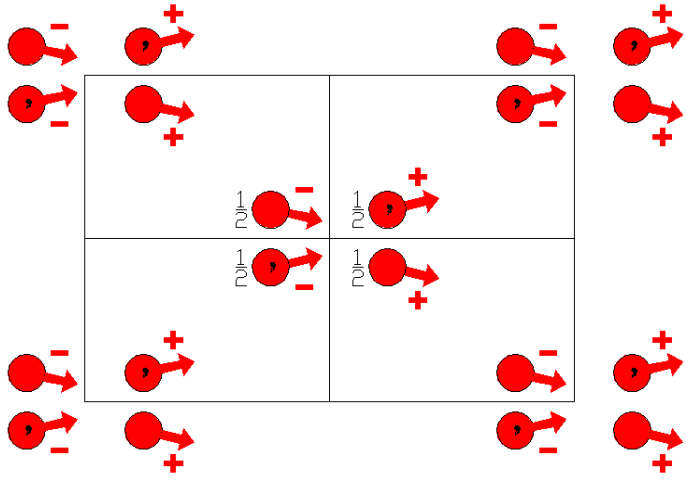
Along [0,1,0] c1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



$Im'm2'$   
44.3.326

$m'm2'$   
 $Im'm2'$

Orthorhombic



**Origin** on  $m'm2'$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2)  $2'_z$  0,0,z  
( $2_z$ |0,0,0)'

(3)  $m_x$  x,0,z  
( $m_y$ |0,0,0)

(4)  $m'_y$  0,y,z  
( $m'_x$ |0,0,0)'

For (1/2,1/2,1/2) + set

(1)  $t(1/2,1/2,1/2)$   
(1|1/2,1/2,1/2)

(2)  $2'_z(0,0,1/2)$  1/4,1/4,z  
( $2_z$ |1/2,1/2,1/2)'

(3)  $n(1/2,0,1/2)$  x,1/4,z  
( $m_y$ |1/2,1/2,1/2)

(4)  $n'(0,1/2,1/2)$  1/4,y,z  
( $m'_x$ |1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

### Positions

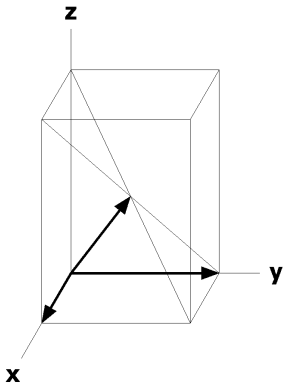
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
8 e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y},z$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) $\bar{x},y,z$ [ $\bar{u}$ ,v,w]
4 d m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0,v, $\bar{w}$ ]		
4 c .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0,v,0]		
2 b m'm2'	0,1/2,z [0,v,0]			
2 a m'm2'	0,0,z [0,v,0]			

### Symmetry of Special Projections

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] c1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

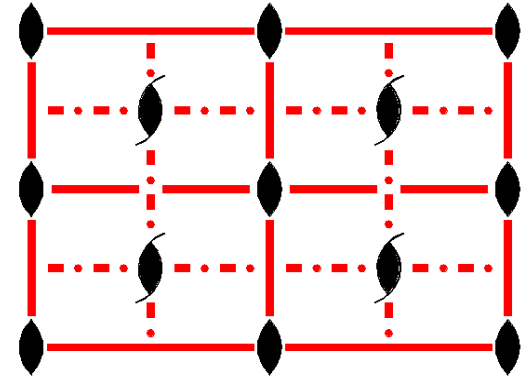
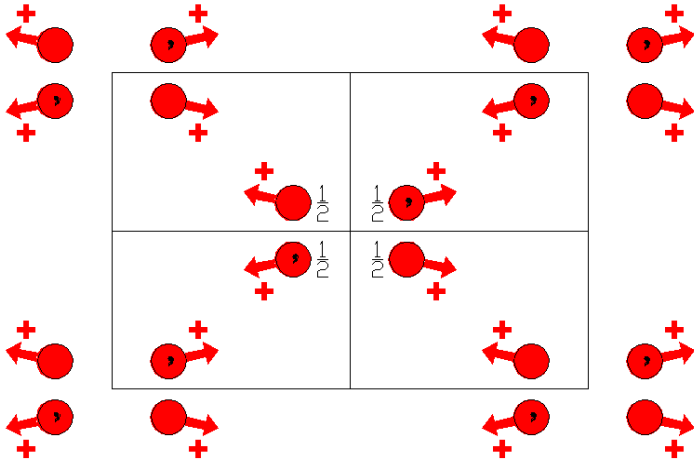
Along [0,1,0] c1m11'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



$Im'm'2$   
44.4.327

$m'm'2$   
 $Im'm'2$

Orthorhombic



**Origin** on  $m'm'2$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- (1) 1  
(1|0,0,0)
- (2) 2  $0,0,z$   
( $2_z$ |0,0,0)
- (3)  $m'$   $x,0,z$   
( $m_y$ |0,0,0)'
- (4)  $m'$   $0,y,z$   
( $m_x$ |0,0,0)'

For  $(1/2,1/2,1/2)$  + set

- (1)  $t$   $(1/2,1/2,1/2)$   
(1| $1/2,1/2,1/2$ )
- (2) 2  $(0,0,1/2) \ 1/4,1/4,z$   
( $2_z$ | $1/2,1/2,1/2$ )
- (3)  $n'$   $(1/2,0,1/2) \ x,1/4,z$   
( $m_y$ | $1/2,1/2,1/2$ )'
- (4)  $n'$   $(0,1/2,1/2) \ 1/4,y,z$   
( $m_x$ | $1/2,1/2,1/2$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

### Positions

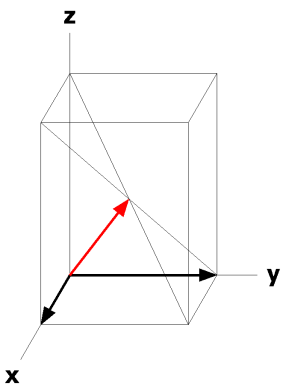
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +		(1/2,1/2,1/2) +	
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
4	d m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]		
4	c .m'.	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]		
2	b m'm'2	0,1/2,z [0,0,w]			
2	a m'm'2	0,0,z [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] c1m'1  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



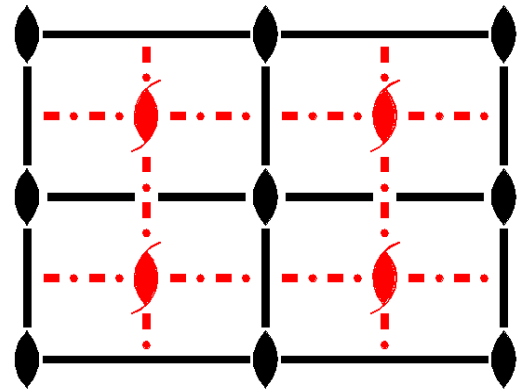
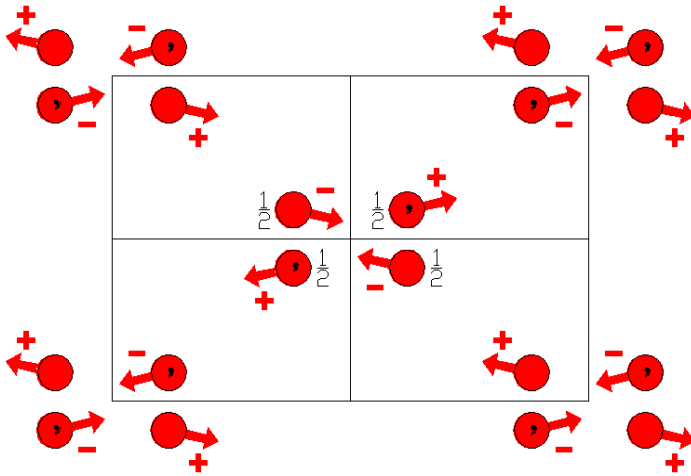
$I_pmm2$

44.5.328

$mm21'$

$I_pmm2$

Orthorhombic



**Origin** on  $mm2$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $m_x,0,z$   
( $m_x$ |0,0,0)

(4)  $m_0,y,z$   
( $m_x$ |0,0,0)

For  $(1/2,1/2,1/2)'$  + set

(1)  $t' (1/2,1/2,1/2)$   
(1| $1/2,1/2,1/2$ )'

(2)  $2' (0,0,1/2) \ 1/4,1/4,z$   
( $2_z$ | $1/2,1/2,1/2$ )'

(3)  $n' (1/2,0,1/2) \ x,1/4,z$   
( $m_y$ | $1/2,1/2,1/2$ )'

(4)  $n' (0,1/2,1/2) \ 1/4,y,z$   
( $m_x$ | $1/2,1/2,1/2$ )'



**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(1/2,1/2,1/2)$ ; (2); (3).

### Positions

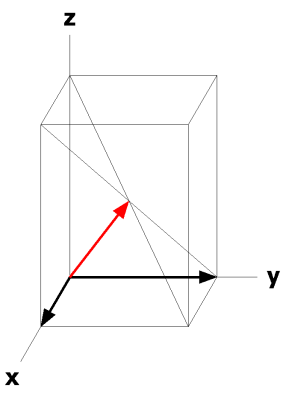
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,1/2)' +		
8	e 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
4	d m..	$0,y,z$ [u,0,0]	$0,\bar{y},z$ [ $\bar{u},0,0$ ]		
4	c .m.	$x,0,z$ [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]		
2	b mm2	$0,1/2,z$ [0,0,0]			
2	a mm2	$0,0,z$ [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1]  $c_p2mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $c1m11'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



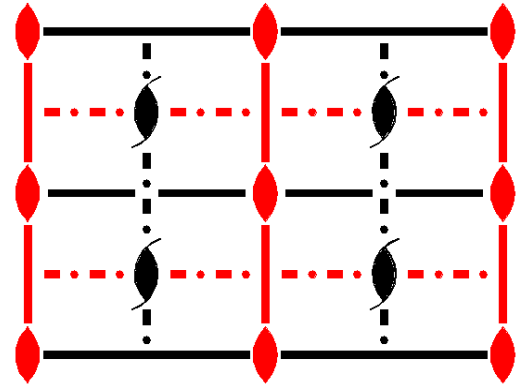
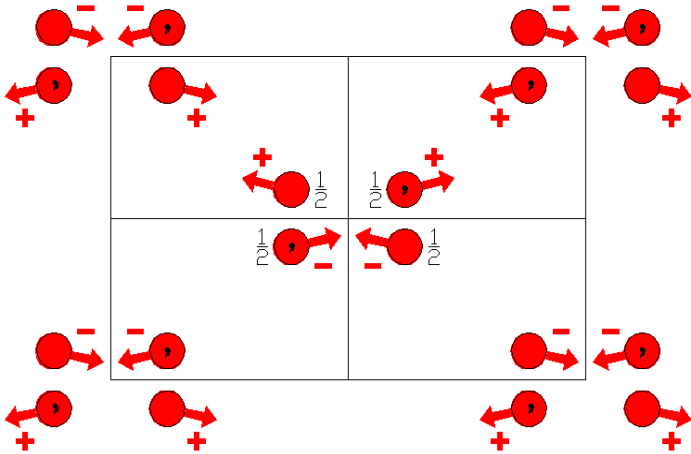
$I_pmm'2'$

44.6.329

$mm21'$

$I_pmm'2'$

Orthorhombic



**Origin** on  $mm'2'$

**Asymmetric unit**  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2)  $2'_z$  0,0,z  
( $2_z$ |0,0,0)'

(3)  $m'_x$  x,0,z  
( $m_x$ |0,0,0)'

(4)  $m'_y$  0,y,z  
( $m_y$ |0,0,0)

For  $(1/2,1/2,1/2)$ ' + set

(1)  $t'$  ( $1/2,1/2,1/2$ )  
(1| $1/2,1/2,1/2$ )'

(2)  $2'_z$  (0,0,1/2)  $1/4,1/4,z$   
( $2_z$ | $1/2,1/2,1/2$ )

(3)  $n'_x$  ( $1/2,0,1/2$ ) x, $1/4,z$   
( $m_y$ | $1/2,1/2,1/2$ )

(4)  $n'_y$  (0, $1/2,1/2$ )  $1/4,y,z$   
( $m_x$ | $1/2,1/2,1/2$ )'

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(1/2,1/2,1/2)$ ; (2); (3).

### Positions

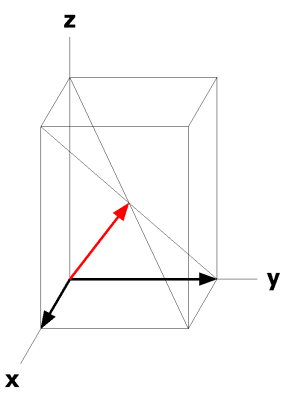
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,1/2)' +		
8	e 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [u,v,\bar{w}]$	(3) $x,\bar{y},z [u,\bar{v},w]$	(4) $\bar{x},y,z [u,\bar{v},\bar{w}]$
4	d m..	$0,y,z [u,0,0]$	$0,\bar{y},z [u,0,0]$		
4	c .m'	$x,0,z [u,0,w]$	$\bar{x},0,z [u,0,\bar{w}]$		
2	b $mm'2'$	$0,1/2,z [u,0,0]$			
2	a $mm'2'$	$0,0,z [u,0,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $c_p2'mm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $c_p1m1$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $0,y,0$



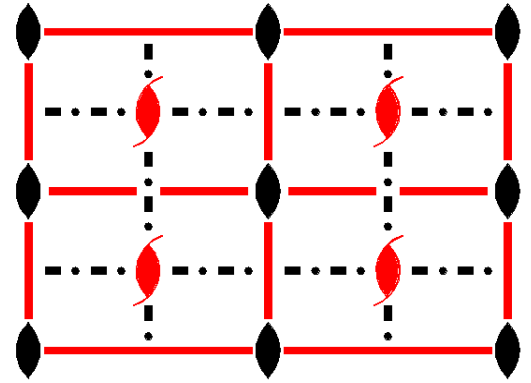
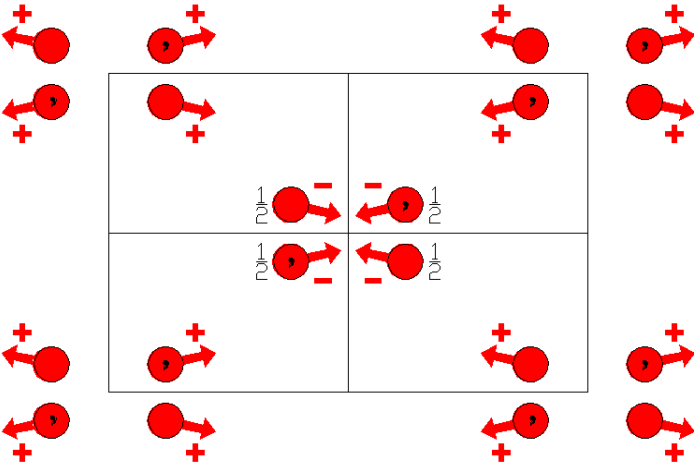
$I_p m' m' 2$

44.7.330

$mm21'$

$I_p m' m' 2$

Orthorhombic



**Origin** on  $m' m' 2$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $m'$   $x,0,z$   
( $m_y$ |0,0,0)'

(4)  $m'$   $0,y,z$   
( $m_x$ |0,0,0)'

For  $(1/2,1/2,1/2)'$  + set

(1)  $t'$   $(1/2,1/2,1/2)$   
(1| $1/2,1/2,1/2$ )'

(2)  $2'$   $(0,0,1/2) \ 1/4,1/4,z$   
( $2_z$ | $1/2,1/2,1/2$ )'

(3)  $n$   $(1/2,0,1/2) \ x,1/4,z$   
( $m_y$ | $1/2,1/2,1/2$ )'

(4)  $n$   $(0,1/2,1/2) \ 1/4,y,z$   
( $m_x$ | $1/2,1/2,1/2$ )'

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,1/2)'$ ; (2); (3).

### Positions

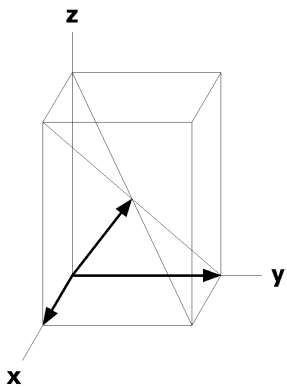
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,1/2)' +		
8	e 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x,\bar{y},z$ [u, $\bar{v},w$ ]	(4) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
4	d $m'..$	$0,y,z$ [0,v,w]	$0,\bar{y},z$ [0, $\bar{v},w$ ]		
4	c $.m'$	$x,0,z$ [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]		
2	b $m' m' 2$	$0,1/2,z$ [0,0,w]			
2	a $m' m' 2$	$0,0,z$ [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1]  $c_p 2m' m'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c_p 1m' 1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

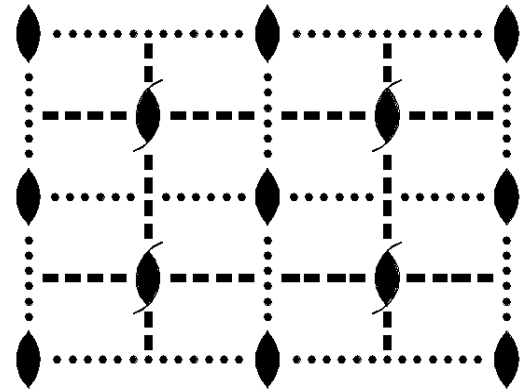
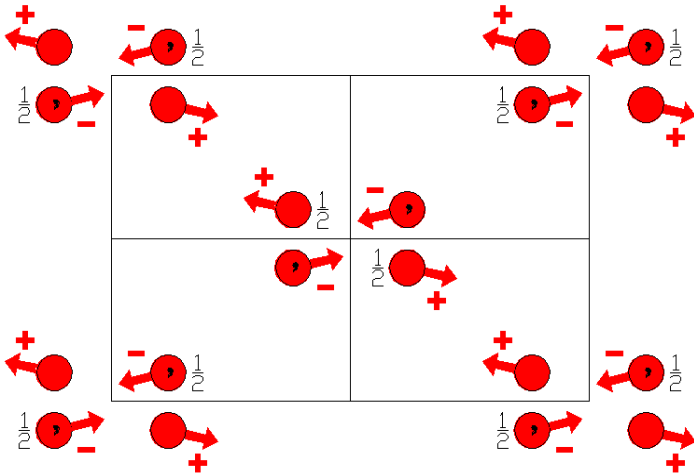
Along [0,1,0]  $c_p 1m' 1$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



lba2  
45.1.331

mm2  
lba2

Orthorhombic



Origin on cc2

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) c $(0,0,1/2)$ $x,0,z$<br>(m <sub>y</sub>  0,0,1/2) | (4) c $(0,0,1/2)$ $0,y,z$<br>(m <sub>x</sub>  0,0,1/2) |
|--------------------|--|--|--|

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t $(1/2,1/2,1/2)$<br>(1 1/2,1/2,1/2) | (2) 2 $(0,0,1/2)$ $1/4,1/4,z$<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) a $(1/2,0,0)$ $x,1/4,z$<br>(m <sub>y</sub>  1/2,1/2,0) | (4) b $(0,1/2,0)$ $1/4,y,z$<br>(m <sub>x</sub>  1/2,1/2,0) |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

### Positions

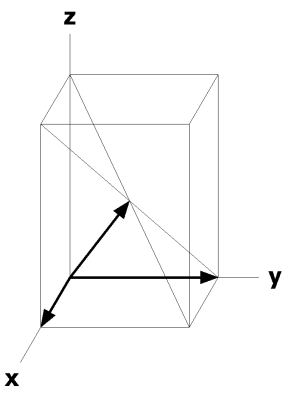
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,1/2) +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y}$ ,z+1/2 [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
4	b ..2	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]		
4	a ..2	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b} \cdot 1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2b} \cdot 1m'1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0

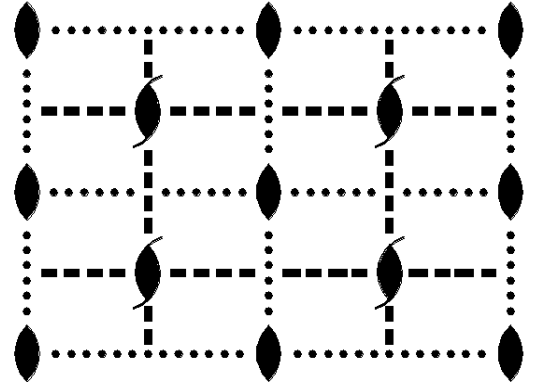
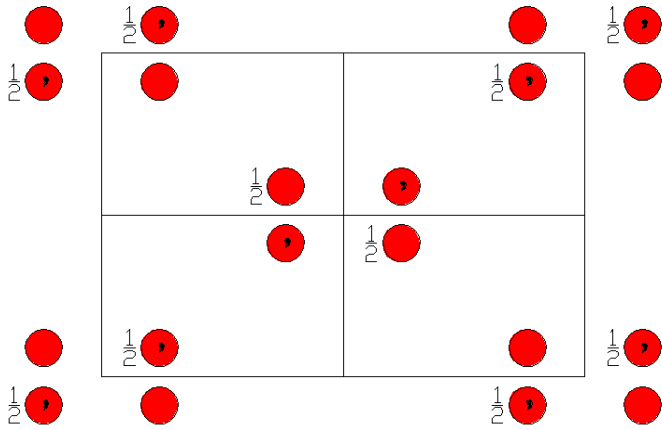


lba21'  
45.2.332

mm21'  
lba21'

Orthorhombic

1'



Origin on cc21'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (4) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) |
|--------------------|--|--|--|

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2) | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (4) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |
|--|--|--|--|

For (0,0,0)' + set

- |                      |  |  |  |
|----------------------|--|--|--|
| (1) 1'<br>(1 0,0,0)' | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (4) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |
|----------------------|--|--|--|

For (1/2,1/2,1/2)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)' | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (4) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |
|--|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); 1'.

### Positions

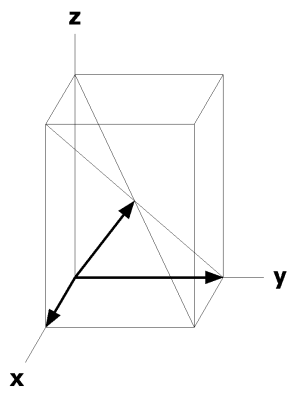
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'		
8	c 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $x,\bar{y},z+1/2$ [0,0,0]	(4) $\bar{x},y,z+1/2$ [0,0,0]
4	b ..21'	0,1/2,z [0,0,0]	0,1/2,z+1/2 [0,0,0]		
4	a ..21'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

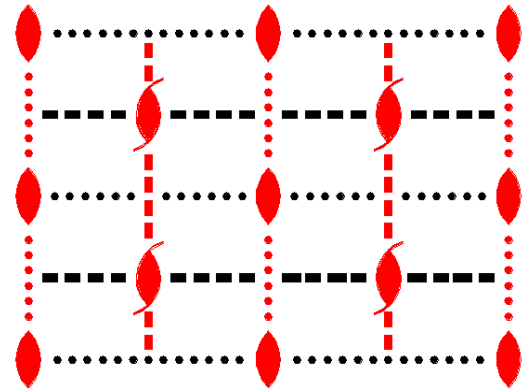
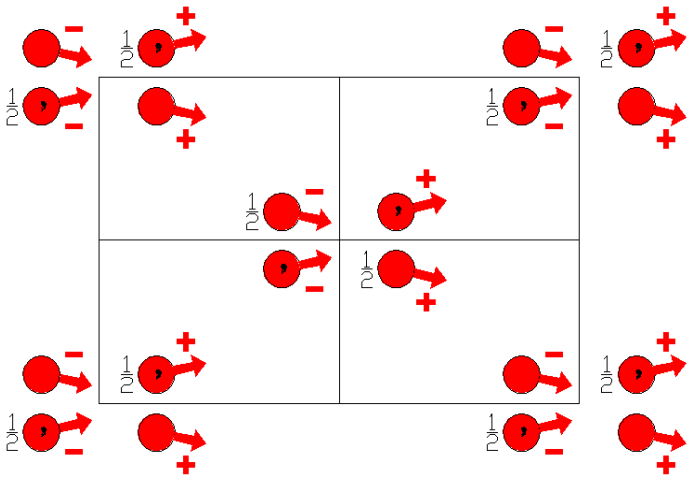
Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



lb'a2'  
45.3.333

m'm2'  
lb'a2'

Orthorhombic



Origin on c'c2'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (4) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |
|--------------------|--|--|--|

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2) | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (4) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

### Positions

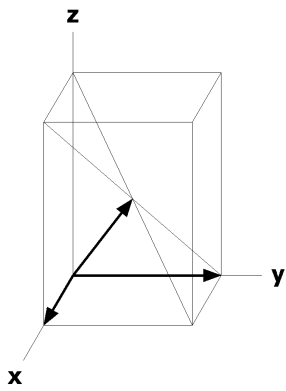
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,1/2) +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y}$ ,z+1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) $\bar{x}$ ,y,z+1/2 [ $\bar{u}$ ,v,w]
4	b ..2'	0,1/2,z [u,v,0]	0,1/2,z+1/2 [ $\bar{u}$ ,v,0]		
4	a ..2'	0,0,z [u,v,0]	0,0,z+1/2 [ $\bar{u}$ ,v,0]		

### Symmetry of Special Projections

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

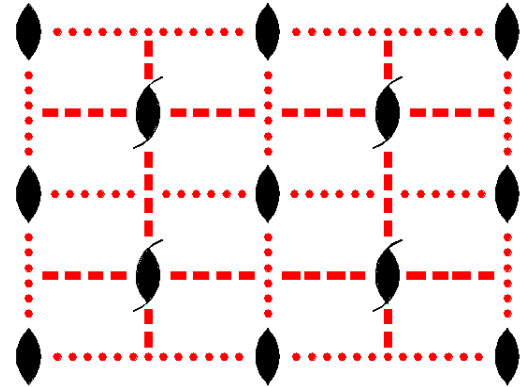
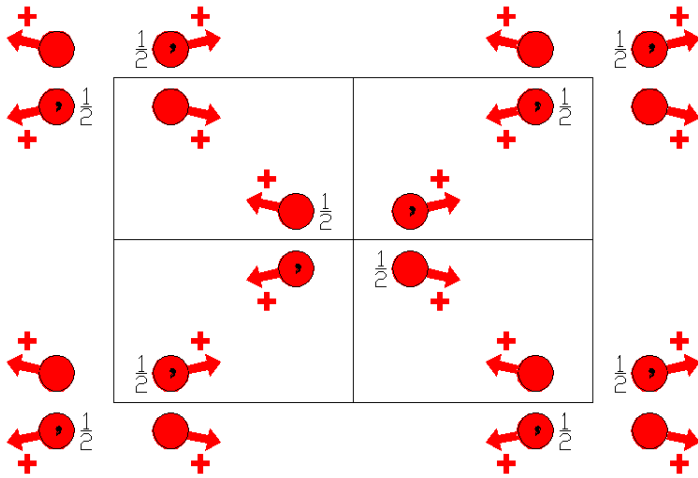
Along [0,1,0] p<sub>2b</sub>-1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



lb'a'2  
45.4.334

m'm'2  
lb'a'2

Orthorhombic



Origin on c'c'2

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (4) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |
|--------------------|--|--|--|

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2) | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (4) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

### Positions

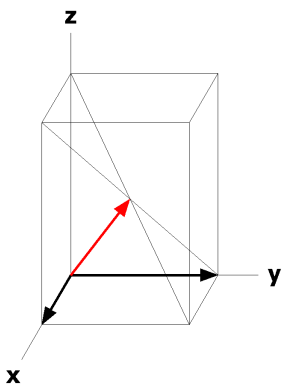
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(1/2,1/2,1/2) +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y}$ ,z+1/2 [u, $\bar{v}$ ,w]	(4) $\bar{x}$ ,y,z+1/2 [ $\bar{u}$ ,v,w]
4	b ..2	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]		
4	a ..2	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p1m'1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



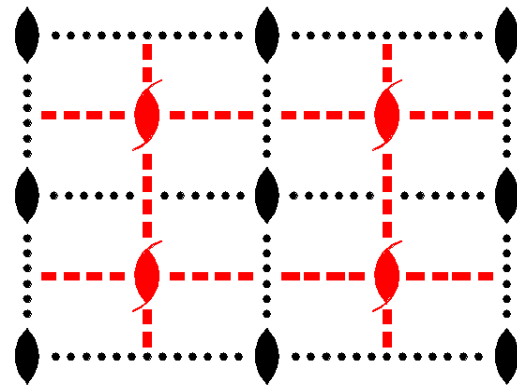
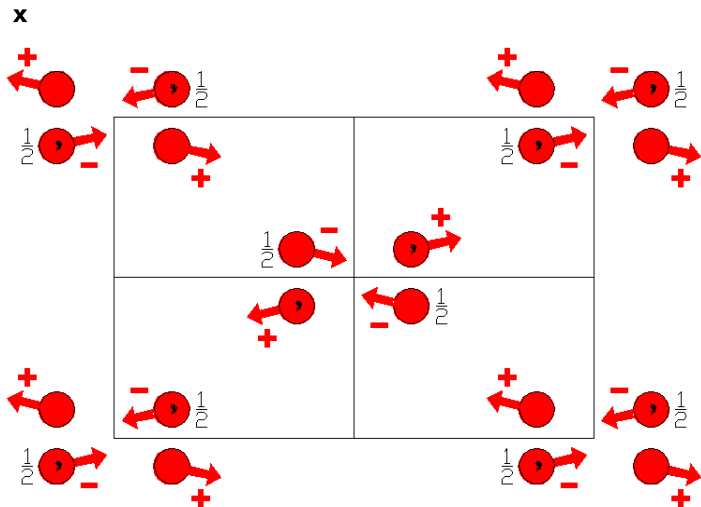
$I_pba2$

45.5.335

$mm2$

$I_pba2$

Orthorhombic



Origin on  $cc2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                  |  |  |
|--------------------|----------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) c $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2) | (4) c $(0,0,1/2)$ $0,y,z$<br>( $m_x$  0,0,1/2) |
|--------------------|----------------------------------|--|--|

For  $(1/2,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t' (1/2,1/2,1/2)$<br>(1  $1/2,1/2,1/2$ )' | (2) $2' (0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1/2$ )' | (3) $a' (1/2,0,0)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,0$ )' | (4) $b' (0,1/2,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

### Positions

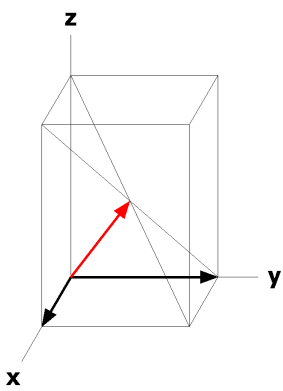
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,1/2)' +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y}$ ,z+1/2 [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
4	b ..2	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]		
4	a ..2	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] c<sub>p</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>-1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

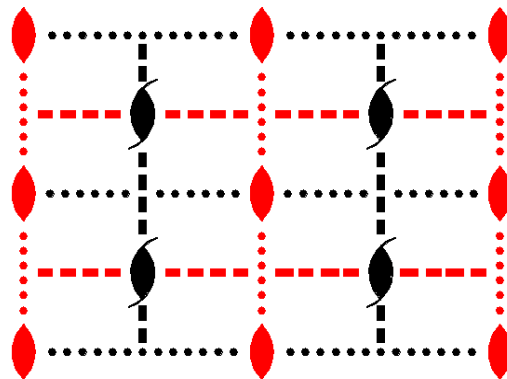
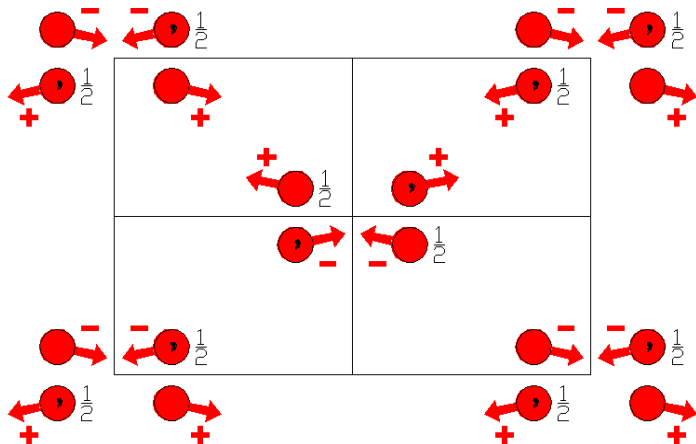
Along [0,1,0] p<sub>2b</sub>-1m'1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$I_pba'2'$   
45.6.336

$mm21'$   
 $I_pba'2'$

Orthorhombic



**Origin** on  $cc'2'$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                      |  |  |
|--------------------|--------------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) $2'$ $0,0,z$<br>( $2_z$  0,0,0)' | (3) $c'$ $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2)' | (4) $c$ $(0,0,1/2)$ $0,y,z$<br>( $m_x$  0,0,1/2) |
|--------------------|--------------------------------------|--|--|

For  $(1/2,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,1/2)$<br>(1 1/2,1/2,1/2)' | (2) $2$ $(0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2) | (3) $a$ $(1/2,0,0)$ $x,1/4,z$<br>( $m_y$  1/2,1/2,0) | (4) $b'$ $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$  1/2,1/2,0)' |
|--|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

### Positions

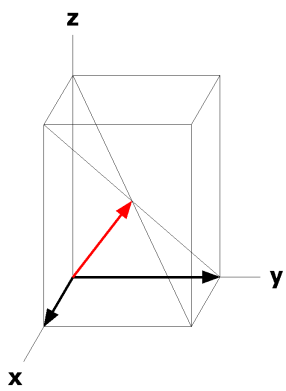
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) + (1/2,1/2,1/2)' +			
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) $\bar{x},y,z+1/2$ [u, $\bar{v},\bar{w}$ ]
4	b ..2'	0,1/2,z [u,v,0]	0,1/2,z+1/2 [u, $\bar{v},0$ ]		
4	a ..2'	0,0,z [u,v,0]	0,0,z+1/2 [u, $\bar{v},0$ ]		

### Symmetry of Special Projections

Along [0,0,1]  $c_p \cdot 2'mm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b} \cdot 1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

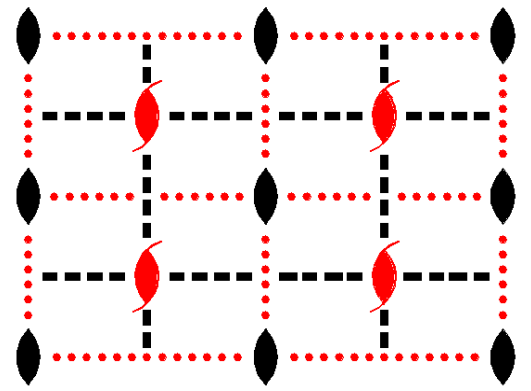
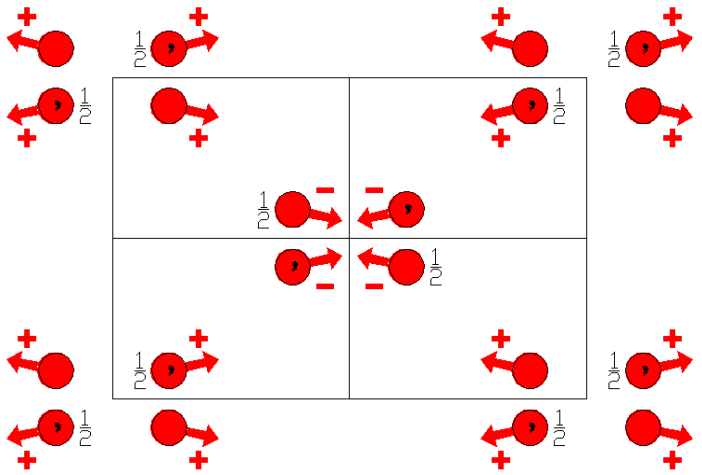
Along [0,1,0]  $p_{2a} \cdot 1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$I_p b' a' 2$   
45.7.337

$mm21'$   
 $I_p b' a' 2$

Orthorhombic



Origin on  $c'c'2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) c' $(0,0,1/2)$ $x,0,z$<br>(m <sub>y</sub>  0,0,1/2)' | (4) c' $(0,0,1/2)$ $0,y,z$<br>(m <sub>x</sub>  0,0,1/2)' |
|--------------------|--|--|--|

For  $(1/2,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' $(1/2,1/2,1/2)$<br>(1 1/2,1/2,1/2)' | (2) 2' $(0,0,1/2)$ $1/4,1/4,z$<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) a $(1/2,0,0)$ $x,1/4,z$<br>(m <sub>y</sub>  1/2,1/2,0) | (4) b $(0,1/2,0)$ $1/4,y,z$<br>(m <sub>x</sub>  1/2,1/2,0) |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

### Positions

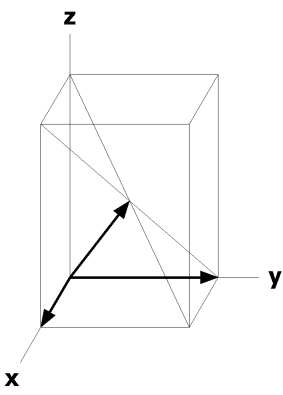
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(1/2,1/2,1/2)' +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) x, $\bar{y}$ ,z+1/2 [u, $\bar{v}$ ,w]	(4) $\bar{x}$ ,y,z+1/2 [ $\bar{u}$ ,v,w]
4	b ..2	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]		
4	a ..2	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1]  $c_p-2m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}-1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

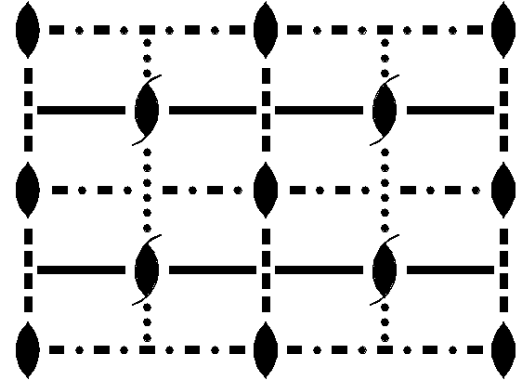
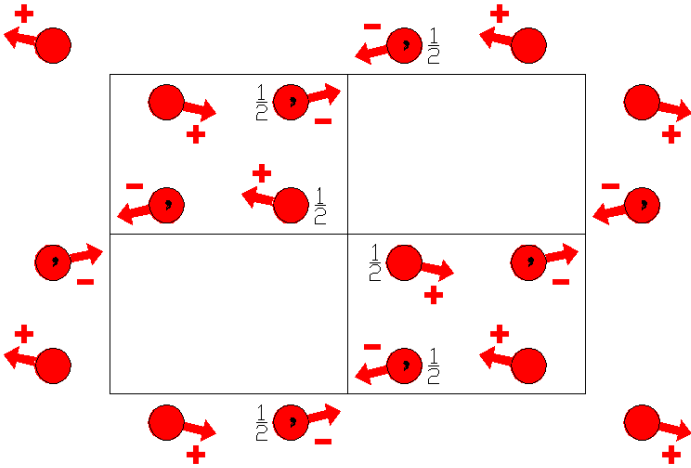
Along [0,1,0]  $p_{2a}-1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 1/4,y,0



Ima2  
46.1.338

mm2  
Ima2

Orthorhombic



Origin on na2

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) a ( $1/2,0,0$ )  $x,0,z$   
( $m_y$ | $1/2,0,0$ )

(4) m  $1/4,y,z$   
( $m_x$ | $1/2,0,0$ )

For (1/2,1/2,1/2) + set

(1) t ( $1/2,1/2,1/2$ )  
(1| $1/2,1/2,1/2$ )

(2) 2 ( $0,0,1/2$ )  $1/4,1/4,z$   
( $2_z$ | $1/2,1/2,1/2$ )

(3) c ( $0,0,1/2$ )  $x,1/4,z$   
( $m_y$ | $0,1/2,1/2$ )

(4) n ( $0,1/2,1/2$ )  $0,y,z$   
( $m_x$ | $0,1/2,1/2$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

### Positions

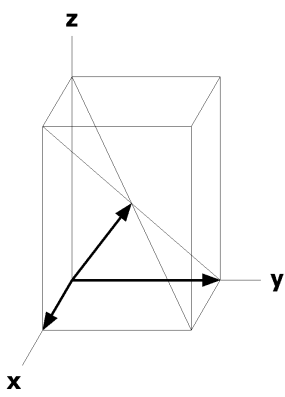
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(1/2,1/2,1/2) +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x+1/2,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x}+1/2,y,z$ [ $u,\bar{v},\bar{w}$ ]
4	b m..	1/4,y,z [u,0,0]	3/4, $\bar{y},z$ [ $\bar{u},0,0$ ]		
4	a ..2	0,0,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,1/4,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a}$ -1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0

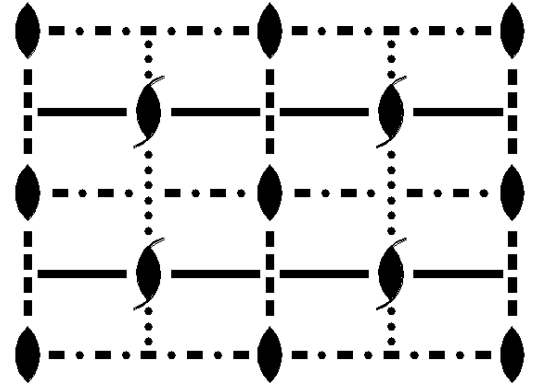
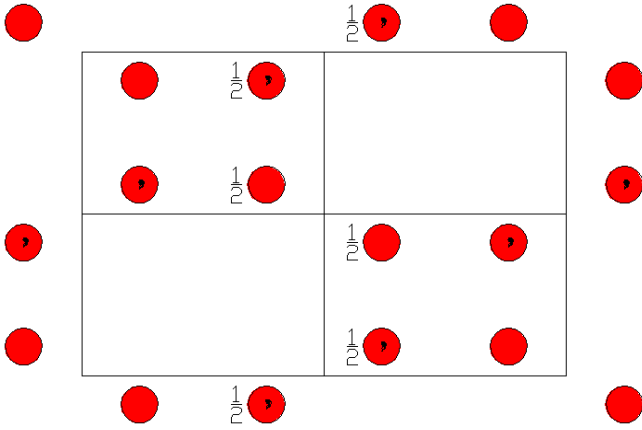


Ima21'  
46.2.339

mm21'  
Ima21'

Orthorhombic

1'



Origin on na21'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- (1) 1 (1|0,0,0)
- (2) 2 (0,0,z) (2<sub>z</sub>|0,0,0)
- (3) a (1/2,0,0) x,0,z (m<sub>y</sub>|1/2,0,0)
- (4) m (1/4,y,z) (m<sub>x</sub>|1/2,0,0)

For (1/2,1/2,1/2) + set

- (1) t (1/2,1/2,1/2) (1|1/2,1/2,1/2)
- (2) 2 (0,0,1/2) 1/4,1/4,z (2<sub>z</sub>|1/2,1/2,1/2)
- (3) c (0,0,1/2) x,1/4,z (m<sub>y</sub>|0,1/2,1/2)
- (4) n (0,1/2,1/2) 0,y,z (m<sub>x</sub>|0,1/2,1/2)

For (0,0,0)' + set

- (1) 1' (1|0,0,0)'
- (2) 2' (0,0,z) (2<sub>z</sub>|0,0,0)'
- (3) a' (1/2,0,0) x,0,z (m<sub>y</sub>|1/2,0,0)'
- (4) m' (1/4,y,z) (m<sub>x</sub>|1/2,0,0)'

For (1/2,1/2,1/2)' + set

- (1) t' (1/2,1/2,1/2) (1|1/2,1/2,1/2)'
- (2) 2' (0,0,1/2) 1/4,1/4,z (2<sub>z</sub>|1/2,1/2,1/2)'
- (3) c' (0,0,1/2) x,1/4,z (m<sub>y</sub>|0,1/2,1/2)'
- (4) n' (0,1/2,1/2) 0,y,z (m<sub>x</sub>|0,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); 1'.

### Positions

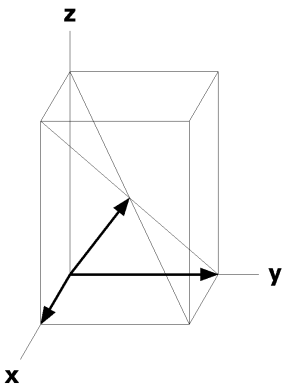
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'		
8	c 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y}, z$ [0,0,0]	(3) $x+1/2, \bar{y}, z$ [0,0,0]	(4) $\bar{x}+1/2, y, z$ [0,0,0]
4	b m..1'	1/4,y,z [0,0,0]	3/4, $\bar{y}$ ,z [0,0,0]		
4	a ..21'	0,0,z [0,0,0]	1/2,0,z [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,1/4,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

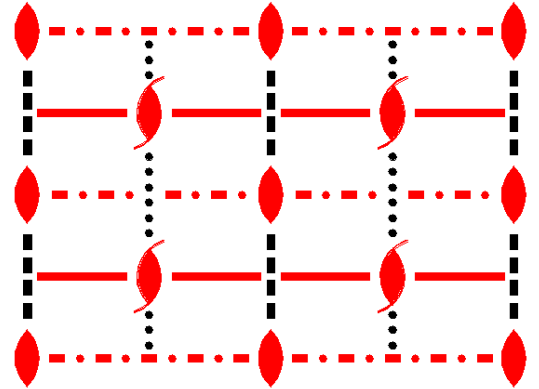
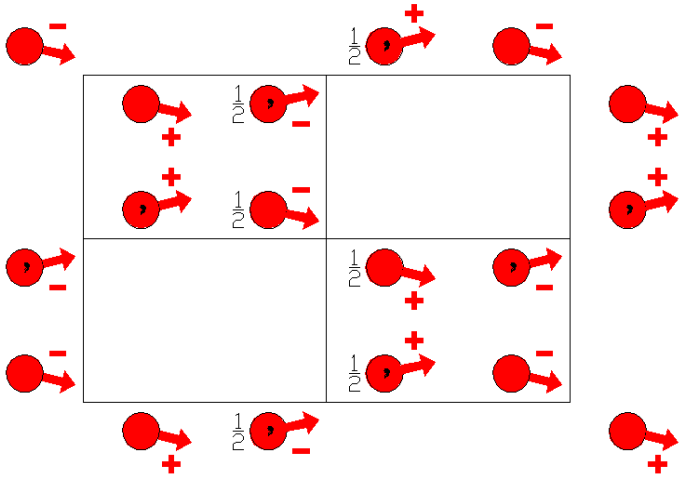
Along [0,1,0] p1m11'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Im'a2'  
46.3.340

m'm2'  
Im'a2'

Orthorhombic



Origin on n'a2'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- (1) 1  
(1|0,0,0)
- (2) 2' 0,0,z  
(2<sub>z</sub>|0,0,0)'
- (3) a (1/2,0,0) x,0,z  
(m<sub>y</sub>|1/2,0,0)
- (4) m' 1/4,y,z  
(m<sub>x</sub>|1/2,0,0)'

For (1/2,1/2,1/2) + set

- (1) t (1/2,1/2,1/2)  
(1|1/2,1/2,1/2)
- (2) 2' (0,0,1/2) 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,1/2)'
- (3) c (0,0,1/2) x,1/4,z  
(m<sub>y</sub>|0,1/2,1/2)
- (4) n' (0,1/2,1/2) 0,y,z  
(m<sub>x</sub>|0,1/2,1/2)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

### Positions

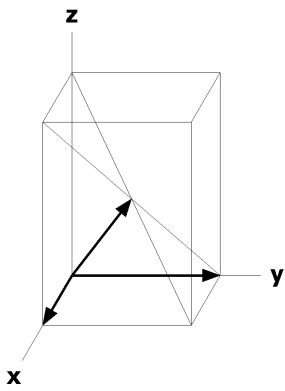
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,1/2) +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x+1/2,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x}+1/2,y,z$ [ $\bar{u},v,w$ ]
4	b m'..	1/4,y,z [0,v,w]	3/4, $\bar{y},z$ [0,v, $\bar{w}$ ]		
4	a ..2'	0,0,z [u,v,0]	1/2,0,z [ $\bar{u},v,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 1/4,1/4,z

Along [1,0,0] c1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

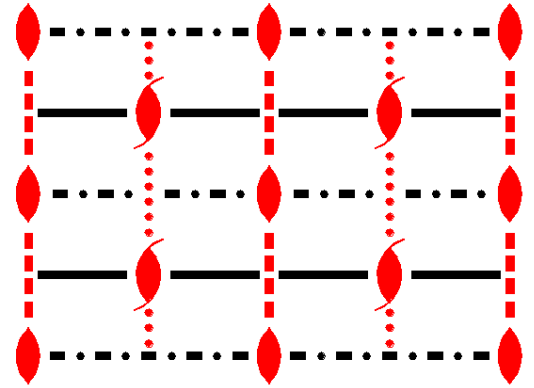
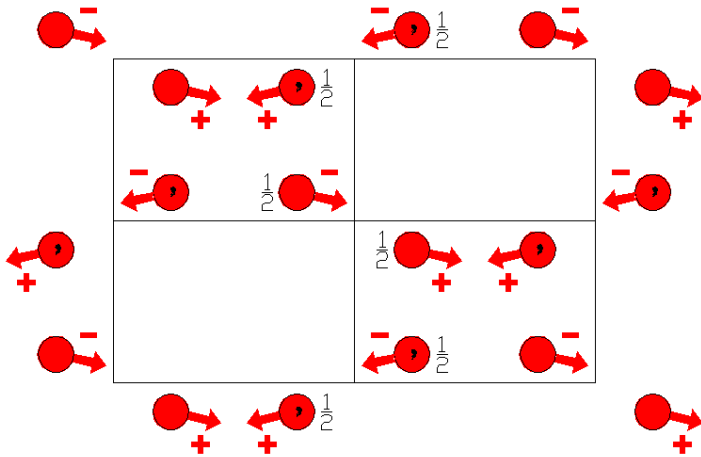
Along [0,1,0]  $p_{2a}$ -1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Ima'2'  
46.4.341

mm'2'  
Ima'2'

Orthorhombic



Origin on na'2'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) a' (1/2,0,0) x,0,z<br>(m <sub>y</sub>  1/2,0,0)' | (4) m 1/4,y,z<br>(m <sub>x</sub>  1/2,0,0) |
|--------------------|--|--|--|

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2) | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (4) n (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>  0,1/2,1/2) |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

### Positions

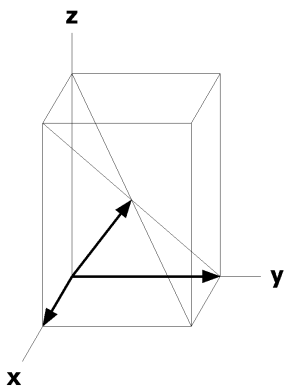
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,1/2) +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x+1/2,\bar{y},z$ [u, $\bar{v}$ ,w]	(4) $\bar{x}+1/2,y,z$ [u, $\bar{v},\bar{w}$ ]
4	b m..	1/4,y,z [u,0,0]	3/4, $\bar{y},z$ [u,0,0]		
4	a ..2'	0,0,z [u,v,0]	1/2,0,z [u, $\bar{v}$ ,0]		

### Symmetry of Special Projections

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,1/4,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

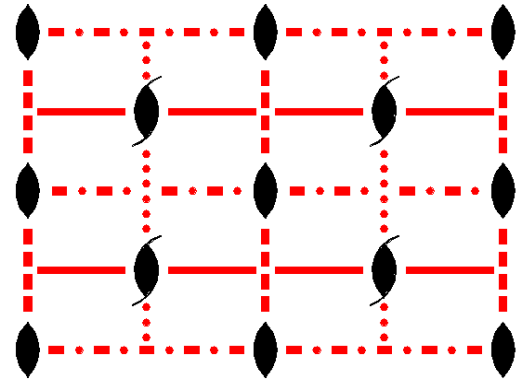
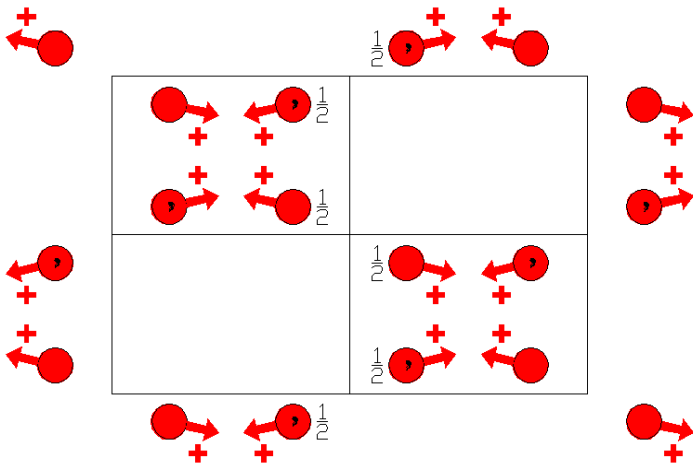
Along [0,1,0] p1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Im'a'2  
46.5.342

m'm'2  
Im'a'2

Orthorhombic



Origin on n'a'2

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |                    |  |  |  |
|--------------------|--|--|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) a' (1/2,0,0) x,0,z<br>(m <sub>y</sub>  1/2,0,0)' | (4) m' 1/4,y,z<br>(m <sub>x</sub>  1/2,0,0)' |
|--------------------|--|--|--|

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2) | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (4) n' (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>  0,1/2,1/2)' |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

### Positions

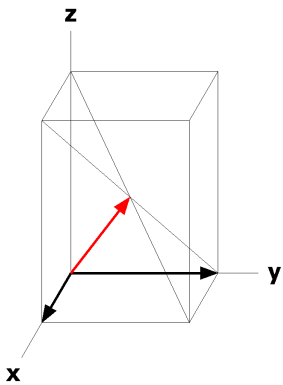
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,1/2) +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x+1/2,\bar{y},z$ [ $u,\bar{v},w$ ]	(4) $\bar{x}+1/2,y,z$ [ $\bar{u},v,w$ ]
4	b m'..	1/4,y,z [0,v,w]	3/4, $\bar{y},z$ [0, $\bar{v},w$ ]		
4	a ..2	0,0,z [0,0,w]	1/2,0,z [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,1/4,z

Along [1,0,0] c1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

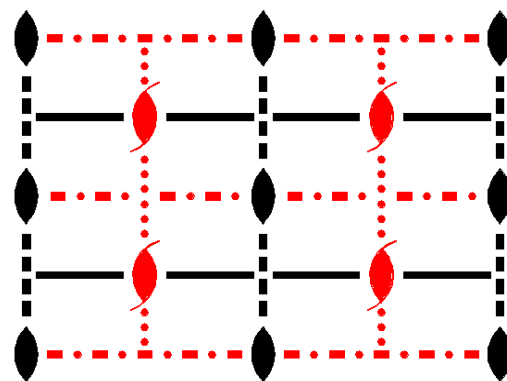
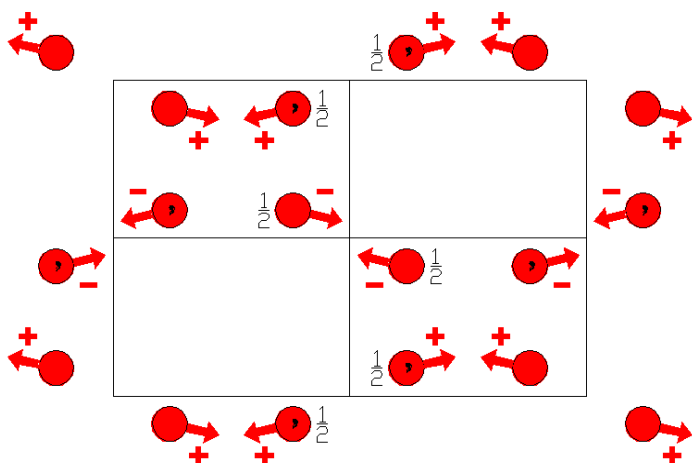
Along [0,1,0] p1m'1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$I_pma2$   
46.6.343

$mm21'$   
 $I_pma2$

Orthorhombic



**Origin** on  $n'a2$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3) a  $(1/2,0,0)$   $x,0,z$   
( $m_y$ | $1/2,0,0$ )

(4) m  $1/4,y,z$   
( $m_x$ | $1/2,0,0$ )

For  $(1/2,1/2,1/2)'$  + set

(1)  $t'$   $(1/2,1/2,1/2)$   
(1| $1/2,1/2,1/2$ )'

(2)  $2'$   $(0,0,1/2)$   $1/4,1/4,z$   
( $2_z$ | $1/2,1/2,1/2$ )'

(3)  $c'$   $(0,0,1/2)$   $x,1/4,z$   
( $m_y$ | $0,1/2,1/2$ )'

(4)  $n'$   $(0,1/2,1/2)$   $0,y,z$   
( $m_x$ | $0,1/2,1/2$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

### Positions

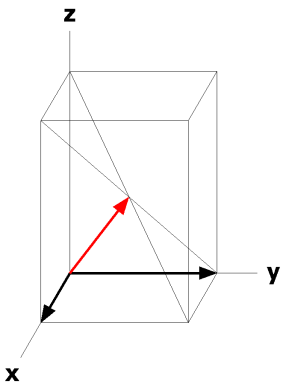
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) + (1/2,1/2,1/2)' +			
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $x+1/2,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $\bar{x}+1/2,y,z$ [ $u,\bar{v},\bar{w}$ ]
4	b m..	1/4,y,z [u,0,0]	3/4, $\bar{y},z$ [ $\bar{u},0,0$ ]		
4	a ..2	0,0,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1]  $c_p \cdot 2'mm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,1/4,z

Along [1,0,0]  $c1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

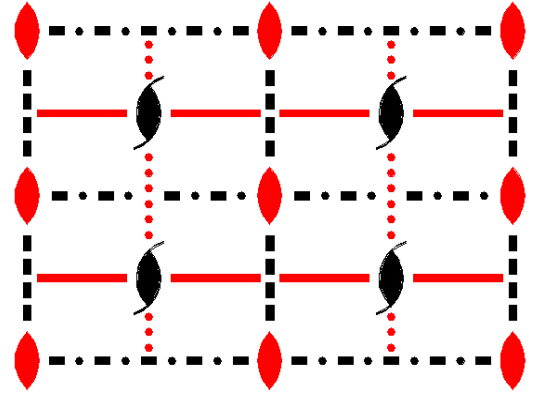
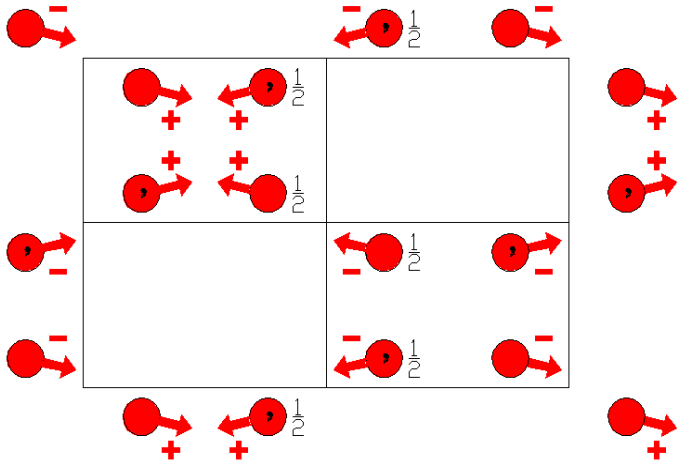
Along [0,1,0]  $p_{2a} \cdot 1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 1/4,y,0



$I_p m' a_2'$   
46.7.344

$mm21'$   
 $I_p m' a_2'$

Orthorhombic



Origin on  $na_2'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |                                      |  |  |
|--------------------|--------------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) $2'$ $0,0,z$<br>( $2_z$  0,0,0)' | (3) a $(1/2,0,0)$ $x,0,z$<br>( $m_y$   $1/2,0,0$ ) | (4) $m'$ $1/4,y,z$<br>( $m_x$   $1/2,0,0$ )' |
|--------------------|--------------------------------------|--|--|

For  $(1/2,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,1/2)$<br>(1  $1/2,1/2,1/2$ )' | (2) 2 $(0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1/2$ ) | (3) $c'$ $(0,0,1/2)$ $x,1/4,z$<br>( $m_y$   $0,1/2,1/2$ )' | (4) n $(0,1/2,1/2)$ $0,y,z$<br>( $m_x$   $0,1/2,1/2$ ) |
|--|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

### Positions

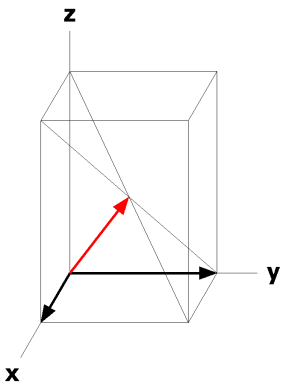
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,1/2)' +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3) $x+1/2, \bar{y}, z$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) $\bar{x}+1/2, y, z$ [ $\bar{u}$ ,v,w]
4	b m'..	1/4,y,z [0,v,w]	3/4, $\bar{y}, z$ [0,v, $\bar{w}$ ]		
4	a ..2'	0,0,z [u,v,0]	1/2,0,z [ $\bar{u}$ ,v,0]		

### Symmetry of Special Projections

Along [0,0,1]  $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,1/4,z

Along [1,0,0]  $c_p \cdot 1m1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a} \cdot 1m1$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



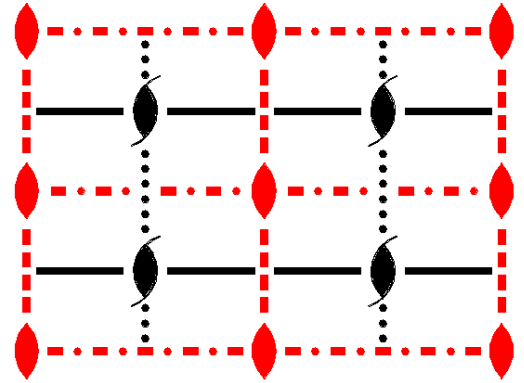
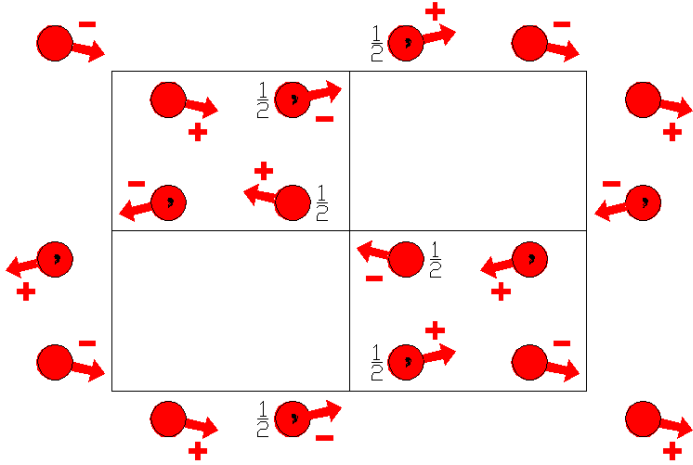
$I_p ma'2'$

46.8.345

$mm21'$

$I_p ma'2'$

Orthorhombic



**Origin** on  $n'a'2'$

**Asymmetric unit**  $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2)  $2'_z$  0,0,z  
( $2_z$ |0,0,0)'

(3)  $a'_x$  (1/2,0,0) x,0,z  
( $m_y$ |1/2,0,0)'

(4)  $m_x$  1/4,y,z  
( $m_x$ |1/2,0,0)

For  $(1/2,1/2,1/2)$ ' + set

(1)  $t'_z$  (1/2,1/2,1/2)  
(1|1/2,1/2,1/2)'

(2)  $2'_z$  (0,0,1/2) 1/4,1/4,z  
( $2_z$ |1/2,1/2,1/2)

(3)  $c_x$  (0,0,1/2) x,1/4,z  
( $m_y$ |0,1/2,1/2)

(4)  $n'_z$  (0,1/2,1/2) 0,y,z  
( $m_x$ |0,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

### Positions

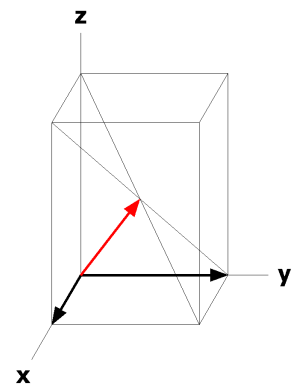
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) + (1/2,1/2,1/2)' +			
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $x+1/2,\bar{y},z$ [u, $\bar{v}$ ,w]	(4) $\bar{x}+1/2,y,z$ [u, $\bar{v},\bar{w}$ ]
4	b m..	1/4,y,z [u,0,0]	3/4, $\bar{y},z$ [u,0,0]		
4	a ..2'	0,0,z [u,v,0]	1/2,0,z [u, $\bar{v}$ ,0]		

### Symmetry of Special Projections

Along [0,0,1]  $c_p$ -2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,1/4,z

Along [1,0,0]  $c1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $p_{2b}$ -1m1  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



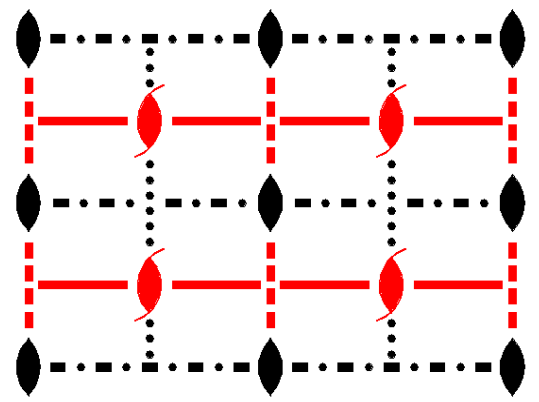
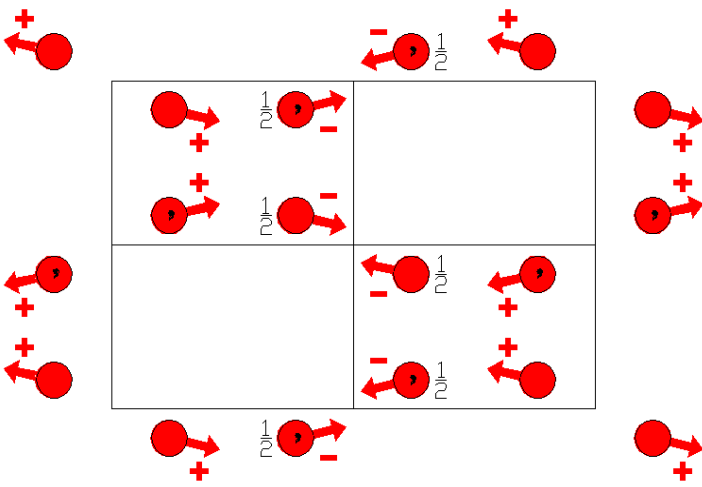
$I_p m' a' 2$

46.9.346

$mm21'$

$I_p m' a' 2$

Orthorhombic



Origin on  $na'2$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- (1) 1  
(1|0,0,0)
- (2) 2  $0,0,z$   
( $2_z$ |0,0,0)
- (3)  $a' (1/2,0,0)$   $x,0,z$   
( $m_y$ | $1/2,0,0$ )'
- (4)  $m' 1/4,y,z$   
( $m_x$ | $1/2,0,0$ )'

For  $(1/2,1/2,1/2)'$  + set

- (1)  $t' (1/2,1/2,1/2)$   
(1| $1/2,1/2,1/2$ )'
- (2)  $2' (0,0,1/2)$   $1/4,1/4,z$   
( $2_z$ | $1/2,1/2,1/2$ )'
- (3)  $c (0,0,1/2)$   $x,1/4,z$   
( $m_y$ | $0,1/2,1/2$ )
- (4)  $n (0,1/2,1/2)$   $0,y,z$   
( $m_x$ | $0,1/2,1/2$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

### Positions

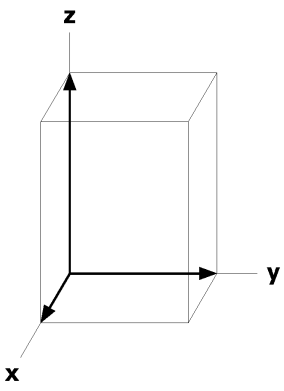
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,1/2)' +		
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $x+1/2, \bar{y}, z$ [ $u, \bar{v}, w$ ]	(4) $\bar{x}+1/2, y, z$ [ $\bar{u}, v, w$ ]
4	b m'..	1/4,y,z [0,v,w]	3/4, $\bar{y}, z$ [0, $\bar{v}, w$ ]		
4	a ..2	0,0,z [0,0,w]	1/2,0,z [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1]  $c_p \cdot 2' m m'$   
 $\mathbf{a}^* = -\mathbf{b}^*/2$   $\mathbf{b}^* = \mathbf{a}^*/2$   
 Origin at 1/4,1/4,z

Along [1,0,0]  $c_p \cdot 1 m' 1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

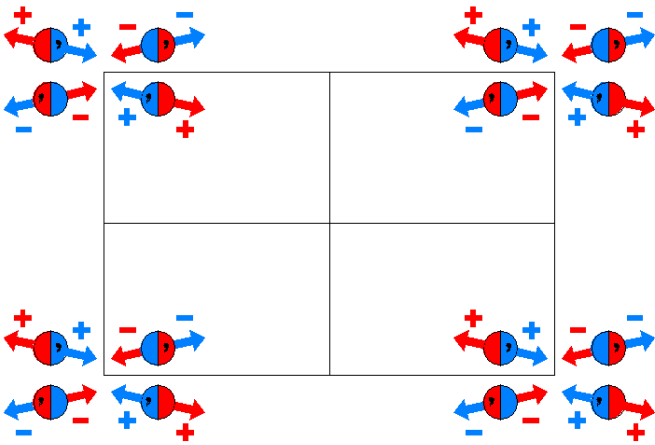
Along [0,1,0]  $p_{2b} \cdot 1 m' 1$   
 $\mathbf{a}^* = -\mathbf{a}^*/2$   $\mathbf{b}^* = \mathbf{c}^*/2$   
 Origin at 0,y,0



Pmmm  
47.1.347

mmm  
P2/m2/m2/m

Orthorhombic

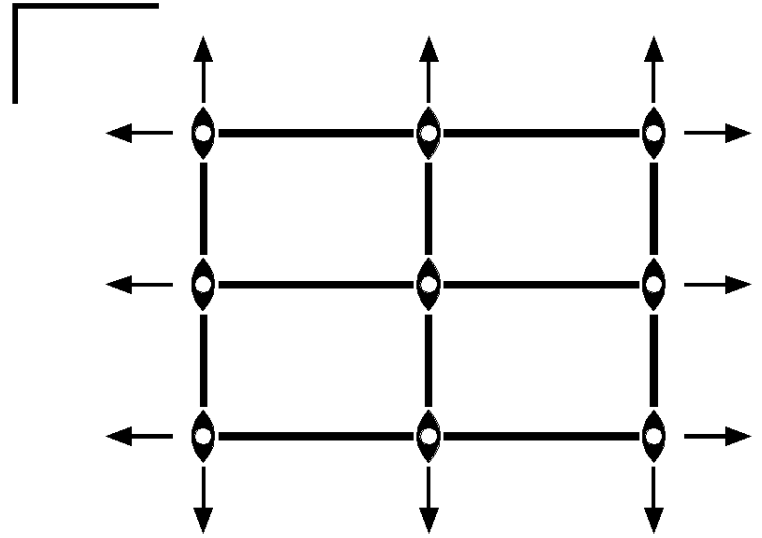


Origin at center (mmm)

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) 1<br>(1 0,0,0)                   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	$\alpha$ 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
4	z ..m	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0,w]	$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
4	y ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0, $\bar{w}$ ]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
4	x .m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v},0$ ]	$\bar{x},1/2,\bar{z}$ [0,v,0]	x,1/2, $\bar{z}$ [0, $\bar{v},0$ ]
4	w .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	$\bar{x},0,\bar{z}$ [0,v,0]	x,0, $\bar{z}$ [0, $\bar{v},0$ ]
4	v m..	1/2,y,z [u,0,0]	1/2, $\bar{y},z$ [ $\bar{u},0,0$ ]	1/2,y, $\bar{z}$ [ $\bar{u},0,0$ ]	1/2, $\bar{y},\bar{z}$ [u,0,0]
4	u m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	0,y, $\bar{z}$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]
2	t mm2	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
2	s mm2	1/2,0,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
2	r mm2	0,1/2,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]		
2	q mm2	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	p m2m	1/2,y,1/2 [0,0,0]	1/2, $\bar{y},1/2$ [0,0,0]		
2	o m2m	1/2,y,0 [0,0,0]	1/2, $\bar{y},0$ [0,0,0]		
2	n m2m	0,y,1/2 [0,0,0]	0, $\bar{y},1/2$ [0,0,0]		
2	m m2m	0,y,0 [0,0,0]	0, $\bar{y},0$ [0,0,0]		
2	l 2mm	x,1/2,1/2 [0,0,0]	$\bar{x},1/2,1/2$ [0,0,0]		
2	k 2mm	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]		
2	j 2mm	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]		
2	i 2mm	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
1	h mmm	1/2,1/2,1/2 [0,0,0]			
1	g mmm	0,1/2,1/2 [0,0,0]			
1	f mmm	1/2,1/2,0 [0,0,0]			
1	e mmm	0,1/2,0 [0,0,0]			

1 d mmm  $1/2, 0, 1/2$  [0,0,0]

1 c mmm  $0, 0, 1/2$  [0,0,0]

1 b mmm  $1/2, 0, 0$  [0,0,0]

1 a mmm  $0, 0, 0$  [0,0,0]

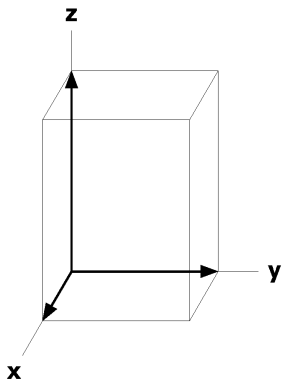
### Symmetry of Special Projections

Along [0,0,1]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0





Pmmm1'

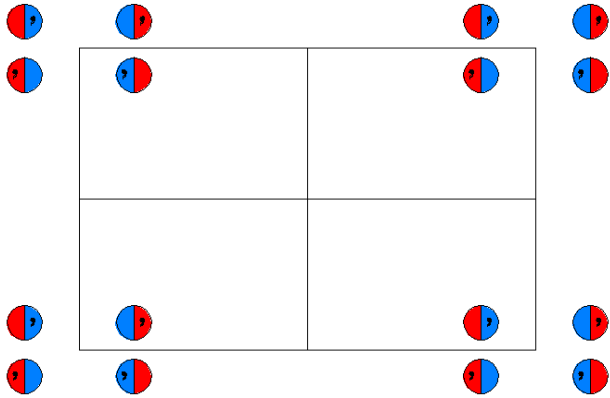
47.2.348

mmm1'

P2/m2/m2/m1'

Orthorhombic

1'

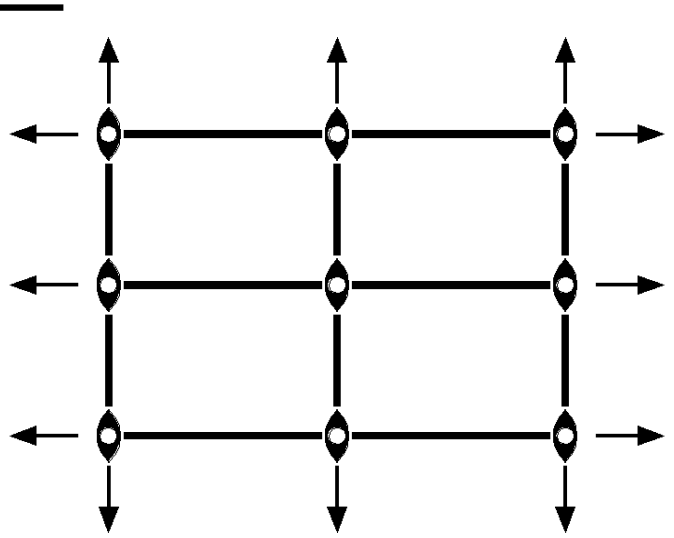


Origin at center (mmm1')

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0)   | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0)   | (7) m x,0,z<br>(m <sub>y</sub>  0,0,0)   | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   |
| For 1' + set                           |  |  |  |
| (1) 1'<br>(1 0,0,0)'                   | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}'$<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |
| For 1' + set                           |  |  |  |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +	1' +		
8 $\alpha$ 11'	(1) x,y,z [0,0,0] (5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0] (6) x,y, $\bar{z}$ [0,0,0]	(3) $\bar{x},y,\bar{z}$ [0,0,0] (7) x, $\bar{y},z$ [0,0,0]	(4) x, $\bar{y},\bar{z}$ [0,0,0] (8) $\bar{x},y,z$ [0,0,0]
4 z ..m1'	x,y,1/2 [0,0,0]	$\bar{x},\bar{y},1/2$ [0,0,0]	$\bar{x},y,1/2$ [0,0,0]	x, $\bar{y},1/2$ [0,0,0]
4 y ..m1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{x},y,0$ [0,0,0]	x, $\bar{y},0$ [0,0,0]
4 x .m.1'	x,1/2,z [0,0,0]	$\bar{x},1/2,z$ [0,0,0]	$\bar{x},1/2,\bar{z}$ [0,0,0]	x,1/2, $\bar{z}$ [0,0,0]
4 w .m.1'	x,0,z [0,0,0]	$\bar{x},0,z$ [0,0,0]	$\bar{x},0,\bar{z}$ [0,0,0]	x,0, $\bar{z}$ [0,0,0]
4 v m..1'	1/2,y,z [0,0,0]	1/2, $\bar{y},z$ [0,0,0]	1/2,y, $\bar{z}$ [0,0,0]	1/2, $\bar{y},\bar{z}$ [0,0,0]
4 u m..1'	0,y,z [0,0,0]	0, $\bar{y},z$ [0,0,0]	0,y, $\bar{z}$ [0,0,0]	0, $\bar{y},\bar{z}$ [0,0,0]
2 t mm21'	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
2 s mm21'	1/2,0,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
2 r mm21'	0,1/2,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]		
2 q mm21'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2 p m2m1'	1/2,y,1/2 [0,0,0]	1/2, $\bar{y},1/2$ [0,0,0]		
2 o m2m1'	1/2,y,0 [0,0,0]	1/2, $\bar{y},0$ [0,0,0]		
2 n m2m1'	0,y,1/2 [0,0,0]	0, $\bar{y},1/2$ [0,0,0]		
2 m m2m1'	0,y,0 [0,0,0]	0, $\bar{y},0$ [0,0,0]		
2 l 2mm1'	x,1/2,1/2 [0,0,0]	$\bar{x},1/2,1/2$ [0,0,0]		
2 k 2mm1'	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]		
2 j 2mm1'	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]		
2 i 2mm1'	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
1 h mmm1'	1/2,1/2,1/2 [0,0,0]			
1 g mmm1'	0,1/2,1/2 [0,0,0]			
1 f mmm1'	1/2,1/2,0 [0,0,0]			
1 e mmm1'	0,1/2,0 [0,0,0]			

1 d mmm1'  $1/2, 0, 1/2$  [0,0,0]

1 c mmm1'  $0, 0, 1/2$  [0,0,0]

1 b mmm1'  $1/2, 0, 0$  [0,0,0]

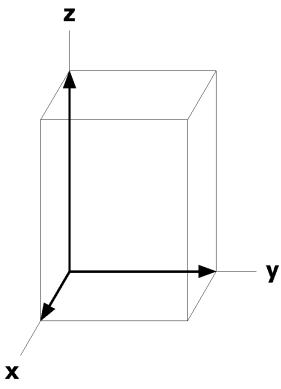
1 a mmm1'  $0, 0, 0$  [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

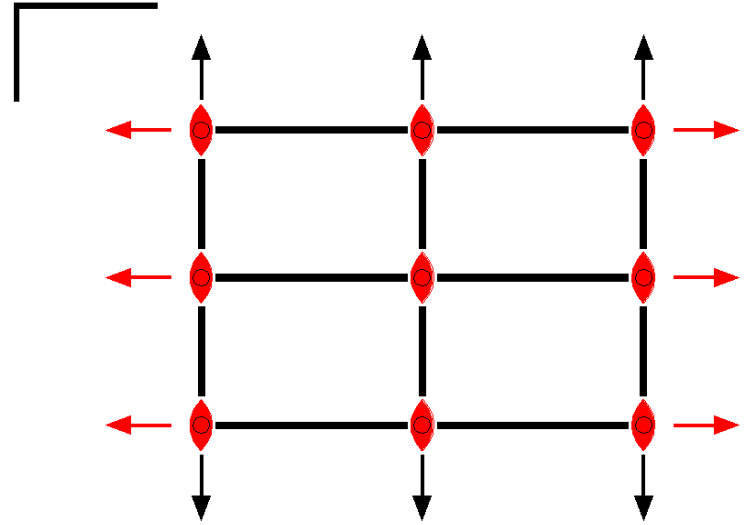
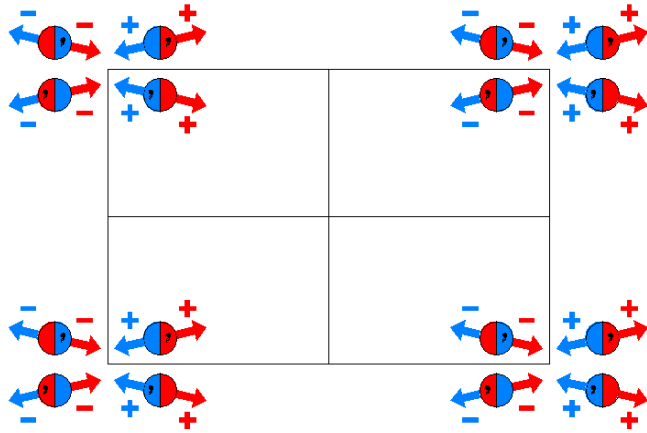
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pm'mm  
47.3.349

m'mm  
P2/m'2'/m2'/m

Orthorhombic



Origin at center (m'mm)

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                      | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)' | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0)   | (7) m x,0,z<br>(m <sub>y</sub>  0,0,0)   | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	$\alpha$ 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
4	z ..m	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0, $\bar{w}$ ]	$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
4	y ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
4	x .m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0,v,0]	$\bar{x},1/2,\bar{z}$ [0, $\bar{v}$ ,0]	x,1/2, $\bar{z}$ [0, $\bar{v}$ ,0]
4	w .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0,v,0]	$\bar{x},0,\bar{z}$ [0, $\bar{v}$ ,0]	x,0, $\bar{z}$ [0, $\bar{v}$ ,0]
4	v m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0,v, $\bar{w}$ ]	1/2,y, $\bar{z}$ [0, $\bar{v},w$ ]	1/2, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
4	u m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0,v, $\bar{w}$ ]	0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
2	t m'm2'	1/2,1/2,z [0,v,0]	1/2,1/2, $\bar{z}$ [0, $\bar{v}$ ,0]		
2	s m'm2'	1/2,0,z [0,v,0]	1/2,0, $\bar{z}$ [0, $\bar{v}$ ,0]		
2	r m'm2'	0,1/2,z [0,v,0]	0,1/2, $\bar{z}$ [0, $\bar{v}$ ,0]		
2	q m'm2'	0,0,z [0,v,0]	0,0, $\bar{z}$ [0, $\bar{v}$ ,0]		
2	p m'2'm	1/2,y,1/2 [0,0,w]	1/2, $\bar{y},1/2$ [0,0, $\bar{w}$ ]		
2	o m'2'm	1/2,y,0 [0,0,w]	1/2, $\bar{y},0$ [0,0, $\bar{w}$ ]		
2	n m'2'm	0,y,1/2 [0,0,w]	0, $\bar{y},1/2$ [0,0,0 $\bar{w}$ ]		
2	m m'2'm	0,y,0 [0,0,w]	0, $\bar{y},0$ [0,0, $\bar{w}$ ]		
2	l 2mm	x,1/2,1/2 [0,0,0]	$\bar{x},1/2,1/2$ [0,0,0]		
2	k 2mm	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]		
2	j 2mm	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]		
2	i 2mm	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
1	h m'mm	1/2,1/2,1/2 [0,0,0]			
1	g m'mm	0,1/2,1/2 [0,0,0]			
1	f m'mm	1/2,1/2,0 [0,0,0]			
1	e m'mm	0,1/2,0 [0,0,0]			

1 d m'mm  $1/2, 0, 1/2$  [0,0,0]

1 c m'mm  $0, 0, 1/2$  [0,0,0]

1 b m'mm  $1/2, 0, 0$  [0,0,0]

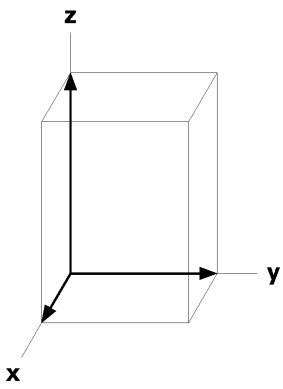
1 a m'mm  $0, 0, 0$  [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
Origin at 0,y,0



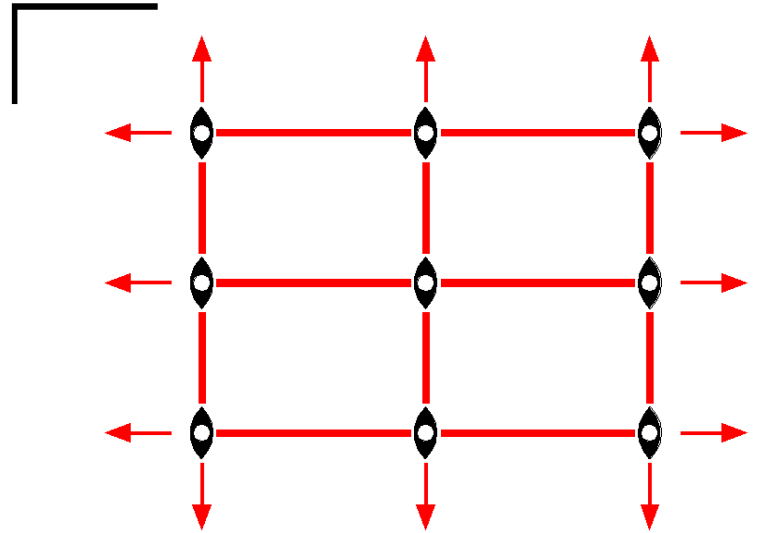
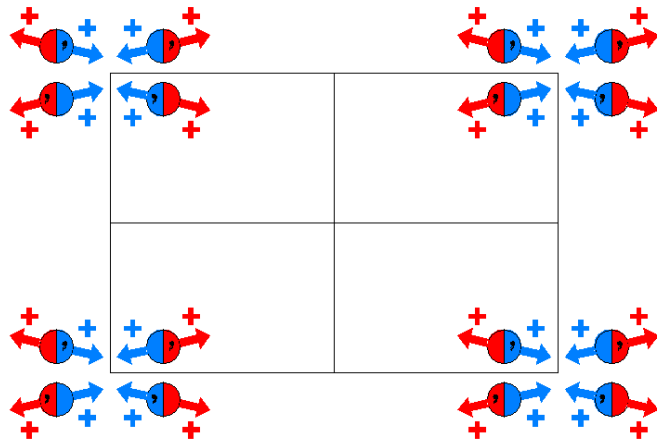
Pm'm'm

47.4.350

m'm'm

P2'/m'2'/m'2'/m

Orthorhombic



Origin at center (m'm'm)

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 2' 0,y,0  
(2<sub>y</sub>|0,0,0)'

(4) 2' x,0,0  
(2<sub>x</sub>|0,0,0)'

(5)  $\bar{1}$   
( $\bar{1}$ |0,0,0)

(6) m x,y,0  
(m<sub>z</sub>|0,0,0)

(7) m' x,0,z  
(m<sub>y</sub>|0,0,0)'

(8) m' 0,y,z  
(m<sub>x</sub>|0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	$\alpha$ 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
4	z ..m	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0,w]	$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0,w]
4	y ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0,w]
4	x .m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ]	$\bar{x},1/2,\bar{z}$ [u,0,w]	x,1/2, $\bar{z}$ [ $\bar{u},0,w$ ]
4	w .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$\bar{x},0,\bar{z}$ [u,0,w]	x,0, $\bar{z}$ [ $\bar{u},0,w$ ]
4	v m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0, $\bar{v},w$ ]	1/2,y, $\bar{z}$ [0, $\bar{v},w$ ]	1/2, $\bar{y},\bar{z}$ [0,v,w]
4	u m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
2	t m'm'2	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
2	s m'm'2	1/2,0,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]		
2	r m'm'2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]		
2	q m'm'2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
2	p m'2'm	1/2,y,1/2 [0,0,w]	1/2, $\bar{y},1/2$ [0,0,w]		
2	o m'2'm	1/2,y,0 [0,0,w]	1/2, $\bar{y},0$ [0,0,w]		
2	n m'2'm	0,y,1/2 [0,0,w]	0, $\bar{y},1/2$ [0,0,w]		
2	m m'2'm	0,y,0 [0,0,w]	0, $\bar{y},0$ [0,0,w]		
2	l 2'm'm	x,1/2,1/2 [0,0,w]	$\bar{x},1/2,1/2$ [0,0,w]		
2	k 2'm'm	x,1/2,0 [0,0,w]	$\bar{x},1/2,0$ [0,0,w]		
2	j 2'm'm	x,0,1/2 [0,0,w]	$\bar{x},0,1/2$ [0,0,w]		
2	i 2'm'm	x,0,0 [0,0,w]	$\bar{x},0,0$ [0,0,w]		
1	h m'm'm	1/2,1/2,1/2 [0,0,w]			
1	g m'm'm	0,1/2,1/2 [0,0,w]			
1	f m'm'm	1/2,1/2,0 [0,0,w]			
1	e m'm'm	0,1/2,0 [0,0,w]			



1 d m'm'm  $1/2, 0, 1/2$  [0,0,w]

1 c m'm'm  $0, 0, 1/2$  [0,0,w]

1 b m'm'm  $1/2, 0, 0$  [0,0,w]

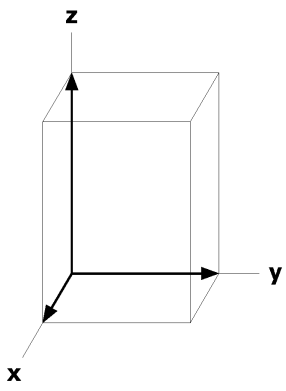
1 a m'm'm  $0, 0, 0$  [0,0,w]

### Symmetry of Special Projections

Along [0,0,1]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0]  $p2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



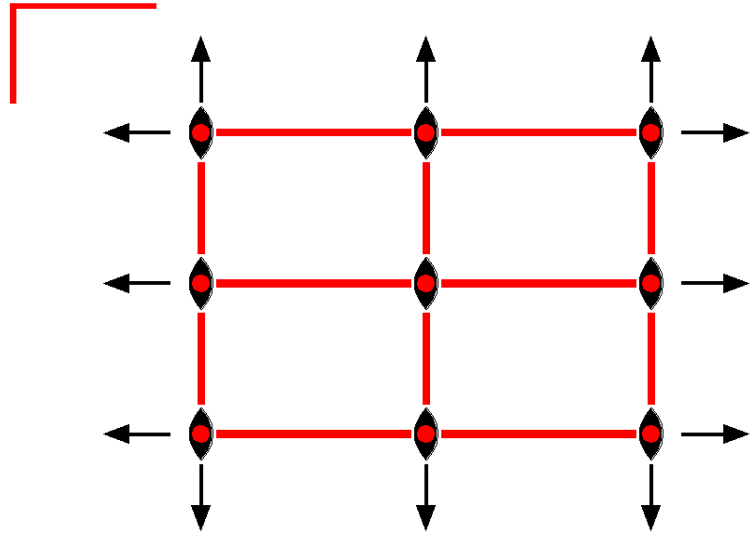
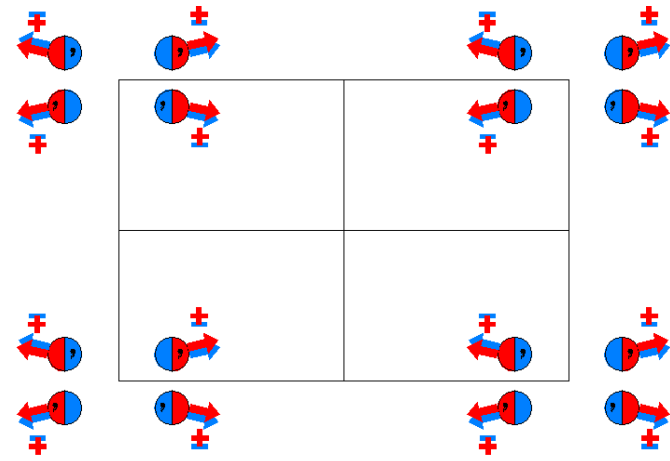
Pm'm'm'

47.5.351

m'm'm'

P2/m'2/m'2/m'

Orthorhombic



Origin at center (m'm'm')

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 2 0,y,0  
(2<sub>y</sub>|0,0,0)

(4) 2 x,0,0  
(2<sub>x</sub>|0,0,0)

(5)  $\bar{1}$ '  
( $\bar{1}$ |0,0,0)'

(6) m' x,y,0  
(m<sub>z</sub>'|0,0,0)'

(7) m' x,0,z  
(m<sub>y</sub>'|0,0,0)'

(8) m' 0,y,z  
(m<sub>x</sub>'|0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	$\alpha$ 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
4	z ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	x, $\bar{y},1/2$ [u, $\bar{v},0$ ]
4	y ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,0$ [ $\bar{u},v,0$ ]	x, $\bar{y},0$ [u, $\bar{v},0$ ]
4	x .m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ]	$\bar{x},1/2,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	x,1/2, $\bar{z}$ [u,0, $\bar{w}$ ]
4	w .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$\bar{x},0,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	x,0, $\bar{z}$ [u,0, $\bar{w}$ ]
4	v m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0, $\bar{v},w$ ]	1/2,y, $\bar{z}$ [0,v, $\bar{w}$ ]	1/2, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
4	u m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	0,y, $\bar{z}$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
2	t m'm'2	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	s m'm'2	1/2,0,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	r m'm'2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	q m'm'2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	p m'2m'	1/2,y,1/2 [0,v,0]	1/2, $\bar{y},1/2$ [0, $\bar{v},0$ ]		
2	o m'2m'	1/2,y,0 [0,v,0]	1/2, $\bar{y},0$ [0, $\bar{v},0$ ]		
2	n m'2m'	0,y,1/2 [0,v,0]	0, $\bar{y},1/2$ [0, $\bar{v},0$ ]		
2	m m'2m'	0,y,0 [0,v,0]	0, $\bar{y},0$ [0, $\bar{v},0$ ]		
2	l 2m'm'	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]		
2	k 2m'm'	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]		
2	j 2m'm'	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]		
2	i 2m'm'	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]		
1	h m'm'm'	1/2,1/2,1/2 [0,0,0]			
1	g m'm'm'	0,1/2,1/2 [0,0,0]			
1	f m'm'm'	1/2,1/2,0 [0,0,0]			
1	e m'm'm'	0,1/2,0 [0,0,0]			

1 d m'm'm'  $1/2, 0, 1/2$  [0,0,0]

1 c m'm'm'  $0, 0, 1/2$  [0,0,0]

1 b m'm'm'  $1/2, 0, 0$  [0,0,0]

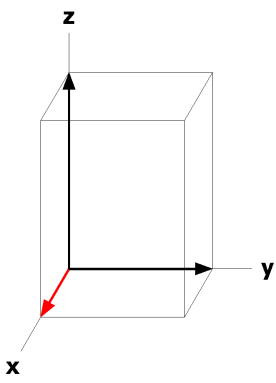
1 a m'm'm'  $0, 0, 0$  [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



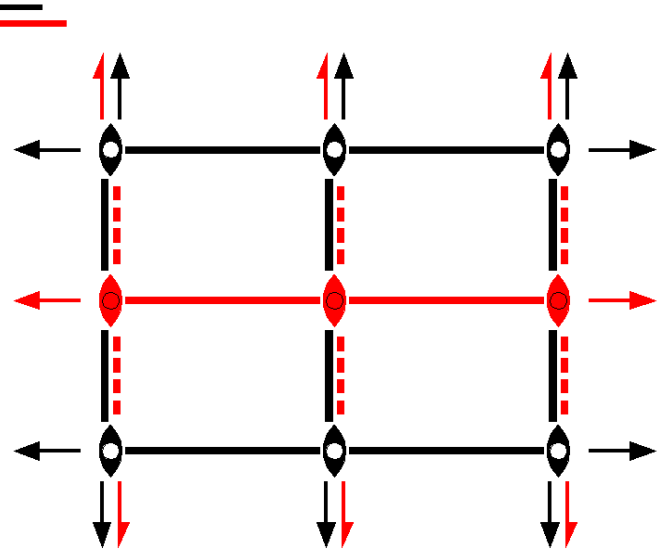
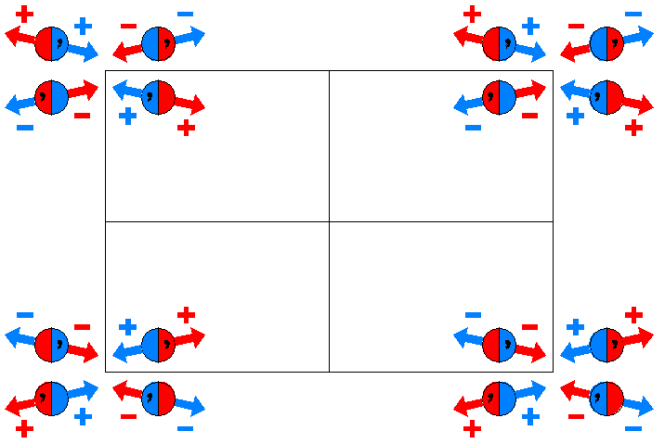
$P_{2a} mmm$

47.6.352

$mmm1'$

$P_{2a} 2/m2/m2/m$

Orthorhombic



**Origin** at center ( $mmm$ )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) 1<br>(1 0,0,0)                   | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) 2 $0,y,0$<br>(2 <sub>y</sub>  0,0,0) | (4) 2 $x,0,0$<br>(2 <sub>x</sub>  0,0,0) |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) m $x,y,0$<br>(m <sub>z</sub>  0,0,0) | (7) m $x,0,z$<br>(m <sub>y</sub>  0,0,0) | (8) m $0,y,z$<br>(m <sub>x</sub>  0,0,0) |

For  $(1,0,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' $(1,0,0)$<br>(1 1,0,0)'                     | (2) 2' $1/2,0,z$<br>(2 <sub>z</sub>  1,0,0)'         | (3) 2' $1/2,y,0$<br>(2 <sub>y</sub>  1,0,0)'         | (4) 2' $(1,0,0)$ $x,0,0$<br>(2 <sub>x</sub>  1,0,0)' |
| (5) $\bar{1}'$ $(1/2,0,0)$<br>( $\bar{1}$  1,0,0)' | (6) a' $(1,0,0)$ $x,y,0$<br>(m <sub>z</sub>  1,0,0)' | (7) a' $(1,0,0)$ $x,0,z$<br>(m <sub>y</sub>  1,0,0)' | (8) m' $1/2,y,z$<br>(m <sub>x</sub>  1,0,0)'         |

**Generators selected** (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
16	$\alpha$ 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8	z ..m	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0,w]	$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
8	y ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0, $\bar{w}$ ]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
8	x .m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v},0$ ]	$\bar{x},1/2,\bar{z}$ [0,v,0]	x,1/2, $\bar{z}$ [0, $\bar{v},0$ ]
8	w .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	$\bar{x},0,\bar{z}$ [0,v,0]	x,0, $\bar{z}$ [0, $\bar{v},0$ ]
8	v m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0,v, $\bar{w}$ ]	1/2,y, $\bar{z}$ [0, $\bar{v},w$ ]	1/2, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8	u m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	0,y, $\bar{z}$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]
4	t m'm2'	1/2,1/2,z [0,v,0]	1/2,1/2, $\bar{z}$ [0, $\bar{v},0$ ]		
4	s m'm2'	1/2,0,z [0,v,0]	1/2,0, $\bar{z}$ [0, $\bar{v},0$ ]		
4	r mm2	0,1/2,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]		
4	q mm2	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4	p m'2'm	1/2,y,1/2 [0,0,w]	1/2, $\bar{y},1/2$ [0,0, $\bar{w}$ ]		
4	o m'2'm	1/2,y,0 [0,0,w]	1/2, $\bar{y},0$ [0,0, $\bar{w}$ ]		
4	n m2m	0,y,1/2 [0,0,0]	0, $\bar{y},1/2$ [0,0,0]		
4	m m2m	0,y,0 [0,0,0]	0, $\bar{y},0$ [0,0,0]		
4	l 2mm	x,1/2,1/2 [0,0,0]	$\bar{x},1/2,1/2$ [0,0,0]		
4	k 2mm	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]		
4	j 2mm	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]		
4	i 2mm	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
2	h m'mm	1/2,1/2,1/2 [0,0,0]			
2	g mmm	0,1/2,1/2 [0,0,0]			
2	f m'mm	1/2,1/2,0 [0,0,0]			
2	e mmm	0,1/2,0 [0,0,0]			

2 d m'mm  $1/2, 0, 1/2$  [0,0,0]

2 c mmm  $0, 0, 1/2$  [0,0,0]

2 b m'mm  $1/2, 0, 0$  [0,0,0]

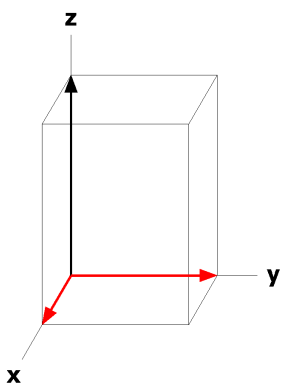
2 a mmm  $0, 0, 0$  [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



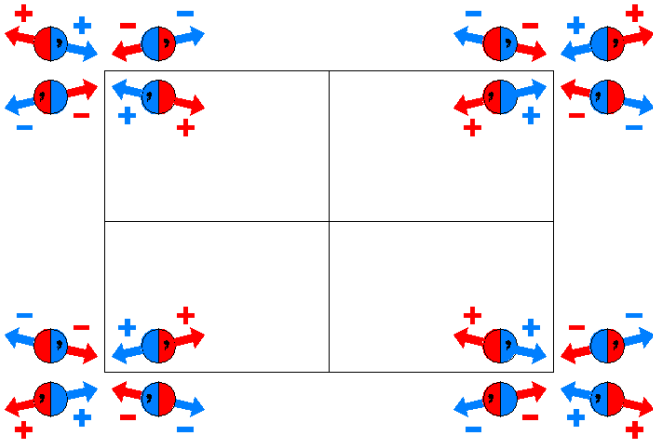
$P_C mmm$

47.7.353

$mmm1'$

$P_C 2/m2/m2/m$

Orthorhombic



**Origin** at center ( $mmm$ )

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

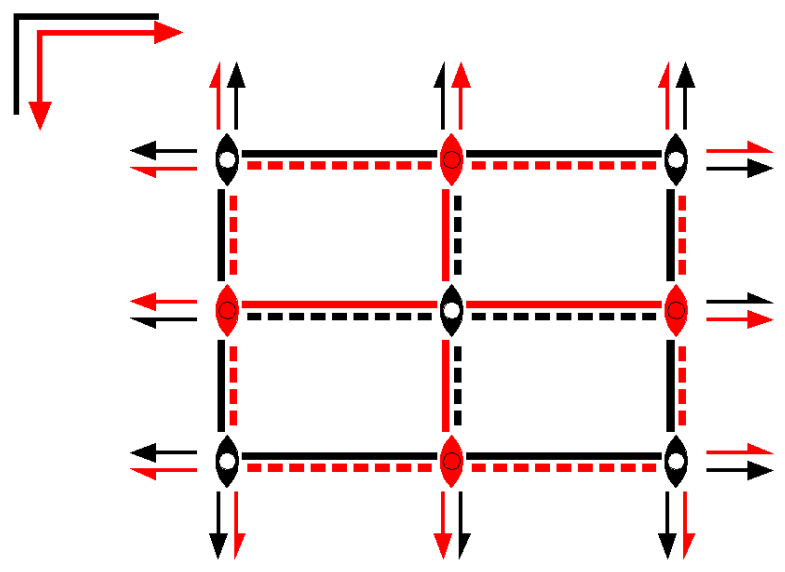
**Symmetry Operations**

For  $(0,0,0)$  + set

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) 1<br>(1 0,0,0)                   | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) 2 $0,y,0$<br>(2 <sub>y</sub>  0,0,0) | (4) 2 $x,0,0$<br>(2 <sub>x</sub>  0,0,0) |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) m $x,y,0$<br>(m <sub>z</sub>  0,0,0) | (7) m $x,0,z$<br>(m <sub>y</sub>  0,0,0) | (8) m $0,y,z$<br>(m <sub>x</sub>  0,0,0) |

For  $(1,0,0)'$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' $(1,0,0)$<br>(1 1,0,0)'                      | (2) 2' $1/2,0,z$<br>(2 <sub>z</sub>  1,0,0)'         | (3) 2' $1/2,y,0$<br>(2 <sub>y</sub>  1,0,0)'         | (4) 2' $(1,0,0)$ $x,0,0$<br>(2 <sub>x</sub>  1,0,0)' |
| (5) $\bar{1}$ ' $(1/2,0,0)$<br>( $\bar{1}$  1,0,0)' | (6) a' $(1,0,0)$ $x,y,0$<br>(m <sub>z</sub>  1,0,0)' | (7) a' $(1,0,0)$ $x,0,z$<br>(m <sub>y</sub>  1,0,0)' | (8) m' $1/2,y,z$<br>(m <sub>x</sub>  1,0,0)'         |





**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 α 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 z ..m	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0,w]	$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
8 y ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0, $\bar{w}$ ]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
8 x .m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [u,0, $\bar{w}$ ]	$\bar{x},1/2,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	x,1/2, $\bar{z}$ [ $\bar{u},0,w$ ]
8 w .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	$\bar{x},0,\bar{z}$ [0,v,0]	x,0, $\bar{z}$ [0, $\bar{v},0$ ]
8 v m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0,v, $\bar{w}$ ]	1/2,y, $\bar{z}$ [0, $\bar{v},w$ ]	1/2, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 u m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	0,y, $\bar{z}$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]
4 t m'm'2	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
4 s m'm2'	1/2,0,z [0,v,0]	1/2,0, $\bar{z}$ [0, $\bar{v},0$ ]		
4 r mm'2'	0,1/2,z [u,0,0]	0,1/2, $\bar{z}$ [ $\bar{u},0,0$ ]		
4 q mm2	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 p m'2'm	1/2,y,1/2 [0,0,w]	1/2, $\bar{y},1/2$ [0,0, $\bar{w}$ ]		
4 o m'2'm	1/2,y,0 [0,0,w]	1/2, $\bar{y},0$ [0,0, $\bar{w}$ ]		
4 n m2m	0,y,1/2 [0,0,0]	0, $\bar{y},1/2$ [0,0,0]		
4 m m2m	0,y,0 [0,0,0]	0, $\bar{y},0$ [0,0,0]		
4 l 2'm'm	x,1/2,1/2 [0,0,w]	$\bar{x},1/2,1/2$ [0,0, $\bar{w}$ ]		
4 k 2'm'm	x,1/2,0 [0,0,w]	$\bar{x},1/2,0$ [0,0, $\bar{w}$ ]		
4 j 2mm	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]		
4 i 2mm	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
2 h m'm'm	1/2,1/2,1/2 [0,0,w]			
2 g mm'm	0,1/2,1/2 [0,0,0]			
2 f m'm'm	1/2,1/2,0 [0,0,w]			
2 e mm'm	0,1/2,0 [0,0,0]			

2 d m'mm  $1/2, 0, 1/2$  [0,0,0]

2 c mmm  $0, 0, 1/2$  [0,0,0]

2 b m'mm  $1/2, 0, 0$  [0,0,0]

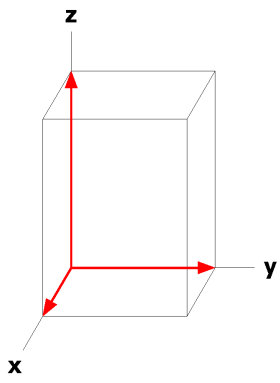
2 a mmm  $0, 0, 0$  [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p_c-2mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



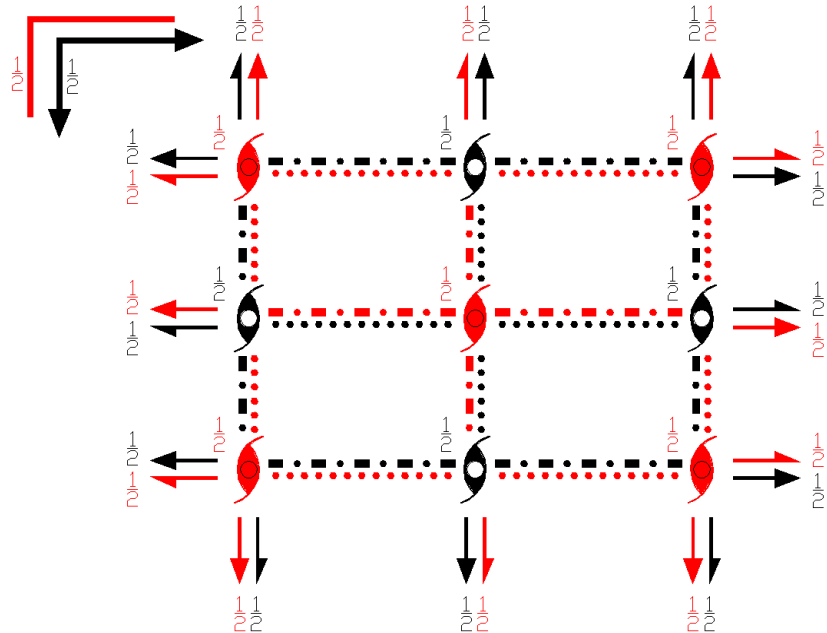
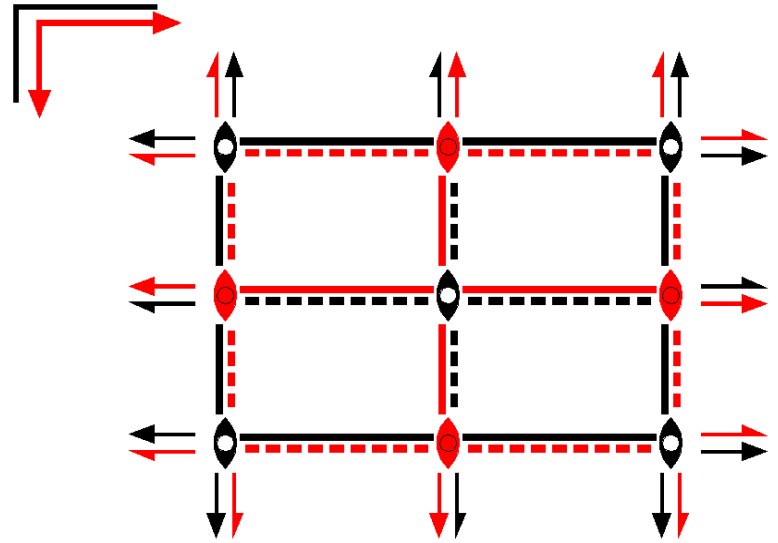
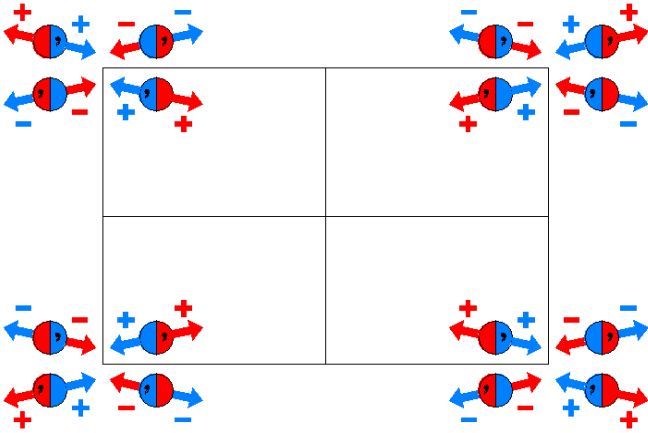
$P_F mmm$

47.8.354

$mmm1'$

$P_F 2/m2/m2/m$

Orthorhombic



**Origin** at center ( $mmm$ )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) +

(1) 1 (1 0,0,0)	(2) 2 <sub>z</sub> 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 2 <sub>y</sub> 0,y,0 (2 <sub>y</sub>  0,0,0)	(4) 2 <sub>x</sub> x,0,0 (2 <sub>x</sub>  0,0,0)
(5) $\bar{1}$ ( $\bar{1}$  0,0,0)	(6) m <sub>x</sub> x,y,0 (m <sub>x</sub>  0,0,0)	(7) m <sub>y</sub> x,0,z (m <sub>y</sub>  0,0,0)	(8) m <sub>z</sub> 0,y,z (m <sub>z</sub>  0,0,0)

For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' <sub>z</sub> 1/2,0,z (2' <sub>z</sub>  1,0,0)'	(3) 2' <sub>y</sub> 1/2,y,0 (2' <sub>y</sub>  1,0,0)'	(4) 2' <sub>x</sub> (1,0,0) x,0,0 (2' <sub>x</sub>  1,0,0)'
(5) $\bar{1}$ ' (1/2,0,0) ( $\bar{1}$  1,0,0)'	(6) a' (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)'	(7) a' (1,0,0) x,0,z (m <sub>y</sub>  1,0,0)'	(8) m' 1/2,y,z (m <sub>x</sub>  1,0,0)'

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 α 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
8 z ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [ $u,\bar{v},0$ ]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]
8 y ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0, $\bar{w}$ ]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
8 x ..m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $u,0,\bar{w}$ ]	$\bar{x},1/2,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	x,1/2, $\bar{z}$ [ $\bar{u},0,w$ ]
8 w .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	$\bar{x},0,\bar{z}$ [0,v,0]	x,0, $\bar{z}$ [0, $\bar{v},0$ ]
8 v m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0, $\bar{v},w$ ]	1/2,y, $\bar{z}$ [0, $\bar{v},w$ ]	1/2, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 u m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	0,y, $\bar{z}$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [ $u,0,0$ ]
4 t m'm'2	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
4 s m'm'2'	1/2,0,z [0,v,0]	1/2,0, $\bar{z}$ [0, $\bar{v},0$ ]		
4 r mm'2'	0,1/2,z [u,0,0]	0,1/2, $\bar{z}$ [ $\bar{u},0,0$ ]		
4 q mm2	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 p m'2m'	1/2,y,1/2 [0,v,0]	1/2, $\bar{y},1/2$ [0,v,0]		
4 o m'2'm	1/2,y,0 [0,0,w]	1/2, $\bar{y},0$ [0,0, $\bar{w}$ ]		
4 n m2'm'	0,y,1/2 [u,0,0]	0, $\bar{y},1/2$ [ $\bar{u},0,0$ ]		

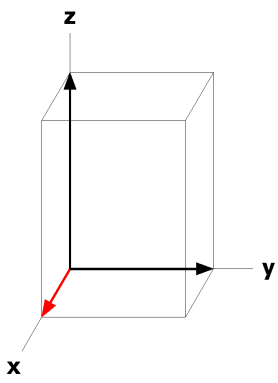
4	m	$m2m$	$0,y,0 [0,0,0]$	$0,\bar{y},0 [0,0,0]$
4	l	$2m'm'$	$x,1/2,1/2 [u,0,0]$	$\bar{x},1/2,1/2 [u,0,0]$
4	k	$2'm'm$	$x,1/2,0 [0,0,w]$	$\bar{x},1/2,0 [0,0,\bar{w}]$
4	j	$2'mm'$	$x,0,1/2 [0,v,0]$	$\bar{x},0,1/2 [0,\bar{v},0]$
4	i	$2mm$	$x,0,0 [0,0,0]$	$\bar{x},0,0 [0,0,0]$
2	h	$m'm'm'$	$1/2,1/2,1/2 [0,0,0]$	
2	g	$mm'm'$	$0,1/2,1/2 [u,0,0]$	
2	f	$m'm'm$	$1/2,1/2,0 [0,0,w]$	
2	e	$mm'm$	$0,1/2,0 [0,0,0]$	
2	d	$m'mm'$	$1/2,0,1/2 [0,v,0]$	
2	c	$mmm'$	$0,0,1/2 [0,0,0]$	
2	b	$m'mm$	$1/2,0,0 [0,0,0]$	
2	a	$mmm$	$0,0,0 [0,0,0]$	

### Symmetry of Special Projections

Along  $[0,0,1]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at  $0,y,0$



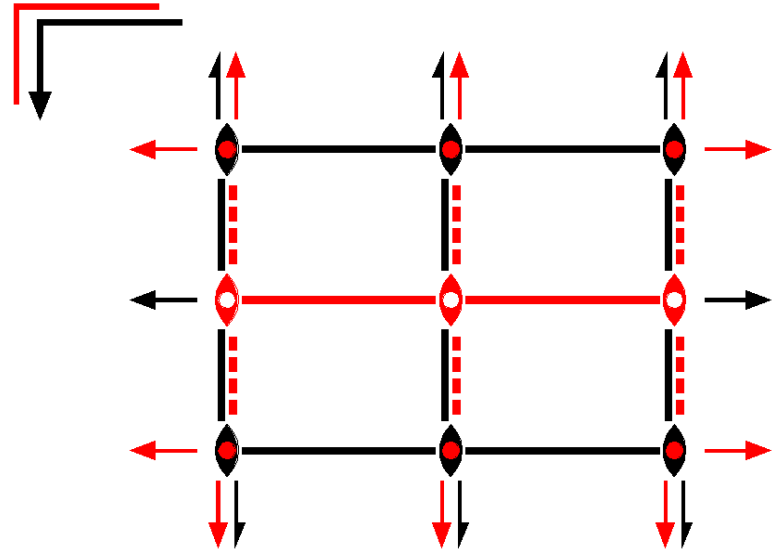
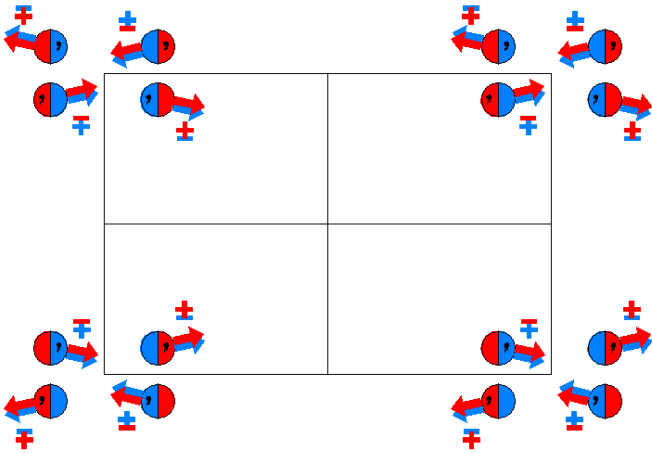
$P_{2a} mmm'$

47.9.355

$mmm1'$

$P_{2a} 2'/m2'/m2'/m'$

Orthorhombic



**Origin** at center ( $mmm'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) m x,0,z<br>(m <sub>y</sub>  0,0,0)   | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   |

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1,0,0)<br>(1 1,0,0)'                     | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'     | (3) 2 1/2,y,0<br>(2 <sub>y</sub>  1,0,0)         | (4) 2 (1,0,0) x,0,0<br>(2 <sub>x</sub>  1,0,0) |
| (5) $\bar{1}$ ' (1/2,0,0)<br>( $\bar{1}$  1,0,0) | (6) a (1,0,0) x,y,0<br>(m <sub>z</sub>  1,0,0) | (7) a' (1,0,0) x,0,z<br>(m <sub>y</sub>  1,0,0)' | (8) m' 1/2,y,z<br>(m <sub>x</sub>  1,0,0)'     |

For (1,0,0)' + set

**Generators selected** (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 α 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 z ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [u, $\bar{v},0$ ]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]
8 y ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,0$ [u, $\bar{v},0$ ]	x, $\bar{y},0$ [ $\bar{u},v,0$ ]
8 x .m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v},0$ ]	$\bar{x},1/2,\bar{z}$ [0, $\bar{v},0$ ]	x,1/2, $\bar{z}$ [0,v,0]
8 w .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	x,0, $\bar{z}$ [0,v,0]
8 v m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0,v, $\bar{w}$ ]	1/2,y, $\bar{z}$ [0,v, $\bar{w}$ ]	1/2, $\bar{y},\bar{z}$ [0,v,w]
8 u m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	0,y, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
4 t m'm2'	1/2,1/2,z [0,v,0]	1/2,1/2, $\bar{z}$ [0,v,0]		
4 s m'm2'	1/2,0,z [0,v,0]	1/2,0, $\bar{z}$ [0,v,0]		
4 r mm2	0,1/2,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]		
4 q mm2	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 p m'2m'	1/2,y,1/2 [0,v,0]	1/2, $\bar{y},1/2$ [0,v,0]		
4 o m'2m'	1/2,y,0 [0,v,0]	1/2, $\bar{y},0$ [0,v,0]		
4 n m2'm'	0,y,1/2 [u,0,0]	0, $\bar{y},1/2$ [ $\bar{u},0,0$ ]		
4 m m2'm'	0,y,0 [u,0,0]	0, $\bar{y},0$ [ $\bar{u},0,0$ ]		
4 l 2'mm'	x,1/2,1/2 [0,v,0]	$\bar{x},1/2,1/2$ [0, $\bar{v},0$ ]		
4 k 2'mm'	x,1/2,0 [0,v,0]	$\bar{x},1/2,0$ [0, $\bar{v},0$ ]		
4 j 2'mm'	x,0,1/2 [0,v,0]	$\bar{x},0,1/2$ [0, $\bar{v},0$ ]		
4 i 2'mm'	x,0,0 [0,v,0]	$\bar{x},0,0$ [0, $\bar{v},0$ ]		
2 h m'mm'	1/2,1/2,1/2 [0,v,0]			
2 g mmm'	0,1/2,1/2 [0,0,0]			
2 f m'mm'	1/2,1/2,0 [0,v,0]			
2 e mmm'	0,1/2,0 [0,0,0]			

2 d  $m'mm'$   $1/2, 0, 1/2$   $[0, v, 0]$

2 c  $mmm'$   $0, 0, 1/2$   $[0, 0, 0]$

2 b  $m'mm'$   $1/2, 0, 0$   $[0, v, 0]$

2 a  $mmm'$   $0, 0, 0$   $[0, 0, 0]$

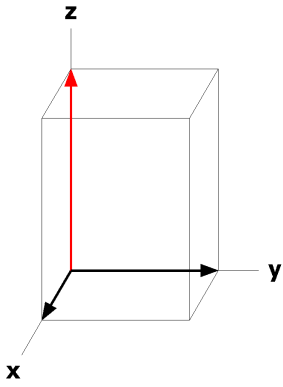
### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p_{2a} 2mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 0, 0$

Along  $[0, 1, 0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at  $0, y, 0$





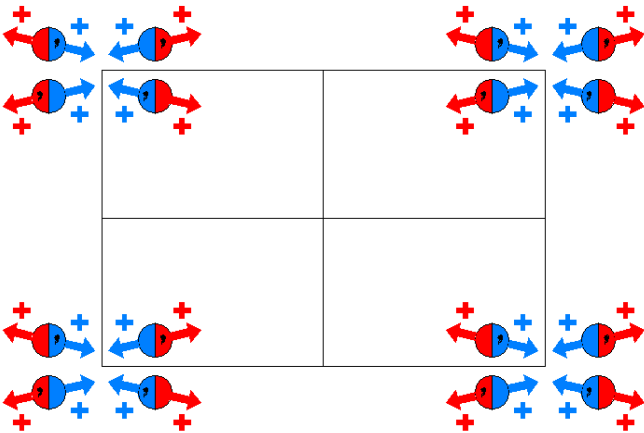
$P_{2c} m'm'm$

47.10.356

$mmm1'$

$P_{2c} 2'/m'2'/m'2/m$

Orthorhombic

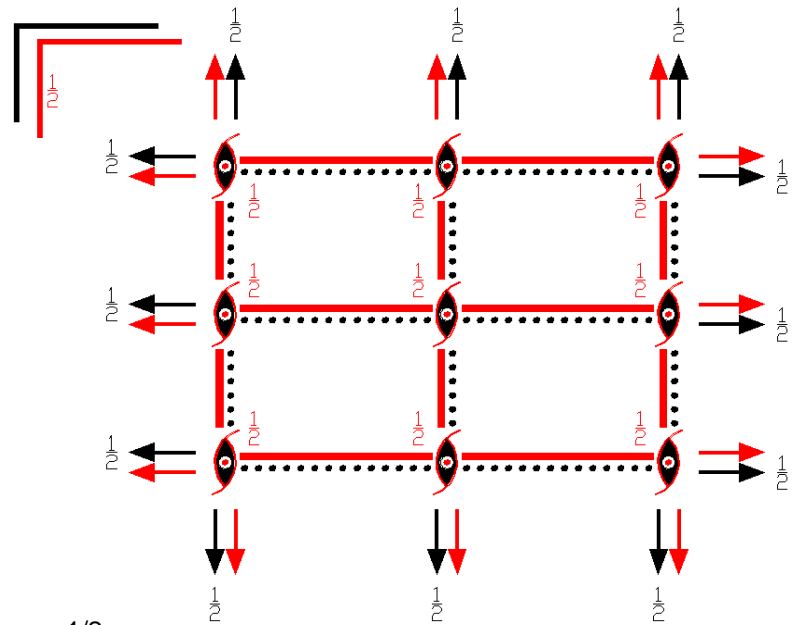


**Origin** at center ( $mm'm'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) 1<br>(1 0,0,0)                   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |
- For (0,0,1)<sup>+</sup> set
- |  |  |  |  |
|--|--|--|--|
| (1) t' (0,0,1)<br>(1 0,0,1)'                     | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)' | (3) 2 0,y,1/2<br>(2 <sub>y</sub>  0,0,1)       | (4) 2 x,0,1/2<br>(2 <sub>x</sub>  0,0,1)       |
| (5) $\bar{1}$ ' 0,0,1/2<br>( $\bar{1}$ ' 0,0,1)' | (6) m' x,y,1/2<br>(m <sub>z</sub> ' 0,0,1)'      | (7) c (0,0,1) x,0,z<br>(m <sub>y</sub>  0,0,1) | (8) c (0,0,1) 0,y,z<br>(m <sub>x</sub>  0,0,1) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
16 α 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(4) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 z ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [ $u,\bar{v},0$ ]	x, $\bar{y},1/2$ [ $u,\bar{v},0$ ]
8 y ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0,w]
8 x .m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ]	$\bar{x},1/2,\bar{z}$ [u,0,w]	x,1/2, $\bar{z}$ [ $\bar{u},0,w$ ]
8 w .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$\bar{x},0,\bar{z}$ [u,0,w]	x,0, $\bar{z}$ [ $\bar{u},0,w$ ]
8 v m'..	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0, $\bar{v},w$ ]	1/2,y, $\bar{z}$ [0, $\bar{v},w$ ]	1/2, $\bar{y},\bar{z}$ [0,v,w]
8 u m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
4 t m'm'2	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
4 s m'm'2	1/2,0,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]		
4 r m'm'2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]		
4 q m'm'2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
4 p m'2m'	1/2,y,1/2 [0,v,0]	1/2, $\bar{y},1/2$ [0, $\bar{v},0$ ]		
4 o m'2m	1/2,y,0 [0,0,w]	1/2, $\bar{y},0$ [0,0,w]		
4 n m'2m'	0,y,1/2 [0,v,0]	0, $\bar{y},1/2$ [0, $\bar{v},0$ ]		
4 m m'2m	0,y,0 [0,0,w]	0, $\bar{y},0$ [0,0,w]		
4 l 2m'm'	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]		
4 k 2'm'm	x,1/2,0 [0,0,w]	$\bar{x},1/2,0$ [0,0,w]		
4 j 2m'm'	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]		
4 i 2'm'm	x,0,0 [0,0,w]	$\bar{x},0,0$ [0,0,w]		
2 h m'm'm'	1/2,1/2,1/2 [0,0,0]			
2 g m'm'm'	0,1/2,1/2 [0,0,0]			
2 f m'm'm	1/2,1/2,0 [0,0,w]			
2 e m'm'm	0,1/2,0 [0,0,w]			

2 d  $m'm'm'$   $1/2, 0, 1/2$   $[0, 0, 0]$

2 c  $m'm'm'$   $0, 0, 1/2$   $[0, 0, 0]$

2 b  $m'm'm'$   $1/2, 0, 0$   $[0, 0, w]$

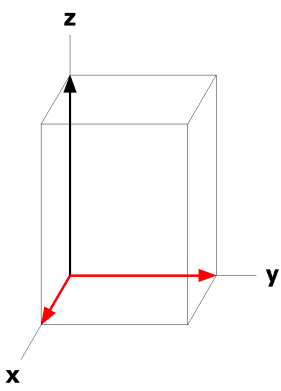
2 a  $m'm'm'$   $0, 0, 0$   $[0, 0, w]$

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$   $p_{2a'} 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $x, 0, 1/2$

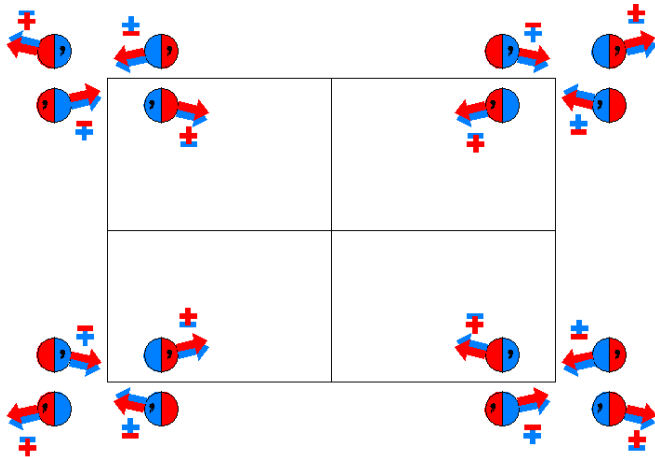
Along  $[0, 1, 0]$   $p_{2a'} 2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at  $0, y, 1/2$



$P_C mmm'$   
47.11.357

$mmm1'$   
 $P_C 2'/m2'/m2/m'$

Orthorhombic



Origin at center ( $mmm'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

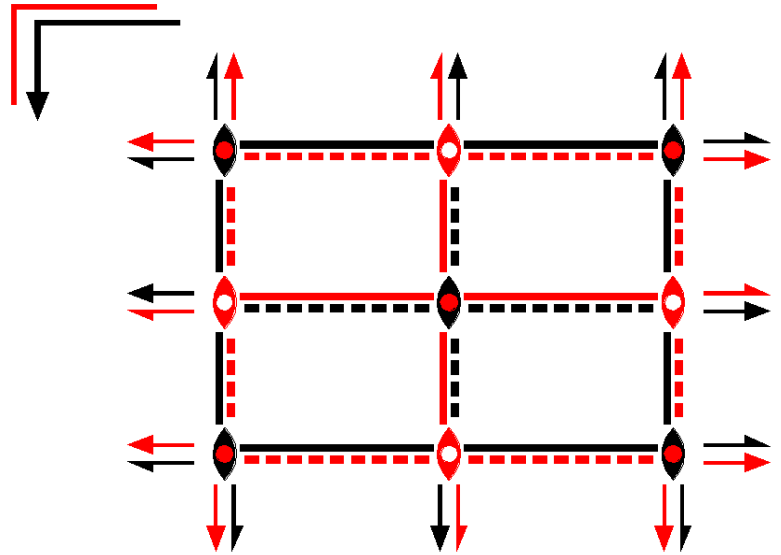
**Symmetry Operations**

- |   |                                      |                                    |                                    |
|---|--------------------------------------|------------------------------------|------------------------------------|
| (1) 1<br>(1 0,0,0)                      | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)     | (3) 2' $0,y,0$<br>( $2_y$  0,0,0)' | (4) 2' $x,0,0$<br>( $2_x$  0,0,0)' |
| (5) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)' | (6) $m'$ $x,y,0$<br>( $m_z$  0,0,0)' | (7) $m$ $x,0,z$<br>( $m_y$  0,0,0) | (8) $m$ $0,y,z$<br>( $m_x$  0,0,0) |

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (1,0,0)<br>(1 1,0,0)'                 | (2) 2' $1/2,0,z$<br>( $2_z$  1,0,0)'       | (3) 2 $1/2,y,0$<br>( $2_y$  1,0,0)           | (4) 2 (1,0,0) $x,0,0$<br>( $2_x$  1,0,0) |
| (5) $\bar{1}$ (1/2,0,0)<br>( $\bar{1}$  1,0,0) | (6) $a$ (1,0,0) $x,y,0$<br>( $m_z$  1,0,0) | (7) $a'$ (1,0,0) $x,0,z$<br>( $m_y$  1,0,0)' | (8) $m'$ $1/2,y,z$<br>( $m_x$  1,0,0)'   |

For (1,0,0)' + set



**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 α 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u, $\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 z ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [u, $\bar{v},0$ ]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]
8 y ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,0$ [u, $\bar{v},0$ ]	x, $\bar{y},0$ [ $\bar{u},v,0$ ]
8 x .m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [u,0, $\bar{w}$ ]	$\bar{x},1/2,\bar{z}$ [u,0,w]	x,1/2, $\bar{z}$ [u,0, $\bar{w}$ ]
8 w .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	x,0, $\bar{z}$ [0,v,0]
8 v m..	1/2,y,z [u,0,0]	1/2, $\bar{y},z$ [ $\bar{u},0,0$ ]	1/2,y, $\bar{z}$ [u,0,0]	1/2, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
8 u m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	0,y, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
4 t m'm'2	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 s m'm'2'	1/2,0,z [0,v,0]	1/2,0, $\bar{z}$ [0,v,0]		
4 r mm'2'	0,1/2,z [u,0,0]	0,1/2, $\bar{z}$ [u,0,0]		
4 q mm2	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 p m'2m'	1/2,y,1/2 [0,v,0]	1/2, $\bar{y},1/2$ [0,v,0]		
4 o m'2m'	1/2,y,0 [0,v,0]	1/2, $\bar{y},0$ [0,v,0]		
4 n m2'm'	0,y,1/2 [u,0,0]	0, $\bar{y},1/2$ [ $\bar{u},0,0$ ]		
4 m m2'm'	0,y,0 [u,0,0]	0, $\bar{y},0$ [ $\bar{u},0,0$ ]		
4 l 2m'm'	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [u,0,0]		
4 k 2m'm'	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [u,0,0]		
4 j 2'mm'	x,0,1/2 [0,v,0]	$\bar{x},0,1/2$ [0, $\bar{v},0$ ]		
4 i 2'mm'	x,0,0 [0,v,0]	$\bar{x},0,0$ [0, $\bar{v},0$ ]		
2 h m'm'm'	1/2,1/2,1/2 [0,0,0]			
2 g mm'm'	0,1/2,1/2 [u,0,0]			
2 f m'm'm'	1/2,1/2,0 [0,0,0]			
2 e mm'm'	0,1/2,0 [u,0,0]			

2 d  $m'mm'$   $1/2, 0, 1/2$   $[0, v, 0]$

2 c  $mmm'$   $0, 0, 1/2$   $[0, 0, 0]$

2 b  $m'mm'$   $1/2, 0, 0$   $[0, v, 0]$

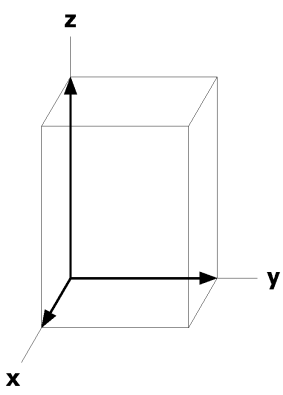
2 a  $mmm'$   $0, 0, 0$   $[0, 0, 0]$

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p_c-2mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 0, 0$

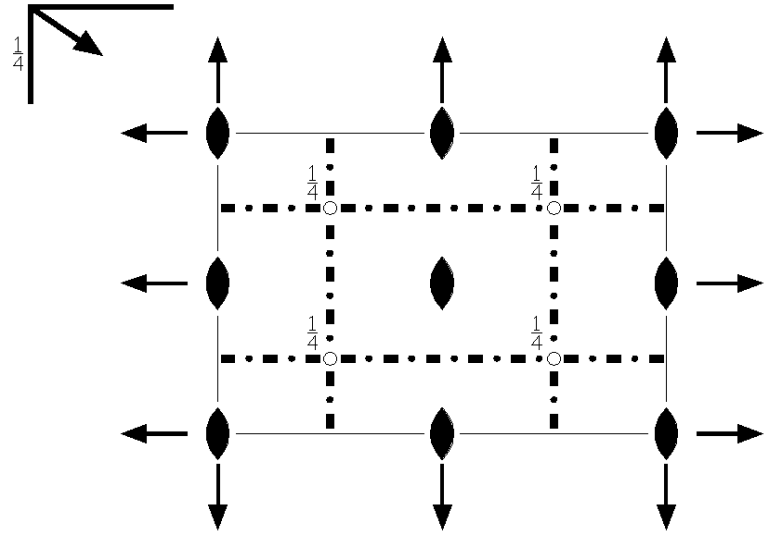
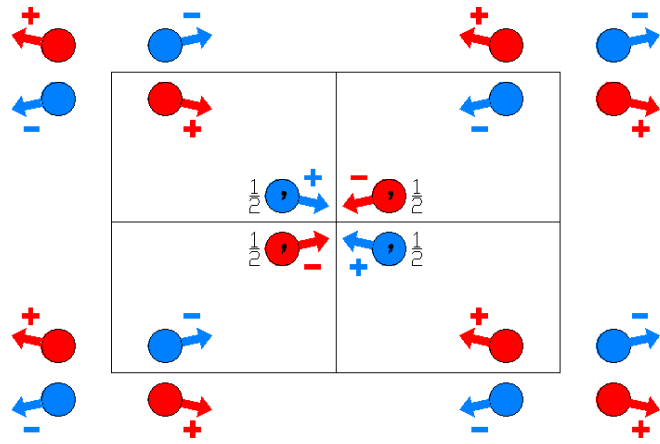
Along  $[0, 1, 0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at  $0, y, 0$



Pnnn  
48.1.358

mmm  
P2/n2/n2/n

Orthorhombic



**Origin** at 222, at  $1/4, 1/4, 1/4$  from  $\bar{1}$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1 | 0,0,0)

(2) 2  $0,0,z$   
( $2_z$  | 0,0,0)

(3) 2  $0,y,0$   
( $2_y$  | 0,0,0)

(4) 2  $x,0,0$   
( $2_x$  | 0,0,0)

(5)  $\bar{1}$   $1/4, 1/4, 1/4$   
( $\bar{1}$  |  $1/2, 1/2, 1/2$ )

(6) n  $(1/2, 1/2, 0)$   $x, y, 1/4$   
( $m_z$  |  $1/2, 1/2, 1/2$ )

(7) n  $(1/2, 0, 1/2)$   $x, 1/4, z$   
( $m_y$  |  $1/2, 1/2, 1/2$ )

(8) n  $(0, 1/2, 1/2)$   $1/4, y, z$   
( $m_x$  |  $1/2, 1/2, 1/2$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	m 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [u,v,w]	(6) x+1/2,y+1/2, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) x+1/2, $\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z+1/2$ [u, $\bar{v},\bar{w}$ ]
4	l ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]
4	k ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]
4	j .2.	1/2,y,0 [0,v,0]	1/2, $\bar{y},0$ [0, $\bar{v},0$ ]	0, $\bar{y}+1/2,1/2$ [0,v,0]	0,y+1/2,1/2 [0, $\bar{v},0$ ]
4	i .2.	0,y,0 [0,v,0]	0, $\bar{y},0$ [0, $\bar{v},0$ ]	1/2, $\bar{y}+1/2,1/2$ [0,v,0]	1/2,y+1/2,1/2 [0, $\bar{v},0$ ]
4	h 2..	X,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	$\bar{x}+1/2,1/2,0$ [u,0,0]	x+1/2,1/2,0 [ $\bar{u},0,0$ ]
4	g 2..	X,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	$\bar{x}+1/2,1/2,1/2$ [u,0,0]	x+1/2,1/2,1/2 [ $\bar{u},0,0$ ]
4	f $\bar{1}$	3/4,3/4,3/4 [u,v,w]	1/4,1/4,3/4 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,1/4 [ $\bar{u},v,\bar{w}$ ]	3/4,1/4,1/4 [u, $\bar{v},\bar{w}$ ]
4	e $\bar{1}$	1/4,1/4,1/4 [u,v,w]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,3/4 [ $\bar{u},v,\bar{w}$ ]	1/4,3/4,3/4 [u, $\bar{v},\bar{w}$ ]
2	d 222	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	c 222	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	b 222	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	a 222	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

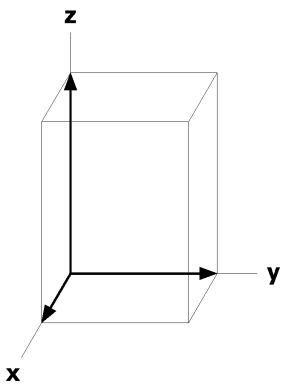
**Symmetry of Special Projections**

Along [0,0,1]  $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0





Pnnn1'

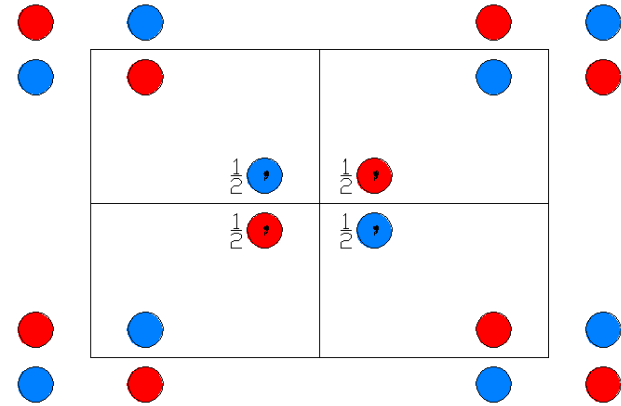
48.2.359

mmm1'

P2/n2/n2/n1'

Orthorhombic

1'



Origin at 2221', at 1/4, 1/4, 1/4 from  $\bar{1}1'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

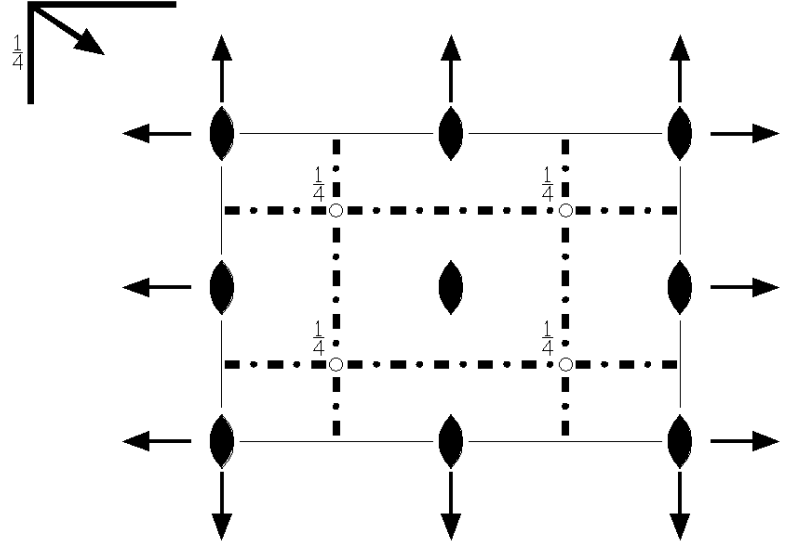
Symmetry Operations

For 1 + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0)                         | (3) 2 0,y,0<br>(2 <sub>y</sub>   0,0,0)                           | (4) 2 x,0,0<br>(2 <sub>x</sub>   0,0,0)                           |
| (5) $\bar{1}$ 1/4, 1/4, 1/4<br>( $\bar{1}$   1/2, 1/2, 1/2) | (6) n (1/2, 1/2, 0) x,y,1/4<br>(m <sub>z</sub>   1/2, 1/2, 1/2) | (7) n (1/2, 0, 1/2) x, 1/4, z<br>(m <sub>y</sub>   1/2, 1/2, 1/2) | (8) n (0, 1/2, 1/2) 1/4, y, z<br>(m <sub>x</sub>   1/2, 1/2, 1/2) |

For 1' + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1'<br>(1   0,0,0)'   | (2) 2' 0,0,z<br>(2 <sub>z</sub>   0,0,0)'                         | (3) 2' 0,y,0<br>(2 <sub>y</sub>   0,0,0)'                           | (4) 2' x,0,0<br>(2 <sub>x</sub>   0,0,0)'                           |
| (5) $\bar{1}'$ 1/4, 1/4, 1/4<br>( $\bar{1}'$   1/2, 1/2, 1/2)' | (6) n' (1/2, 1/2, 0) x,y,1/4<br>(m <sub>z</sub>   1/2, 1/2, 1/2)' | (7) n' (1/2, 0, 1/2) x, 1/4, z<br>(m <sub>y</sub>   1/2, 1/2, 1/2)' | (8) n' (0, 1/2, 1/2) 1/4, y, z<br>(m <sub>x</sub>   1/2, 1/2, 1/2)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5), 1'.

**Positions**

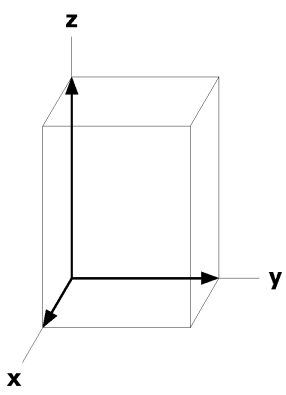
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +	1' +		
8 m 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]		
	(3) $\bar{x},y,\bar{z}$ [0,0,0]	(4) x, $\bar{y},\bar{z}$ [0,0,0]		
	(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [0,0,0]	(6) x+1/2,y+1/2, $\bar{z}+1/2$ [0,0,0]		
	(7) x+1/2, $\bar{y}+1/2,z+1/2$ [0,0,0]	(8) $\bar{x}+1/2,y+1/2,z+1/2$ [0,0,0]		
4 l ..21'	0,1/2,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	1/2,0,z+1/2 [0,0,0]
4 k ..21'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,1/2,z+1/2 [0,0,0]
4 j .2.1'	1/2,y,0 [0,0,0]	1/2, $\bar{y}$ ,0 [0,0,0]	0, $\bar{y}+1/2,1/2$ [0,0,0]	0,y+1/2,1/2 [0,0,0]
4 i .2.1'	0,y,0 [0,0,0]	0, $\bar{y}$ ,0 [0,0,0]	1/2, $\bar{y}+1/2,1/2$ [0,0,0]	1/2,y+1/2,1/2 [0,0,0]
4 h 2..1'	X,0,1/2 [0,0,0]	$\bar{x}$ ,0,1/2 [0,0,0]	$\bar{x}+1/2,1/2,0$ [0,0,0]	x+1/2,1/2,0 [0,0,0]
4 g 2..1'	X,0,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0]	$\bar{x}+1/2,1/2,1/2$ [0,0,0]	x+1/2,1/2,1/2 [0,0,0]
4 f $\bar{1}1'$	3/4,3/4,3/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
4 e $\bar{1}1'$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]
2 d 2221'	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2 c 2221'	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2 b 2221'	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
2 a 2221'	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

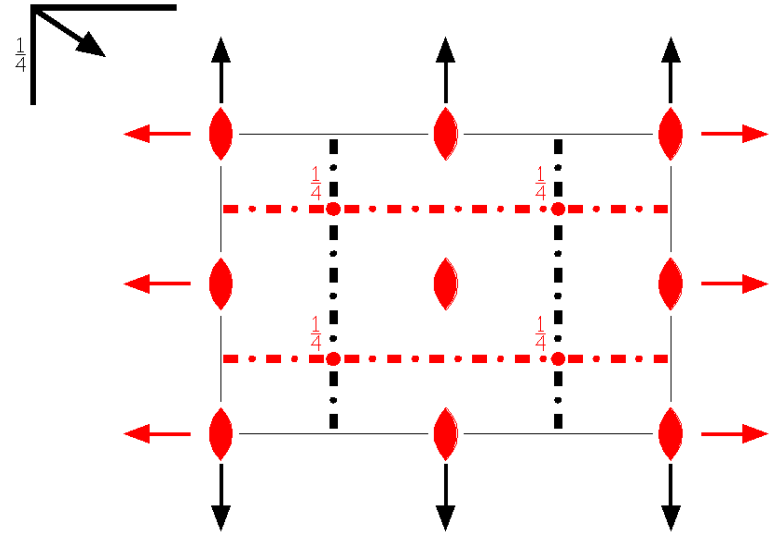
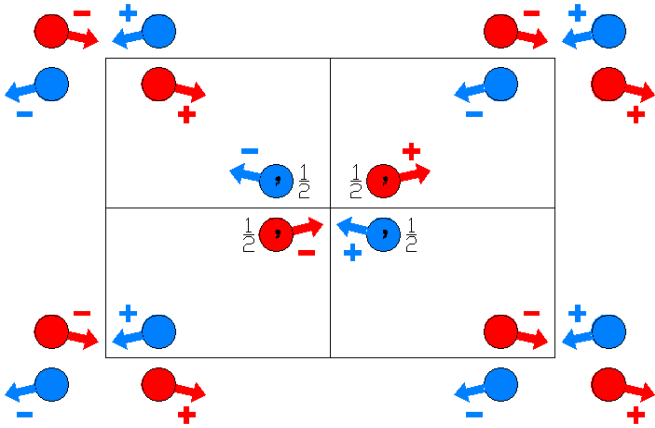
Along [0,1,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pn'nn  
48.3.360

m'mm  
P2/n'2'/n2'/n

Orthorhombic



**Origin** at 22'2', at  $1/4, 1/4, 1/4$  from  $\bar{1}'$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                       | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                   | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                       |
| (5) $\bar{1}'$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)' | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (7) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

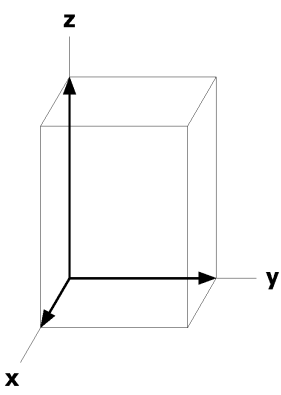
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	m 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x+1/2,y+1/2, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) x+1/2, $\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]
4	l ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}$ [u, $\bar{v}$ ,0]	1/2,0, $\bar{z}+1/2$ [ $\bar{u},\bar{v}$ ,0]	1/2,0,z+1/2 [ $\bar{u},v,0$ ]
4	k ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [u, $\bar{v}$ ,0]	1/2,1/2, $\bar{z}+1/2$ [ $\bar{u},\bar{v}$ ,0]	1/2,1/2,z+1/2 [ $\bar{u},v,0$ ]
4	j .2'	1/2,y,0 [u,0,w]	1/2, $\bar{y}$ ,0 [u,0, $\bar{w}$ ]	0, $\bar{y}+1/2,1/2$ [ $\bar{u},0,\bar{w}$ ]	0,y+1/2,1/2 [ $\bar{u},0,w$ ]
4	i .2'	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [u,0, $\bar{w}$ ]	1/2, $\bar{y}+1/2,1/2$ [ $\bar{u},0,\bar{w}$ ]	1/2,y+1/2,1/2 [ $\bar{u},0,w$ ]
4	h 2..	X,0,1/2 [u,0,0]	$\bar{x}$ ,0,1/2 [u,0,0]	$\bar{x}+1/2,1/2,0$ [ $\bar{u},0,0$ ]	x+1/2,1/2,0 [ $\bar{u},0,0$ ]
4	g 2..	X,0,0 [u,0,0]	$\bar{x}$ ,0,0 [u,0,0]	$\bar{x}+1/2,1/2,1/2$ [ $\bar{u},0,0$ ]	x+1/2,1/2,1/2 [ $\bar{u},0,0$ ]
4	f $\bar{1}$	3/4,3/4,3/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
4	e $\bar{1}$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]
2	d 22'2'	0,1/2,0 [u,0,0]	1/2,0,1/2 [ $\bar{u},0,0$ ]		
2	c 22'2'	0,0,1/2 [u,0,0]	1/2,1/2,0 [ $\bar{u},0,0$ ]		
2	b 22'2'	1/2,0,0 [u,0,0]	0,1/2,1/2 [ $\bar{u},0,0$ ]		
2	a 22'2'	0,0,0 [u,0,0]	1/2,1/2,1/2 [ $\bar{u},0,0$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $c_p^*2'mm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c2mm$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

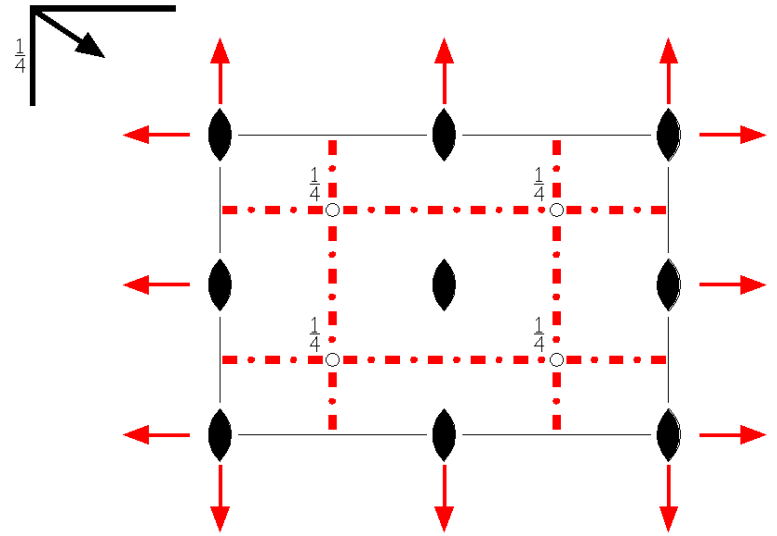
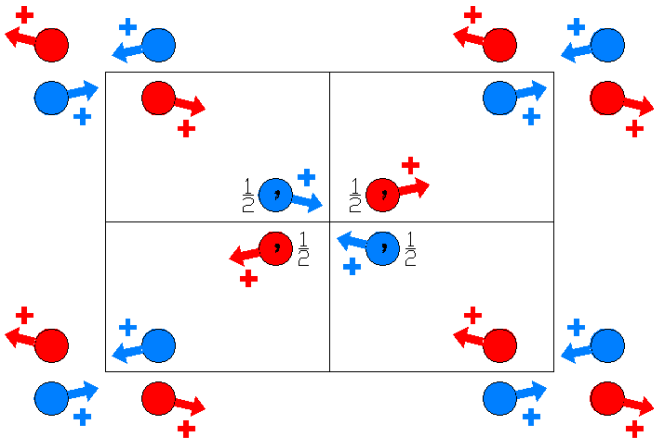
Along [0,1,0]  $c_p^*2'mm'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pn'n'n  
48.4.361

m'm'm  
P2'n'2'/n'2'/n

Orthorhombic



**Origin** at 2'2'2, at 1/4, 1/4, 1/4 from  $\bar{1}$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                     | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                     |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2) | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (7) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

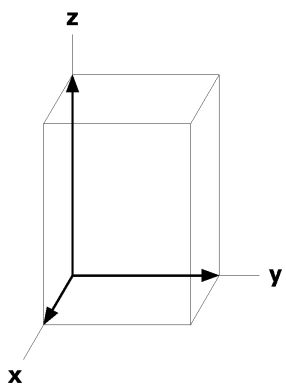
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	m 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
		(3) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]		
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [u,v,w]	(6) x+1/2,y+1/2, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]		
		(7) x+1/2, $\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(8) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]		
4	l ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0,z+1/2 [0,0,w]
4	k ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,1/2,z+1/2 [0,0,w]
4	j .2'	1/2,y,0 [u,0,w]	1/2, $\bar{y},0$ [ $\bar{u},0,w$ ]	0, $\bar{y}+1/2,1/2$ [u,0,w]	0,y+1/2,1/2 [ $\bar{u},0,w$ ]
4	i .2'	0,y,0 [u,0,w]	0, $\bar{y},0$ [ $\bar{u},0,w$ ]	1/2, $\bar{y}+1/2,1/2$ [u,0,w]	1/2,y+1/2,1/2 [ $\bar{u},0,w$ ]
4	h 2'..	X,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	$\bar{x}+1/2,1/2,0$ [0,v,w]	x+1/2,1/2,0 [0, $\bar{v},w$ ]
4	g 2'..	X,0,0 [0,v,w]	$\bar{x},0,0$ [0, $\bar{v},w$ ]	$\bar{x}+1/2,1/2,1/2$ [0,v,w]	x+1/2,1/2,1/2 [0, $\bar{v},w$ ]
4	f $\bar{1}$	3/4,3/4,3/4 [u,v,w]	1/4,1/4,3/4 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,1/4 [ $u,\bar{v},w$ ]	3/4,1/4,1/4 [ $\bar{u},v,w$ ]
4	e $\bar{1}$	1/4,1/4,1/4 [u,v,w]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,3/4 [ $u,\bar{v},w$ ]	1/4,3/4,3/4 [ $\bar{u},v,w$ ]
2	d 2'2'2	0,1/2,0 [0,0,w]	1/2,0,1/2 [0,0,w]		
2	c 2'2'2	0,0,1/2 [0,0,w]	1/2,1/2,0 [0,0,w]		
2	b 2'2'2	1/2,0,0 [0,0,w]	0,1/2,1/2 [0,0,w]		
2	a 2'2'2	0,0,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] c2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



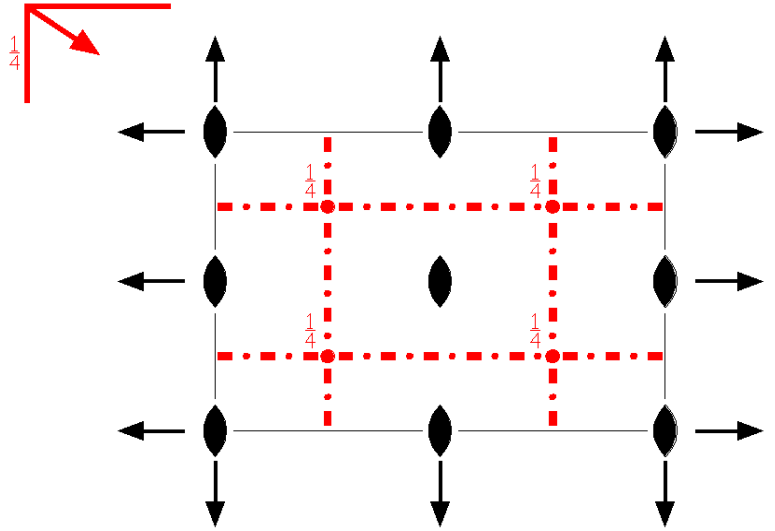
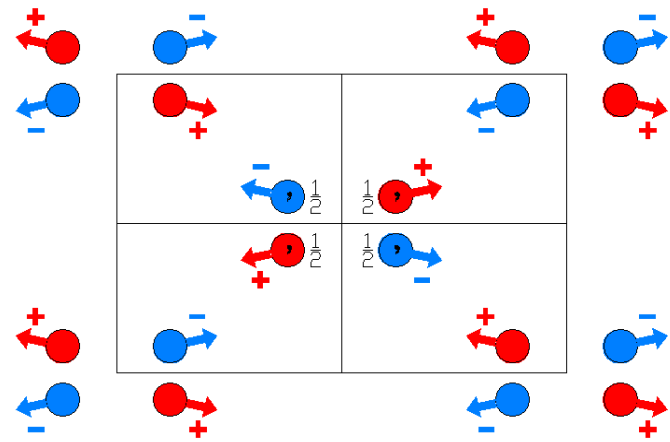
Pn'n'n'

48.5.362

m'm'm'

P2/n'2/n'2/n'

Orthorhombic



Origin at 222, at 1/4,1/4,1/4 from  $\bar{1}$ '

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                       | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                       | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                       |
| (5) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$ ' 1/2,1/2,1/2)' | (6) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (7) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	m 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x+1/2,y+1/2, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(7) x+1/2, $\bar{y}+1/2,z+1/2$ [u, $\bar{v},w$ ]	(8) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]
4	l ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0,w]
4	k ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0,w]
4	j .2.	1/2,y,0 [0,v,0]	1/2, $\bar{y},0$ [0, $\bar{v},0$ ]	0, $\bar{y}+1/2,1/2$ [0, $\bar{v},0$ ]	0,y+1/2,1/2 [0,v,0]
4	i .2.	0,y,0 [0,v,0]	0, $\bar{y},0$ [0, $\bar{v},0$ ]	1/2, $\bar{y}+1/2,1/2$ [0, $\bar{v},0$ ]	1/2,y+1/2,1/2 [0,v,0]
4	h 2..	X,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	$\bar{x}+1/2,1/2,0$ [ $\bar{u},0,0$ ]	x+1/2,1/2,0 [u,0,0]
4	g 2..	X,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	$\bar{x}+1/2,1/2,1/2$ [ $\bar{u},0,0$ ]	x+1/2,1/2,1/2 [u,0,0]
4	f $\bar{1}'$	3/4,3/4,3/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
4	e $\bar{1}'$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]
2	d 222	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	c 222	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	b 222	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	a 222	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

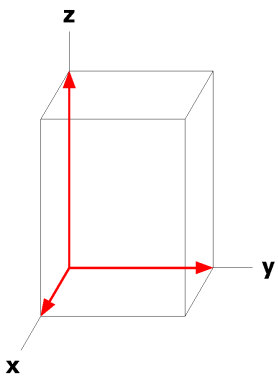
**Symmetry of Special Projections**

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0

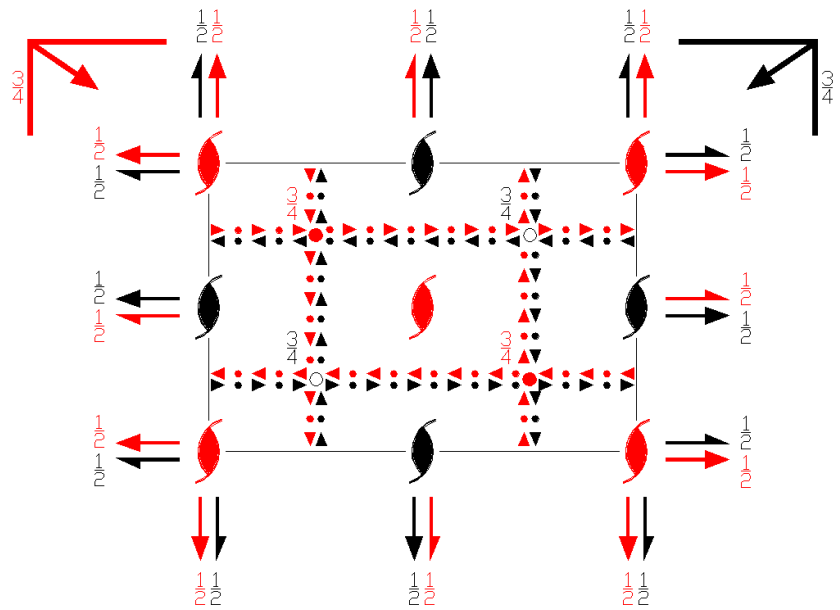
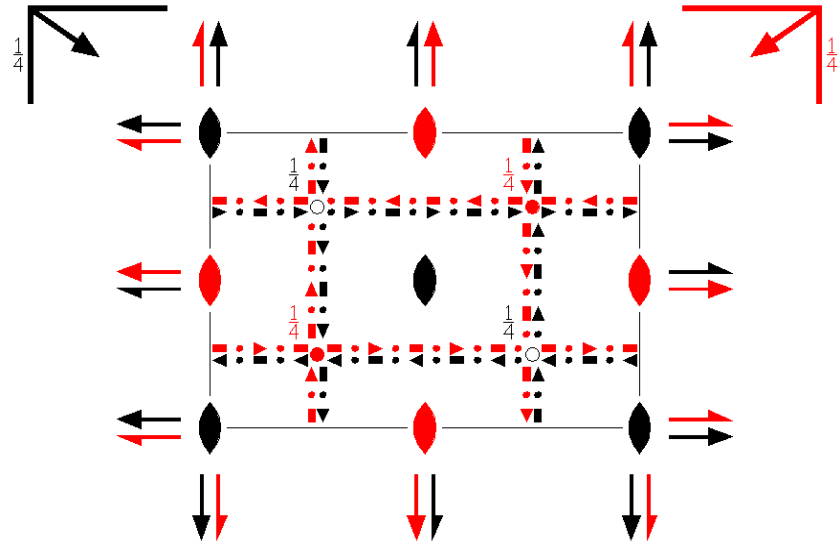
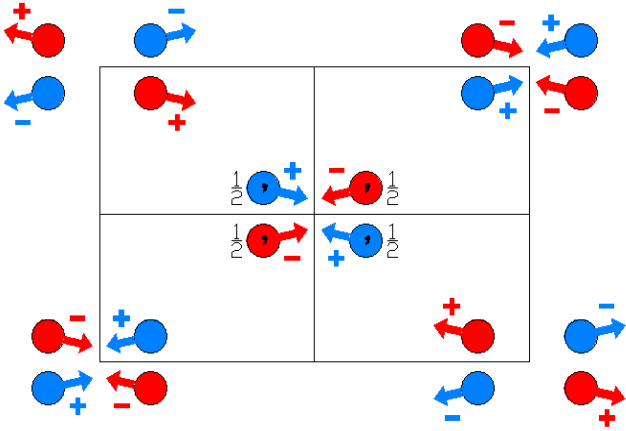




$P_F nnn$   
48.6.363

$mmm1'$   
 $P_F 2/n2/n2/n$

Orthorhombic



Origin at 222, at  $1/4, 1/4, 1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 2 0,y,0 (2 <sub>y</sub>  0,0,0)	(4) 2 x,0,0 (2 <sub>x</sub>  0,0,0)
(5) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$  1/2,1/2,1/2)	(6) n (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>  1/2,1/2,1/2)	(7) n (1/2,0,1/2) x,1/4,z (m <sub>y</sub>  1/2,1/2,1/2)	(8) n (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1/2)

For (1,0,0)' + set

(1) t' (1,0,0) (1 0,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 2' 1/2,y,0 (2 <sub>y</sub>  1,0,0)'	(4) 2' (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)'
(5) $\bar{1}$ ' 3/4,1/4,1/4 ( $\bar{1}$ ' 3/2,1/2,1/2)'	(6) n' (3/2,1/2,0) x,y,1/4 (m <sub>z</sub> ' 3/2,1/2,1/2)'	(7) n' (3/2,0,1/2) x,1/4,z (m <sub>y</sub> ' 3/2,1/2,1/2)'	(8) n' (0,1/2,1/2) 3/4,y,z (m <sub>x</sub> ' 3/2,1/2,1/2)'

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).**Positions**

		Coordinates			
		(0,0,0) +		(1,0,0)' +	
Multiplicity,	Wyckoff letter,	Site Symmetry.			
16	m 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [u,v,w]	(6) x+1/2,y+1/2, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) x+1/2, $\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z+1/2$ [u, $\bar{v},\bar{w}$ ]
8	l ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]
8	k ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]
8	j .2.	1/2,y,0 [0,v,0]	1/2, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]	0, $\bar{y}+1/2,1/2$ [0,v,0]	0,y+1/2,1/2 [0, $\bar{v}$ ,0]
8	i .2.	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]	1/2, $\bar{y}+1/2,1/2$ [0,v,0]	1/2,y+1/2,1/2 [0, $\bar{v}$ ,0]
8	h 2..	X,0,1/2 [u,0,0]	$\bar{x}$ ,0,1/2 [ $\bar{u}$ ,0,0]	$\bar{x}+1/2,1/2,0$ [u,0,0]	x+1/2,1/2,0 [ $\bar{u}$ ,0,0]
8	g 2..	X,0,0 [u,0,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0]	$\bar{x}+1/2,1/2,1/2$ [u,0,0]	x+1/2,1/2,1/2 [ $\bar{u}$ ,0,0]
8	f $\bar{1}$	3/4,3/4,3/4 [u,v,w]	1/4,1/4,3/4 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,1/4 [ $\bar{u},v,\bar{w}$ ]	3/4,1/4,1/4 [u, $\bar{v},\bar{w}$ ]
8	e $\bar{1}$	1/4,1/4,1/4 [u,v,w]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,3/4 [ $\bar{u},v,\bar{w}$ ]	1/4,3/4,3/4 [u, $\bar{v},\bar{w}$ ]
4	d 222	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
4	c 222	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
4	b 222	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]		

4 a 222 0,0,0 [0,0,0]

1/2,1/2,1/2 [0,0,0]

**Symmetry of Special Projections**Along [0,0,1]  $c2mm1'$  $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$ 

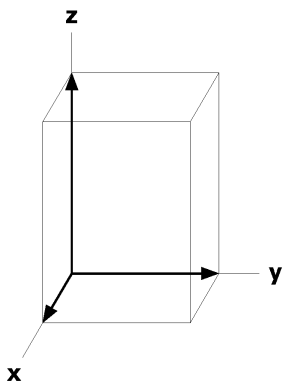
Origin at 0,0,z

Along [1,0,0]  $c2mm1'$  $\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}$ 

Origin at x,0,0

Along [0,1,0]  $c2mm1'$  $\mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{a}$ 

Origin at 0,y,0



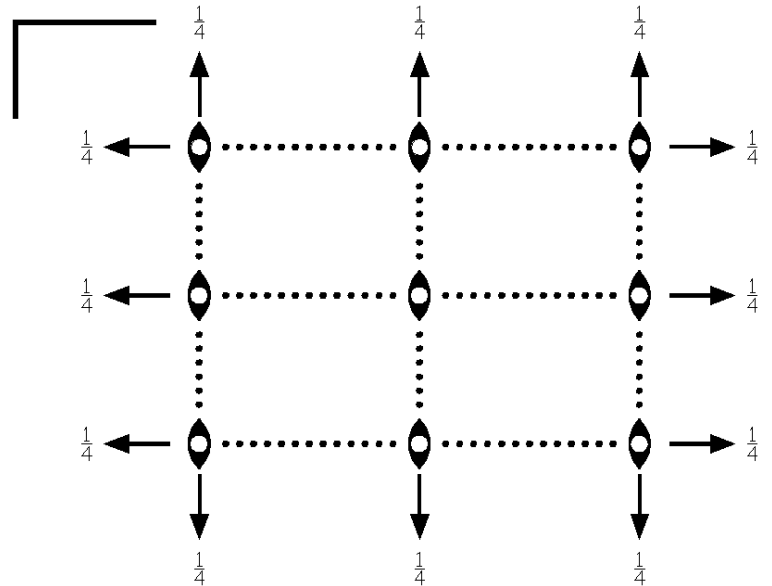
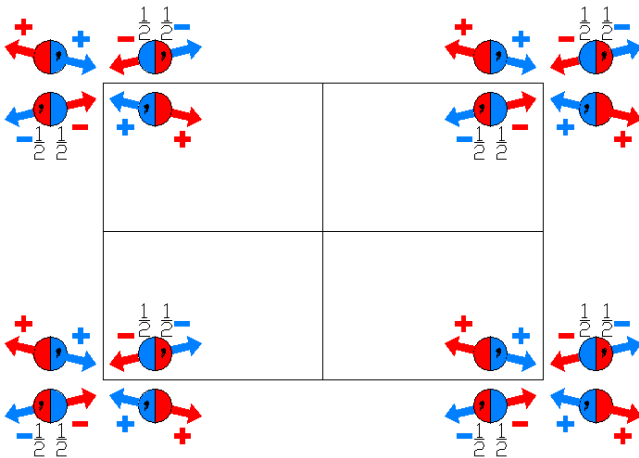
Pccm

49.1.364

mmm

P2/c2/c2/m

Orthorhombic



Origin at center ( 2/m ) at cc2/m

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 2 0,y,1/4  
(2<sub>y</sub>|0,0,1/2)

(4) 2 x,0,1/4  
(2<sub>x</sub>|0,0,1/2)

(5)  $\bar{1}$   
( $\bar{1}$ |0,0,0)

(6) m x,y,0  
(m<sub>z</sub>|0,0,0)

(7) c (0,0,1/2) x,0,z  
(m<sub>y</sub>|0,0,1/2)

(8) c (0,0,1/2) 0,y,z  
(m<sub>x</sub>|0,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

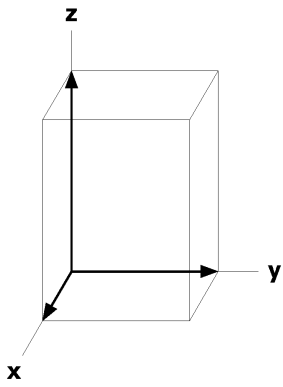
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	r 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
4	q ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	$x,\bar{y},1/2$ [0,0, $\bar{w}$ ]
4	p ..2	1/2,0,z [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]
4	o ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
4	n ..2	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]
4	m ..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]
4	l ..2	1/2,y,1/4 [0,v,0]	1/2, $\bar{y},1/4$ [0, $\bar{v},0$ ]	1/2, $\bar{y},3/4$ [0,v,0]	1/2,y,3/4 [0, $\bar{v},0$ ]
4	k ..2	0,y,1/4 [0,v,0]	0, $\bar{y},1/4$ [0, $\bar{v},0$ ]	0, $\bar{y},3/4$ [0,v,0]	0,y,3/4 [0, $\bar{v},0$ ]
4	j 2..	x,1/2,1/4 [u,0,0]	$\bar{x},1/2,1/4$ [ $\bar{u},0,0$ ]	$\bar{x},1/2,3/4$ [u,0,0]	x,1/2,3/4 [ $\bar{u},0,0$ ]
4	i 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	$\bar{x},0,3/4$ [u,0,0]	x,0,3/4 [ $\bar{u},0,0$ ]
2	h 222	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	g 222	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]		
2	f 222	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]		
2	e 222	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	d ..2/m	1/2,0,0 [0,0,w]	1/2,0,1/2 [0,0, $\bar{w}$ ]		
2	c ..2/m	0,1/2,0 [0,0,w]	0,1/2,1/2 [0,0, $\bar{w}$ ]		
2	b ..2/m	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		
2	a ..2/m	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a'}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a'}2m'm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pccm1'

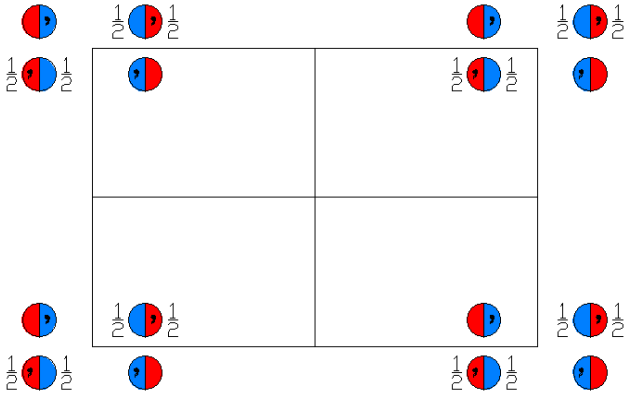
49.2.365

mmm1'

P2/c2/c2/m1'

Orthorhombic

1'



Origin at center ( 2/m1' ) at cc2/m1'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                      | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 2 <sub>y</sub> 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)            | (4) 2 <sub>x</sub> x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)            |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0)    | (6) m <sub>x</sub> x,y,0<br>(m <sub>x</sub>  0,0,0)    | (7) c <sub>z</sub> (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)    | (8) c <sub>y</sub> (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)    |
| (1) 1'<br>(1 0,0,0)'                    | (2) 2' <sub>z</sub> 0,0,z<br>(2' <sub>z</sub>  0,0,0)' | (3) 2' <sub>y</sub> 0,y,1/4<br>(2' <sub>y</sub>  0,0,1/2)'         | (4) 2' <sub>x</sub> x,0,1/4<br>(2' <sub>x</sub>  0,0,1/2)'         |
| (5) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)' | (6) m' <sub>x</sub> x,y,0<br>(m' <sub>x</sub>  0,0,0)' | (7) c' <sub>z</sub> (0,0,1/2) x,0,z<br>(m' <sub>y</sub>  0,0,1/2)' | (8) c' <sub>y</sub> (0,0,1/2) 0,y,z<br>(m' <sub>x</sub>  0,0,1/2)' |

For 1 + set

For 1' + set

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

### Positions

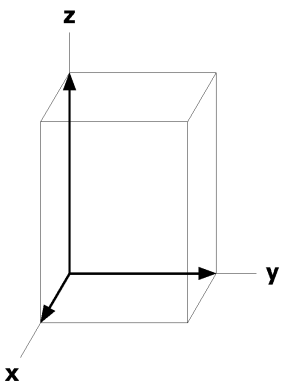
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +		1' +	
8 r 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{x},y,\bar{z}+1/2$ [0,0,0]	(4) $x,\bar{y},\bar{z}+1/2$ [0,0,0]
	(5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(6) $x,y,\bar{z}$ [0,0,0]	(7) $x,\bar{y},z+1/2$ [0,0,0]	(8) $\bar{x},y,z+1/2$ [0,0,0]
4 q ..m1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{x},y,1/2$ [0,0,0]	$x,\bar{y},1/2$ [0,0,0]
4 p ..21'	1/2,0,z [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	1/2,0,z+1/2 [0,0,0]
4 o ..21'	0,1/2,z [0,0,0]	0,1/2, $\bar{z}+1/2$ [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	0,1/2,z+1/2 [0,0,0]
4 n ..21'	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	1/2,1/2,z+1/2 [0,0,0]
4 m ..21'	0,0,z [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0,z+1/2 [0,0,0]
4 l .2.1'	1/2,y,1/4 [0,0,0]	1/2, $\bar{y},1/4$ [0,0,0]	1/2, $\bar{y},3/4$ [0,0,0]	1/2,y,3/4 [0,0,0]
4 k .2.1'	0,y,1/4 [0,0,0]	0, $\bar{y},1/4$ [0,0,0]	0, $\bar{y},3/4$ [0,0,0]	0,y,3/4 [0,0,0]
4 j 2..1'	x,1/2,1/4 [0,0,0]	$\bar{x},1/2,1/4$ [0,0,0]	$\bar{x},1/2,3/4$ [0,0,0]	x,1/2,3/4 [0,0,0]
4 i 2..1'	x,0,1/4 [0,0,0]	$\bar{x},0,1/4$ [0,0,0]	$\bar{x},0,3/4$ [0,0,0]	x,0,3/4 [0,0,0]
2 h 2221'	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2 g 2221'	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]		
2 f 2221'	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]		
2 e 2221'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2 d ..2/m1'	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2 c ..2/m1'	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
2 b ..2/m1'	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2 a ..2/m1'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

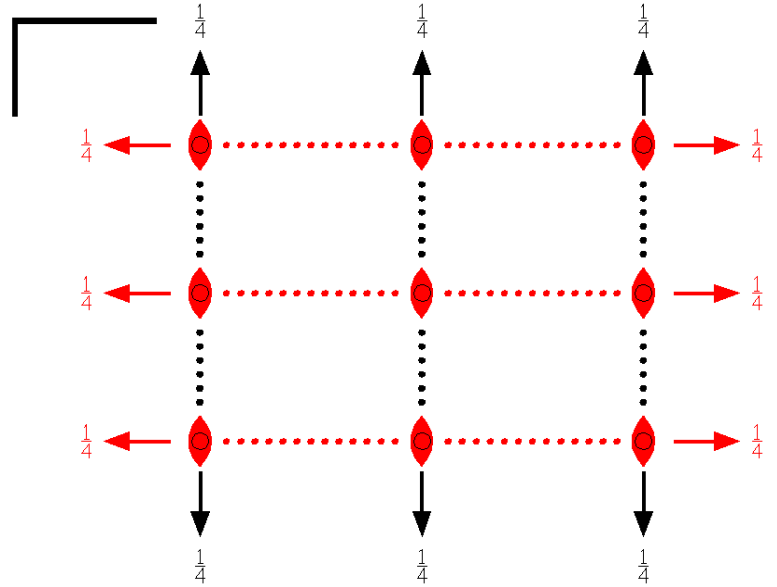
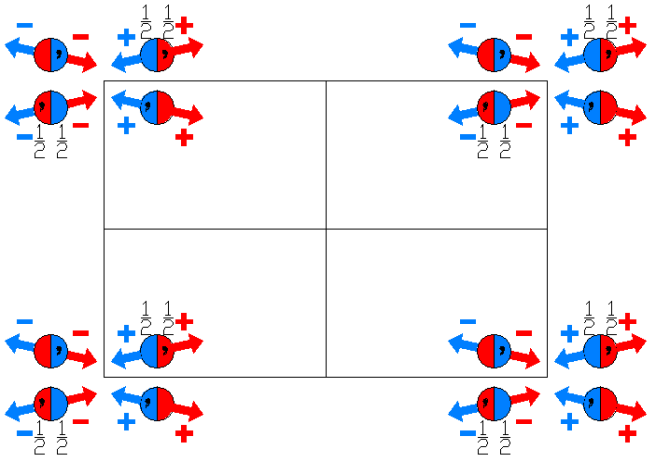
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pc'cm  
49.3.366

m'mm  
P2/c'2'/c2'/m

Orthorhombic



**Origin** at center ( 2'/m ) at c'c2'/m

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                      | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'       | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)           |
| (5) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)' | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0)   | (7) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (8) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

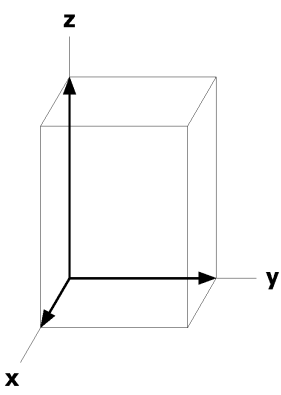
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	r 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
4	q ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
4	p ..2'	1/2,0,z [u,v,0]	1/2,0, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	1/2,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/2,0,z+1/2 [ $\bar{u},v,0$ ]
4	o ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	0,1/2, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	0,1/2,z+1/2 [ $\bar{u},v,0$ ]
4	n ..2'	1/2,1/2,z [u,v,0]	1/2,1/2, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	1/2,1/2, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/2,1/2,z+1/2 [ $\bar{u},v,0$ ]
4	m ..2'	0,0,z [u,v,0]	0,0, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	0,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	0,0,z+1/2 [ $\bar{u},v,0$ ]
4	l ..2'	1/2,y,1/4 u,0,w]	1/2, $\bar{y},1/4$ [u,0, $\bar{w}$ ]	1/2, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,3/4 [ $\bar{u},0,w$ ]
4	k ..2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [u,0, $\bar{w}$ ]	0, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	0,y,3/4 [ $\bar{u},0,w$ ]
4	j 2..	x,1/2,1/4 [u,0,0]	$\bar{x},1/2,1/4$ [u,0,0]	$\bar{x},1/2,3/4$ [ $\bar{u},0,0$ ]	x,1/2,3/4 [ $\bar{u},0,0$ ]
4	i 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [u,0,0]	$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [ $\bar{u},0,0$ ]
2	h 22'2'	1/2,1/2,1/4 [u,0,0]	1/2,1/2,3/4 [ $\bar{u},0,0$ ]		
2	g 22'2'	0,1/2,1/4 [u,0,0]	0,1/2,3/4 [ $\bar{u},0,0$ ]		
2	f 22'2'	1/2,0,1/4 [u,0,0]	1/2,0,3/4 [ $\bar{u},0,0$ ]		
2	e 22'2'	0,0,1/4 [u,0,0]	0,0,3/4 [ $\bar{u},0,0$ ]		
2	d ..2'/m	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	c ..2'/m	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	b ..2'/m	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a ..2'/m	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

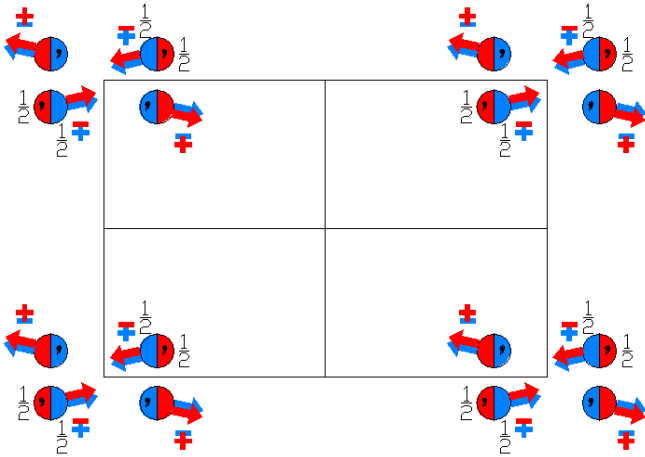
Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pccm'  
49.4.367

mmm'  
P2'/c2'/c2/m'

Orthorhombic

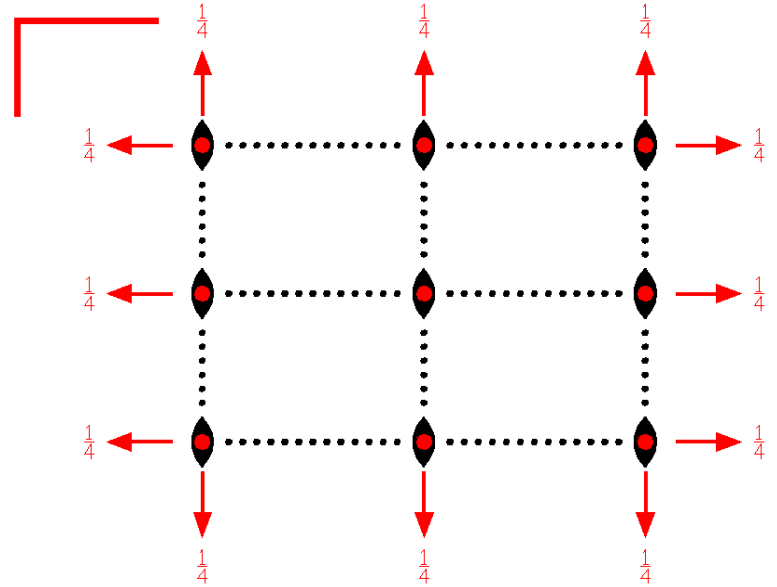


Origin at center ( $2/m'$ ) at  $cc2/m'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'       | (4) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'       |
| (5) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (8) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

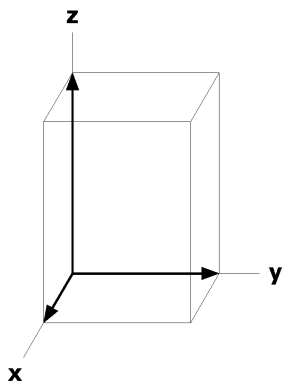
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	r 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(4) $x,\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(7) $x,\bar{y},z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(8) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
4	q ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [ $\bar{u},\bar{v},0$ ]	$x,\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]
4	p ..2	1/2,0,z [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]
4	o ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
4	n ..2	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]
4	m ..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]
4	l .2'	1/2,y,1/4 [u,0,w]	1/2, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	1/2, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,3/4 [u,0, $\bar{w}$ ]
4	k .2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	0, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	0,y,3/4 [u,0, $\bar{w}$ ]
4	j 2'..	x,1/2,1/4 [0,v,w]	$\bar{x},1/2,1/4$ [0, $\bar{v},w$ ]	$\bar{x},1/2,3/4$ [0,v, $\bar{w}$ ]	x,1/2,3/4 [0, $\bar{v},\bar{w}$ ]
4	i 2'..	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	$\bar{x},0,3/4$ [0,v, $\bar{w}$ ]	x,0,3/4 [0, $\bar{v},\bar{w}$ ]
2	h 2'2'2	1/2,1/2,1/4 [0,0,w]	1/2,1/2,3/4 [0,0, $\bar{w}$ ]		
2	g 2'2'2	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0, $\bar{w}$ ]		
2	f 2'2'2	1/2,0,1/4 [0,0,w]	1/2,0,3/4 [0,0, $\bar{w}$ ]		
2	e 2'2'2	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		
2	d ..2/m'	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	c ..2/m'	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	b ..2/m'	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a ..2/m'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a^*}2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

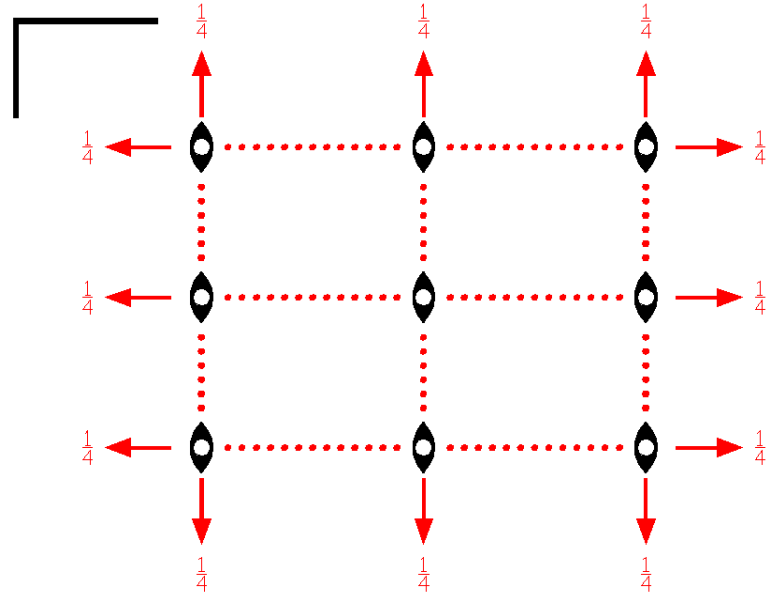
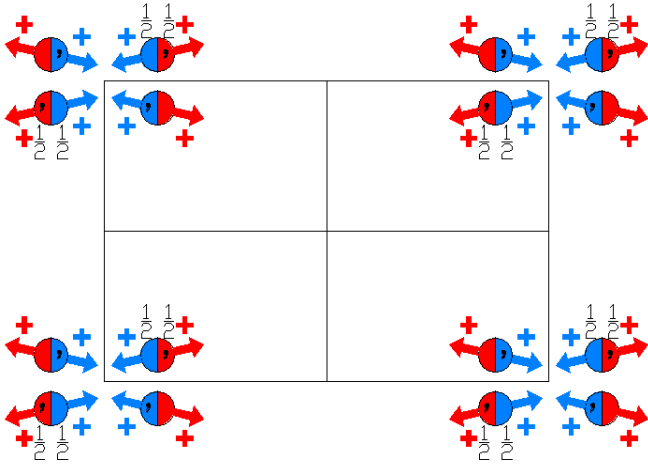
Along [0,1,0]  $p_{2a^*}2'mm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pc'c'm  
49.5.368

m'm'm  
P2'/c'2'/c'2'/m

Orthorhombic



Origin at center (2/m) at c'c'2'/m

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) 1<br>(1 0,0,0)                   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'         | (4) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'         |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (8) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

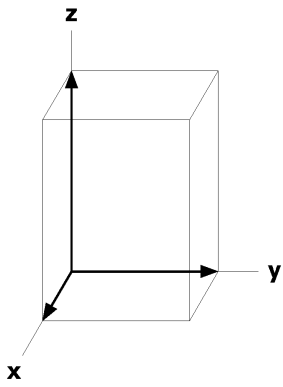
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	r 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(4) $x,\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(8) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
4	q ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,1/2$ [0,0,w]	$x,\bar{y},1/2$ [0,0,w]
4	p ..2	1/2,0,z [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	1/2,0,z+1/2 [0,0,w]
4	o ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	0,1/2,z+1/2 [0,0,w]
4	n ..2	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2,z+1/2 [0,0,w]
4	m ..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0,w]
4	l .2'	1/2,y,1/4 [u,0,w]	1/2, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	1/2, $\bar{y},3/4$ [u,0,w]	1/2,y,3/4 [ $\bar{u},0,w$ ]
4	k .2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	0, $\bar{y},3/4$ [u,0,w]	0,y,3/4 [ $\bar{u},0,w$ ]
4	j 2'..	x,1/2,1/4 [0,v,w]	$\bar{x},1/2,1/4$ [0, $\bar{v},w$ ]	$\bar{x},1/2,3/4$ [0,v,w]	x,1/2,3/4 [0, $\bar{v},w$ ]
4	i 2'..	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	$\bar{x},0,3/4$ [0,v,w]	x,0,3/4 [0, $\bar{v},w$ ]
2	h 2'2'2	1/2,1/2,1/4 [0,0,w]	1/2,1/2,3/4 [0,0,w]		
2	g 2'2'2	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0,w]		
2	f 2'2'2	1/2,0,1/4 [0,0,w]	1/2,0,3/4 [0,0,w]		
2	e 2'2'2	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		
2	d ..2/m	1/2,0,0 [0,0,w]	1/2,0,1/2 [0,0,w]		
2	c ..2/m	0,1/2,0 [0,0,w]	0,1/2,1/2 [0,0,w]		
2	b ..2/m	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]		
2	a ..2/m	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

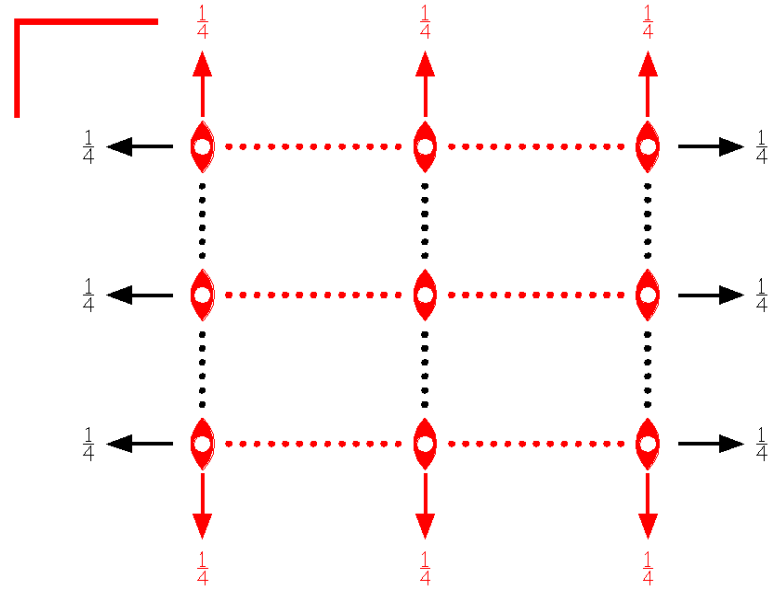
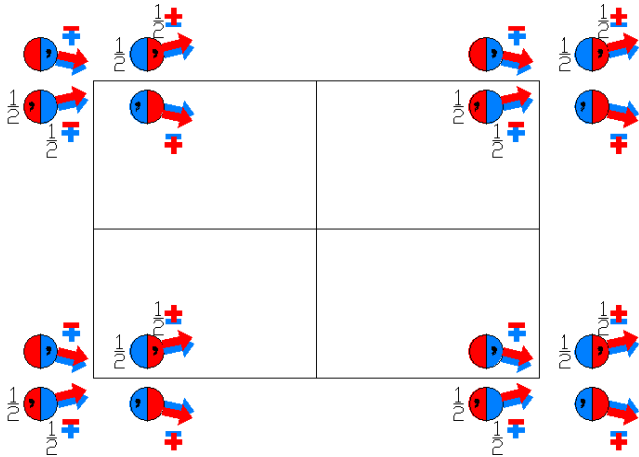
Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pc'cm'  
49.6.369

m'mm'  
P2'/c'2/c2'/m'

Orthorhombic



**Origin** at center ( $2'/m'$ ) at  $c'c2'/m'$

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |                                      |                                      |   |   |
|--------------------------------------|--------------------------------------|---|---|
| (1) 1<br>(1 0,0,0)                   | (2) $2'_z$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $2_{yz}$ 0,y,1/4<br>( $2_y$  0,0,1/2)         | (4) $2'_{xz}$ x,0,1/4<br>( $2_x$  0,0,1/2)'         |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) $m'_x$ x,y,0<br>( $m_z$  0,0,0)' | (7) $c_{yz}$ (0,0,1/2) x,0,z<br>( $m_y$  0,0,1/2) | (8) $c'_{xz}$ (0,0,1/2) 0,y,z<br>( $m_x$  0,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

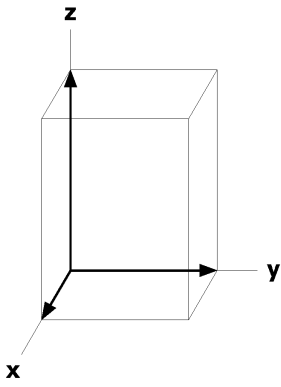
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	r 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
4	q ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [u,v,0]	$\bar{x},y,1/2$ [ $\bar{u},v,0$ ]]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]
4	p ..2'	1/2,0,z [u,v,0]	1/2,0, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	1/2,0, $\bar{z}$ [u,v,0]	1/2,0,z+1/2 [ $\bar{u},v,0$ ]
4	o ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	0,1/2, $\bar{z}$ [u,v,0]	0,1/2,z+1/2 [ $\bar{u},v,0$ ]
4	n ..2'	1/2,1/2,z [u,v,0]	1/2,1/2, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	1/2,1/2, $\bar{z}$ [u,v,0]	1/2,1/2,z+1/2 [ $\bar{u},v,0$ ]
4	m ..2'	0,0,z [u,v,0]	0,0, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	0,0, $\bar{z}$ [u,v,0]	0,0,z+1/2 [ $\bar{u},v,0$ ]
4	l ..2.	1/2,y,1/4 [0,v,0]	1/2, $\bar{y},1/4$ [0,v,0]	1/2, $\bar{y},3/4$ [0,v,0]	1/2,y,3/4 [0,v,0]
4	k ..2.	0,y,1/4 [0,v,0]	0, $\bar{y},1/4$ [0,v,0]	0, $\bar{y},3/4$ [0,v,0]	0,y,3/4 [0,v,0]
4	j 2'..	x,1/2,1/4 [0,v,w]	$\bar{x},1/2,1/4$ [0,v, $\bar{w}$ ]	$\bar{x},1/2,3/4$ [0,v,w]	x,1/2,3/4 [0,v, $\bar{w}$ ]
4	i 2'..	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0,v, $\bar{w}$ ]	$\bar{x},0,3/4$ [0,v,w]	x,0,3/4 [0,v, $\bar{w}$ ]
2	h 2'22'	1/2,1/2,1/4 [0,v,0]	1/2,1/2,3/4 [0,v,0]		
2	g 2'22'	0,1/2,1/4 [0,v,0]	0,1/2,3/4 [0,v,0]		
2	f 2'22'	1/2,0,1/4 [0,v,0]	1/2,0,3/4 [0,v,0]		
2	e 2'22'	0,0,1/4 [0,v,0]	0,0,3/4 [0,v,0]		
2	d ..2'/m'	1/2,0,0 [u,v,0]	1/2,0,1/2 [ $\bar{u},v,0$ ]]		
2	c ..2'/m'	0,1/2,0 [u,v,0]	0,1/2,1/2 [ $\bar{u},v,0$ ]		
2	b ..2'/m'	1/2,1/2,0 [u,v,0]	1/2,1/2,1/2 [ $\bar{u},v,0$ ]		
2	a ..2'/m'	0,0,0 [u,v,0]	0,0,1/2 [ $\bar{u},v,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = -\mathbf{c}/2$   
 Origin at x,0,0

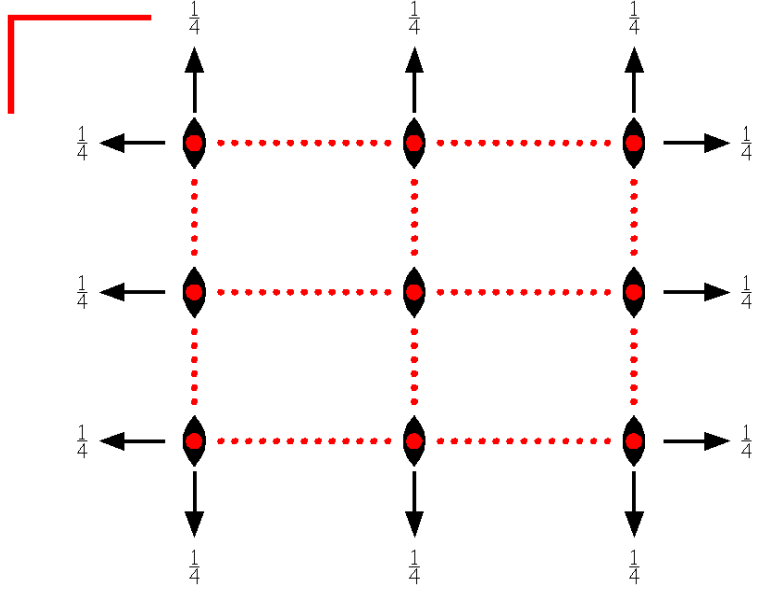
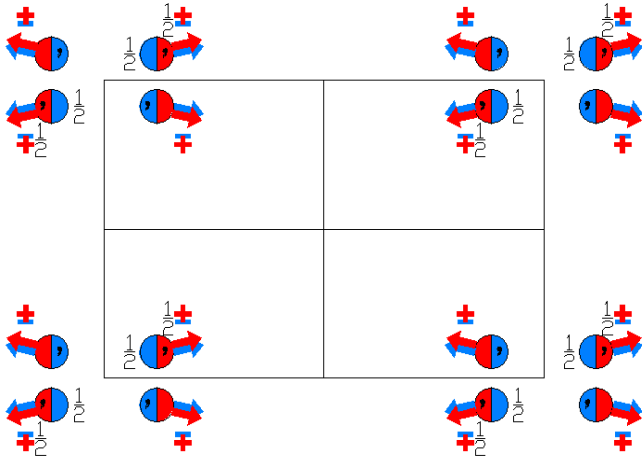
Along [0,1,0] p<sub>2a'</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pc'c'm'  
49.7.370

m'm'm'  
P2/c'2/c'2/m'

Orthorhombic



Origin at center ( 2/m' ) at c'c'2/m'

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

- (1) 1  
(1|0,0,0)
- (2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)
- (3) 2 0,y,1/4  
(2<sub>y</sub>|0,0,1/2)
- (4) 2 x,0,1/4  
(2<sub>x</sub>|0,0,1/2)
- (5)  $\bar{1}'$   
( $\bar{1}$ |0,0,0)'
- (6) m' x,y,0  
(m<sub>z</sub>|0,0,0)'
- (7) c' (0,0,1/2) x,0,z  
(m<sub>y</sub>|0,0,1/2)'
- (8) c' (0,0,1/2) 0,y,z  
(m<sub>x</sub>|0,0,1/2)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

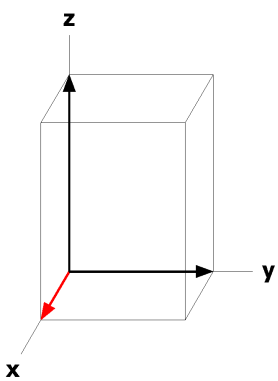
		Coordinates				
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	r	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ]
			(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) x, $\bar{y},\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ]	(8) $\bar{x},\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]
4	q	..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	x, $\bar{y},1/2$ [u, $\bar{v},0$ ]
4	p	..2	1/2,0,z [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0,w]
4	o	..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0,w]
4	n	..2	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0,w]
4	m	..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]
4	l	..2	1/2,y,1/4 [0,v,0]	1/2, $\bar{y},1/4$ [0, $\bar{v},0$ ]	1/2, $\bar{y},3/4$ [0, $\bar{v},0$ ]	1/2,y,3/4 [0,v,0]
4	k	..2	0,y,1/4 [0,v,0]	0, $\bar{y},1/4$ [0, $\bar{v},0$ ]	0, $\bar{y},3/4$ [0, $\bar{v},0$ ]	0,y,3/4 [0,v,0]
4	j	2..	x,1/2,1/4 [u,0,0]	$\bar{x},1/2,1/4$ [ $\bar{u},0,0$ ]	$\bar{x},1/2,3/4$ [ $\bar{u},0,0$ ]	x,1/2,3/4 [u,0,0]
4	i	2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [u,0,0]
2	h	222	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	g	222	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]		
2	f	222	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]		
2	e	222	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	d	..2/m'	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	c	..2/m'	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	b	..2/m'	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a	..2/m'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



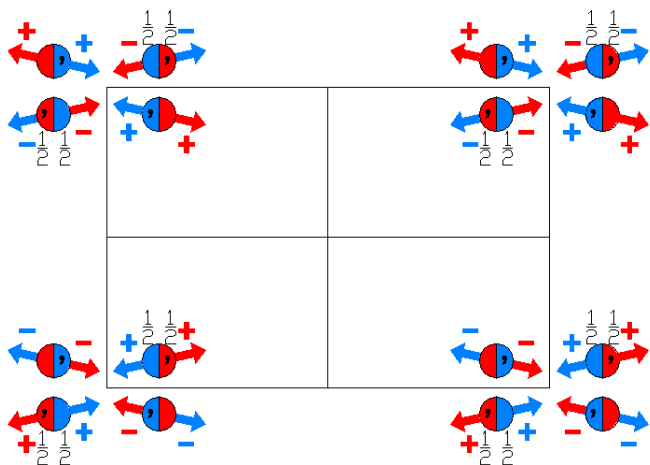
$P_{2a} ccm$

49.8.371

$mmm1'$

$P_{2a} 2/c2/c2/m$

Orthorhombic



**Origin** at center ( $2/m$ ) at  $cc2/m$

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

(1) 1  
(1 | 0,0,0)

(2) 2  $0,0,z$   
( $2_z$  | 0,0,0)

(3) 2  $0,y,1/4$   
( $2_y$  | 0,0,1/2)

(4) 2  $x,0,1/4$   
( $2_x$  | 0,0,1/2)

(5)  $\bar{1}$   
( $\bar{1}$  | 0,0,0)

(6) m  $x,y,0$   
( $m_z$  | 0,0,0)

(7) c  $(0,0,1/2)$   $x,0,z$   
( $m_y$  | 0,0,1/2)

(8) c  $(0,0,1/2)$   $0,y,z$   
( $m_x$  | 0,0,1/2)

For (0,0,0) + set

For (1,0,0)' + set

(1)  $t'$  (1,0,0)  
(1 | 1,0,0)'

(2)  $2'$   $1/2,0,z$   
( $2_z$  | 1,0,0)'

(3)  $2'$   $1/2,y,1/4$   
( $2_y$  | 1,0,1/2)'

(4)  $2'$  (1,0,0)  $x,0,1/4$   
( $2_x$  | 1,0,1/2)'

(5)  $\bar{1}'$   $1/2,0,0$   
( $\bar{1}$  | 1,0,0)'

(6)  $a'$  (1,0,0)  $x,y,0$   
( $m_z$  | 1,0,0)'

(7)  $n'$  (1,0,1/2)  $x,0,z$   
( $m_y$  | 1,0,1/2)'

(8)  $c'$  (0,0,1/2)  $1/2,y,z$   
( $m_x$  | 1,0,1/2)'

**Generators selected** (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

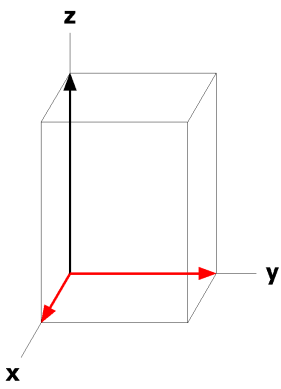
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 r 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(6) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
8 q ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	$x,\bar{y},1/2$ [0,0, $\bar{w}$ ]
8 p ..2'	1/2,0,z [u,v,0]	1/2,0, $\bar{z}+1/2$ [ $u,\bar{v},0$ ]	1/2,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/2,0,z+1/2 [ $\bar{u},v,0$ ]
8 o ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
8 n ..2'	1/2,1/2,z [u,v,0]	1/2,1/2, $\bar{z}+1/2$ [ $u,\bar{v},0$ ]	1/2,1/2, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/2,1/2,z+1/2 [ $\bar{u},v,0$ ]
8 m ..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]
8 l ..2'	1/2,y,1/4 [u,0,w]	1/2, $\bar{y},1/4$ [ $u,0,\bar{w}$ ]	1/2, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,3/4 [ $\bar{u},0,w$ ]
8 k ..2	0,y,1/4 [0,v,0]	0, $\bar{y},1/4$ [0, $\bar{v},0$ ]	0, $\bar{y},3/4$ [0,v,0]	0,y,3/4 [0, $\bar{v},0$ ]
8 j 2..	x,1/2,1/4 [u,0,0]	$\bar{x},1/2,1/4$ [ $\bar{u},0,0$ ]	$\bar{x},1/2,3/4$ [u,0,0]	x,1/2,3/4 [ $\bar{u},0,0$ ]
8 i 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	$\bar{x},0,3/4$ [u,0,0]	x,0,3/4 [ $\bar{u},0,0$ ]
4 h 222	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
4 g 222	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]		
4 f 222	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]		
4 e 222	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
4 d ..2'/m	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 c ..2/m'	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 b ..2'/m	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a ..2/m'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



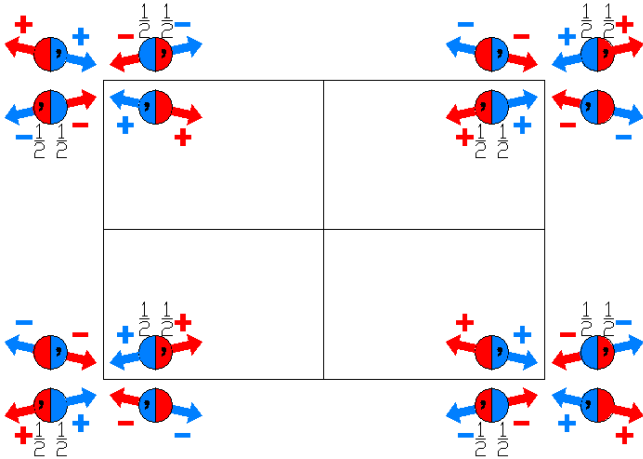
$P_C$  ccm

49.9.372

mmm1'

$P_C 2/c2/c2/m$

Orthorhombic

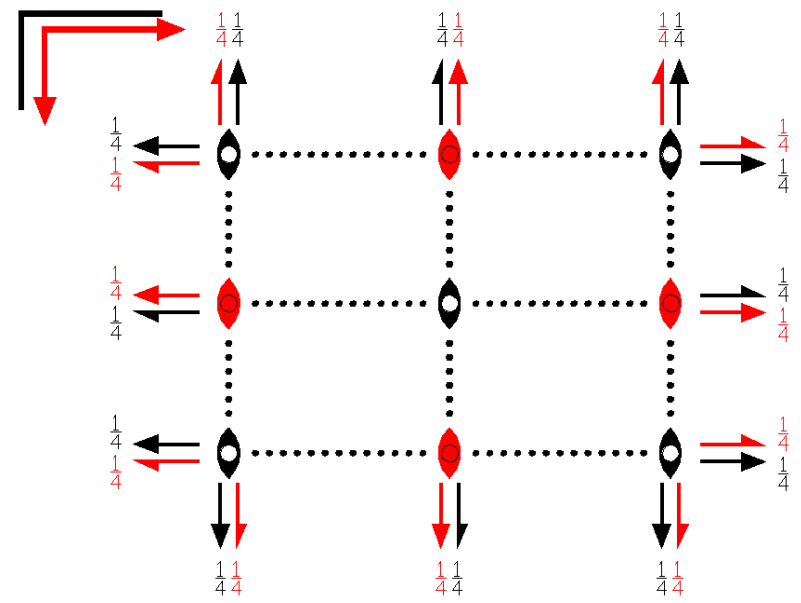


**Origin** at center ( $2/m$ ) at  $cc2/m$

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |                                      |                                  |  |  |
|--------------------------------------|----------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) 2 $0,y,1/4$<br>( $2_y$  0,0,1/2)         | (4) 2 $x,0,1/4$<br>( $2_x$  0,0,1/2)         |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) m $x,y,0$<br>( $m_z$  0,0,0) | (7) c (0,0,1/2) $x,0,z$<br>( $m_y$  0,0,1/2) | (8) c (0,0,1/2) $0,y,z$<br>( $m_x$  0,0,1/2) |
- 
- |   |  |  |  |
|---|--|--|--|
| (1) $t'$ (1,0,0)<br>(1 1,0,0)'                    | (2) $2'$ $1/2,0,z$<br>( $2_z$  1,0,0)'       | (3) $2'$ $1/2,y,1/4$<br>( $2_y$  1,0,1/2)'       | (4) $2'$ (1,0,0) $x,0,1/4$<br>( $2_x$  1,0,1/2)'   |
| (5) $\bar{1}'$ $1/2,0,0$<br>( $\bar{1}'$  1,0,0)' | (6) $a'$ (1,0,0) $x,y,0$<br>( $m_z$  1,0,0)' | (7) $n'$ (1,0,1/2) $x,0,z$<br>( $m_y$  1,0,1/2)' | (8) $c'$ (0,0,1/2) $1/2,y,z$<br>( $m_x$  1,0,1/2)' |



**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

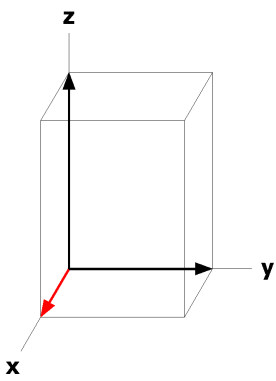
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 r 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
8 q ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	$x,\bar{y},1/2$ [0,0, $\bar{w}$ ]
8 p ..2'	1/2,0,z [u,v,0]	1/2,0, $\bar{z}+1/2$ [ $u,\bar{v},0$ ]	1/2,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/2,0,z+1/2 [ $\bar{u},v,0$ ]
8 o ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	0,1/2, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	0,1/2,z+1/2 [ $u,\bar{v},0$ ]
8 n ..2	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2,z+1/2 [0,0,w]
8 m ..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]
8 l ..2'	1/2,y,1/4 [u,0,w]	1/2, $\bar{y},1/4$ [ $u,0,\bar{w}$ ]	1/2, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,3/4 [ $\bar{u},0,w$ ]
8 k ..2	0,y,1/4 [0,v,0]	0, $\bar{y},1/4$ [0, $\bar{v},0$ ]	0, $\bar{y},3/4$ [0,v,0]	0,y,3/4 [0, $\bar{v},0$ ]
8 j 2'..	x,1/2,1/4 [0,v,w]	$\bar{x},1/2,1/4$ [0,v, $\bar{w}$ ]	$\bar{x},1/2,3/4$ [0, $\bar{v},\bar{w}$ ]	x,1/2,3/4 [0, $\bar{v},w$ ]
8 i 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	$\bar{x},0,3/4$ [u,0,0]	x,0,3/4 [ $\bar{u},0,0$ ]
4 h 2'2'2	1/2,1/2,1/4 [0,0,w]	1/2,1/2,3/4 [0,0,w]		
4 g 2'22'	0,1/2,1/4 [0,v,0]	0,1/2,3/4 [0, $\bar{v},0$ ]		
4 f 22'2'	1/2,0,1/4 [u,0,0]	1/2,0,3/4 [ $\bar{u},0,0$ ]		
4 e 222	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
4 d ..2'/m	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 c ..2'/m	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 b ..2'/m	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]		
4 a ..2'/m	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



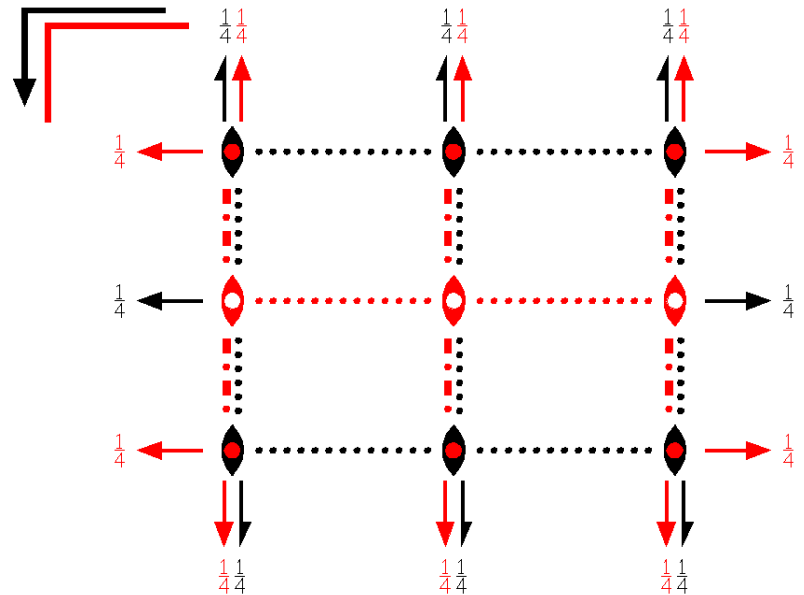
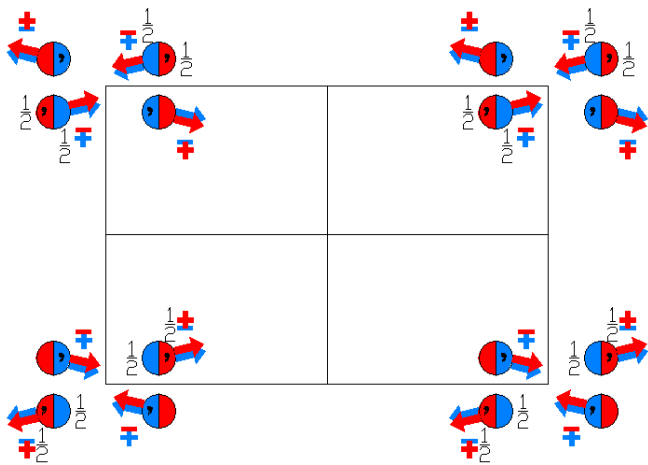
$P_{2a} ccm'$

49.10.373

$mmm1'$

$P_{2a} 2'/c2'/c2/m'$

Orthorhombic



**Origin** at center ( $2/m'$ ) at  $cc2/m'$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'       | (4) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'       |
| (5) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (8) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) |
- 
- |  |  |  |  |
|--|--|--|--|
| For (1,0,0)' + set                           |  |  |  |
| (1) t' (1,0,0)<br>(1 1,0,0)'                 | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'     | (3) 2 1/2,y,1/4<br>(2 <sub>y</sub>  1,0,1/2)         | (4) 2 (1,0,0) x,0,1/4<br>(2 <sub>x</sub>  1,0,1/2)     |
| (5) $\bar{1}$ 1/2,0,0<br>( $\bar{1}$  1,0,0) | (6) a (1,0,0) x,y,0<br>(m <sub>z</sub>  1,0,0) | (7) n' (1,0,1/2) x,0,z<br>(m <sub>y</sub>  1,0,1/2)' | (8) c' (0,0,1/2) 1/2,y,z<br>(m <sub>x</sub>  1,0,1/2)' |

**Generators selected** (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

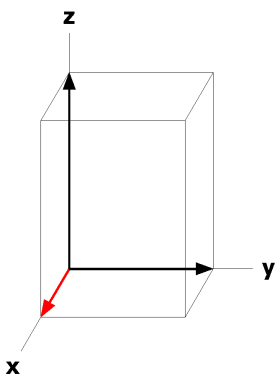
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z+1/2$ [u, $\bar{v},\bar{w}$ ]
8 q ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [u, $\bar{v},0$ ]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]
8 p ..2'	1/2,0,z [u,v,0]	1/2,0, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	1/2,0, $\bar{z}$ [u,v,0]	1/2,0,z+1/2 [ $\bar{u},v,0$ ]
8 o ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
8 n ..2'	1/2,1/2,z [u,v,0]	1/2,1/2, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	1/2,1/2, $\bar{z}$ [u,v,0]	1/2,1/2,z+1/2 [ $\bar{u},v,0$ ]
8 m ..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]
8 l ..2.	1/2,y,1/4 [0,v,0]	1/2, $\bar{y},1/4$ [0,v,0]	1/2, $\bar{y},3/4$ [0,v,0]	1/2,y,3/4 [0,v,0]
8 k ..2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	0, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	0,y,3/4 [u,0, $\bar{w}$ ]
8 j 2'..	x,1/2,1/4 [0,v,w]	$\bar{x},1/2,1/4$ [0, $\bar{v},w$ ]	$\bar{x},1/2,3/4$ [0, $\bar{v},\bar{w}$ ]	x,1/2,3/4 [0,v, $\bar{w}$ ]
8 i 2'..	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	$\bar{x},0,3/4$ [0, $\bar{v},\bar{w}$ ]	x,0,3/4 [0,v, $\bar{w}$ ]
4 h 2'22'	1/2,1/2,1/4 [0,v,0]	1/2,1/2,3/4 [0,v,0]		
4 g 2'2'2	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0, $\bar{w}$ ]		
4 f 2'22'	1/2,0,1/4 [0,v,0]	1/2,0,3/4 [0,v,0]		
4 e 2'2'2	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		
4 d ..2'/m'	1/2,0,0 [u,v,0]	1/2,0,1/2 [ $\bar{u},v,0$ ]		
4 c ..2/m'	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 b ..2'/m'	1/2,1/2,0 [u,v,0]	1/2,1/2,1/2 [ $\bar{u},v,0$ ]		
4 a ..2/m'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2mm</sub>1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 1/2,y,0



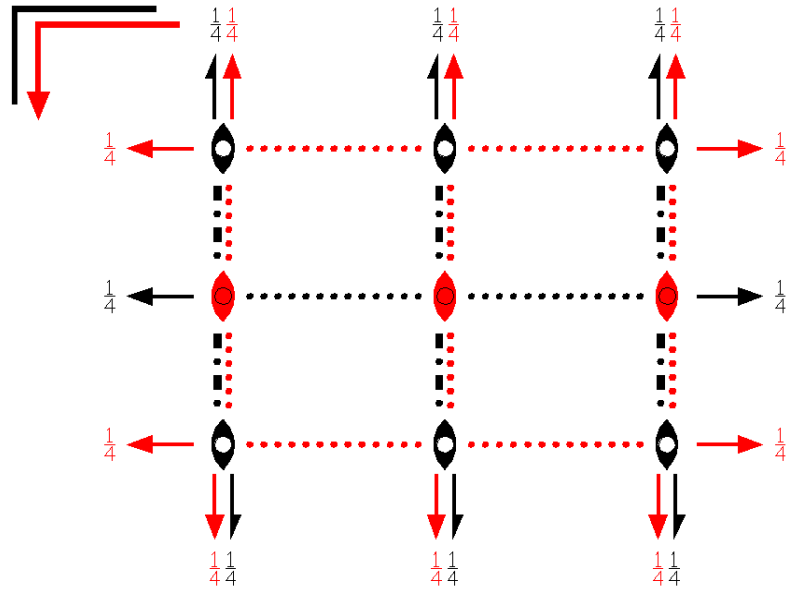
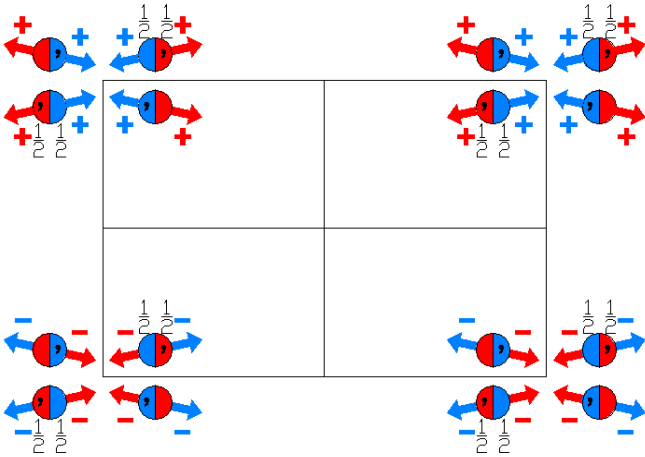
$P_{2a} c'c'm$

49.11.374

$mmm1'$

$P_{2a} 2'/c'2'/c'2'/m$

Orthorhombic



**Origin** at center ( $2/m$ ) at  $c'c'2'/m$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) 1<br>(1 0,0,0)                   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'         | (4) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'         |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (8) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |
- 
- |  |   |   |   |
|--|---|---|---|
| For (1,0,0)' + set                               |   |   |   |
| (1) t' (1,0,0)<br>(1 1,0,0)'                     | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'        | (3) 2 1/2,y,1/4<br>(2 <sub>y</sub>  1,0,1/2)        | (4) 2 (1,0,0) x,0,1/4<br>(2 <sub>x</sub>  1,0,1/2)    |
| (5) $\bar{1}$ ' 1/2,0,0<br>( $\bar{1}$ ' 1,0,0)' | (6) a' (1,0,0) x,y,0<br>(m <sub>z</sub> ' 1,0,0)' | (7) n (1,0,1/2) x,0,z<br>(m <sub>y</sub> ' 1,0,1/2) | (8) c (0,0,1/2) 1/2,y,z<br>(m <sub>x</sub> ' 1,0,1/2) |



**Generators selected** (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

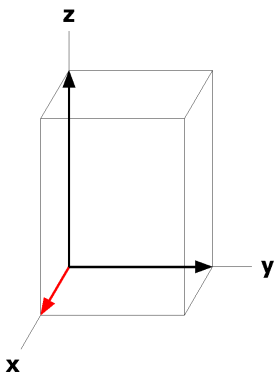
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
8 q ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0,w]
8 p ..2'	1/2,0,z [u,v,0]	1/2,0, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	1/2,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/2,0,z+1/2 [u, $\bar{v},0$ ]
8 o ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	0,1/2,z+1/2 [0,0,w]
8 n ..2'	1/2,1/2,z [u,v,0]	1/2,1/2, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	1/2,1/2, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/2,1/2,z+1/2 [u, $\bar{v},0$ ]
8 m ..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0,w]
8 l ..2.	1/2,y,1/4 [0,v,0]	1/2, $\bar{y},1/4$ [0,v,0]	1/2, $\bar{y},3/4$ [0, $\bar{v},0$ ]	1/2,y,3/4 [0, $\bar{v},0$ ]
8 k ..2'.	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	0, $\bar{y},3/4$ [u,0,w]	0,y,3/4 [ $\bar{u},0,w$ ]
8 j 2'..	x,1/2,1/4 [0,v,w]	$\bar{x},1/2,1/4$ [0, $\bar{v},w$ ]	$\bar{x},1/2,3/4$ [0,v,w]	x,1/2,3/4 [0, $\bar{v},w$ ]
8 i 2'..	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	$\bar{x},0,3/4$ [0,v,w]	x,0,3/4 [0, $\bar{v},w$ ]
4 h 2'22'	1/2,1/2,1/4 [0,v,0]	1/2,1/2,3/4 [0, $\bar{v},0$ ]		
4 g 2'2'2	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0,w]		
4 f 2'22'	1/2,0,1/4 [0,v,0]	1/2,0,3/4 [0, $\bar{v},0$ ]		
4 e 2'2'2	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		
4 d ..2'/m	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 c ..2/m	0,1/2,0 [0,0,w]	0,1/2,1/2 [0,0,w]		
4 b ..2'/m	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a ..2/m	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2b</sub>2mm  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



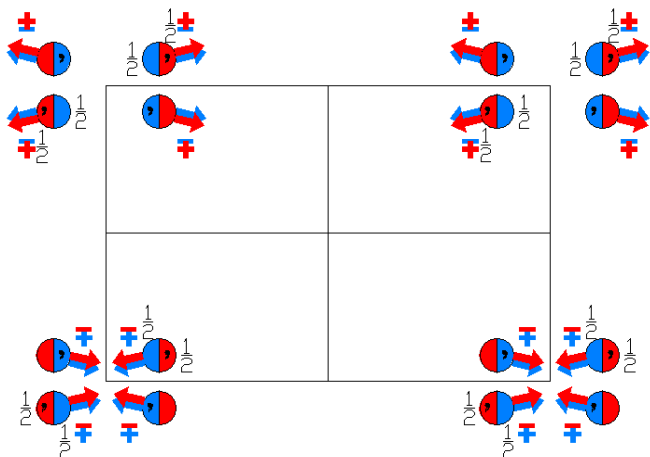
$P_{2a} c'c'm'$

49.12.375

$mmm1'$

$P_{2a} 2/c'2/c'2/m'$

Orthorhombic

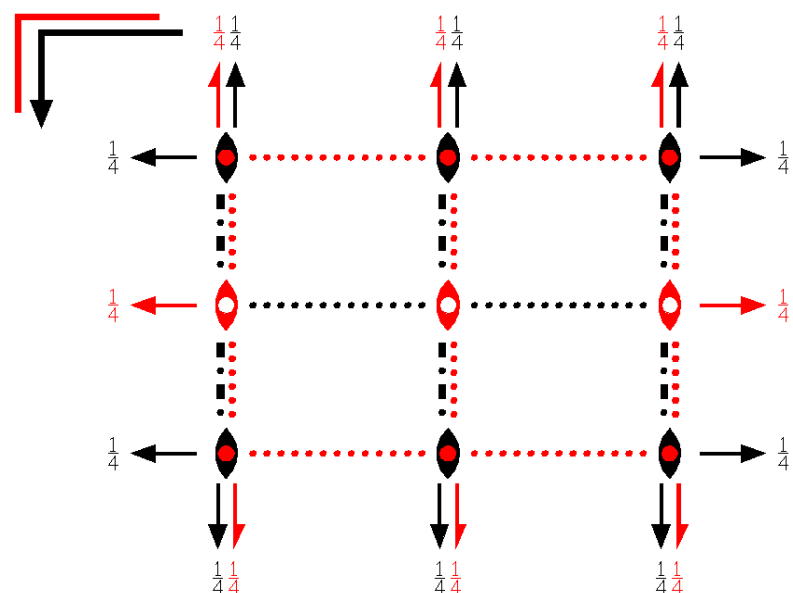


**Origin** at center ( $2/m'$ ) at  $c'c'2/m'$

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)     | (3) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)     | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)           |
| (5) $\bar{1}'$<br>( $\bar{1}$  0,0,0)'       | (6) $m'$ x,y,0<br>( $m_z$  0,0,0)'         | (7) $c'$ (0,0,1/2) x,0,z<br>( $m_y$  0,0,1/2)' | (8) $c'$ (0,0,1/2) 0,y,z<br>( $m_x$  0,0,1/2)'       |
| For (1,0,0)' + set                           |  |  |  |
| (1) $t'$ (1,0,0)<br>(1 1,0,0)'               | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)' | (3) 2' 1/2,y,1/4<br>(2 <sub>y</sub>  1,0,1/2)' | (4) 2' (1,0,0) x,0,1/4<br>(2 <sub>x</sub>  1,0,1/2)' |
| (5) $\bar{1}$ 1/2,0,0<br>( $\bar{1}$  1,0,0) | (6) $a$ (1,0,0) x,y,0<br>( $m_z$  1,0,0)   | (7) $n$ (1,0,1/2) x,0,z<br>( $m_y$  1,0,1/2)   | (8) $c$ (0,0,1/2) 1/2,y,z<br>( $m_x$  1,0,1/2)       |



**Generators selected** (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

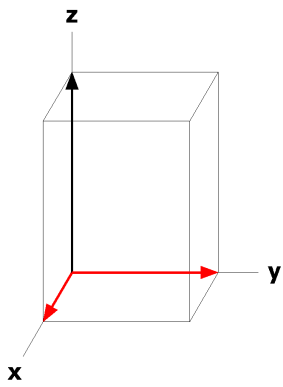
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
8 q ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	x, $\bar{y},1/2$ [u, $\bar{v},0$ ]
8 p ..2'	1/2,0,z [u,v,0]	1/2,0, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	1/2,0, $\bar{z}$ [u,v,0]	1/2,0,z+1/2 [u, $\bar{v},0$ ]
8 o ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0,w]
8 n ..2'	1/2,1/2,z [u,v,0]	1/2,1/2, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	1/2,1/2, $\bar{z}$ [u,v,0]	1/2,1/2,z+1/2 [u, $\bar{v},0$ ]
8 m ..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]
8 l ..2'	1/2,y,1/4 [u,0,w]	1/2, $\bar{y},1/4$ [u,0, $\bar{w}$ ]	1/2, $\bar{y},3/4$ [u,0,w]	1/2,y,3/4 [u,0, $\bar{w}$ ]
8 k ..2	0,y,1/4 [0,v,0]	0, $\bar{y},1/4$ [0, $\bar{v},0$ ]	0, $\bar{y},3/4$ [0, $\bar{v},0$ ]	0,y,3/4 [0,v,0]
8 j 2..	x,1/2,1/4 [u,0,0]	$\bar{x},1/2,1/4$ [ $\bar{u},0,0$ ]	$\bar{x},1/2,3/4$ [ $\bar{u},0,0$ ]	x,1/2,3/4 [u,0,0]
8 i 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [u,0,0]
4 h 22'2'	1/2,1/2,1/4 [u,0,0]	1/2,1/2,3/4 [u,0,0]		
4 g 222	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]		
4 f 22'2'	1/2,0,1/4 [u,0,0]	1/2,0,3/4 [u,0,0]		
4 e 222	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
4 d ..2'/m'	1/2,0,0 [u,v,0]	1/2,0,1/2 [u, $\bar{v},0$ ]		
4 c ..2/m'	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 b ..2'/m'	1/2,1/2,0 [u,v,0]	1/2,1/2,1/2 [u, $\bar{v},0$ ]		
4 a ..2/m'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>'-2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

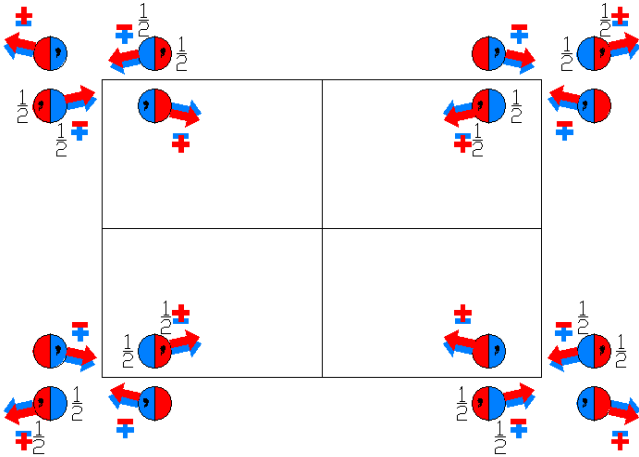
Along [0,1,0] p<sub>2a</sub>'-2m'm'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$P_C ccm'$   
49.13.376

$mmm1'$   
 $P_C 2'/c2'/c2/m'$

Orthorhombic

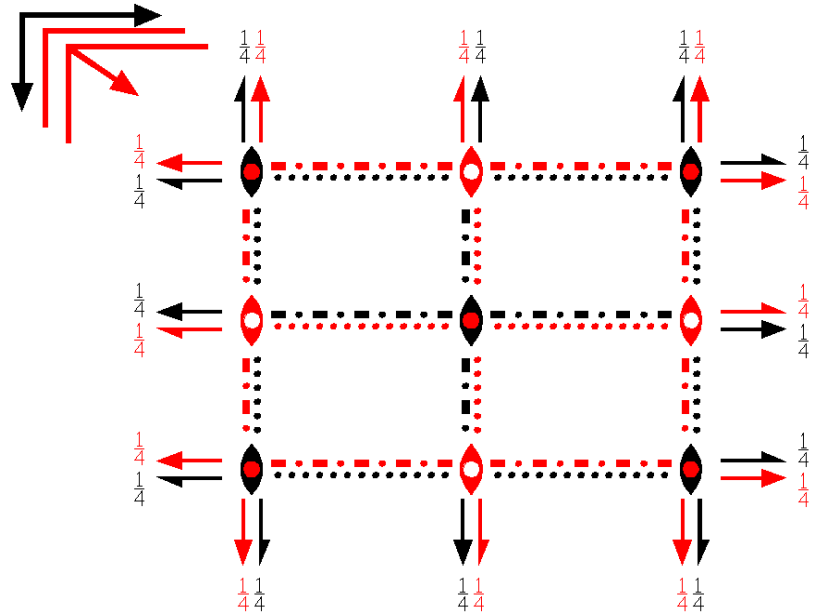


**Origin** at center ( $2/m'$ ) at  $cc2/m'$

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 <sub>0,0,z</sub><br>(2 <sub>z</sub>  0,0,0)   | (3) 2' <sub>0,y,1/4</sub><br>(2 <sub>y</sub>  0,0,1/2)'       | (4) 2' <sub>x,0,1/4</sub><br>(2 <sub>x</sub>  0,0,1/2)'       |
| (5) $\bar{1}'$<br>( $\bar{1}$  0,0,0)' | (6) m' <sub>x,y,0</sub><br>(m <sub>z</sub>  0,0,0)' | (7) c (0,0,1/2) <sub>x,0,z</sub><br>(m <sub>y</sub>  0,0,1/2) | (8) c (0,0,1/2) <sub>0,y,z</sub><br>(m <sub>x</sub>  0,0,1/2) |
- 
- |  |   |   |   |
|--|---|---|---|
| For (1,0,0)' + set                           |   |   |   |
| (1) t' (1,0,0)<br>(1 1,0,0)'                 | (2) 2' <sub>1/2,0,z</sub><br>(2 <sub>z</sub>  1,0,0)'     | (3) 2 <sub>1/2,y,1/4</sub><br>(2 <sub>y</sub>  1,0,1/2)         | (4) 2 (1,0,0) <sub>x,0,1/4</sub><br>(2 <sub>x</sub>  1,0,1/2)     |
| (5) $\bar{1}$ 1/2,0,0<br>( $\bar{1}$  1,0,0) | (6) a (1,0,0) <sub>x,y,0</sub><br>(m <sub>z</sub>  1,0,0) | (7) n' (1,0,1/2) <sub>x,0,z</sub><br>(m <sub>y</sub>  1,0,1/2)' | (8) c' (0,0,1/2) <sub>1/2,y,z</sub><br>(m <sub>x</sub>  1,0,1/2)' |



**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

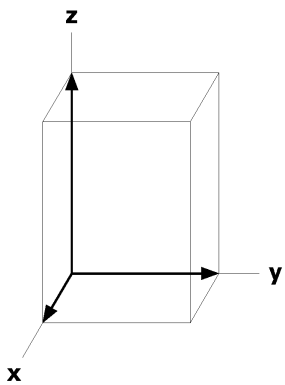
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z+1/2$ [u, $\bar{v},\bar{w}$ ]
8 q ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [u, $\bar{v},0$ ]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]
8 p ..2'	1/2,0,z [u,v,0]	1/2,0, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	1/2,0, $\bar{z}$ [u,v,0]	1/2,0,z+1/2 [ $\bar{u},v,0$ ]
8 o ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	0,1/2, $\bar{z}$ [u,v,0]	0,1/2,z+1/2 [u, $\bar{v},0$ ]
8 n ..2	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]
8 m ..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]
8 l ..2.	1/2,y,1/4 [0,v,0]	1/2, $\bar{y},1/4$ [0,v,0]	1/2, $\bar{y},3/4$ [0,v,0]	1/2,y,3/4 [0,v,0]
8 k ..2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	0, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	0,y,3/4 [u,0, $\bar{w}$ ]
8 j 2..	x,1/2,1/4 [u,0,0]	$\bar{x},1/2,1/4$ [u,0,0]	$\bar{x},1/2,3/4$ [u,0,0]	x,1/2,3/4 [u,0,0]
8 i 2'..	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	$\bar{x},0,3/4$ [0, $\bar{v},\bar{w}$ ]	x,0,3/4 [0,v, $\bar{w}$ ]
4 h 222	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
4 g 22'2'	0,1/2,1/4 [u,0,0]	0,1/2,3/4 [u,0,0]		
4 f 2'22'	1/2,0,1/4 [0,v,0]	1/2,0,3/4 [0,v,0]		
4 e 2'2'2	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		
4 d ..2'/m'	1/2,0,0 [u,v,0]	1/2,0,1/2 [ $\bar{u},v,0$ ]		
4 c ..2'/m'	0,1/2,0 [u,v,0]	0,1/2,1/2 [u, $\bar{v},0$ ]		
4 b ..2/m'	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a ..2/m'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

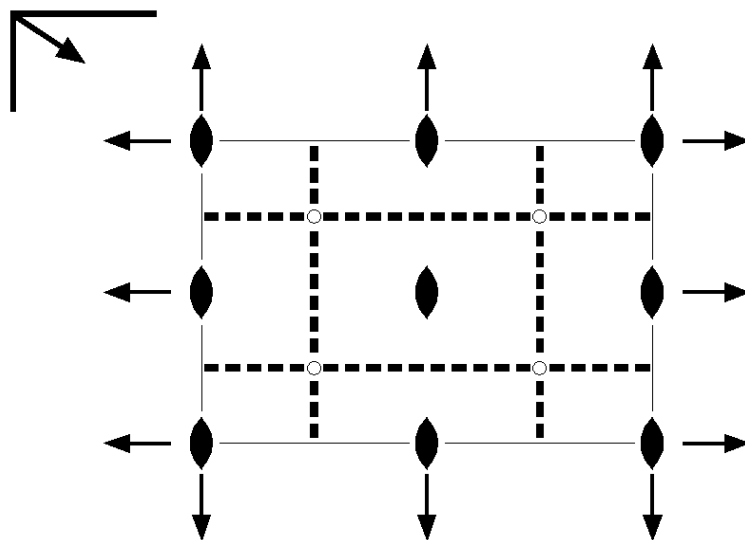
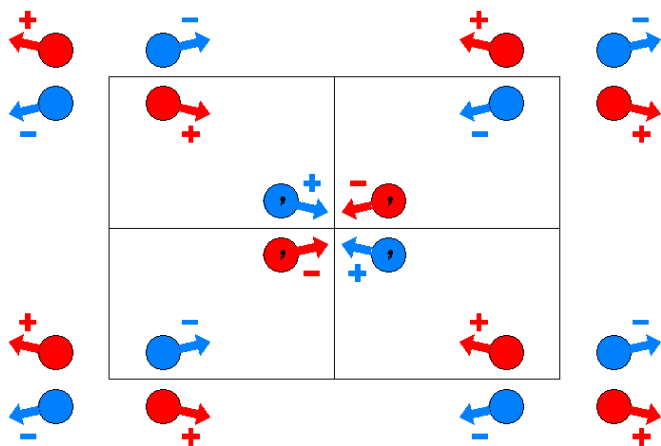
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pban  
50.1.377

mmm  
P2/b2/a2/n

Orthorhombic



**Origin** at 222/n, at  $1/4, 1/4, 0$  from  $\bar{1}$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                 | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                 |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

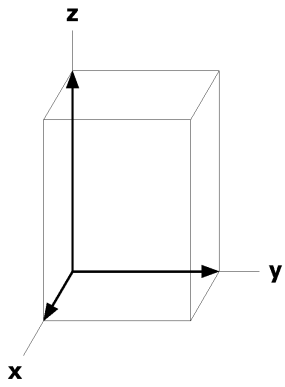
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	m 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
		(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]		
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [u,v,w]	(6) x+1/2,y+1/2, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]		
		(7) x+1/2, $\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z$ [u, $\bar{v},\bar{w}$ ]		
4	l ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]
4	k ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]
4	j .2.	0,y,1/2 [0,v,0]	0, $\bar{y}$ ,1/2 [0, $\bar{v}$ ,0]	1/2, $\bar{y}+1/2$ ,1/2 [0,v,0]	1/2,y+1/2,1/2 [0, $\bar{v}$ ,0]
4	i .2.	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]	1/2, $\bar{y}+1/2$ ,0 [0,v,0]	1/2,y+1/2,0 [0, $\bar{v}$ ,0]
4	h 2..	x,0,1/2 [u,0,0]	$\bar{x}$ ,0,1/2 [ $\bar{u}$ ,0,0]	$\bar{x}+1/2$ ,1/2,1/2 [u,0,0]	x+1/2,1/2,1/2 [ $\bar{u}$ ,0,0]
4	g 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0]	$\bar{x}+1/2$ ,1/2,0 [u,0,0]	x+1/2,1/2,0 [ $\bar{u}$ ,0,0]
4	f $\bar{1}$	1/4,1/4,1/2 [u,v,w]	3/4,3/4,1/2 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,1/2 [ $\bar{u},v,\bar{w}$ ]	1/4,3/4,1/2 [u, $\bar{v},\bar{w}$ ]
4	e $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,0 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,0 [ $\bar{u},v,\bar{w}$ ]	1/4,3/4,0 [u, $\bar{v},\bar{w}$ ]
2	d 222	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	c 222	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	b 222	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
2	a 222	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0

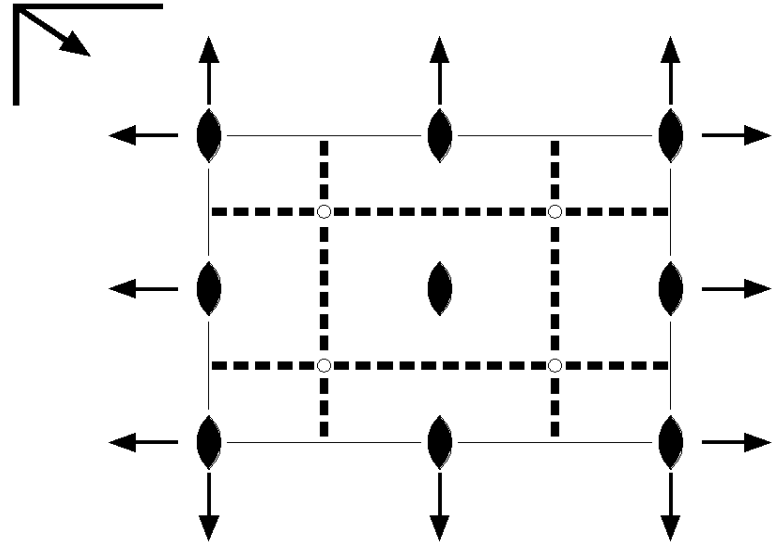
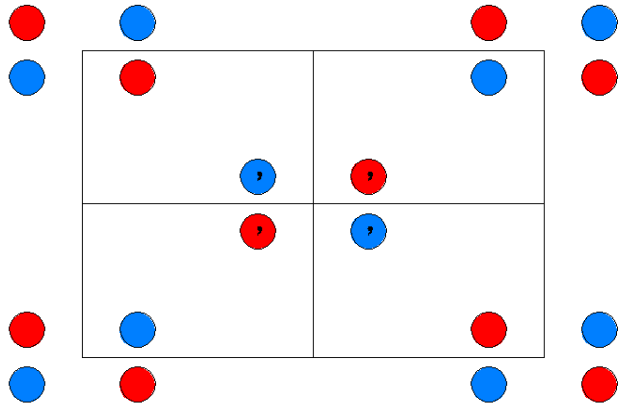


Pban1'  
50.2.378

mmm1'  
P2/b2/a2/n1'

Orthorhombic

1'



Origin at 222/n1', at 1/4,1/4,0 from  $\bar{1}1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For 1 + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                 | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                 |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |

For 1' + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1'<br>(1 0,0,0)'                                  | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                  | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                  | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                  |
| (5) $\bar{1}'$ 1/4,1/4,0<br>( $\bar{1}'$  1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub> ' 1/2,1/2,0)' | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub> ' 1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub> ' 1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

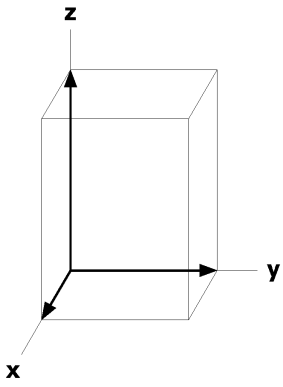
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +	1' +		
8 m 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]		
	(3) $\bar{x},y,\bar{z}$ [0,0,0]	(4) x, $\bar{y},\bar{z}$ [0,0,0]		
	(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [0,0,0]	(6) x+1/2,y+1/2, $\bar{z}$ [0,0,0]		
	(7) x+1/2, $\bar{y}+1/2,z$ [0,0,0]	(8) $\bar{x}+1/2,y+1/2,z$ [0,0,0]		
4 l ..21'	0,1/2,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	1/2,0,z [0,0,0]
4 k ..21'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	1/2,1/2,z [0,0,0]
4 j .2.1'	0,y,1/2 [0,0,0]	0, $\bar{y}$ ,1/2 [0,0,0]	1/2, $\bar{y}+1/2$ ,1/2 [0,0,0]	1/2,y+1/2,1/2 [0,0,0]
4 i .2.1'	0,y,0 [0,0,0]	0, $\bar{y}$ ,0 [0,0,0]	1/2, $\bar{y}+1/2$ ,0 [0,0,0]	1/2,y+1/2,0 [0,0,0]
4 h 2..1'	x,0,1/2 [0,0,0]	$\bar{x}$ ,0,1/2 [0,0,0]	$\bar{x}+1/2$ ,1/2,1/2 [0,0,0]	x+1/2,1/2,1/2 [0,0,0]
4 g 2..1'	x,0,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0]	$\bar{x}+1/2$ ,1/2,0 [0,0,0]	x+1/2,1/2,0 [0,0,0]
4 f $\bar{1}1'$	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]
4 e $\bar{1}1'$	1/4,1/4,0 [0,0,0]	3/4,3/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]	1/4,3/4,0 [0,0,0]
2 d 2221'	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2 c 2221'	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
2 b 2221'	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
2 a 2221'	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

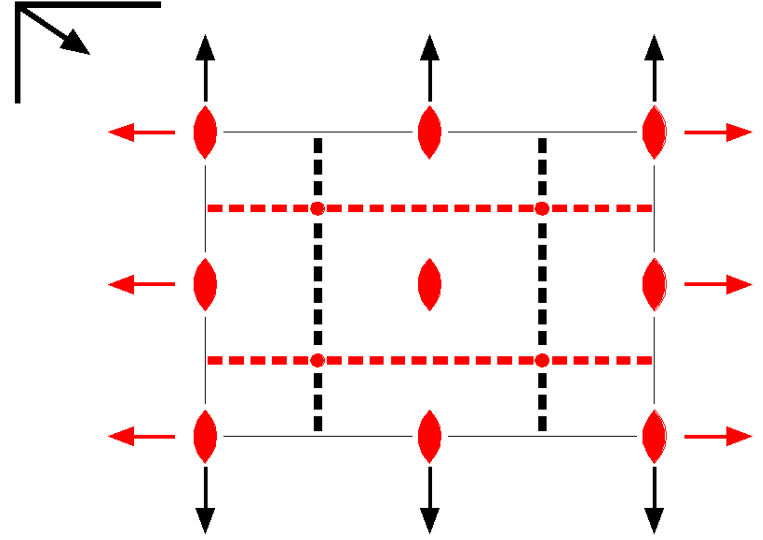
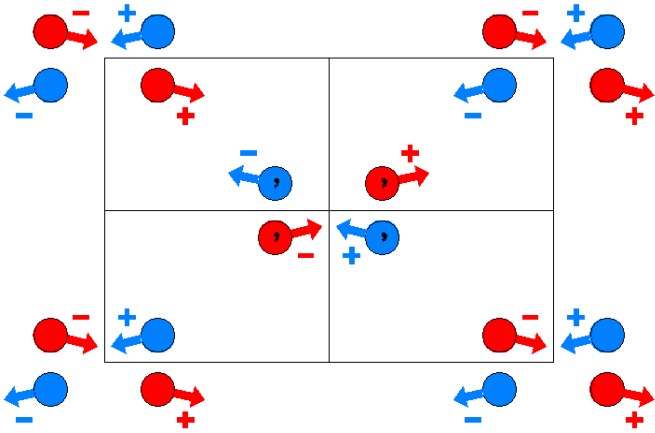
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Pb'an  
50.3.379

m'mm  
P2/b'2'/a'2'/n

Orthorhombic



**Origin** at  $22'2'/n$ , at  $1/4, 1/4, 0$  from  $\bar{1}'$

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)   | (2) $2'_z$ 0,0,z<br>( $2_z$  0,0,0)'                       | (3) $2'_y$ 0,y,0<br>( $2_y$  0,0,0)'                           | (4) $2'_x$ x,0,0<br>( $2_x$  0,0,0)                           |
| (5) $\bar{1}'$ $1/4, 1/4, 0$<br>( $\bar{1}$   $1/2, 1/2, 0$ )' | (6) n ( $1/2, 1/2, 0$ ) x,y,0<br>( $m_z$   $1/2, 1/2, 0$ ) | (7) a ( $1/2, 0, 0$ ) x, $1/4$ ,z<br>( $m_y$   $1/2, 1/2, 0$ ) | (8) b' (0, $1/2$ ,0) $1/4$ ,y,z<br>( $m_x$   $1/2, 1/2, 0$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

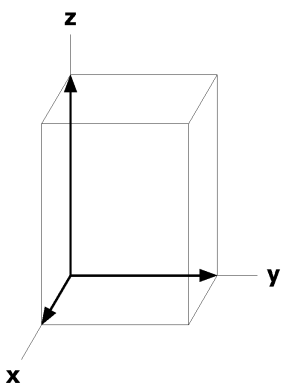
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	m 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]		
		(3) $\bar{x},y,\bar{z}$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]		
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x+1/2,y+1/2, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]		
		(7) x+1/2, $\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]		
4	l ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}$ [u, $\bar{v}$ ,0]	1/2,0, $\bar{z}$ [ $\bar{u},\bar{v}$ ,0]	1/2,0,z [ $\bar{u},v,0$ ]
4	k ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [u, $\bar{v}$ ,0]	1/2,1/2, $\bar{z}$ [ $\bar{u},\bar{v}$ ,0]	1/2,1/2,z [ $\bar{u},v,0$ ]
4	j .2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ ,1/2 [u,0, $\bar{w}$ ]	1/2, $\bar{y}+1/2$ ,1/2 [ $\bar{u},0,\bar{w}$ ]	1/2,y+1/2,1/2 [ $\bar{u},0,w$ ]
4	i .2'	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [u,0, $\bar{w}$ ]	1/2, $\bar{y}+1/2$ ,0 [ $\bar{u},0,\bar{w}$ ]	1/2,y+1/2,0 [ $\bar{u},0,w$ ]
4	h 2..	x,0,1/2 [u,0,0]	$\bar{x}$ ,0,1/2 [u,0,0]	$\bar{x}+1/2$ ,1/2,1/2 [ $\bar{u},0,0$ ]	x+1/2,1/2,1/2 [ $\bar{u},0,0$ ]
4	g 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [u,0,0]	$\bar{x}+1/2$ ,1/2,0 [ $\bar{u},0,0$ ]	x+1/2,1/2,0 [ $\bar{u},0,0$ ]
4	f $\bar{1}'$	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]
4	e $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]	1/4,3/4,0 [0,0,0]
2	d 22'2'	0,0,1/2 [u,0,0]	1/2,1/2,1/2 [ $\bar{u},0,0$ ]		
2	c 22'2'	1/2,0,1/2 [u,0,0]	0,1/2,1/2 [ $\bar{u},0,0$ ]		
2	b 22'2'	1/2,0,0 [u,0,0]	0,1/2,0 [ $\bar{u},0,0$ ]		
2	a 22'2'	0,0,0 [u,0,0]	1/2,1/2,0 [ $\bar{u},0,0$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $c_p \cdot 2'mm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

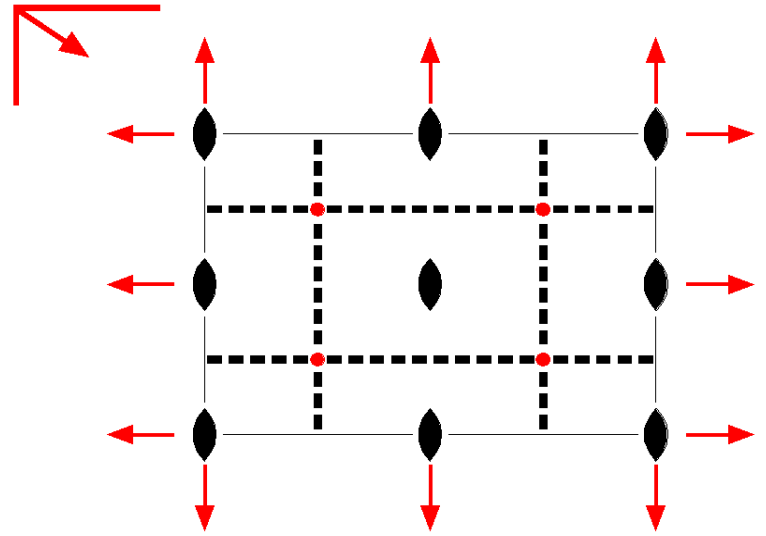
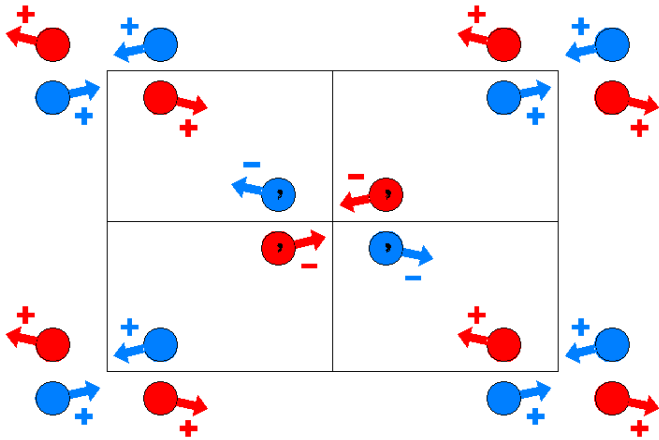
Along [0,1,0]  $p_{2a} \cdot 2mm$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/2



Pban'  
50.4.380

mmm'  
P2'/b2'/a2/n'

Orthorhombic



Origin at 2'2'2'/n', at 1/4,1/4,0 from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                                    | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                   | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'               | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'               |
| (5) $\bar{1}'$ 1/4,1/4,0<br>( $\bar{1}'$  1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

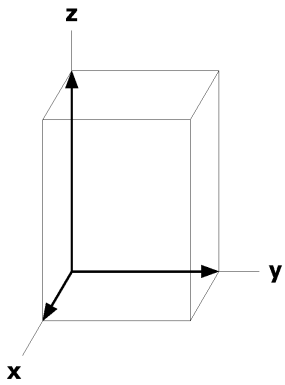
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	m 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x+1/2,y+1/2, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) x+1/2, $\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z$ [u, $\bar{v},\bar{w}$ ]
4	l ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0,z [0,0, $\bar{w}$ ]
4	k ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2,z [0,0, $\bar{w}$ ]
4	j .2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ ,1/2 [ $\bar{u}$ ,0,w]	1/2, $\bar{y}+1/2$ ,1/2 [ $\bar{u}$ ,0, $\bar{w}$ ]	1/2,y+1/2,1/2 [u,0, $\bar{w}$ ]
4	i .2'	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [ $\bar{u}$ ,0,w]	1/2, $\bar{y}+1/2$ ,0 [ $\bar{u}$ ,0, $\bar{w}$ ]	1/2,y+1/2,0 [u,0, $\bar{w}$ ]
4	h 2'..	x,0,1/2 [0,v,w]	$\bar{x}$ ,0,1/2 [0, $\bar{v}$ ,w]	$\bar{x}+1/2$ ,1/2,1/2 [0, $\bar{v}$ , $\bar{w}$ ]	x+1/2,1/2,1/2 [0,v, $\bar{w}$ ]
4	g 2'..	x,0,0 [0,v,w]	$\bar{x}$ ,0,0 [0, $\bar{v}$ ,w]	$\bar{x}+1/2$ ,1/2,0 [0, $\bar{v}$ , $\bar{w}$ ]	x+1/2,1/2,0 [0,v, $\bar{w}$ ]
4	f $\bar{1}'$	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]
4	e $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]	1/4,3/4,0 [0,0,0]
2	d 2'2'2	0,0,1/2 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		
2	c 2'2'2	1/2,0,1/2 [0,0,w]	0,1/2,1/2 [0,0, $\bar{w}$ ]		
2	b 2'2'2	1/2,0,0 [0,0,w]	0,1/2,0 [0,0, $\bar{w}$ ]		
2	a 2'2'2	0,0,0 [0,0,w]	1/2,1/2,0 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}$  2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

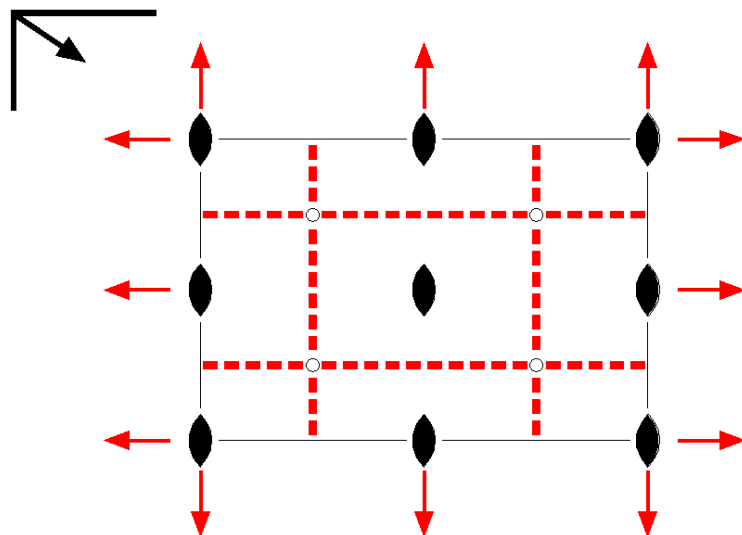
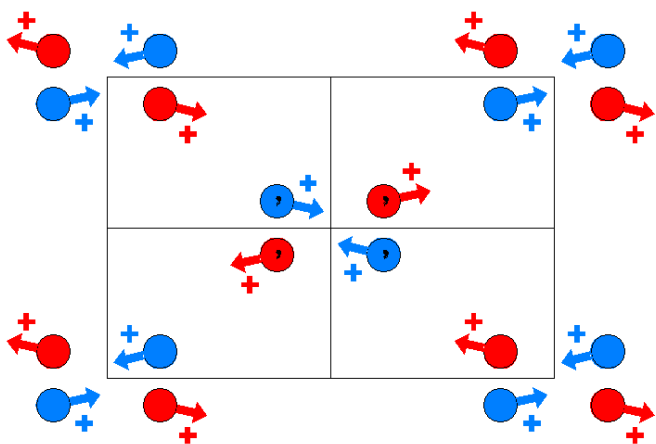
Along [0,1,0]  $p_{2a}$  2mm  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



Pb'a'n  
50.5.381

m'm'm  
P2'/b'2'/a'2'/n

Orthorhombic



**Origin** at 2'2'2'/n, at 1/4,1/4,0 from  $\bar{1}$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                 | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                 |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

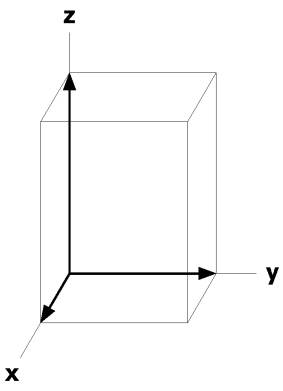
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	m 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
		(3) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]		
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [u,v,w]	(6) x+1/2,y+1/2, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]		
		(7) x+1/2, $\bar{y}+1/2,z$ [ $u,\bar{v},w$ ]	(8) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]		
4	l ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	1/2,0,z [0,0,w]
4	k ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2,z [0,0,w]
4	j .2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ ,1/2 [ $\bar{u}$ ,0,w]	1/2, $\bar{y}+1/2$ ,1/2 [u,0,w]	1/2,y+1/2,1/2 [ $\bar{u}$ ,0,w]
4	i .2'	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [ $\bar{u}$ ,0,w]	1/2, $\bar{y}+1/2$ ,0 [u,0,w]	1/2,y+1/2,0 [ $\bar{u}$ ,0,w]
4	h 2'..	x,0,1/2 [0,v,w]	$\bar{x}$ ,0,1/2 [0, $\bar{v}$ ,w]	$\bar{x}+1/2$ ,1/2,1/2 [0,v,w]	x+1/2,1/2,1/2 [0, $\bar{v}$ ,w]
4	g 2'..	x,0,0 [0,v,w]	$\bar{x}$ ,0,0 [0, $\bar{v}$ ,w]	$\bar{x}+1/2$ ,1/2,0 [0,v,w]	x+1/2,1/2,0 [0, $\bar{v}$ ,w]
4	f $\bar{1}$	1/4,1/4,1/2 [u,v,w]	3/4,3/4,1/2 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,1/2 [u, $\bar{v},w$ ]	1/4,3/4,1/2 [ $\bar{u},v,w$ ]
4	e $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,0 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,0 [u, $\bar{v},w$ ]	1/4,3/4,0 [ $\bar{u},v,w$ ]
2	d 2'2'2	0,0,1/2 [0,0,w]	1/2,1/2,1/2 [0,0,w]		
2	c 2'2'2	1/2,0,1/2 [0,0,w]	0,1/2,1/2 [0,0,w]		
2	b 2'2'2	1/2,0,0 [0,0,w]	0,1/2,0 [0,0,w]		
2	a 2'2'2	0,0,0 [0,0,w]	1/2,1/2,0 [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1]  $c_p \cdot 2mm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = -\mathbf{b}/2$   
 Origin at x,0,0

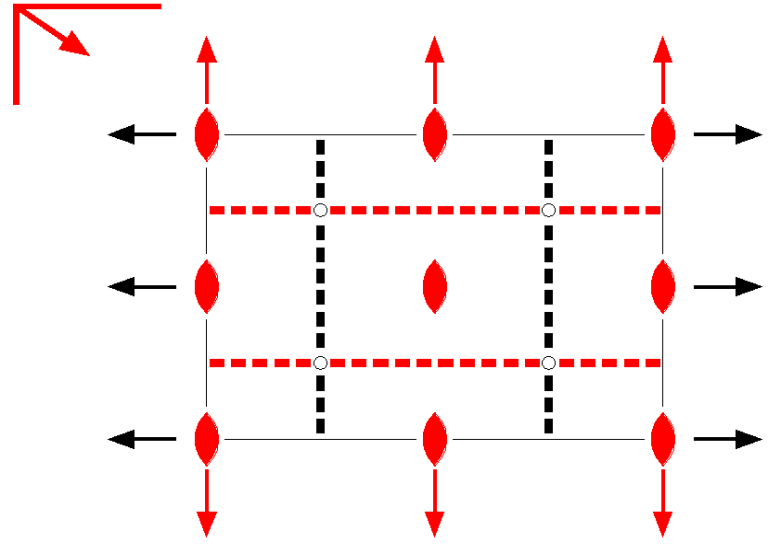
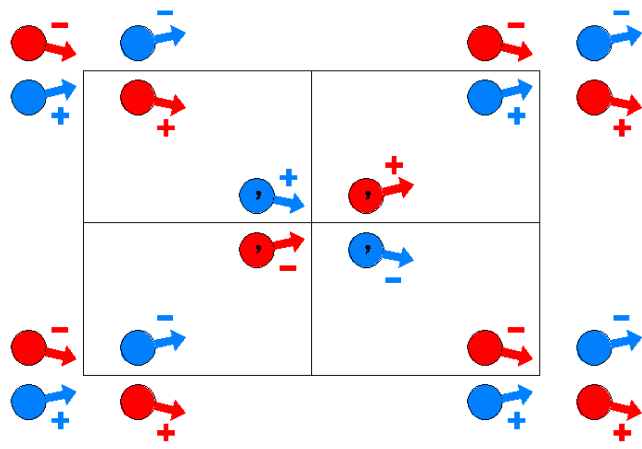
Along [0,1,0]  $p2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Pb'an'  
50.6.382

mmm  
P2'/b'2'/a2'/n'

Orthorhombic



**Origin** at 2'22'/n', at 1/4,1/4,0 from  $\bar{1}$

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                 | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                 | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                 |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

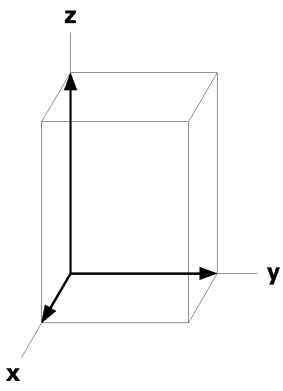
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	m 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [u,v,w]	(6) x+1/2,y+1/2, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) x+1/2, $\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]
4	l ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}$ [ $\bar{u},v,0$ ]	1/2,0, $\bar{z}$ [u,v,0]	1/2,0,z [ $\bar{u},v,0$ ]
4	k ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [ $\bar{u},v,0$ ]	1/2,1/2, $\bar{z}$ [u,v,0]	1/2,1/2,z [ $\bar{u},v,0$ ]
4	j .2.	0,y,1/2 [0,v,0]	0, $\bar{y}$ ,1/2 [0,v,0]	1/2, $\bar{y}+1/2$ ,1/2 [0,v,0]	1/2,y+1/2,1/2 [0,v,0]
4	i .2.	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0,v,0]	1/2, $\bar{y}+1/2$ ,0 [0,v,0]	1/2,y+1/2,0 [0,v,0]
4	h 2..	x,0,1/2 [0,v,w]	$\bar{x}$ ,0,1/2 [0,v, $\bar{w}$ ]	$\bar{x}+1/2$ ,1/2,1/2 [0,v,w]	x+1/2,1/2,1/2 [0,v, $\bar{w}$ ]
4	g 2..	x,0,0 [0,v,w]	$\bar{x}$ ,0,0 [0,v, $\bar{w}$ ]	$\bar{x}+1/2$ ,1/2,0 [0,v,w]	x+1/2,1/2,0 [0,v, $\bar{w}$ ]
4	f $\bar{1}$	1/4,1/4,1/2 [u,v,w]	3/4,3/4,1/2 [u,v, $\bar{w}$ ]	3/4,1/4,1/2 [ $\bar{u},v,\bar{w}$ ]	1/4,3/4,1/2 [ $\bar{u},v,w$ ]
4	e $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,0 [u,v, $\bar{w}$ ]	3/4,1/4,0 [ $\bar{u},v,\bar{w}$ ]	1/4,3/4,0 [ $\bar{u},v,w$ ]
2	d 2'22'	0,0,1/2 [0,v,0]	1/2,1/2,1/2 [0,v,0]		
2	c 2'22'	1/2,0,1/2 [0,v,0]	0,1/2,1/2 [0,v,0]		
2	b 2'22'	1/2,0,0 [0,v,0]	0,1/2,0 [0,v,0]		
2	a 2'22'	0,0,0 [0,v,0]	1/2,1/2,0 [0,v,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

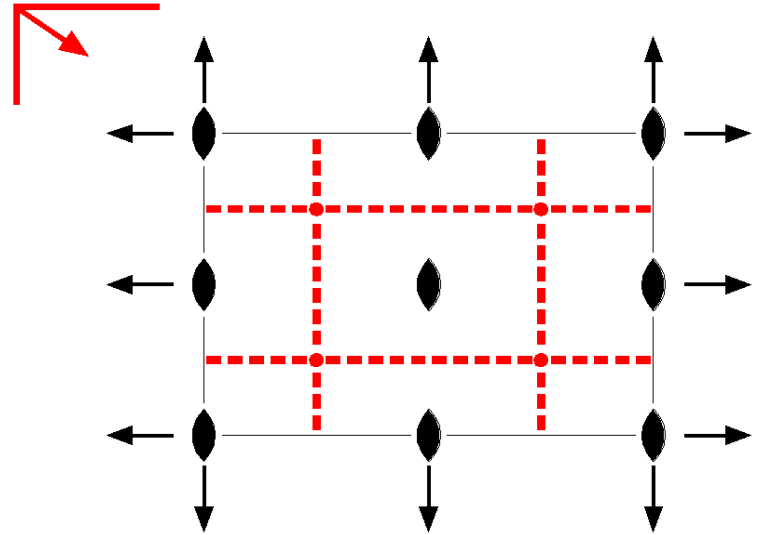
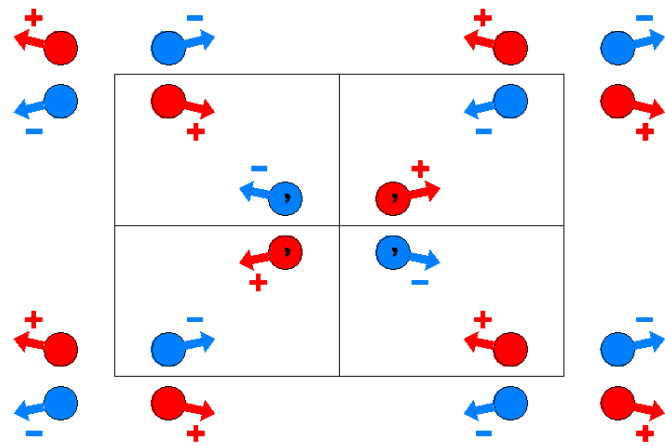
Along [0,1,0] p<sub>2a</sub>'2mm  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pb'a'n'  
50.7.383

m'm'm'  
P2/b'2/a'2/n'

Orthorhombic



Origin at 222/n', at 1/4,1/4,0 from  $\bar{1}$ '

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                   |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$ ' 1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

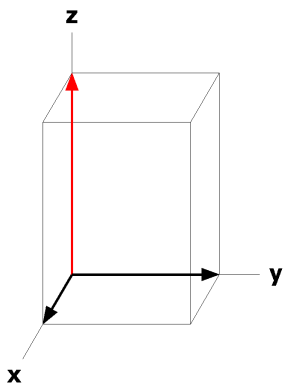
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	m 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
		(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]		
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x+1/2,y+1/2, $\bar{z}$ [u,v, $\bar{w}$ ]		
		(7) x+1/2, $\bar{y}+1/2,z$ [u, $\bar{v},w$ ]	(8) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]		
4	l ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0,z [0,0,w]
4	k ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2,z [0,0,w]
4	j .2.	0,y,1/2 [0,v,0]	0, $\bar{y}$ ,1/2 [0, $\bar{v}$ ,0]	1/2, $\bar{y}+1/2$ ,1/2 [0, $\bar{v}$ ,0]	1/2,y+1/2,1/2 [0,v,0]
4	i .2.	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]	1/2, $\bar{y}+1/2$ ,0 [0, $\bar{v}$ ,0]	1/2,y+1/2,0 [0,v,0]
4	h 2..	x,0,1/2 [u,0,0]	$\bar{x}$ ,0,1/2 [ $\bar{u}$ ,0,0]	$\bar{x}+1/2$ ,1/2,1/2 [ $\bar{u}$ ,0,0]	x+1/2,1/2,1/2 [u,0,0]
4	g 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0]	$\bar{x}+1/2$ ,1/2,0 [ $\bar{u}$ ,0,0]	x+1/2,1/2,0 [u,0,0]
4	f $\bar{1}'$	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]
4	e $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]	1/4,3/4,0 [0,0,0]
2	d 222	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	c 222	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	b 222	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
2	a 222	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



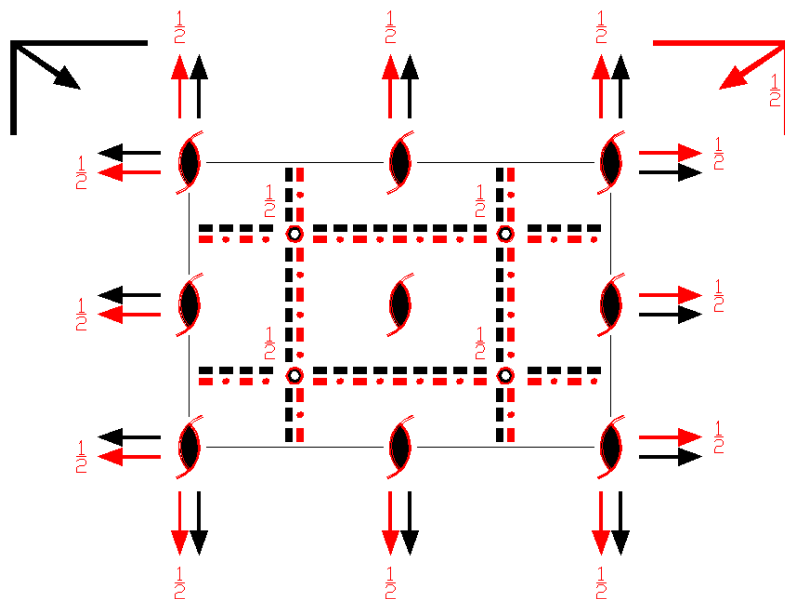
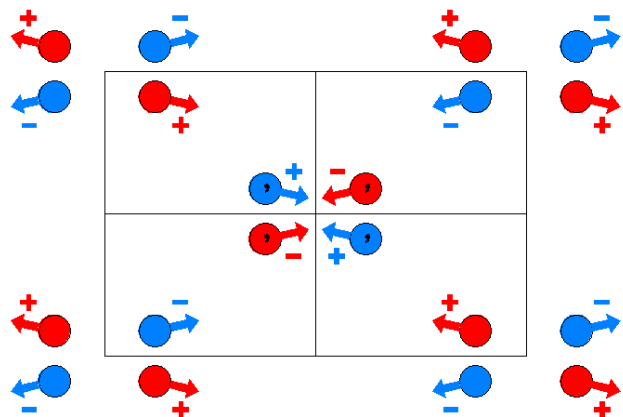
$P_{2c}$  ban

50.8.384

$mmm1'$

$P_{2c} 2/b2/a2/n$

Orthorhombic



**Origin** at  $222/n$ , at  $1/4, 1/4, 0$  from  $\bar{1}$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $1$<br>$(1 0,0,0)$                             | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                   | (3) $2$ $0,y,0$<br>$(2_y 0,0,0)$                   | (4) $2$ $x,0,0$<br>$(2_x 0,0,0)$                   |
| (5) $\bar{1}$ $1/4,1/4,0$<br>$(\bar{1} 1/2,1/2,0)$ | (6) $n$ $(1/2,1/2,0)$ $x,y,0$<br>$(m_z 1/2,1/2,0)$ | (7) $a$ $(1/2,0,0)$ $x,1/4,z$<br>$(m_y 1/2,1/2,0)$ | (8) $b$ $(0,1/2,0)$ $1/4,y,z$<br>$(m_x 1/2,1/2,0)$ |

For  $(0,0,1)'$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t'$ $(0,0,1)$<br>$(1 0,0,1)'$                      | (2) $2'$ $(0,0,1)$ $0,0,z$<br>$(2_z 0,0,1)'$           | (3) $2'$ $0,y,1/2$<br>$(2_y 0,0,1)'$                 | (4) $2'$ $x,0,1/2$<br>$(2_x 0,0,1)'$                 |
| (5) $\bar{1}'$ $1/4,1/4,1/2$<br>$(\bar{1}' 1/2,1/2,1)'$ | (6) $n'$ $(1/2,1/2,0)$ $x,y,1/2$<br>$(m_z 1/2,1/2,1)'$ | (7) $n'$ $(1/2,0,1)$ $x,1/4,z$<br>$(m_y 1/2,1/2,1)'$ | (8) $n'$ $(0,1/2,1)$ $1/4,y,z$<br>$(m_x 1/2,1/2,1)'$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

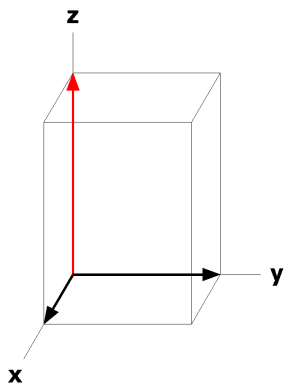
		Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.			
		(0,0,0) +	(0,0,1)' +
16	m 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$
		(3) $\bar{x},y,\bar{z} [\bar{u},v,\bar{w}]$	(4) $x,\bar{y},\bar{z} [u,\bar{v},\bar{w}]$
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z} [u,v,w]$	(6) $x+1/2,y+1/2,\bar{z} [\bar{u},\bar{v},w]$
		(7) $x+1/2,\bar{y}+1/2,z [\bar{u},v,\bar{w}]$	(8) $\bar{x}+1/2,y+1/2,z [u,\bar{v},\bar{w}]$
8	l ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]
			1/2,0, $\bar{z}$ [0,0,w]
8	k ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
			1/2,1/2, $\bar{z}$ [0,0,w]
8	j .2'	0,y,1/2 [u,0,w]	0, $\bar{y}$ ,1/2 [ $\bar{u}$ ,0,w]
			1/2, $\bar{y}+1/2$ ,1/2 [ $\bar{u}$ ,0, $\bar{w}$ ]
8	i .2.	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]
			1/2, $\bar{y}+1/2$ ,0 [0,v,0]
8	h 2'..	x,0,1/2 [0,v,w]	$\bar{x}$ ,0,1/2 [0, $\bar{v}$ ,w]
			$\bar{x}+1/2$ ,1/2,1/2 [0, $\bar{v}$ , $\bar{w}$ ]
8	g 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0]
			$\bar{x}+1/2$ ,1/2,0 [u,0,0]
8	f $\bar{1}$ '	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]
			3/4,1/4,1/2 [0,0,0]
8	e $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,0 [ $\bar{u},\bar{v},w]$ ]
			3/4,1/4,0 [ $\bar{u},v,\bar{w}]$ ]
4	d 2'2'2	0,0,1/2 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]
4	c 2'2'2	1/2,0,1/2 [0,0,w]	0,1/2,1/2 [0,0, $\bar{w}$ ]
4	b 222	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]
4	a 222	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>c</sub>\*2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/2

Along [0,1,0] p<sub>c</sub>\*2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,1/2



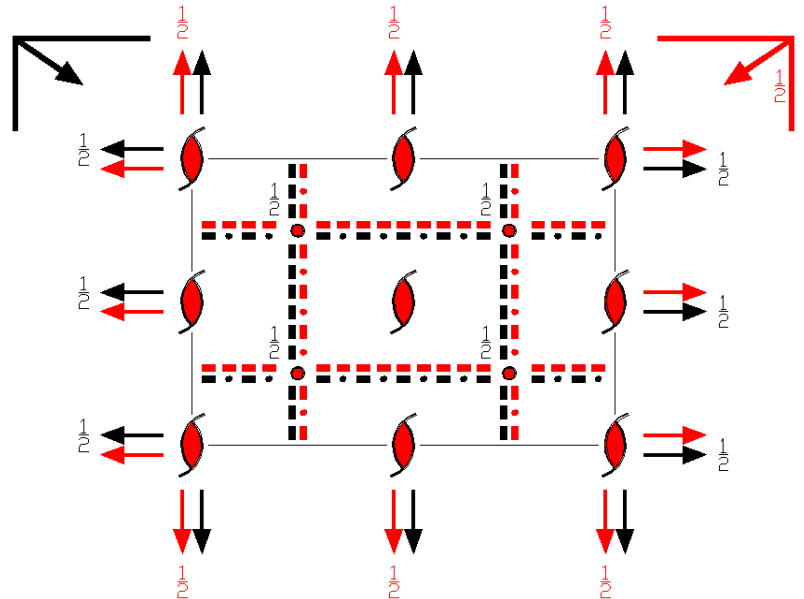
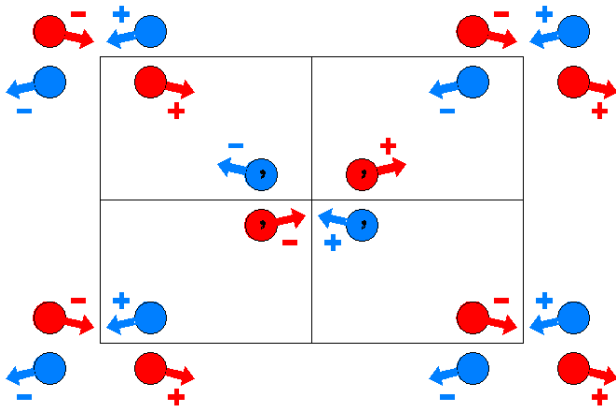
$P_{2c} b'an$

50.9.385

$mmm1'$

$P_{2c} 2/b'2'/a2'/n$

Orthorhombic



**Origin** at  $22'2'/n$ , at  $1/4, 1/4, 0$  from  $\bar{1}'$

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)'                         | (3) $2'$ 0,y,0<br>( $2_y$  0,0,0)'                             | (4) $2$ x,0,0<br>( $2_x$  0,0,0)                                   |
| (5) $\bar{1}'$ $1/4, 1/4, 0$<br>( $\bar{1}'$   $1/2, 1/2, 0$ )' | (6) n ( $1/2, 1/2, 0$ ) x,y,0<br>( $m_z$   $1/2, 1/2, 0$ ) | (7) a ( $1/2, 0, 0$ ) x, $1/4, z$<br>( $m_y$   $1/2, 1/2, 0$ ) | (8) $b'$ ( $0, 1/2, 0$ ) $1/4, y, z$<br>( $m_x$   $1/2, 1/2, 0$ )' |

For  $(0,0,1)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'                                 | (2) $2$ (0,0,1) 0,0,z<br>( $2_z$  0,0,1)                         | (3) $2$ 0,y,1/2<br>( $2_y$  0,0,1)                                 | (4) $2'$ x,0,1/2<br>( $2_x$  0,0,1)'                           |
| (5) $\bar{1}$ $1/4, 1/4, 1/2$<br>( $\bar{1}$   $1/2, 1/2, 1$ ) | (6) $n'$ ( $1/2, 1/2, 0$ ) x,y,1/2<br>( $m_z$   $1/2, 1/2, 1$ )' | (7) $n'$ ( $1/2, 0, 1$ ) x, $1/4, z$<br>( $m_y$   $1/2, 1/2, 1$ )' | (8) n ( $0, 1/2, 1$ ) $1/4, y, z$<br>( $m_x$   $1/2, 1/2, 1$ ) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

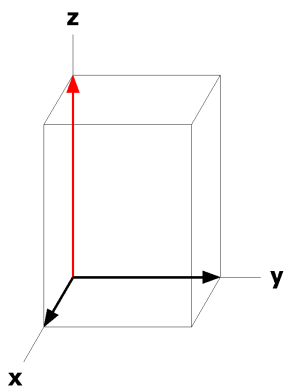
Multiplicity, Wyckoff letter, Site Symmetry.		Coordinates			
		(0,0,0) +		(0,0,1)' +	
16	m 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]		
		(3) $\bar{x},y,\bar{z}$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]		
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x+1/2,y+1/2, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]		
		(7) x+1/2, $\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]		
8	i ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}$ [u, $\bar{v}$ ,0]	1/2,0, $\bar{z}$ [ $\bar{u},\bar{v}$ ,0]	1/2,0,z [ $\bar{u},v,0$ ]
8	k ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [u, $\bar{v}$ ,0]	1/2,1/2, $\bar{z}$ [ $\bar{u},\bar{v}$ ,0]	1/2,1/2,z [ $\bar{u},v,0$ ]
8	j .2.	0,y,1/2 [0,v,0]	0, $\bar{y}$ ,1/2 [0,v,0]	1/2, $\bar{y}+1/2$ ,1/2 [0,v,0]	1/2,y+1/2,1/2 0,v,0]
8	i .2'	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [u,0, $\bar{w}$ ]	1/2, $\bar{y}+1/2$ ,0 [ $\bar{u}$ ,0, $\bar{w}$ ]	1/2,y+1/2,0 [ $\bar{u}$ ,0,w]
8	h 2'..	x,0,1/2 [0,v,w]	$\bar{x}$ ,0,1/2 [0,v, $\bar{w}$ ]	$\bar{x}+1/2$ ,1/2,1/2 [0,v,w]	x+1/2,1/2,1/2 [0,v, $\bar{w}$ ]
8	g 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [u,0,0]	$\bar{x}+1/2$ ,1/2,0 [ $\bar{u}$ ,0,0]	x+1/2,1/2,0 [ $\bar{u}$ ,0,0]
8	f $\bar{1}$	1/4,1/4,1/2 [u,v,w]	3/4,3/4,1/2 [u,v, $\bar{w}$ ]	3/4,1/4,1/2 [ $\bar{u},v,\bar{w}$ ]	1/4,3/4,1/2 [ $\bar{u},v,w$ ]
8	e $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]	1/4,3/4,0 [0,0,0]
4	d 2'22'	0,0,1/2 [0,v,0]	1/2,1/2,1/2 [0,v,0]		
4	c 2'22'	1/2,0,1/2 [0,v,0]	0,1/2,1/2 [0,v,0]		
4	b 22'2'	1/2,0,0 [u,0,0]	0,1/2,0 [ $\bar{u}$ ,0,0]		
4	a 22'2'	0,0,0 [u,0,0]	1/2,1/2,0 [ $\bar{u}$ ,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>\*2mm  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>c</sub>\*2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/2



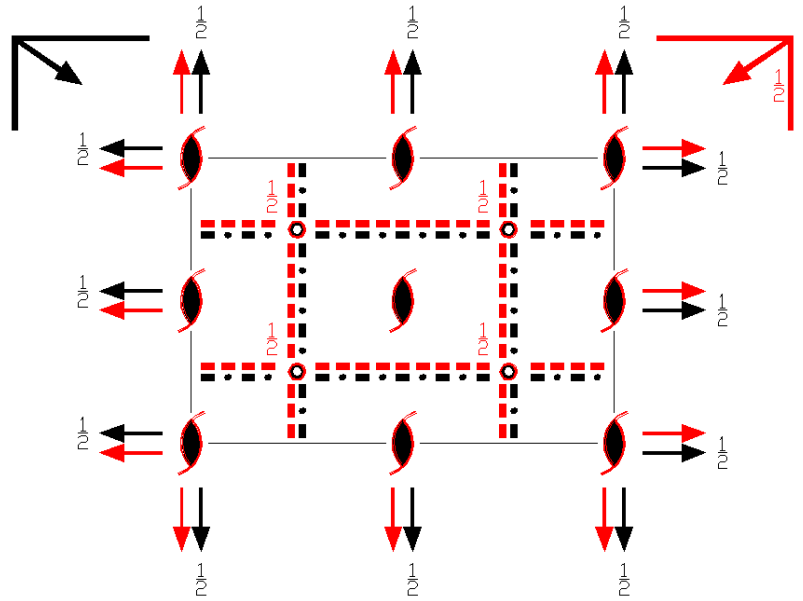
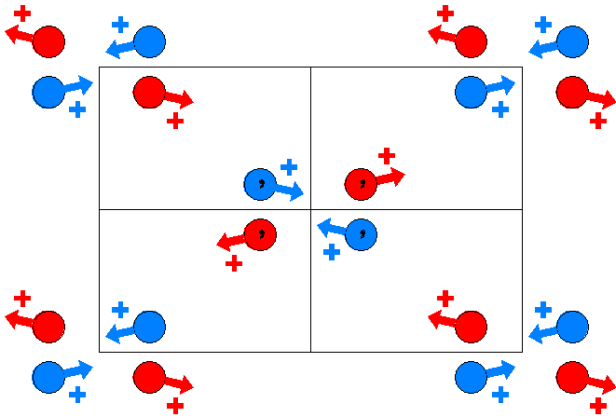
$P_{2c} b'a'n$

50.10.386

$mmm1'$

$P_{2c} 2'/b'2'/a'2'/n$

Orthorhombic



**Origin** at  $2'2'2'/n$ , at  $1/4, 1/4, 0$  from  $\bar{1}$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |   |  |  |
|--|---|--|--|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                 | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                 |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)       | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)      | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |
| For (0,0,1)' + set                                       |   |  |  |
| (1) t' (0,0,1)<br>(1 0,0,1)'                             | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)'            | (3) 2 0,y,1/2<br>(2 <sub>y</sub>  0,0,1)                 | (4) 2 x,0,1/2<br>(2 <sub>x</sub>  0,0,1)                 |
| (5) $\bar{1}$ ' 1/4,1/4,1/2<br>( $\bar{1}$ ' 1/2,1/2,1)' | (6) n' (1/2,1/2,0) x,y,1/2<br>(m <sub>z</sub> ' 1/2,1/2,1)' | (7) n (1/2,0,1) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1)   | (8) n (0,1/2,1) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1)   |



**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

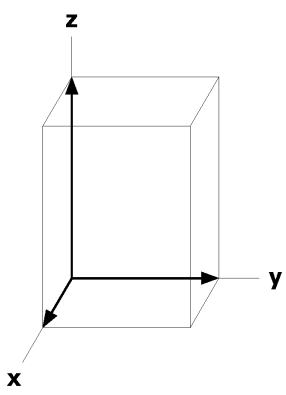
Multiplicity, Wyckoff letter, Site Symmetry.		Coordinates			
		(0,0,0) +	(0,0,1)' +		
16	m 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
		(3) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]		
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [u,v,w]	(6) x+1/2,y+1/2, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]		
		(7) x+1/2, $\bar{y}+1/2,z$ [u, $\bar{v},w$ ]	(8) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]		
8	l ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	1/2,0,z [0,0,w]
8	k ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2,z [0,0,w]
8	j .2.	0,y,1/2 [0,v,0]	0, $\bar{y}$ ,1/2 [0, $\bar{v}$ ,0]	1/2, $\bar{y}+1/2$ ,1/2 [0, $\bar{v}$ ,0]	1/2,y+1/2,1/2 [0,v,0]
8	i .2'	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [ $\bar{u}$ ,0,w]	1/2, $\bar{y}+1/2$ ,0 [u,0,w]	1/2,y+1/2,0 [ $\bar{u}$ ,0,w]
8	h 2..	x,0,1/2 [u,0,0]	$\bar{x}$ ,0,1/2 [ $\bar{u}$ ,0,0]	$\bar{x}+1/2$ ,1/2,1/2 [ $\bar{u}$ ,0,0]	x+1/2,1/2,1/2 [u,0,0]
8	g 2'..	x,0,0 [0,v,w]	$\bar{x}$ ,0,0 [0, $\bar{v}$ ,w]	$\bar{x}+1/2$ ,1/2,0 [0,v,w]	x+1/2,1/2,0 [0, $\bar{v}$ ,w]
8	f $\bar{1}$ '	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]
8	e $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,0 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,0 [u, $\bar{v},w$ ]	1/4,3/4,0 [ $\bar{u},v,w$ ]
4	d 222	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4	c 222	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
4	b 2'2'2	1/2,0,0 [0,0,w]	0,1/2,0 [0,0,w]		
4	a 2'2'2	0,0,0 [0,0,w]	1/2,1/2,0 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,1/2

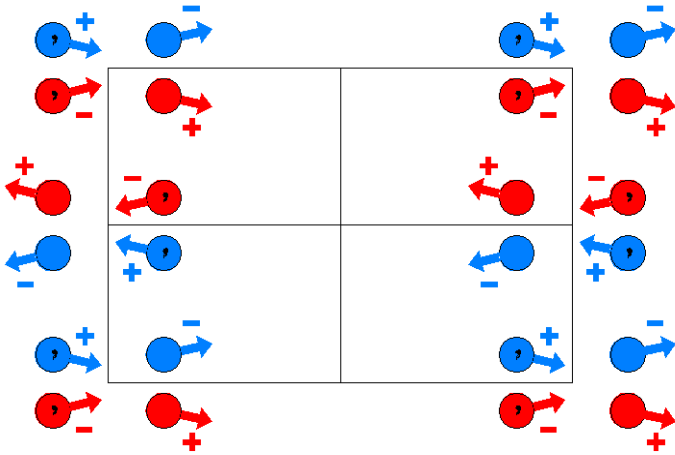
Along [0,1,0] p<sub>2a</sub>'2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Pmma  
51.1.387

mmm  
P2<sub>1</sub>/m2/m2/a

Orthorhombic

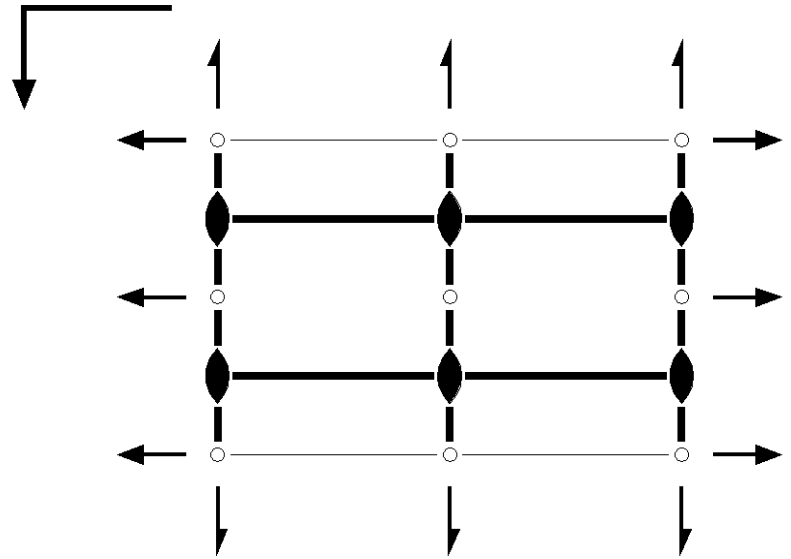


Origin at center ( 2/m ) at 2, 2/ma

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

### Symmetry Operations

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) 1<br>(1 0,0,0)                   | (2) 2 $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)           | (3) 2 $0,y,0$<br>(2 <sub>y</sub>  0,0,0) | (4) 2 $(1/2,0,0)$ $x,0,0$<br>(2 <sub>x</sub>  1/2,0,0) |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) a $(1/2,0,0)$ $x,y,0$<br>(m <sub>z</sub>  1/2,0,0) | (7) m $x,0,z$<br>(m <sub>y</sub>  0,0,0) | (8) m $1/4,y,z$<br>(m <sub>x</sub>  1/2,0,0)           |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

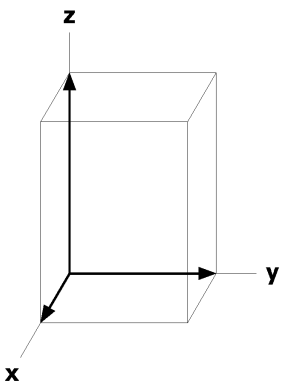
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	l 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(4) $x+1/2, \bar{y}, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]
		(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(7) $x, \bar{y}, z$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(8) $\bar{x}+1/2, y, z$ [ $u, \bar{v}, \bar{w}$ ]
4	k m..	1/4,y,z [u,0,0]	1/4, $\bar{y}$ ,z [ $\bar{u}, 0, 0$ ]	3/4,y, $\bar{z}$ [ $\bar{u}, 0, 0$ ]	3/4, $\bar{y}$ , $\bar{z}$ [u,0,0]
4	j .m.	x,1/2,z [0,v,0]	$\bar{x}+1/2, 1/2, z$ [0, $\bar{v}, 0$ ]	$\bar{x}, 1/2, \bar{z}$ [0,v,0]	$x+1/2, 1/2, \bar{z}$ [0, $\bar{v}, 0$ ]
4	i .m.	x,0,z [0,v,0]	$\bar{x}+1/2, 0, z$ [0, $\bar{v}, 0$ ]	$\bar{x}, 0, \bar{z}$ [0,v,0]	$x+1/2, 0, \bar{z}$ [0, $\bar{v}, 0$ ]
4	h .2.	0,y,1/2 [0,v,0]	1/2, $\bar{y}$ ,1/2 [0, $\bar{v}, 0$ ]	0, $\bar{y}$ ,1/2 [0,v,0]	1/2,y,1/2 [0, $\bar{v}, 0$ ]
4	g .2.	0,y,0 [0,v,0]	1/2, $\bar{y}$ ,0 [0, $\bar{v}, 0$ ]	0, $\bar{y}$ ,0 [0,v,0]	1/2,y,0 [0, $\bar{v}, 0$ ]
2	f mm2	1/4,1/2,z [0,0,0]	3/4,1/2, $\bar{z}$ [0,0,0]		
2	e mm2	1/4,0,z [0,0,0]	3/4,0, $\bar{z}$ [0,0,0]		
2	d .2/m.	0,1/2,1/2 [0,v,0]	1/2,1/2,1/2 [0, $\bar{v}, 0$ ]		
2	c .2/m.	0,0,1/2 [0,v,0]	1/2,0,1/2 [0, $\bar{v}, 0$ ]		
2	b .2/m.	0,1/2,0 [0,v,0]	1/2,1/2,0 [0, $\bar{v}, 0$ ]		
2	a .2/m.	0,0,0 [0,v,0]	1/2,0,0 [0, $\bar{v}, 0$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2a}$ -2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $p2mg1'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pmma1'

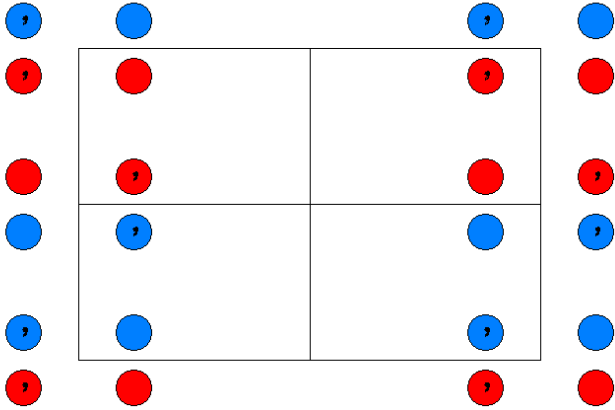
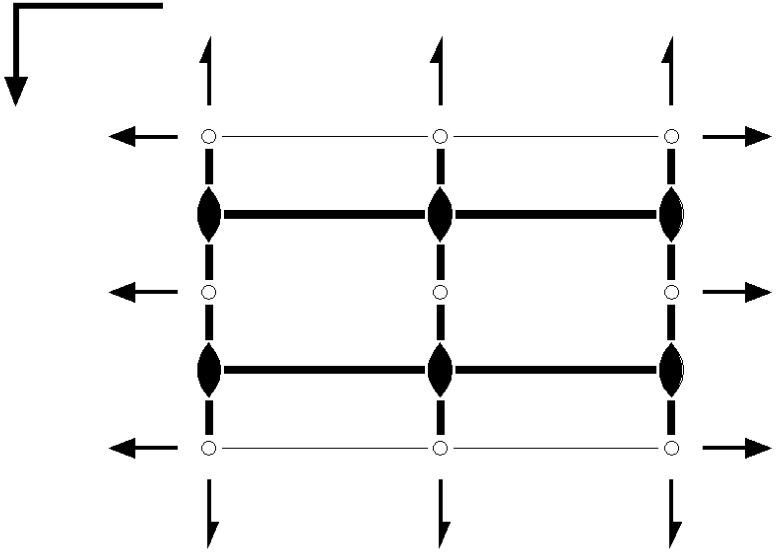
51.2.388

mmm1'

P2<sub>1</sub>/m2/m2/a1'

Orthorhombic

1'



Origin at center ( 2/m1' ) at 2, 2/ma1'

Asymmetric unit  $0 \leq x \leq 1/4;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,0)            | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)    | (4) 2 (1/2,0,0) x,0,0<br>(2 <sub>x</sub>  1/2,0,0)    |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0)     | (6) a (1/2,0,0) x,y,0<br>(m <sub>z</sub>  1/2,0,0)    | (7) m x,0,z<br>(m <sub>y</sub>  0,0,0)    | (8) m 1/4,y,z<br>(m <sub>x</sub>  1/2,0,0)            |
| For 1' + set                             |   |   |   |
| (1) 1'<br>(1 0,0,0)'                     | (2) 2' 1/4,0,z<br>(2 <sub>z</sub> ' 1/2,0,0)'         | (3) 2' 0,y,0<br>(2 <sub>y</sub> ' 0,0,0)' | (4) 2' (1/2,0,0) x,0,0<br>(2 <sub>x</sub> ' 1/2,0,0)' |
| (5) $\bar{1}$ '<br>( $\bar{1}$ ' 0,0,0)' | (6) a' (1/2,0,0) x,y,0<br>(m <sub>z</sub> ' 1/2,0,0)' | (7) m' x,0,z<br>(m <sub>y</sub> ' 0,0,0)' | (8) m' 1/4,y,z<br>(m <sub>x</sub> ' 1/2,0,0)'         |
| For 1' + set                             |   |   |   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

### Positions

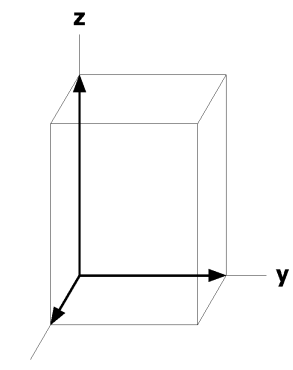
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
8 l 11'	(1) x,y,z [0,0,0] (5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(2) $\bar{x}+1/2,\bar{y},z$ [0,0,0] (6) $x+1/2,y,\bar{z}$ [0,0,0]	(3) $\bar{x},y,\bar{z}$ [0,0,0] (7) $x,\bar{y},z$ [0,0,0]	(4) $x+1/2,\bar{y},\bar{z}$ [0,0,0] (8) $\bar{x}+1/2,y,z$ [0,0,0]
4 k m..1'	1/4,y,z [0,0,0]	1/4, $\bar{y},z$ [0,0,0]	3/4,y, $\bar{z}$ [0,0,0]	3/4, $\bar{y},\bar{z}$ [0,0,0]
4 j .m.1'	x,1/2,z [0,0,0]	$\bar{x}+1/2,1/2,z$ [0,0,0]	$\bar{x},1/2,\bar{z}$ [0,0,0]	$x+1/2,1/2,\bar{z}$ [0,0,0]
4 i .m.1'	x,0,z [0,0,0]	$\bar{x}+1/2,0,z$ [0,0,0]	$\bar{x},0,\bar{z}$ [0,0,0]	$x+1/2,0,\bar{z}$ [0,0,0]
4 h .2.1'	0,y,1/2 [0,0,0]	1/2, $\bar{y},1/2$ [0,0,0]	0, $\bar{y},1/2$ [0,0,0]	1/2,y,1/2 [0,0,0]
4 g .2.1'	0,y,0 [0,0,0]	1/2, $\bar{y},0$ [0,0,0]	0, $\bar{y},0$ [0,0,0]	1/2,y,0 [0,0,0]
2 f mm21'	1/4,1/2,z [0,0,0]	3/4,1/2, $\bar{z}$ [0,0,0]		
2 e mm21'	1/4,0,z [0,0,0]	3/4,0, $\bar{z}$ [0,0,0]		
2 d .2/m.1'	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2 c .2/m.1'	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
2 b .2/m.1'	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]		
2 a .2/m.1'	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

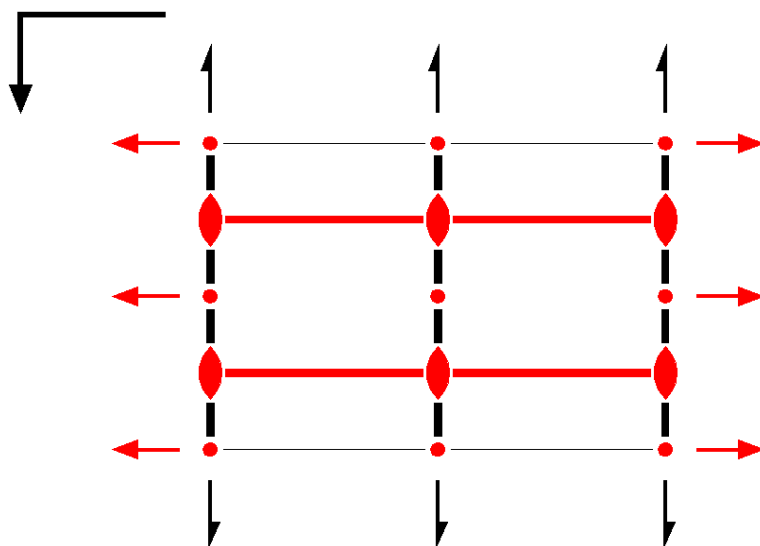
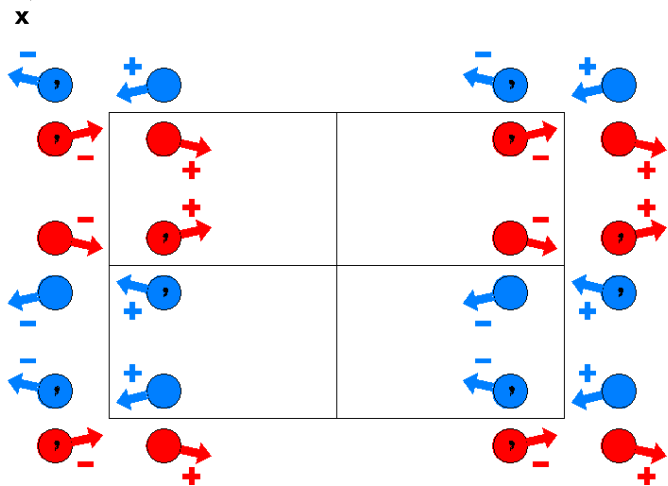
Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pm'ma  
51.3.389

m'mm  
P2<sub>1</sub>/m'2'/m2'/a

Orthorhombic



**Origin** at center ( 2'/m ) at 2, 2'/ma

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                      | (2) 2' 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,0)'       | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (4) 2 (1/2,0,0) x,0,0<br>(2 <sub>x</sub>  1/2,0,0) |
| (5) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)' | (6) a (1/2,0,0) x,y,0<br>(m <sub>z</sub>  1/2,0,0) | (7) m x,0,z<br>(m <sub>y</sub>  0,0,0)   | (8) m' 1/4,y,z<br>(m <sub>x</sub>  1/2,0,0)'       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

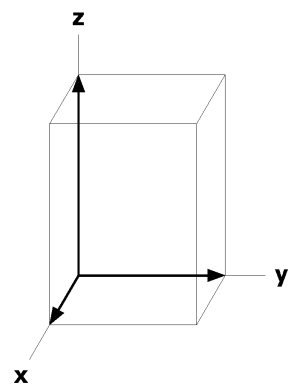
		Coordinates				
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	l	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [u,v, $\bar{w}$ ] (6) $x+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x}+1/2,y,z$ [ $\bar{u},v,w$ ]
4	k	m'..	1/4,y,z [0,v,w]	1/4, $\bar{y},z$ [0,v, $\bar{w}$ ]	3/4,y, $\bar{z}$ [0, $\bar{v},w$ ]	3/4, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
4	j	.m.	x,1/2,z [0,v,0]	$\bar{x}+1/2,1/2,z$ [0,v,0]	$\bar{x},1/2,\bar{z}$ [0, $\bar{v},0$ ]	$x+1/2,1/2,\bar{z}$ [0, $\bar{v},0$ ]
4	i	.m.	x,0,z [0,v,0]	$\bar{x}+1/2,0,z$ [0,v,0]	$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	$x+1/2,0,\bar{z}$ [0, $\bar{v},0$ ]
4	h	.2'	0,y,1/2 u,0,w]	1/2, $\bar{y},1/2$ [u,0, $\bar{w}$ ]	0, $\bar{y},1/2$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,1/2 [ $\bar{u},0,w$ ]
4	g	.2'	0,y,0 [u,0,w]	1/2, $\bar{y},0$ [u,0, $\bar{w}$ ]	0, $\bar{y},0$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,0 [ $\bar{u},0,w$ ]
2	f	m'm2'	1/4,1/2,z [0,v,0]	3/4,1/2, $\bar{z}$ [0, $\bar{v},0$ ]		
2	e	m'm2'	1/4,0,z [0,v,0]	3/4,0, $\bar{z}$ [0, $\bar{v},0$ ]		
2	d	.2'/m.	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	c	.2'/m.	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	b	.2'/m.	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a	.2'/m.	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2a}$ -2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



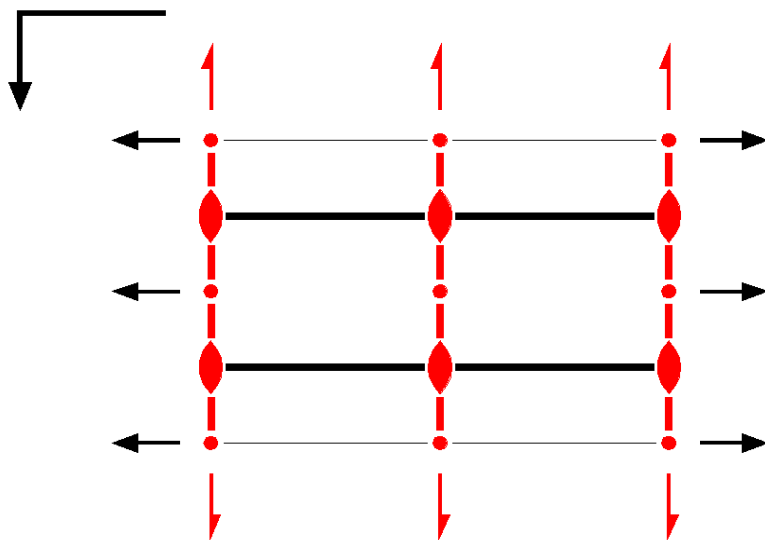
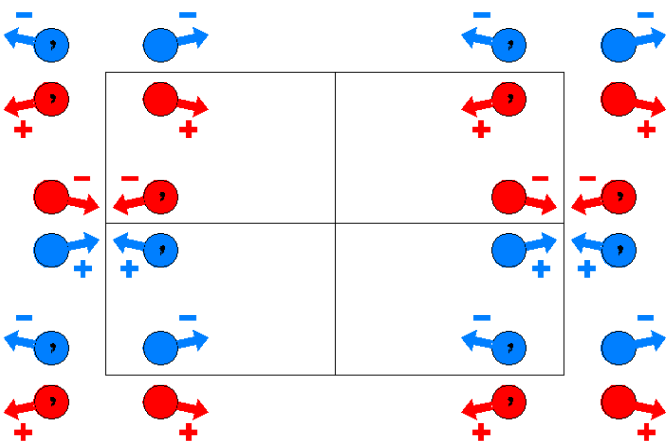
Pmm'a

51.4.390

mm'm

P2<sub>1</sub>'/m2/m'2'/a

Orthorhombic



**Origin** at center ( $2/m'$ ) at  $2, '2/m'a$

**Asymmetric unit**  $0 \leq x \leq 1/4;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

- |   |                                      |                                    |                                      |
|---|--------------------------------------|------------------------------------|--------------------------------------|
| (1) 1<br>(1 0,0,0)                      | (2) 2'<br>(2 <sub>z</sub>  1/2,0,0)' | (3) 2<br>(2 <sub>y</sub>  0,0,0)   | (4) 2'<br>(2 <sub>x</sub>  1/2,0,0)' |
| (5) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)' | (6) a<br>(m <sub>z</sub>  1/2,0,0)   | (7) m'<br>(m <sub>y</sub>  0,0,0)' | (8) m<br>(m <sub>x</sub>  1/2,0,0)   |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

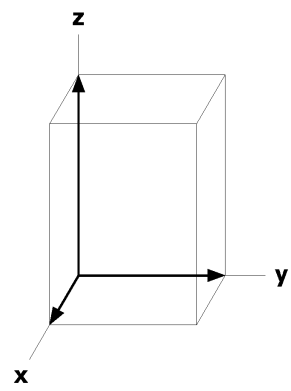
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	l 1	(1) x,y,z [u,v,w] (5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(2) $\bar{x}+1/2, \bar{y}, \bar{z}$ [u,v, $\bar{w}$ ] (6) $x+1/2, y, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ] (7) $x, \bar{y}, z$ [u, $\bar{v}, w$ ]	(4) $x+1/2, \bar{y}, \bar{z}$ [ $\bar{u}, v, w$ ] (8) $\bar{x}+1/2, y, z$ [u, $\bar{v}, \bar{w}$ ]
4	k m..	1/4,y,z [u,0,0]	1/4, $\bar{y}$ ,z [u,0,0]	3/4,y, $\bar{z}$ [ $\bar{u}, 0, 0$ ]	3/4, $\bar{y}$ , $\bar{z}$ [ $\bar{u}, 0, 0$ ]
4	j .m'	x,1/2,z [u,0,w]	$\bar{x}+1/2, 1/2, z$ [u,0, $\bar{w}$ ]	$\bar{x}, 1/2, \bar{z}$ [ $\bar{u}, 0, \bar{w}$ ]	$x+1/2, 1/2, \bar{z}$ [ $\bar{u}, 0, w$ ]
4	i .m'	x,0,z [u,0,w]	$\bar{x}+1/2, 0, z$ [u,0, $\bar{w}$ ]	$\bar{x}, 0, \bar{z}$ [ $\bar{u}, 0, \bar{w}$ ]	$x+1/2, 0, \bar{z}$ [ $\bar{u}, 0, w$ ]
4	h .2.	0,y,1/2 [0,v,0]	1/2, $\bar{y}$ ,1/2 [0,v,0]	0, $\bar{y}$ ,1/2 [0, $\bar{v}$ ,0]	1/2,y,1/2 [0, $\bar{v}$ ,0]
4	g .2.	0,y,0 [0,v,0]	1/2, $\bar{y}$ ,0 [0,v,0]	0, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]	1/2,y,0 [0, $\bar{v}$ ,0]
2	f mm'2'	1/4,1/2,z [u,0,0]	3/4,1/2, $\bar{z}$ [ $\bar{u}, 0, 0$ ]		
2	e mm'2'	1/4,0,z [u,0,0]	3/4,0, $\bar{z}$ [ $\bar{u}, 0, 0$ ]		
2	d .2/m'	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	c .2/m'	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	b .2/m'	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a .2/m'	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2a} \cdot 2m' m'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

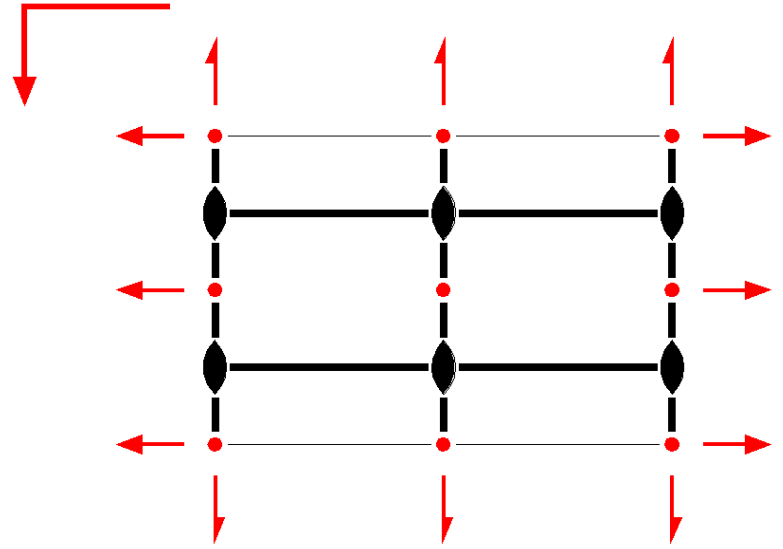
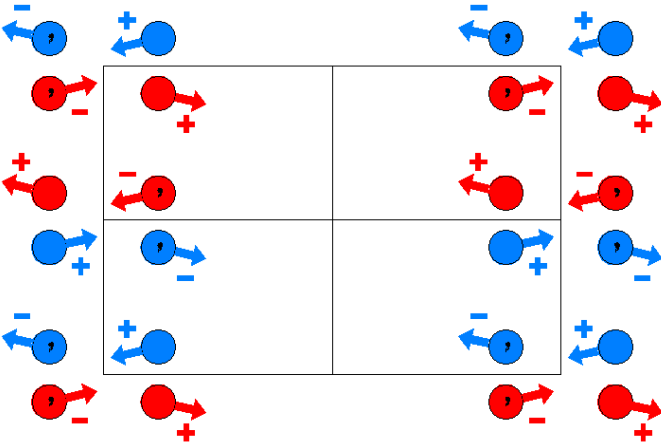
Along [0,1,0]  $p2mg$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pmma'  
51.5.391

mmm'  
P2<sub>1</sub>'/m2'/m2/a'

Orthorhombic



Origin at center ( 2'/m ) at 2, '2'/ma'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

### Symmetry Operations

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                      | (2) 2 $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)             | (3) 2' $0,y,0$<br>(2 <sub>y</sub>  0,0,0)' | (4) 2' $(1/2,0,0)$ $x,0,0$<br>(2 <sub>x</sub>  1/2,0,0)' |
| (5) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)' | (6) a' $(1/2,0,0)$ $x,y,0$<br>(m <sub>z</sub>  1/2,0,0)' | (7) m $x,0,z$<br>(m <sub>y</sub>  0,0,0)   | (8) m $1/4,y,z$<br>(m <sub>x</sub>  1/2,0,0)             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

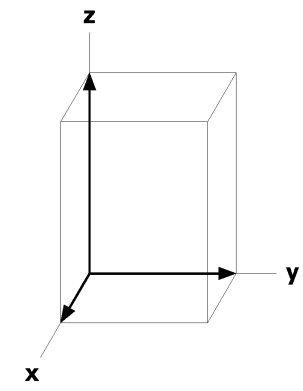
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
8	l	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x}+1/2,y,z$ [u, $\bar{v},\bar{w}$ ]
4	k	m..	1/4,y,z [u,0,0]	1/4, $\bar{y},z$ [ $\bar{u},0,0$ ]	3/4,y, $\bar{z}$ [u,0,0]	3/4, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
4	j	.m.	x,1/2,z [0,v,0]	$\bar{x}+1/2,1/2,z$ [0, $\bar{v},0$ ]	$\bar{x},1/2,\bar{z}$ [0, $\bar{v},0$ ]	$x+1/2,1/2,\bar{z}$ [0,v,0]
4	i	.m.	x,0,z [0,v,0]	$\bar{x}+1/2,0,z$ [0, $\bar{v},0$ ]	$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	$x+1/2,0,\bar{z}$ [0,v,0]
4	h	.2'	0,y,1/2 [u,0,w]	1/2, $\bar{y},1/2$ [ $\bar{u},0,w$ ]	0, $\bar{y},1/2$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,1/2 [u,0, $\bar{w}$ ]
4	g	.2'	0,y,0 [u,0,w]	1/2, $\bar{y},0$ [ $\bar{u},0,w$ ]	0, $\bar{y},0$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,0 [u,0, $\bar{w}$ ]
2	f	mm2	1/4,1/2,z [0,0,0]	3/4,1/2, $\bar{z}$ [0,0,0]		
2	e	mm2	1/4,0,z [0,0,0]	3/4,0, $\bar{z}$ [0,0,0]		
2	d	.2'/m.	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	c	.2'/m.	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	b	.2'/m.	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a	.2'/m.	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



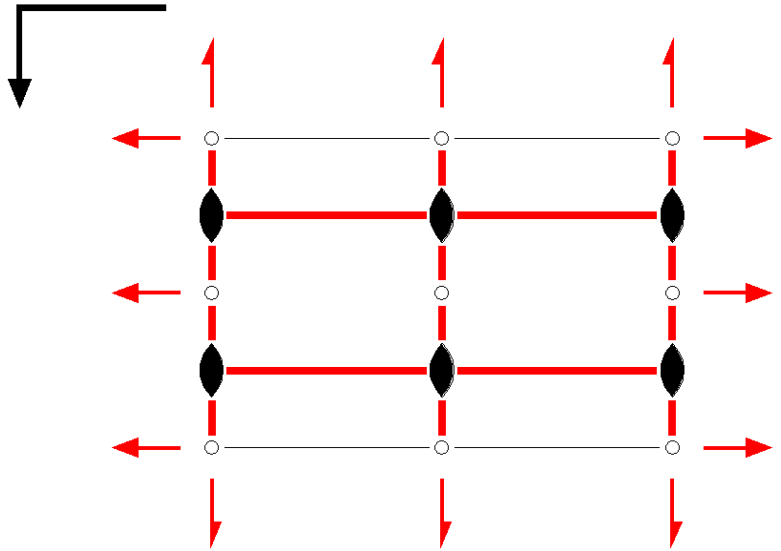
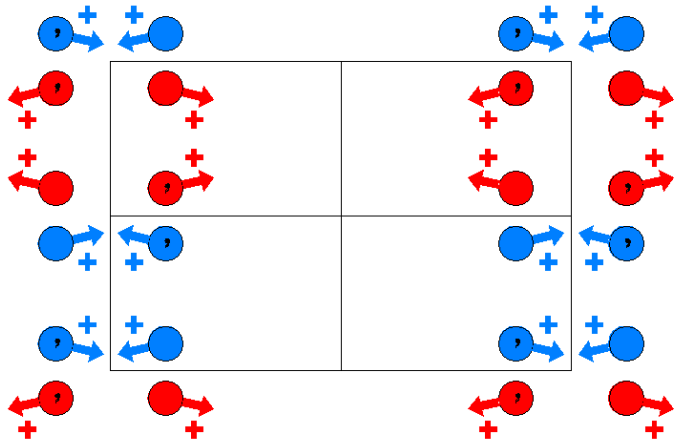
Pm'm'a

51.6.392

m'm'm

P2<sub>1</sub>'/m'2'/m'2/a

Orthorhombic



**Origin** at center ( $2'/m'$ ) at  $2_1'2'/m'a$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) 1<br>(1 0,0,0)                   | (2) 2 $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)           | (3) 2' $0,y,0$<br>(2 <sub>y</sub>  0,0,0)' | (4) 2' $(1/2,0,0)$ $x,0,0$<br>(2 <sub>x</sub>  1/2,0,0)' |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) a $(1/2,0,0)$ $x,y,0$<br>(m <sub>z</sub>  1/2,0,0) | (7) m' $x,0,z$<br>(m <sub>y</sub>  0,0,0)' | (8) m' $1/4,y,z$<br>(m <sub>x</sub>  1/2,0,0)'           |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

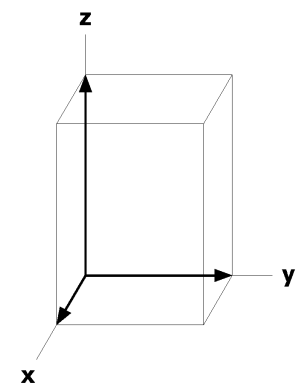
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	l	1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, \bar{y}, \bar{z}$ [u, $\bar{v}, w$ ]	(4) $x+1/2, \bar{y}, \bar{z}$ [ $\bar{u}, v, w$ ]
			(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(7) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, w$ ]	(8) $\bar{x}+1/2, y, z$ [ $\bar{u}, v, w$ ]
4	k	m'..	1/4,y,z [0,v,w]	1/4, $\bar{y}, z$ [0, $\bar{v}, w$ ]	3/4,y, $\bar{z}$ [0, $\bar{v}, w$ ]	3/4, $\bar{y}, \bar{z}$ [0,v,w]
4	j	.m'.	x,1/2,z [u,0,w]	$\bar{x}+1/2, 1/2, z$ [ $\bar{u}, 0, w$ ]	$\bar{x}, 1/2, \bar{z}$ [u,0,w]	$x+1/2, 1/2, \bar{z}$ [ $\bar{u}, 0, w$ ]
4	i	.m'.	x,0,z [u,0,w]	$\bar{x}+1/2, 0, z$ [ $\bar{u}, 0, w$ ]	$\bar{x}, 0, \bar{z}$ [u,0,w]	$x+1/2, 0, \bar{z}$ [ $\bar{u}, 0, w$ ]
4	h	.2'.	0,y,1/2 [u,0,w]	1/2, $\bar{y}, 1/2$ [ $\bar{u}, 0, w$ ]	0, $\bar{y}, 1/2$ [u,0,w]	1/2,y,1/2 [ $\bar{u}, 0, w$ ]
4	g	.2'.	0,y,0 [u,0,w]	1/2, $\bar{y}, 0$ [ $\bar{u}, 0, w$ ]	0, $\bar{y}, 0$ [u,0,w]	1/2,y,0 [ $\bar{u}, 0, w$ ]
2	f	m'm'2	1/4,1/2,z [0,0,w]	3/4,1/2, $\bar{z}$ [0,0,w]		
2	e	m'm'2	1/4,0,z [0,0,w]	3/4,0, $\bar{z}$ [0,0,w]		
2	d	.2'/m'.	0,1/2,1/2 [u,0,w]	1/2,1/2,1/2 [ $\bar{u}, 0, w$ ]		
2	c	.2'/m'.	0,0,1/2 [u,0,w]	1/2,0,1/2 [ $\bar{u}, 0, w$ ]		
2	b	.2'/m'.	0,1/2,0 [u,0,w]	1/2,1/2,0 [ $\bar{u}, 0, w$ ]		
2	a	.2'/m'.	0,0,0 [u,0,w]	1/2,0,0 [ $\bar{u}, 0, w$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,0,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at x,0,0

Along [0,1,0]  $p2'm'g$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



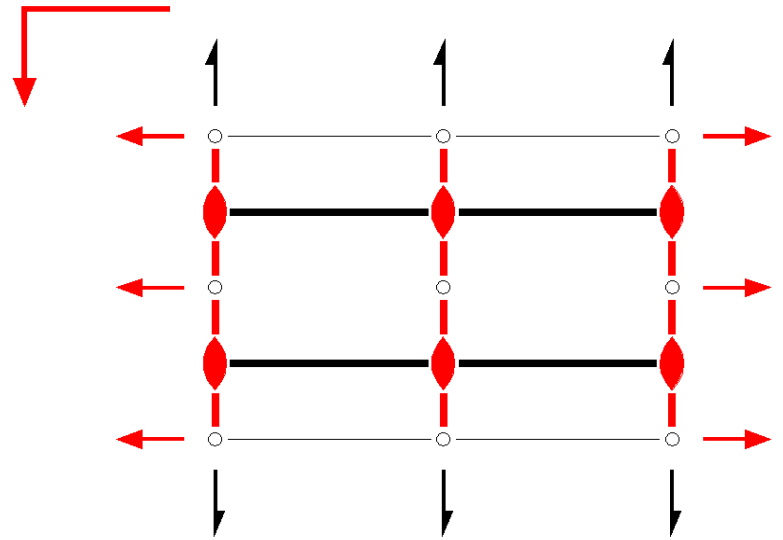
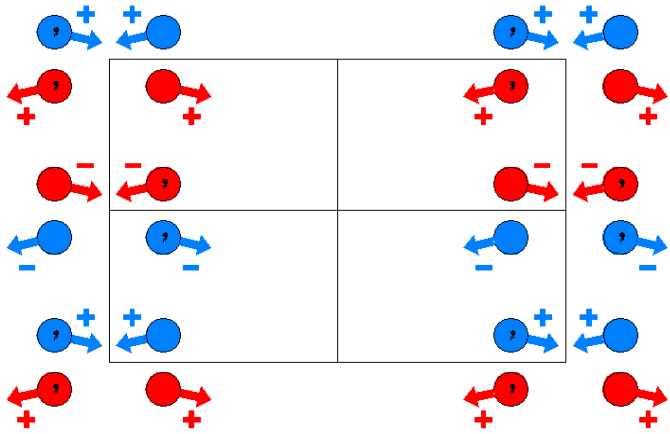
Pmm'a'

51.7.393

mm'm'

P2<sub>1</sub>/m2'/m'2'/a'

Orthorhombic



**Origin** at center ( $2'/m'$ ) at  $2, 2/m'a'$

**Asymmetric unit**  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

- |                                      |  |                                    |  |
|--------------------------------------|--|------------------------------------|--|
| (1) 1<br>(1 0,0,0)                   | (2) 2'<br>(2 <sub>z</sub>  1/2,0,0)'                 | (3) 2'<br>(2 <sub>y</sub>  0,0,0)' | (4) 2 (1/2,0,0) x,0,0<br>(2 <sub>x</sub>  1/2,0,0) |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) a' (1/2,0,0) x,y,0<br>(m <sub>z</sub>  1/2,0,0)' | (7) m'<br>(m <sub>y</sub>  0,0,0)' | (8) m 1/4,y,z<br>(m <sub>x</sub>  1/2,0,0)         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

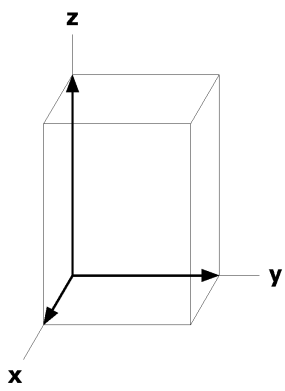
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	l	1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}, y, \bar{z}$ [u, $\bar{v}$ ,w]	(4) $x+1/2, \bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
			(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y, \bar{z}$ [u,v, $\bar{w}$ ]	(7) $x, \bar{y}, z$ [u, $\bar{v}$ ,w]	(8) $\bar{x}+1/2, y, z$ [u, $\bar{v}, \bar{w}$ ]
4	k	m..	1/4,y,z [u,0,0]	1/4, $\bar{y}$ ,z [u,0,0]	3/4,y, $\bar{z}$ [u,0,0]	3/4, $\bar{y}, \bar{z}$ [u,0,0]
4	j	.m'	x,1/2,z [u,0,w]	$\bar{x}+1/2, 1/2, z$ [u,0, $\bar{w}$ ]	$\bar{x}, 1/2, \bar{z}$ [u,0,w]	$x+1/2, 1/2, \bar{z}$ [u,0, $\bar{w}$ ]
4	i	.m'	x,0,z [u,0,w]	$\bar{x}+1/2, 0, z$ [u,0, $\bar{w}$ ]	$\bar{x}, 0, \bar{z}$ [u,0,w]	$x+1/2, 0, \bar{z}$ [u,0, $\bar{w}$ ]
4	h	.2'	0,y,1/2 [u,0,w]	1/2, $\bar{y}, 1/2$ [u,0, $\bar{w}$ ]	0, $\bar{y}, 1/2$ [u,0,w]	1/2,y,1/2 [u,0, $\bar{w}$ ]
4	g	.2'	0,y,0 [u,0,w]	1/2, $\bar{y}, 0$ [u,0, $\bar{w}$ ]	0, $\bar{y}, 0$ [u,0,w]	1/2,y,0 [u,0, $\bar{w}$ ]
2	f	mm'2'	1/4,1/2,z [u,0,0]	3/4,1/2, $\bar{z}$ [u,0,0]		
2	e	mm'2'	1/4,0,z [u,0,0]	3/4,0, $\bar{z}$ [u,0,0]		
2	d	.2'/m'	0,1/2,1/2 [u,0,w]	1/2,1/2,1/2 [u,0, $\bar{w}$ ]		
2	c	.2'/m'	0,0,1/2 [u,0,w]	1/2,0,1/2 [u,0, $\bar{w}$ ]		
2	b	.2'/m'	0,1/2,0 [u,0,w]	1/2,1/2,0 [u,0, $\bar{w}$ ]		
2	a	.2'/m'	0,0,0 [u,0,w]	1/2,0,0 [u,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

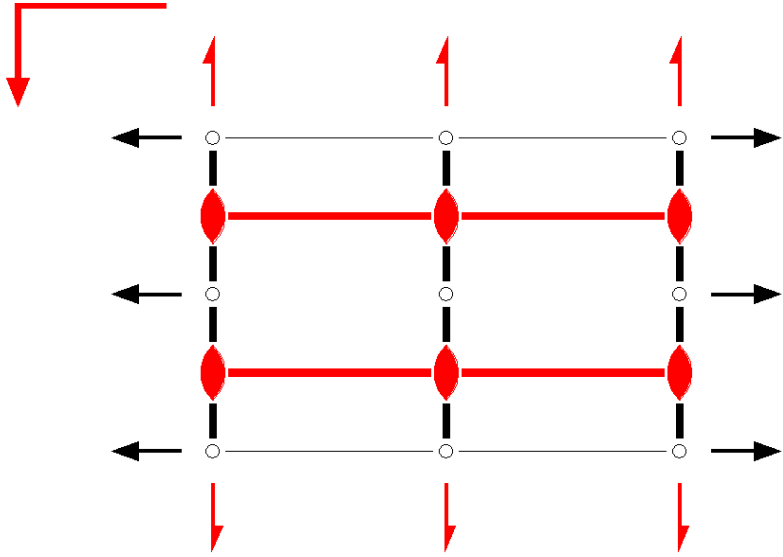
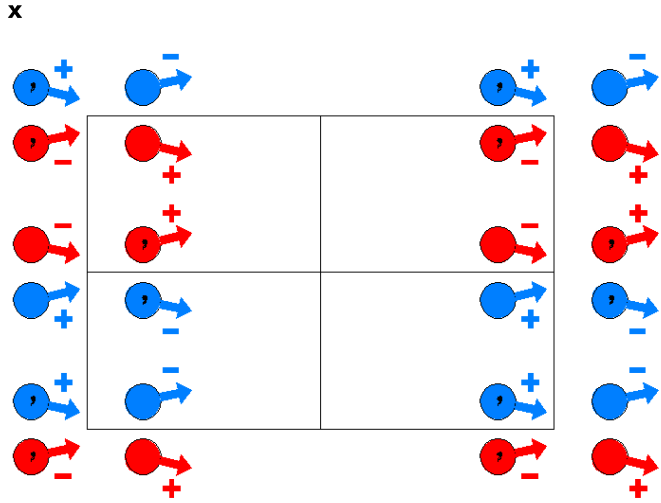
Along [0,1,0] p2'mg'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pm'ma'  
51.8.394

m'mm'  
P2<sub>1</sub>'/m'2/m2'/a'

Orthorhombic



**Origin** at center ( $2/m$ ) at  $2, '2/ma'$

**Asymmetric unit**  $0 \leq x \leq 1/4;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

- |                                      |                                      |                                  |                                      |
|--------------------------------------|--------------------------------------|----------------------------------|--------------------------------------|
| (1) 1<br>(1 0,0,0)                   | (2) 2'<br>(2 <sub>z</sub>  1/2,0,0)' | (3) 2<br>(2 <sub>y</sub>  0,0,0) | (4) 2'<br>(2 <sub>x</sub>  1/2,0,0)' |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) a'<br>(m <sub>z</sub>  1/2,0,0)' | (7) m<br>(m <sub>y</sub>  0,0,0) | (8) m'<br>(m <sub>x</sub>  1/2,0,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

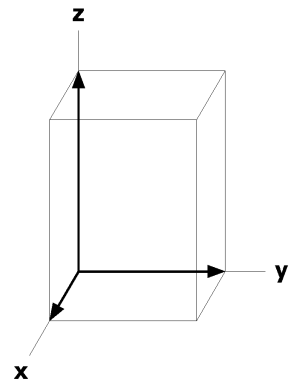
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	l	1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x+1/2, \bar{y}, \bar{z}$ [ $\bar{u}, v, w$ ]
			(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y, \bar{z}$ [u,v, $\bar{w}$ ]	(7) $x, \bar{y}, z$ [ $\bar{u}, v, \bar{w}$ ]	(8) $\bar{x}+1/2, y, z$ [ $\bar{u}, v, w$ ]
4	k	m'..	1/4,y,z [0,v,w]	1/4, $\bar{y}, z$ [0,v, $\bar{w}$ ]	3/4,y, $\bar{z}$ [0,v, $\bar{w}$ ]	3/4, $\bar{y}, \bar{z}$ [0,v,w]
4	j	.m.	x,1/2,z [0,v,0]	$\bar{x}+1/2, 1/2, z$ [0,v,0]	$\bar{x}, 1/2, \bar{z}$ [0,v,0]	$x+1/2, 1/2, \bar{z}$ [0,v,0]
4	i	.m.	x,0,z [0,v,0]	$\bar{x}+1/2, 0, z$ [0,v,0]	$\bar{x}, 0, \bar{z}$ [0,v,0]	$x+1/2, 0, \bar{z}$ [0,v,0]
4	h	.2.	0,y,1/2 [0,v,0]	1/2, $\bar{y}, 1/2$ [0,v,0]	0, $\bar{y}, 1/2$ [0,v,0]	1/2,y,1/2 [0,v,0]
4	g	.2.	0,y,0 [0,v,0]	1/2, $\bar{y}, 0$ [0,v,0]	0, $\bar{y}, 0$ [0,v,0]	1/2,y,0 [0,v,0]
2	f	m'm2'	1/4,1/2,z [0,v,0]	3/4,1/2, $\bar{z}$ [0,v,0]		
2	e	m'm2'	1/4,0,z [0,v,0]	3/4,0, $\bar{z}$ [0,v,0]		
2	d	.2/m.	0,1/2,1/2 [0,v,0]	1/2,1/2,1/2 [0,v,0]		
2	c	.2/m.	0,0,1/2 [0,v,0]	1/2,0,1/2 [0,v,0]		
2	b	.2/m.	0,1/2,0 [0,v,0]	1/2,1/2,0 [0,v,0]		
2	a	.2/m.	0,0,0 [0,v,0]	1/2,0,0 [0,v,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



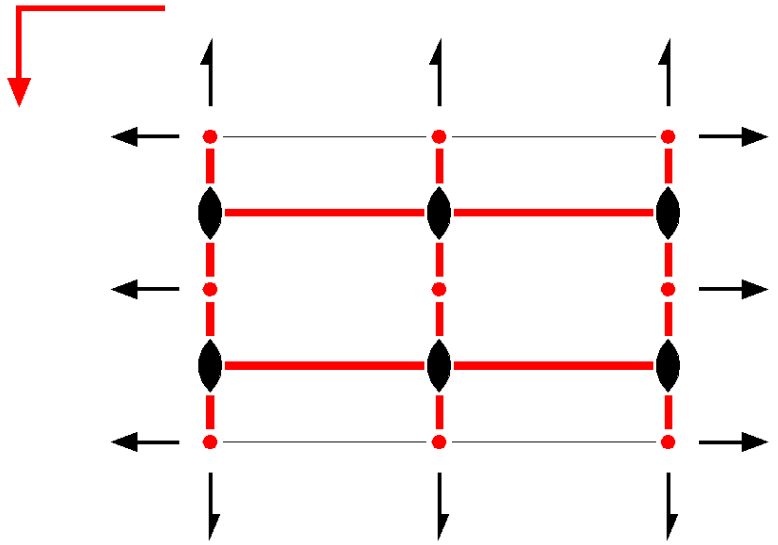
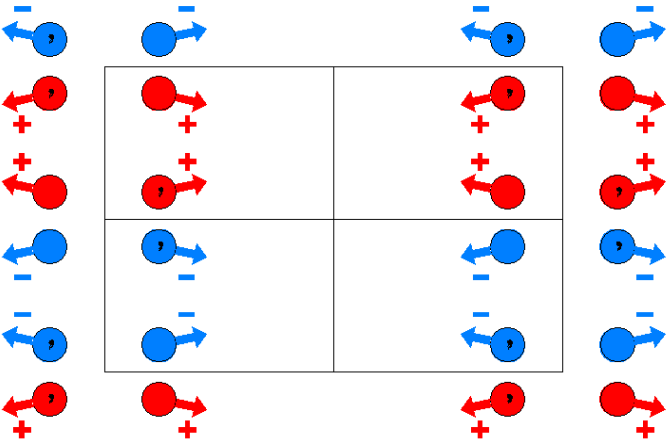
Pm'm'a'

51.9.395

m'm'm'

P2<sub>1</sub>/m'2/m'2/a'

Orthorhombic



**Origin** at center ( 2/m' ) at 2, 2/m'a'

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                      | (2) 2 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,0)           | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 (1/2,0,0) x,0,0<br>(2 <sub>x</sub>  1/2,0,0) |
| (5) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)' | (6) a' (1/2,0,0) x,y,0<br>(m <sub>z</sub>  1/2,0,0)' | (7) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (8) m' 1/4,y,z<br>(m <sub>x</sub>  1/2,0,0)'       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

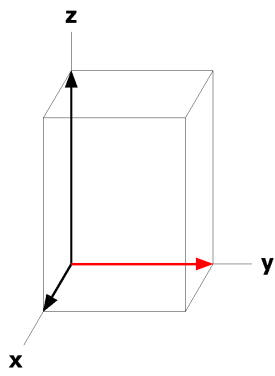
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	l	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
			(6) $x+1/2,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(7) $x,\bar{y},z$ [ $u,\bar{v},w$ ]	(8) $\bar{x}+1/2,y,z$ [ $\bar{u},v,w$ ]	
4	k	m'..	1/4,y,z [0,v,w]	1/4, $\bar{y},z$ [0, $\bar{v},w$ ]	3/4,y, $\bar{z}$ [0,v, $\bar{w}$ ]	3/4, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
4	j	.m'.	x,1/2,z [u,0,w]	$\bar{x}+1/2,1/2,z$ [ $\bar{u},0,w$ ]	$\bar{x},1/2,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	$x+1/2,1/2,\bar{z}$ [ $u,0,\bar{w}$ ]
4	i	.m'.	x,0,z [u,0,w]	$\bar{x}+1/2,0,z$ [ $\bar{u},0,w$ ]	$\bar{x},0,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	$x+1/2,0,\bar{z}$ [ $u,0,\bar{w}$ ]
4	h	.2.	0,y,1/2 [0,v,0]	1/2, $\bar{y},1/2$ [0, $\bar{v},0$ ]	0, $\bar{y},1/2$ [0, $\bar{v},0$ ]	1/2,y,1/2 [0,v,0]
4	g	.2.	0,y,0 [0,v,0]	1/2, $\bar{y},0$ [0, $\bar{v},0$ ]	0, $\bar{y},0$ [0, $\bar{v},0$ ]	1/2,y,0 [0,v,0]
2	f	m'm'2	1/4,1/2,z [0,0,w]	3/4,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	e	m'm'2	1/4,0,z [0,0,w]	3/4,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	d	.2/m'.	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	c	.2/m'.	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	b	.2/m'.	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a	.2/m'.	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

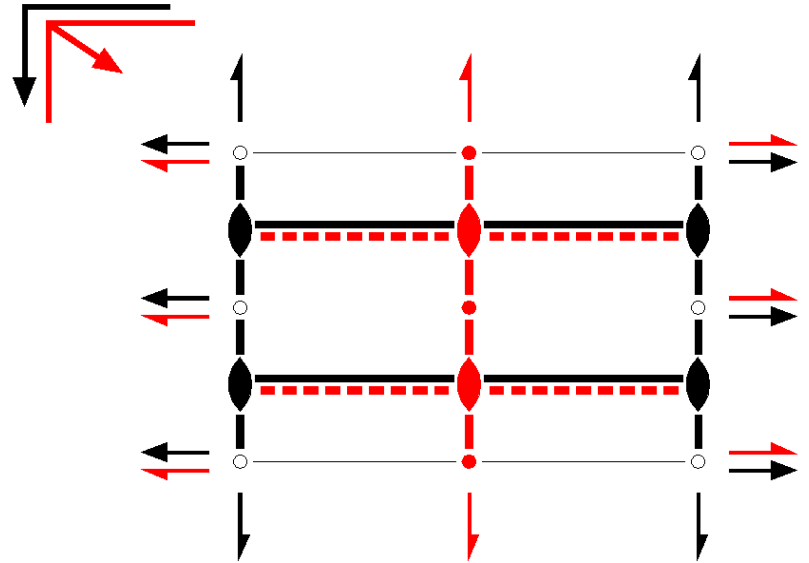
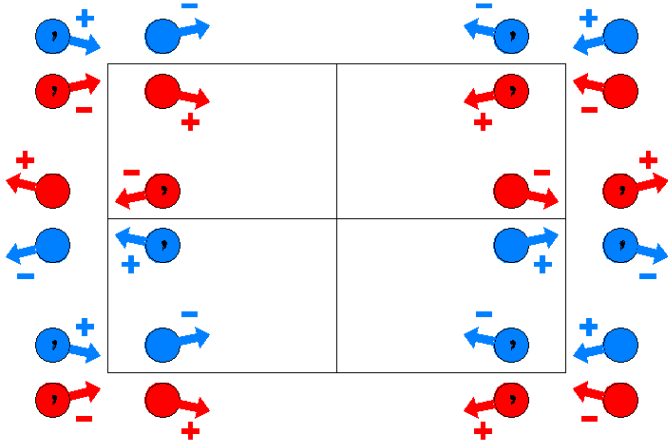
Along [0,1,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



$P_{2b}$  mma  
51.10.396

mmm1'  
 $P_{2b} 2_1/m2/m2/a$

Orthorhombic



**Origin** at center ( $2/m$ ) at  $2, 2/ma$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)      (2) 2  $1/4, 0, z$   
( $2_z$ | $1/2, 0, 0$ )      (3) 2  $0, y, 0$   
( $2_y$ | $0, 0, 0$ )      (4) 2  $(1/2, 0, 0)$   $x, 0, 0$   
( $2_x$ | $1/2, 0, 0$ )

(5)  $\bar{1}$   
( $\bar{1}$ |0,0,0)      (6) a  $(1/2, 0, 0)$   $x, y, 0$   
( $m_z$ | $1/2, 0, 0$ )      (7) m  $x, 0, z$   
( $m_y$ | $0, 0, 0$ )      (8) m  $1/4, y, z$   
( $m_x$ | $1/2, 0, 0$ )

For  $(0, 1, 0)'$  + set

(1)  $t'$   $(0, 1, 0)$   
(1| $0, 1, 0$ )'      (2)  $2'$   $1/4, 1/2, z$   
( $2_z$ | $1/2, 1, 0$ )'      (3)  $2'$   $(0, 1, 0)$   $0, y, 0$   
( $2_y$ | $0, 1, 0$ )'      (4)  $2'$   $(1/2, 0, 0)$   $x, 1/2, 0$   
( $2_x$ | $1/2, 1, 0$ )'

(5)  $\bar{1}'$   $0, 1/2, 0$   
( $\bar{1}$ | $0, 1, 0$ )'      (6)  $n'$   $(1/2, 1, 0)$   $x, y, 0$   
( $m_z$ | $1/2, 1, 0$ )'      (7)  $m'$   $x, 1/2, z$   
( $m_y$ | $0, 1, 0$ )'      (8)  $b'$   $(0, 1, 0)$   $1/4, y, z$   
( $m_x$ | $1/2, 1, 0$ )'

**Generators selected** (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

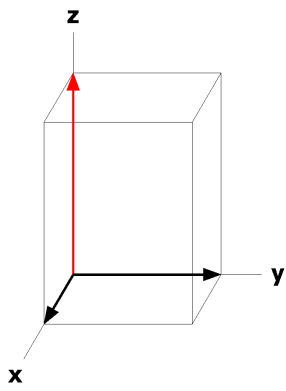
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
16 l 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x}+1/2,y,z$ [ $\bar{u},\bar{v},\bar{w}$ ]
8 k m..	1/4,y,z [u,0,0]	1/4, $\bar{y},z$ [ $\bar{u},0,0$ ]	3/4,y, $\bar{z}$ [ $\bar{u},0,0$ ]	3/4, $\bar{y},\bar{z}$ [u,0,0]
8 j .m'	x,1/2,z [u,0,w]	$\bar{x}+1/2,1/2,z$ [u,0, $\bar{w}$ ]	$\bar{x},1/2,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	$x+1/2,1/2,\bar{z}$ [ $\bar{u},0,w$ ]
8 i .m.	x,0,z [0,v,0]	$\bar{x}+1/2,0,z$ [0, $\bar{v},0$ ]	$\bar{x},0,\bar{z}$ [0,v,0]	$x+1/2,0,\bar{z}$ [0, $\bar{v},0$ ]
8 h .2.	0,y,1/2 [0,v,0]	1/2, $\bar{y},1/2$ [0, $\bar{v},0$ ]	0, $\bar{y},1/2$ [0,v,0]	1/2,y,1/2 [0, $\bar{v},0$ ]
8 g .2.	0,y,0 [0,v,0]	1/2, $\bar{y},0$ [0, $\bar{v},0$ ]	0, $\bar{y},0$ [0,v,0]	1/2,y,0 [0, $\bar{v},0$ ]
4 f mm'2'	1/4,1/2,z [u,0,0]	3/4,1/2, $\bar{z}$ [ $\bar{u},0,0$ ]		
4 e mm2	1/4,0,z [0,0,0]	3/4,0, $\bar{z}$ [0,0,0]		
4 d .2/m'	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 c .2/m.	0,0,1/2 [0,v,0]	1/2,0,1/2 [0, $\bar{v},0$ ]		
4 b .2/m'	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]		
4 a .2/m.	0,0,0 [0,v,0]	1/2,0,0 [0, $\bar{v},0$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>-2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

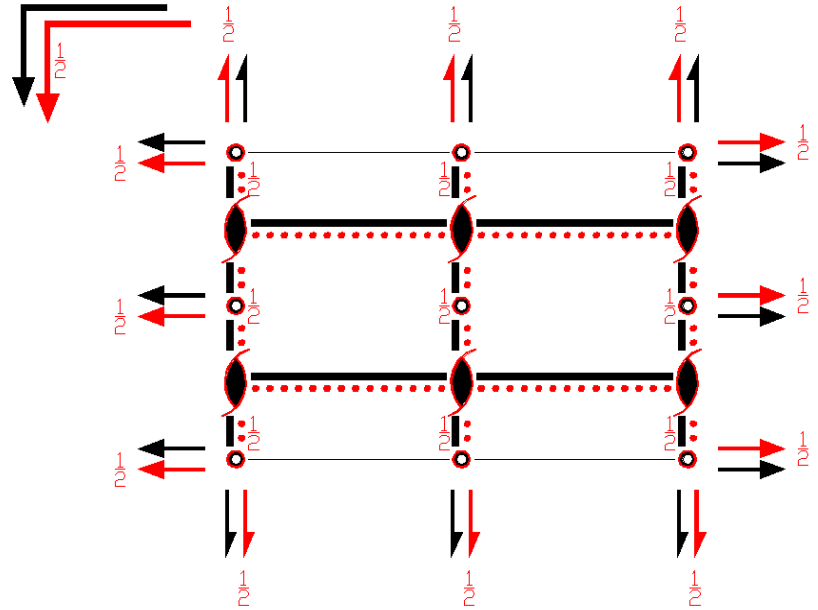
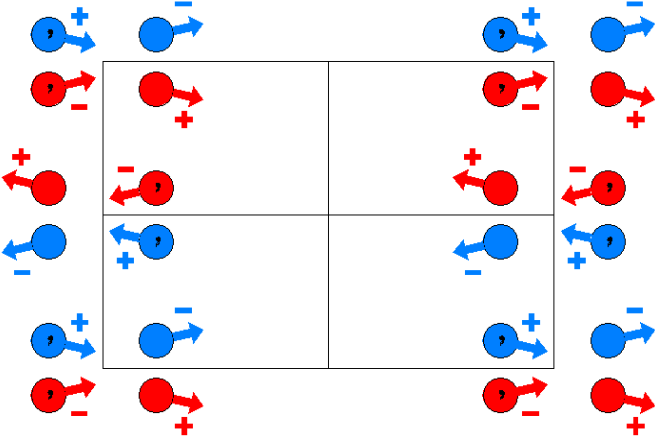
Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



$P_{2c} mma$   
51.11.397

$mmm1'$   
 $P_{2c} 2_1/m2/m2/a$

Orthorhombic



**Origin** at center ( $2/m$ ) at  $2, 2/ma$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2)  $2 \quad 1/4, 0, z$   
( $2_z$ | $1/2, 0, 0$ )

(3)  $2 \quad 0, y, 0$   
( $2_y$ | $0, 0, 0$ )

(4)  $2 \quad (1/2, 0, 0) \quad x, 0, 0$   
( $2_x$ | $1/2, 0, 0$ )

(5)  $\bar{1}$   
( $\bar{1}$ |0,0,0)

(6)  $a \quad (1/2, 0, 0) \quad x, y, 0$   
( $m_z$ | $1/2, 0, 0$ )

(7)  $m \quad x, 0, z$   
( $m_y$ | $0, 0, 0$ )

(8)  $m \quad 1/4, y, z$   
( $m_x$ | $1/2, 0, 0$ )

For (0,0,0) + set

For (0,0,1)' + set

(1)  $t' \quad (0, 0, 1)$   
(1|0,0,1)'

(2)  $2' \quad (0, 0, 1) \quad 1/4, 0, z$   
( $2_z$ | $1/2, 0, 1$ )'

(3)  $2' \quad 0, y, 1/2$   
( $2_y$ | $0, 0, 1$ )'

(4)  $2' \quad (1/2, 0, 0) \quad x, 0, 1/2$   
( $2_x$ | $1/2, 0, 1$ )'

(5)  $\bar{1}' \quad 0, 0, 1/2$   
( $\bar{1}$ |0,0,1)'

(6)  $a' \quad (1/2, 0, 0) \quad x, y, 1/2$   
( $m_z$ | $1/2, 0, 1$ )'

(7)  $c' \quad (0, 0, 1) \quad x, 0, z$   
( $m_y$ | $0, 0, 1$ )'

(8)  $c' \quad (0, 0, 1) \quad 1/4, y, z$   
( $m_x$ | $1/2, 0, 1$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

### Positions

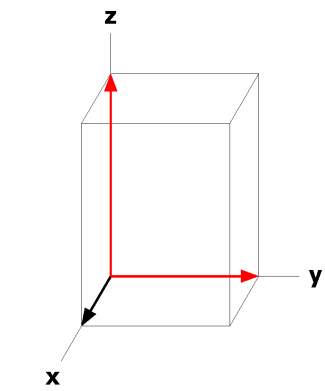
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
16 l 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x}+1/2,y,z$ [ $\bar{u},\bar{v},\bar{w}$ ]
8 k m..	1/4,y,z [u,0,0]	1/4, $\bar{y},z$ [ $\bar{u},0,0$ ]	3/4,y, $\bar{z}$ [ $\bar{u},0,0$ ]	3/4, $\bar{y},\bar{z}$ [u,0,0]
8 j .m.	x,1/2,z [0,v,0]	$\bar{x}+1/2,1/2,z$ [0, $\bar{v},0$ ]	$\bar{x},1/2,\bar{z}$ [0,v,0]	$x+1/2,1/2,\bar{z}$ [0, $\bar{v},0$ ]
8 i .m.	x,0,z [0,v,0]	$\bar{x}+1/2,0,z$ [0, $\bar{v},0$ ]	$\bar{x},0,\bar{z}$ [0,v,0]	$x+1/2,0,\bar{z}$ [0, $\bar{v},0$ ]
8 h .2'	0,y,1/2 [u,0,w]	1/2, $\bar{y},1/2$ [ $\bar{u},0,w$ ]	0, $\bar{y},1/2$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,1/2 [u,0, $\bar{w}$ ]
8 g .2.	0,y,0 [0,v,0]	1/2, $\bar{y},0$ [0, $\bar{v},0$ ]	0, $\bar{y},0$ [0,v,0]	1/2,y,0 [0, $\bar{v},0$ ]
4 f mm2	1/4,1/2,z [0,0,0]	3/4,1/2, $\bar{z}$ [0,0,0]		
4 e mm2	1/4,0,z [0,0,0]	3/4,0, $\bar{z}$ [0,0,0]		
4 d .2'/m.	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 c .2'/m.	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 b .2/m.	0,1/2,0 [0,v,0]	1/2,1/2,0 [0, $\bar{v},0$ ]		
4 a .2/m.	0,0,0 [0,v,0]	1/2,0,0 [0, $\bar{v},0$ ]		

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

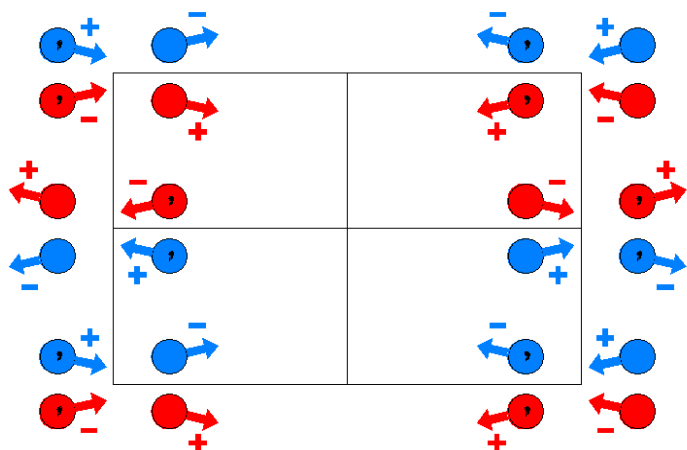
Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



$P_A mma$

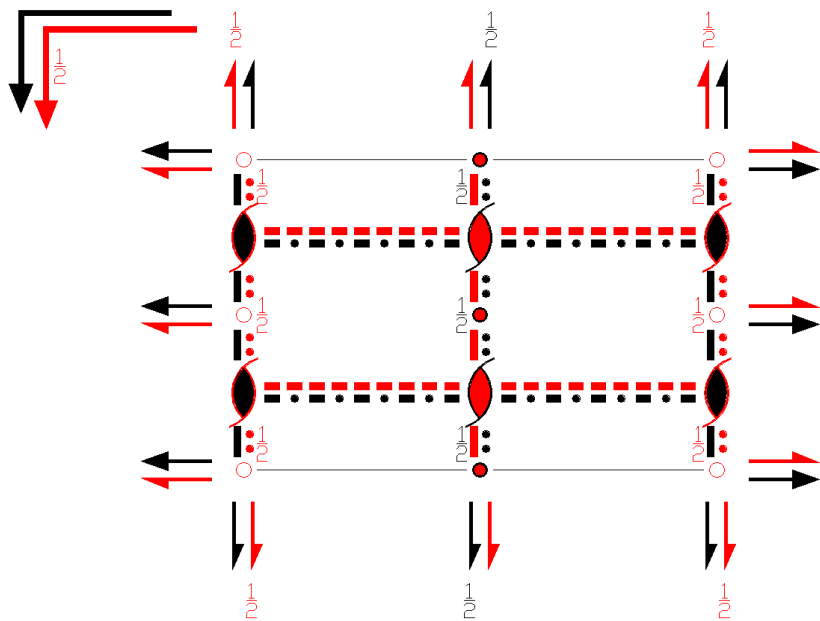
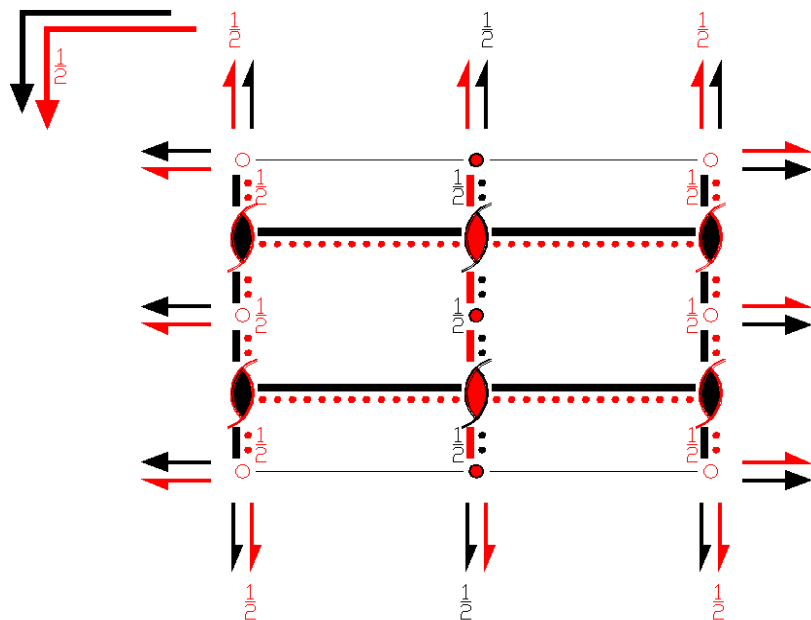
51.12.398



$mmm1'$

$P_A 2_1/m2/m2/a$

Orthorhombic



**Origin** at center ( $2/m$ ) at  $2, 2/ma$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$



**Symmetry Operations**

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 <sub>z</sub> 1/4,0,z (2 <sub>z</sub>  1/2,0,0)	(3) 2 <sub>y</sub> 0,y,0 (2 <sub>y</sub>  0,0,0)	(4) 2 <sub>x</sub> (1/2,0,0) x,0,0 (2 <sub>x</sub>  1/2,0,0)
(5) $\bar{1}$ ( $\bar{1}$  0,0,0)	(6) a (1/2,0,0) x,y,0 (m <sub>z</sub>  1/2,0,0)	(7) m <sub>y</sub> x,0,z (m <sub>y</sub>  0,0,0)	(8) m <sub>x</sub> 1/4,y,z (m <sub>x</sub>  1/2,0,0)

For (0,1,0)' + set

(1) t' (0,1,0) (1 0,1,0)'	(2) 2' <sub>z</sub> 1/4,1/2,z (2' <sub>z</sub>  1/2,1,0)'	(3) 2' (0,1,0) 0,y,0 (2' <sub>y</sub>  0,1,0)'	(4) 2' (1/2,0,0) x,1/2,0 (2' <sub>x</sub>  1/2,1,0)'
(5) $\bar{1}$ ' 0,1/2,0 ( $\bar{1}$  0,1,0)'	(6) n' (1/2,1,0) x,y,0 (m <sub>z</sub>  1/2,1,0)'	(7) m' <sub>y</sub> x,1/2,z (m' <sub>y</sub>  0,1,0)'	(8) b' (0,1,0) 1/4,y,z (m <sub>x</sub>  1/2,1,0)'

**Generators selected** (1); t(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).**Positions**

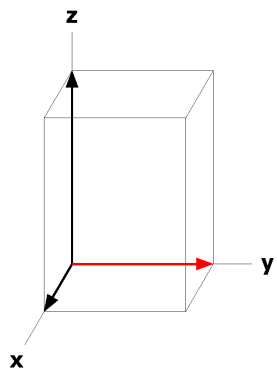
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
16 l 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x}+1/2,y,z$ [ $\bar{u},\bar{v},\bar{w}$ ]
8 k m..	1/4,y,z [u,0,0]	1/4, $\bar{y},z$ [ $\bar{u},0,0$ ]	3/4,y, $\bar{z}$ [ $\bar{u},0,0$ ]	3/4, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
8 j .m'.	x,1/2,z [u,0,w]	$\bar{x}+1/2,1/2,z$ [u,0, $\bar{w}$ ]	$\bar{x},1/2,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	$x+1/2,1/2,\bar{z}$ [ $\bar{u},0,w$ ]
8 i .m.	x,0,z [0,v,0]	$\bar{x}+1/2,0,z$ [0, $\bar{v},0$ ]	$\bar{x},0,\bar{z}$ [0,v,0]	$x+1/2,0,\bar{z}$ [0, $\bar{v},0$ ]
8 h .2'.	0,y,1/2 [u,0,w]	1/2, $\bar{y},1/2$ [ $\bar{u},0,w$ ]	0, $\bar{y},1/2$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,1/2 [u,0, $\bar{w}$ ]
8 g .2.	0,y,0 [0,v,0]	1/2, $\bar{y},0$ [0, $\bar{v},0$ ]	0, $\bar{y},0$ [0,v,0]	1/2,y,0 [0, $\bar{v},0$ ]
4 f mm'2'	1/4,1/2,z [u,0,0]	3/4,1/2, $\bar{z}$ [ $\bar{u},0,0$ ]		
4 e mm2	1/4,0,z [0,0,0]	3/4,0, $\bar{z}$ [0,0,0]		
4 d .2'/m'.	0,1/2,1/2 [u,0,w]	1/2,1/2,1/2 [u,0, $\bar{w}$ ]		
4 c .2'/m.	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 b .2'/m'.	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]		
4 a .2/m.	0,0,0 [0,v,0]	1/2,0,0 [0, $\bar{v},0$ ]		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,0,0$

Along  $[0,1,0]$   $p2mg1'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $0,y,0$



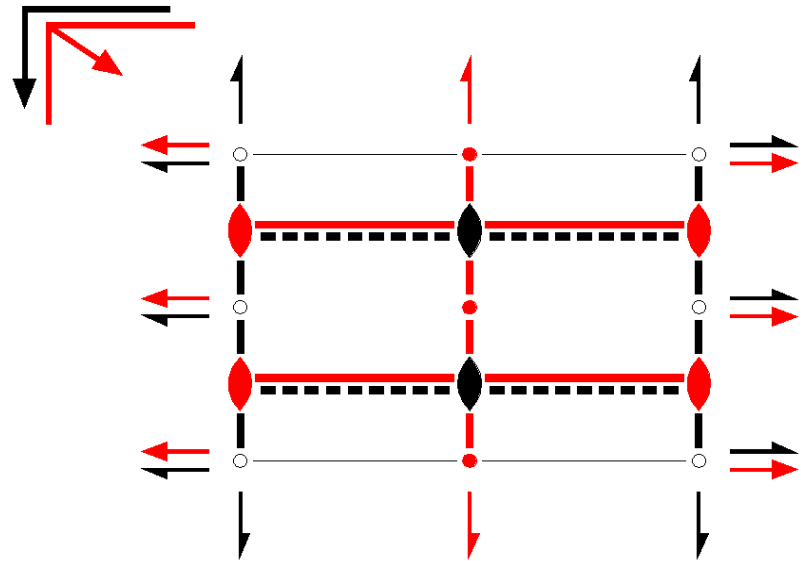
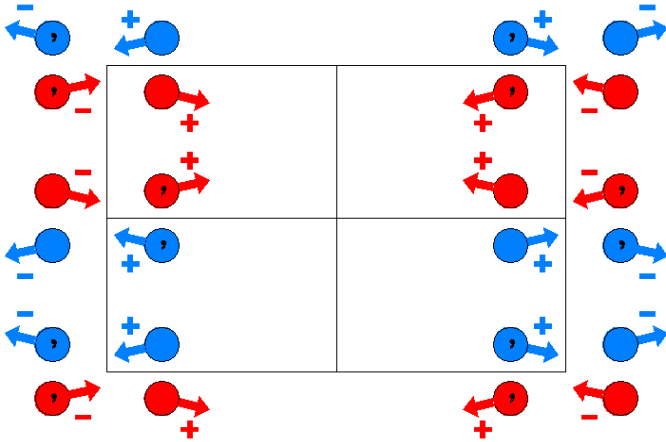
$P_{2b} m'ma$

51.13.399

$mmm1'$

$P_{2b} 2_1/m'2'/m2'/a$

Orthorhombic



**Origin** at center ( $2/m$ ) at  $2, 2/ma$

**Asymmetric unit**  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) $2'$ $1/4, 0, z$<br>( $2_z$   $1/2, 0, 0$ )'             | (3) $2'$ $0, y, 0$<br>( $2_y$   $0, 0, 0$ )' | (4) $2$ ( $1/2, 0, 0$ ) $x, 0, 0$<br>( $2_x$   $1/2, 0, 0$ ) |
| (5) $\bar{1}'$<br>( $\bar{1}$   $0, 0, 0$ )' | (6) $a$ ( $1/2, 0, 0$ ) $x, y, 0$<br>( $m_z$   $1/2, 0, 0$ ) | (7) $m$ $x, 0, z$<br>( $m_y$   $0, 0, 0$ )   | (8) $m'$ $1/4, y, z$<br>( $m_x$   $1/2, 0, 0$ )'             |

For (0,0,0) + set

For (0,1,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (0,1,0)<br>(1 0,1,0)'                         | (2) $2$ $1/4, 1/2, z$<br>( $2_z$   $1/2, 1, 0$ )               | (3) $2$ (0,1,0) $0, y, 0$<br>( $2_y$   $0, 1, 0$ ) | (4) $2'$ ( $1/2, 0, 0$ ) $x, 1/2, 0$<br>( $2_x$   $1/2, 1, 0$ )' |
| (5) $\bar{1}$ $0, 1/2, 0$<br>( $\bar{1}$   $0, 1, 0$ ) | (6) $n'$ ( $1/2, 1, 0$ ) $x, y, 0$<br>( $m_z$   $1/2, 1, 0$ )' | (7) $m'$ $x, 1/2, z$<br>( $m_y$   $0, 1, 0$ )'     | (8) $b$ (0,1,0) $1/4, y, z$<br>( $m_x$   $1/2, 1, 0$ )           |

**Generators selected** (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

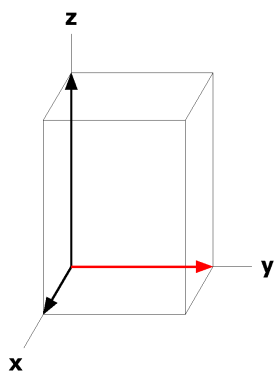
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
16 l 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [u,v, $\bar{w}$ ] (6) $x+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x}+1/2,y,z$ [ $\bar{u},v,w$ ]
8 k m'..	1/4,y,z [0,v,w]	1/4, $\bar{y},z$ [0,v, $\bar{w}$ ]	3/4,y, $\bar{z}$ [0, $\bar{v},w$ ]	3/4, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 j .m'.	x,1/2,z [u,0,w]	$\bar{x}+1/2,1/2,z$ [ $\bar{u},0,w$ ]	$\bar{x},1/2,\bar{z}$ [u,0,w]	$x+1/2,1/2,\bar{z}$ [ $\bar{u},0,w$ ]
8 i .m.	x,0,z [0,v,0]	$\bar{x}+1/2,0,z$ [0,v,0]	$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	$x+1/2,0,\bar{z}$ [0, $\bar{v},0$ ]
8 h .2'.	0,y,1/2 [u,0,w]	1/2, $\bar{y},1/2$ [u,0, $\bar{w}$ ]	0, $\bar{y},1/2$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,1/2 [ $\bar{u},0,w$ ]
8 g .2'.	0,y,0 [u,0,w]	1/2, $\bar{y},0$ [u,0, $\bar{w}$ ]	0, $\bar{y},0$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,0 [ $\bar{u},0,w$ ]
4 f m'm'2	1/4,1/2,z [0,0,w]	3/4,1/2, $\bar{z}$ [0,0,w]		
4 e m'm'2'	1/4,0,z [0,v,0]	3/4,0, $\bar{z}$ [0, $\bar{v},0$ ]		
4 d .2'/m'.	0,1/2,1/2 [u,0,w]	1/2,1/2,1/2 [ $\bar{u},0,w$ ]		
4 c .2'/m.	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 b .2'/m'.	0,1/2,0 [u,0,w]	1/2,1/2,0 [ $\bar{u},0,w$ ]		
4 a .2'/m.	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



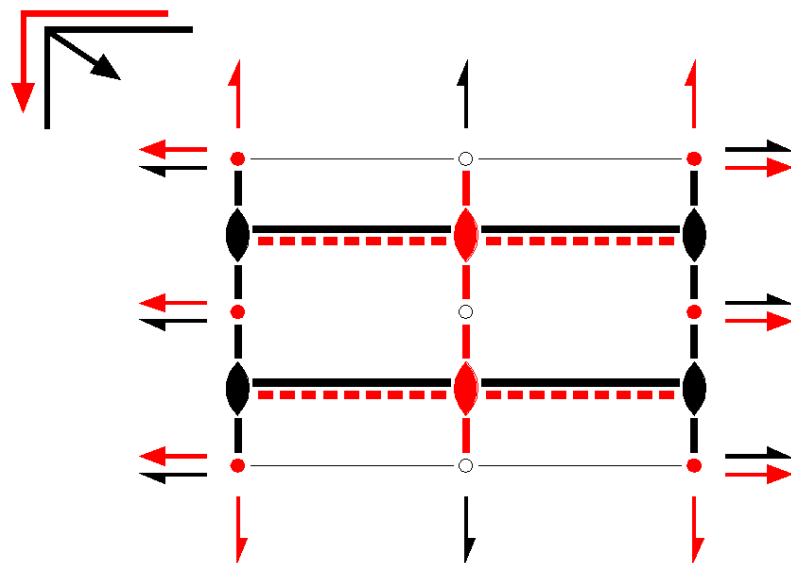
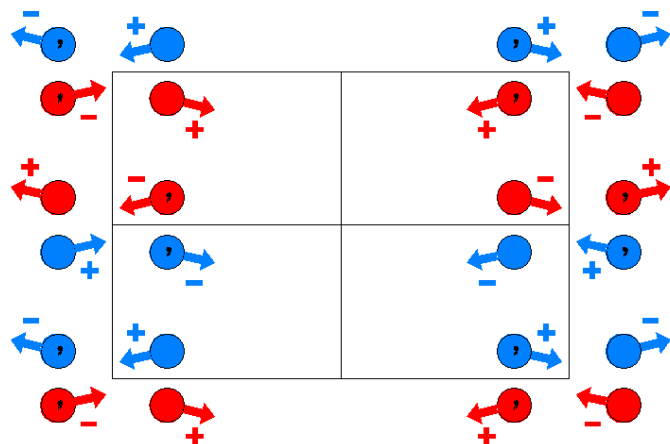
$P_{2b} mma'$

51.14.400

$mmm1'$

$P_{2b} 2_1' / m2' / m2' / a'$

Orthorhombic



**Origin** at center ( $2/m$ ) at  $2_1' 2' / ma'$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )               | (3) $2'$ $0,y,0$<br>( $2_y$   $0,0,0$ )' | (4) $2'$ $(1/2,0,0)$ $x,0,0$<br>( $2_x$   $1/2,0,0$ )' |
| (5) $\bar{1}'$<br>( $\bar{1}$   $0,0,0$ )' | (6) $a'$ $(1/2,0,0)$ $x,y,0$<br>( $m_z$   $1/2,0,0$ )' | (7) $m$ $x,0,z$<br>( $m_y$   $0,0,0$ )   | (8) $m$ $1/4,y,z$<br>( $m_x$   $1/2,0,0$ )             |

For  $(0,1,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(0,1,0)$<br>(1  $0,1,0$ )'               | (2) $2'$ $1/4,1/2,z$<br>( $2_z$   $1/2,1,0$ )'       | (3) 2 $(0,1,0)$ $0,y,0$<br>( $2_y$   $0,1,0$ ) | (4) 2 $(1/2,0,0)$ $x,1/2,0$<br>( $2_x$   $1/2,1,0$ )   |
| (5) $\bar{1}$ $0,1/2,0$<br>( $\bar{1}$   $0,1,0$ ) | (6) $n$ $(1/2,1,0)$ $x,y,0$<br>( $m_z$   $1/2,1,0$ ) | (7) $m'$ $x,1/2,z$<br>( $m_y$   $0,1,0$ )'     | (8) $b'$ $(0,1,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1,0$ )' |

**Generators selected** (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

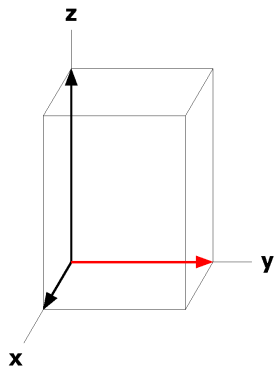
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
16 l 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x}+1/2,y,z$ [u, $\bar{v},\bar{w}$ ]
8 k m..	1/4,y,z [u,0,0]	1/4, $\bar{y},z$ [ $\bar{u},0,0$ ]	3/4,y, $\bar{z}$ [u,0,0]	3/4, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
8 j .m'	x,1/2,z [u,0,w]	$\bar{x}+1/2,1/2,z$ [u,0, $\bar{w}$ ]	$\bar{x},1/2,\bar{z}$ [u,0,w]	$x+1/2,1/2,\bar{z}$ [u,0, $\bar{w}$ ]
8 i .m.	x,0,z [0,v,0]	$\bar{x}+1/2,0,z$ [0, $\bar{v},0$ ]	$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	$x+1/2,0,\bar{z}$ [0,v,0]
8 h .2'	0,y,1/2 [u,0,w]	1/2, $\bar{y},1/2$ [ $\bar{u},0,w$ ]	0, $\bar{y},1/2$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,1/2 [u,0, $\bar{w}$ ]
8 g .2'	0,y,0 [u,0,w]	1/2, $\bar{y},0$ [ $\bar{u},0,w$ ]	0, $\bar{y},0$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,0 [u,0, $\bar{w}$ ]
4 f mm'2'	1/4,1/2,z [u,0,0]	3/4,1/2, $\bar{z}$ [u,0,0]		
4 e mm2	1/4,0,z [0,0,0]	3/4,0, $\bar{z}$ [0,0,0]		
4 d .2'/m'	0,1/2,1/2 [u,0,w]	1/2,1/2,1/2 [u,0, $\bar{w}$ ]		
4 c .2'/m.	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 b .2'/m'	0,1/2,0 [u,0,w]	1/2,1/2,0 [u,0, $\bar{w}$ ]		
4 a .2'/m.	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



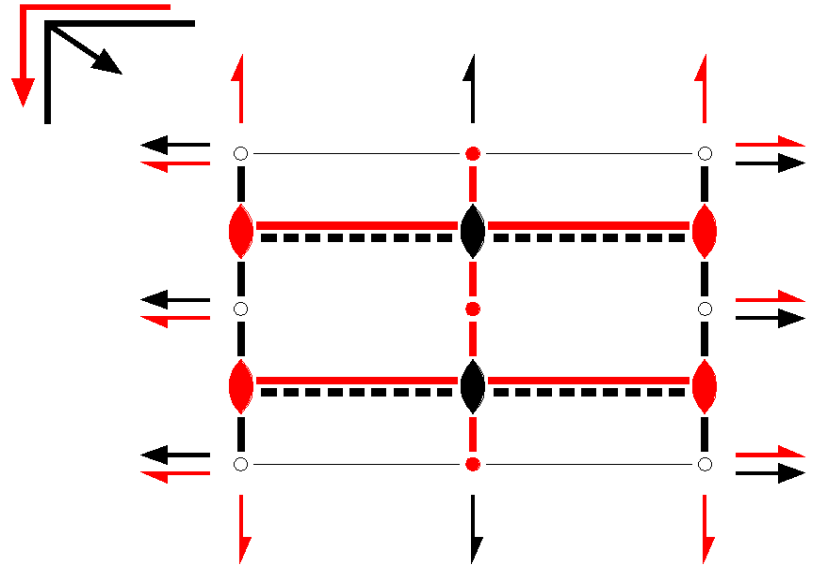
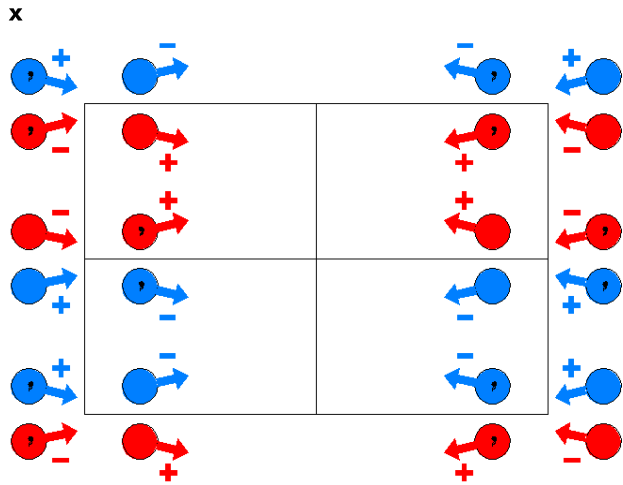
$P_{2b} m'ma'$

51.15.401

$mmm1'$

$P_{2b} 2_1'/m'2/m'2'/a'$

Orthorhombic



**Origin** at center ( $2/m$ ) at  $2_1' 2'/ma'$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

- |                                      |  |  |  |
|--------------------------------------|--|--|--|
| (1) 1<br>(1 0,0,0)                   | (2) $2'_z$ $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )'           | (3) $2_y$ $0,y,0$<br>( $2_y$   $0,0,0$ ) | (4) $2'_x$ $(1/2,0,0)$ $x,0,0$<br>( $2_x$   $1/2,0,0$ )' |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) $a'_z$ $(1/2,0,0)$ $x,y,0$<br>( $m_z$   $1/2,0,0$ )' | (7) $m_y$ $x,0,z$<br>( $m_y$   $0,0,0$ ) | (8) $m'_x$ $1/4,y,z$<br>( $m_x$   $1/2,0,0$ )'           |

For (0,0,0) + set

For (0,1,0)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) $t'_z$ $(0,1,0)$<br>(1 0,1,0)'               | (2) $2'_z$ $1/4,1/2,z$<br>( $2_z$   $1/2,1,0$ )        | (3) $2'_y$ $(0,1,0)$ $0,y,0$<br>( $2_y$   $0,1,0$ )' | (4) $2'_x$ $(1/2,0,0)$ $x,1/2,0$<br>( $2_x$   $1/2,1,0$ ) |
| (5) $\bar{1}'$ $0,1/2,0$<br>( $\bar{1}$  0,1,0)' | (6) $n_z$ $(1/2,1,0)$ $x,y,0$<br>( $m_z$   $1/2,1,0$ ) | (7) $m'_y$ $x,1/2,z$<br>( $m_y$   $0,1,0$ )'         | (8) $b'_x$ $(0,1,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1,0$ )   |

**Generators selected** (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
16 l 1	(1) x,y,z [u,v,w] (5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z$ [u,v, $\bar{w}$ ] (6) $x+1/2, y, \bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ] (7) $x, \bar{y}, z$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x+1/2, \bar{y}, \bar{z}$ [ $\bar{u}, v, w$ ] (8) $\bar{x}+1/2, y, z$ [ $\bar{u}, v, w$ ]
8 k m'..	1/4,y,z [0,v,w]	1/4, $\bar{y}$ ,z [0,v, $\bar{w}$ ]	3/4,y, $\bar{z}$ [0,v, $\bar{w}$ ]	3/4, $\bar{y}$ , $\bar{z}$ [0,v,w]
8 j .m'.	x,1/2,z [u,0,w]	$\bar{x}+1/2, 1/2, z$ [ $\bar{u}, 0, w$ ]	$\bar{x}, 1/2, \bar{z}$ [ $\bar{u}, 0, \bar{w}$ ]	$x+1/2, 1/2, \bar{z}$ [u,0, $\bar{w}$ ]
8 i .m.	x,0,z [0,v,0]	$\bar{x}+1/2, 0, z$ [0,v,0]	$\bar{x}, 0, \bar{z}$ [0,v,0]	$x+1/2, 0, \bar{z}$ [0,v,0]
8 h .2.	0,y,1/2 [0,v,0]	1/2, $\bar{y}$ ,1/2 [0,v,0]	0, $\bar{y}$ ,1/2 [0,v,0]	1/2,y,1/2 [0,v,0]
8 g .2.	0,y,0 [0,v,0]	1/2, $\bar{y}$ ,0 [0,v,0]	0, $\bar{y}$ ,0 [0,v,0]	1/2,y,0 [0,v,0]
4 f m'm'2	1/4,1/2,z [0,0,w]	3/4,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 e m'm'2'	1/4,0,z [0,v,0]	3/4,0, $\bar{z}$ [0,v,0]		
4 d .2/m'.	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 c .2/m.	0,0,1/2 [0,v,0]	1/2,0,1/2 [0,v,0]		
4 b .2/m'.	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]		
4 a .2/m.	0,0,0 [0,v,0]	1/2,0,0 [0,v,0]		

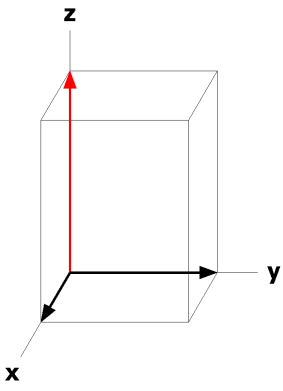
### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>'2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'2'mm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0

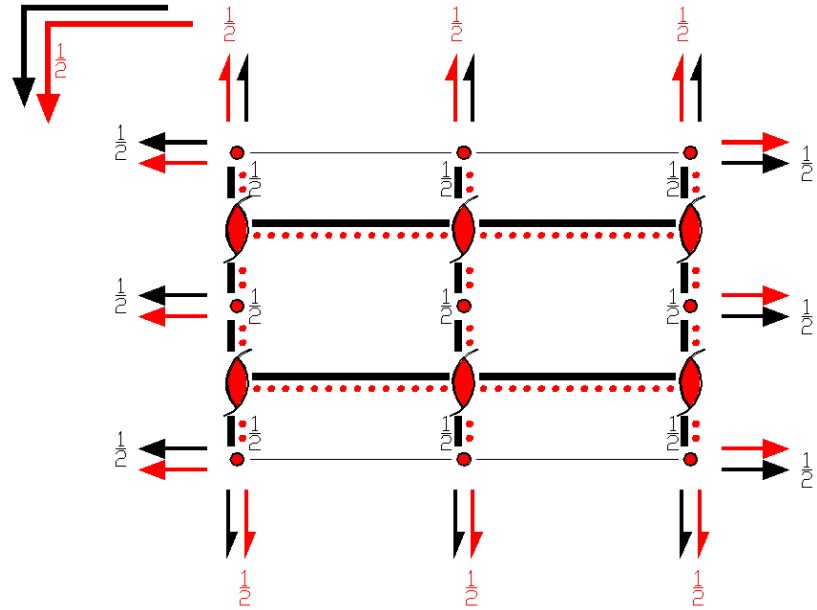
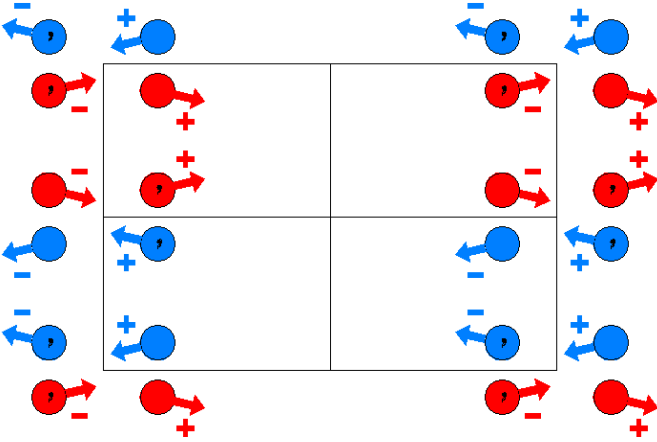




$P_{2c} m'ma$   
51.16.402

$mmm1'$   
 $P_{2c} 2_1/m'2'/m2'/a$

Orthorhombic



**Origin** at center ( $2'/m$ ) at  $2_1' 2'/ma'$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) $2'$ $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )'           | (3) $2'$ $0,y,0$<br>( $2_y$   $0,0,0$ )' | (4) $2$ ( $1/2,0,0$ ) $x,0,0$<br>( $2_x$   $1/2,0,0$ ) |
| (5) $\bar{1}'$<br>( $\bar{1}$   $0,0,0$ )' | (6) $a$ ( $1/2,0,0$ ) $x,y,0$<br>( $m_z$   $1/2,0,0$ ) | (7) $m$ $x,0,z$<br>( $m_y$   $0,0,0$ )   | (8) $m'$ $1/4,y,z$<br>( $m_x$   $1/2,0,0$ )'           |

For (0,0,1)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'                     | (2) $2$ (0,0,1) $1/4,0,z$<br>( $2_z$   $1/2,0,1$ )         | (3) $2$ $0,y,1/2$<br>( $2_y$   $0,0,1$ )         | (4) $2'$ ( $1/2,0,0$ ) $x,0,1/2$<br>( $2_x$   $1/2,0,1$ )' |
| (5) $\bar{1}$ $0,0,1/2$<br>( $\bar{1}$   $0,0,1$ ) | (6) $a'$ ( $1/2,0,0$ ) $x,y,1/2$<br>( $m_z$   $1/2,0,1$ )' | (7) $c'$ (0,0,1) $x,0,z$<br>( $m_y$   $0,0,1$ )' | (8) $c$ (0,0,1) $1/4,y,z$<br>( $m_x$   $1/2,0,1$ )         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

### Positions

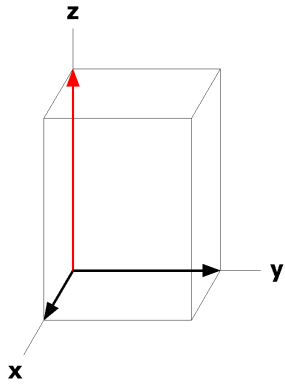
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
16 l 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [u,v, $\bar{w}$ ] (6) $x+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x}+1/2,y,z$ [ $\bar{u},v,w$ ]
8 k m'..	1/4,y,z [u,v,0]	1/4, $\bar{y},z$ [ $\bar{u},v,0$ ]	3/4,y, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	3/4, $\bar{y},\bar{z}$ [u, $\bar{v},0$ ]
8 j .m.	x,1/2,z [0,v,0]	$\bar{x}+1/2,1/2,z$ [0,v,0]	$\bar{x},1/2,\bar{z}$ [0, $\bar{v},0$ ]	$x+1/2,1/2,\bar{z}$ [0, $\bar{v},0$ ]
8 i .m.	x,0,z [0,v,0]	$\bar{x}+1/2,0,z$ [0,v,0]	$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	$x+1/2,0,\bar{z}$ [0, $\bar{v},0$ ]
8 h .2.	0,y,1/2 [0,v,0]	1/2, $\bar{y},1/2$ [0, $\bar{v},0$ ]	0, $\bar{y},1/2$ [0,v,0]	1/2,y,1/2 [0, $\bar{v},0$ ]
8 g .2'	0,y,0 [u,0,w]	1/2, $\bar{y},0$ [u,0, $\bar{w}$ ]	0, $\bar{y},0$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,0 [ $\bar{u},0,w$ ]
4 f m'm2'	1/4,1/2,z [0,v,0]	3/4,1/2, $\bar{z}$ [0, $\bar{v},0$ ]		
4 e m'm2'	1/4,0,z [0,v,0]	3/4,0, $\bar{z}$ [0, $\bar{v},0$ ]		
4 d .2/m.	0,1/2,1/2 [0,v,0]	1/2,1/2,1/2 [0,v,0]		
4 c .2/m.	0,0,1/2 [0,v,0]	1/2,0,1/2 [0,v,0]		
4 b .2'/m.	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]		
4 a .2'/m.	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>\*2mm  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

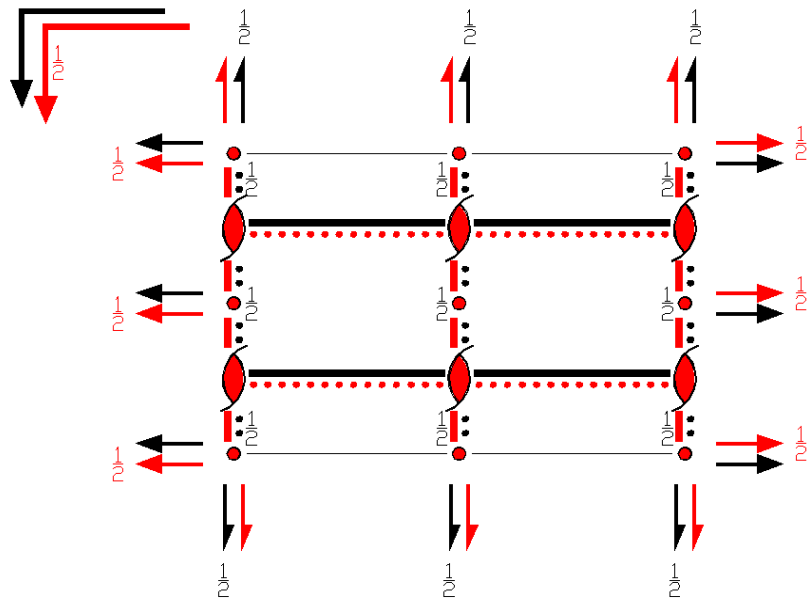
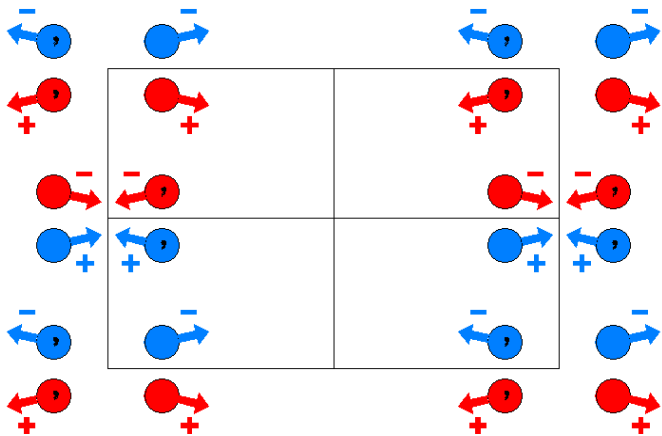
Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



$P_{2c}mm'a$   
51.17.403

$mmm1'$   
 $P_{2c}2_1'm2/m'2'/a$

Orthorhombic



**Origin** at center ( $2/m'$ ) at  $2_1'2/m'a$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) $2_1'$ $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )'       | (3) 2 $0,y,0$<br>( $2_y$   $0,0,0$ )     | (4) $2_1'$ ( $1/2,0,0$ ) $x,0,0$<br>( $2_x$   $1/2,0,0$ )' |
| (5) $\bar{1}'$<br>( $\bar{1}$   $0,0,0$ )' | (6) a ( $1/2,0,0$ ) $x,y,0$<br>( $m_z$   $1/2,0,0$ ) | (7) $m'$ $x,0,z$<br>( $m_y$   $0,0,0$ )' | (8) m $1/4,y,z$<br>( $m_x$   $1/2,0,0$ )                   |

For (0,0,1) + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'                     | (2) 2 (0,0,1) $1/4,0,z$<br>( $2_z$   $1/2,0,1$ )         | (3) $2_1'$ $0,y,1/2$<br>( $2_y$   $0,0,1$ )' | (4) 2 ( $1/2,0,0$ ) $x,0,1/2$<br>( $2_x$   $1/2,0,1$ ) |
| (5) $\bar{1}$ $0,0,1/2$<br>( $\bar{1}$   $0,0,1$ ) | (6) a' ( $1/2,0,0$ ) $x,y,1/2$<br>( $m_z$   $1/2,0,1$ )' | (7) c (0,0,1) $x,0,z$<br>( $m_y$   $0,0,1$ ) | (8) c' (0,0,1) $1/4,y,z$<br>( $m_x$   $1/2,0,1$ )'     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

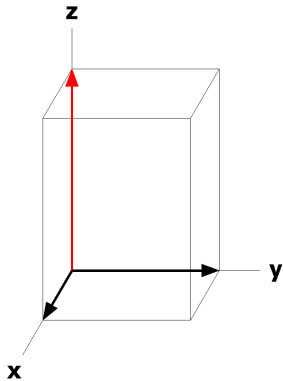
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
16 l 1	(1) x,y,z [u,v,w] (5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(2) $\bar{x}+1/2, \bar{y}, z$ [u,v, $\bar{w}$ ] (6) x+1/2,y, $\bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ] (7) x, $\bar{y}, z$ [u, $\bar{v}, w$ ]	(4) x+1/2, $\bar{y}, \bar{z}$ [ $\bar{u}, v, w$ ] (8) $\bar{x}+1/2, y, z$ [u, $\bar{v}, \bar{w}$ ]
8 k m..	1/4,y,z [u,0,0]	1/4, $\bar{y}, z$ [u,0,0]	3/4,y, $\bar{z}$ [ $\bar{u}, 0, 0$ ]	3/4, $\bar{y}, \bar{z}$ [ $\bar{u}, 0, 0$ ]
8 j .m'	x,1/2,z [u,0,w]	$\bar{x}+1/2, 1/2, z$ [u,0, $\bar{w}$ ]	$\bar{x}, 1/2, \bar{z}$ [ $\bar{u}, 0, \bar{w}$ ]	x+1/2,1/2, $\bar{z}$ [ $\bar{u}, 0, w$ ]
8 i .m'	x,0,z [u,0,w]	$\bar{x}+1/2, 0, z$ [u,0, $\bar{w}$ ]	$\bar{x}, 0, \bar{z}$ [ $\bar{u}, 0, \bar{w}$ ]	x+1/2,0, $\bar{z}$ [ $\bar{u}, 0, w$ ]
8 h .2'	0,y,1/2 [u,0,w]	1/2, $\bar{y}, 1/2$ [u,0, $\bar{w}$ ]	0, $\bar{y}, 1/2$ [u,0,w]	1/2,y,1/2 [u,0, $\bar{w}$ ]
8 g .2	0,y,0 [0,v,0]	1/2, $\bar{y}, 0$ [0,v,0]	0, $\bar{y}, 0$ [0, $\bar{v}, 0$ ]	1/2,y,0 [0, $\bar{v}, 0$ ]
4 f mm'2'	1/4,1/2,z [u,0,0]	3/4,1/2, $\bar{z}$ [ $\bar{u}, 0, 0$ ]		
4 e mm'2'	1/4,0,z [u,0,0]	3/4,0, $\bar{z}$ [ $\bar{u}, 0, 0$ ]		
4 d .2'/m'	0,1/2,1/2 [u,0,w]	1/2,1/2,1/2 [u,0, $\bar{w}$ ]		
4 c .2'/m'	0,0,1/2 [u,0,w]	1/2,0,1/2 [u,0, $\bar{w}$ ]		
4 b .2'/m'	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]		
4 a .2'/m'	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2b</sub>-2mg  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



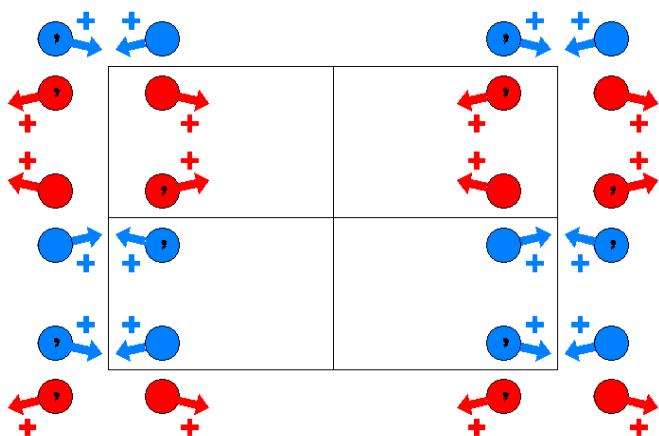
$P_{2c} m'm'a$

51.18.404

$mmm1'$

$P_{2c} 2_1' / m'2' / m'2' / a$

Orthorhombic



**Origin** at center ( $2'/m'$ ) at  $2_1' 2'/m'a$

**Asymmetric unit**  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

- |                                      |   |  |  |
|--------------------------------------|---|--|--|
| (1) 1<br>(1 0,0,0)                   | (2) $2 \quad 1/4,0,z$<br>( $2_z$   $1/2,0,0$ )          | (3) $2' \quad 0,y,0$<br>( $2_y$   $0,0,0$ )' | (4) $2' \quad (1/2,0,0) \quad x,0,0$<br>( $2_x$   $1/2,0,0$ )' |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) a ( $1/2,0,0) \quad x,y,0$<br>( $m_z$   $1/2,0,0$ ) | (7) $m' \quad x,0,z$<br>( $m_y$   $0,0,0$ )' | (8) $m' \quad 1/4,y,z$<br>( $m_x$   $1/2,0,0$ )'               |

For (0,0,0) + set

For (0,0,1)' + set

- |  |  |   |  |
|--|--|---|--|
| (1) $t' \quad (0,0,1)$<br>(1 0,0,1)'                 | (2) $2' \quad (0,0,1) \quad 1/4,0,z$<br>( $2_z$   $1/2,0,1$ )' | (3) $2 \quad 0,y,1/2$<br>( $2_y$   $0,0,1$ )        | (4) $2 \quad (1/2,0,0) \quad x,0,1/2$<br>( $2_x$   $1/2,0,1$ ) |
| (5) $\bar{1}' \quad 0,0,1/2$<br>( $\bar{1}$  0,0,1)' | (6) a' ( $1/2,0,0) \quad x,y,1/2$<br>( $m_z$   $1/2,0,1$ )'    | (7) c ( $0,0,1) \quad x,0,z$<br>( $m_y$   $0,0,1$ ) | (8) c ( $0,0,1) \quad 1/4,y,z$<br>( $m_x$   $1/2,0,1$ )        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

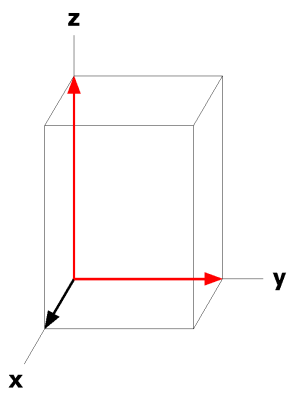
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
16 l 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) $x,\bar{y},z$ [u, $\bar{v},w$ ]	(4) $x+1/2,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x}+1/2,y,z$ [ $\bar{u},v,w$ ]
8 k m'..	1/4,y,z [0,v,w]	1/4, $\bar{y},z$ [0, $\bar{v},w$ ]	3/4,y, $\bar{z}$ [0, $\bar{v},w$ ]	3/4, $\bar{y},\bar{z}$ [0,v,w]
8 j .m'.	x,1/2,z [u,0,w]	$\bar{x}+1/2,1/2,z$ [ $\bar{u},0,w$ ]	$\bar{x},1/2,\bar{z}$ [u,0,w]	$x+1/2,1/2,\bar{z}$ [ $\bar{u},0,w$ ]
8 i .m'.	x,0,z [u,0,w]	$\bar{x}+1/2,0,z$ [ $\bar{u},0,w$ ]	$\bar{x},0,\bar{z}$ [u,0,w]	$x+1/2,0,\bar{z}$ [ $\bar{u},0,w$ ]
8 h .2.	0,y,1/2 [0,v,0]	1/2, $\bar{y},1/2$ [0, $\bar{v},0$ ]	0, $\bar{y},1/2$ [0, $\bar{v},0$ ]	1/2,y,1/2 [0,v,0]
8 g .2'.	0,y,0 [u,0,w]	1/2, $\bar{y},0$ [ $\bar{u},0,w$ ]	0, $\bar{y},0$ [u,0,w]	1/2,y,0 [ $\bar{u},0,w$ ]
4 f m'm'2	1/4,1/2,z [0,0,w]	3/4,1/2, $\bar{z}$ [0,0,w]		
4 e m'm'2	1/4,0,z [0,0,w]	3/4,0, $\bar{z}$ [0,0,w]		
4 d .2/m'.	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 c .2/m'.	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 b .2'/m'.	0,1/2,0 [u,0,w]	1/2,1/2,0 [ $\bar{u},0,w$ ]		
4 a .2'/m'.	0,0,0 [u,0,w]	1/2,0,0 [ $\bar{u},0,w$ ]		

**Symmetry of Special Projections**

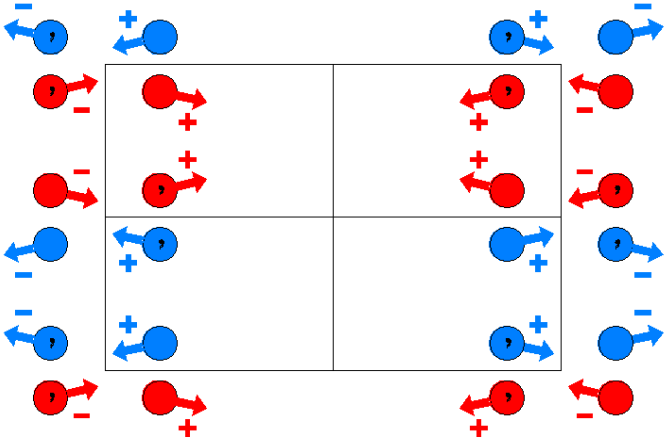
Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'-2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2b</sub>'-2m'g'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,1/2

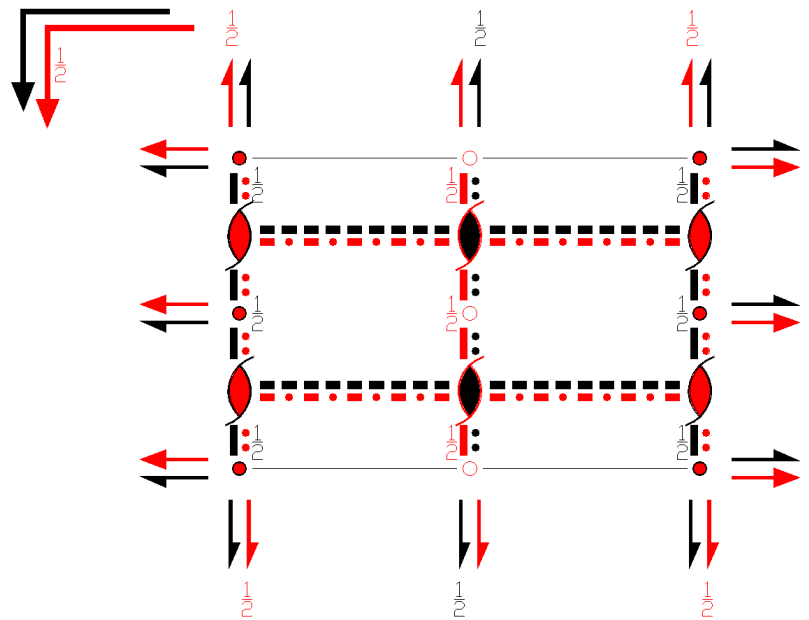
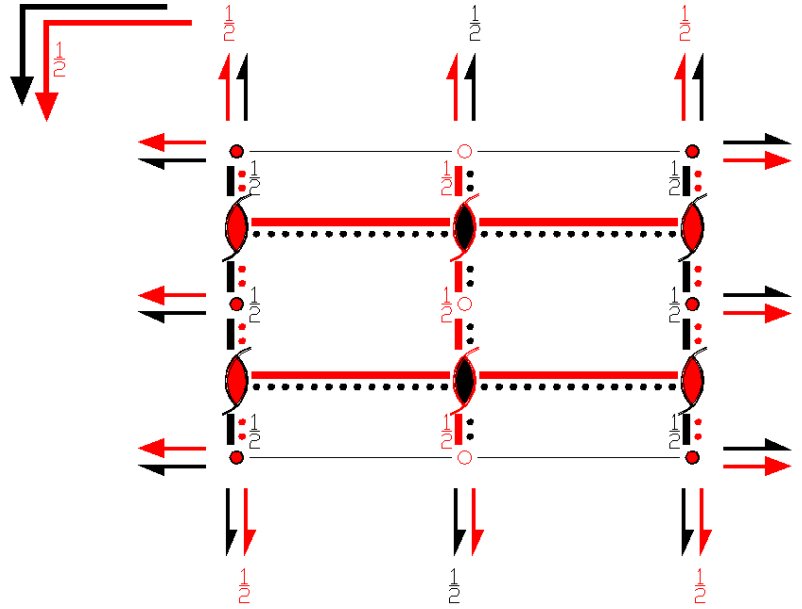


$P_A m'ma$   
51.19.405



$mmm1'$   
 $P_A 2_1/m'2'/m2'/a$

Orthorhombic



**Origin** at center ( $2/m$ ) at  $2, 2'/ma$

**Asymmetric unit**  $0 \leq x \leq 1/4;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2' 1/4,0,z (2 <sub>z</sub>  1/2,0,0)'	(3) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(4) 2 (1/2,0,0) x,0,0 (2 <sub>x</sub>  1/2,0,0)
(5) $\bar{1}$ ' ( $\bar{1}$  0,0,0)'	(6) a (1/2,0,0) x,y,0 (m <sub>z</sub>  1/2,0,0)	(7) m x,0,z (m <sub>y</sub>  0,0,0)	(8) m' 1/4,y,z (m <sub>x</sub>  1/2,0,0)'

For (0,1,0)' + set

(1) t' (0,1,0) (1 0,1,0)'	(2) 2 1/4,1/2,z (2 <sub>z</sub>  1/2,1,0)	(3) 2 (0,1,0) 0,y,0 (2 <sub>y</sub>  0,1,0)	(4) 2' (1/2,0,0) x,1/2,0 (2 <sub>x</sub>  1/2,1,0)'
(5) $\bar{1}$ 0,1/2,0 ( $\bar{1}$  0,1,0)	(6) n' (1/2,1,0) x,y,0 (m <sub>z</sub>  1/2,1,0)'	(7) m' x,1/2,z (m <sub>y</sub>  0,1,0)'	(8) b (0,1,0) 1/4,y,z (m <sub>x</sub>  1/2,1,0)

**Generators selected** (1); t(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
16 l 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [u,v, $\bar{w}$ ] (6) $x+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x}+1/2,y,z$ [ $\bar{u},v,w$ ]
8 k m'..	1/4,y,z [0,v,w]	1/4, $\bar{y},z$ [0,v, $\bar{w}$ ]	3/4,y, $\bar{z}$ [0, $\bar{v},w$ ]	3/4, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 j .m'.	x,1/2,z [u,0,w]	$\bar{x}+1/2,1/2,z$ [ $\bar{u},0,w$ ]	$\bar{x},1/2,\bar{z}$ [u,0,w]	$x+1/2,1/2,\bar{z}$ [ $\bar{u},0,w$ ]
8 i .m.	x,0,z [0,v,0]	$\bar{x}+1/2,0,z$ [0,v,0]	$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	$x+1/2,0,\bar{z}$ [0, $\bar{v},0$ ]
8 h .2.	0,y,1/2 [0,v,0]	1/2, $\bar{y},1/2$ [0,v,0]	0, $\bar{y},1/2$ [0,v,0]	1/2,y,1/2 [0,v,0]
8 g .2'.	0,y,0 [u,0,w]	1/2, $\bar{y},0$ [u,0, $\bar{w}$ ]	0, $\bar{y},0$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,0 [ $\bar{u},0,w$ ]
4 f m'm'2	1/4,1/2,z [0,0,w]	3/4,1/2, $\bar{z}$ [0,0,w]		
4 e m'm'2'	1/4,0,z [0,v,0]	3/4,0, $\bar{z}$ [0, $\bar{v},0$ ]		
4 d .2/m'.	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 c .2/m.	0,0,1/2 [0,v,0]	1/2,0,1/2 [0,v,0]		
4 b .2'/m'.	0,1/2,0 [u,0,w]	1/2,1/2,0 [ $\bar{u},0,w$ ]		
4 a .2'/m.	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]		

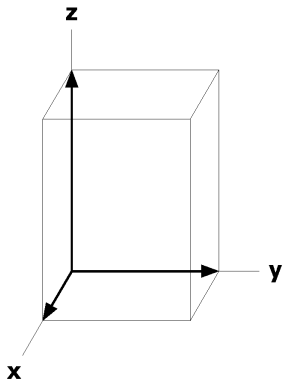


**Symmetry of Special Projections**

Along  $[0,0,1]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p_c \cdot 2mm$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,0,0$

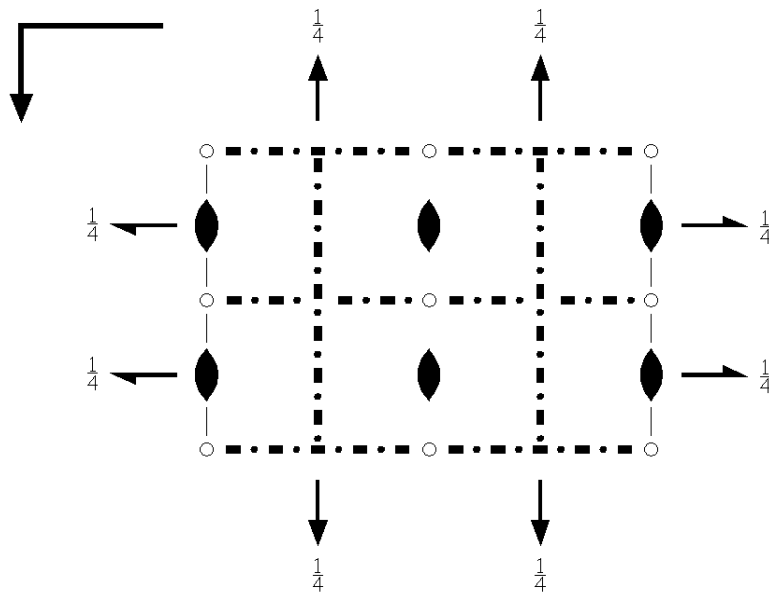
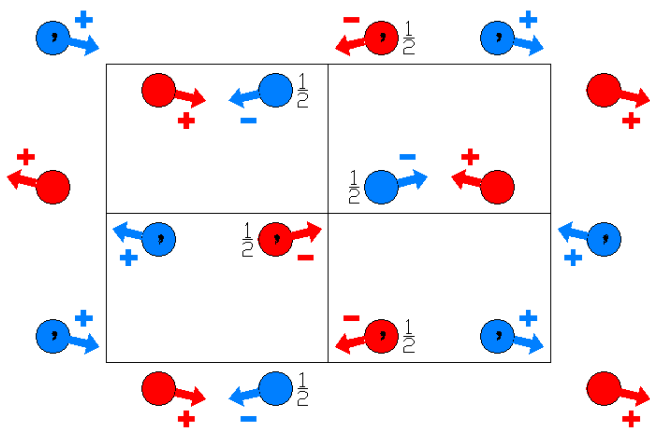
Along  $[0,1,0]$   $p2mg1'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $0,y,0$



Pnna  
52.1.406

mmm  
P2/n2<sub>1</sub>/n2/a

Orthorhombic



Origin at  $\bar{1}$  on n1a

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)         | (3) 2 (0,1/2,0) $1/4,y,1/4$<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (4) 2 $x,1/4,1/4$<br>(2 <sub>x</sub>  0,1/2,1/2)         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a (1/2,0,0) $x,y,0$<br>(m <sub>z</sub>  1/2,0,0) | (7) n (1/2,0,1/2) $x,1/4,z$<br>(m <sub>y</sub>  1/2,1/2,1/2) | (8) n (0,1/2,1/2) $0,y,z$<br>(m <sub>x</sub>  0,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

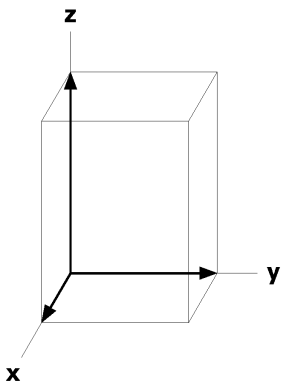
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}+1/2, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) x, $\bar{y}+1/2, \bar{z}+1/2$ [ $u, \bar{v}, \bar{w}$ ]
		(5) $\bar{x}, \bar{y}, \bar{z}$ [ $u, v, w$ ]	(6) $x+1/2, y, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(7) $x+1/2, \bar{y}+1/2, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(8) $\bar{x}, y+1/2, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]
4	d 2..	x, 1/4, 1/4 [u,0,0]	$\bar{x}+1/2, 3/4, 1/4$ [ $\bar{u}, 0, 0$ ]	$\bar{x}, 3/4, 3/4$ [u,0,0]	$x+1/2, 1/4, 3/4$ [ $\bar{u}, 0, 0$ ]
4	c ..2	1/4, 0, z [0,0,w]	1/4, 1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	3/4, 0, $\bar{z}$ [0,0,w]	3/4, 1/2, $z+1/2$ [0,0, $\bar{w}$ ]
4	b $\bar{1}$	0, 0, 1/2 [u,v,w]	1/2, 0, 1/2 [ $\bar{u}, \bar{v}, w$ ]	1/2, 1/2, 0 [ $\bar{u}, v, \bar{w}$ ]	0, 1/2, 0 [ $u, \bar{v}, \bar{w}$ ]
4	a $\bar{1}$	0, 0, 0 [u,v,w]	1/2, 0, 0 [ $\bar{u}, \bar{v}, w$ ]	1/2, 1/2, 1/2 [ $\bar{u}, v, \bar{w}$ ]	0, 1/2, 1/2 [ $u, \bar{v}, \bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2b} \cdot 2m'g'$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4, 0, z

Along [1,0,0]  $c_p \cdot 2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x, 0, 0

Along [0,1,0]  $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 1/4, y, 1/4

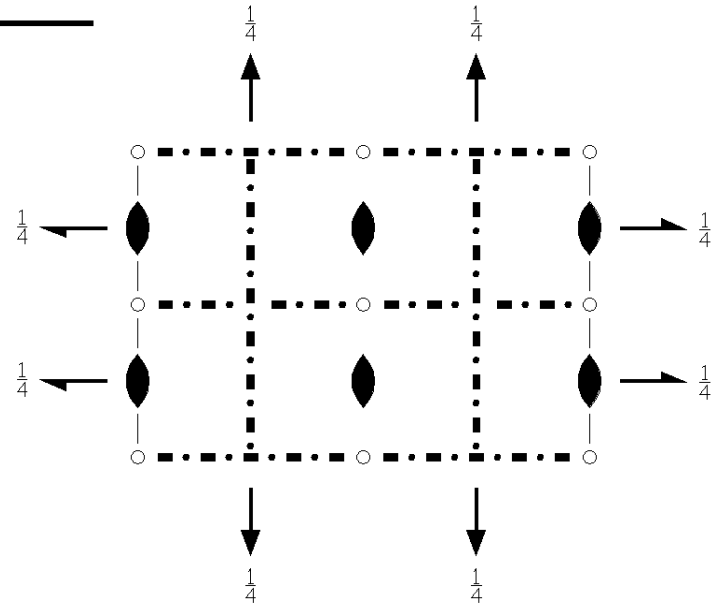
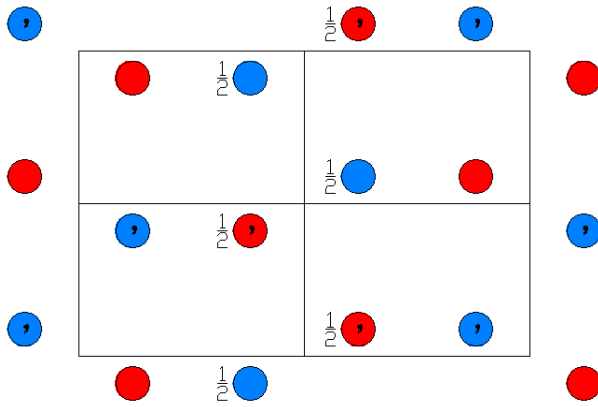


Pnna1'  
52.2.407

mmm1'  
P2/n2<sub>1</sub>/n2/a1'

Orthorhombic

1'



Origin at  $\bar{1}1'$  on  $n1a1'$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For 1 + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)         | (3) 2 (0,1/2,0) $1/4,y,1/4$<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (4) 2 $x,1/4,1/4$<br>(2 <sub>x</sub>  0,1/2,1/2)         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a (1/2,0,0) $x,y,0$<br>(m <sub>z</sub>  1/2,0,0) | (7) n (1/2,0,1/2) $x,1/4,z$<br>(m <sub>y</sub>  1/2,1/2,1/2) | (8) n (0,1/2,1/2) $0,y,z$<br>(m <sub>x</sub>  0,1/2,1/2) |

For 1' + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1'<br>(1 0,0,0)'                          | (2) 2' $1/4,0,z$<br>(2' <sub>z</sub>  1/2,0,0)'         | (3) 2' (0,1/2,0) $1/4,y,1/4$<br>(2' <sub>y</sub>  1/2,1/2,1/2)' | (4) 2' $x,1/4,1/4$<br>(2' <sub>x</sub>  0,1/2,1/2)'         |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}'$  0,0,0)' | (6) a' (1/2,0,0) $x,y,0$<br>(m' <sub>z</sub>  1/2,0,0)' | (7) n' (1/2,0,1/2) $x,1/4,z$<br>(m' <sub>y</sub>  1/2,1/2,1/2)' | (8) n' (0,1/2,1/2) $0,y,z$<br>(m' <sub>x</sub>  0,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

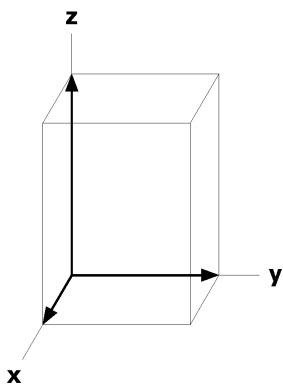
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1+	1' +	
8 e 11'	(1) x,y,z [0,0,0] (5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(2) $\bar{x}+1/2,\bar{y},z$ [0,0,0] (6) $x+1/2,y,\bar{z}$ [0,0,0]	(3) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [0,0,0] (7) $x+1/2,\bar{y}+1/2,z+1/2$ [0,0,0]	(4) $x,\bar{y}+1/2,\bar{z}+1/2$ [0,0,0] (8) $\bar{x},y+1/2,z+1/2$ [0,0,0]
4 d 2..1'	x,1/4,1/4 [0,0,0]	$\bar{x}+1/2,3/4,1/4$ [0,0,0]	$\bar{x},3/4,3/4$ [0,0,0]	$x+1/2,1/4,3/4$ [0,0,0]
4 c ..21'	1/4,0,z [0,0,0]	1/4,1/2, $\bar{z}+1/2$ [0,0,0]	3/4,0, $\bar{z}$ [0,0,0]	3/4,1/2,z+1/2 [0,0,0]
4 b $\bar{1}1'$	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	0,1/2,0 [0,0,0]
4 a $\bar{1}1'$	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p2mg1'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

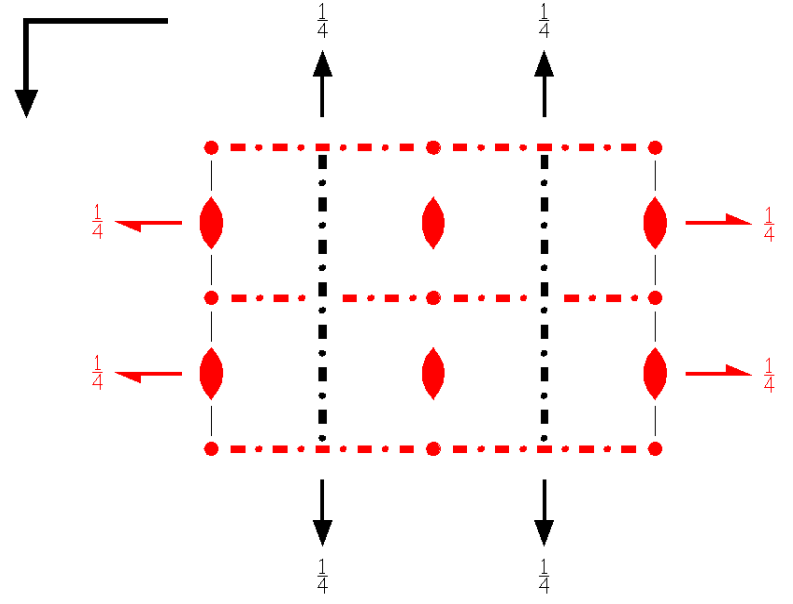
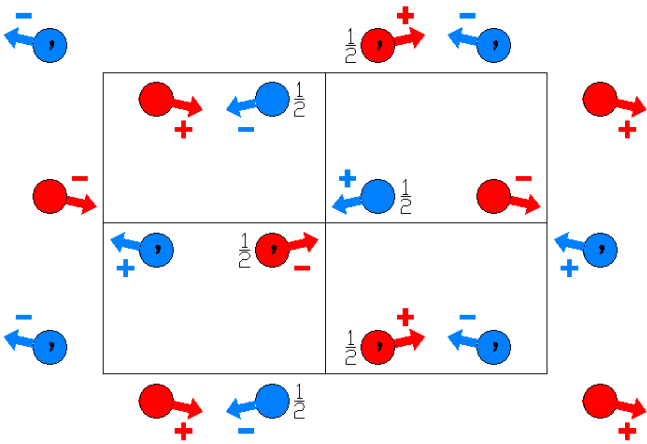
Along [0,1,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 1/4,y,1/4



Pn'na  
52.3.408

m'mm  
P2/n'2<sub>1</sub>'/n2'/a

Orthorhombic



Origin at  $\bar{1}$ ' on n'1a

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2' $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)'       | (3) 2' (0,1/2,0) $1/4,y,1/4$<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (4) 2 $x,1/4,1/4$<br>(2 <sub>x</sub>  0,1/2,1/2)           |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a (1/2,0,0) $x,y,0$<br>(m <sub>z</sub>  1/2,0,0) | (7) n (1/2,0,1/2) $x,1/4,z$<br>(m <sub>y</sub>  1/2,1/2,1/2)   | (8) n' (0,1/2,1/2) $0,y,z$<br>(m <sub>x</sub>  0,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

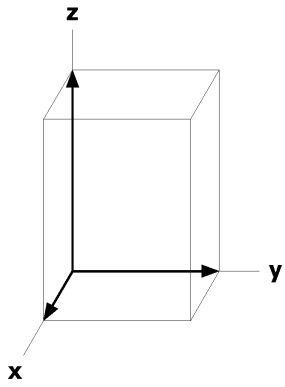
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y}+1/2,\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x+1/2,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) x+1/2, $\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y+1/2,z+1/2$ [ $\bar{u},v,w$ ]
4	d 2..	x,1/4,1/4 [u,0,0]	$\bar{x}+1/2,3/4,1/4$ [u,0,0]	$\bar{x},3/4,3/4$ [ $\bar{u},0,0$ ]	x+1/2,1/4,3/4 [ $\bar{u},0,0$ ]
4	c ..2'	1/4,0,z [u,v,0]	1/4,1/2, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	3/4,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	3/4,1/2,z+1/2 [ $\bar{u},v,0$ ]
4	b $\bar{1}'$	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	0,1/2,0 [0,0,0]
4	a $\bar{1}'$	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2b}\cdot 2m'g'$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2mm$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

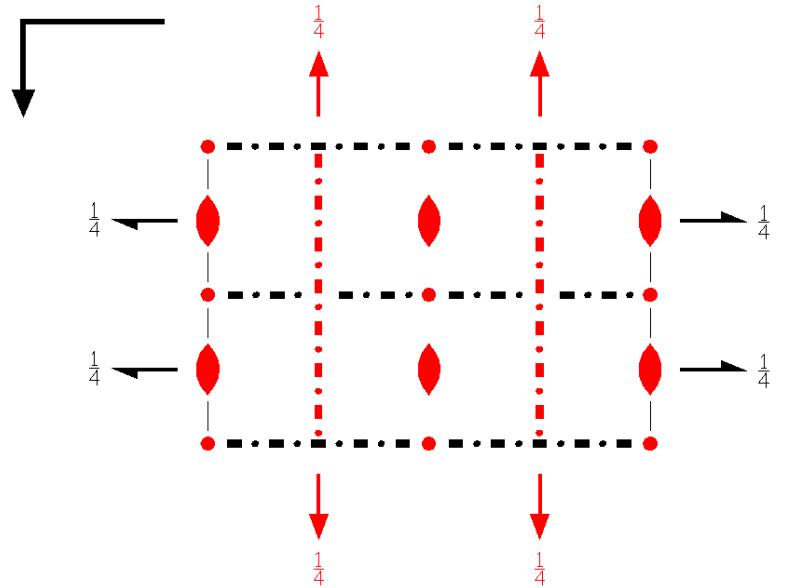
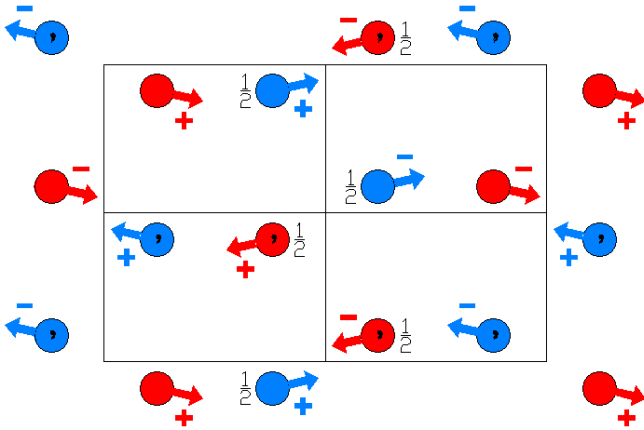
Along [0,1,0]  $c_p\cdot 2'mm'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,1/4



Pnn'a  
52.4.409

mm'm  
P2'/n2<sub>1</sub>/n'2'/a

Orthorhombic



Origin at  $\bar{1}$ ' on n1a

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2' $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)'       | (3) 2 (0,1/2,0) $1/4,y,1/4$<br>(2 <sub>y</sub>  1/2,1/2,1/2)   | (4) 2' $x,1/4,1/4$<br>(2 <sub>x</sub>  0,1/2,1/2)'       |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a (1/2,0,0) $x,y,0$<br>(m <sub>z</sub>  1/2,0,0) | (7) n' (1/2,0,1/2) $x,1/4,z$<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (8) n (0,1/2,1/2) $0,y,z$<br>(m <sub>x</sub>  0,1/2,1/2) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

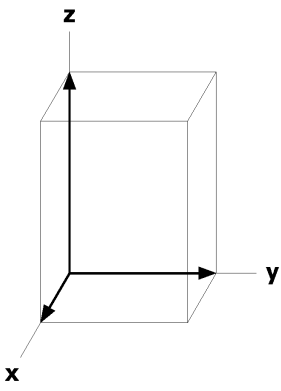
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x+1/2,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) x+1/2, $\bar{y}+1/2,z+1/2$ [u, $\bar{v},w$ ]	(8) $\bar{x},y+1/2,z+1/2$ [u, $\bar{v},\bar{w}$ ]
4	d 2'..	x,1/4,1/4 [0,v,w]	$\bar{x}+1/2,3/4,1/4$ [0,v, $\bar{w}$ ]	$\bar{x},3/4,3/4$ [0, $\bar{v},\bar{w}$ ]	x+1/2,1/4,3/4 [0, $\bar{v},w$ ]
4	c ..2'	1/4,0,z [u,v,0]	1/4,1/2, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	3/4,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	3/4,1/2,z+1/2 [u, $\bar{v},0$ ]
4	b $\bar{1}'$	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	0,1/2,0 [0,0,0]
4	a $\bar{1}'$	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2b} \cdot 2mg$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 2mm$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

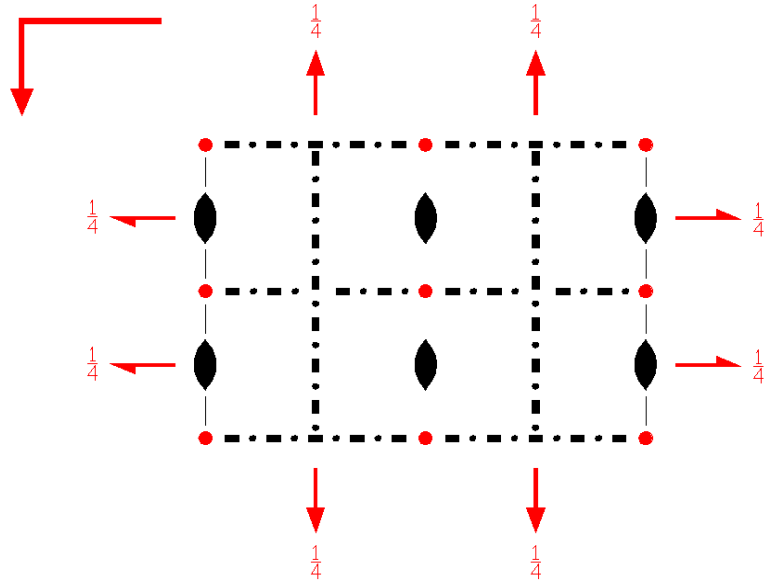
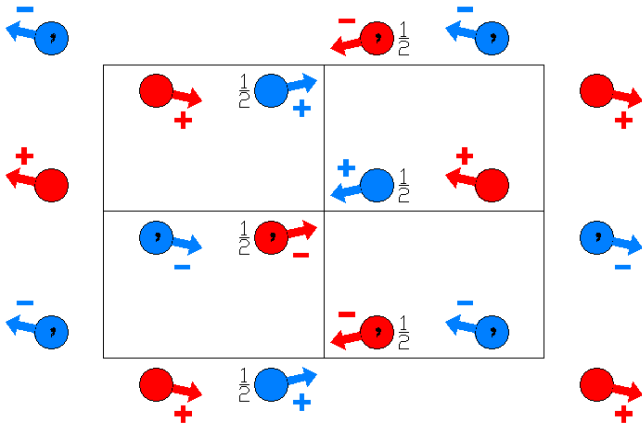
Along [0,1,0]  $c \cdot 2mm$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 1/4,y,1/4



Pnna'  
52.5.410

mmm'  
P2'/n2<sub>1</sub>'/n2/a'

Orthorhombic



Origin at  $\bar{1}'$  on  $n1a'$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)           | (3) 2' (0,1/2,0) $1/4,y,1/4$<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (4) 2' $x,1/4,1/4$<br>(2 <sub>x</sub>  0,1/2,1/2)'       |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a' (1/2,0,0) $x,y,0$<br>(m <sub>z</sub>  1/2,0,0)' | (7) n (1/2,0,1/2) $x,1/4,z$<br>(m <sub>y</sub>  1/2,1/2,1/2)   | (8) n (0,1/2,1/2) $0,y,z$<br>(m <sub>x</sub>  0,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

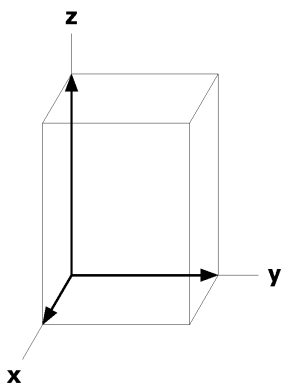
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	e 1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(4) $x,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(7) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
4	d 2'..	$x,1/4,1/4$ [ $0,v,w$ ]	$\bar{x}+1/2,3/4,1/4$ [ $0,\bar{v},w$ ]	$\bar{x},3/4,3/4$ [ $0,\bar{v},\bar{w}$ ]	$x+1/2,1/4,3/4$ [ $0,v,\bar{w}$ ]
4	c ..2	$1/4,0,z$ [ $0,0,w$ ]	$1/4,1/2,\bar{z}+1/2$ [ $0,0,w$ ]	$3/4,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$3/4,1/2,z+1/2$ [ $0,0,\bar{w}$ ]
4	b $\bar{1}'$	$0,0,1/2$ [ $0,0,0$ ]	$1/2,0,1/2$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]	$0,1/2,0$ [ $0,0,0$ ]
4	a $\bar{1}'$	$0,0,0$ [ $0,0,0$ ]	$1/2,0,0$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]	$0,1/2,1/2$ [ $0,0,0$ ]

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p2mg$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

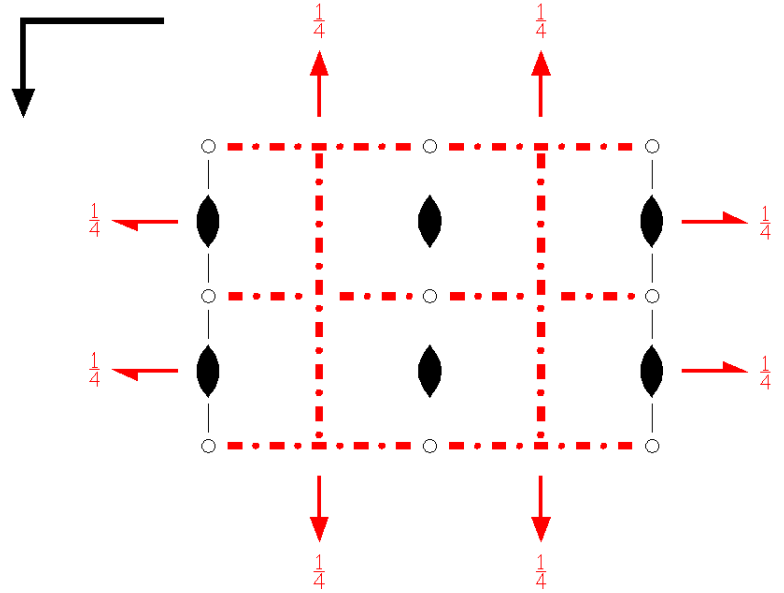
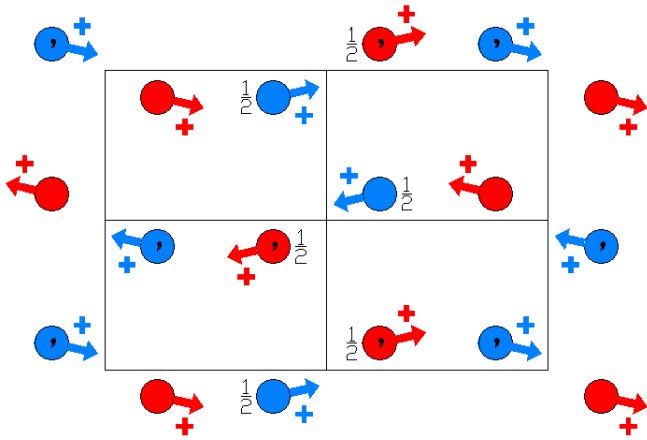
Along  $[0,1,0]$   $c_p \cdot 2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at  $1/4,y,1/4$



Pn'n'a  
52.6.411

m'm'm  
P2'/n'2<sub>1</sub>'/n'2/a

Orthorhombic



Origin at  $\bar{1}$  on n'1a

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)         | (3) 2' (0,1/2,0) $1/4,y,1/4$<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (4) 2' $x,1/4,1/4$<br>(2 <sub>x</sub>  0,1/2,1/2)'         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a (1/2,0,0) $x,y,0$<br>(m <sub>z</sub>  1/2,0,0) | (7) n' (1/2,0,1/2) $x,1/4,z$<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (8) n' (0,1/2,1/2) $0,y,z$<br>(m <sub>x</sub>  0,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

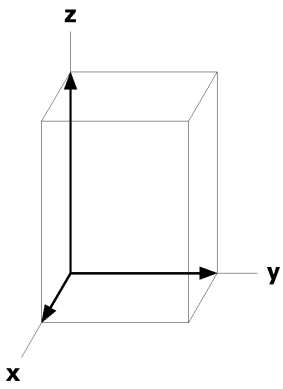
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}+1/2, y+1/2, \bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y}+1/2, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]
		(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) x+1/2,y, $\bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(7) x+1/2, $\bar{y}+1/2, z+1/2$ [u, $\bar{v}$ ,w]	(8) $\bar{x}, y+1/2, z+1/2$ [ $\bar{u}, v, w$ ]
4	d 2'..	x,1/4,1/4 [0,v,w]	$\bar{x}+1/2, 3/4, 1/4$ [0, $\bar{v}$ ,w]	$\bar{x}, 3/4, 3/4$ [0,v,w]	x+1/2,1/4,3/4 [0, $\bar{v}$ ,w]
4	c ..2	1/4,0,z [0,0,w]	1/4,1/2, $\bar{z}+1/2$ [0,0,w]	3/4,0, $\bar{z}$ [0,0,w]	3/4,1/2,z+1/2 [0,0,w]
4	b $\bar{1}$	0,0,1/2 [u,v,w]	1/2,0,1/2 [ $\bar{u}, \bar{v}, w$ ]	1/2,1/2,0 [u, $\bar{v}$ ,w]	0,1/2,0 [ $\bar{u}, v, w$ ]
4	a $\bar{1}$	0,0,0 [u,v,w]	1/2,0,0 [ $\bar{u}, \bar{v}, w$ ]	1/2,1/2,1/2 [u, $\bar{v}$ ,w]	0,1/2,1/2 [ $\bar{u}, v, w$ ]

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2b}2mg$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,0,z

Along [1,0,0]  $c2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

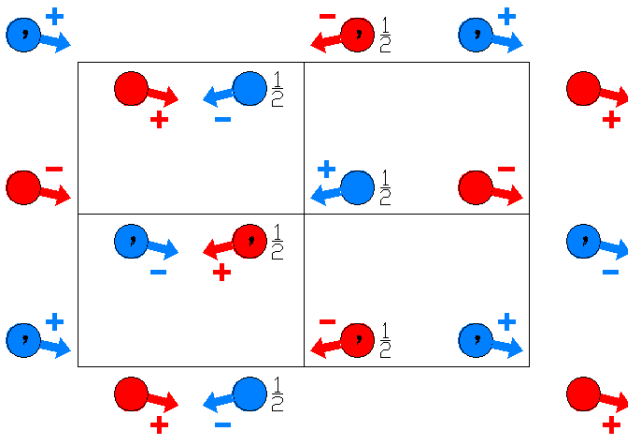
Along [0,1,0]  $c2'mm'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,1/4



Pnn'a'  
52.7.412

mm'm'  
P2/n2<sub>1</sub>'/n'2'/a'

Orthorhombic

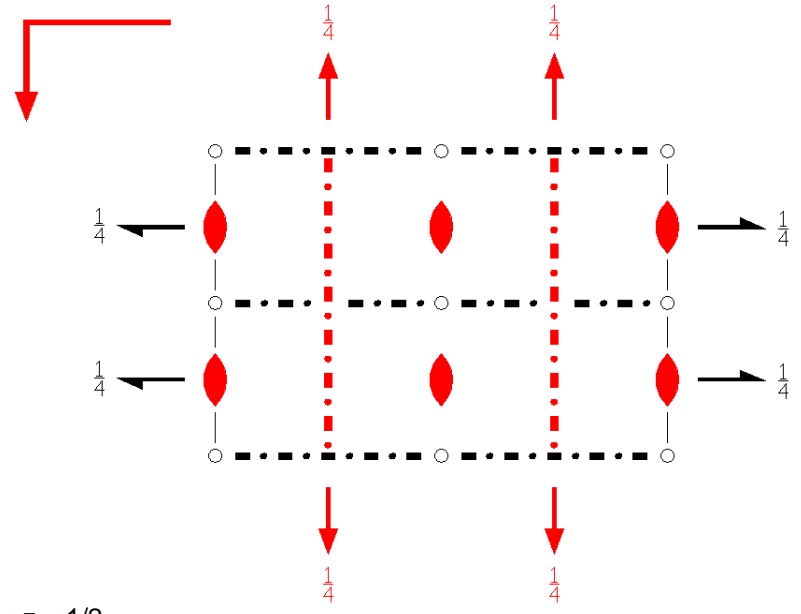


Origin at  $\bar{1}$  on  $n1a'$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/4;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2' $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)'         | (3) 2' (0,1/2,0) $1/4,y,1/4$<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (4) 2 $x,1/4,1/4$<br>(2 <sub>x</sub>  0,1/2,1/2)         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a' (1/2,0,0) $x,y,0$<br>(m <sub>z</sub>  1/2,0,0)' | (7) n' (1/2,0,1/2) $x,1/4,z$<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (8) n (0,1/2,1/2) $0,y,z$<br>(m <sub>x</sub>  0,1/2,1/2) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

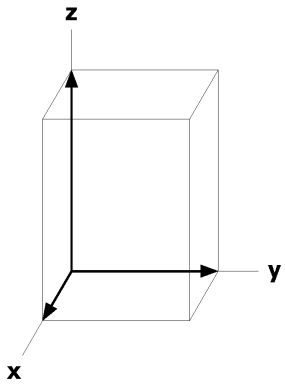
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y}+1/2,\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x+1/2,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) x+1/2, $\bar{y}+1/2,z+1/2$ [u, $\bar{v}$ ,w]	(8) $\bar{x},y+1/2,z+1/2$ [u, $\bar{v},\bar{w}$ ]
4	d 2..	x,1/4,1/4 [u,0,0]	$\bar{x}+1/2,3/4,1/4$ [u,0,0]	$\bar{x},3/4,3/4$ [u,0,0]	x+1/2,1/4,3/4 [u,0,0]
4	c ..2'	1/4,0,z [u,v,0]	1/4,1/2, $\bar{z}+1/2$ [u, $\bar{v}$ ,0]	3/4,0, $\bar{z}$ [u,v,0]	3/4,1/2,z+1/2 [u, $\bar{v}$ ,0]
4	b $\bar{1}$	0,0,1/2 [u,v,w]	1/2,0,1/2 [u,v, $\bar{w}$ ]	1/2,1/2,0 [u, $\bar{v}$ ,w]	0,1/2,0 [u, $\bar{v},\bar{w}$ ]
4	a $\bar{1}$	0,0,0 [u,v,w]	1/2,0,0 [u,v, $\bar{w}$ ]	1/2,1/2,1/2 [u, $\bar{v}$ ,w]	0,1/2,1/2 [u, $\bar{v},\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p2'm'g  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 2'mm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

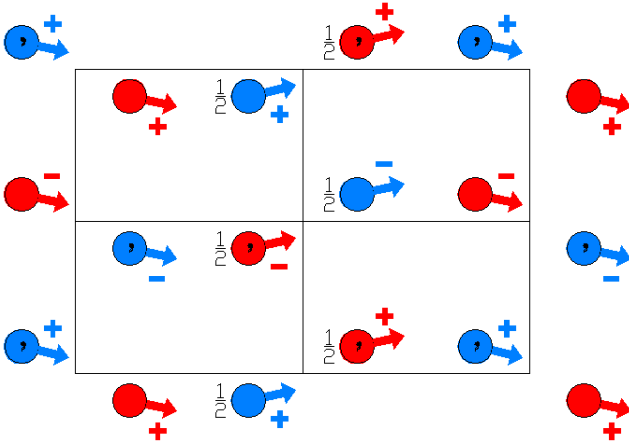
Along [0,1,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,1/4



Pn'na'  
52.8.413

m'mm'  
P2'/n'2<sub>1</sub>/n2'/a'

Orthorhombic

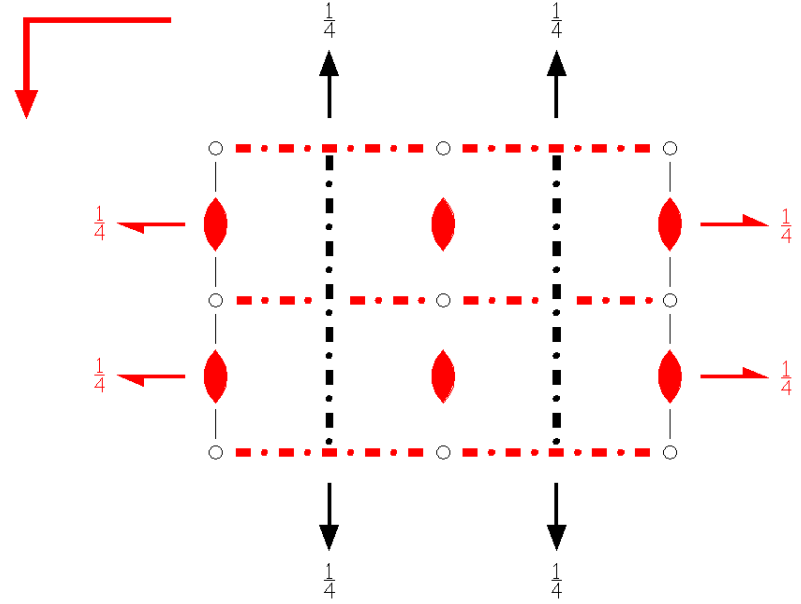


Origin at  $\bar{1}$  on n'1a'

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2' $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)'         | (3) 2 (0,1/2,0) $1/4,y,1/4$<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (4) 2' $x,1/4,1/4$<br>(2 <sub>x</sub>  0,1/2,1/2)'         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a' (1/2,0,0) $x,y,0$<br>(m <sub>z</sub>  1/2,0,0)' | (7) n (1/2,0,1/2) $x,1/4,z$<br>(m <sub>y</sub>  1/2,1/2,1/2) | (8) n' (0,1/2,1/2) $0,y,z$<br>(m <sub>x</sub>  0,1/2,1/2)' |





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

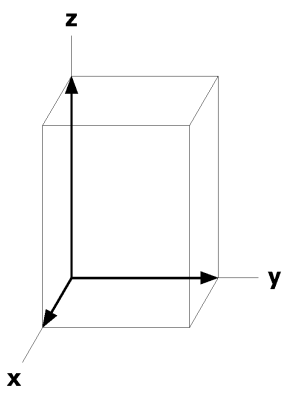
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x+1/2,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) x+1/2, $\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y+1/2,z+1/2$ [ $\bar{u},v,w$ ]
4	d 2'..	x,1/4,1/4 [0,v,w]	$\bar{x}+1/2,3/4,1/4$ [0,v, $\bar{w}$ ]	$\bar{x},3/4,3/4$ [0,v,w]	x+1/2,1/4,3/4 [0,v, $\bar{w}$ ]
4	c ..2'	1/4,0,z [u,v,0]	1/4,1/2, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	3/4,0, $\bar{z}$ [u,v,0]	3/4,1/2,z+1/2 [ $\bar{u},v,0$ ]
4	b $\bar{1}$	0,0,1/2 [u,v,w]	1/2,0,1/2 [u,v, $\bar{w}$ ]	1/2,1/2,0 [ $\bar{u},v,\bar{w}$ ]	0,1/2,0 [ $\bar{u},v,w$ ]
4	a $\bar{1}$	0,0,0 [u,v,w]	1/2,0,0 [u,v, $\bar{w}$ ]	1/2,1/2,1/2 [ $\bar{u},v,\bar{w}$ ]	0,1/2,1/2 [ $\bar{u},v,w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p2'mg'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

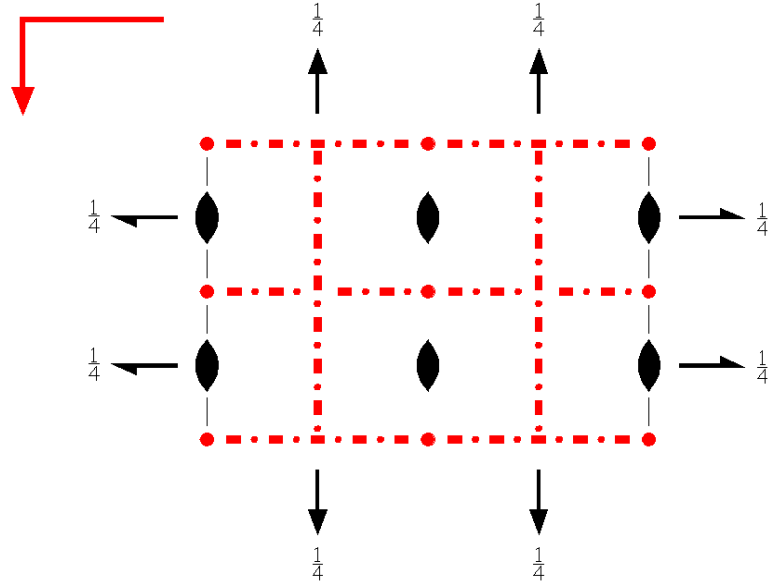
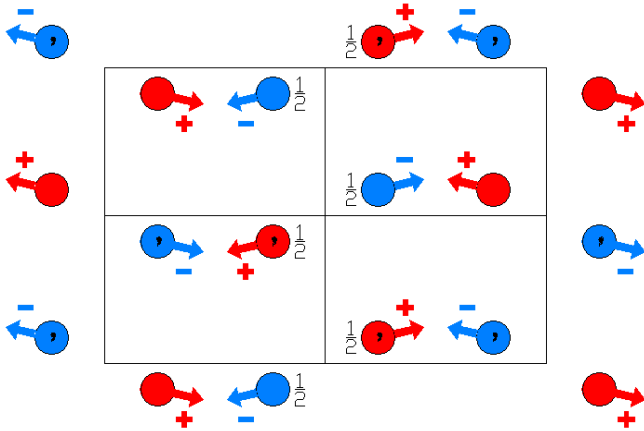
Along [0,1,0]  $c_p$ .2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 1/4,y,1/4



Pn'n'a'  
52.9.414

m'm'm'  
P2/n'2<sub>1</sub>/n'2/a'

Orthorhombic



Origin at  $\bar{1}$ ' on n'1a'

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                             | (2) 2 $1/4, 0, z$<br>(2 <sub>z</sub>  1/2, 0, 0)             | (3) 2 (0, 1/2, 0) $1/4, y, 1/4$<br>(2 <sub>y</sub>  1/2, 1/2, 1/2)   | (4) 2 $x, 1/4, 1/4$<br>(2 <sub>x</sub>  0, 1/2, 1/2)             |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$ ' 0,0,0)' | (6) a' (1/2, 0, 0) $x, y, 0$<br>(m <sub>z</sub>  1/2, 0, 0)' | (7) n' (1/2, 0, 1/2) $x, 1/4, z$<br>(m <sub>y</sub>  1/2, 1/2, 1/2)' | (8) n' (0, 1/2, 1/2) $0, y, z$<br>(m <sub>x</sub>  0, 1/2, 1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

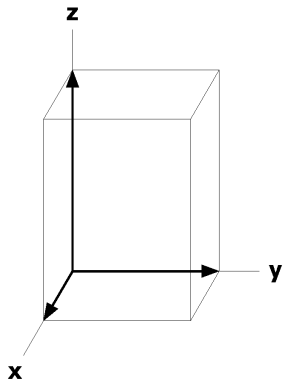
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}+1/2, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x, \bar{y}+1/2, \bar{z}+1/2$ [ $u, \bar{v}, \bar{w}$ ]
		(5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(6) $x+1/2, y, \bar{z}$ [ $u, v, \bar{w}$ ]	(7) $x+1/2, \bar{y}+1/2, z+1/2$ [ $u, \bar{v}, w$ ]	(8) $\bar{x}, y+1/2, z+1/2$ [ $\bar{u}, v, w$ ]
4	d 2..	$x, 1/4, 1/4$ [u,0,0]	$\bar{x}+1/2, 3/4, 1/4$ [ $\bar{u}, 0, 0$ ]	$\bar{x}, 3/4, 3/4$ [ $\bar{u}, 0, 0$ ]	$x+1/2, 1/4, 3/4$ [u,0,0]
4	c ..2	$1/4, 0, z$ [0,0,w]	$1/4, 1/2, \bar{z}+1/2$ [0,0, $\bar{w}$ ]	$3/4, 0, \bar{z}$ [0,0, $\bar{w}$ ]	$3/4, 1/2, z+1/2$ [0,0,w]
4	b $\bar{1}'$	$0, 0, 1/2$ [0,0,0]	$1/2, 0, 1/2$ [0,0,0]	$1/2, 1/2, 0$ [0,0,0]	$0, 1/2, 0$ [0,0,0]
4	a $\bar{1}'$	$0, 0, 0$ [0,0,0]	$1/2, 0, 0$ [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]	$0, 1/2, 1/2$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p2m'g'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

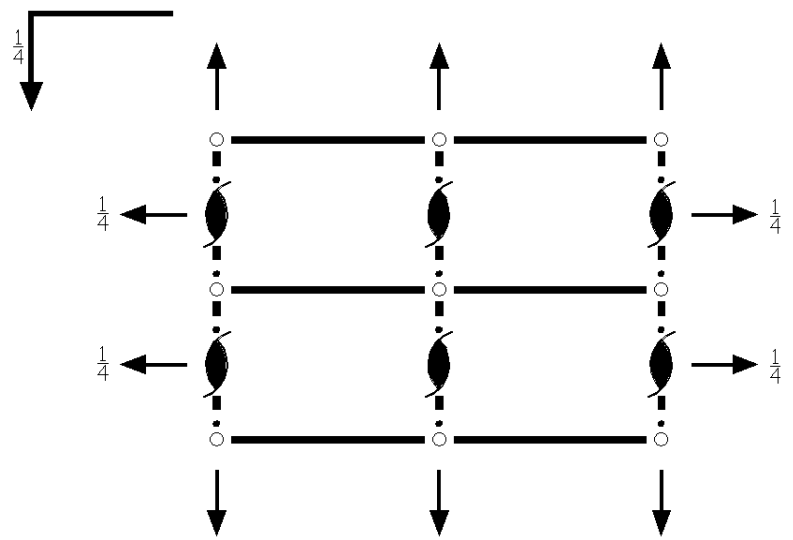
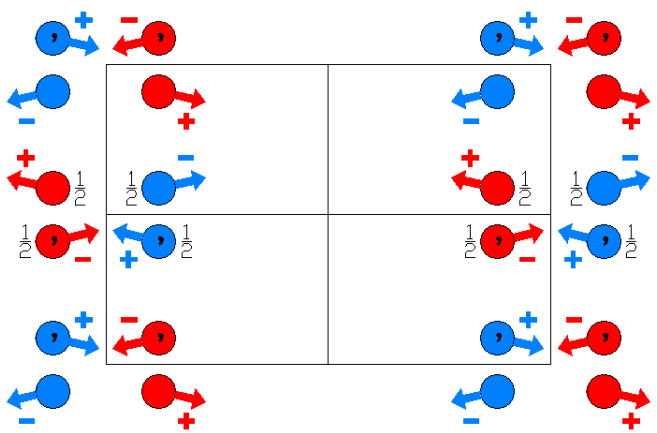
Along [0,1,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 1/4,y,1/4



Pmna  
53.1.415

mmm  
P2/m2/n2<sub>1</sub>/a

Orthorhombic



Origin at center ( 2/m ) at 2/mn1

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)         | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2) | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2) | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

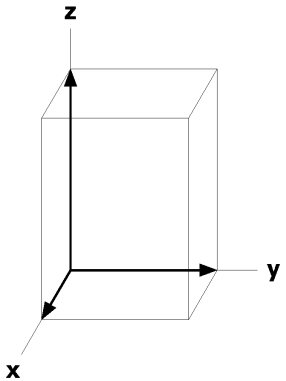
			Coordinates				
Multiplicity,	Wyckoff letter,	Site Symmetry.					
8	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	
			(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x+1/2,y, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) x+1/2, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]	
4	h	m..	0,y,z [u,0,0]	1/2, $\bar{y},z+1/2$ [ $\bar{u},0,0$ ]	1/2,y, $\bar{z}+1/2$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]	
4	g	.2.	1/4,y,1/4 [0,v,0]	1/4, $\bar{y},3/4$ [0, $\bar{v},0$ ]	3/4, $\bar{y},3/4$ [0,v,0]	3/4,y,1/4 [0, $\bar{v},0$ ]	
4	f	2..	x,1/2,0 [u,0,0]	$\bar{x}+1/2,1/2,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},1/2,0$ [u,0,0]	x+1/2,1/2,1/2 [ $\bar{u},0,0$ ]	
4	e	2..	x,0,0 [u,0,0]	$\bar{x}+1/2,0,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},0,0$ [u,0,0]	x+1/2,0,1/2 [ $\bar{u},0,0$ ]	
2	d	2/m..	0,1/2,0 [u,0,0]	1/2,1/2,1/2 [ $\bar{u},0,0$ ]			
2	c	2/m..	1/2,1/2,0 [u,0,0]	0,1/2,1/2 [ $\bar{u},0,0$ ]			
2	b	2/m..	1/2,0,0 [u,0,0]	0,0,1/2 [ $\bar{u},0,0$ ]			
2	a	2/m..	0,0,0 [u,0,0]	1/2,0,1/2 [ $\bar{u},0,0$ ]			

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,0,0]  $p2mg1'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0]  $c_p2'mm'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0

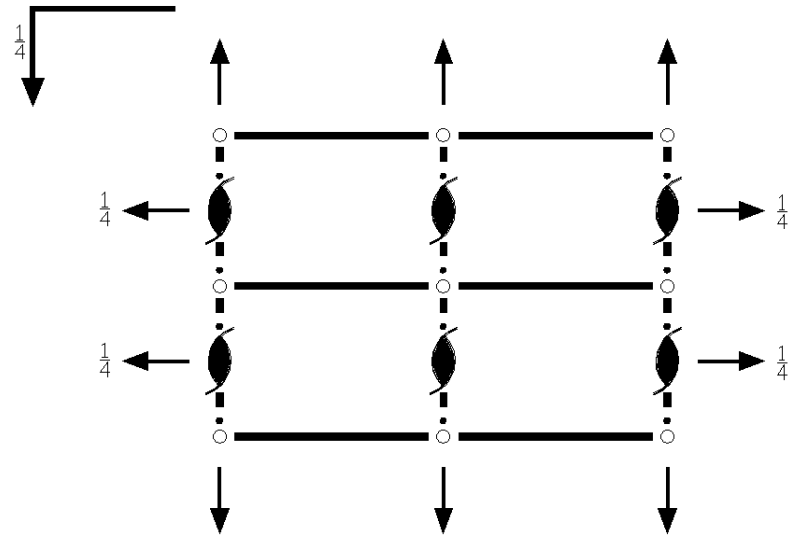
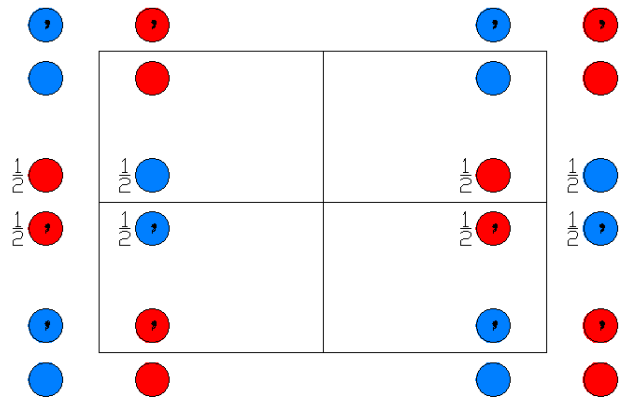


Pmna1'  
53.2.416

mmm1'  
P2/m2/n2<sub>1</sub>/a1'

Orthorhombic

1'



Origin at center ( 2/m1' ) at 2/mn11'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

Symmetry Operations

For 1 + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                        | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>   1/2,0,1/2) | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,0,1/2)         | (4) 2 x,0,0<br>(2 <sub>x</sub>   0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>   1/2,0,1/2) | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>   1/2,0,1/2) | (8) m 0,y,z<br>(m <sub>x</sub>   0,0,0) |

For 1' + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1'<br>(1   0,0,0)'                         | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>   1/2,0,1/2)' | (3) 2' 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,0,1/2)'         | (4) 2' x,0,0<br>(2 <sub>x</sub>   0,0,0)' |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$   0,0,0)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>   1/2,0,1/2)' | (7) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>   1/2,0,1/2)' | (8) m' 0,y,z<br>(m <sub>x</sub>   0,0,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

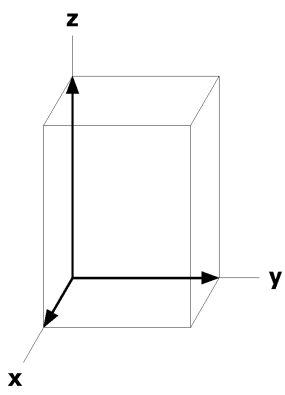
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +	1' +		
8 i 11'	(1) x,y,z [0,0,0] (5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [0,0,0] (6) $x+1/2,y,\bar{z}+1/2$ [0,0,0]	(3) $\bar{x}+1/2,y,\bar{z}+1/2$ [0,0,0] (7) $x+1/2,\bar{y},z+1/2$ [0,0,0]	(4) $x,\bar{y},\bar{z}$ [0,0,0] (8) $\bar{x},y,z$ [0,0,0]
4 h m..1'	0,y,z [0,0,0]	$1/2,\bar{y},z+1/2$ [0,0,0]	$1/2,y,\bar{z}+1/2$ [0,0,0]	$0,\bar{y},\bar{z}$ [0,0,0]
4 g .2.1'	$1/4,y,1/4$ [0,0,0]	$1/4,\bar{y},3/4$ [0,0,0]	$3/4,\bar{y},3/4$ [0,0,0]	$3/4,y,1/4$ [0,0,0]
4 f 2..1'	$x,1/2,0$ [0,0,0]	$\bar{x}+1/2,1/2,1/2$ [0,0,0]	$\bar{x},1/2,0$ [0,0,0]	$x+1/2,1/2,1/2$ [0,0,0]
4 e 2..1'	$x,0,0$ [0,0,0]	$\bar{x}+1/2,0,1/2$ [0,0,0]	$\bar{x},0,0$ [0,0,0]	$x+1/2,0,1/2$ [0,0,0]
2 d 2/m..1'	$0,1/2,0$ [0,0,0]	$1/2,1/2,1/2$ [0,0,0]		
2 c 2/m..1'	$1/2,1/2,0$ [0,0,0]	$0,1/2,1/2$ [0,0,0]		
2 b 2/m..1'	$1/2,0,0$ [0,0,0]	$0,0,1/2$ [0,0,0]		
2 a 2/m..1'	$0,0,0$ [0,0,0]	$1/2,0,1/2$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

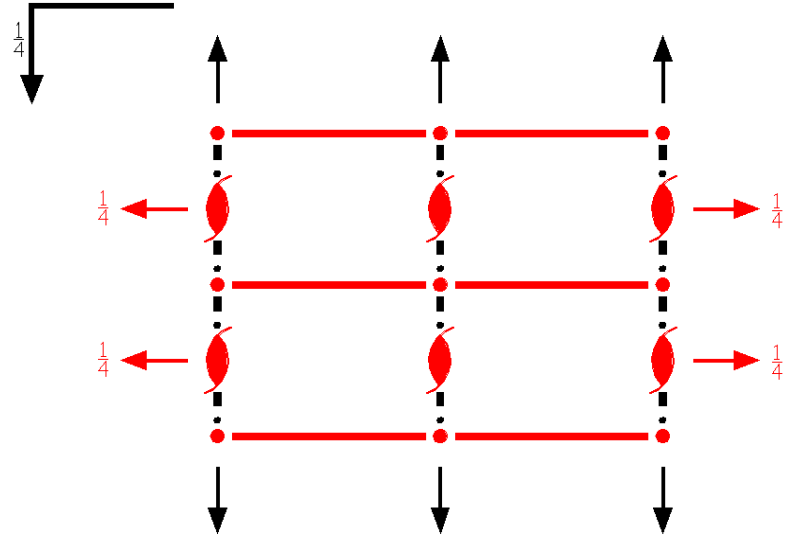
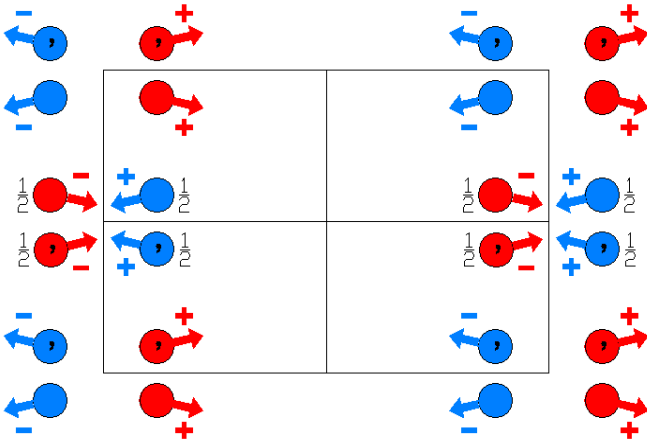
Along [0,1,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pm'na  
53.3.417

m'mm  
P2/m'2'/n2<sub>1</sub>'/a

Orthorhombic



Origin at center ( 2/m' ) at 2/m'n1

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/4$

### Symmetry Operations

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) 2' 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)'       | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)   | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2) | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

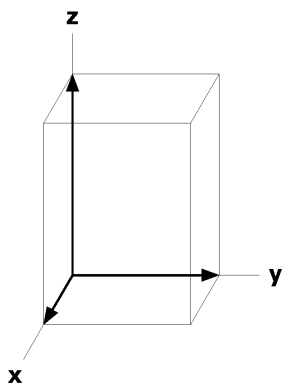
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	i 1	(1) x,y,z [u,v,w] (5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [u,v, $\bar{w}$ ] (6) x+1/2,y, $\bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}+1/2, y, \bar{z}+1/2$ [u, $\bar{v}, w$ ] (7) x+1/2, $\bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ] (8) $\bar{x}, y, z$ [ $\bar{u}, v, w$ ]
4	h m'..	0,y,z [0,v,w]	1/2, $\bar{y}, z+1/2$ [0,v, $\bar{w}$ ]	1/2,y, $\bar{z}+1/2$ [0, $\bar{v}, w$ ]	0, $\bar{y}, \bar{z}$ [0, $\bar{v}, \bar{w}$ ]
4	g .2'	1/4,y,1/4 [u,0,w]	1/4, $\bar{y}, 3/4$ [u,0, $\bar{w}$ ]	3/4, $\bar{y}, 3/4$ [ $\bar{u}, 0, \bar{w}$ ]	3/4,y,1/4 [ $\bar{u}, 0, w$ ]
4	f 2..	x,1/2,0 [u,0,0]	$\bar{x}+1/2, 1/2, 1/2$ [u,0,0]	$\bar{x}, 1/2, 0$ [ $\bar{u}, 0, 0$ ]	x+1/2,1/2,1/2 [ $\bar{u}, 0, 0$ ]
4	e 2..	x,0,0 [u,0,0]	$\bar{x}+1/2, 0, 1/2$ [u,0,0]	$\bar{x}, 0, 0$ [ $\bar{u}, 0, 0$ ]	x+1/2,0,1/2 [ $\bar{u}, 0, 0$ ]
2	d 2/m'..	0,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	c 2/m'..	1/2,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	b 2/m'..	1/2,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
2	a 2/m'..	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2a} \cdot 2m' m'$   
 $\mathbf{a}^* = \mathbf{a}/2 \quad \mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p 2mg$   
 $\mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

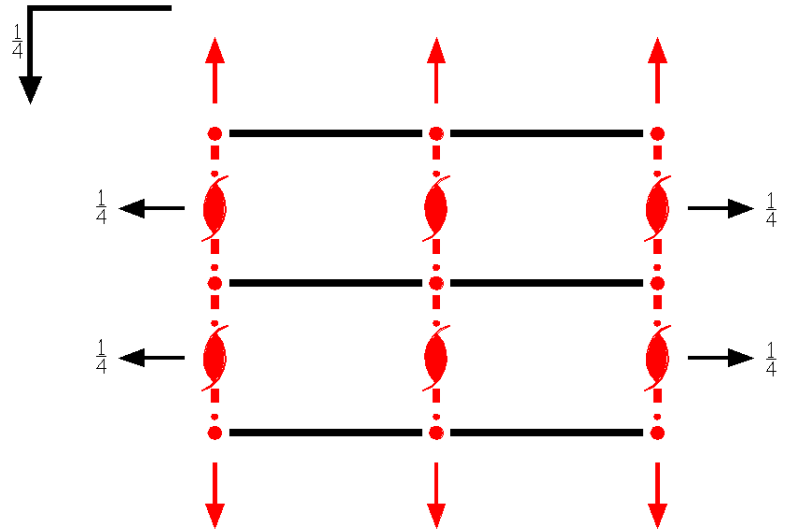
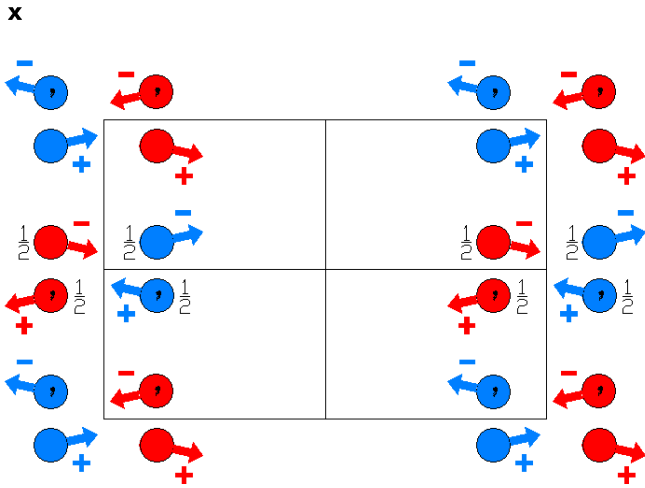
Along [0,1,0]  $c_p \cdot 2m' m'$   
 $\mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pmn'a  
53.4.418

mm'm  
P2'/m2/n'2<sub>1</sub>'/a

Orthorhombic



Origin at center ( 2'/m ) at 2'/mn'1

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)           | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)   | (7) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2)' | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

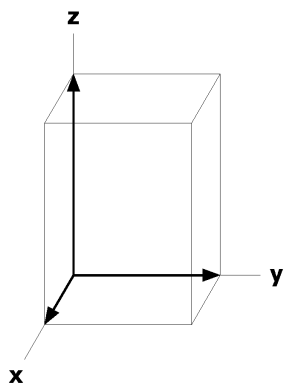
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	i 1	(1) x,y,z [u,v,w] (5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [u,v, $\bar{w}$ ] (6) x+1/2,y, $\bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}+1/2, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ] (7) x+1/2, $\bar{y}, z+1/2$ [u, $\bar{v}, w$ ]	(4) x, $\bar{y}, \bar{z}$ [ $\bar{u}, v, w$ ] (8) $\bar{x}, y, z$ [u, $\bar{v}, \bar{w}$ ]
4	h m..	0,y,z [u,0,0]	1/2, $\bar{y}, z+1/2$ [u,0,0]	1/2,y, $\bar{z}+1/2$ [ $\bar{u}, 0, 0$ ]	0, $\bar{y}, \bar{z}$ [ $\bar{u}, 0, 0$ ]
4	g .2.	1/4,y,1/4 [0,v,0]	1/4, $\bar{y}, 3/4$ [0,v,0]	3/4, $\bar{y}, 3/4$ [0, $\bar{v}, 0$ ]	3/4,y,1/4 [0, $\bar{v}, 0$ ]
4	f 2'..	x,1/2,0 [0,v,w]	$\bar{x}+1/2, 1/2, 1/2$ [0,v, $\bar{w}$ ]	$\bar{x}, 1/2, 0$ [0, $\bar{v}, \bar{w}$ ]	x+1/2,1/2,1/2 [0, $\bar{v}, w$ ]
4	e 2'..	x,0,0 [0,v,w]	$\bar{x}+1/2, 0, 1/2$ [0,v, $\bar{w}$ ]	$\bar{x}, 0, 0$ [0, $\bar{v}, \bar{w}$ ]	x+1/2,0,1/2 [0, $\bar{v}, w$ ]
2	d 2'/m..	0,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	c 2'/m..	1/2,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	b 2'/m..	1/2,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
2	a 2'/m..	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2a}2mm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2mg1'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

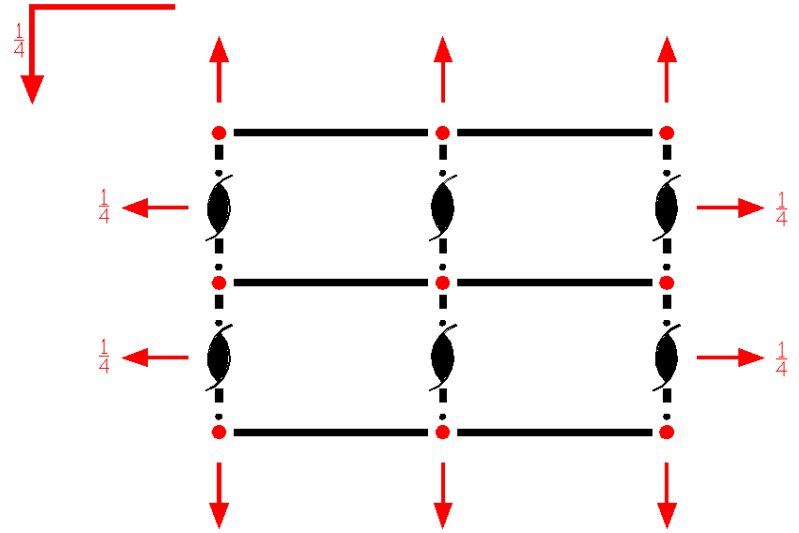
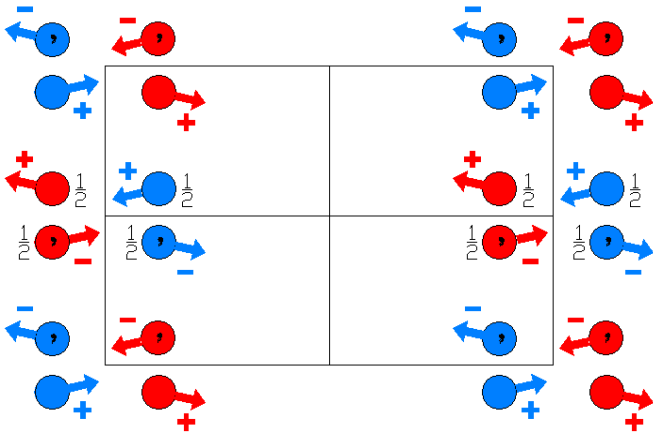
Along [0,1,0]  $c2mm$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pmna'  
53.5.419

mmm'  
P2'/m2'/n2<sub>1</sub>/a'

Orthorhombic



Origin at center ( $2'/m$ ) at  $2'/mn1$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2' 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)'       | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2) | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

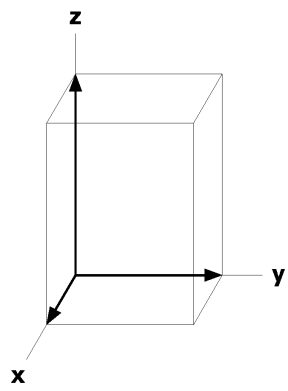
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	i 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x}+1/2,y,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) $x+1/2,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
4	h m..	0,y,z [u,0,0]	$1/2,\bar{y},z+1/2$ [ $\bar{u},0,0$ ]	$1/2,y,\bar{z}+1/2$ [u,0,0]	$0,\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
4	g .2'	$1/4,y,1/4$ [u,0,w]	$1/4,\bar{y},3/4$ [ $\bar{u},0,w$ ]	$3/4,\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	$3/4,y,1/4$ [u,0, $\bar{w}$ ]
4	f 2'..	$x,1/2,0$ [0,v,w]	$\bar{x}+1/2,1/2,1/2$ [0, $\bar{v},w$ ]	$\bar{x},1/2,0$ [0, $\bar{v},\bar{w}$ ]	$x+1/2,1/2,1/2$ [0,v, $\bar{w}$ ]
4	e 2'..	$x,0,0$ [0,v,w]	$\bar{x}+1/2,0,1/2$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0, $\bar{v},\bar{w}$ ]	$x+1/2,0,1/2$ [0,v, $\bar{w}$ ]
2	d 2'/m..	$0,1/2,0$ [0,0,0]	$1/2,1/2,1/2$ [0,0,0]		
2	c 2'/m..	$1/2,1/2,0$ [0,0,0]	$0,1/2,1/2$ [0,0,0]		
2	b 2'/m..	$1/2,0,0$ [0,0,0]	$0,0,1/2$ [0,0,0]		
2	a 2'/m..	$0,0,0$ [0,0,0]	$1/2,0,1/2$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

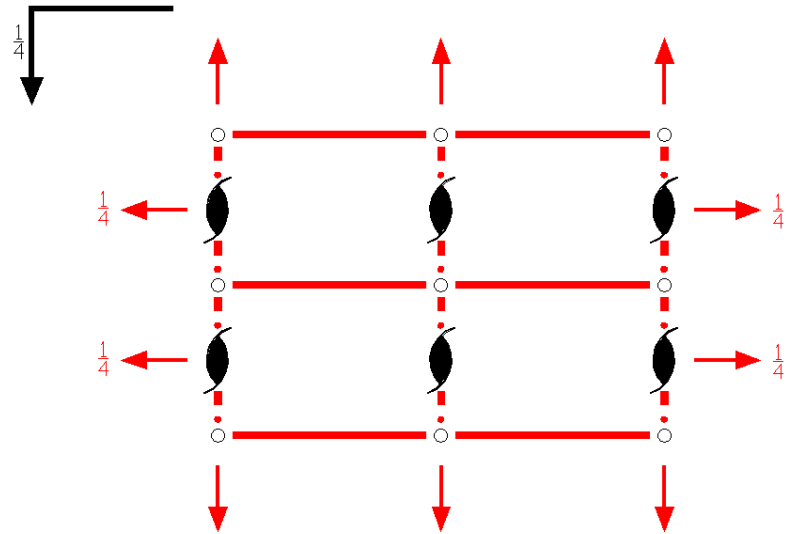
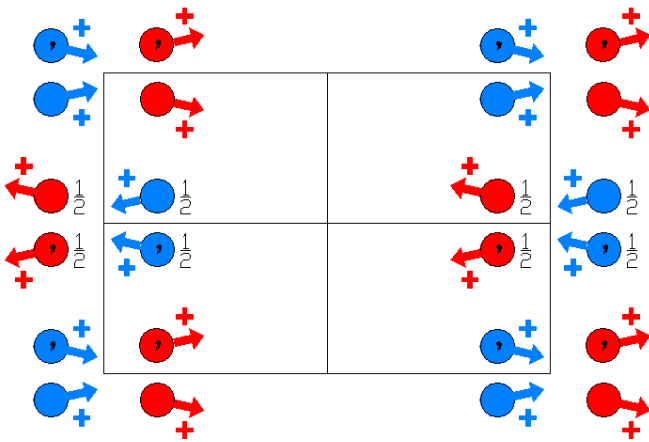
Along [0,1,0]  $c_p$ -2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pm'n'a  
53.6.420

m'm'm  
P2'/m'2'/n'2<sub>1</sub>/a

Orthorhombic



Origin at center ( $2'/m'$ ) at  $2'/m'n'1$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) 2' 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)'         | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2) | (7) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2)' | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

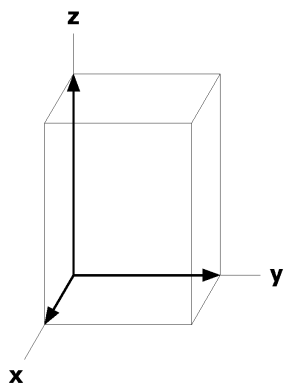
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	i 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ] (7) $x+1/2,\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
4	h m'..	0,y,z [0,v,w]	$1/2,\bar{y},z+1/2$ [0, $\bar{v},w$ ]	$1/2,y,\bar{z}+1/2$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
4	g .2'	$1/4,y,1/4$ [u,0,w]	$1/4,\bar{y},3/4$ [ $\bar{u},0,w$ ]	$3/4,\bar{y},3/4$ [u,0,w]	$3/4,y,1/4$ [ $\bar{u},0,w$ ]
4	f 2'..	x,1/2,0 [0,v,w]	$\bar{x}+1/2,1/2,1/2$ [0, $\bar{v},w$ ]	$\bar{x},1/2,0$ [0,v,w]	$x+1/2,1/2,1/2$ [0, $\bar{v},w$ ]
4	e 2'..	x,0,0 [0,v,w]	$\bar{x}+1/2,0,1/2$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0,v,w]	$x+1/2,0,1/2$ [0, $\bar{v},w$ ]
2	d 2'/m'..	0,1/2,0 [0,v,w]	$1/2,1/2,1/2$ [0, $\bar{v},w$ ]		
2	c 2'/m'..	$1/2,1/2,0$ [0,v,w]	$0,1/2,1/2$ [0, $\bar{v},w$ ]		
2	b 2'/m'..	$1/2,0,0$ [0,v,w]	$0,0,1/2$ [0, $\bar{v},w$ ]		
2	a 2'/m'..	0,0,0 [0,v,w]	$1/2,0,1/2$ [0, $\bar{v},w$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2'mg'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

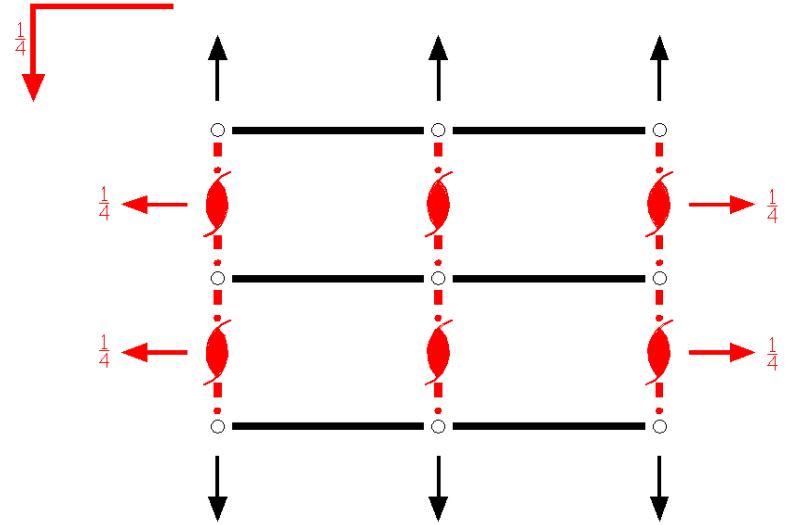
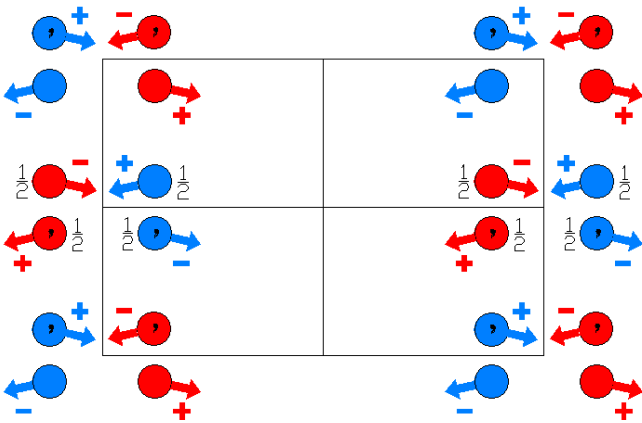
Along [0,1,0]  $c_p, 2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pmn'a'  
53.7.421

mm'm'  
P2/m2'/n'2<sub>1</sub>'/a'

Orthorhombic



Origin at center ( 2/m ) at 2/mn'1

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) 2' 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)'         | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2)' | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

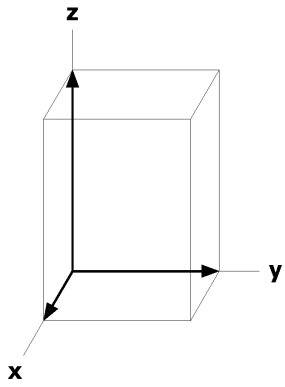
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	i 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x}+1/2, y, \bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
		(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) x+1/2,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(7) x+1/2, $\bar{y}, z+1/2$ [u, $\bar{v}$ ,w]	(8) $\bar{x}, y, z$ [u, $\bar{v}, \bar{w}$ ]
4	h m..	0,y,z [u,0,0]	1/2, $\bar{y}, z+1/2$ [u,0,0]	1/2,y, $\bar{z}+1/2$ [u,0,0]	0, $\bar{y}, \bar{z}$ [u,0,0]
4	g .2'	1/4,y,1/4 [u,0,w]	1/4, $\bar{y}, 3/4$ [u,0, $\bar{w}$ ]	3/4, $\bar{y}, 3/4$ [u,0,w]	3/4,y,1/4 [u,0, $\bar{w}$ ]
4	f 2..	x,1/2,0 [u,0,0]	$\bar{x}+1/2, 1/2, 1/2$ [u,0,0]	$\bar{x}, 1/2, 0$ [u,0,0]	x+1/2,1/2,1/2 [u,0,0]
4	e 2..	x,0,0 [u,0,0]	$\bar{x}+1/2, 0, 1/2$ [u,0,0]	$\bar{x}, 0, 0$ [u,0,0]	x+1/2,0,1/2 [u,0,0]
2	d 2/m..	0,1/2,0 [u,0,0]	1/2,1/2,1/2 [u,0,0]		
2	c 2/m..	1/2,1/2,0 [u,0,0]	0,1/2,1/2 [u,0,0]		
2	b 2/m..	1/2,0,0 [u,0,0]	0,0,1/2 [u,0,0]		
2	a 2/m..	0,0,0 [u,0,0]	1/2,0,1/2 [u,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



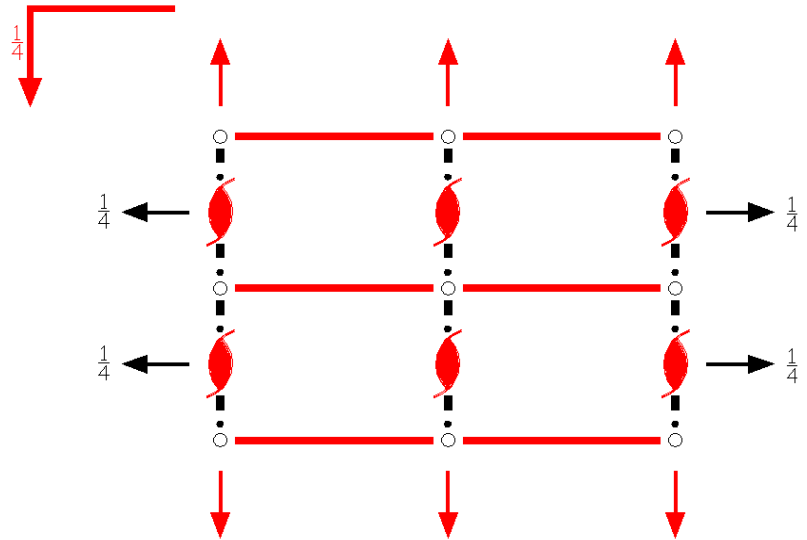
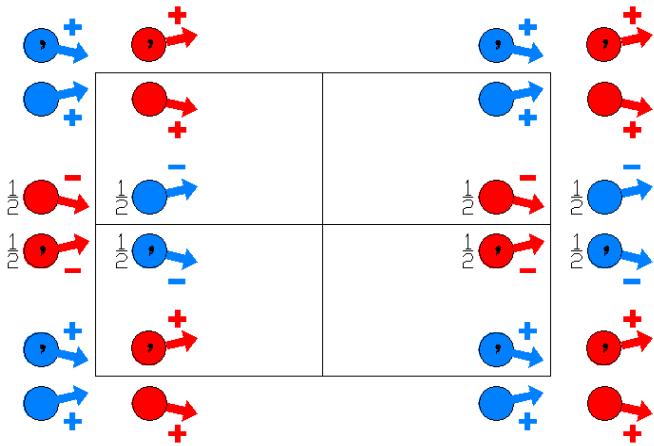
Pm'na'

53.8.422

m'mm'

P2'/m'2/n2<sub>1</sub>'/a'

Orthorhombic



Origin at center ( 2'/m' ) at 2'/m'n1

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)         | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2) | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

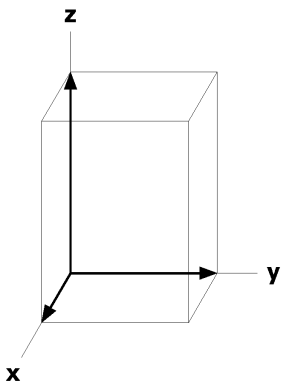
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	i 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x}+1/2,y,\bar{z}+1/2$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u}$ ,v,w]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x+1/2,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(7) x+1/2, $\bar{y},z+1/2$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(8) $\bar{x},y,z$ [ $\bar{u}$ ,v,w]
4	h m'..	0,y,z [0,v,w]	1/2, $\bar{y},z+1/2$ [0,v, $\bar{w}$ ]	1/2,y, $\bar{z}+1/2$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
4	g .2.	1/4,y,1/4 [0,v,0]	1/4, $\bar{y},3/4$ [0,v,0]	3/4, $\bar{y},3/4$ [0,v,0]	3/4,y,1/4 [0,v,0]
4	f 2'..	x,1/2,0 [0,v,w]	$\bar{x}+1/2,1/2,1/2$ [0,v, $\bar{w}$ ]	$\bar{x},1/2,0$ [0,v,w]	x+1/2,1/2,1/2 [0,v, $\bar{w}$ ]
4	e 2'..	x,0,0 [0,v,w]	$\bar{x}+1/2,0,1/2$ [0,v, $\bar{w}$ ]	$\bar{x},0,0$ [0,v,w]	x+1/2,0,1/2 [0,v, $\bar{w}$ ]
2	d 2'/m'..	0,1/2,0 [0,v,w]	1/2,1/2,1/2 [0,v, $\bar{w}$ ]		
2	c 2'/m'..	1/2,1/2,0 [0,v,w]	0,1/2,1/2 [0,v, $\bar{w}$ ]		
2	b 2'/m'..	1/2,0,0 [0,v,w]	0,0,1/2 [0,v, $\bar{w}$ ]		
2	a 2'/m'..	0,0,0 [0,v,w]	1/2,0,1/2 [0,v, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

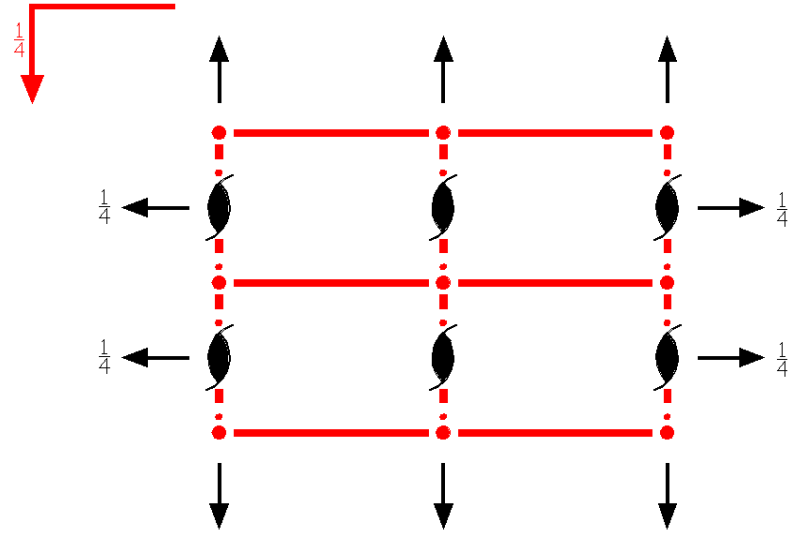
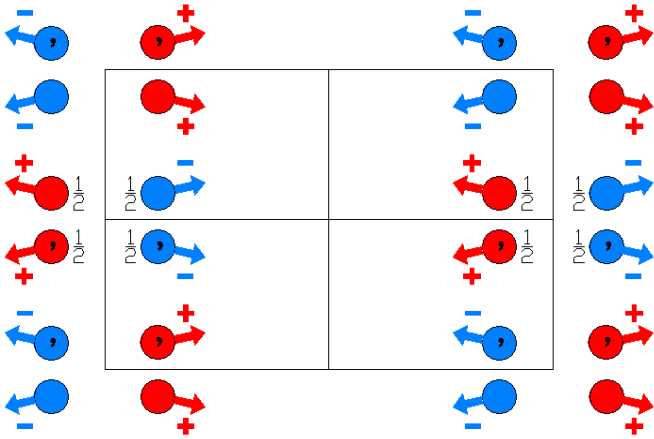
Along [0,1,0]  $c_p$ .2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pm'n'a'  
53.9.423

m'm'm'  
P2/m'2/n'2<sub>1</sub>/a'

Orthorhombic



Origin at center ( $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ ) at  $2/m'n'1$

Asymmetric unit  $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

### Symmetry Operations

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)           | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2)' | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

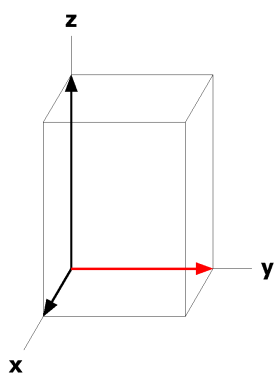
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	i 1	(1) x,y,z [u,v,w] (5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ] (6) $x+1/2, y, \bar{z}+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x}+1/2, y, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ] (7) $x+1/2, \bar{y}, z+1/2$ [u, $\bar{v}, w$ ]	(4) $x, \bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ] (8) $\bar{x}, y, z$ [ $\bar{u}, v, w$ ]
4	h m'..	0,y,z [0,v,w]	$1/2, \bar{y}, z+1/2$ [0, $\bar{v}, w$ ]	$1/2, y, \bar{z}+1/2$ [0,v, $\bar{w}$ ]	$0, \bar{y}, \bar{z}$ [0, $\bar{v}, \bar{w}$ ]
4	g .2.	$1/4, y, 1/4$ [0,v,0]	$1/4, \bar{y}, 3/4$ [0, $\bar{v}, 0$ ]	$3/4, \bar{y}, 3/4$ [0, $\bar{v}, 0$ ]	$3/4, y, 1/4$ [0,v,0]
4	f 2..	$x, 1/2, 0$ [u,0,0]	$\bar{x}+1/2, 1/2, 1/2$ [ $\bar{u}, 0, 0$ ]	$\bar{x}, 1/2, 0$ [ $\bar{u}, 0, 0$ ]	$x+1/2, 1/2, 1/2$ [u,0,0]
4	e 2..	$x, 0, 0$ [u,0,0]	$\bar{x}+1/2, 0, 1/2$ [ $\bar{u}, 0, 0$ ]	$\bar{x}, 0, 0$ [ $\bar{u}, 0, 0$ ]	$x+1/2, 0, 1/2$ [u,0,0]
2	d $2/m'..$	$0, 1/2, 0$ [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]		
2	c $2/m'..$	$1/2, 1/2, 0$ [0,0,0]	$0, 1/2, 1/2$ [0,0,0]		
2	b $2/m'..$	$1/2, 0, 0$ [0,0,0]	$0, 0, 1/2$ [0,0,0]		
2	a $2/m'..$	$0, 0, 0$ [0,0,0]	$1/2, 0, 1/2$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2m'g'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

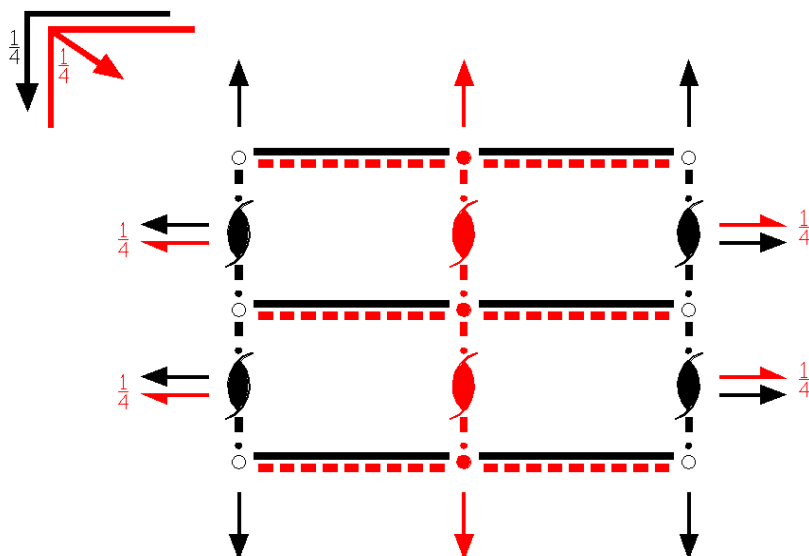
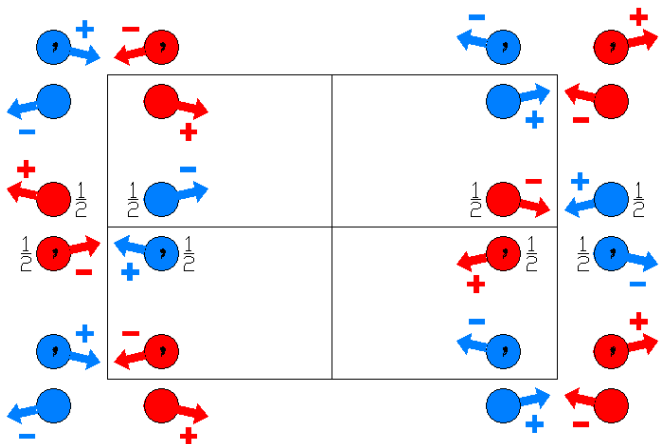
Along [0,1,0]  $c2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



$P_{2b} mna$   
53.10.424

$mmm1'$   
 $P_{2b} 2/m2/n2_1/a$

Orthorhombic



Origin at center ( $2/m$ ) at  $2/mn1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |  |                                      |
|--|--|--|--------------------------------------|
| (1) 1<br>(1 0,0,0)                               | (2) 2 $(0,0,1/2)$ $1/4,0,z$<br>( $2_z$   $1/2,0,1/2$ ) | (3) 2 $1/4,y,1/4$<br>( $2_y$   $1/2,0,1/2$ )           | (4) 2 $x,0,0$<br>( $2_x$   $0,0,0$ ) |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ ) | (6) a $(1/2,0,0)$ $x,y,1/4$<br>( $m_z$   $1/2,0,1/2$ ) | (7) n $(1/2,0,1/2)$ $x,0,z$<br>( $m_y$   $1/2,0,1/2$ ) | (8) m $0,y,z$<br>( $m_x$   $0,0,0$ ) |

For  $(0,1,0)'$  + set

- |   |   |   |   |
|---|---|---|---|
| (1) $t'$ $(0,1,0)$<br>(1  $0,1,0$ )'                  | (2) $2'$ $(0,0,1/2)$ $1/4,1/2,z$<br>( $2'_z$   $1/2,1,1/2$ )' | (3) $2'$ $(0,1,0)$ $1/4,y,1/4$<br>( $2'_y$   $1/2,1,1/2$ )'   | (4) $2'$ $x,1/2,0$<br>( $2'_x$   $0,1,0$ )'         |
| (5) $\bar{1}'$ $0,1/2,0$<br>( $\bar{1}'$   $0,1,0$ )' | (6) $n'$ $(1/2,1,0)$ $x,y,1/4$<br>( $m'_z$   $1/2,1,1/2$ )'   | (7) $n'$ $(1/2,0,1/2)$ $x,1/2,z$<br>( $m'_y$   $1/2,1,1/2$ )' | (8) $b'$ $(0,1,0)$ $0,y,z$<br>( $m'_x$   $0,1,0$ )' |

**Generators selected** (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

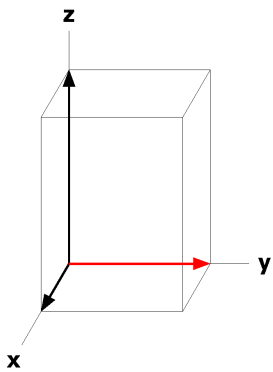
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
16 i 1	(1) x,y,z [u,v,w] (5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ] (6) $x+1/2, y, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}+1/2, y, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ] (7) $x+1/2, \bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x, \bar{y}, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ] (8) $\bar{x}, y, z$ [ $u, \bar{v}, \bar{w}$ ]
8 h m..	0,y,z [u,0,0]	$1/2, \bar{y}, z+1/2$ [ $\bar{u}, 0, 0$ ]	$1/2, y, \bar{z}+1/2$ [ $\bar{u}, 0, 0$ ]	$0, \bar{y}, \bar{z}$ [u,0,0]
8 g .2.	$1/4, y, 1/4$ [0,v,0]	$1/4, \bar{y}, 3/4$ [0, $\bar{v}$ ,0]	$3/4, \bar{y}, 3/4$ [0,v,0]	$3/4, y, 1/4$ [0, $\bar{v}$ ,0]
8 f 2'..	$x, 1/2, 0$ [0,v,w]	$\bar{x}+1/2, 1/2, 1/2$ [0,v, $\bar{w}$ ]	$\bar{x}, 1/2, 0$ [0, $\bar{v}$ , $\bar{w}$ ]	$x+1/2, 1/2, 1/2$ [0, $\bar{v}$ ,w]
8 e 2..	$x, 0, 0$ [u,0,0]	$\bar{x}+1/2, 0, 1/2$ [ $\bar{u}, 0, 0$ ]	$\bar{x}, 0, 0$ [u,0,0]	$x+1/2, 0, 1/2$ [ $\bar{u}, 0, 0$ ]
4 d 2'/m..	$0, 1/2, 0$ [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]		
4 c 2'/m..	$1/2, 1/2, 0$ [0,0,0]	$0, 1/2, 1/2$ [0,0,0]		
4 b 2'/m..	$1/2, 0, 0$ [u,0,0]	$0, 0, 1/2$ [ $\bar{u}, 0, 0$ ]		
4 a 2'/m..	$0, 0, 0$ [u,0,0]	$1/2, 0, 1/2$ [ $\bar{u}, 0, 0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p 2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



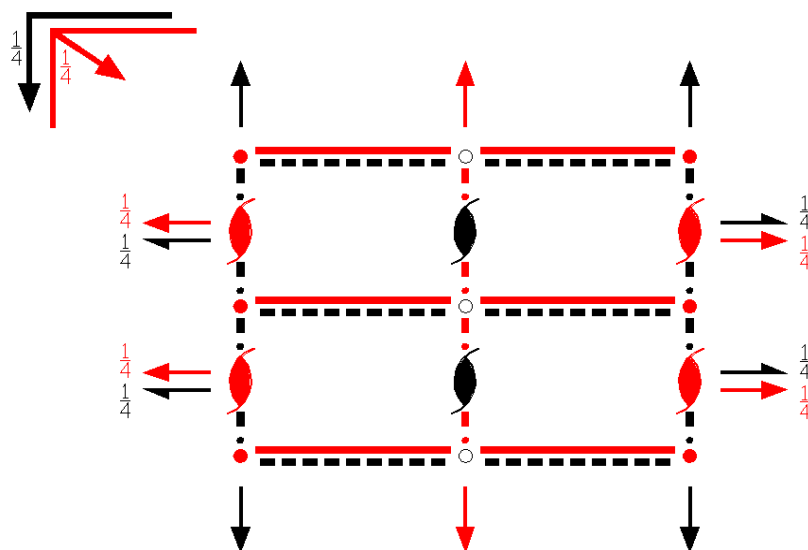
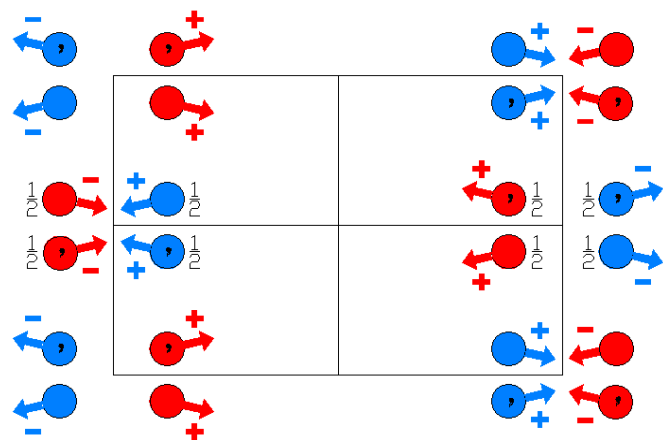
$P_{2b} m'na$

53.11.425

$mmm1'$

$P_{2b} 2/m'2'/n2_1'/a$

Orthorhombic



Origin at center ( $2/m'$ ) at  $2/m'n1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                               | (2) $2' (0,0,1/2)$ $1/4,0,z$<br>( $2_z$   $1/2,0,1/2$ )' | (3) $2' 1/4,y,1/4$<br>( $2_y$   $1/2,0,1/2$ )'           | (4) 2 $x,0,0$<br>( $2_x$   $0,0,0$ )   |
| (5) $\bar{1}' 0,0,0$<br>( $\bar{1}$   $0,0,0$ )' | (6) a ( $1/2,0,0$ ) $x,y,1/4$<br>( $m_z$   $1/2,0,1/2$ ) | (7) n ( $1/2,0,1/2$ ) $x,0,z$<br>( $m_y$   $1/2,0,1/2$ ) | (8) $m' 0,y,z$<br>( $m_x$   $0,0,0$ )' |

For (0,1,0)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t' (0,1,0)$<br>(1  $0,1,0$ )'                | (2) 2 ( $0,0,1/2$ ) $1/4,1/2,z$<br>( $2_z$   $1/2,1,1/2$ ) | (3) 2 ( $0,1,0$ ) $1/4,y,1/4$<br>( $2_y$   $1/2,1,1/2$ )   | (4) $2' x,1/2,0$<br>( $2_x$   $0,1,0$ )'         |
| (5) $\bar{1}' 0,1/2,0$<br>( $\bar{1}$   $0,1,0$ ) | (6) $n' (1/2,1,0)$ $x,y,1/4$<br>( $m_z$   $1/2,1,1/2$ )'   | (7) $n' (1/2,0,1/2)$ $x,1/2,z$<br>( $m_y$   $1/2,1,1/2$ )' | (8) b ( $0,1,0$ ) $0,y,z$<br>( $m_x$   $0,1,0$ ) |



**Generators selected** (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

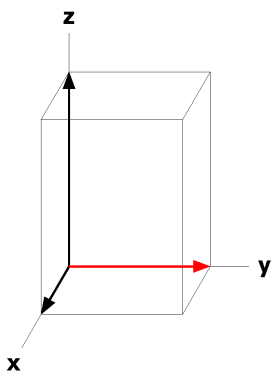
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +		(0,1,0)' +	
16	i 1	(1) x,y,z [u,v,w] (5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(2) $\bar{x}+1/2, \bar{y}, \bar{z}+1/2$ [u,v, $\bar{w}$ ] (6) x+1/2,y, $\bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}+1/2, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ] (7) x+1/2, $\bar{y}, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ] (8) $\bar{x}, y, z$ [ $\bar{u}, v, w$ ]
8	h m'..	0,y,z [0,v,w]	1/2, $\bar{y}, \bar{z}+1/2$ [0,v, $\bar{w}$ ]	1/2,y, $\bar{z}+1/2$ [0, $\bar{v}, w$ ]	0, $\bar{y}, \bar{z}$ [0, $\bar{v}, \bar{w}$ ]
8	g .2.	1/4,y,1/4 [0,v,0]	1/4, $\bar{y}, 3/4$ [0,v,0]	3/4, $\bar{y}, 3/4$ [0, $\bar{v}, 0$ ]	3/4,y,1/4 [0, $\bar{v}, 0$ ]
8	f 2'..	x,1/2,0 [0,v,w]	$\bar{x}+1/2, 1/2, 1/2$ [0, $\bar{v}, w$ ]	$\bar{x}, 1/2, 0$ [0,v,w]	x+1/2,1/2,1/2 [0, $\bar{v}, w$ ]
8	e 2..	x,0,0 [u,0,0]	$\bar{x}+1/2, 0, 1/2$ [u,0,0]	$\bar{x}, 0, 0$ [ $\bar{u}, 0, 0$ ]	x+1/2,0,1/2 [ $\bar{u}, 0, 0$ ]
4	d 2'/m'..	0,1/2,0 [0,v,w]	1/2,1/2,1/2 [0, $\bar{v}, w$ ]		
4	c 2'/m'..	1/2,1/2,0 [0,v,w]	0,1/2,1/2 [0, $\bar{v}, w$ ]		
4	b 2'/m'..	1/2,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
4	a 2'/m'..	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,1/2,z

Along [1,0,0] p<sub>2b</sub>-2mg  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

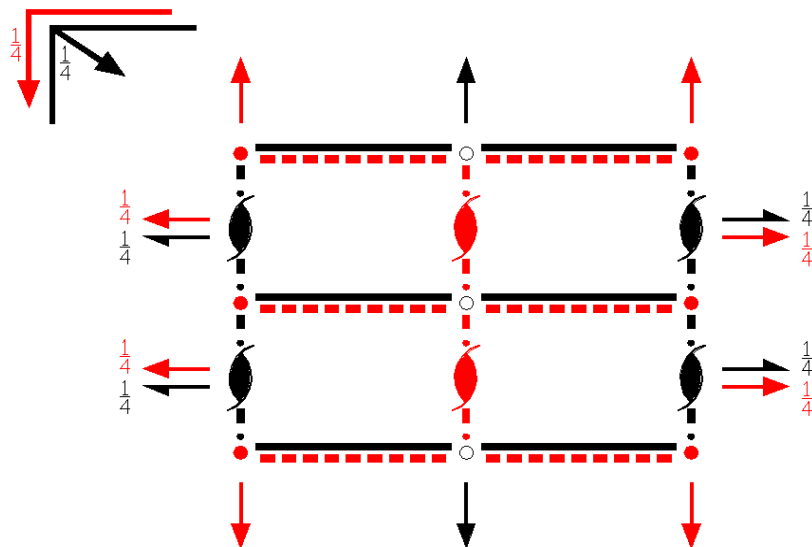
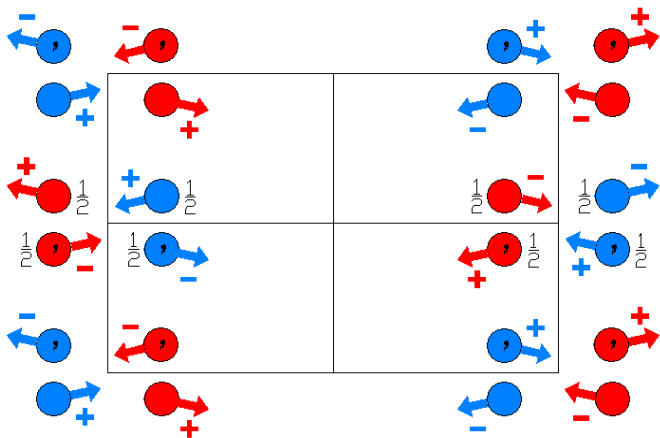
Along [0,1,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



$P_{2b} mna'$   
53.12.426

$mmm1'$   
 $P_{2b} 2'/m2'/n2_1/a'$

Orthorhombic



Origin at center ( $2'/m$ ) at  $2'/mn1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 $(0,0,1/2)$ $1/4,0,z$<br>( $2_z$   $1/2,0,1/2$ )     | (3) $2'$ $1/4,y,1/4$<br>( $2_y$   $1/2,0,1/2$ )'         | (4) $2'$ $x,0,0$<br>( $2_x$   $0,0,0$ )' |
| (5) $\bar{1}'$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ )' | (6) $a'$ $(1/2,0,0)$ $x,y,1/4$<br>( $m_z$   $1/2,0,1/2$ )' | (7) $n$ $(1/2,0,1/2)$ $x,0,z$<br>( $m_y$   $1/2,0,1/2$ ) | (8) $m$ $0,y,z$<br>( $m_x$   $0,0,0$ )   |

For  $(0,1,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(0,1,0)$<br>(1  $0,1,0$ )'               | (2) $2'$ $(0,0,1/2)$ $1/4,1/2,z$<br>( $2_z$   $1/2,1,1/2$ )' | (3) 2 $(0,1,0)$ $1/4,y,1/4$<br>( $2_y$   $1/2,1,1/2$ )       | (4) 2 $x,1/2,0$<br>( $2_x$   $0,1,0$ )             |
| (5) $\bar{1}$ $0,1/2,0$<br>( $\bar{1}$   $0,1,0$ ) | (6) $n$ $(1/2,1,0)$ $x,y,1/4$<br>( $m_z$   $1/2,1,1/2$ )     | (7) $n'$ $(1/2,0,1/2)$ $x,1/2,z$<br>( $m_y$   $1/2,1,1/2$ )' | (8) $b'$ $(0,1,0)$ $0,y,z$<br>( $m_x$   $0,1,0$ )' |

**Generators selected** (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

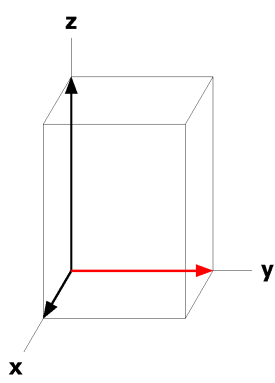
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
16 i 1	(1) x,y,z [u,v,w] (5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ] (6) $x+1/2, y, \bar{z}+1/2$ [ $u, v, \bar{w}$ ]	(3) $\bar{x}+1/2, y, \bar{z}+1/2$ [ $u, \bar{v}, w$ ] (7) $x+1/2, \bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x, \bar{y}, \bar{z}$ [ $\bar{u}, v, w$ ] (8) $\bar{x}, y, z$ [ $u, \bar{v}, \bar{w}$ ]
8 h m..	0,y,z [u,0,0]	1/2, $\bar{y}$ ,z+1/2 [ $\bar{u}, 0, 0$ ]	1/2,y, $\bar{z}+1/2$ [u,0,0]	0, $\bar{y}, \bar{z}$ [ $\bar{u}, 0, 0$ ]
8 g .2'	1/4,y,1/4 [u,0,w]	1/4, $\bar{y}, 3/4$ [ $\bar{u}, 0, w$ ]	3/4, $\bar{y}, 3/4$ [ $\bar{u}, 0, \bar{w}$ ]	3/4,y,1/4 [u,0, $\bar{w}$ ]
8 f 2..	x,1/2,0 [u,0,0]	$\bar{x}+1/2, 1/2, 1/2$ [u,0,0]	$\bar{x}, 1/2, 0$ [u,0,0]	x+1/2, 1/2, 1/2 [u,0,0]
8 e 2'..	x,0,0 [0,v,w]	$\bar{x}+1/2, 0, 1/2$ [0, $\bar{v}, w$ ]	$\bar{x}, 0, 0$ [0, $\bar{v}, \bar{w}$ ]	x+1/2, 0, 1/2 [0,v, $\bar{w}$ ]
4 d 2/m..	0,1/2,0 [u,0,0]	1/2,1/2,1/2 [u,0,0]		
4 c 2/m..	1/2,1/2,0 [u,0,0]	0,1/2,1/2 [u,0,0]		
4 b 2'/m..	1/2,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
4 a 2'/m..	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

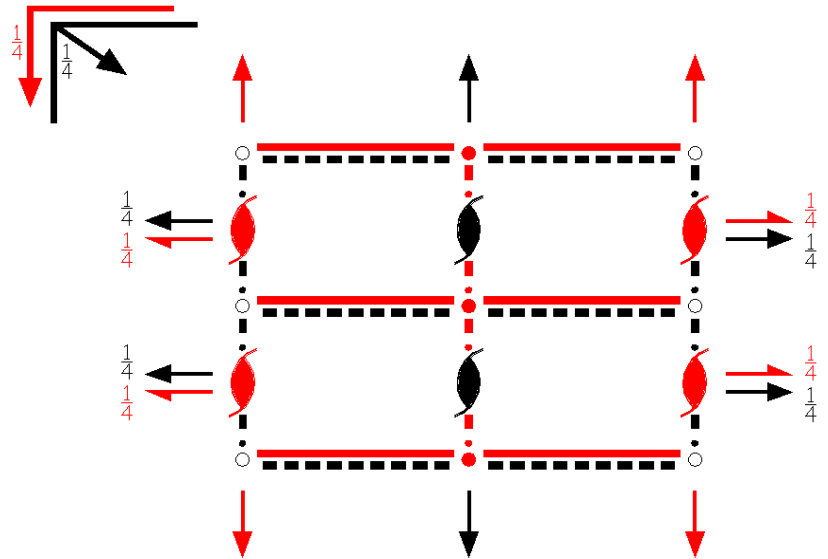
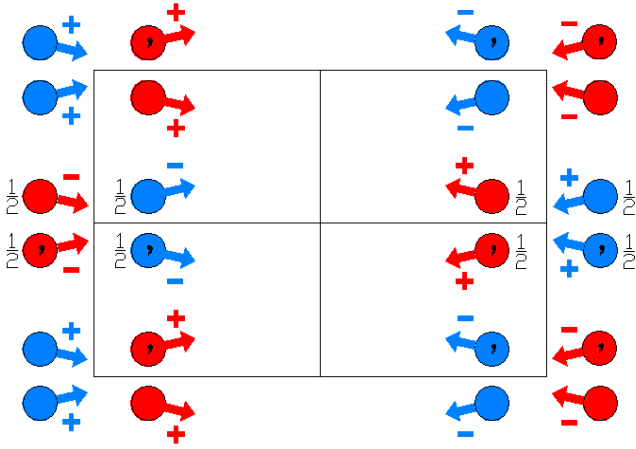
Along [0,1,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



$P_{2b} m'na'$   
53.13.427

$mmm1'$   
 $P_{2b} 2'/m'2/n2_1'/a'$

Orthorhombic



Origin at center ( $2'/m'$ ) at  $2'/m'n1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                   | (2) $2' (0,0,1/2) \quad 1/4,0,z$<br>( $2_z$   $1/2,0,1/2$ )' | (3) $2 \quad 1/4,y,1/4$<br>( $2_y$   $1/2,0,1/2$ )         | (4) $2' \quad x,0,0$<br>( $2_x$   $0,0,0$ )' |
| (5) $\bar{1} \quad 0,0,0$<br>( $\bar{1}$   $0,0,0$ ) | (6) $a' (1/2,0,0) \quad x,y,1/4$<br>( $m_z$   $1/2,0,1/2$ )' | (7) $n (1/2,0,1/2) \quad x,0,z$<br>( $m_y$   $1/2,0,1/2$ ) | (8) $m' \quad 0,y,z$<br>( $m_x$   $0,0,0$ )' |

For (0,1,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t' (0,1,0)$<br>(1  $0,1,0$ )'                       | (2) $2 (0,0,1/2) \quad 1/4,1/2,z$<br>( $2_z$   $1/2,1,1/2$ ) | (3) $2' (0,1,0) \quad 1/4,y,1/4$<br>( $2_y$   $1/2,1,1/2$ )'   | (4) $2 \quad x,1/2,0$<br>( $2_x$   $0,1,0$ )       |
| (5) $\bar{1}' \quad 0,1/2,0$<br>( $\bar{1}$   $0,1,0$ )' | (6) $n (1/2,1,0) \quad x,y,1/4$<br>( $m_z$   $1/2,1,1/2$ )   | (7) $n' (1/2,0,1/2) \quad x,1/2,z$<br>( $m_y$   $1/2,1,1/2$ )' | (8) $b (0,1,0) \quad 0,y,z$<br>( $m_x$   $0,1,0$ ) |

**Generators selected** (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

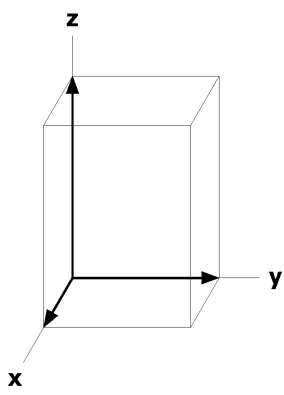
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
16 i 1	(1) x,y,z [u,v,w] (5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [u,v, $\bar{w}$ ] (6) $x+1/2, y, \bar{z}+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x}+1/2, y, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ] (7) $x+1/2, \bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) x, $\bar{y}, \bar{z}$ [ $\bar{u}, v, w$ ] (8) $\bar{x}, y, z$ [ $\bar{u}, v, w$ ]
8 h m'..	0,y,z [0,v,w]	1/2, $\bar{y}, z+1/2$ [0,v, $\bar{w}$ ]	1/2,y, $\bar{z}+1/2$ [0,v, $\bar{w}$ ]	0, $\bar{y}, \bar{z}$ [0,v,w]
8 g .2.	1/4,y,1/4 [0,v,0]	1/4, $\bar{y}, 3/4$ [0,v,0]	3/4, $\bar{y}, 3/4$ [0,v,0]	3/4,y,1/4 [0,v,0]
8 f 2..	x,1/2,0 [u,0,0]	$\bar{x}+1/2, 1/2, 1/2$ [ $\bar{u}, 0, 0$ ]	$\bar{x}, 1/2, 0$ [ $\bar{u}, 0, 0$ ]	x+1/2, 1/2, 1/2 [u,0,0]
8 e 2'..	x,0,0 [0,v,w]	$\bar{x}+1/2, 0, 1/2$ [0,v, $\bar{w}$ ]	$\bar{x}, 0, 0$ [0,v,w]	x+1/2, 0, 1/2 [0,v, $\bar{w}$ ]
4 d 2/m'..	0,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 c 2/m'..	1/2,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 b 2'/m'..	1/2,0,0 [0,v,w]	0,0,1/2 [0,v, $\bar{w}$ ]		
4 a 2'/m'..	0,0,0 [0,v,w]	1/2,0,1/2 [0,v, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,1/2,z

Along [1,0,0] p<sub>2b</sub>-2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,1/4,0

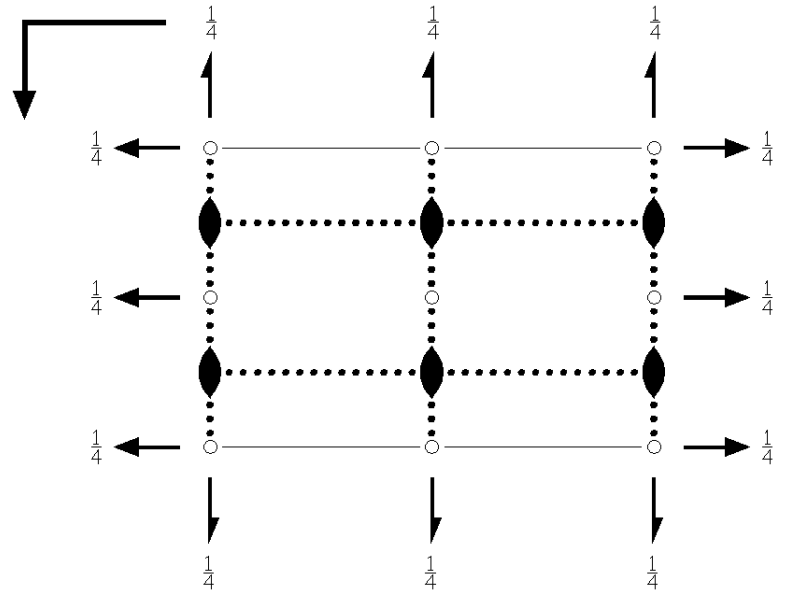
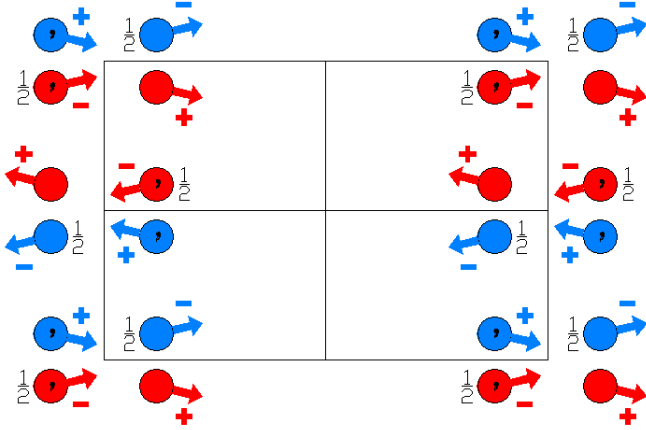
Along [0,1,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pcca  
54.1.428

mmm  
 $P2_1/c2/c2/a$

Orthorhombic



Origin at  $\bar{1}$  on 1ca

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                               | (2) 2 $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )           | (3) 2 $0,y,1/4$<br>( $2_y$   $0,0,1/2$ )           | (4) 2 $(1/2,0,0)$ $x,0,1/4$<br>( $2_x$   $1/2,0,1/2$ ) |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ ) | (6) a $(1/2,0,0)$ $x,y,0$<br>( $m_z$   $1/2,0,0$ ) | (7) c $(0,0,1/2)$ $x,0,z$<br>( $m_y$   $0,0,1/2$ ) | (8) c $(0,0,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,0,1/2$ ) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

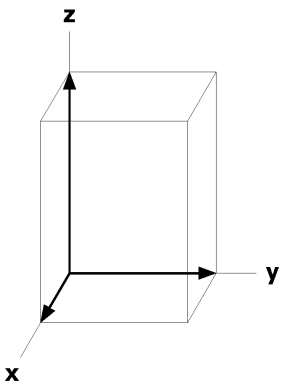
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	f	1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x+1/2, \bar{y}, \bar{z}+1/2$ [ $u, \bar{v}, \bar{w}$ ]
			(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(7) $x, \bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(8) $\bar{x}+1/2, y, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]
4	e	..2	1/4, 1/2, z [0,0,w]	3/4, 1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	3/4, 1/2, $\bar{z}$ [0,0,w]	1/4, 1/2, z+1/2 [0,0, $\bar{w}$ ]
4	d	..2	1/4, 0, z [0,0,w]	3/4, 0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	3/4, 0, $\bar{z}$ [0,0,w]	1/4, 0, z+1/2 [0,0, $\bar{w}$ ]
4	c	.2.	0, y, 1/4 [0,v,0]	1/2, $\bar{y}, 1/4$ [0, $\bar{v}, 0$ ]	0, $\bar{y}, 3/4$ [0,v,0]	1/2, y, 3/4 [0, $\bar{v}, 0$ ]
4	b	$\bar{1}$	0, 1/2, 0 [u,v,w]	1/2, 1/2, 0 [ $\bar{u}, \bar{v}, w$ ]	0, 1/2, 1/2 [ $\bar{u}, v, \bar{w}$ ]	1/2, 1/2, 1/2 [ $u, \bar{v}, \bar{w}$ ]
4	a	$\bar{1}$	0, 0, 0 [u,v,w]	1/2, 0, 0 [ $\bar{u}, \bar{v}, w$ ]	0, 0, 1/2 [ $\bar{u}, v, \bar{w}$ ]	1/2, 0, 1/2 [ $u, \bar{v}, \bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2a} \cdot 2mm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,0,0]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x, 1/2, 0

Along [0,1,0]  $p_{2b} \cdot 2m'g'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0, y, 1/4

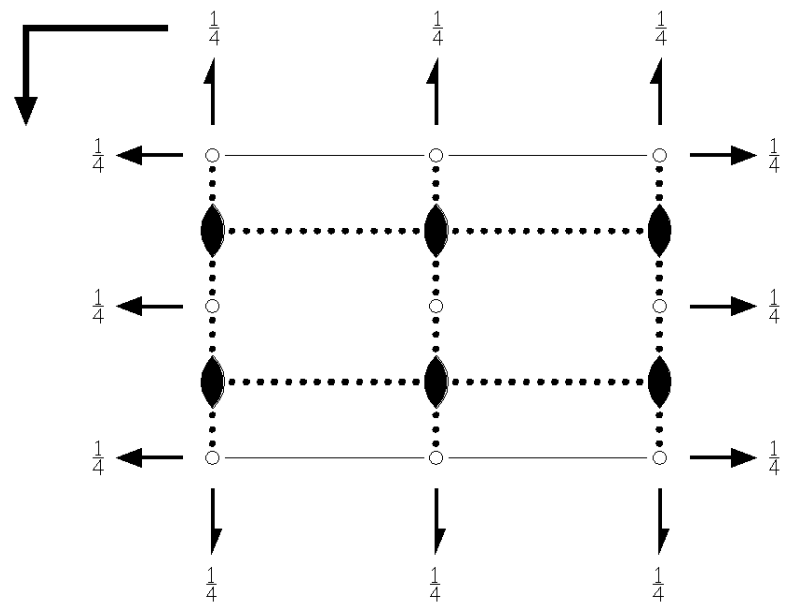
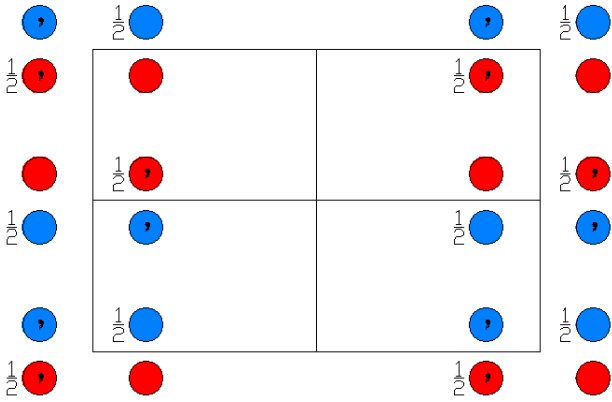


Pcca1'  
54.2.429

mmm1'  
P2<sub>1</sub>/c2/c2/a1'

Orthorhombic

1'



Origin at  $\bar{1}1'$  on  $1ca1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For 1 + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)           | (3) 2 $0,y,1/4$<br>(2 <sub>y</sub>  0,0,1/2)           | (4) 2 $(1/2,0,0)$ $x,0,1/4$<br>(2 <sub>x</sub>  1/2,0,1/2) |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0) | (6) a $(1/2,0,0)$ $x,y,0$<br>(m <sub>z</sub>  1/2,0,0) | (7) c $(0,0,1/2)$ $x,0,z$<br>(m <sub>y</sub>  0,0,1/2) | (8) c $(0,0,1/2)$ $1/4,y,z$<br>(m <sub>x</sub>  1/2,0,1/2) |

For 1' + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1'<br>(1 0,0,0)'                           | (2) 2' $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)'           | (3) 2' $0,y,1/4$<br>(2 <sub>y</sub>  0,0,1/2)'           | (4) 2' $(1/2,0,0)$ $x,0,1/4$<br>(2 <sub>x</sub>  1/2,0,1/2)' |
| (5) $\bar{1}'$ $0,0,0$<br>( $\bar{1}$  0,0,0)' | (6) a' $(1/2,0,0)$ $x,y,0$<br>(m <sub>z</sub>  1/2,0,0)' | (7) c' $(0,0,1/2)$ $x,0,z$<br>(m <sub>y</sub>  0,0,1/2)' | (8) c' $(0,0,1/2)$ $1/4,y,z$<br>(m <sub>x</sub>  1/2,0,1/2)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

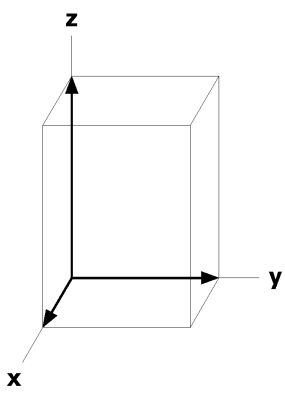
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +	1' +		
8 f 11'	(1) x,y,z [0,0,0] (5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(2) $\bar{x}+1/2,\bar{y},z$ [0,0,0] (6) $x+1/2,y,\bar{z}$ [0,0,0]	(3) $\bar{x},y,\bar{z}+1/2$ [0,0,0] (7) $x,\bar{y},z+1/2$ [0,0,0]	(4) $x+1/2,\bar{y},\bar{z}+1/2$ [0,0,0] (8) $\bar{x}+1/2,y,z+1/2$ [0,0,0]
4 e ..21'	1/4,1/2,z [0,0,0]	3/4,1/2, $\bar{z}+1/2$ [0,0,0]	3/4,1/2, $\bar{z}$ [0,0,0]	1/4,1/2,z+1/2 [0,0,0]
4 d ..21'	1/4,0,z [0,0,0]	3/4,0, $\bar{z}+1/2$ [0,0,0]	3/4,0, $\bar{z}$ [0,0,0]	1/4,0,z+1/2 [0,0,0]
4 c .2.1'	0,y,1/4 [0,0,0]	1/2, $\bar{y}$ ,1/4 [0,0,0]	0, $\bar{y}$ ,3/4 [0,0,0]	1/2,y,3/4 [0,0,0]
4 b $\bar{1}1'$	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]
4 a $\bar{1}1'$	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

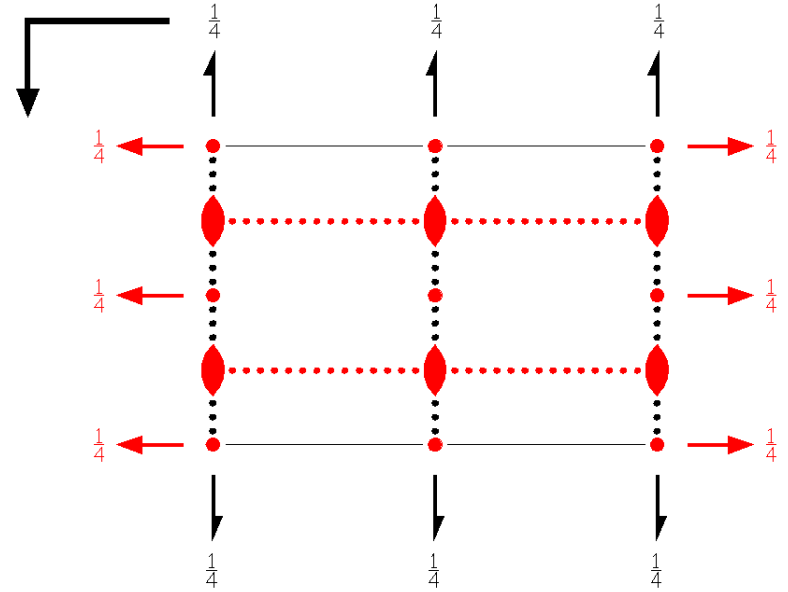
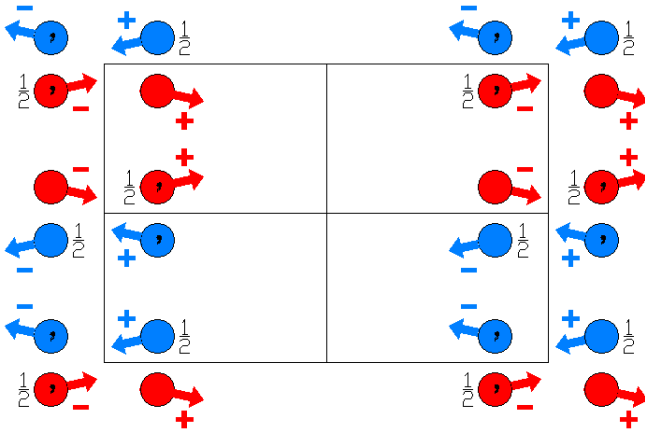
Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pc'ca  
54.3.430

m'mm  
P2<sub>1</sub>/c'2'/c2'/a

Orthorhombic



Origin at  $\bar{1}$ ' on 1ca

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                              | (2) 2' $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)'       | (3) 2' $0,y,1/4$<br>(2 <sub>y</sub>  0,0,1/2)'       | (4) 2 (1/2,0,0) $x,0,1/4$<br>(2 <sub>x</sub>  1/2,0,1/2)   |
| (5) $\bar{1}$ ' $0,0,0$<br>( $\bar{1}$  0,0,0)' | (6) a (1/2,0,0) $x,y,0$<br>(m <sub>z</sub>  1/2,0,0) | (7) c (0,0,1/2) $x,0,z$<br>(m <sub>y</sub>  0,0,1/2) | (8) c' (0,0,1/2) $1/4,y,z$<br>(m <sub>x</sub>  1/2,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

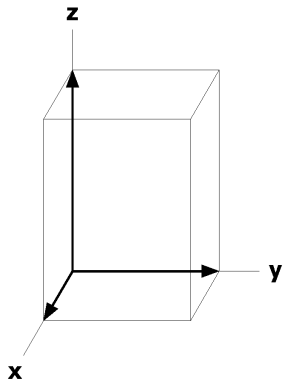
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	f 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [u, $\bar{v},w$ ]	(4) $x+1/2,\bar{y},\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,\bar{y},z+1/2$ [ $\bar{u},v,w$ ]
4	e ..2'	1/4,1/2,z [u,v,0]	3/4,1/2, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	3/4,1/2, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,1/2,z+1/2 [ $\bar{u},v,0$ ]
4	d ..2'	1/4,0,z [u,v,0]	3/4,0, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	3/4,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,0,z+1/2 [ $\bar{u},v,0$ ]
4	c .2'	0,y,1/4 [u,0,w]	1/2, $\bar{y},1/4$ [u,0, $\bar{w}$ ]	0, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,3/4 [ $\bar{u},0,w$ ]
4	b $\bar{1}'$	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]
4	a $\bar{1}'$	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

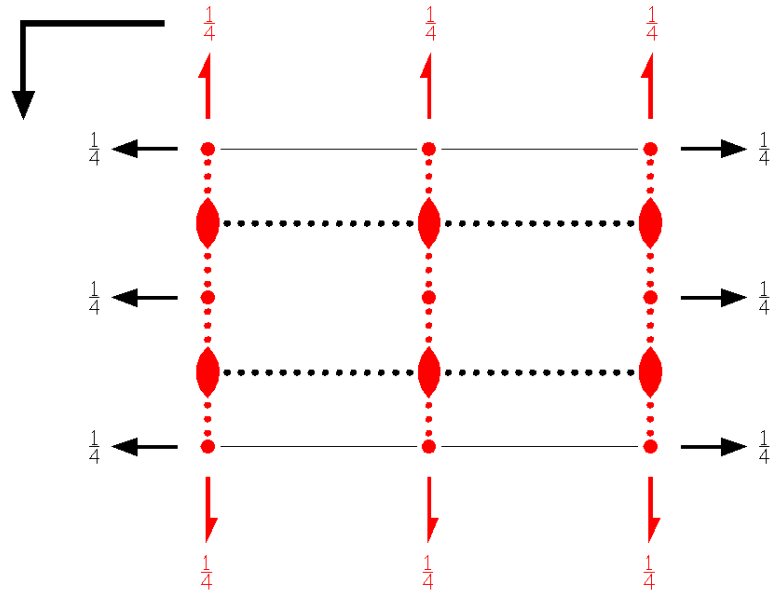
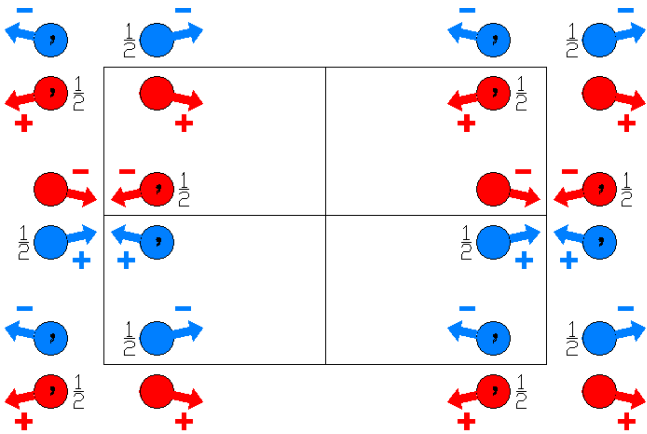
Along [0,1,0] p<sub>2b</sub>'2mg  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pcc'a  
54.4.431

mm'm  
 $P2_1'/c2/c'2'/a$

Orthorhombic



Origin at  $\bar{1}'$  on  $1c'a$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) $2'$ $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )'         | (3) 2 $0,y,1/4$<br>( $2_y$   $0,0,1/2$ )                 | (4) $2'$ ( $1/2,0,0$ ) $x,0,1/4$<br>( $2_x$   $1/2,0,1/2$ )' |
| (5) $\bar{1}'$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ )' | (6) a ( $1/2,0,0$ ) $x,y,0$<br>( $m_z$   $1/2,0,0$ ) | (7) $c'$ ( $0,0,1/2$ ) $x,0,z$<br>( $m_y$   $0,0,1/2$ )' | (8) c ( $0,0,1/2$ ) $1/4,y,z$<br>( $m_x$   $1/2,0,1/2$ )     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

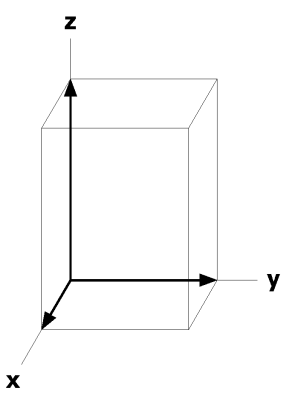
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	f 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(8) $\bar{x}+1/2,y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
4	e ..2'	1/4,1/2,z [u,v,0]	3/4,1/2, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	3/4,1/2, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,1/2,z+1/2 [ $u,\bar{v},0$ ]
4	d ..2'	1/4,0,z [u,v,0]	3/4,0, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	3/4,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,0,z+1/2 [ $u,\bar{v},0$ ]
4	c .2.	0,y,1/4 [0,v,0]	1/2, $\bar{y}$ ,1/4 [0,v,0]	0, $\bar{y}$ ,3/4 [0, $\bar{v}$ ,0]	1/2,y,3/4 [0, $\bar{v}$ ,0]
4	b $\bar{1}'$	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]
4	a $\bar{1}'$	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}2mm$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

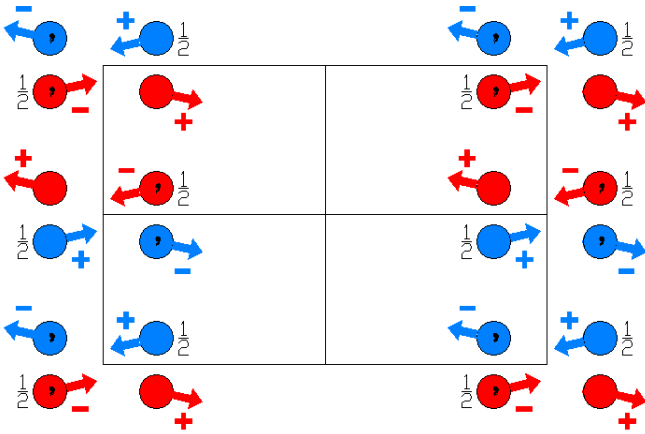
Along [0,1,0]  $p_{2b}2m'g'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pcca'  
54.5.432

mmm'  
P2<sub>1</sub>'/c2'/c2/a'

Orthorhombic

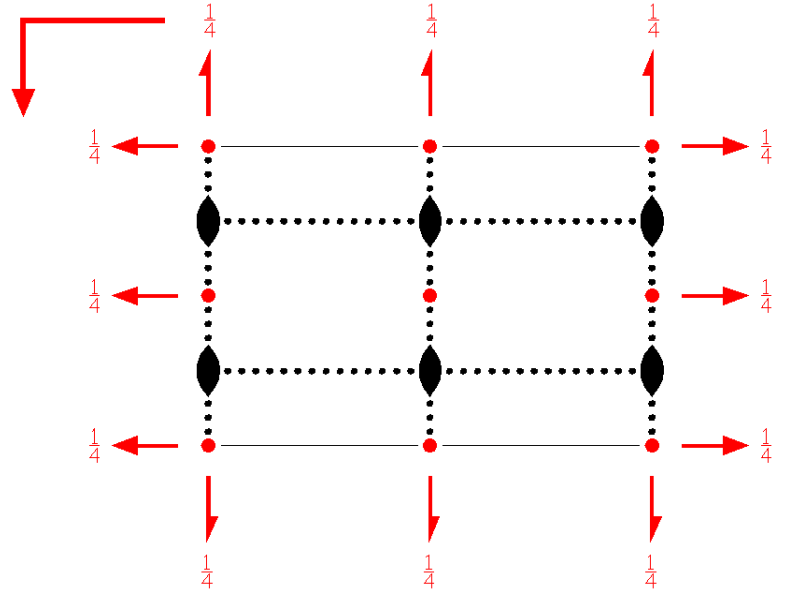


Origin at  $\bar{1}'$  on  $1ca'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                             | (2) 2 $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)             | (3) 2' $0,y,1/4$<br>(2 <sub>y</sub>  0,0,1/2)'         | (4) 2' $(1/2,0,0)$ $x,0,1/4$<br>(2 <sub>x</sub>  1/2,0,1/2)' |
| (5) $\bar{1}'$ $0,0,0$<br>( $\bar{1}$  0,0,0)' | (6) a' $(1/2,0,0)$ $x,y,0$<br>(m <sub>z</sub>  1/2,0,0)' | (7) c $(0,0,1/2)$ $x,0,z$<br>(m <sub>y</sub>  0,0,1/2) | (8) c $(0,0,1/2)$ $1/4,y,z$<br>(m <sub>x</sub>  1/2,0,1/2)   |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

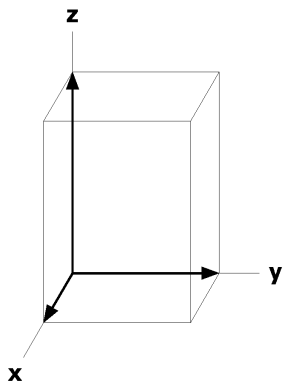
		Coordinates				
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	f	1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(4) $x+1/2, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]
			(5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(6) $x+1/2, y, \bar{z}$ [ $u, v, \bar{w}$ ]	(7) $x, \bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(8) $\bar{x}+1/2, y, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]
4	e	..2	1/4, 1/2, z [0,0,w]	3/4, 1/2, $\bar{z}+1/2$ [0,0,w]	3/4, 1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4, 1/2, z+1/2 [0,0, $\bar{w}$ ]
4	d	..2	1/4, 0, z [0,0,w]	3/4, 0, $\bar{z}+1/2$ [0,0,w]	3/4, 0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4, 0, z+1/2 [0,0, $\bar{w}$ ]
4	c	.2'	0, y, 1/4 [u,0,w]	1/2, $\bar{y}, 1/4$ [ $\bar{u}, 0, w$ ]	0, $\bar{y}, 3/4$ [ $\bar{u}, 0, \bar{w}$ ]	1/2, y, 3/4 [u,0, $\bar{w}$ ]
4	b	$\bar{1}'$	0, 1/2, 0 [0,0,0]	1/2, 1/2, 0 [0,0,0]	0, 1/2, 1/2 [0,0,0]	1/2, 1/2, 1/2 [0,0,0]
4	a	$\bar{1}'$	0, 0, 0 [0,0,0]	1/2, 0, 0 [0,0,0]	0, 0, 1/2 [0,0,0]	1/2, 0, 1/2 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a^*} 2m' m'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

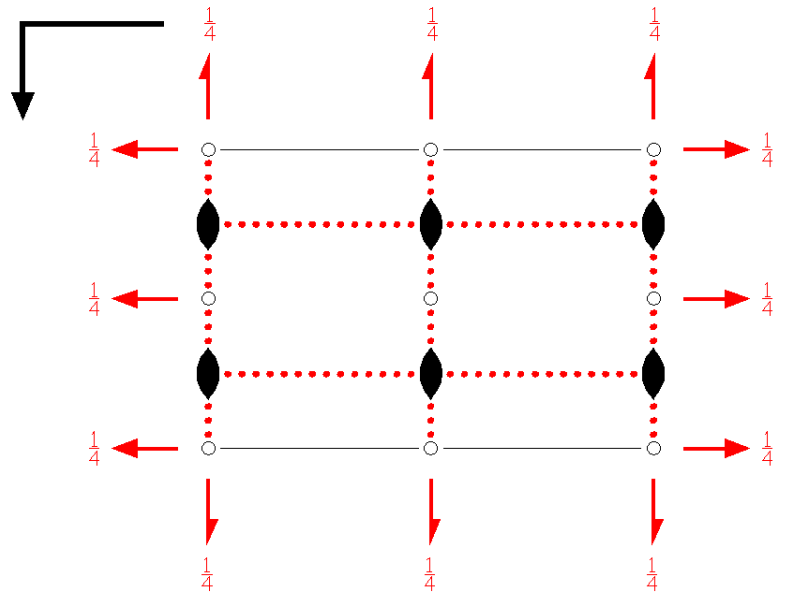
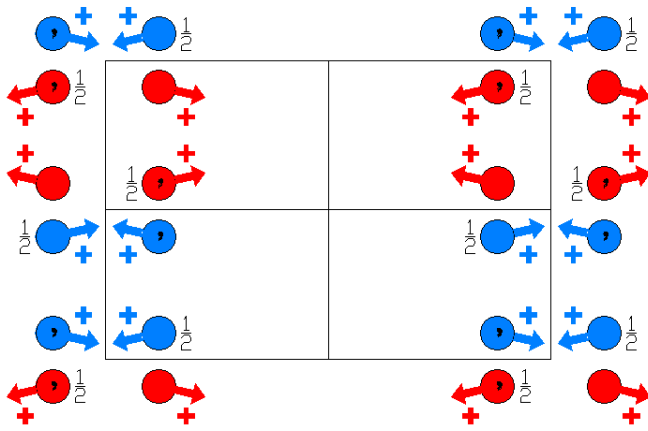
Along [0,1,0]  $p_{2b^*} 2m' g'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pc'c'a  
54.6.433

m'm'm  
P2<sub>1</sub>'/c'2'/c'2/a

Orthorhombic



Origin at  $\bar{1}$  on 1c'a

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)           | (3) 2' $0,y,1/4$<br>(2 <sub>y</sub>  0,0,1/2)'           | (4) 2' $(1/2,0,0)$ $x,0,1/4$<br>(2 <sub>x</sub>  1/2,0,1/2)' |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0) | (6) a $(1/2,0,0)$ $x,y,0$<br>(m <sub>z</sub>  1/2,0,0) | (7) c' $(0,0,1/2)$ $x,0,z$<br>(m <sub>y</sub>  0,0,1/2)' | (8) c' $(0,0,1/2)$ $1/4,y,z$<br>(m <sub>x</sub>  1/2,0,1/2)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

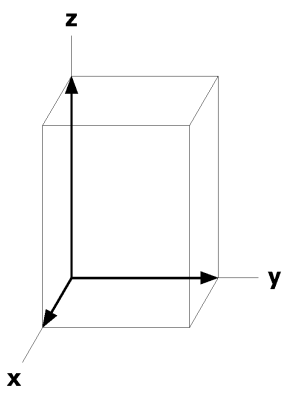
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	f	1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, \bar{y}, \bar{z}+1/2$ [u, $\bar{v}, w$ ]	(4) $x+1/2, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]
			(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(7) $x, \bar{y}, z+1/2$ [u, $\bar{v}, w$ ]	(8) $\bar{x}+1/2, y, z+1/2$ [ $\bar{u}, v, w$ ]
4	e	..2	1/4,1/2,z [0,0,w]	3/4,1/2, $\bar{z}+1/2$ [0,0,w]	3/4,1/2, $\bar{z}$ [0,0,w]	1/4,1/2,z+1/2 [0,0,w]
4	d	..2	1/4,0,z [0,0,w]	3/4,0, $\bar{z}+1/2$ [0,0,w]	3/4,0, $\bar{z}$ [0,0,w]	1/4,0,z+1/2 [0,0,w]
4	c	.2'	0,y,1/4 [u,0,w]	1/2, $\bar{y}, 1/4$ [ $\bar{u}, 0, w$ ]	0, $\bar{y}, 3/4$ [u,0,w]	1/2,y,3/4 [ $\bar{u}, 0, w$ ]
4	b	$\bar{1}$	0,1/2,0 [u,v,w]	1/2,1/2,0 [ $\bar{u}, \bar{v}, w$ ]	0,1/2,1/2 [u, $\bar{v}, w$ ]	1/2,1/2,1/2 [ $\bar{u}, v, w$ ]
4	a	$\bar{1}$	0,0,0 [u,v,w]	1/2,0,0 [ $\bar{u}, \bar{v}, w$ ]	0,0,1/2 [u, $\bar{v}, w$ ]	1/2,0,1/2 [ $\bar{u}, v, w$ ]

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,0,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

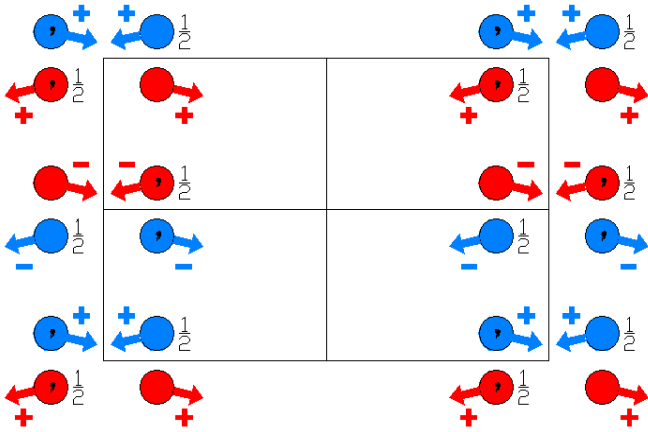
Along [0,1,0]  $p2'm'g$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pcc'a'  
54.7.434

mm'm'  
P2<sub>1</sub>/c2'/c2'/a'

Orthorhombic

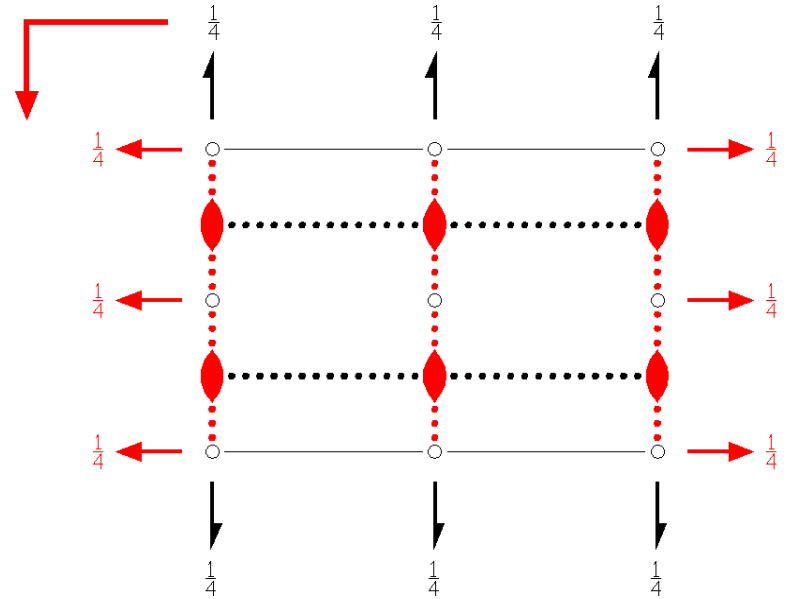


Origin at  $\bar{1}$  on 1c'a'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2' 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,0)'         | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'         | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>  1/2,0,1/2) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a' (1/2,0,0) x,y,0<br>(m <sub>z</sub>  1/2,0,0)' | (7) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (8) c (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,0,1/2) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

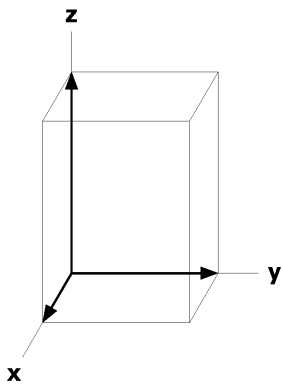
		Coordinates				
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	f	1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}, \bar{y}, \bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) $x+1/2, \bar{y}, \bar{z}+1/2$ [u, $\bar{v}, \bar{w}$ ]
			(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y, \bar{z}$ [u,v, $\bar{w}$ ]	(7) $x, \bar{y}, z+1/2$ [u, $\bar{v}$ ,w]	(8) $\bar{x}+1/2, y, z+1/2$ [u, $\bar{v}, \bar{w}$ ]
4	e	..2'	1/4,1/2,z [u,v,0]	3/4,1/2, $\bar{z}+1/2$ [u, $\bar{v}$ ,0]	3/4,1/2, $\bar{z}$ [u,v,0]	1/4,1/2,z+1/2 [u, $\bar{v}$ ,0]
4	d	..2'	1/4,0,z [u,v,0]	3/4,0, $\bar{z}+1/2$ [u, $\bar{v}$ ,0]	3/4,0, $\bar{z}$ [u,v,0]	1/4,0,z+1/2 [u, $\bar{v}$ ,0]
4	c	.2'	0,y,1/4 [u,0,w]	1/2, $\bar{y}$ ,1/4 [u,0, $\bar{w}$ ]	0, $\bar{y}$ ,3/4 [u,0,w]	1/2,y,3/4 [u,0, $\bar{w}$ ]
4	b	$\bar{1}$	0,1/2,0 [u,v,w]	1/2,1/2,0 [u,v, $\bar{w}$ ]	0,1/2,1/2 [u, $\bar{v}$ ,w]	1/2,1/2,1/2 [u, $\bar{v}, \bar{w}$ ]
4	a	$\bar{1}$	0,0,0 [u,v,w]	1/2,0,0 [u,v, $\bar{w}$ ]	0,0,1/2 [u, $\bar{v}$ ,w]	1/2,0,1/2 [u, $\bar{v}, \bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1]  $p2'mm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a'}2mm$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

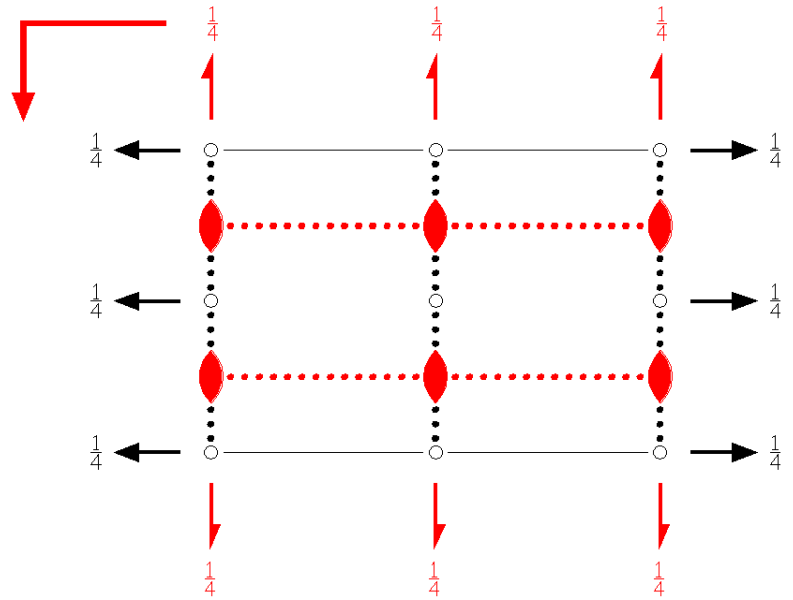
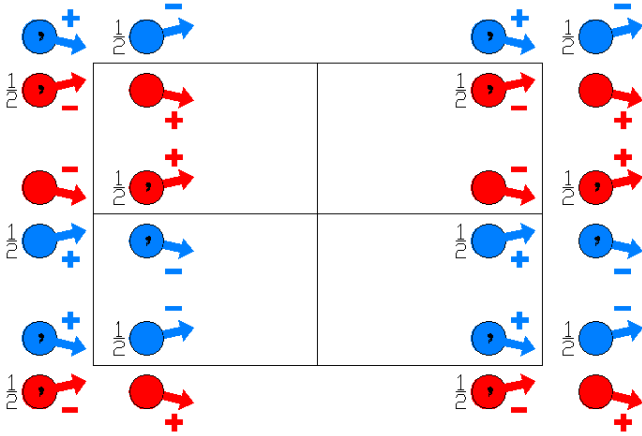
Along [0,1,0]  $p2'mg'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pc'ca'  
54.8.435

m'mm'  
P2<sub>1</sub>'/c2'/c2'/a'

Orthorhombic



Origin at  $\bar{1}$  on 1ca'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2' $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)'           | (3) 2 $0,y,1/4$<br>(2 <sub>y</sub>  0,0,1/2)           | (4) 2' $(1/2,0,0)$ $x,0,1/4$<br>(2 <sub>x</sub>  1/2,0,1/2)' |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0) | (6) a' $(1/2,0,0)$ $x,y,0$<br>(m <sub>z</sub>  1/2,0,0)' | (7) c $(0,0,1/2)$ $x,0,z$<br>(m <sub>y</sub>  0,0,1/2) | (8) c' $(0,0,1/2)$ $1/4,y,z$<br>(m <sub>x</sub>  1/2,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

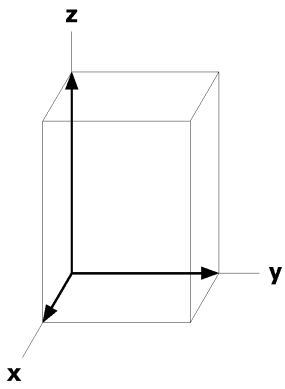
		Coordinates				
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	f	1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x+1/2, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]
			(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y, \bar{z}$ [u,v, $\bar{w}$ ]	(7) $x, \bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(8) $\bar{x}+1/2, y, z+1/2$ [ $\bar{u}, v, w$ ]
4	e	..2'	1/4, 1/2, z [u,v,0]	3/4, 1/2, $\bar{z}+1/2$ [ $\bar{u}, v, 0$ ]	3/4, 1/2, $\bar{z}$ [u,v,0]	1/4, 1/2, $z+1/2$ [ $\bar{u}, v, 0$ ]
4	d	..2'	1/4, 0, z [u,v,0]	3/4, 0, $\bar{z}+1/2$ [ $\bar{u}, v, 0$ ]	3/4, 0, $\bar{z}$ [u,v,0]	1/4, 0, $z+1/2$ [ $\bar{u}, v, 0$ ]
4	c	.2.	0, y, 1/4 [0,v,0]	1/2, $\bar{y}, 1/4$ [0,v,0]	0, $\bar{y}, 3/4$ [0,v,0]	1/2, y, 3/4 [0,v,0]
4	b	$\bar{1}$	0, 1/2, 0 [u,v,w]	1/2, 1/2, 0 [u,v, $\bar{w}$ ]	0, 1/2, 1/2 [ $\bar{u}, v, \bar{w}$ ]	1/2, 1/2, 1/2 [ $\bar{u}, v, w$ ]
4	a	$\bar{1}$	0, 0, 0 [u,v,w]	1/2, 0, 0 [u,v, $\bar{w}$ ]	0, 0, 1/2 [ $\bar{u}, v, \bar{w}$ ]	1/2, 0, 1/2 [ $\bar{u}, v, w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

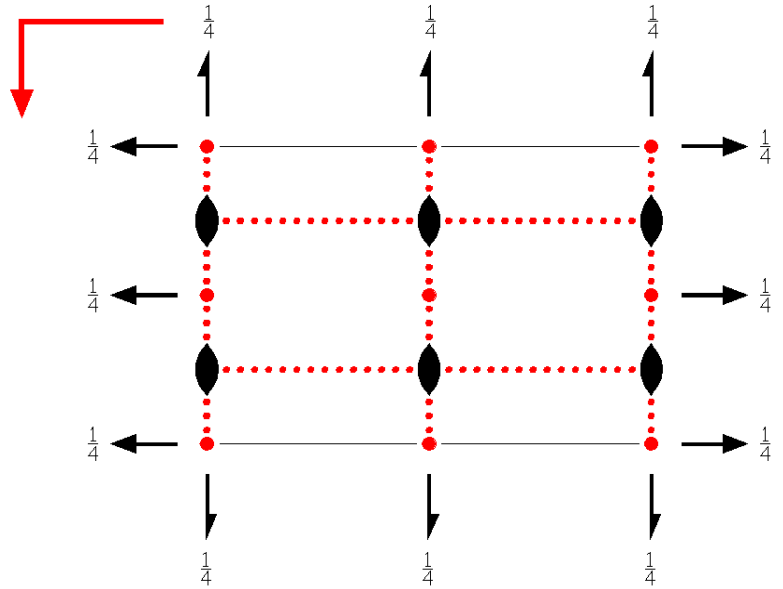
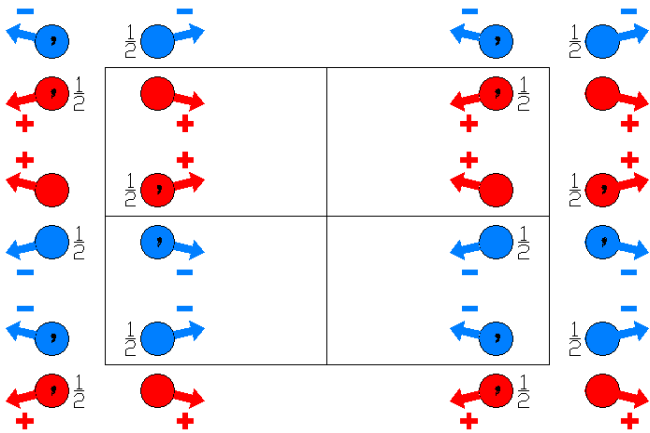
Along [0,1,0] p<sub>2b</sub>'2m'g'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pc'c'a'  
54.9.436

m'm'm'  
P2<sub>1</sub>/c'2/c'2/a'

Orthorhombic



Origin at  $\bar{1}$ ' on 1c'a'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                              | (2) 2 $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)             | (3) 2 $0,y,1/4$<br>(2 <sub>y</sub>  0,0,1/2)             | (4) 2 $(1/2,0,0)$ $x,0,1/4$<br>(2 <sub>x</sub>  1/2,0,1/2)   |
| (5) $\bar{1}$ ' $0,0,0$<br>( $\bar{1}$  0,0,0)' | (6) a' $(1/2,0,0)$ $x,y,0$<br>(m <sub>z</sub>  1/2,0,0)' | (7) c' $(0,0,1/2)$ $x,0,z$<br>(m <sub>y</sub>  0,0,1/2)' | (8) c' $(0,0,1/2)$ $1/4,y,z$<br>(m <sub>x</sub>  1/2,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

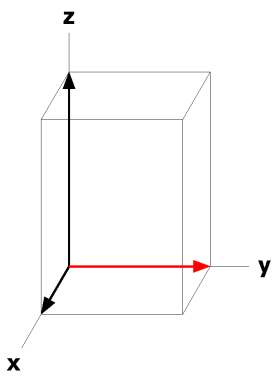
		Coordinates				
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	f	1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(4) $x+1/2, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]
			(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y, \bar{z}$ [u,v,w]	(7) $x, \bar{y}, z+1/2$ [u,v,w]	(8) $\bar{x}+1/2, y, z+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]
4	e	..2	1/4, 1/2, z [0,0,w]	3/4, 1/2, $\bar{z}+1/2$ [0,0,w]	3/4, 1/2, $\bar{z}$ [0,0,w]	1/4, 1/2, z+1/2 [0,0,w]
4	d	..2	1/4, 0, z [0,0,w]	3/4, 0, $\bar{z}+1/2$ [0,0,w]	3/4, 0, $\bar{z}$ [0,0,w]	1/4, 0, z+1/2 [0,0,w]
4	c	.2.	0, y, 1/4 [0,v,0]	1/2, $\bar{y}, 1/4$ [0,v,0]	0, $\bar{y}, 3/4$ [0,v,0]	1/2, y, 3/4 [0,v,0]
4	b	$\bar{1}'$	0, 1/2, 0 [0,0,0]	1/2, 1/2, 0 [0,0,0]	0, 1/2, 1/2 [0,0,0]	1/2, 1/2, 1/2 [0,0,0]
4	a	$\bar{1}'$	0, 0, 0 [0,0,0]	1/2, 0, 0 [0,0,0]	0, 0, 1/2 [0,0,0]	1/2, 0, 1/2 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

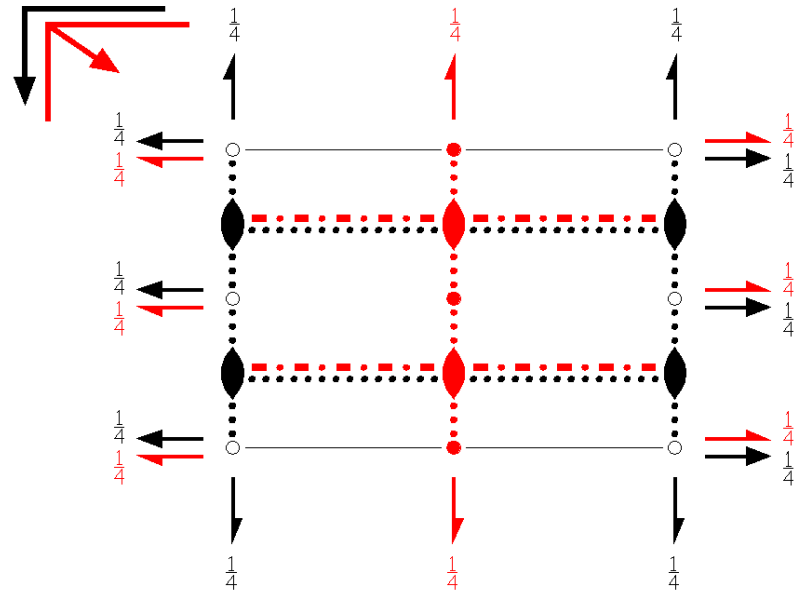
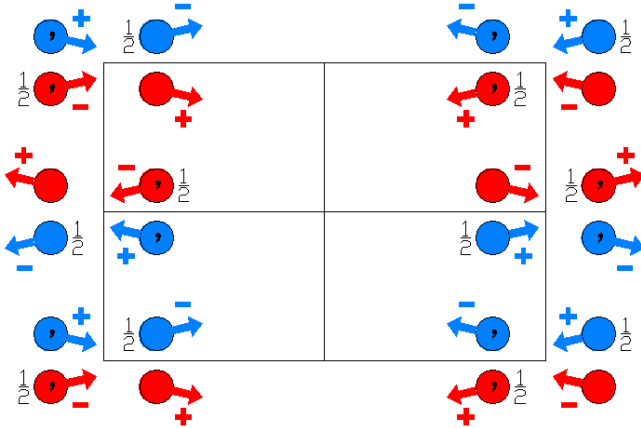
Along [0,1,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$P_{2b} cca$   
54.10.437

$mmm1'$   
 $P_{2b} 2_1/c2/c2/a$

Orthorhombic



Origin at  $\bar{1}$  on  $1ca$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                               | (2) 2 $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )           | (3) 2 $0,y,1/4$<br>( $2_y$   $0,0,1/2$ )           | (4) 2 $(1/2,0,0)$ $x,0,1/4$<br>( $2_x$   $1/2,0,1/2$ ) |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ ) | (6) a $(1/2,0,0)$ $x,y,0$<br>( $m_z$   $1/2,0,0$ ) | (7) c $(0,0,1/2)$ $x,0,z$<br>( $m_y$   $0,0,1/2$ ) | (8) c $(0,0,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,0,1/2$ ) |

For  $(0,1,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(0,1,0)$<br>(1  $0,1,0$ )'                 | (2) $2'$ $1/4,1/2,z$<br>( $2_z$   $1/2,1,0$ )'         | (3) $2'$ $(0,1,0)$ $0,y,1/4$<br>( $2_y$   $0,1,1/2$ )'   | (4) $2'$ $(1/2,0,0)$ $x,1/2,1/4$<br>( $2_x$   $1/2,1,1/2$ )' |
| (5) $\bar{1}'$ $0,1/2,0$<br>( $\bar{1}$   $0,1,0$ )' | (6) $n'$ $(1/2,1,0)$ $x,y,0$<br>( $m_z$   $1/2,1,0$ )' | (7) $c'$ $(0,0,1/2)$ $x,1/2,z$<br>( $m_y$   $0,1,1/2$ )' | (8) $n'$ $(0,1,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,1,1/2$ )'   |



**Generators selected** (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

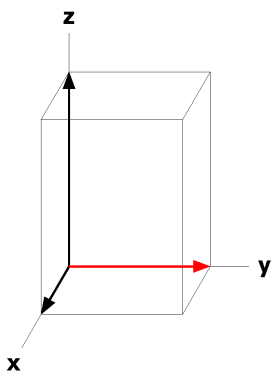
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
16 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x+1/2, \bar{y}, \bar{z}+1/2$ [ $u, \bar{v}, \bar{w}$ ]
	(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(7) $x, \bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(8) $\bar{x}+1/2, y, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]
8 e ..2'	1/4, 1/2, z [u,v,0]	3/4, 1/2, $\bar{z}+1/2$ [ $\bar{u}, v, 0$ ]	3/4, 1/2, $\bar{z}$ [ $\bar{u}, \bar{v}, 0$ ]	1/4, 1/2, z+1/2 [ $u, \bar{v}, 0$ ]
8 d ..2	1/4, 0, z [0,0,w]	3/4, 0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	3/4, 0, $\bar{z}$ [0,0,w]	1/4, 0, z+1/2 [0,0, $\bar{w}$ ]
8 c .2.	0, y, 1/4 [0,v,0]	1/2, $\bar{y}, 1/4$ [0, $\bar{v}, 0$ ]	0, $\bar{y}, 3/4$ [0,v,0]	1/2, y, 3/4 [0, $\bar{v}, 0$ ]
8 b $\bar{1}'$	0, 1/2, 0 [0,0,0]	1/2, 1/2, 0 [0,0,0]	0, 1/2, 1/2 [0,0,0]	1/2, 1/2, 1/2 [0,0,0]
8 a $\bar{1}$	0, 0, 0 [u,v,w]	1/2, 0, 0 [ $\bar{u}, \bar{v}, w$ ]	0, 0, 1/2 [ $\bar{u}, v, \bar{w}$ ]	1/2, 0, 1/2 [ $u, \bar{v}, \bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,0,0] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/2,0

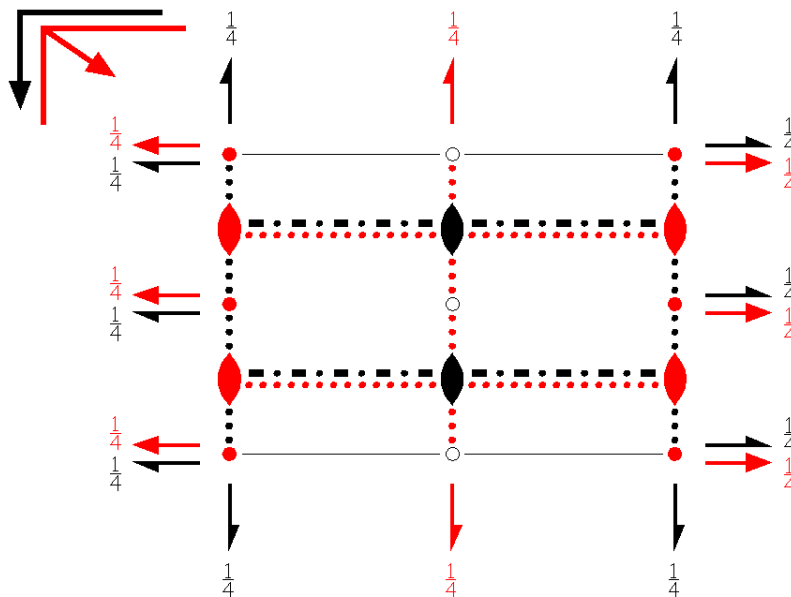
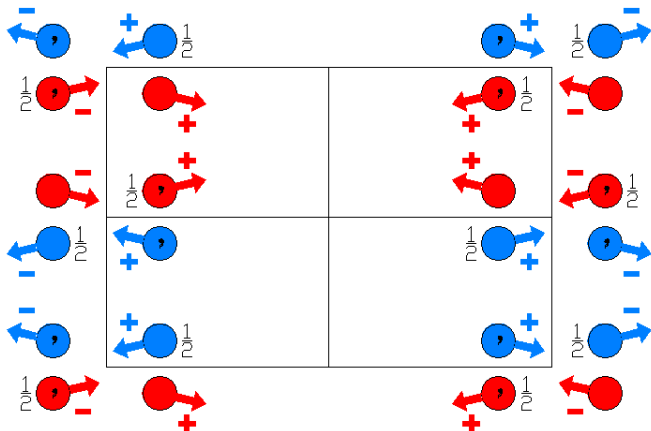
Along [0,1,0] p 2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$P_{2b} c'ca$   
54.11.438

$mmm1'$   
 $P_{2b} 2_1/c'2'/c2'/a$

Orthorhombic



Origin at  $\bar{1}'$  on  $1ca$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For  $(0,0,0) +$  set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) $2'$ $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )'         | (3) $2'$ $0,y,1/4$<br>( $2_y$   $0,0,1/2$ )'         | (4) $2$ $(1/2,0,0)$ $x,0,1/4$<br>( $2_x$   $1/2,0,1/2$ )   |
| (5) $\bar{1}'$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ )' | (6) $a$ $(1/2,0,0)$ $x,y,0$<br>( $m_z$   $1/2,0,0$ ) | (7) $c$ $(0,0,1/2)$ $x,0,z$<br>( $m_y$   $0,0,1/2$ ) | (8) $c'$ $(0,0,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,0,1/2$ )' |

For  $(0,1,0) +$  set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(0,1,0)$<br>(1  $0,1,0$ )'               | (2) $2$ $1/4,1/2,z$<br>( $2_z$   $1/2,1,0$ )           | (3) $2$ $(0,1,0)$ $0,y,1/4$<br>( $2_y$   $0,1,1/2$ )     | (4) $2'$ $(1/2,0,0)$ $x,1/2,1/4$<br>( $2_x$   $1/2,1,1/2$ )' |
| (5) $\bar{1}$ $0,1/2,0$<br>( $\bar{1}$   $0,1,0$ ) | (6) $n'$ $(1/2,1,0)$ $x,y,0$<br>( $m_z$   $1/2,1,0$ )' | (7) $c'$ $(0,0,1/2)$ $x,1/2,z$<br>( $m_y$   $0,1,1/2$ )' | (8) $n$ $(0,1,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,1,1/2$ )     |

**Generators selected** (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

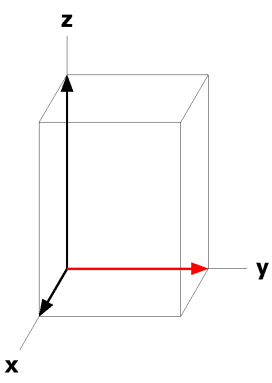
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
16 f 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [u,v, $\bar{w}$ ] (6) x+1/2,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x+1/2, $\bar{y},\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x}+1/2,y,z+1/2$ [ $\bar{u},v,w$ ]
8 e ..2	1/4,1/2,z [0,0,w]	3/4,1/2, $\bar{z}+1/2$ [0,0,w]	3/4,1/2, $\bar{z}$ [0,0,w]	1/4,1/2,z+1/2 [0,0,w]
8 d ..2'	1/4,0,z [u,v,0]	3/4,0, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	3/4,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,0,z+1/2 [ $\bar{u},v,0$ ]
8 c .2'	0,y,1/4 [u,0,w]	1/2, $\bar{y},1/4$ [u,0, $\bar{w}$ ]	0, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,3/4 [ $\bar{u},0,w$ ]
8 b $\bar{1}$	0,1/2,0 [u,v,w]	1/2,1/2,0 [ $\bar{u},\bar{v},w$ ]	0,1/2,1/2 [u, $\bar{v},w$ ]	1/2,1/2,1/2 [ $\bar{u},v,w$ ]
8 a $\bar{1}'$	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

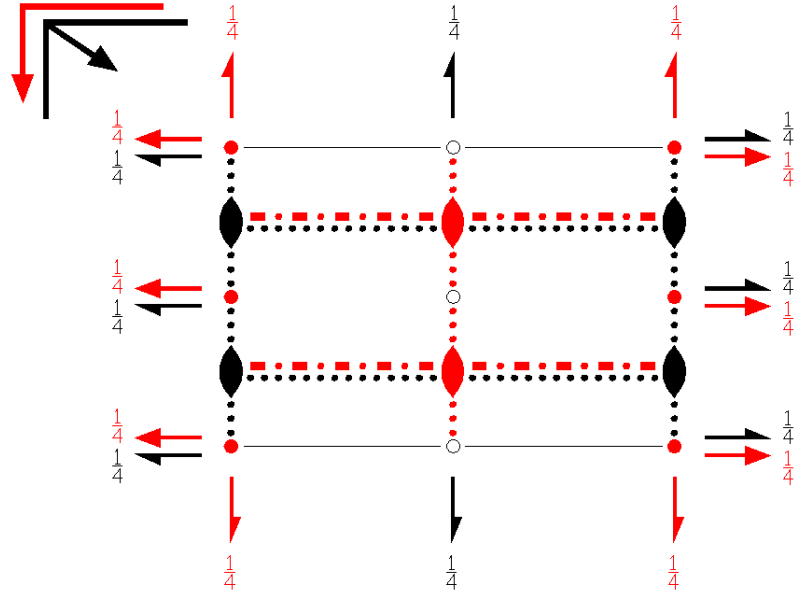
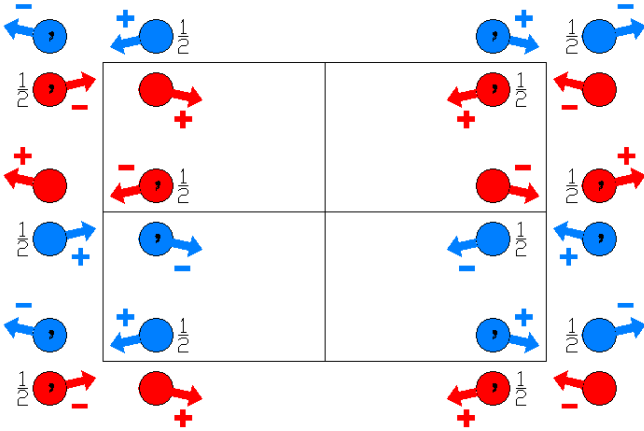
Along [0,1,0] p 2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$P_{2b} cca'$   
54.12.439

$mmm1'$   
 $P_{2b} 2_1' / c2' / c2' / a'$

Orthorhombic



Origin at  $\bar{1}'$  on  $1ca'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0) +$  set

- |   |  |  |  |
|---|--|--|--|
| (1) $1$<br>$(1 0,0,0)$                        | (2) $2$ $1/4,0,z$<br>$(2_z 1/2,0,0)$             | (3) $2'$ $0,y,1/4$<br>$(2_y 0,0,1/2)'$         | (4) $2'$ $(1/2,0,0)$ $x,0,1/4$<br>$(2_x 1/2,0,1/2)'$ |
| (5) $\bar{1}'$ $0,0,0$<br>$(\bar{1}' 0,0,0)'$ | (6) $a'$ $(1/2,0,0)$ $x,y,0$<br>$(m_z 1/2,0,0)'$ | (7) $c$ $(0,0,1/2)$ $x,0,z$<br>$(m_y 0,0,1/2)$ | (8) $c$ $(0,0,1/2)$ $1/4,y,z$<br>$(m_x 1/2,0,1/2)$   |

For  $(0,1,0) +$  set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(0,1,0)$<br>$(1 0,1,0)'$           | (2) $2'$ $1/4,1/2,z$<br>$(2_z 1/2,1,0)'$       | (3) $2$ $(0,1,0)$ $0,y,1/4$<br>$(2_y 0,1,1/2)$     | (4) $2$ $(1/2,0,0)$ $x,1/2,1/4$<br>$(2_x 1/2,1,1/2)$ |
| (5) $\bar{1}$ $0,1/2,0$<br>$(\bar{1} 0,1,0)$ | (6) $n$ $(1/2,1,0)$ $x,y,0$<br>$(m_z 1/2,1,0)$ | (7) $c'$ $(0,0,1/2)$ $x,1/2,z$<br>$(m_y 0,1,1/2)'$ | (8) $n'$ $(0,1,1/2)$ $1/4,y,z$<br>$(m_x 1/2,1,1/2)'$ |

**Generators selected** (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

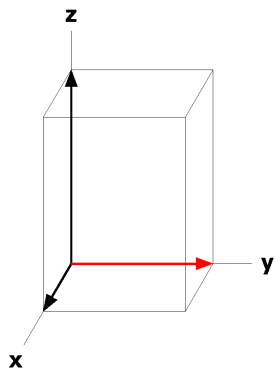
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
16 f 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $u,\bar{v},w$ ] (7) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ] (8) $\bar{x}+1/2,y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
8 e ..2'	1/4,1/2,z [u,v,0]	3/4,1/2, $\bar{z}+1/2$ [ $u,\bar{v},0$ ]	3/4,1/2, $\bar{z}$ [u,v,0]	1/4,1/2,z+1/2 [ $u,\bar{v},0$ ]
8 d ..2	1/4,0,z [0,0,w]	3/4,0, $\bar{z}+1/2$ [0,0,w]	3/4,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,0,z+1/2 [0,0, $\bar{w}$ ]
8 c .2'	0,y,1/4 [u,0,w]	1/2, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	0, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,3/4 [u,0, $\bar{w}$ ]
8 b $\bar{1}$	0,1/2,0 [u,v,w]	1/2,1/2,0 [u,v, $\bar{w}$ ]	0,1/2,1/2 [u, $\bar{v},w$ ]	1/2,1/2,1/2 [u, $\bar{v},\bar{w}$ ]
8 a $\bar{1}'$	0,0,0 [0,0,0]	1/2,0,0 [0,0,0]	0,0,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>·2mm  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>c</sub>·2mm  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/2,1/4

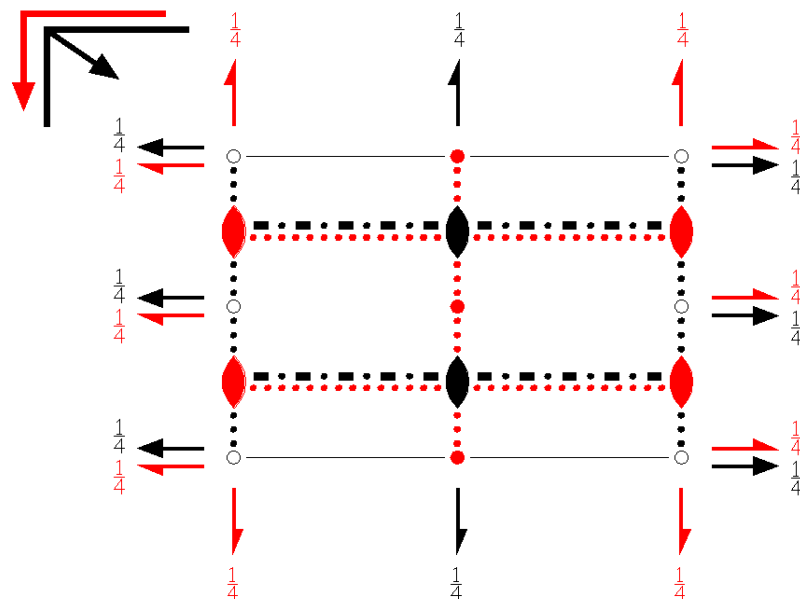
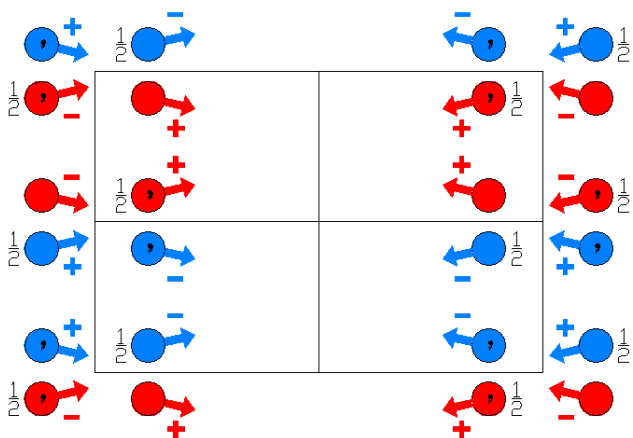
Along [0,1,0] p 2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$P_{2b} c'ca'$   
54.13.440

$mmm1'$   
 $P_{2b} 2_1' c'2/c2'/a'$

Orthorhombic



Origin at  $\bar{1}$  on  $1ca'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |                                      |                                      |                                    |  |
|--------------------------------------|--------------------------------------|------------------------------------|--|
| (1) 1<br>(1 0,0,0)                   | (2) 2'<br>(2 <sub>z</sub>  1/2,0,0)' | (3) 2<br>(2 <sub>y</sub>  0,0,1/2) | (4) 2'<br>(2 <sub>x</sub>  1/2,0,1/2)' |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) a'<br>(m <sub>z</sub>  1/2,0,0)' | (7) c<br>(m <sub>y</sub>  0,0,1/2) | (8) c'<br>(m <sub>x</sub>  1/2,0,1/2)' |

For (0,1,0) + set

- |   |                                    |                                      |                                      |
|---|------------------------------------|--------------------------------------|--------------------------------------|
| (1) t'<br>(1 0,1,0)'                    | (2) 2<br>(2 <sub>z</sub>  1/2,1,0) | (3) 2'<br>(2 <sub>y</sub>  0,1,1/2)' | (4) 2<br>(2 <sub>x</sub>  1/2,1,1/2) |
| (5) $\bar{1}$ '<br>( $\bar{1}$  0,1,0)' | (6) n<br>(m <sub>z</sub>  1/2,1,0) | (7) c'<br>(m <sub>y</sub>  0,1,1/2)' | (8) n<br>(m <sub>x</sub>  1/2,1,1/2) |

**Generators selected** (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

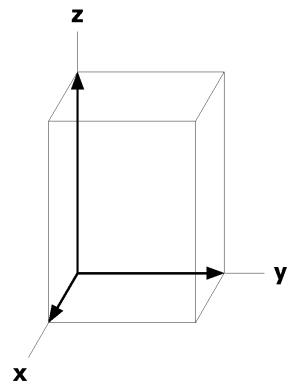
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1,0)' +		
16 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x+1/2, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]
	(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y, \bar{z}$ [u,v, $\bar{w}$ ]	(7) $x, \bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(8) $\bar{x}+1/2, y, z+1/2$ [ $\bar{u}, v, w$ ]
8 e ..2	1/4, 1/2, z [0,0,w]	3/4, 1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	3/4, 1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4, 1/2, z+1/2 [0,0,w]
8 d ..2'	1/4, 0, z [u,v,0]	3/4, 0, $\bar{z}+1/2$ [ $\bar{u}, v, 0$ ]	3/4, 0, $\bar{z}$ [u,v,0]	1/4, 0, z+1/2 [ $\bar{u}, v, 0$ ]
8 c .2.	0, y, 1/4 [0,v,0]	1/2, $\bar{y}, 1/4$ [0,v,0]	0, $\bar{y}, 3/4$ [0,v,0]	1/2, y, 3/4 [0,v,0]
8 b $\bar{1}'$	0, 1/2, 0 [0,0,0]	1/2, 1/2, 0 [0,0,0]	0, 1/2, 1/2 [0,0,0]	1/2, 1/2, 1/2 [0,0,0]
8 a $\bar{1}$	0, 0, 0 [u,v,w]	1/2, 0, 0 [u,v, $\bar{w}$ ]	0, 0, 1/2 [ $\bar{u}, v, \bar{w}$ ]	1/2, 0, 1/2 [ $\bar{u}, v, w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>·2m'm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>·2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x, 1/2, 0

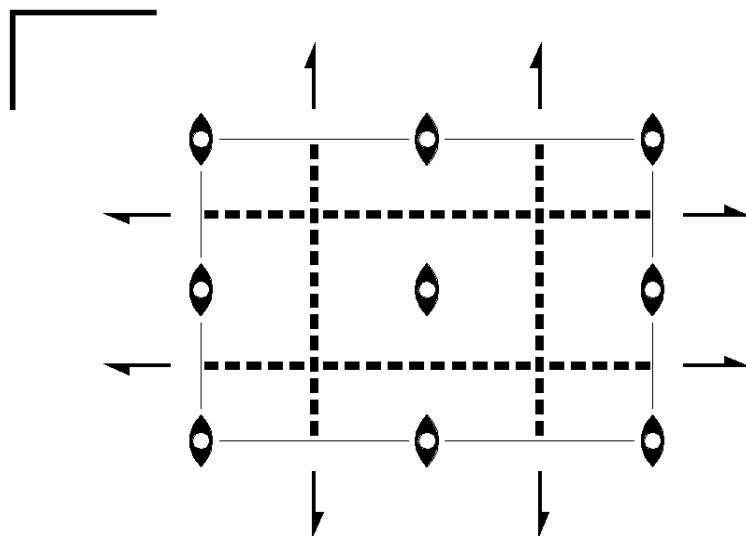
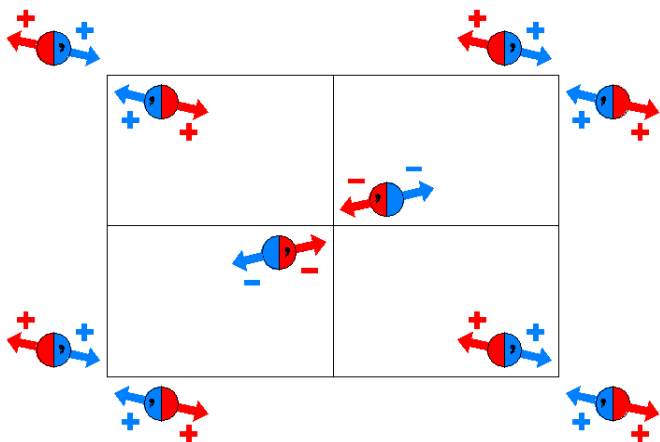
Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pbam  
55.1.441

mmm  
 $P2_1/b 2_1/a2/m$

Orthorhombic



Origin at center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

- |  |                                  |  |  |
|--|----------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) 2 $(0,1/2,0) 1/4,y,0$<br>( $2_y$   $1/2,1/2,0$ ) | (4) 2 $(1/2,0,0) x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ ) |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0) | (6) m $x,y,0$<br>( $m_z$  0,0,0) | (7) a $(1/2,0,0) x,1/4,z$<br>( $m_y$   $1/2,1/2,0$ ) | (8) b $(0,1/2,0) 1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ ) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

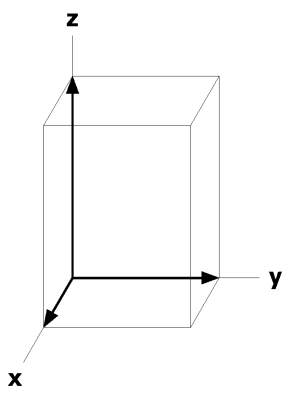
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z$ [u, $\bar{v},\bar{w}$ ]
4	h ..m	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0,w]	$\bar{x}+1/2,y+1/2,1/2$ [0,0, $\bar{w}$ ]	$x+1/2,\bar{y}+1/2,1/2$ [0,0, $\bar{w}$ ]
4	g ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x}+1/2,y+1/2,0$ [0,0, $\bar{w}$ ]	$x+1/2,\bar{y}+1/2,0$ [0,0, $\bar{w}$ ]
4	f ..2	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]
4	e ..2	0,0,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]
2	d ..2/m	0,1/2,1/2 [0,0,w]	1/2,0,1/2 [0,0, $\bar{w}$ ]		
2	c ..2/m	0,1/2,0 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]		
2	b ..2/m	0,0,1/2 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		
2	a ..2/m	0,0,0 [0,0,w]	1/2,1/2,0 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p2gg1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a'}2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0]  $p_{2a'}2mm$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



Pbam1'

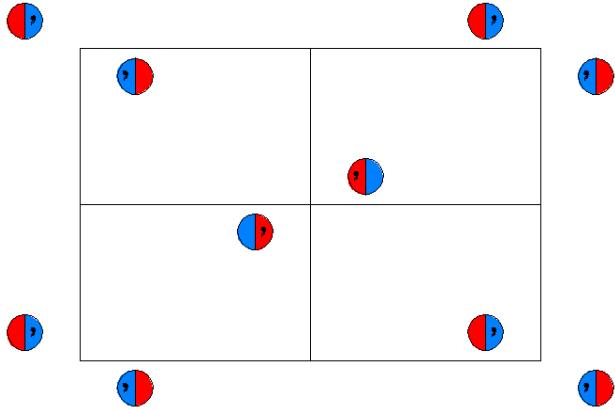
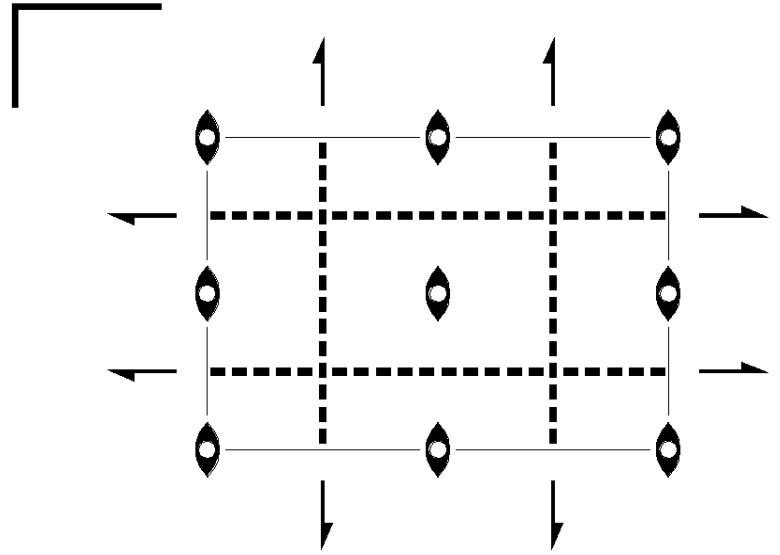
55.2.442

mmm1'

P2<sub>1</sub>/b 2<sub>1</sub>/a2/m1'

Orthorhombic

1'



Origin at center ( 2/m1' )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

For 1 + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |

For 1' + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1'<br>(1 0,0,0)'                          | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

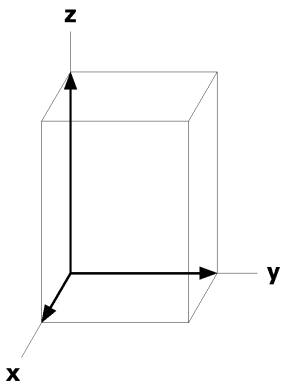
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +	1' +		
8 i 11'	(1) x,y,z [0,0,0] (5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0] (6) x,y, $\bar{z}$ [0,0,0]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [0,0,0] (7) x+1/2, $\bar{y}+1/2,z$ [0,0,0]	(4) x+1/2, $\bar{y}+1/2,\bar{z}$ [0,0,0] (8) $\bar{x}+1/2,y+1/2,z$ [0,0,0]
4 h ..m1'	x,y,1/2 [0,0,0]	$\bar{x},\bar{y},1/2$ [0,0,0]	$\bar{x}+1/2,y+1/2,1/2$ [0,0,0]	x+1/2, $\bar{y}+1/2,1/2$ [0,0,0]
4 g ..m1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{x}+1/2,y+1/2,0$ [0,0,0]	x+1/2, $\bar{y}+1/2,0$ [0,0,0]
4 f ..21'	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0,z [0,0,0]
4 e ..21'	0,0,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2,z [0,0,0]
2 d ..2/m1'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
2 c ..2/m1'	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
2 b ..2/m1'	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2 a ..2/m1'	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



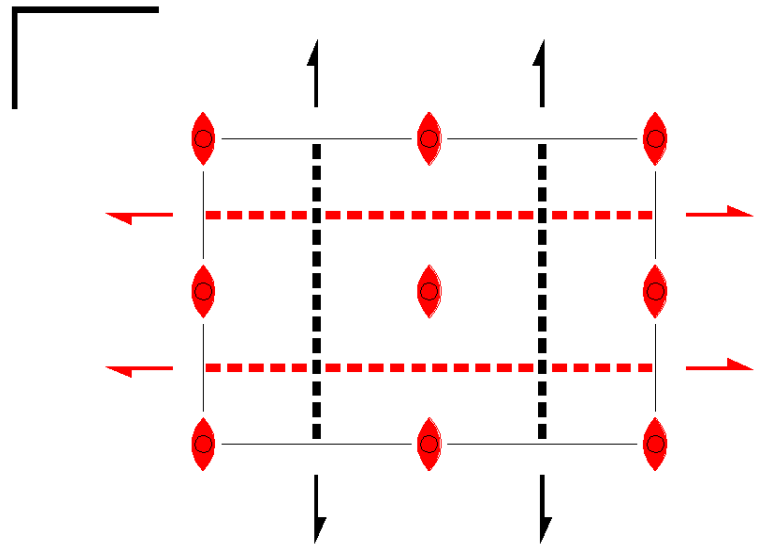
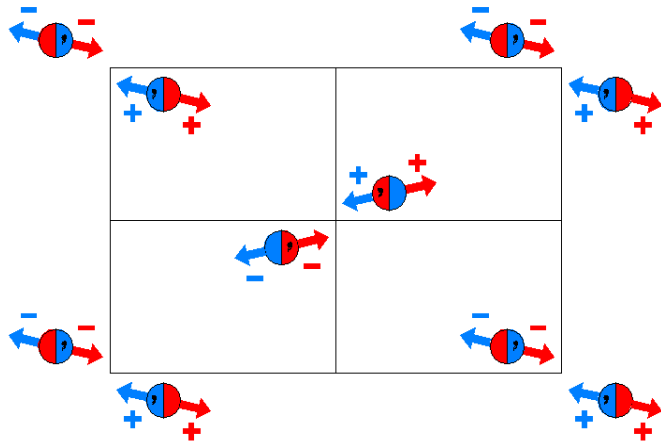
Pb'am

55.3.443

m'mm

$P2_1/b' 2_1'/a2'/m$

Orthorhombic



Origin at center ( $2'/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |                                      |  |  |
|---|--------------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                          | (2) $2'_z$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $2'_y$ (0,1/2,0) $1/4,y,0$<br>( $2_y$  1/2,1/2,0)' | (4) 2 ( $1/2,0,0$ ) $x,1/4,0$<br>( $2_x$  1/2,1/2,0)   |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m $x,y,0$<br>( $m_z$  0,0,0)     | (7) a ( $1/2,0,0$ ) $x,1/4,z$<br>( $m_y$  1/2,1/2,0)   | (8) $b'_x$ (0,1/2,0) $1/4,y,z$<br>( $m_x$  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

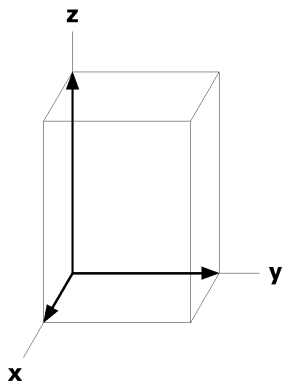
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [u, $\bar{v}$ ,w]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [u, $\bar{v}$ , $\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v}$ ,w]	(7) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]
4	h ..m	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0, $\bar{w}$ ]	$\bar{x}+1/2,y+1/2,1/2$ [0,0,w]	$x+1/2,\bar{y}+1/2,1/2$ [0,0, $\bar{w}$ ]
4	g ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{x}+1/2,y+1/2,0$ [0,0,w]	$x+1/2,\bar{y}+1/2,0$ [0,0, $\bar{w}$ ]
4	f ..2'	0,1/2,z [u,v,0]	1/2,0, $\bar{z}$ [u, $\bar{v}$ ,0]	0,1/2, $\bar{z}$ [ $\bar{u},\bar{v}$ ,0]	1/2,0,z [ $\bar{u},v,0$ ]
4	e ..2'	0,0,z [u,v,0]	1/2,1/2, $\bar{z}$ [u, $\bar{v}$ ,0]	0,0, $\bar{z}$ [ $\bar{u},\bar{v}$ ,0]	1/2,1/2,z [ $\bar{u},v,0$ ]
2	d ..2'/m	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	c ..2'/m	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
2	b ..2'/m	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a ..2'/m	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

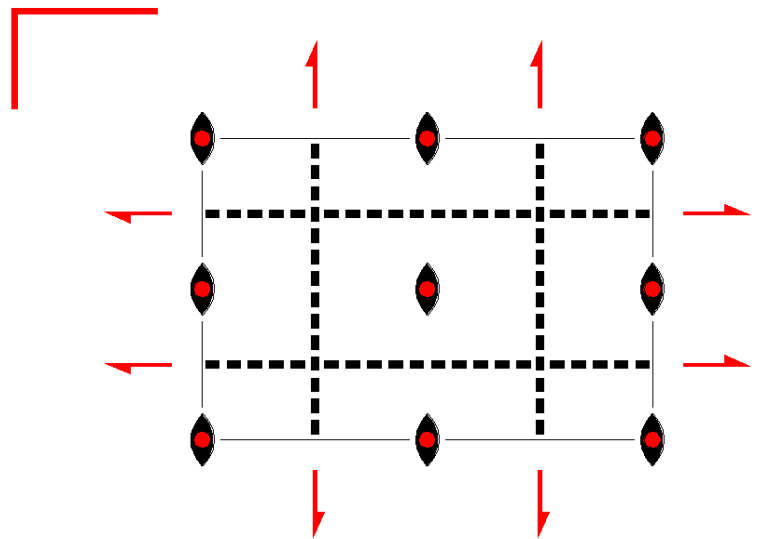
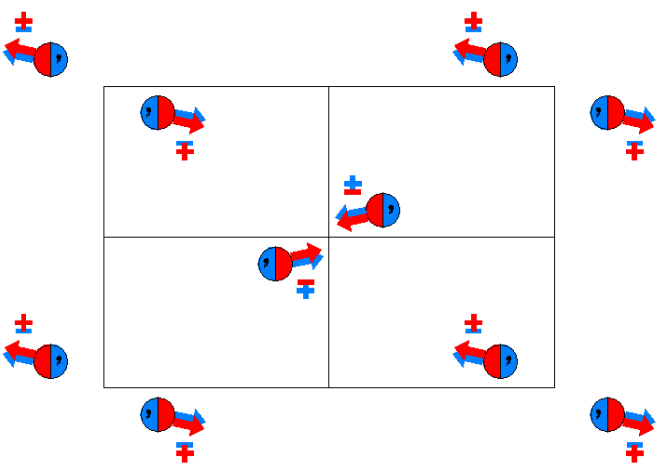
Along [0,1,0] p<sub>2a'</sub>2mm  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pbam'  
55.4.444

mmm'  
P2<sub>1</sub>'/b 2<sub>1</sub>'/a2/m'

Orthorhombic



Origin at center ( 2/m' )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)   | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

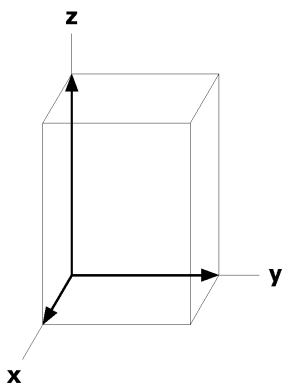
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z$ [u, $\bar{v},\bar{w}$ ]
4	h ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{x}+1/2,y+1/2,1/2$ [u, $\bar{v},0$ ]	$x+1/2,\bar{y}+1/2,1/2$ [ $\bar{u},\bar{v},0$ ]
4	g ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x}+1/2,y+1/2,0$ [u, $\bar{v},0$ ]	$x+1/2,\bar{y}+1/2,0$ [ $\bar{u},\bar{v},0$ ]
4	f ..2	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]
4	e ..2	0,0,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]
2	d ..2/m'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	c ..2/m'	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
2	b ..2/m'	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a ..2/m'	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a'}-2m'm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

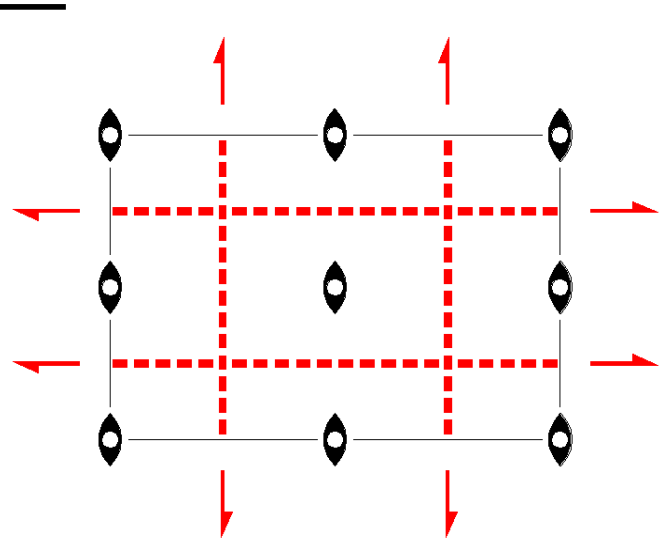
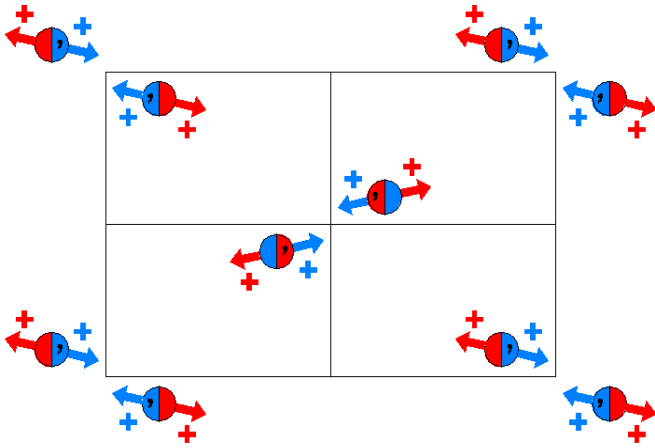
Along [0,1,0]  $p_{2a'}-2m'm'$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pb'a'm  
55.5.445

m'm'm  
P2<sub>1</sub>'/b' 2<sub>1</sub>'/a'2/m

Orthorhombic



Origin at center ( 2/m )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

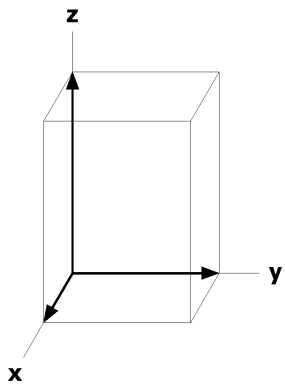
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $u,\bar{v},w$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x+1/2,\bar{y}+1/2,z$ [ $u,\bar{v},w$ ]	(8) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]
4	h ..m	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0,w]	$\bar{x}+1/2,y+1/2,1/2$ [0,0,w]	$x+1/2,\bar{y}+1/2,1/2$ [0,0,w]
4	g ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x}+1/2,y+1/2,0$ [0,0,w]	$x+1/2,\bar{y}+1/2,0$ [0,0,w]
4	f ..2	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0,z [0,0,w]
4	e ..2	0,0,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	1/2,1/2,z [0,0,w]
2	d ..2/m	0,1/2,1/2 [0,0,w]	1/2,0,1/2 [0,0,w]		
2	c ..2/m	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]		
2	b ..2/m	0,0,1/2 [0,0,w]	1/2,1/2,1/2 [0,0,w]		
2	a ..2/m	0,0,0 [0,0,w]	1/2,1/2,0 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

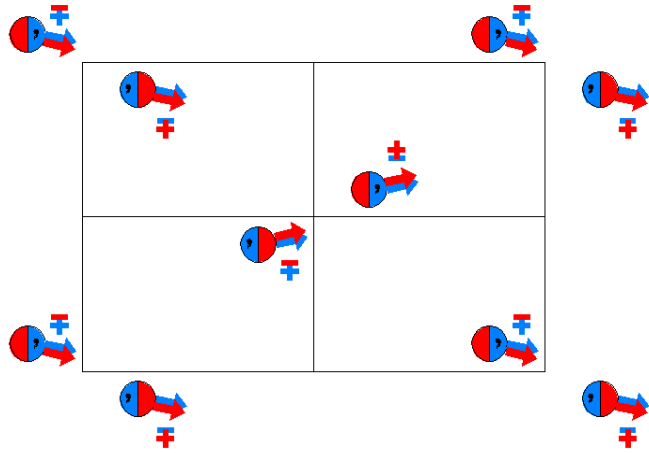
Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Pb'am'  
55.6.446

m'mm'  
P2<sub>1</sub>'/b' 2<sub>1</sub>/a<sub>2</sub>'/m'

Orthorhombic

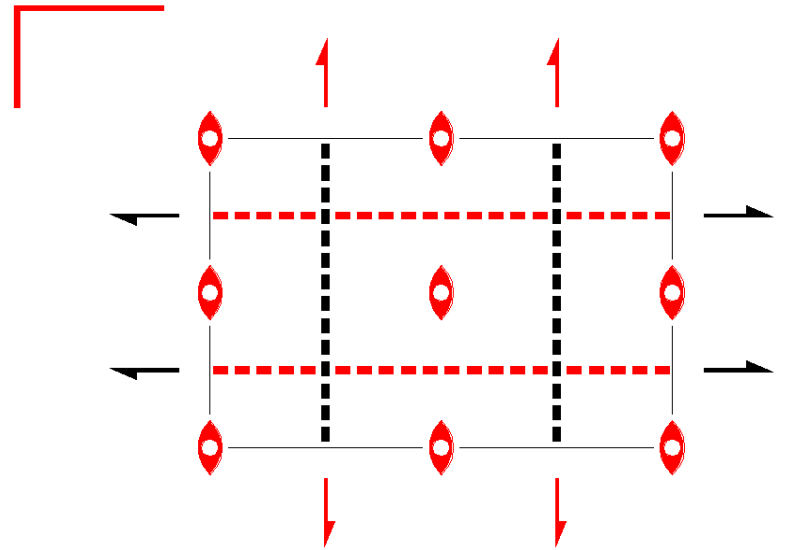


Origin at center ( 2'/m' )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

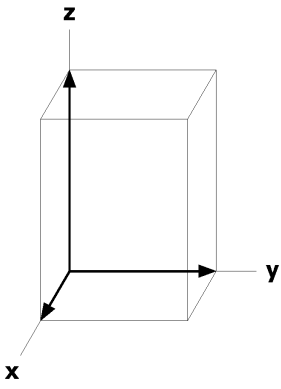
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]
4	h ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [u,v,0]	$\bar{x}+1/2,y+1/2,1/2$ [ $\bar{u},v,0$ ]	$x+1/2,\bar{y}+1/2,1/2$ [ $\bar{u},v,0$ ]
4	g ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [u,v,0]	$\bar{x}+1/2,y+1/2,0$ [ $\bar{u},v,0$ ]	$x+1/2,\bar{y}+1/2,0$ [ $\bar{u},v,0$ ]
4	f ..2'	0,1/2,z [u,v,0]	1/2,0, $\bar{z}$ [ $\bar{u},v,0$ ]	0,1/2, $\bar{z}$ [u,v,0]	1/2,0,z [ $\bar{u},v,0$ ]
4	e ..2'	0,0,z [u,v,0]	1/2,1/2, $\bar{z}$ [ $\bar{u},v,0$ ]	0,0, $\bar{z}$ [u,v,0]	1/2,1/2,z [ $\bar{u},v,0$ ]
2	d ..2'/m'	0,1/2,1/2 [u,v,0]	1/2,0,1/2 [ $\bar{u},v,0$ ]		
2	c ..2'/m'	0,1/2,0 [u,v,0]	1/2,0,0 [ $\bar{u},v,0$ ]		
2	b ..2'/m'	0,0,1/2 [u,v,0]	1/2,1/2,1/2 [ $\bar{u},v,0$ ]		
2	a ..2'/m'	0,0,0 [u,v,0]	1/2,1/2,0 [ $\bar{u},v,0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2'gg'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

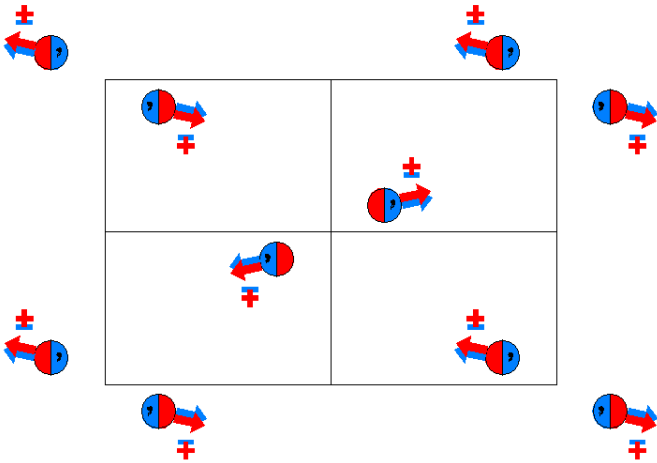
Along [0,1,0] p<sub>2a'</sub>2m'm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



Pb'a'm'  
55.7.447

m'm'm'  
P2<sub>1</sub>/b'2<sub>1</sub>/a'2/m'

Orthorhombic

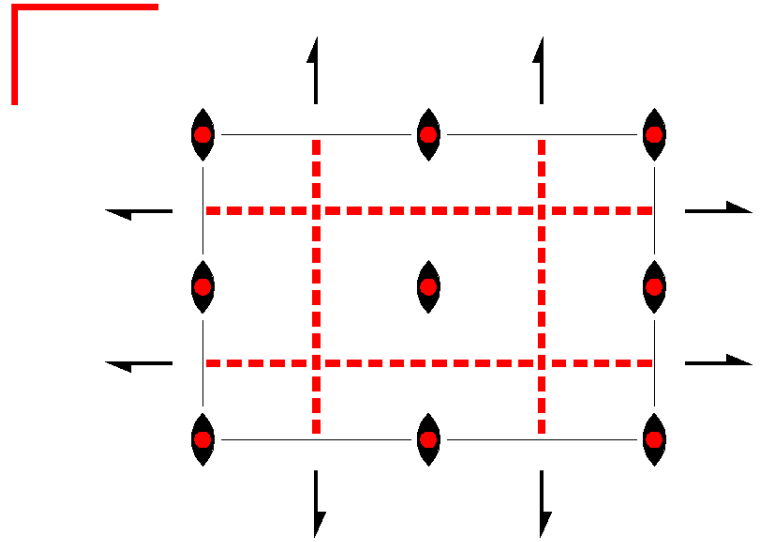


Origin at center ( 2/m' )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                             | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)    | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)    |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$ ' 0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub> ' 0,0,0)' | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub> ' 1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub> ' 1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) $x+1/2,\bar{y}+1/2,z$ [u, $\bar{v},w$ ]	(8) $\bar{x}+1/2,\bar{y}+1/2,z$ [ $\bar{u},\bar{v},w$ ]
4	h ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{x}+1/2,\bar{y}+1/2,1/2$ [ $\bar{u},\bar{v},0$ ]	$x+1/2,\bar{y}+1/2,1/2$ [u, $\bar{v},0$ ]
4	g ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x}+1/2,\bar{y}+1/2,0$ [ $\bar{u},\bar{v},0$ ]	$x+1/2,\bar{y}+1/2,0$ [u, $\bar{v},0$ ]
4	f ..2	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0,z [0,0,w]
4	e ..2	0,0,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2,z [0,0,w]
2	d ..2/m'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	c ..2/m'	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
2	b ..2/m'	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a ..2/m'	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2g'g'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0

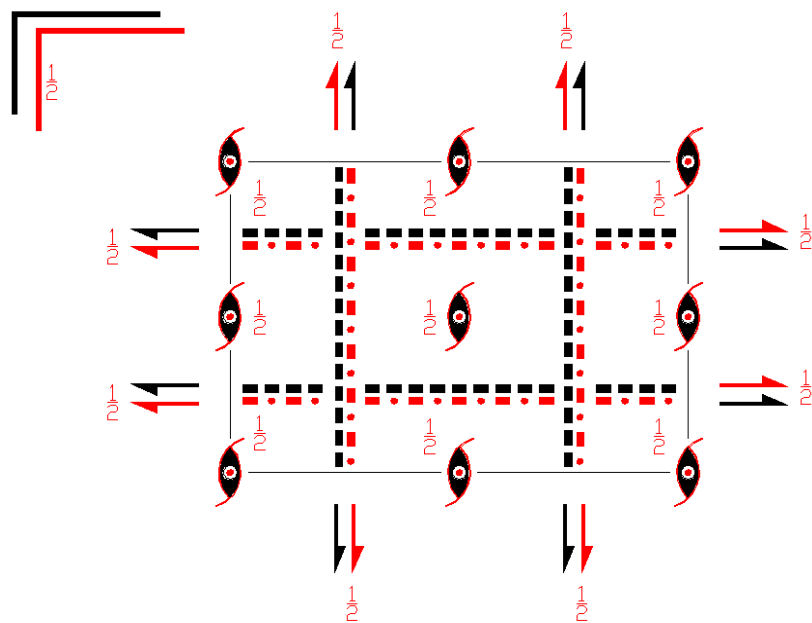
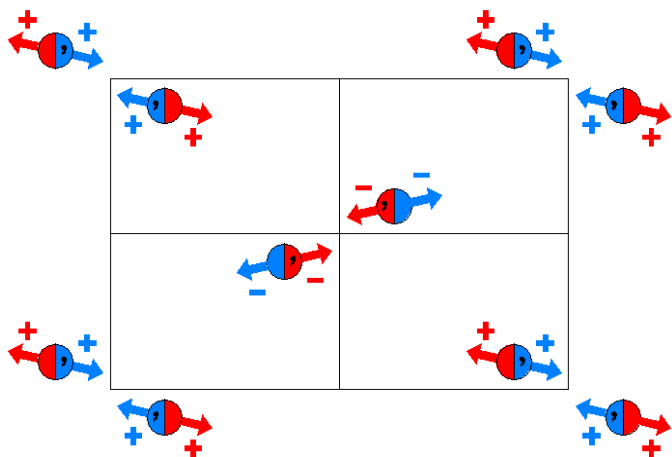
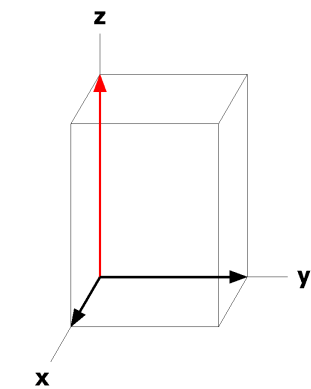
$P_{2c}$  bam

55.8.448

mmm1'

$P_{2c} 2_1/b 2_1/a 2/m$

Orthorhombic



Origin at center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |

For (0,0,1)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' (0,0,1)<br>(1 0,0,1)'                    | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)' | (3) 2' (0,1/2,0) 1/4,y,1/2<br>(2 <sub>y</sub>  1/2,1/2,1)' | (4) 2' (1/2,0,0) x,1/4,1/2<br>(2 <sub>x</sub>  1/2,1/2,1)' |
| (5) $\bar{1}$ ' 0,0,1/2<br>( $\bar{1}$  0,0,1)' | (6) m' x,y,1/2<br>(m <sub>z</sub>  0,0,1)'       | (7) n' (1/2,0,1) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1)'   | (8) n' (0,1/2,1) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1)'   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
16 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]
8 h ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{x}+1/2,y+1/2,1/2$ [ $u,\bar{v},0$ ]	$x+1/2,\bar{y}+1/2,1/2$ [ $\bar{u},v,0$ ]
8 g ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x}+1/2,y+1/2,0$ [0,0, $\bar{w}$ ]	$x+1/2,\bar{y}+1/2,0$ [0,0, $\bar{w}$ ]
8 f ..2	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]
8 e ..2	0,0,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]
4 d ..2/m'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 c ..2/m	0,1/2,0 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]		
4 b ..2/m'	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a ..2/m	0,0,0 [0,0,w]	1/2,1/2,0 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>c</sub> 2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0] p<sub>c</sub> 2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,0

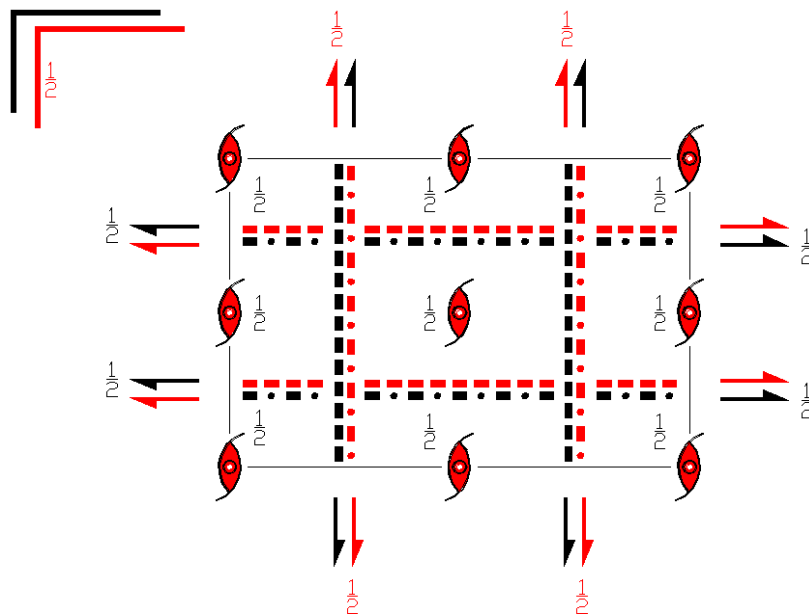
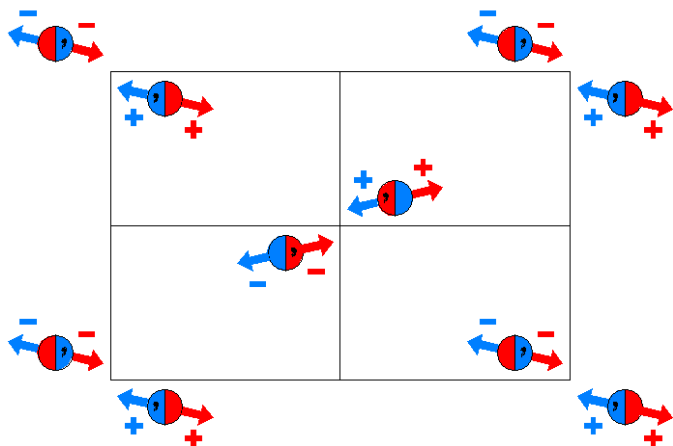
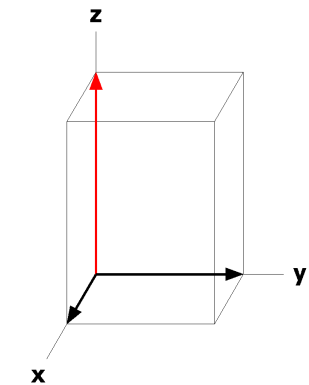
$P_{2c} b'am$

55.9.449

$mmm1'$

$P_{2c} 2_1/b' 2_1/a2'/m$

Orthorhombic



Origin at center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |                                      |  |   |
|---|--------------------------------------|--|---|
| (1) 1<br>(1 0,0,0)                          | (2) $2'_z$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $2'_y$ (0,1/2,0) $1/4,y,0$<br>( $2_y$  1/2,1/2,0)' | (4) $2'_x$ (1/2,0,0) $x,1/4,0$<br>( $2_x$  1/2,1/2,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) $m_x$ x,y,0<br>( $m_x$  0,0,0)   | (7) $a$ (1/2,0,0) $x,1/4,z$<br>( $m_y$  1/2,1/2,0)     | (8) $b'$ (0,1/2,0) $1/4,y,z$<br>( $m_x$  1/2,1/2,0)'  |

For (0,0,1) + set

- |  |   |   |  |
|--|---|---|--|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'               | (2) $2'_z$ (0,0,1) 0,0,z<br>( $2_z$  0,0,1) | (3) $2'_y$ (0,1/2,0) $1/4,y,1/2$<br>( $2_y$  1/2,1/2,1) | (4) $2'_x$ (1/2,0,0) $x,1/4,1/2$<br>( $2_x$  1/2,1/2,1)' |
| (5) $\bar{1}$ 0,0,1/2<br>( $\bar{1}$  0,0,1) | (6) $m'_x$ x,y,1/2<br>( $m_x$  0,0,1)'      | (7) $n'$ (1/2,0,1) $x,1/4,z$<br>( $m_y$  1/2,1/2,1)'    | (8) $n$ (0,1/2,1) $1/4,y,z$<br>( $m_x$  1/2,1/2,1)       |



**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

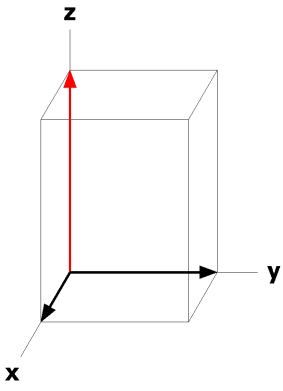
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
16 i 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [u, $\bar{v},w$ ] (7) x+1/2, $\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(4) x+1/2, $\bar{y}+1/2,\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]
8 h ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [u,v,0]	$\bar{x}+1/2,y+1/2,1/2$ [ $\bar{u},v,0$ ]	x+1/2, $\bar{y}+1/2,1/2$ [ $\bar{u},v,0$ ]
8 g ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{x}+1/2,y+1/2,0$ [0,0,w]	x+1/2, $\bar{y}+1/2,0$ [0,0, $\bar{w}$ ]
8 f ..2'	0,1/2,z [u,v,0]	1/2,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	0,1/2, $\bar{z}$ [u, $\bar{v},0$ ]	1/2,0,z [ $\bar{u},v,0$ ]
8 e ..2'	0,0,z [u,v,0]	1/2,1/2, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	0,0, $\bar{z}$ [u, $\bar{v},0$ ]	1/2,1/2,z [ $\bar{u},v,0$ ]
4 d ..2/m'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 c ..2/m	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
4 b ..2/m'	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a ..2'/m	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a'</sub>2mm  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>c'</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



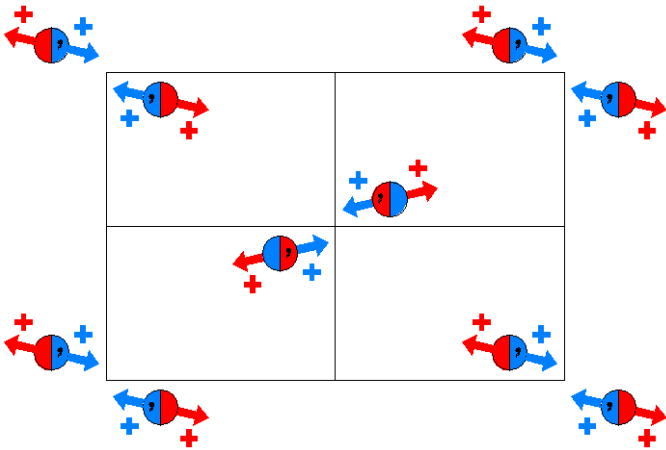
$P_{2c} b'a'm$

55.10.450

$mmm1'$

$P_{2c} 2_1' / b' 2_1' / a' 2/m$

Orthorhombic



Origin at center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

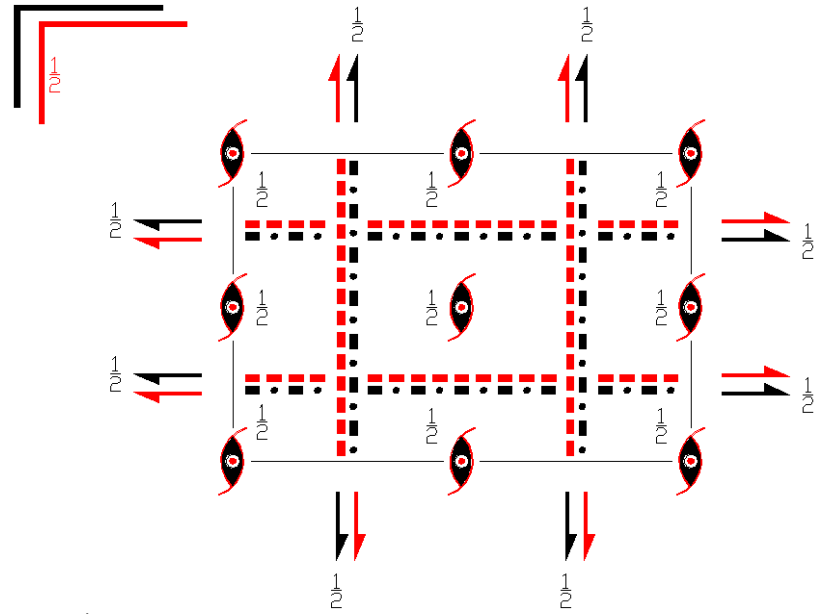
Symmetry Operations

For (0,0,0) + set

- |  |                                  |  |  |
|--|----------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) 2' (0,1/2,0) $1/4,y,0$<br>( $2_y$  1/2,1/2,0)' | (4) 2' (1/2,0,0) $x,1/4,0$<br>( $2_x$  1/2,1/2,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m $x,y,0$<br>( $m_z$  0,0,0) | (7) a' (1/2,0,0) $x,1/4,z$<br>( $m_y$  1/2,1/2,0)' | (8) b' (0,1/2,0) $1/4,y,z$<br>( $m_x$  1/2,1/2,0)' |

For (0,0,1)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' (0,0,1)<br>(1 0,0,1)'                    | (2) 2' (0,0,1) $0,0,z$<br>( $2_z$  0,0,1)' | (3) 2 (0,1/2,0) $1/4,y,1/2$<br>( $2_y$  1/2,1/2,1) | (4) 2 (1/2,0,0) $x,1/4,1/2$<br>( $2_x$  1/2,1/2,1) |
| (5) $\bar{1}$ ' 0,0,1/2<br>( $\bar{1}$  0,0,1)' | (6) m' $x,y,1/2$<br>( $m_z$  0,0,1)'       | (7) n (1/2,0,1) $x,1/4,z$<br>( $m_y$  1/2,1/2,1)   | (8) n (0,1/2,1) $1/4,y,z$<br>( $m_x$  1/2,1/2,1)   |



**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

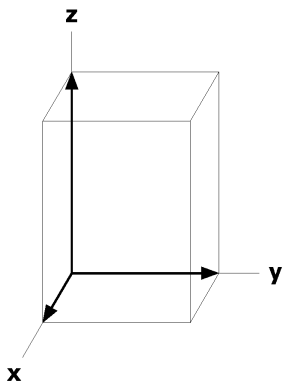
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
16 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $u,\bar{v},w$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x+1/2,\bar{y}+1/2,z$ [u, $\bar{v},w$ ]	(8) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]
8 h ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{x}+1/2,y+1/2,1/2$ [ $\bar{u},v,0$ ]	$x+1/2,\bar{y}+1/2,1/2$ [u, $\bar{v},0$ ]
8 g ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x}+1/2,y+1/2,0$ [0,0,w]	$x+1/2,\bar{y}+1/2,0$ [0,0,w]
8 f ..2	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0,z [0,0,w]
8 e ..2	0,0,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	1/2,1/2,z [0,0,w]
4 d ..2/m'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 c ..2/m	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]		
4 b ..2/m'	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a ..2/m	0,0,0 [0,0,w]	1/2,1/2,0 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a'</sub>-2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,1/2

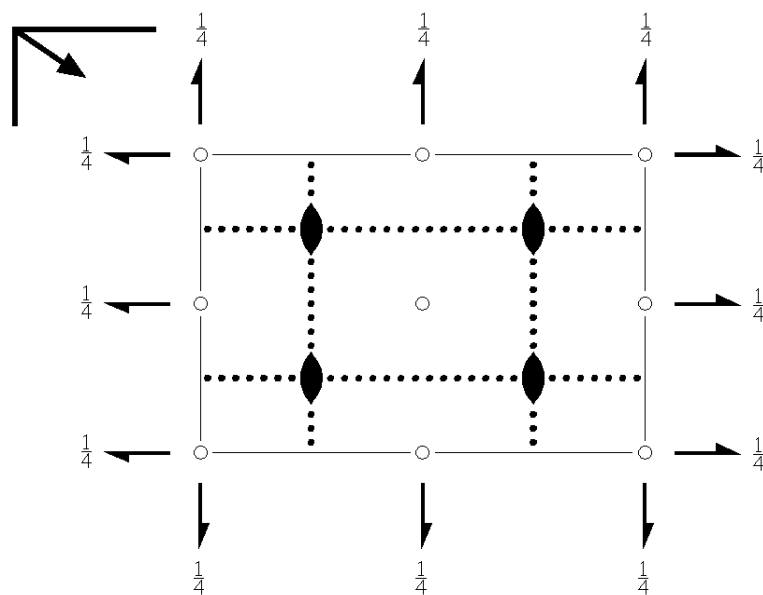
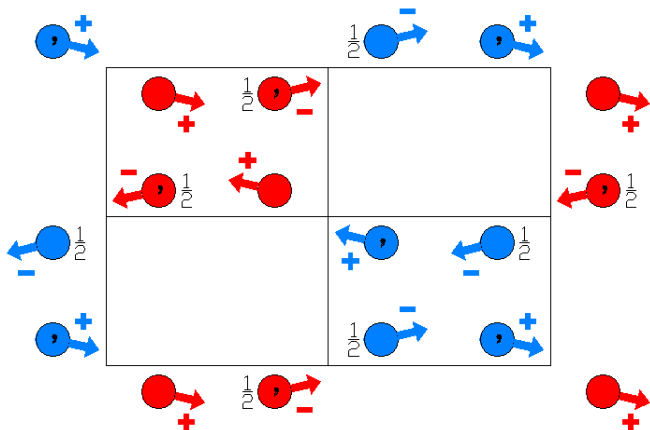
Along [0,1,0] p<sub>2a'</sub>-2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,1/2



Pccn  
56.1.451

mmm  
 $P2_1/c2_1/c2/n$

Orthorhombic



Origin at  $\bar{1}$  on 11n

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 $1/4, 1/4, z$<br>( $2_z$   $1/2, 1/2, 0$ )         | (3) 2 (0,1/2,0) $0, y, 1/4$<br>( $2_y$   $0, 1/2, 1/2$ ) | (4) 2 (1/2,0,0) $x, 0, 1/4$<br>( $2_x$   $1/2, 0, 1/2$ ) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) n (1/2,1/2,0) $x, y, 0$<br>( $m_z$   $1/2, 1/2, 0$ ) | (7) c (0,0,1/2) $x, 1/4, z$<br>( $m_y$   $0, 1/2, 1/2$ ) | (8) c (0,0,1/2) $1/4, y, z$<br>( $m_x$   $1/2, 0, 1/2$ ) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

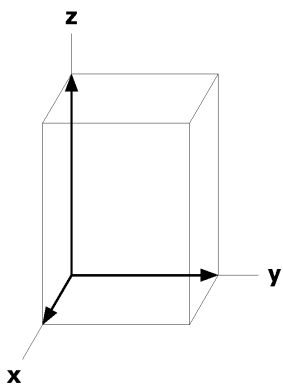
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}+1/2, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, \bar{y}+1/2, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(4) $x+1/2, \bar{y}, \bar{z}+1/2$ [ $u, \bar{v}, \bar{w}$ ]
		(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y+1/2, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(7) $x, \bar{y}+1/2, z+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(8) $\bar{x}+1/2, y, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]
4	d ..2	1/4,3/4,z [0,0,w]	3/4,1/4, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	3/4,1/4, $\bar{z}$ [0,0,w]	1/4,3/4,z+1/2 [0,0, $\bar{w}$ ]
4	c ..2	1/4,1/4,z [0,0,w]	3/4,3/4, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	3/4,3/4, $\bar{z}$ [0,0,w]	1/4,1/4,z+1/2 [0,0, $\bar{w}$ ]
4	b $\bar{1}$	0,0,1/2 [u,v,w]	1/2,1/2,1/2 [ $\bar{u}, \bar{v}, w$ ]	0,1/2,0 [ $\bar{u}, \bar{v}, \bar{w}$ ]	1/2,0,0 [ $u, \bar{v}, \bar{w}$ ]
4	a $\bar{1}$	0,0,0 [u,v,w]	1/2,1/2,0 [ $\bar{u}, \bar{v}, w$ ]	0,1/2,1/2 [ $\bar{u}, \bar{v}, \bar{w}$ ]	1/2,0,1/2 [ $u, \bar{v}, \bar{w}$ ]

**Symmetry of Special Projections**

Along [0,01]  $c_p$ -2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,1/4,z

Along [1,0,0]  $p_{2b}$ -2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,1/4

Along [0,1,0]  $p_{2b}$ -2m'g'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0

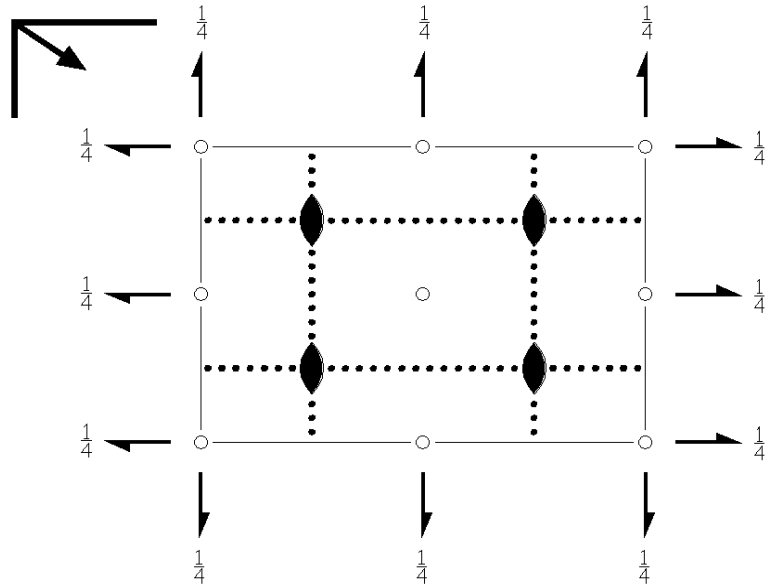
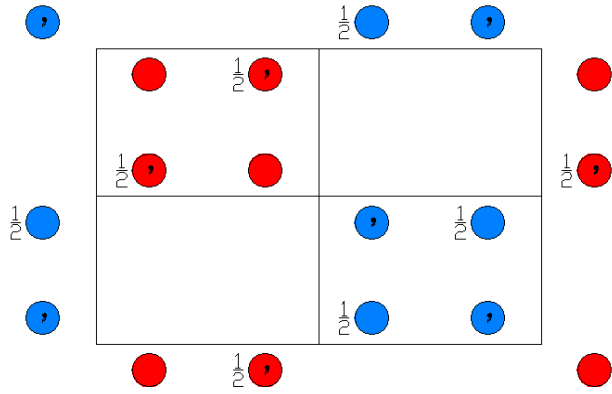


Pccn1'  
56.2.452

mmm1'  
P2<sub>1</sub>/c2<sub>1</sub>/c2/n1'

Orthorhombic

1'



Origin at  $\bar{1}1'$  on  $11n1'$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1; 0 \leq z \leq 1/2$

Symmetry Operations

For 1 + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 $1/4, 1/4, z$<br>(2 <sub>z</sub>  1/2, 1/2, 0)           | (3) 2 (0, 1/2, 0) $0, y, 1/4$<br>(2 <sub>y</sub>  0, 1/2, 1/2) | (4) 2 (1/2, 0, 0) $x, 0, 1/4$<br>(2 <sub>x</sub>  1/2, 0, 1/2) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) n (1/2, 1/2, 0) $x, y, 0$<br>(m <sub>z</sub>  1/2, 1/2, 0) | (7) c (0, 0, 1/2) $x, 1/4, z$<br>(m <sub>y</sub>  0, 1/2, 1/2) | (8) c (0, 0, 1/2) $1/4, y, z$<br>(m <sub>x</sub>  1/2, 0, 1/2) |

For 1' + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1'<br>(1 0,0,0)'                         | (2) 2' $1/4, 1/4, z$<br>(2 <sub>z</sub>  1/2, 1/2, 0)'           | (3) 2' (0, 1/2, 0) $0, y, 1/4$<br>(2 <sub>y</sub>  0, 1/2, 1/2)' | (4) 2' (1/2, 0, 0) $x, 0, 1/4$<br>(2 <sub>x</sub>  1/2, 0, 1/2)' |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) n' (1/2, 1/2, 0) $x, y, 0$<br>(m <sub>z</sub>  1/2, 1/2, 0)' | (7) c' (0, 0, 1/2) $x, 1/4, z$<br>(m <sub>y</sub>  0, 1/2, 1/2)' | (8) c' (0, 0, 1/2) $1/4, y, z$<br>(m <sub>x</sub>  1/2, 0, 1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

### Positions

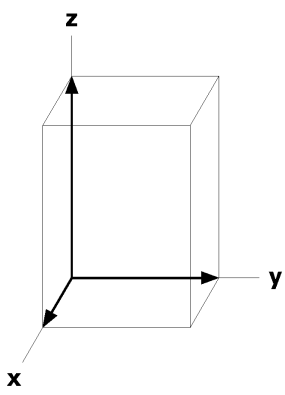
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +		1' +	
8 e 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}+1/2, \bar{y}+1/2, z$ [0,0,0]	(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [0,0,0]	(4) $x+1/2, \bar{y}, \bar{z}+1/2$ [0,0,0]
	(5) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]	(6) $x+1/2, y+1/2, \bar{z}$ [0,0,0]	(7) $x, \bar{y}+1/2, z+1/2$ [0,0,0]	(8) $\bar{x}+1/2, y, z+1/2$ [0,0,0]
4 d ..21'	1/4,3/4,z [0,0,0]	3/4,1/4, $\bar{z}+1/2$ [0,0,0]	3/4,1/4, $\bar{z}$ [0,0,0]	1/4,3/4,z+1/2 [0,0,0]
4 c ..21'	1/4,1/4,z [0,0,0]	3/4,3/4, $\bar{z}+1/2$ [0,0,0]	3/4,3/4, $\bar{z}$ [0,0,0]	1/4,1/4,z+1/2 [0,0,0]
4 b $\bar{1}1'$	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]
4 a $\bar{1}1'$	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]

### Symmetry of Special Projections

Along [0,01] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,1/4,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

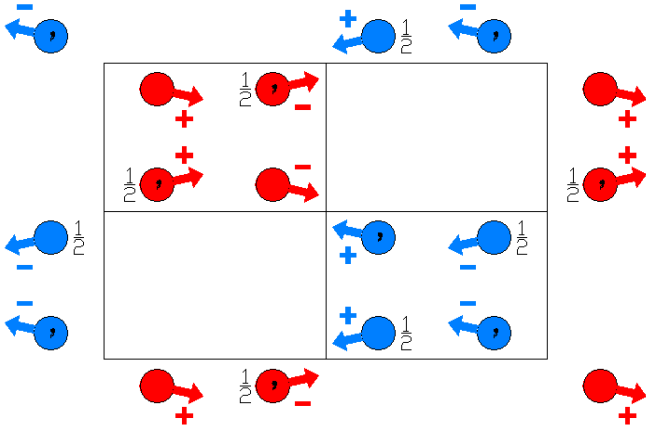
Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pc'cn  
56.3.453

m'mm  
P2<sub>1</sub>/c'2<sub>1</sub>'/c2'/n

Orthorhombic

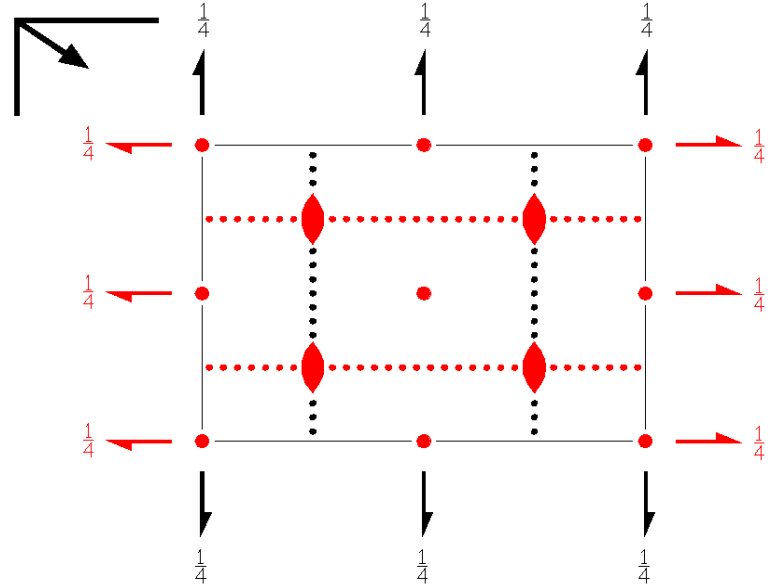


Origin at  $\bar{1}$ ' on 11n

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2' $1/4, 1/4, z$<br>(2 <sub>z</sub>  1/2, 1/2, 0)'         | (3) 2' (0, 1/2, 0) $0, y, 1/4$<br>(2 <sub>y</sub>  0, 1/2, 1/2)' | (4) 2 (1/2, 0, 0) $x, 0, 1/4$<br>(2 <sub>x</sub>  1/2, 0, 1/2)   |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) n (1/2, 1/2, 0) $x, y, 0$<br>(m <sub>z</sub>  1/2, 1/2, 0) | (7) c (0, 0, 1/2) $x, 1/4, z$<br>(m <sub>y</sub>  0, 1/2, 1/2)   | (8) c' (0, 0, 1/2) $1/4, y, z$<br>(m <sub>x</sub>  1/2, 0, 1/2)' |





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

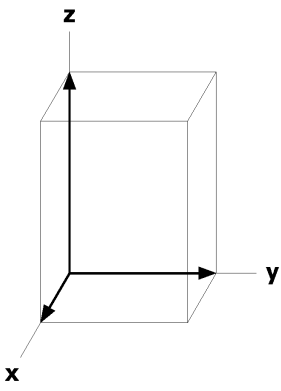
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}+1/2, z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) $x+1/2, \bar{y}, \bar{z}+1/2$ [u, $\bar{v}, \bar{w}$ ]
		(5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(6) $x+1/2, y+1/2, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(7) $x, \bar{y}+1/2, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(8) $\bar{x}+1/2, y, z+1/2$ [ $\bar{u}, v, w$ ]
4	d ..2'	1/4,3/4,z [u,v,0]	3/4,1/4, $\bar{z}+1/2$ [u, $\bar{v}$ ,0]	3/4,1/4, $\bar{z}$ [ $\bar{u}, \bar{v}$ ,0]	1/4,3/4,z+1/2 [ $\bar{u}, v$ ,0]
4	c ..2'	1/4,1/4,z [u,v,0]	3/4,3/4, $\bar{z}+1/2$ [u, $\bar{v}$ ,0]	3/4,3/4, $\bar{z}$ [ $\bar{u}, \bar{v}$ ,0]	1/4,1/4,z+1/2 [ $\bar{u}, v$ ,0]
4	b $\bar{1}'$	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]
4	a $\bar{1}'$	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]

**Symmetry of Special Projections**

Along [0,01]  $c_p \cdot 2' mm'$   
 $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,1/4,z

Along [1,0,0]  $p 2mg$   
 $\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

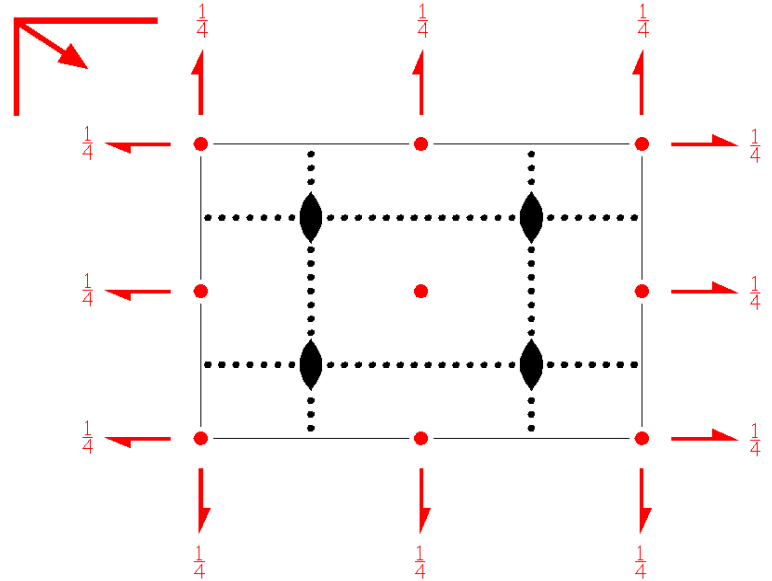
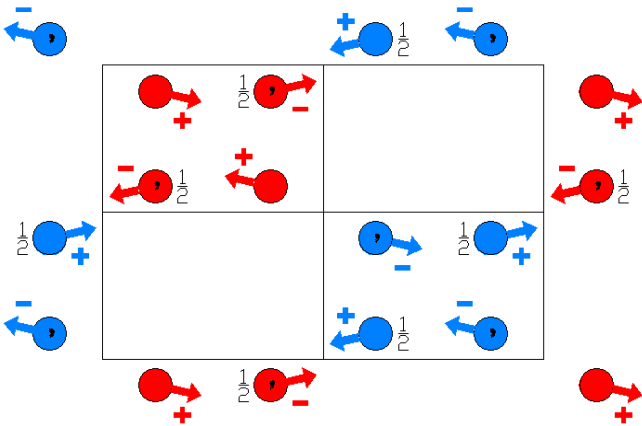
Along [0,1,0]  $p_{2b} \cdot 2mg$   
 $\mathbf{a}^* = -\mathbf{a} \quad \mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pccn'  
56.4.454

mmm'  
P2<sub>1</sub>'/c2<sub>1</sub>'/c2/n'

Orthorhombic



Origin at  $\bar{1}'$  on 11n'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $1/4, 1/4, z$<br>(2 <sub>z</sub>  1/2, 1/2, 0)             | (3) 2' (0, 1/2, 0) $0, y, 1/4$<br>(2 <sub>y</sub>  0, 1/2, 1/2)' | (4) 2' (1/2, 0, 0) $x, 0, 1/4$<br>(2 <sub>x</sub>  1/2, 0, 1/2)' |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) n' (1/2, 1/2, 0) $x, y, 0$<br>(m <sub>z</sub>  1/2, 1/2, 0)' | (7) c (0, 0, 1/2) $x, 1/4, z$<br>(m <sub>y</sub>  0, 1/2, 1/2)   | (8) c (0, 0, 1/2) $1/4, y, z$<br>(m <sub>x</sub>  1/2, 0, 1/2)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

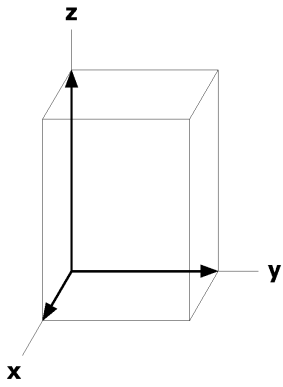
		Coordinates							
Multiplicity, Wyckoff letter, Site Symmetry.									
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2,\bar{y}+1/2,z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(4) $x+1/2,\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,y+1/2,\bar{z}$ [ $u,v,\bar{w}$ ]	(7) $x,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
4	d ..2	1/4,3/4,z [0,0,w]	3/4,1/4, $\bar{z}+1/2$ [0,0,w]	3/4,1/4, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,3/4,z+1/2 [0,0, $\bar{w}$ ]				
4	c ..2	1/4,1/4,z [0,0,w]	3/4,3/4, $\bar{z}+1/2$ [0,0,w]	3/4,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,1/4,z+1/2 [0,0, $\bar{w}$ ]				
4	b $\bar{1}'$	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]				
4	a $\bar{1}'$	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]				

**Symmetry of Special Projections**

Along [0,01] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,1/4,z

Along [1,0,0]  $p_{2b} \cdot 2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

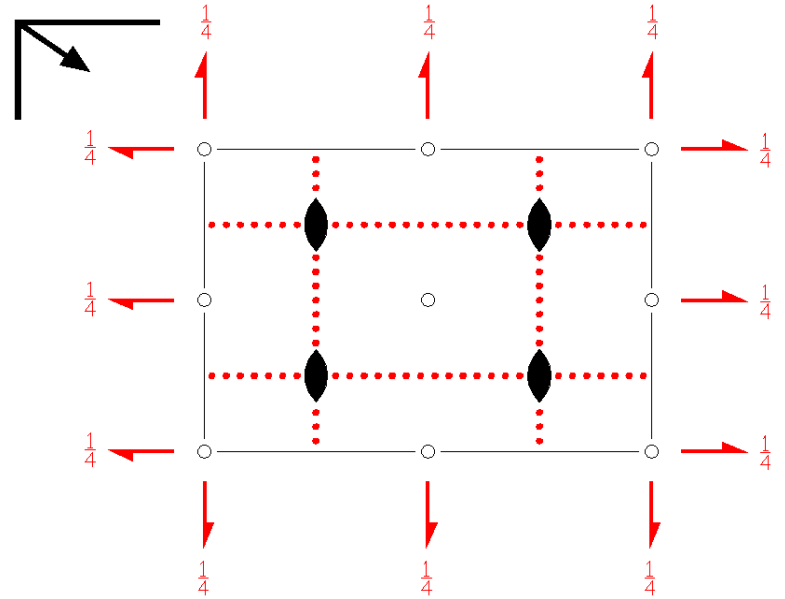
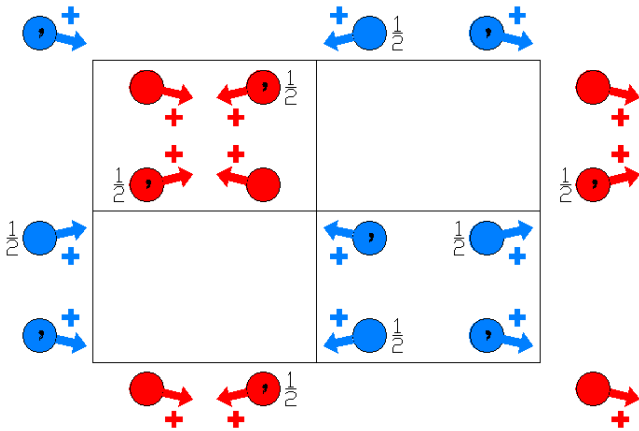
Along [0,1,0]  $p_{2b} \cdot 2m'g'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pc'c'n  
56.5.455

m'm'm  
P2<sub>1</sub>'/c2<sub>1</sub>'/c2/n

Orthorhombic



Origin at  $\bar{1}$  on 11n

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 $1/4, 1/4, z$<br>(2 <sub>z</sub>  1/2, 1/2, 0)           | (3) 2' (0, 1/2, 0) $0, y, 1/4$<br>(2 <sub>y</sub>  0, 1/2, 1/2)' | (4) 2' (1/2, 0, 0) $x, 0, 1/4$<br>(2 <sub>x</sub>  1/2, 0, 1/2)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) n (1/2, 1/2, 0) $x, y, 0$<br>(m <sub>z</sub>  1/2, 1/2, 0) | (7) c' (0, 0, 1/2) $x, 1/4, z$<br>(m <sub>y</sub>  0, 1/2, 1/2)' | (8) c' (0, 0, 1/2) $1/4, y, z$<br>(m <sub>x</sub>  1/2, 0, 1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

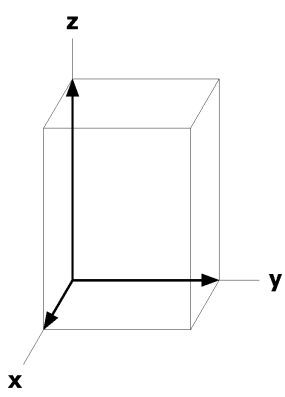
		Coordinates							
Multiplicity, Wyckoff letter, Site Symmetry.									
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}+1/2, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [ $u, \bar{v}, w$ ]	(4) $x+1/2, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]	(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y+1/2, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(7) $x, \bar{y}+1/2, z+1/2$ [ $u, \bar{v}, w$ ]	(8) $\bar{x}+1/2, y, z+1/2$ [ $\bar{u}, v, w$ ]
4	d ..2	1/4,3/4,z [0,0,w]	3/4,1/4, $\bar{z}+1/2$ [0,0,w]	3/4,1/4, $\bar{z}$ [0,0,w]	1/4,3/4,z+1/2 [0,0,w]				
4	c ..2	1/4,1/4,z [0,0,w]	3/4,3/4, $\bar{z}+1/2$ [0,0,w]	3/4,3/4, $\bar{z}$ [0,0,w]	1/4,1/4,z+1/2 [0,0,w]				
4	b $\bar{1}$	0,0,1/2 [u,v,w]	1/2,1/2,1/2 [ $\bar{u}, \bar{v}, w$ ]	0,1/2,0 [ $u, \bar{v}, w$ ]	1/2,0,0 [ $\bar{u}, v, w$ ]				
4	a $\bar{1}$	0,0,0 [u,v,w]	1/2,1/2,0 [ $\bar{u}, \bar{v}, w$ ]	0,1/2,1/2 [ $u, \bar{v}, w$ ]	1/2,0,1/2 [ $\bar{u}, v, w$ ]				

**Symmetry of Special Projections**

Along [0,01] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,1/4,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

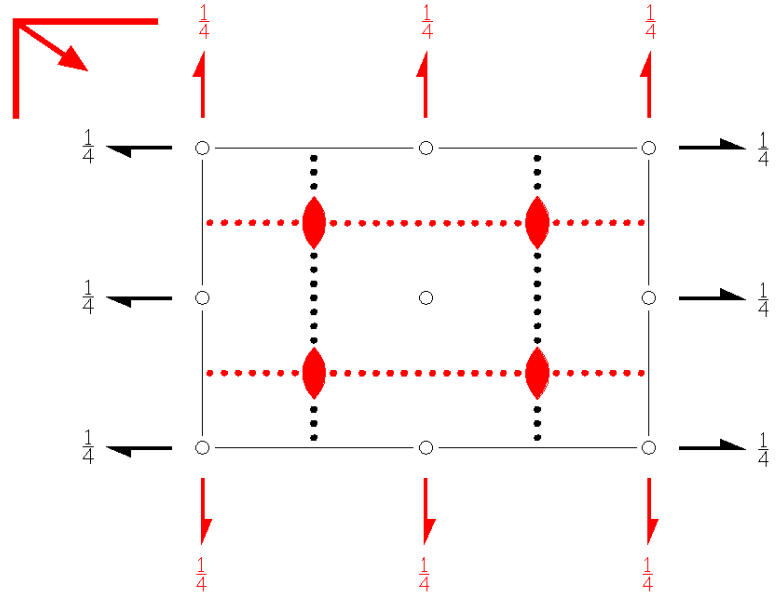
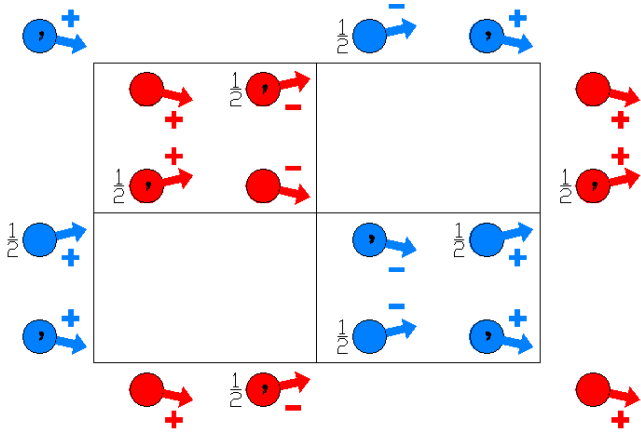
Along [0,1,0] p2'm'g  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pc'cn'  
56.6.456

m'mm'  
P2<sub>1</sub>'/c'2<sub>1</sub>/c2'/n'

Orthorhombic



Origin at  $\bar{1}$  on 11n'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2' $1/4, 1/4, z$<br>(2 <sub>z</sub>  1/2, 1/2, 0)'           | (3) 2 (0, 1/2, 0) $0, y, 1/4$<br>(2 <sub>y</sub>  0, 1/2, 1/2) | (4) 2' (1/2, 0, 0) $x, 0, 1/4$<br>(2 <sub>x</sub>  1/2, 0, 1/2)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) n' (1/2, 1/2, 0) $x, y, 0$<br>(m <sub>z</sub>  1/2, 1/2, 0)' | (7) c (0, 0, 1/2) $x, 1/4, z$<br>(m <sub>y</sub>  0, 1/2, 1/2) | (8) c' (0, 0, 1/2) $1/4, y, z$<br>(m <sub>x</sub>  1/2, 0, 1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

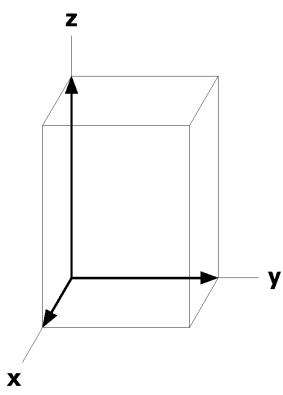
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}+1/2, z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x+1/2, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]
		(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y+1/2, \bar{z}$ [u,v, $\bar{w}$ ]	(7) $x, \bar{y}+1/2, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(8) $\bar{x}+1/2, y, z+1/2$ [ $\bar{u}, v, w$ ]
4	d ..2'	1/4,3/4,z [u,v,0]	3/4,1/4, $\bar{z}+1/2$ [ $\bar{u}, v, 0$ ]	3/4,1/4, $\bar{z}$ [u,v,0]	1/4,3/4,z+1/2 [ $\bar{u}, v, 0$ ]
4	c ..2'	1/4,1/4,z [u,v,0]	3/4,3/4, $\bar{z}+1/2$ [ $\bar{u}, v, 0$ ]	3/4,3/4, $\bar{z}$ [u,v,0]	1/4,1/4,z+1/2 [ $\bar{u}, v, 0$ ]
4	b $\bar{1}$	0,0,1/2 [u,v,w]	1/2,1/2,1/2 [u,v, $\bar{w}$ ]	0,1/2,0 [ $\bar{u}, v, \bar{w}$ ]	1/2,0,0 [ $\bar{u}, v, w$ ]
4	a $\bar{1}$	0,0,0 [u,v,w]	1/2,1/2,0 [u,v, $\bar{w}$ ]	0,1/2,1/2 [ $\bar{u}, v, \bar{w}$ ]	1/2,0,1/2 [ $\bar{u}, v, w$ ]

**Symmetry of Special Projections**

Along [0,01] c2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 1/4,1/4,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

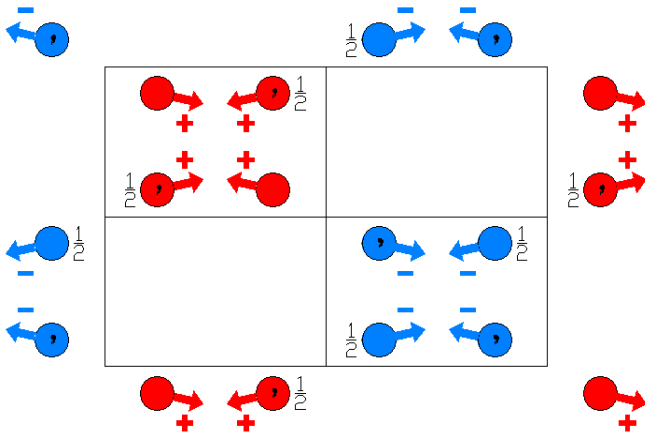
Along [0,1,0] p<sub>2b</sub>'2mg  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pc'c'n'  
56.7.457

m'm'm'  
P2<sub>1</sub>/c'2<sub>1</sub>/c'2/n'

Orthorhombic

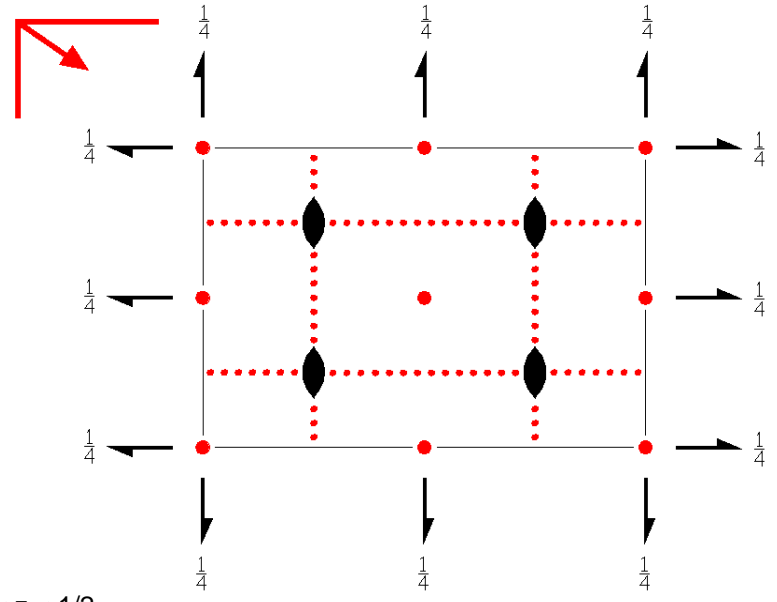


Origin at  $\bar{1}'$  on 11n'

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $1/4, 1/4, z$<br>(2 <sub>z</sub>  1/2, 1/2, 0)             | (3) 2 (0, 1/2, 0) $0, y, 1/4$<br>(2 <sub>y</sub>  0, 1/2, 1/2) | (4) 2 (1/2, 0, 0) $x, 0, 1/4$<br>(2 <sub>x</sub>  1/2, 0, 1/2) |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) n' (1/2, 1/2, 0) $x, y, 0$<br>(m <sub>z</sub>  1/2, 1/2, 0)' | (7) c' (0,0,1/2) $x, 1/4, z$<br>(m <sub>y</sub>  0, 1/2, 1/2)' | (8) c' (0,0,1/2) $1/4, y, z$<br>(m <sub>x</sub>  1/2, 0, 1/2)' |





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

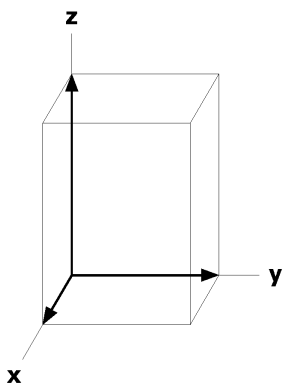
		Coordinates							
Multiplicity, Wyckoff letter, Site Symmetry.									
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}+1/2, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x+1/2, \bar{y}, \bar{z}+1/2$ [ $u, \bar{v}, \bar{w}$ ]	(5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(6) $x+1/2, y+1/2, \bar{z}$ [ $u, v, \bar{w}$ ]	(7) $x, \bar{y}+1/2, z+1/2$ [ $u, \bar{v}, w$ ]	(8) $\bar{x}+1/2, y, z+1/2$ [ $\bar{u}, v, w$ ]
4	d ..2	1/4,3/4,z [0,0,w]	3/4,1/4, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	3/4,1/4, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,3/4,z+1/2 [0,0,w]				
4	c ..2	1/4,1/4,z [0,0,w]	3/4,3/4, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	3/4,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,1/4,z+1/2 [0,0,w]				
4	b $\bar{1}'$	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]				
4	a $\bar{1}'$	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]				

### Symmetry of Special Projections

Along [0,01] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,1/4,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

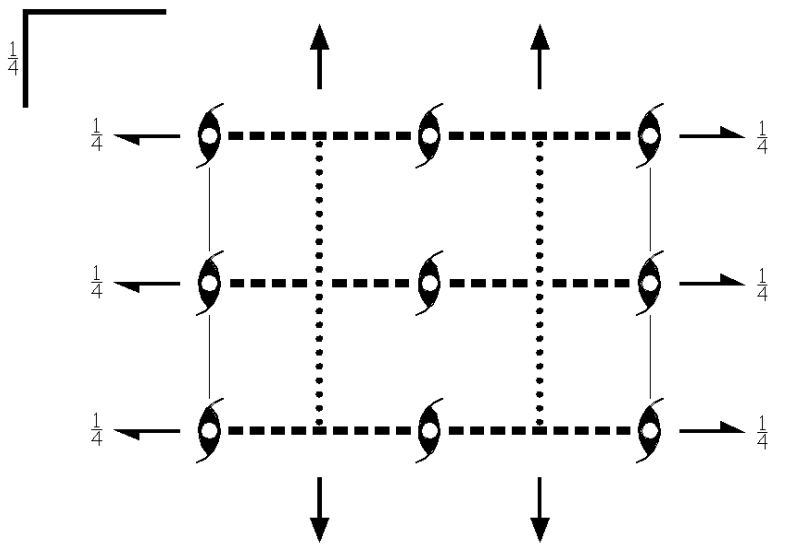
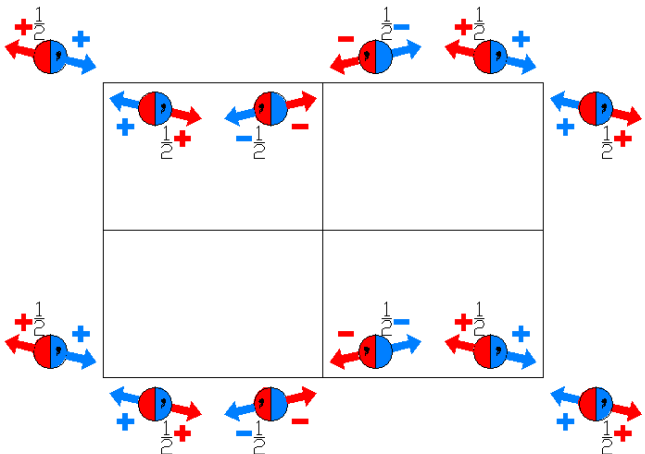
Along [0,1,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pbcm  
57.1.458

mmm  
P2/b<sub>2</sub><sub>1</sub>/c<sub>2</sub><sub>1</sub>/m

Orthorhombic



Origin at  $\bar{1}$  on b<sub>12</sub>

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2) | (4) 2 x,1/4,0<br>(2 <sub>x</sub>  0,1/2,0)         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,1/4<br>(m <sub>z</sub>  0,0,1/2)         | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2) | (8) b (0,1/2,0) 0,y,z<br>(m <sub>x</sub>  0,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

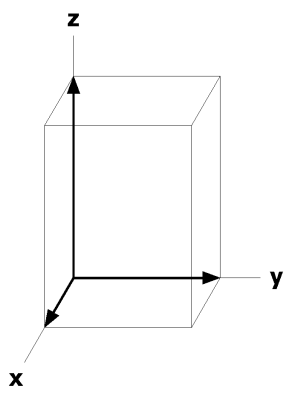
		Coordinates							
Multiplicity, Wyckoff letter, Site Symmetry.									
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(5) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(6) $x,y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]
4	d ..m	x,y,1/4 [0,0,w]	$\bar{x},\bar{y},3/4$ [0,0,w]	$\bar{x},y+1/2,1/4$ [0,0, $\bar{w}$ ]	$x,\bar{y}+1/2,3/4$ [0,0, $\bar{w}$ ]				
4	c 2..	x,1/4,0 [u,0,0]	$\bar{x},3/4,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},3/4,0$ [u,0,0]	x,1/4,1/2 [ $\bar{u},0,0$ ]				
4	b $\bar{1}$	1/2,0,0 [u,v,w]	1/2,0,1/2 [ $\bar{u},\bar{v},w$ ]	1/2,1/2,1/2 [ $\bar{u},v,\bar{w}$ ]	1/2,1/2,0 [u, $\bar{v},\bar{w}$ ]				
4	a $\bar{1}$	0,0,0 [u,v,w]	0,0,1/2 [ $\bar{u},\bar{v},w$ ]	0,1/2,1/2 [ $\bar{u},v,\bar{w}$ ]	0,1/2,0 [u, $\bar{v},\bar{w}$ ]				

**Symmetry of Special Projections**

Along [0,01]  $p2mg1'$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b}2mg$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,1/4,0

Along [0,1,0]  $p_{2a}2mm$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



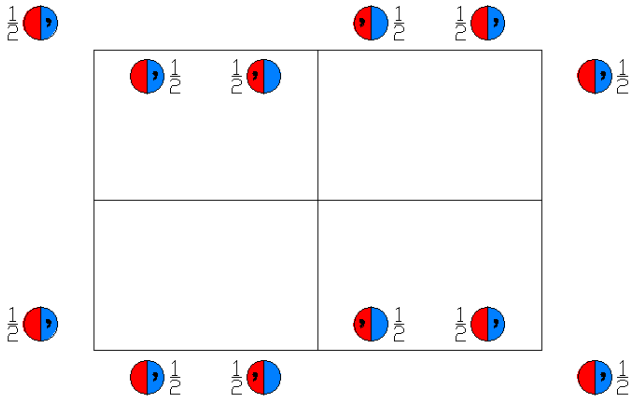
Pbcm1'

57.2.459

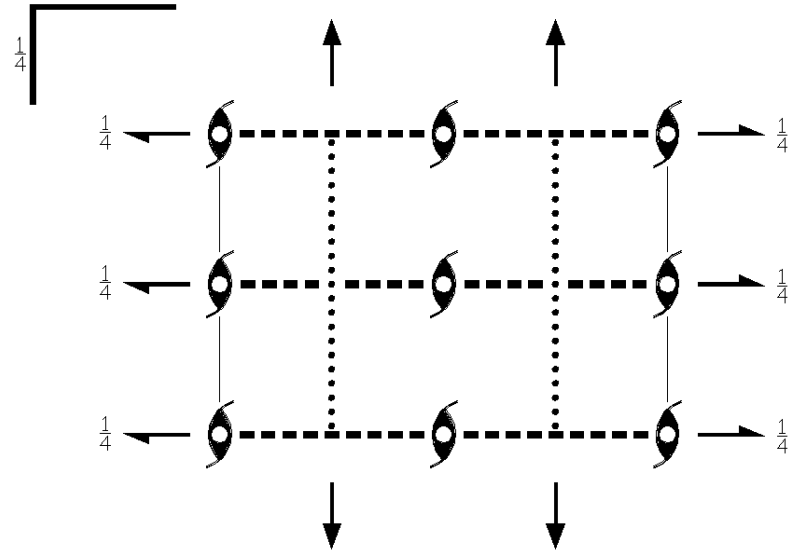
mmm1'

P2/b2<sub>1</sub>/c2<sub>1</sub>/m1'

Orthorhombic



1'



Origin at  $\bar{1}1'$  on b12,1'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

For 1 + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2) | (4) 2 x,1/4,0<br>(2 <sub>x</sub>  0,1/2,0)         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,1/4<br>(m <sub>z</sub>  0,0,1/2)         | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2) | (8) b (0,1/2,0) 0,y,z<br>(m <sub>x</sub>  0,1/2,0) |

For 1' + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1'<br>(1 0,0,0)'                         | (2) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)' | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2' x,1/4,0<br>(2 <sub>x</sub>  0,1/2,0)'         |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,1/4<br>(m <sub>z</sub>  0,0,1/2)'         | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) b' (0,1/2,0) 0,y,z<br>(m <sub>x</sub>  0,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

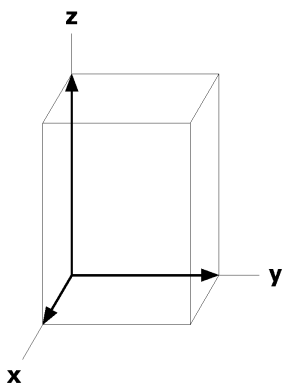
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +	1 +	1' +	1' +
8 e 11'	(1) x,y,z [0,0,0] (5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(2) $\bar{x},\bar{y},z+1/2$ [0,0,0] (6) x,y, $\bar{z}+1/2$ [0,0,0]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [0,0,0] (7) x, $\bar{y}+1/2,z+1/2$ [0,0,0]	(4) x, $\bar{y}+1/2,\bar{z}$ [0,0,0] (8) $\bar{x},y+1/2,z$ [0,0,0]
4 d ..m1'	x,y,1/4 [0,0,0]	$\bar{x},\bar{y},3/4$ [0,0,0]	$\bar{x},y+1/2,1/4$ [0,0,0]	x, $\bar{y}+1/2,3/4$ [0,0,0]
4 c 2..1'	x,1/4,0 [0,0,0]	$\bar{x},3/4,1/2$ [0,0,0]	$\bar{x},3/4,0$ [0,0,0]	x,1/4,1/2 [0,0,0]
4 b $\bar{1}1'$	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
4 a $\bar{1}1'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	0,1/2,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,01] p2mg1'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

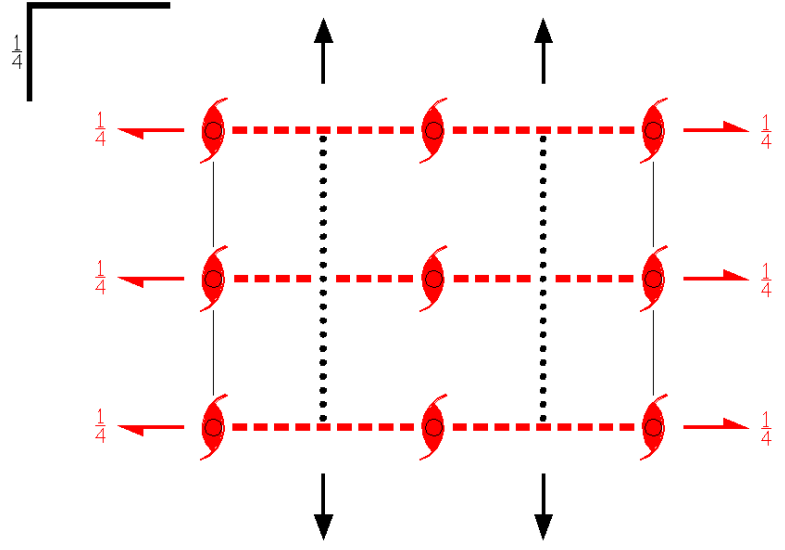
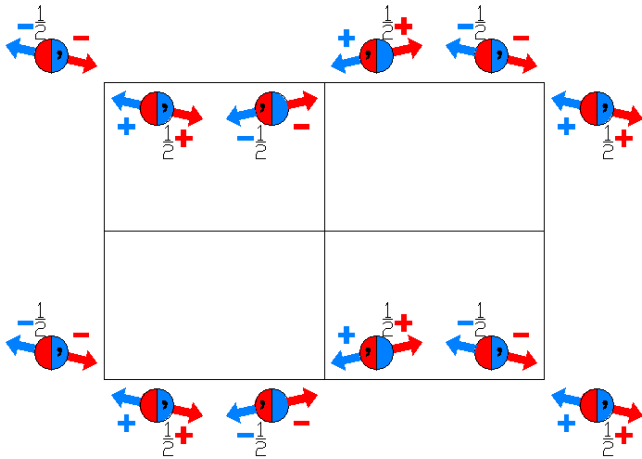
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pb'cm  
57.3.460

m'mm  
P2/b'2<sub>1</sub>'/c2<sub>1</sub>'/m

Orthorhombic



Origin at  $\bar{1}'$  on  $b'12_1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)' | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2 x,1/4,0<br>(2 <sub>x</sub>  0,1/2,0)           |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m x,y,1/4<br>(m <sub>z</sub>  0,0,1/2)           | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)   | (8) b' (0,1/2,0) 0,y,z<br>(m <sub>x</sub>  0,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

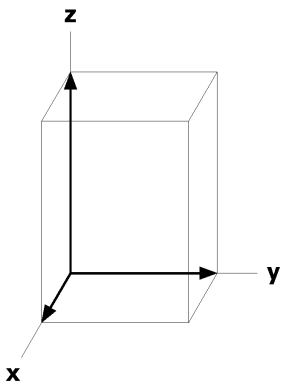
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	e 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) $x,\bar{y}+1/2,\bar{z}$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y+1/2,z$ [ $\bar{u},v,w$ ]
4	d ..m	$x,y,1/4$ [0,0,w]	$\bar{x},\bar{y},3/4$ [0,0, $\bar{w}$ ]	$\bar{x},y+1/2,1/4$ [0,0,w]	$x,\bar{y}+1/2,3/4$ [0,0, $\bar{w}$ ]
4	c 2..	$x,1/4,0$ [u,0,0]	$\bar{x},3/4,1/2$ [u,0,0]	$\bar{x},3/4,0$ [ $\bar{u},0,0$ ]	$x,1/4,1/2$ [ $\bar{u},0,0$ ]
4	b $\bar{1}'$	$1/2,0,0$ [0,0,0]	$1/2,0,1/2$ [0,0,0]	$1/2,1/2,1/2$ [0,0,0]	$1/2,1/2,0$ [0,0,0]
4	a $\bar{1}'$	$0,0,0$ [0,0,0]	$0,0,1/2$ [0,0,0]	$0,1/2,1/2$ [0,0,0]	$0,1/2,0$ [0,0,0]

**Symmetry of Special Projections**

Along [0,01]  $p2mg1'$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0]  $p2mg$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

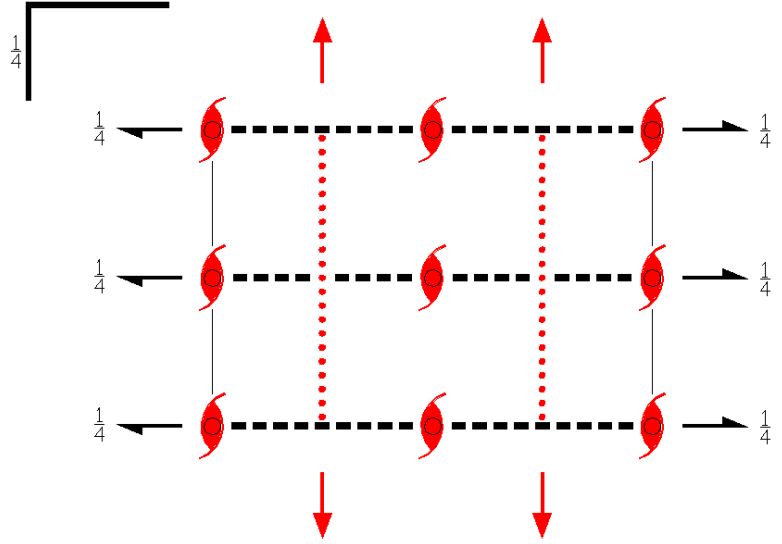
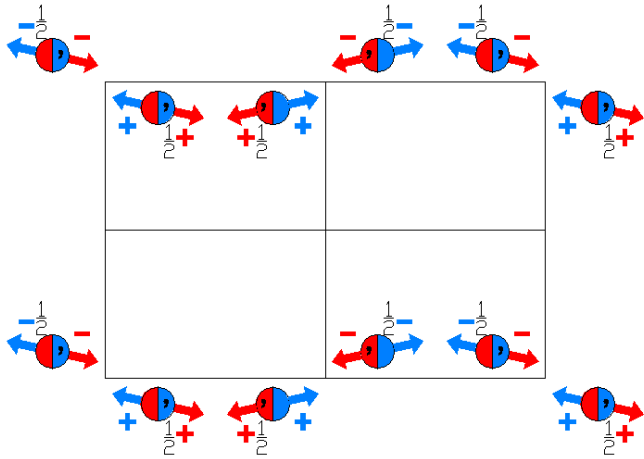
Along [0,1,0]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pbc'm  
57.4.461

mm'm  
P2'/b2<sub>1</sub>/c'2<sub>1</sub>'/m

Orthorhombic



Origin at  $\bar{1}'$  on  $b12_1'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)' | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2' x,1/4,0<br>(2 <sub>x</sub>  0,1/2,0)'       |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m x,y,1/4<br>(m <sub>z</sub>  0,0,1/2)           | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) b (0,1/2,0) 0,y,z<br>(m <sub>x</sub>  0,1/2,0) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

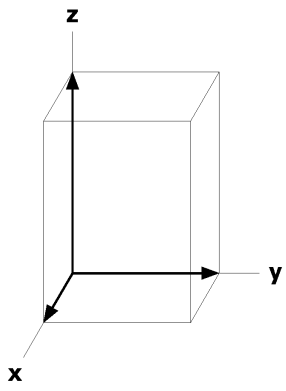
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	e 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y}+1/2,z+1/2$ [u, $\bar{v},w$ ]	(8) $\bar{x},y+1/2,z$ [u, $\bar{v},\bar{w}$ ]
4	d ..m	$x,y,1/4$ [0,0,w]	$\bar{x},\bar{y},3/4$ [0,0, $\bar{w}$ ]	$\bar{x},y+1/2,1/4$ [0,0, $\bar{w}$ ]	$x,\bar{y}+1/2,3/4$ [0,0,w]
4	c 2'..	$x,1/4,0$ [0,v,w]	$\bar{x},3/4,1/2$ [0,v, $\bar{w}$ ]	$\bar{x},3/4,0$ [0, $\bar{v},\bar{w}$ ]	$x,1/4,1/2$ [0, $\bar{v},w$ ]
4	b $\bar{1}'$	$1/2,0,0$ [0,0,0]	$1/2,0,1/2$ [0,0,0]	$1/2,1/2,1/2$ [0,0,0]	$1/2,1/2,0$ [0,0,0]
4	a $\bar{1}'$	$0,0,0$ [0,0,0]	$0,0,1/2$ [0,0,0]	$0,1/2,1/2$ [0,0,0]	$0,1/2,0$ [0,0,0]

**Symmetry of Special Projections**

Along [0,01]  $p2mg1'$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b}2mg$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

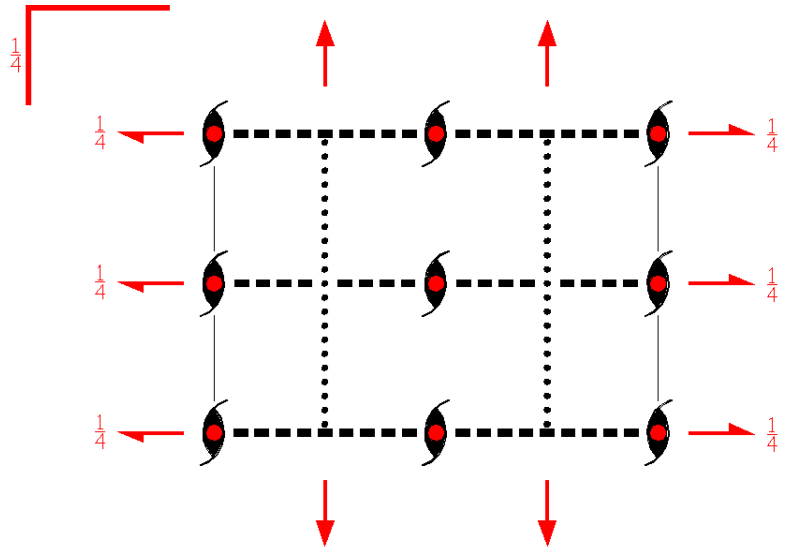
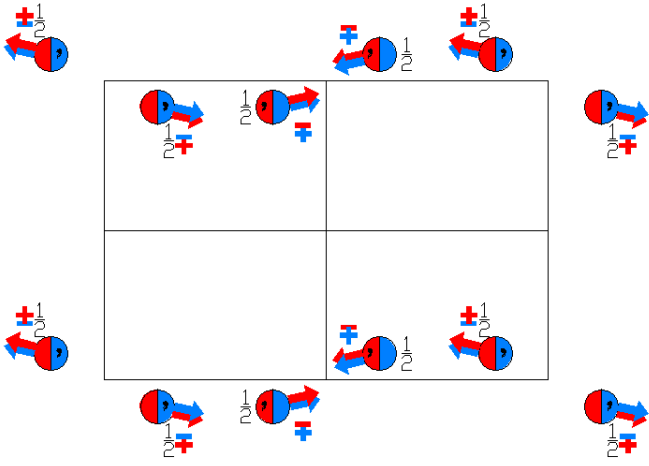
Along [0,1,0]  $p2mm$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pbcm'  
57.5.462

mmm'  
P2'/b2<sub>1</sub>'/c2<sub>1</sub>'/m'

Orthorhombic



Origin at  $\bar{1}'$  on b12<sub>1</sub>

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2' x,1/4,0<br>(2 <sub>x</sub>  0,1/2,0)'       |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,1/4<br>(m <sub>z</sub>  0,0,1/2)'       | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)   | (8) b (0,1/2,0) 0,y,z<br>(m <sub>x</sub>  0,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

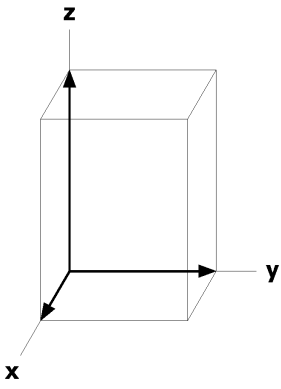
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	e 1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) $x, \bar{y}+1/2, \bar{z}$ [ $\bar{u}, v, w$ ]
		(5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(6) $x, y, \bar{z}+1/2$ [u,v, $\bar{w}$ ]	(7) $x, \bar{y}+1/2, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(8) $\bar{x}, y+1/2, z$ [u, $\bar{v}, \bar{w}$ ]
4	d ..m'	$x, y, 1/4$ [u,v,0]	$\bar{x}, \bar{y}, 3/4$ [ $\bar{u}, \bar{v}, 0$ ]	$\bar{x}, y+1/2, 1/4$ [u, $\bar{v}, 0$ ]	$x, \bar{y}+1/2, 3/4$ [ $\bar{u}, v, 0$ ]
4	c 2'..	$x, 1/4, 0$ [0,v,w]	$\bar{x}, 3/4, 1/2$ [0, $\bar{v}, w$ ]	$\bar{x}, 3/4, 0$ [0, $\bar{v}, \bar{w}$ ]	$x, 1/4, 1/2$ [0,v, $\bar{w}$ ]
4	b $\bar{1}'$	$1/2, 0, 0$ [0,0,0]	$1/2, 0, 1/2$ [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]	$1/2, 1/2, 0$ [0,0,0]
4	a $\bar{1}'$	$0, 0, 0$ [0,0,0]	$0, 0, 1/2$ [0,0,0]	$0, 1/2, 1/2$ [0,0,0]	$0, 1/2, 0$ [0,0,0]

**Symmetry of Special Projections**

Along [0,01]  $p2mg$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b} 2mg$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x, 1/4, 0$

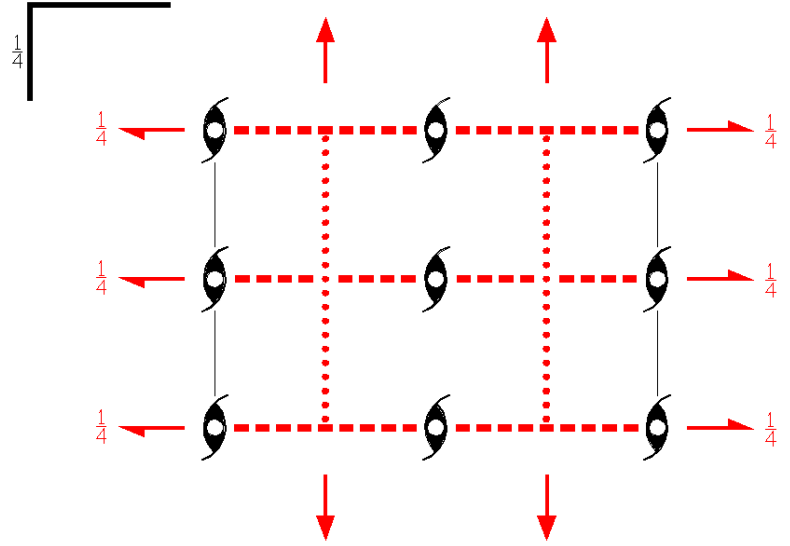
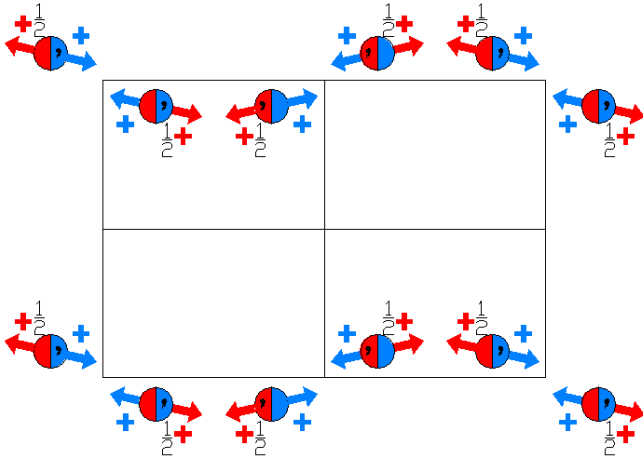
Along [0,1,0]  $p_{2a} 2mm$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pb'c'm  
57.6.463

m'm'm  
P2'/b'2<sub>1</sub>'/c'2<sub>1</sub>/m

Orthorhombic



Origin at  $\bar{1}$  on b'12<sub>1</sub>

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2' x,1/4,0<br>(2 <sub>x</sub>  0,1/2,0)'         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,1/4<br>(m <sub>z</sub>  0,0,1/2)         | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) b' (0,1/2,0) 0,y,z<br>(m <sub>x</sub>  0,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

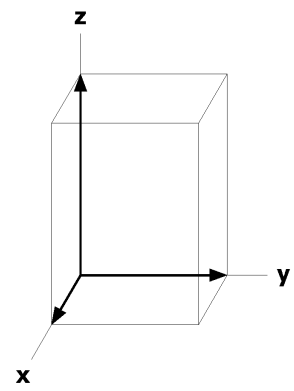
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(4) $x,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) $x,y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(8) $\bar{x},y+1/2,z$ [ $\bar{u},v,w$ ]
4	d ..m	x,y,1/4 [0,0,w]	$\bar{x},\bar{y},3/4$ [0,0,w]	$\bar{x},y+1/2,1/4$ [0,0,w]	$x,\bar{y}+1/2,3/4$ [0,0,w]
4	c 2'..	x,1/4,0 [0,v,w]	$\bar{x},3/4,1/2$ [0, $\bar{v},w$ ]	$\bar{x},3/4,0$ [0,v,w]	$x,1/4,1/2$ [0, $\bar{v},w$ ]
4	b $\bar{1}$	1/2,0,0 [u,v,w]	1/2,0,1/2 [ $\bar{u},\bar{v},w$ ]	1/2,1/2,1/2 [ $u,\bar{v},w$ ]	1/2,1/2,0 [ $\bar{u},v,w$ ]
4	a $\bar{1}$	0,0,0 [u,v,w]	0,0,1/2 [ $\bar{u},\bar{v},w$ ]	0,1/2,1/2 [ $u,\bar{v},w$ ]	0,1/2,0 [ $\bar{u},v,w$ ]

**Symmetry of Special Projections**

Along [0,01] p2mg1'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

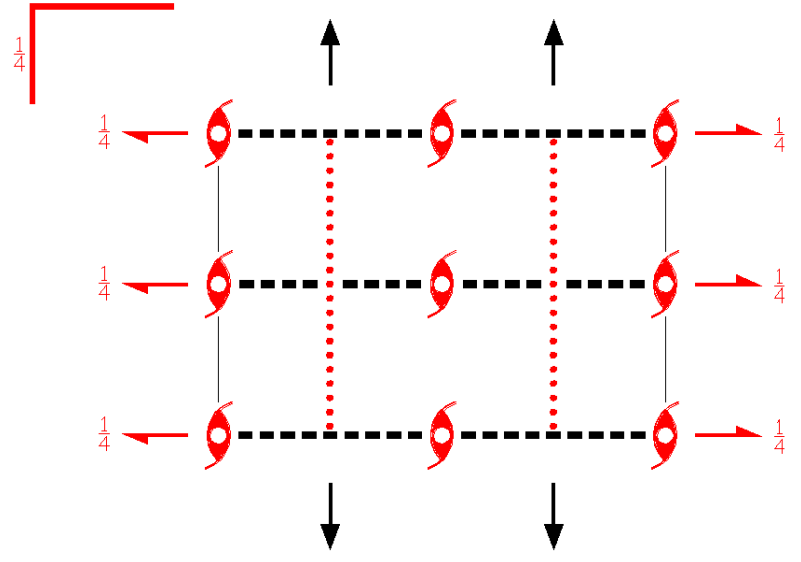
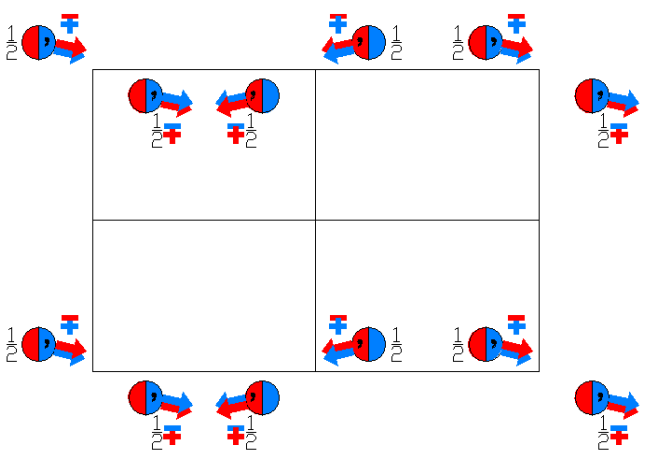
Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pbc'm'  
57.7.464

mm'm'  
P2/b2<sub>1</sub>'/c'2<sub>1</sub>'/m'

Orthorhombic



Origin at  $\bar{1}$  on b12<sub>1</sub>'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)' | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2 x,1/4,0<br>(2 <sub>x</sub>  0,1/2,0)         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m' x,y,1/4<br>(m <sub>z</sub>  0,0,1/2)'         | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) b (0,1/2,0) 0,y,z<br>(m <sub>x</sub>  0,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

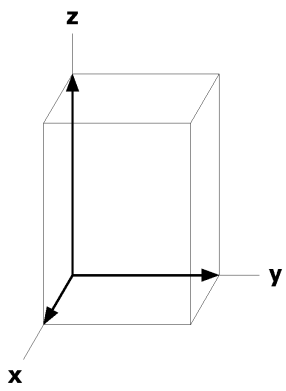
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) $x,\bar{y}+1/2,\bar{z}$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) $x,y,\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(7) $x,\bar{y}+1/2,z+1/2$ [u, $\bar{v}$ ,w]	(8) $\bar{x},y+1/2,z$ [u, $\bar{v},\bar{w}$ ]
4	d ..m'	x,y,1/4 [u,v,0]	$\bar{x},\bar{y},3/4$ [u,v,0]	$\bar{x},y+1/2,1/4$ [u, $\bar{v}$ ,0]	$x,\bar{y}+1/2,3/4$ [u, $\bar{v}$ ,0]
4	c 2..	x,1/4,0 [u,0,0]	$\bar{x},3/4,1/2$ [u,0,0]	$\bar{x},3/4,0$ [u,0,0]	x,1/4,1/2 [u,0,0]
4	b $\bar{1}$	1/2,0,0 [u,v,w]	1/2,0,1/2 [u,v, $\bar{w}$ ]	1/2,1/2,1/2 [u, $\bar{v}$ ,w]	1/2,1/2,0 [u, $\bar{v},\bar{w}$ ]
4	a $\bar{1}$	0,0,0 [u,v,w]	0,0,1/2 [u,v, $\bar{w}$ ]	0,1/2,1/2 [u, $\bar{v}$ ,w]	0,1/2,0 [u, $\bar{v},\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,01] p2'm'g  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>'2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,1/4,0

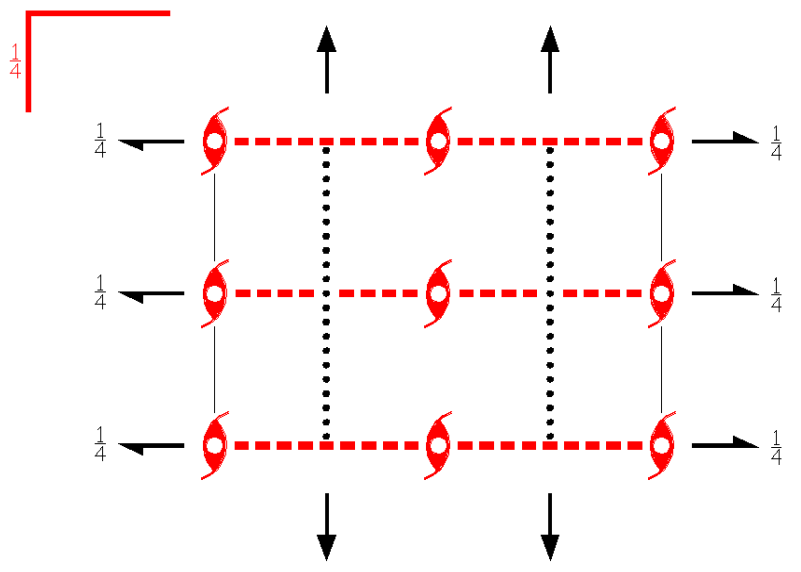
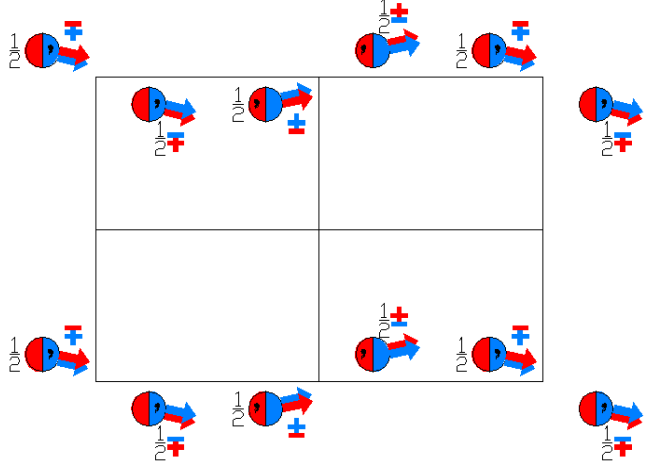
Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pb'cm'  
57.8.465

m'mm'  
P2'/b'2<sub>1</sub>/c2<sub>1</sub>'/m'

Orthorhombic



Origin at  $\bar{1}$  on b'12,'

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)' | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2) | (4) 2' x,1/4,0<br>(2 <sub>x</sub>  0,1/2,0)'         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m' x,y,1/4<br>(m <sub>z</sub>  0,0,1/2)'         | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2) | (8) b' (0,1/2,0) 0,y,z<br>(m <sub>x</sub>  0,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

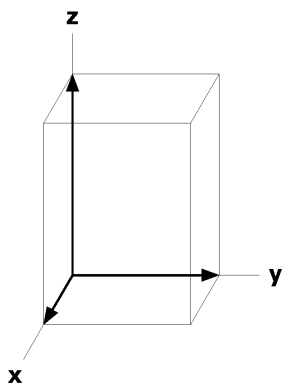
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) $x,y,\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(7) $x,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y+1/2,z$ [ $\bar{u},v,w$ ]
4	d ..m'	x,y,1/4 [u,v,0]	$\bar{x},\bar{y},3/4$ [u,v,0]	$\bar{x},y+1/2,1/4$ [ $\bar{u},v,0$ ]	$x,\bar{y}+1/2,3/4$ [ $\bar{u},v,0$ ]
4	c 2'..	x,1/4,0 [0,v,w]	$\bar{x},3/4,1/2$ [0,v, $\bar{w}$ ]	$\bar{x},3/4,0$ [0,v,w]	x,1/4,1/2 [0,v, $\bar{w}$ ]
4	b $\bar{1}$	1/2,0,0 [u,v,w]	1/2,0,1/2 [u,v, $\bar{w}$ ]	1/2,1/2,1/2 [ $\bar{u},v,\bar{w}$ ]	1/2,1/2,0 [ $\bar{u},v,w$ ]
4	a $\bar{1}$	0,0,0 [u,v,w]	0,0,1/2 [u,v, $\bar{w}$ ]	0,1/2,1/2 [ $\bar{u},v,\bar{w}$ ]	0,1/2,0 [ $\bar{u},v,w$ ]

**Symmetry of Special Projections**

Along [0,01] p2'mg'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>'2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



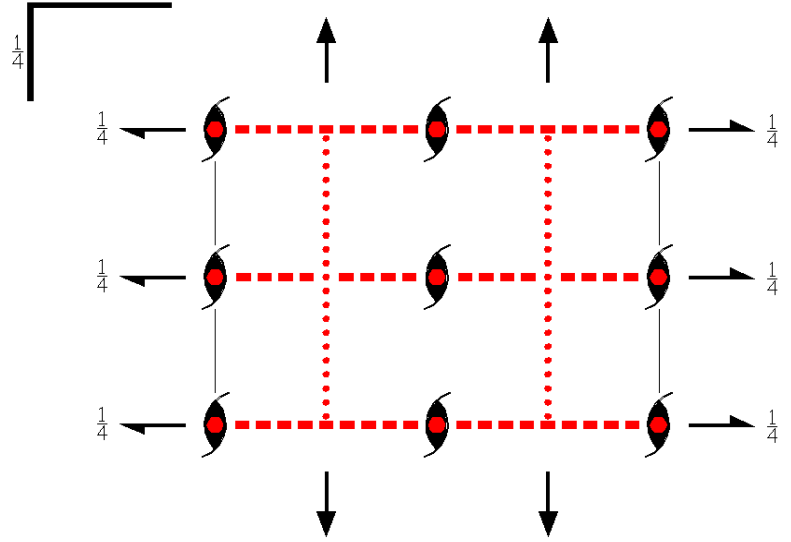
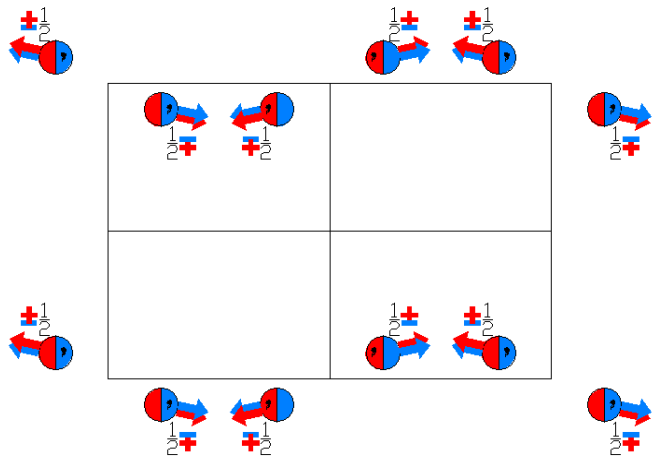
Pb'c'm'

57.9.466

m'm'm'

P2/b'2<sub>1</sub>/c'2<sub>1</sub>/m'

Orthorhombic



Origin at  $\bar{1}'$  on  $b'12_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2 x,1/4,0<br>(2 <sub>x</sub>  0,1/2,0)           |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,1/4<br>(m <sub>z</sub>  0,0,1/2)'       | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) b' (0,1/2,0) 0,y,z<br>(m <sub>x</sub>  0,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

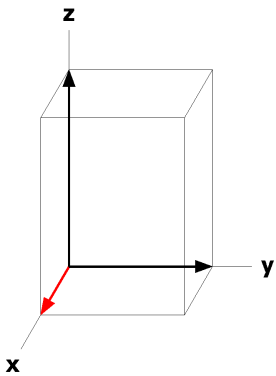
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,y,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]	(7) $x,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(8) $\bar{x},y+1/2,z$ [ $\bar{u},v,w$ ]
4	d ..m'	x,y,1/4 [u,v,0]	$\bar{x},\bar{y},3/4$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y+1/2,1/4$ [ $\bar{u},v,0$ ]	$x,\bar{y}+1/2,3/4$ [ $u,\bar{v},0$ ]
4	c 2..	x,1/4,0 [u,0,0]	$\bar{x},3/4,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},3/4,0$ [ $\bar{u},0,0$ ]	x,1/4,1/2 [u,0,0]
4	b $\bar{1}'$	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
4	a $\bar{1}'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	0,1/2,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,01] p2m'g'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

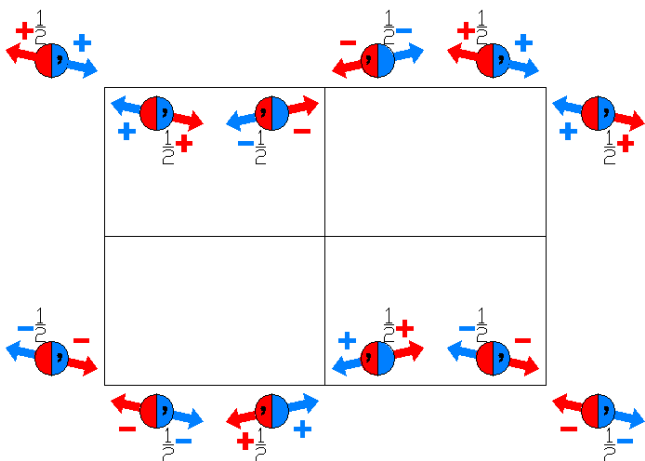
Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



$P_{2a}bcm$   
57.10.467

$mmm1'$   
 $P_{2a}2/b2_1/c2_1/m$

Orthorhombic



Origin at  $\bar{1}$  on  $b12$ ,

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

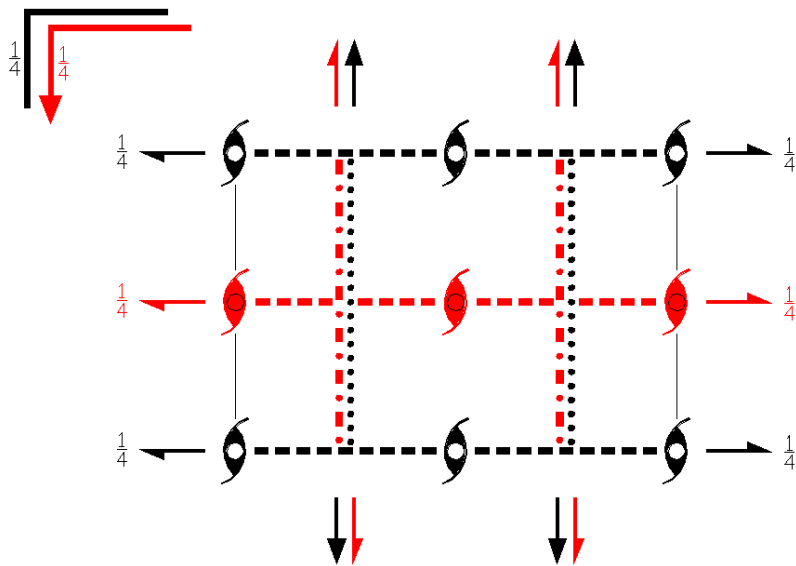
### Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $(0,0,1/2)$ $0,0,z$<br>( $2_z$  0,0,1/2) | (3) 2 $(0,1/2,0)$ $0,y,1/4$<br>( $2_y$  0,1/2,1/2) | (4) 2 $x,1/4,0$<br>( $2_x$  0,1/2,0)           |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0) | (6) m $x,y,1/4$<br>( $m_z$  0,0,1/2)           | (7) c $(0,0,1/2)$ $x,1/4,z$<br>( $m_y$  0,1/2,1/2) | (8) b $(0,1/2,0)$ $0,y,z$<br>( $m_x$  0,1/2,0) |

For  $(1,0,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1,0,0)$<br>(1 1,0,0)'                 | (2) $2'$ $(0,0,1/2)$ $1/2,0,z$<br>( $2_z$  1,0,1/2)' | (3) $2'$ $(0,1/2,0)$ $1/2,y,1/4$<br>( $2_y$  1,1/2,1/2)' | (4) $2'$ $(1,0,0)$ $x,1/4,0$<br>( $2_x$  1,1/2,0)'   |
| (5) $\bar{1}'$ $1/2,0,0$<br>( $\bar{1}$  1,0,0)' | (6) $a'$ $(1,0,0)$ $x,y,1/4$<br>( $m_z$  1,0,1/2)'   | (7) $n'$ $(1,0,1/2)$ $x,1/4,z$<br>( $m_y$  1,1/2,1/2)'   | (8) $b'$ $(0,1/2,0)$ $1/2,y,z$<br>( $m_x$  1,1/2,0)' |



**Generators selected** (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

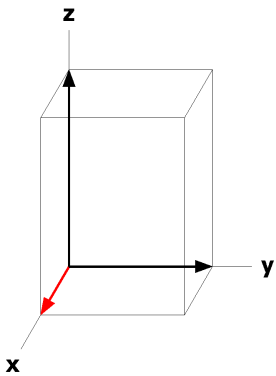
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(6) $x,y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]
8 d ..m	x,y,1/4 [0,0,w]	$\bar{x},\bar{y},3/4$ [0,0,w]	$\bar{x},y+1/2,1/4$ [0,0, $\bar{w}$ ]	$x,\bar{y}+1/2,3/4$ [0,0, $\bar{w}$ ]
8 c 2..	x,1/4,0 [u,0,0]	$\bar{x},3/4,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},3/4,0$ [u,0,0]	x,1/4,1/2 [ $\bar{u},0,0$ ]
8 b $\bar{1}'$	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
8 a $\bar{1}$	0,0,0 [u,v,w]	0,0,1/2 [ $\bar{u},\bar{v},w$ ]	0,1/2,1/2 [ $\bar{u},v,\bar{w}$ ]	0,1/2,0 [ $u,\bar{v},\bar{w}$ ]

### Symmetry of Special Projections

Along [0,01] p2mg1'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

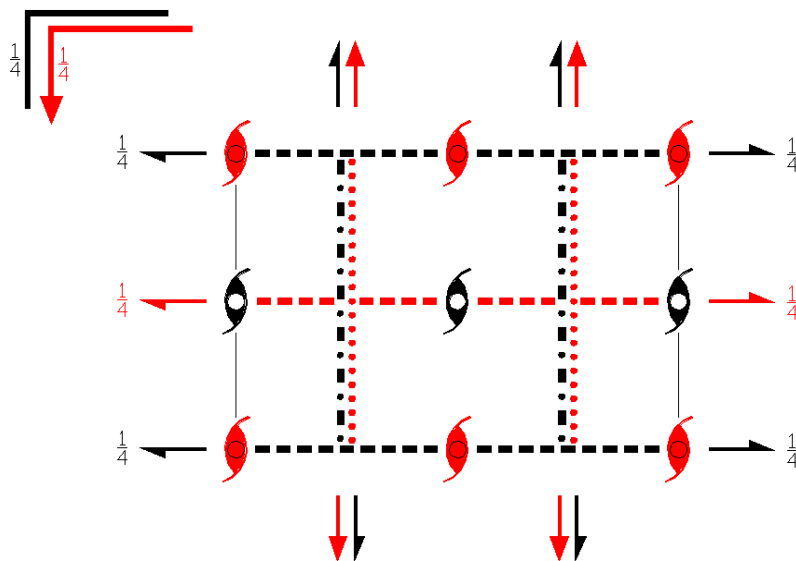
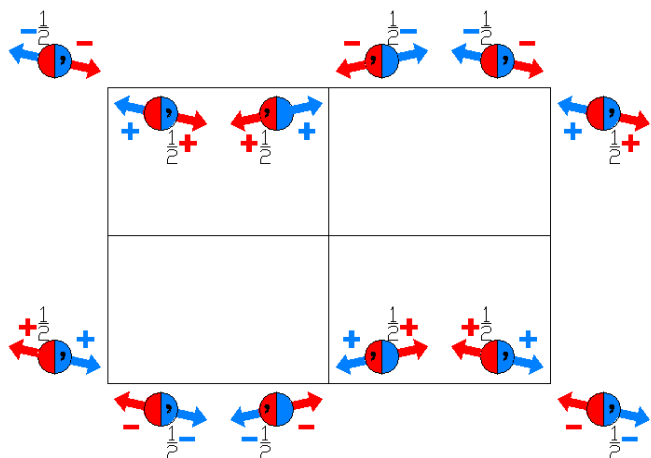
Along [0,1,0] p<sub>c</sub>·2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,1/4



$P_{2a}bc'm$   
57.11.468

$mmm1'$   
 $P_{2a}2'/b2_1/c'2_1'/m$

Orthorhombic



Origin at  $\bar{1}'$  on  $b12_1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) $2'$ $(0,0,1/2)$<br>( $2_z$  0,0,1/2)' | (3) $2$ $(0,1/2,0)$<br>( $2_y$  0,1/2,1/2)   | (4) $2'$ $x,1/4,0$<br>( $2_x$  0,1/2,0)' |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) $m$ $x,y,1/4$<br>( $m_z$  0,0,1/2)     | (7) $c'$ $(0,0,1/2)$<br>( $m_y$  0,1/2,1/2)' | (8) $b$ $(0,1/2,0)$<br>( $m_x$  0,1/2,0) |

For  $(1,0,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1,0,0)$<br>(1 1,0,0)'               | (2) $2$ $(0,0,1/2)$<br>( $2_z$  1,0,1/2) | (3) $2'$ $(0,1/2,0)$<br>( $2_y$  1,1/2,1/2)' | (4) $2$ $(1,0,0)$<br>( $2_x$  1,1/2,0)     |
| (5) $\bar{1}$ $1/2,0,0$<br>( $\bar{1}$  1,0,0) | (6) $a'$ $(1,0,0)$<br>( $m_z$  1,0,1/2)' | (7) $n$ $(1,0,1/2)$<br>( $m_y$  1,1/2,1/2)   | (8) $b'$ $(0,1/2,0)$<br>( $m_x$  1,1/2,0)' |

**Generators selected** (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

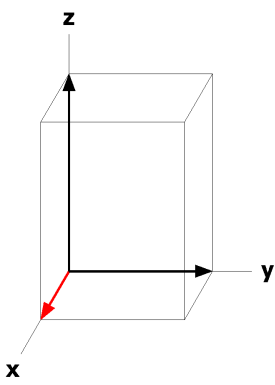
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 e 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y}+1/2,z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y+1/2,z$ [u, $\bar{v},\bar{w}$ ]
8 d ..m	x,y,1/4 [0,0,w]	$\bar{x},\bar{y},3/4$ [0,0, $\bar{w}$ ]	$\bar{x},y+1/2,1/4$ [0,0, $\bar{w}$ ]	x, $\bar{y}+1/2,3/4$ [0,0,w]
8 c 2'..	x,1/4,0 [0,v,w]	$\bar{x},3/4,1/2$ [0,v, $\bar{w}$ ]	$\bar{x},3/4,0$ [0, $\bar{v},\bar{w}$ ]	x,1/4,1/2 [0, $\bar{v},w$ ]
8 b $\bar{1}$	1/2,0,0 [u,v,w]	1/2,0,1/2 [ $\bar{u},\bar{v},w$ ]	1/2,1/2,1/2 [u, $\bar{v},w$ ]	1/2,1/2,0 [ $\bar{u},v,w$ ]
8 a $\bar{1}'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	0,1/2,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,01] p2mg1'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

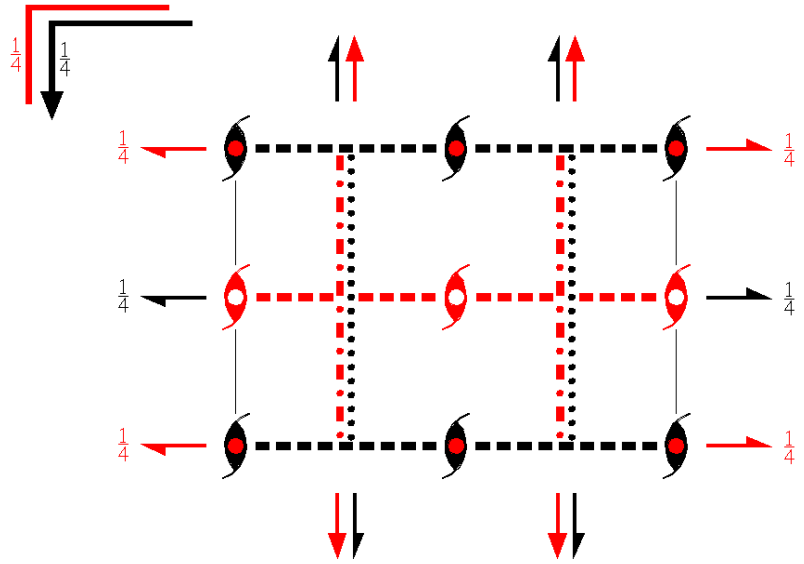
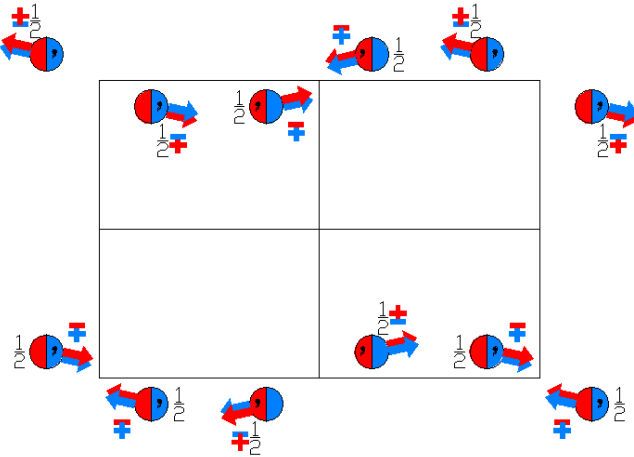
Along [0,1,0] p<sub>2a</sub>'2mm  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$P_{2a}bcm'$   
57.12.469

$mmm1'$   
 $P_{2a}2'/b2_1'/c2_1'/m'$

Orthorhombic



Origin at  $\bar{1}'$  on  $b12_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2' x,1/4,0<br>(2 <sub>x</sub>  0,1/2,0)'       |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,1/4<br>(m <sub>z</sub>  0,0,1/2)'       | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)   | (8) b (0,1/2,0) 0,y,z<br>(m <sub>x</sub>  0,1/2,0) |

For (1,0,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1,0,0)<br>(1 1,0,0)'                 | (2) 2' (0,0,1/2) 1/2,0,z<br>(2 <sub>z</sub>  1,0,1/2)' | (3) 2 (0,1/2,0) 1/2,y,1/4<br>(2 <sub>y</sub>  1,1/2,1/2) | (4) 2 (1,0,0) x,1/4,0<br>(2 <sub>x</sub>  1,1/2,0)     |
| (5) $\bar{1}$ 1/2,0,0<br>( $\bar{1}$  1,0,0) | (6) a (1,0,0) x,y,1/4<br>(m <sub>z</sub>  1,0,1/2)     | (7) n' (1,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1,1/2,1/2)' | (8) b' (0,1/2,0) 1/2,y,z<br>(m <sub>x</sub>  1,1/2,0)' |



**Generators selected** (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

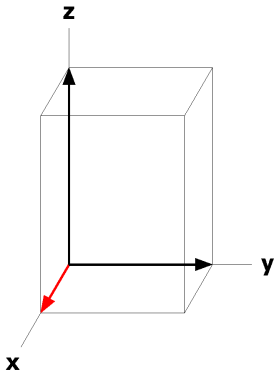
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 e 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ] (7) x, $\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y+1/2,z$ [u, $\bar{v},\bar{w}$ ]
8 d ..m'	x,y,1/4 [u,v,0]	$\bar{x},\bar{y},3/4$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y+1/2,1/4$ [u, $\bar{v},0$ ]	x, $\bar{y}+1/2,3/4$ [ $\bar{u},v,0$ ]
8 c 2'..	x,1/4,0 [0,v,w]	$\bar{x},3/4,1/2$ [0, $\bar{v},w$ ]	$\bar{x},3/4,0$ [0, $\bar{v},\bar{w}$ ]	x,1/4,1/2 [0,v, $\bar{w}$ ]
8 b $\bar{1}$	1/2,0,0 [u,v,w]	1/2,0,1/2 [u,v, $\bar{w}$ ]	1/2,1/2,1/2 [ $\bar{u},v,\bar{w}$ ]	1/2,1/2,0 [ $\bar{u},v,w$ ]
8 a $\bar{1}'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	0,1/2,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,01] p<sub>2b</sub>·2mg  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>c</sub>·2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



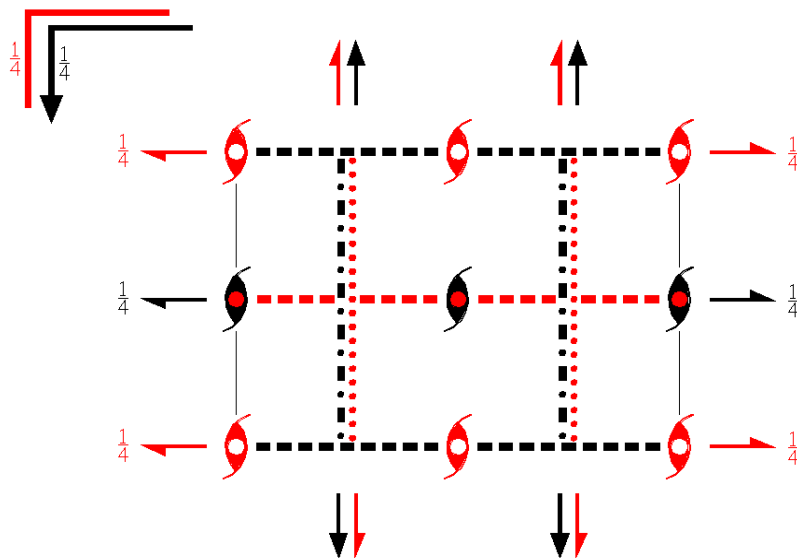
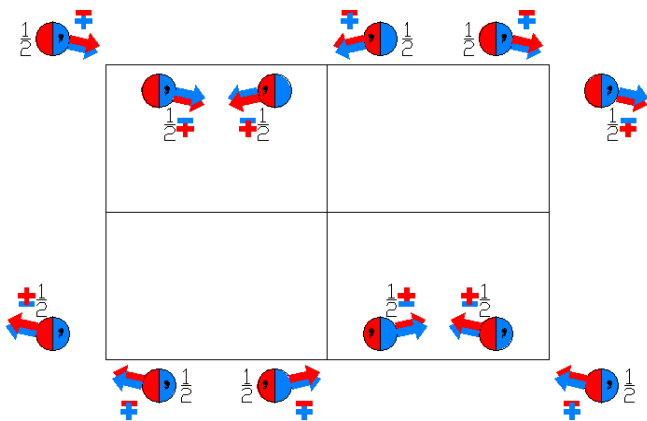
$P_{2a}bc'm'$

57.13.470

$mmm1'$

$P_{2a}2/b2_1'/c'2_1'/m'$

Orthorhombic



Origin at  $\bar{1}$  on  $b12_1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                               | (2) $2' (0,0,1/2) \quad 0,0,z$<br>( $2_z$  0,0,1/2)' | (3) $2' (0,1/2,0) \quad 0,y,1/4$<br>( $2_y$  0,1/2,1/2)' | (4) $2 \quad x,1/4,0$<br>( $2_x$  0,1/2,0)         |
| (5) $\bar{1} \quad 0,0,0$<br>( $\bar{1}$  0,0,0) | (6) $m' \quad x,y,1/4$<br>( $m_z$  0,0,1/2)'         | (7) $c' (0,0,1/2) \quad x,1/4,z$<br>( $m_y$  0,1/2,1/2)' | (8) $b (0,1/2,0) \quad 0,y,z$<br>( $m_x$  0,1/2,0) |

For (1,0,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t' (1,0,0)$<br>(1 1,0,0)'                       | (2) $2 (0,0,1/2) \quad 1/2,0,z$<br>( $2_z$  1,0,1/2) | (3) $2 (0,1/2,0) \quad 1/2,y,1/4$<br>( $2_y$  1,1/2,1/2) | (4) $2' (1,0,0) \quad x,1/4,0$<br>( $2_x$  1,1/2,0)'   |
| (5) $\bar{1}' \quad 1/2,0,0$<br>( $\bar{1}$  1,0,0)' | (6) $a (1,0,0) \quad x,y,1/4$<br>( $m_z$  1,0,1/2)   | (7) $n (1,0,1/2) \quad x,1/4,z$<br>( $m_y$  1,1/2,1/2)   | (8) $b' (0,1/2,0) \quad 1/2,y,z$<br>( $m_x$  1,1/2,0)' |

**Generators selected** (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

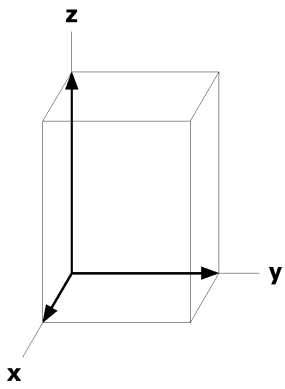
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 e 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) $x,\bar{y}+1/2,\bar{z}$ [u, $\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) $x,y,\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(7) $x,\bar{y}+1/2,z+1/2$ [u, $\bar{v}$ ,w]	(8) $\bar{x},y+1/2,z$ [u, $\bar{v},\bar{w}$ ]
8 d ..m'	x,y,1/4 [u,v,0]	$\bar{x},\bar{y},3/4$ [u,v,0]	$\bar{x},y+1/2,1/4$ [u, $\bar{v}$ ,0]	$x,\bar{y}+1/2,3/4$ [u, $\bar{v}$ ,0]
8 c 2..	x,1/4,0 [u,0,0]	$\bar{x},3/4,1/2$ [u,0,0]	$\bar{x},3/4,0$ [u,0,0]	x,1/4,1/2 [u,0,0]
8 b $\bar{1}'$	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
8 a $\bar{1}$	0,0,0 [u,v,w]	0,0,1/2 [u,v, $\bar{w}$ ]	0,1/2,1/2 [u, $\bar{v}$ ,w]	0,1/2,0 [u, $\bar{v},\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,01] p<sub>2b</sub>'2m'g'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 1/4,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

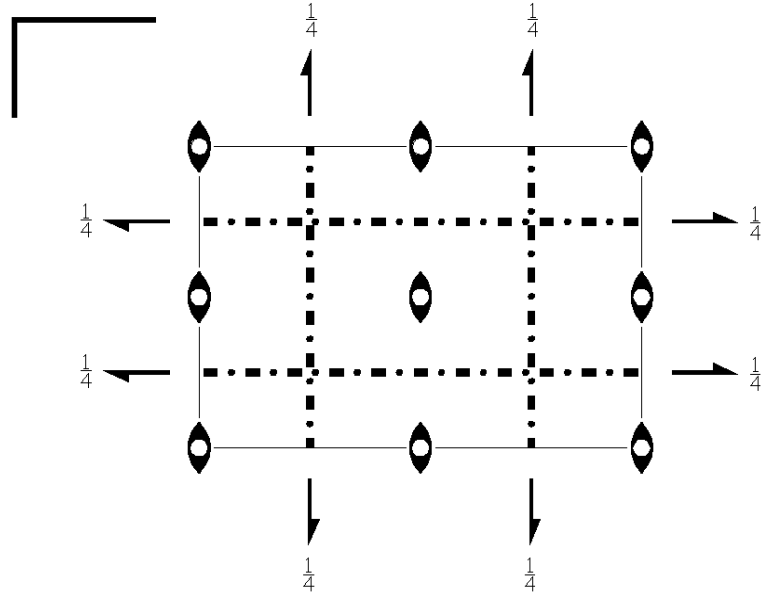
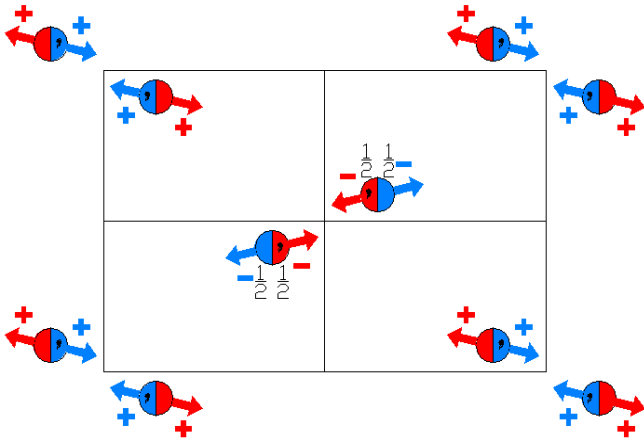
Along [0,1,0] p<sub>2a</sub>'2m'm'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 1/4,y,1/4



Pnmm  
58.1.471

mmm  
 $P2_1/n2_1/n2/m$

Orthorhombic



Origin at center (  $2/m$  )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

- |  |                                  |  |  |
|--|----------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) 2 (0,1/2,0) $1/4,y,1/4$<br>( $2_y$  1/2,1/2,1/2) | (4) 2 (1/2,0,0) $x,1/4,1/4$<br>( $2_x$  1/2,1/2,1/2) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m $x,y,0$<br>( $m_z$  0,0,0) | (7) n (1/2,0,1/2) $x,1/4,z$<br>( $m_y$  1/2,1/2,1/2) | (8) n (0,1/2,1/2) $1/4,y,z$<br>( $m_x$  1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

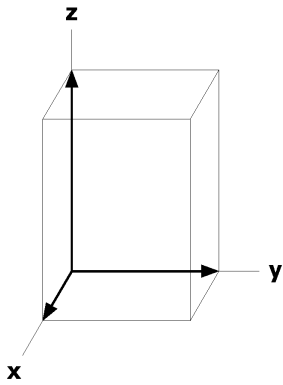
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	h 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z+1/2$ [u, $\bar{v},\bar{w}$ ]
4	g ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x}+1/2,y+1/2,1/2$ [0,0, $\bar{w}$ ]	$x+1/2,\bar{y}+1/2,1/2$ [0,0, $\bar{w}$ ]
4	f ..2	0,1/2,z [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]
4	e ..2	0,0,z [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]
2	d ..2/m	0,1/2,1/2 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]		
2	c ..2/m	0,1/2,0 [0,0,w]	1/2,0,1/2 [0,0, $\bar{w}$ ]		
2	b ..2/m	0,0,1/2 [0,0,w]	1/2,1/2,0 [0,0, $\bar{w}$ ]		
2	a ..2/m	0,0,0 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c_p$ -2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0]  $c_p$ -2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pnnm1'

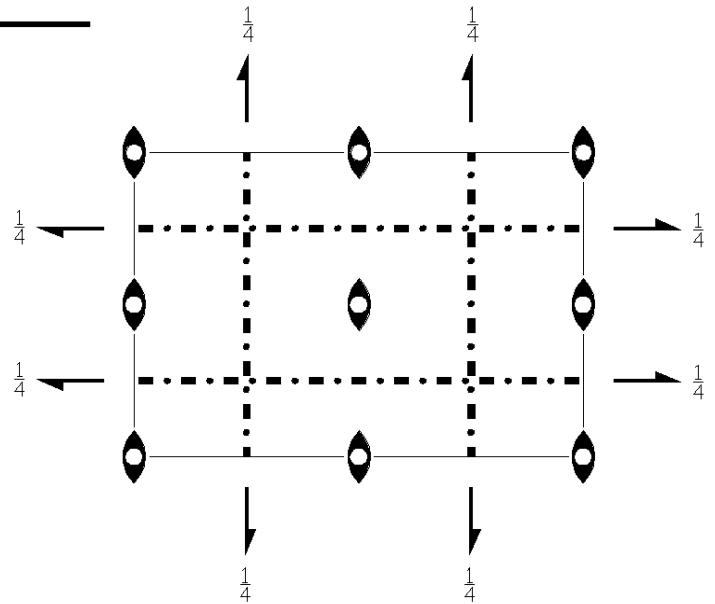
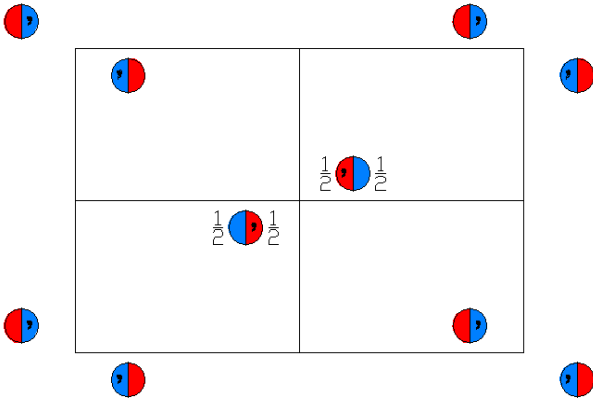
58.2.472

mmm1'

P2<sub>1</sub>/n2<sub>1</sub>/n2/m1'

Orthorhombic

1'



Origin at center ( 2/m1' )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For 1 + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (4) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (8) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) |

For 1' + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1'<br>(1 0,0,0)'                          | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (4) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

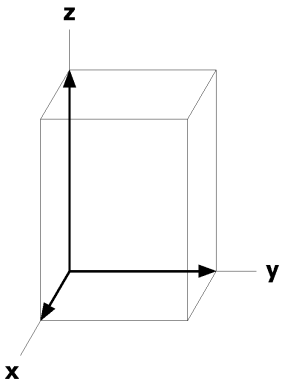
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +	1 +	1' +	1' +
8 h 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [0,0,0]	(4) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [0,0,0]
	(5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(6) x,y, $\bar{z}$ [0,0,0]	(7) $x+1/2,\bar{y}+1/2,z+1/2$ [0,0,0]	(8) $\bar{x}+1/2,y+1/2,z+1/2$ [0,0,0]
4 g ..m1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{x}+1/2,y+1/2,1/2$ [0,0,0]	$x+1/2,\bar{y}+1/2,1/2$ [0,0,0]
4 f ..21'	0,1/2,z [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0,z+1/2 [0,0,0]
4 e ..21'	0,0,z [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2,z+1/2 [0,0,0]
2 d ..2/m1'	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]		
2 c ..2/m1'	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2 b ..2/m1'	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2 a ..2/m1'	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

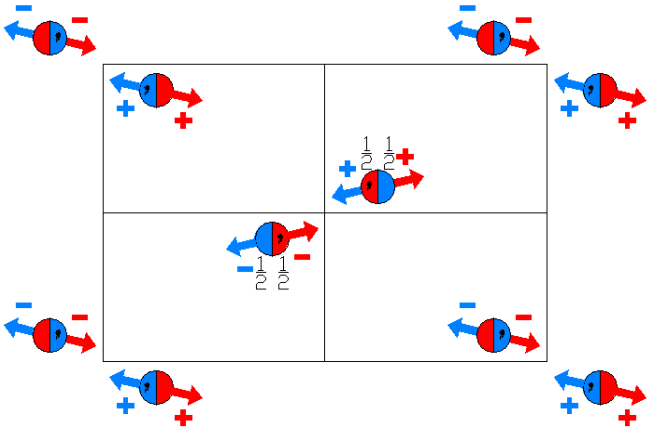
Along [0,1,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pn'm  
58.3.473

m'mm  
P<sub>2</sub><sub>1</sub>/n'2<sub>1</sub>'/n2'/m

Orthorhombic

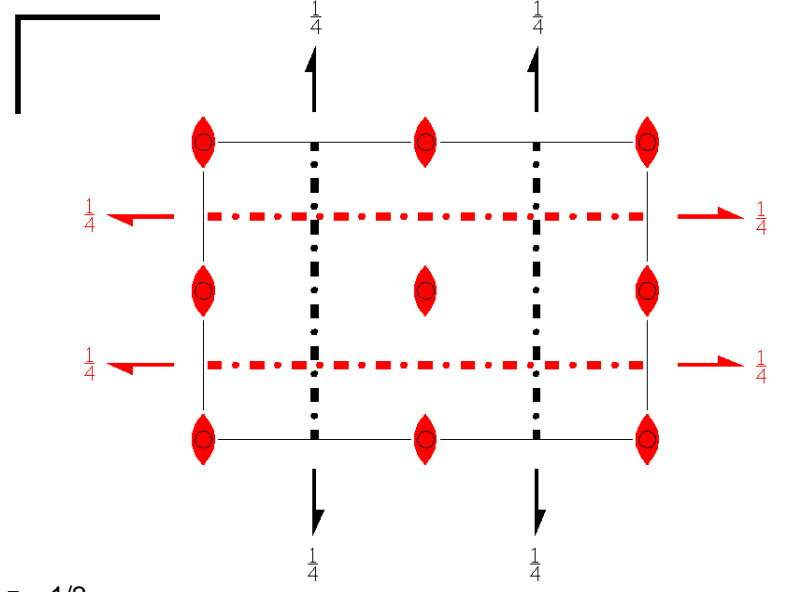


Origin at center ( 2'/m )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (4) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)   |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0)   | (7) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)   | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

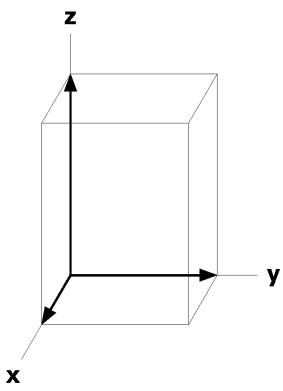
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	h 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [u,v,\bar{w}]$	(3) $\bar{x}+1/2,y+1/2,\bar{z}+1/2 [u,\bar{v},w]$	(4) $x+1/2,\bar{y}+1/2,\bar{z}+1/2 [u,\bar{v},\bar{w}]$
		(5) $\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$	(6) $x,y,\bar{z} [\bar{u},\bar{v},w]$	(7) $x+1/2,\bar{y}+1/2,z+1/2 [\bar{u},v,\bar{w}]$	(8) $\bar{x}+1/2,y+1/2,z+1/2 [\bar{u},v,w]$
4	g ..m	$x,y,0 [0,0,w]$	$\bar{x},\bar{y},0 [0,0,\bar{w}]$	$\bar{x}+1/2,y+1/2,1/2 [0,0,w]$	$x+1/2,\bar{y}+1/2,1/2 [0,0,\bar{w}]$
4	f ..2'	$0,1/2,z [u,v,0]$	$1/2,0,\bar{z}+1/2 [u,\bar{v},0]$	$0,1/2,\bar{z} [\bar{u},\bar{v},0]$	$1/2,0,z+1/2 [\bar{u},v,0]$
4	e ..2'	$0,0,z [u,v,0]$	$1/2,1/2,\bar{z}+1/2 [u,\bar{v},0]$	$0,0,\bar{z} [\bar{u},\bar{v},0]$	$1/2,1/2,z+1/2 [\bar{u},v,0]$
2	d ..2'/m	$0,1/2,1/2 [0,0,0]$	$1/2,0,0 [0,0,0]$		
2	c ..2'/m	$0,1/2,0 [0,0,0]$	$1/2,0,1/2 [0,0,0]$		
2	b ..2'/m	$0,0,1/2 [0,0,0]$	$1/2,1/2,0 [0,0,0]$		
2	a ..2'/m	$0,0,0 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p2gg1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c2mm$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

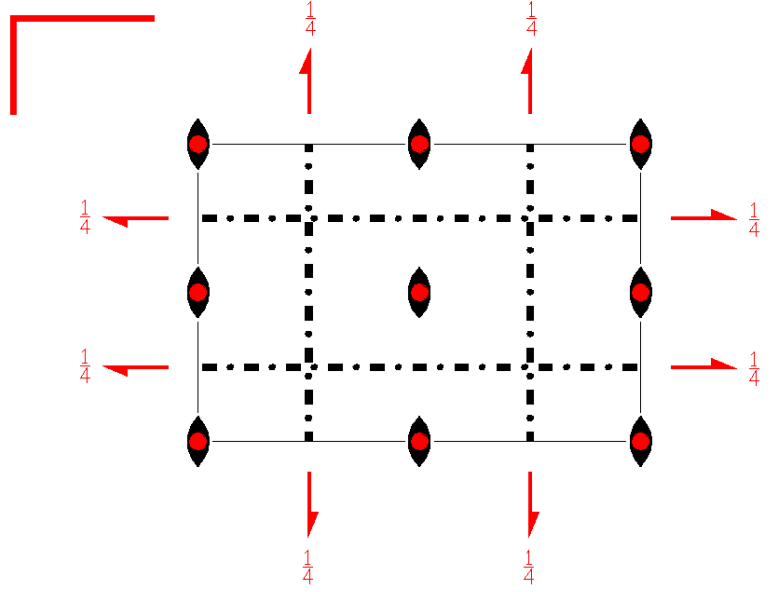
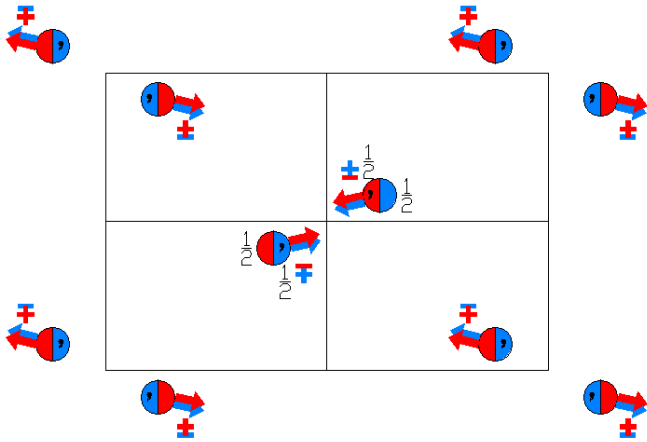
Along  $[0,1,0]$   $c_p-2mm$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at  $0,y,0$



Pnnm'  
58.4.474

mmm'  
P2<sub>1</sub>'/n2<sub>1</sub>'/n2/m'

Orthorhombic



Origin at center ( 2/m' )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (4) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)   | (8) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

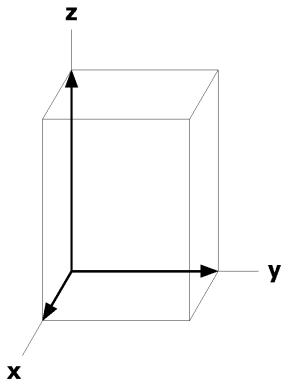
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	h 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [u, $\bar{v},w$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,y,\bar{z}$ [u,v, $\bar{w}$ ]	(7) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z+1/2$ [u, $\bar{v},\bar{w}$ ]
4	g ..m'	$x,y,0$ [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x}+1/2,y+1/2,1/2$ [u, $\bar{v},0$ ]	$x+1/2,\bar{y}+1/2,1/2$ [ $\bar{u},v,0$ ]
4	f ..2	$0,1/2,z$ [0,0,w]	$1/2,0,\bar{z}+1/2$ [0,0,w]	$0,1/2,\bar{z}$ [0,0, $\bar{w}$ ]	$1/2,0,z+1/2$ [0,0, $\bar{w}$ ]
4	e ..2	$0,0,z$ [0,0,w]	$1/2,1/2,\bar{z}+1/2$ [0,0,w]	$0,0,\bar{z}$ [0,0, $\bar{w}$ ]	$1/2,1/2,z+1/2$ [0,0, $\bar{w}$ ]
2	d ..2/m'	$0,1/2,1/2$ [0,0,0]	$1/2,0,0$ [0,0,0]		
2	c ..2/m'	$0,1/2,0$ [0,0,0]	$1/2,0,1/2$ [0,0,0]		
2	b ..2/m'	$0,0,1/2$ [0,0,0]	$1/2,1/2,0$ [0,0,0]		
2	a ..2/m'	$0,0,0$ [0,0,0]	$1/2,1/2,1/2$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

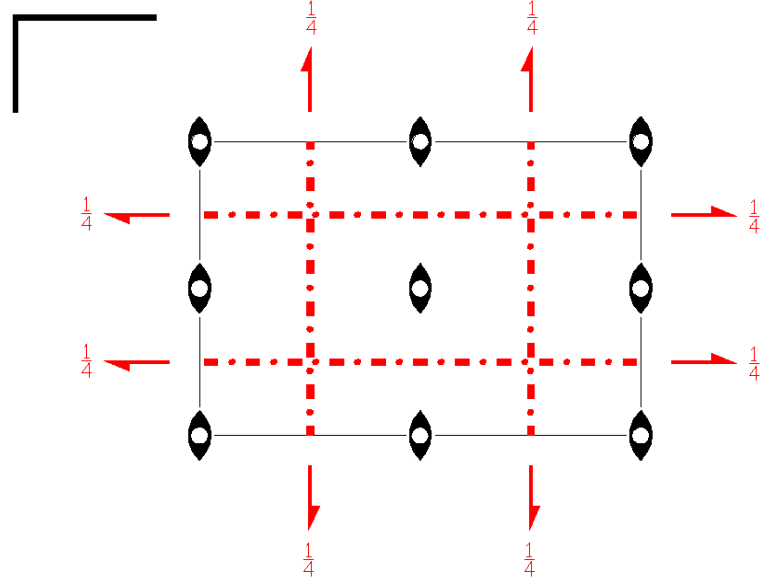
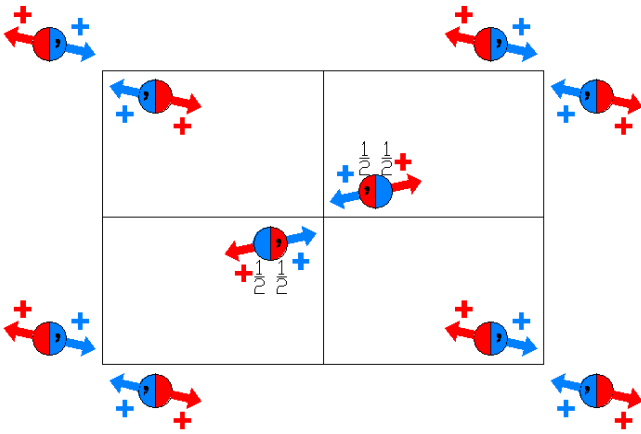
Along [0,1,0]  $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pn'n'm  
58.5.475

m'm'm  
P2<sub>1</sub>'/n2<sub>1</sub>'/n2/m

Orthorhombic



Origin at center ( 2/m )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (4) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

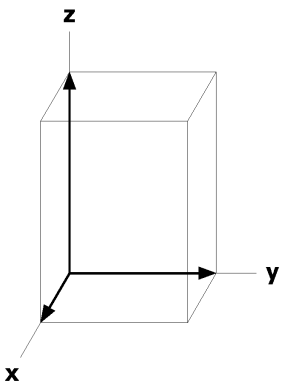
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	h 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [u, $\bar{v},w$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x+1/2,\bar{y}+1/2,z+1/2$ [u, $\bar{v},w$ ]	(8) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]
4	g ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x}+1/2,y+1/2,1/2$ [0,0,w]	$x+1/2,\bar{y}+1/2,1/2$ [0,0,w]
4	f ..2	0,1/2,z [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0,z+1/2 [0,0,w]
4	e ..2	0,0,z [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	1/2,1/2,z+1/2 [0,0,w]
2	d ..2/m	0,1/2,1/2 [0,0,w]	1/2,0,0 [0,0,w]		
2	c ..2/m	0,1/2,0 [0,0,w]	1/2,0,1/2 [0,0,w]		
2	b ..2/m	0,0,1/2 [0,0,w]	1/2,1/2,0 [0,0,w]		
2	a ..2/m	0,0,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

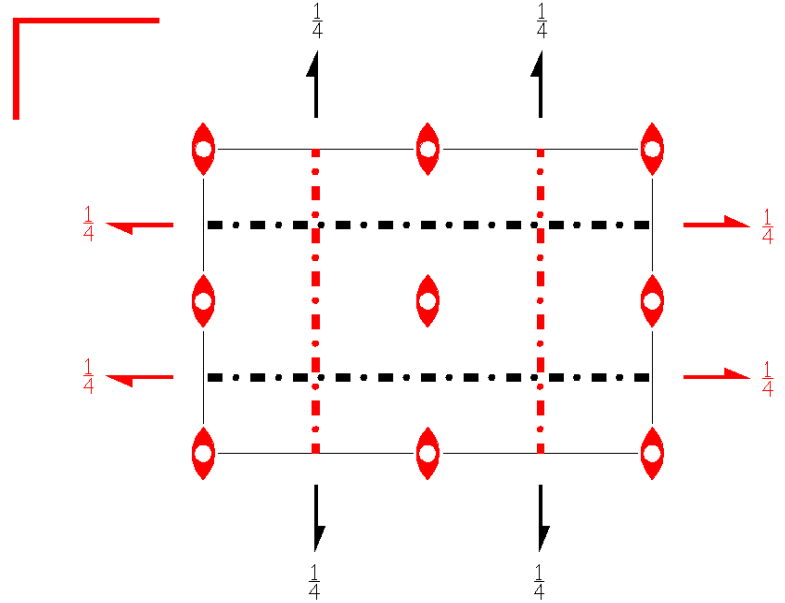
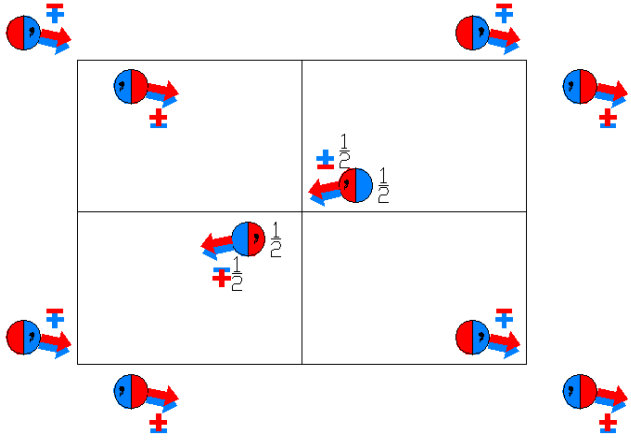
Along [0,1,0] c2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pnn'm'  
58.6.476

mm'm'  
P2<sub>1</sub>/n2<sub>1</sub>'/n'2'/m'

Orthorhombic



Origin at center (2'/m')

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (4) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (8) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

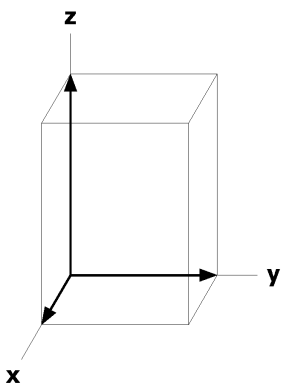
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	h 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) $x+1/2,\bar{y}+1/2,z+1/2$ [u, $\bar{v}$ ,w]	(8) $\bar{x}+1/2,y+1/2,z+1/2$ [u, $\bar{v},\bar{w}$ ]
4	g ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [u,v,0]	$\bar{x}+1/2,y+1/2,1/2$ [u, $\bar{v}$ ,0]	$x+1/2,\bar{y}+1/2,1/2$ [u, $\bar{v}$ ,0]
4	f ..2'	0,1/2,z [u,v,0]	1/2,0, $\bar{z}+1/2$ [u, $\bar{v}$ ,0]	0,1/2, $\bar{z}$ [u,v,0]	1/2,0,z+1/2 [u, $\bar{v}$ ,0]
4	e ..2'	0,0,z [u,v,0]	1/2,1/2, $\bar{z}+1/2$ [u, $\bar{v}$ ,0]	0,0, $\bar{z}$ [u,v,0]	1/2,1/2,z+1/2 [u, $\bar{v}$ ,0]
2	d ..2'/m'	0,1/2,1/2 [u,v,0]	1/2,0,0 [u, $\bar{v}$ ,0]		
2	c ..2'/m'	0,1/2,0 [u,v,0]	1/2,0,1/2 [u, $\bar{v}$ ,0]		
2	b ..2'/m'	0,0,1/2 [u,v,0]	1/2,1/2,0 [u, $\bar{v}$ ,0]		
2	a ..2'/m'	0,0,0 [u,v,0]	1/2,1/2,1/2 [u, $\bar{v}$ ,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2'gg'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c<sub>p</sub>-2'mm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

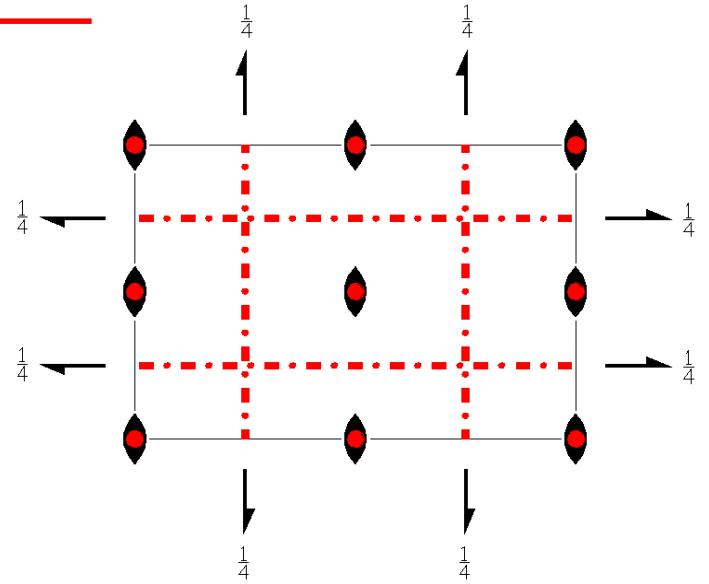
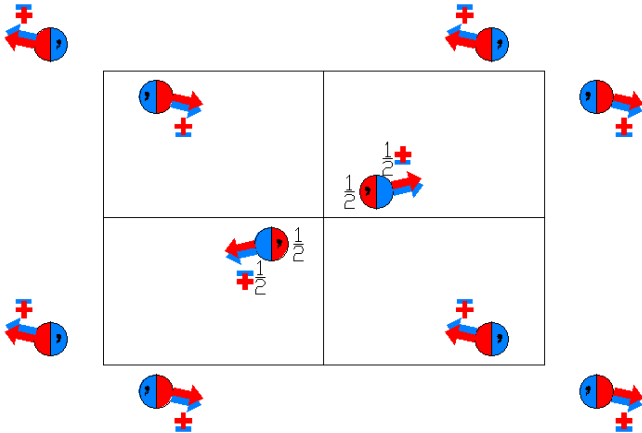
Along [0,1,0] c 2'mm'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



$Pn'n'm'$   
58.7.477

$m'm'm'$   
 $P2_1/n'2_1/n'2/m'$

Orthorhombic



Origin at center ( $2/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

- |  |                                      |  |  |
|--|--------------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)     | (3) 2 (0,1/2,0) $1/4,y,1/4$<br>( $2_y$  1/2,1/2,1/2)     | (4) 2 (1/2,0,0) $x,1/4,1/4$<br>( $2_x$  1/2,1/2,1/2)     |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) $m'$ $x,y,0$<br>( $m_z$  0,0,0)' | (7) $n'$ (1/2,0,1/2) $x,1/4,z$<br>( $m_y$  1/2,1/2,1/2)' | (8) $n'$ (0,1/2,1/2) $1/4,y,z$<br>( $m_x$  1/2,1/2,1/2)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

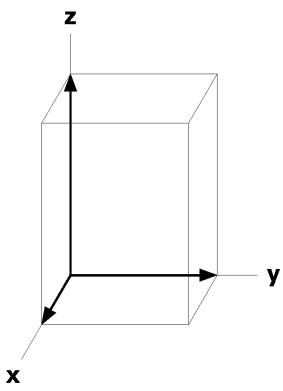
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	h 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]
4	g ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x}+1/2,y+1/2,1/2$ [ $\bar{u},v,0$ ]	$x+1/2,\bar{y}+1/2,1/2$ [ $u,\bar{v},0$ ]
4	f ..2	0,1/2,z [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0,w]
4	e ..2	0,0,z [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0,w]
2	d ..2/m'	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]		
2	c ..2/m'	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	b ..2/m'	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a ..2/m'	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2g'g'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

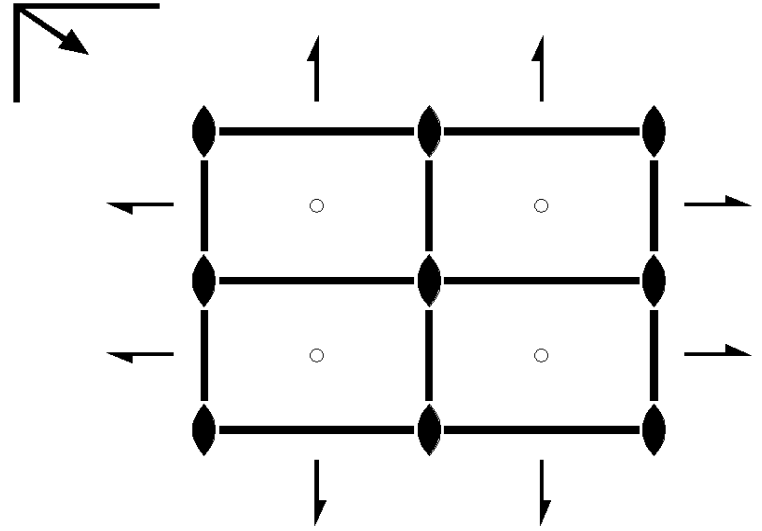
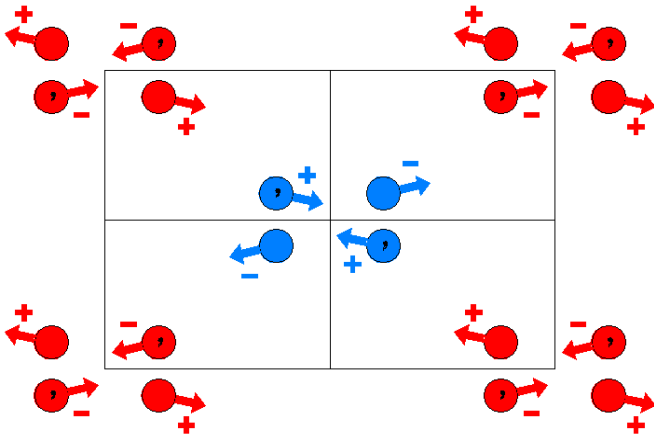
Along [0,1,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pmmn  
59.1.478

mmm  
 $P2_1/m2_1/m2/n$

Orthorhombic



Origin at  $mm2/n$  at  $1/4, 1/4, 0$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                       | (3) 2 $(0,1/2,0)$ $1/4,y,0$<br>( $2_y$   $1/2,1/2,0$ ) | (4) 2 $(1/2,0,0)$ $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ ) |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ ) | (6) n $(1/2,1/2,0)$ $x,y,0$<br>( $m_z$   $1/2,1/2,0$ ) | (7) m $x,0,z$<br>( $m_y$  0,0,0)                       | (8) m $0,y,z$<br>( $m_x$  0,0,0)                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

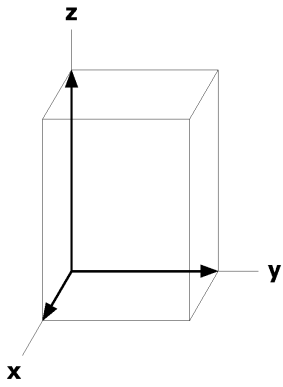
		Coordinates			
		Multiplicity, Wyckoff letter, Site Symmetry.			
8	g 1				
(1)	x,y,z [u,v,w]	(2)	$\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3)	$\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]
(4)	$x+1/2,\bar{y}+1/2,\bar{z}$ [u,v,w]	(5)	$\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [u,v,w]	(6)	$x+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]
(7)	x,y,z [ $\bar{u},v,\bar{w}$ ]	(8)	$\bar{x},y,z$ [u,v,w]		
4	f .m. x,0,z [0,v,0]	$\bar{x},0,z$ [0,v,0]	$\bar{x}+1/2,1/2,\bar{z}$ [0,v,0]	$x+1/2,1/2,\bar{z}$ [0,v,0]	
4	e m.. 0,y,z [u,0,0]	$0,\bar{y},z$ [ $\bar{u},0,0$ ]	$1/2,y+1/2,\bar{z}$ [ $\bar{u},0,0$ ]	$1/2,\bar{y}+1/2,\bar{z}$ [u,0,0]	
4	d $\bar{1}$ 1/4,1/4,1/2 [u,v,w]	$3/4,3/4,1/2$ [ $\bar{u},\bar{v},w$ ]	$1/4,3/4,1/2$ [ $\bar{u},v,\bar{w}$ ]	$3/4,1/4,1/2$ [u,v,w]	
4	c $\bar{1}$ 1/4,1/4,0 [u,v,w]	$3/4,3/4,0$ [ $\bar{u},\bar{v},w$ ]	$1/4,3/4,0$ [ $\bar{u},v,\bar{w}$ ]	$3/4,1/4,0$ [u,v,w]	
2	b mm2 0,1/2,z [0,0,0]	$1/2,0,\bar{z}$ [0,0,0]			
2	a mm2 0,0,z [0,0,0]	$1/2,1/2,\bar{z}$ [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $c_p$ -2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2mg1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0]  $p2mg1'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



Pmmn1'

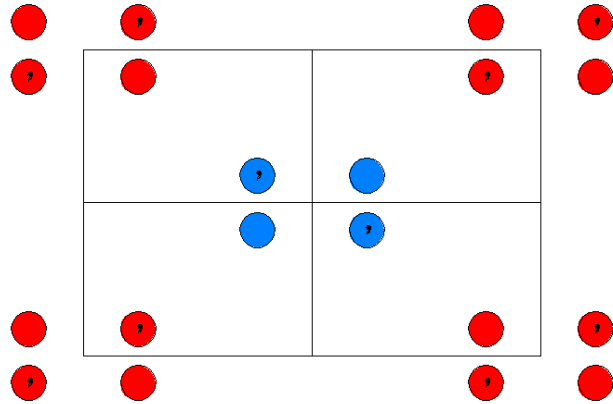
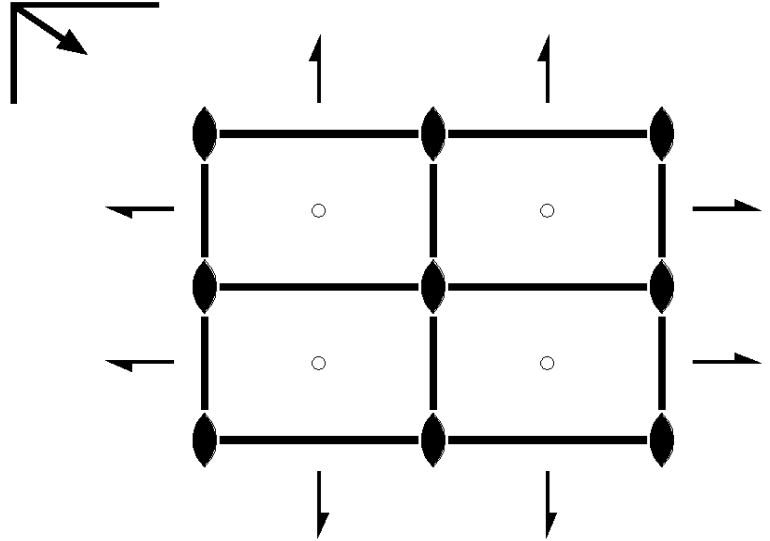
59.2.479

mmm1'

P2<sub>1</sub>/m2<sub>1</sub>/m2/n1'

Orthorhombic

1'



Origin at mm2/n1' at 1/4,1/4,0 from  $\bar{1}1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For 1 + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (7) m x,0,z<br>(m <sub>y</sub>  0,0,0)                 | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0)                 |

For 1' + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1'<br>(1 0,0,0)'                                  | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                 | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}'$ 1/4,1/4,0<br>( $\bar{1}'$  1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (7) m' x,0,z<br>(m <sub>y</sub>  0,0,0)'                 | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)'                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

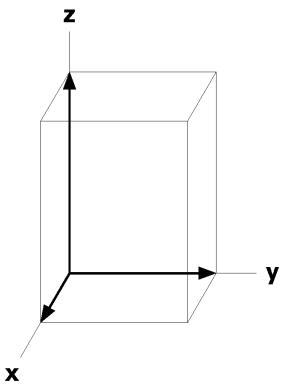
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	g 11'				
(1)	x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [0,0,0]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [0,0,0]	
(5)	$\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [0,0,0]	(6) $x+1/2,y+1/2,\bar{z}$ [0,0,0]	(7) $x,\bar{y},z$ [0,0,0]	(8) $\bar{x},y,z$ [0,0,0]	
4	f .m.1' x,0,z [0,0,0]	$\bar{x},0,z$ [0,0,0]	$\bar{x}+1/2,1/2,\bar{z}$ [0,0,0]	$x+1/2,1/2,\bar{z}$ [0,0,0]	
4	e m..1' 0,y,z [0,0,0]	$0,\bar{y},z$ [0,0,0]	$1/2,y+1/2,\bar{z}$ [0,0,0]	$1/2,\bar{y}+1/2,\bar{z}$ [0,0,0]	
4	d $\bar{1}1'$ 1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	
4	c $\bar{1}1'$ 1/4,1/4,0 [0,0,0]	3/4,3/4,0 [0,0,0]	1/4,3/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]	
2	b mm21' 0,1/2,z [0,0,0]	$1/2,0,\bar{z}$ [0,0,0]			
2	a mm21' 0,0,z [0,0,0]	$1/2,1/2,\bar{z}$ [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

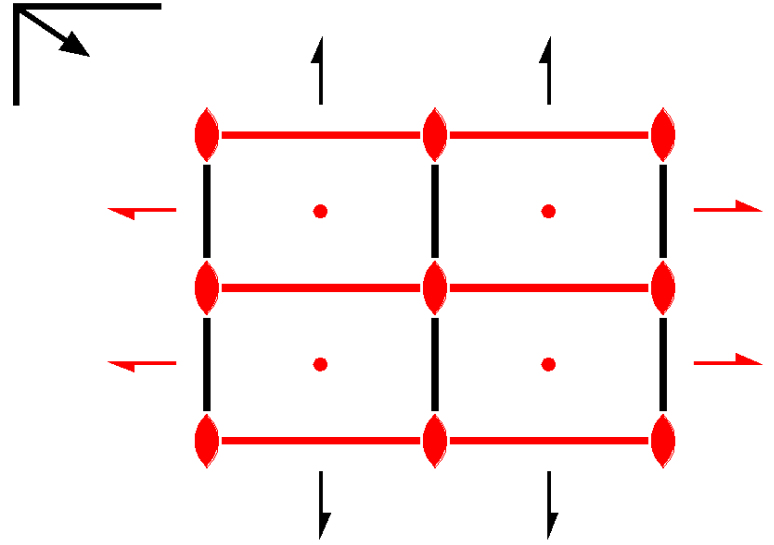
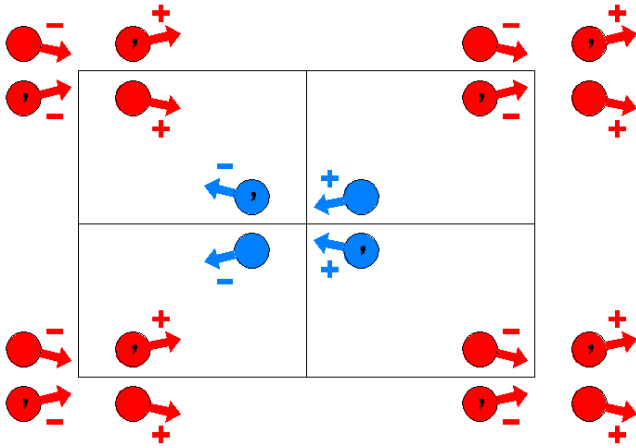
Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



Pm'mn  
59.3.480

m'mm  
P<sub>2</sub><sub>1</sub>/m'<sub>2</sub><sub>1</sub>'/m<sub>2</sub><sub>1</sub>'/n

Orthorhombic



Origin at m'm<sub>2</sub>'/n at 1/4,1/4,0 from  $\bar{1}$ '

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                                    | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'               | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (7) m x,0,z<br>(m <sub>y</sub>  0,0,0)                   | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)'               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

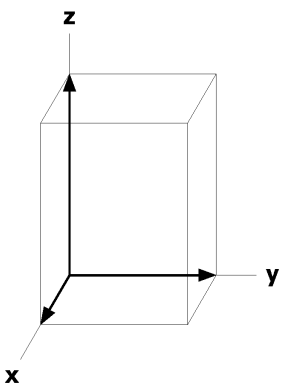
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	g 1				
(1)	x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [u, $\bar{v}$ ,w]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [u, $\bar{v},\bar{w}$ ]	
(5)	$\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	
4	f .m. x,0,z [0,v,0]	$\bar{x},0,z$ [0,v,0]	$\bar{x}+1/2,1/2,\bar{z}$ [0, $\bar{v}$ ,0]	$x+1/2,1/2,\bar{z}$ [0, $\bar{v}$ ,0]	
4	e m'. 0,y,z [0,v,w]	$0,\bar{y},z$ [0,v, $\bar{w}$ ]	$1/2,y+1/2,\bar{z}$ [0, $\bar{v}$ ,w]	$1/2,\bar{y}+1/2,\bar{z}$ [0, $\bar{v},\bar{w}$ ]	
4	d $\bar{1}'$ 1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	
4	c $\bar{1}'$ 1/4,1/4,0 [0,0,0]	3/4,3/4,0 [0,0,0]	1/4,3/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]	
2	b m'm2' 0,1/2,z [0,v,0]	$1/2,0,\bar{z}$ [0, $\bar{v}$ ,0]			
2	a m'm2' 0,0,z [0,v,0]	$1/2,1/2,\bar{z}$ [0, $\bar{v}$ ,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $c_p$ -2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

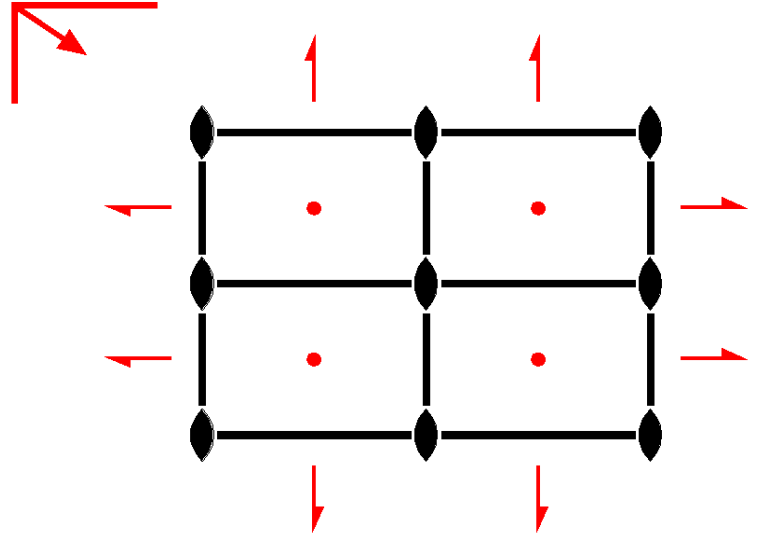
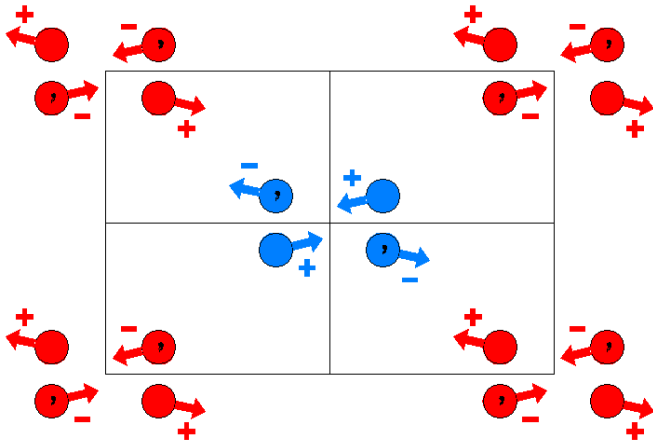
Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



Pmmn'  
59.4.481

mmm'  
P2<sub>1</sub>'/m2<sub>1</sub>'/m2/n'

Orthorhombic



Origin at mm2/n' at 1/4,1/4,0 from  $\bar{1}$ '

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                                    | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                   | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (7) m x,0,z<br>(m <sub>y</sub>  0,0,0)                   | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0)                   |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

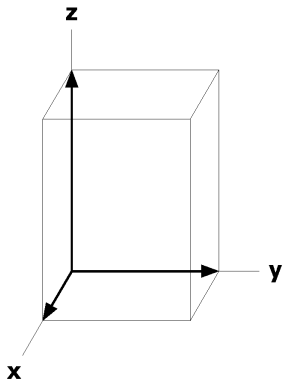
		Coordinates			
		Multiplicity, Wyckoff letter, Site Symmetry.			
8	g 1				
(1)	x,y,z [u,v,w]	(2)	$\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3)	$\bar{x}+1/2,y+1/2,\bar{z}$ [ $u,\bar{v},w$ ]
(4)	$x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]	(5)	$\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6)	$x+1/2,y+1/2,\bar{z}$ [ $u,v,\bar{w}$ ]
(7)	$x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(8)	$\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]		
4	f .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]	$\bar{x}+1/2,1/2,\bar{z}$ [0, $\bar{v}$ ,0]	$x+1/2,1/2,\bar{z}$ [0,v,0]
4	e m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	1/2,y+1/2, $\bar{z}$ [u,0,0]	1/2, $\bar{y}+1/2,\bar{z}$ [ $\bar{u},0,0$ ]
4	d $\bar{1}'$	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]
4	c $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,0 [0,0,0]	1/4,3/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]
2	b mm2	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
2	a mm2	0,0,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



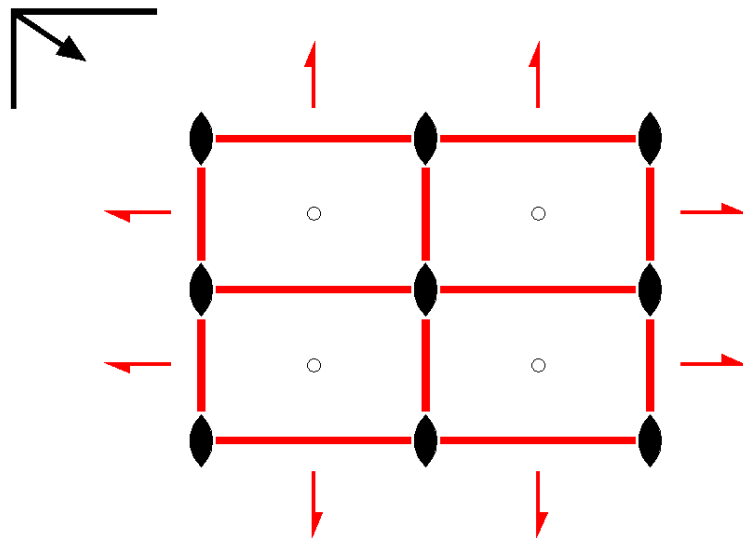
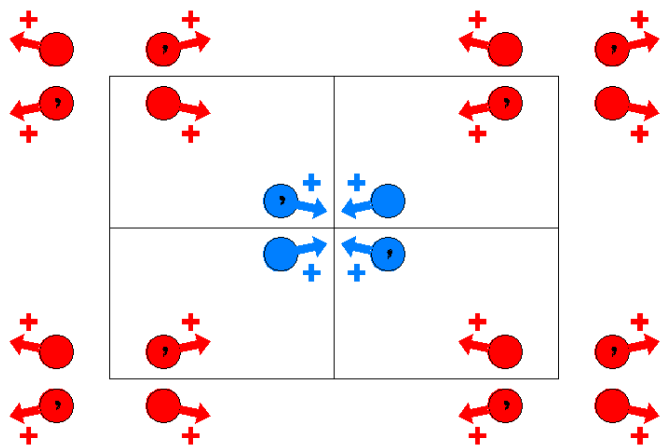
Pm'm'n

59.5.482

m'm'm

P2<sub>1</sub>'/m'2<sub>1</sub>'/m'2/n

Orthorhombic



Origin at m'm'2/n at 1/4,1/4,0 from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (7) m' x,0,z<br>(m <sub>y</sub>  0,0,0)'                 | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)'                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

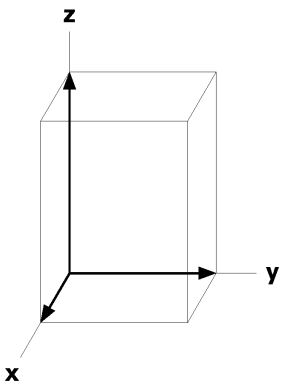
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	g 1				
(1)	x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $u,\bar{v},w$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]	
(5)	$\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [u,v,w]	(6) $x+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y},z$ [ $u,\bar{v},w$ ]	(8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	
4	f .m'. x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$\bar{x}+1/2,1/2,\bar{z}$ [u,0,w]	$x+1/2,1/2,\bar{z}$ [ $\bar{u},0,w$ ]	
4	e m'.. 0,y,z [0,v,w]	$0,\bar{y},z$ [0, $\bar{v},w$ ]	$1/2,y+1/2,\bar{z}$ [0, $\bar{v},w$ ]	$1/2,\bar{y}+1/2,\bar{z}$ [0,v,w]	
4	d $\bar{1}$ 1/4,1/4,1/2 [u,v,w]	$3/4,3/4,1/2$ [ $\bar{u},\bar{v},w$ ]	$1/4,3/4,1/2$ [ $u,\bar{v},w$ ]	$3/4,1/4,1/2$ [ $\bar{u},v,w$ ]	
4	c $\bar{1}$ 1/4,1/4,0 [u,v,w]	$3/4,3/4,0$ [ $\bar{u},\bar{v},w$ ]	$1/4,3/4,0$ [ $u,\bar{v},w$ ]	$3/4,1/4,0$ [ $\bar{u},v,w$ ]	
2	b m'm'2 0,1/2,z [0,0,w]	$1/2,0,\bar{z}$ [0,0,w]			
2	a m'm'2 0,0,z [0,0,w]	$1/2,1/2,\bar{z}$ [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1]  $c_p$ -2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2'mg'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0]  $p2'm'g$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



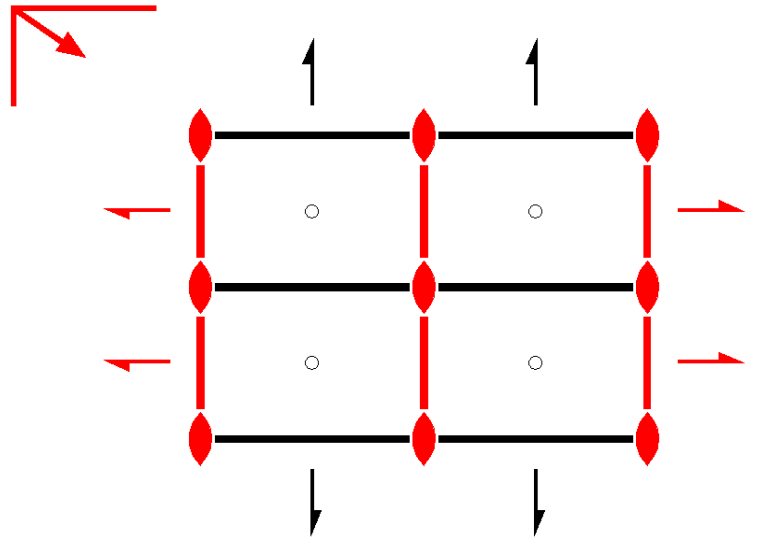
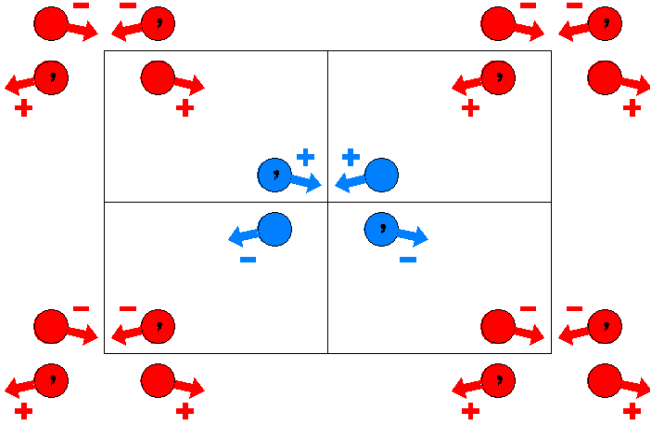
Pmm'n'

59.6.483

mm'm'

$P2_1/m2_1'/m'2'/n'$

Orthorhombic



Origin at mm'2'/n' at 1/4,1/4,0 from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                 | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (7) m' x,0,z<br>(m <sub>y</sub>  0,0,0)'                 | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0)                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

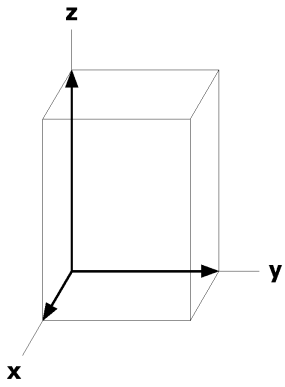
		Coordinates					
Multiplicity, Wyckoff letter, Site Symmetry.							
8 g 1							
(1)	x,y,z [u,v,w]	(2)	$\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3)	$\bar{x}+1/2, y+1/2, \bar{z}$ [u, $\bar{v}$ ,w]	(4)	$x+1/2, \bar{y}+1/2, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
(5)	$\bar{x}+1/2, \bar{y}+1/2, \bar{z}$ [u,v,w]	(6)	$x+1/2, y+1/2, \bar{z}$ [u,v, $\bar{w}$ ]	(7)	$x, \bar{y}, z$ [u, $\bar{v}$ ,w]	(8)	$\bar{x}, y, z$ [u, $\bar{v}, \bar{w}$ ]
4	f .m'	x,0,z [u,0,w]	$\bar{x}, 0, z$ [u,0, $\bar{w}$ ]	$\bar{x}+1/2, 1/2, \bar{z}$ [u,0,w]	$x+1/2, 1/2, \bar{z}$ [u,0, $\bar{w}$ ]		
4	e m..	0,y,z [u,0,0]	$0, \bar{y}, z$ [u,0,0]	$1/2, y+1/2, \bar{z}$ [u,0,0]	$1/2, \bar{y}+1/2, \bar{z}$ [u,0,0]		
4	d $\bar{1}$	1/4,1/4,1/2 [u,v,w]	3/4,3/4,1/2 [u,v, $\bar{w}$ ]	1/4,3/4,1/2 [u, $\bar{v}$ ,w]	3/4,1/4,1/2 [u, $\bar{v}, \bar{w}$ ]		
4	c $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,0 [u,v, $\bar{w}$ ]	1/4,3/4,0 [u, $\bar{v}$ ,w]	3/4,1/4,0 [u, $\bar{v}, \bar{w}$ ]		
2	b mm'2'	0,1/2,z [u,0,0]	$1/2, 0, \bar{z}$ [u,0,0]				
2	a mm'2'	0,0,z [u,0,0]	$1/2, 1/2, \bar{z}$ [u,0,0]				

**Symmetry of Special Projections**

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0] p2'mg'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



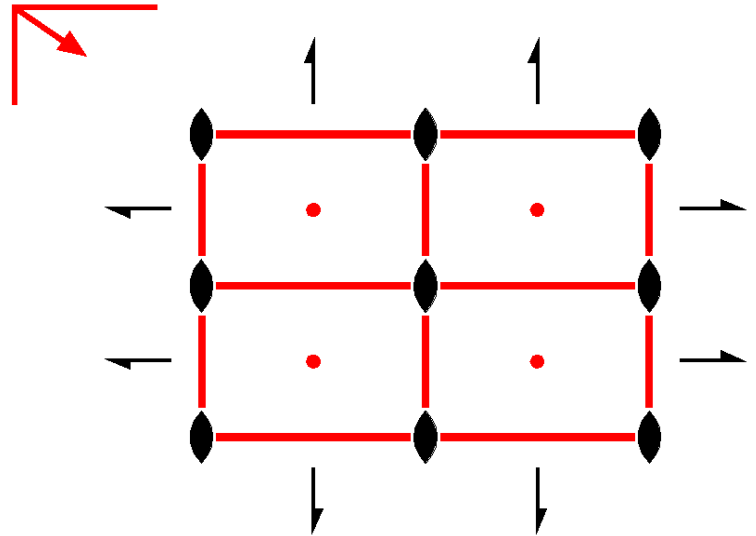
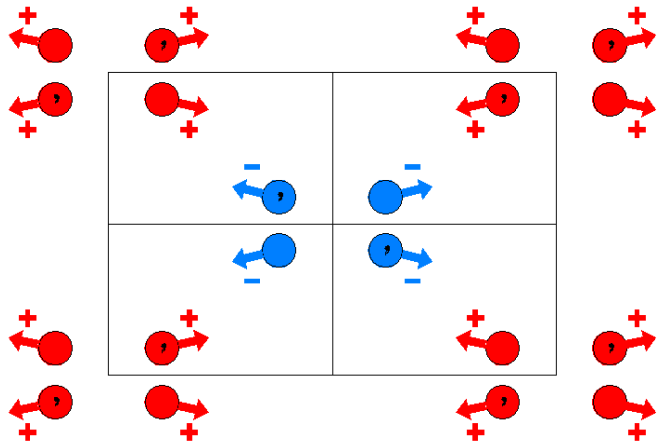
Pm'm'n'

59.7.484

m'm'm'

P2<sub>1</sub>/m'2<sub>1</sub>/m'2/n'

Orthorhombic



Origin at m'm'2/n' at 1/4,1/4,0 from  $\bar{1}$ '

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                   | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$ ' 1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (7) m' x,0,z<br>(m <sub>y</sub>  0,0,0)'               | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)'               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

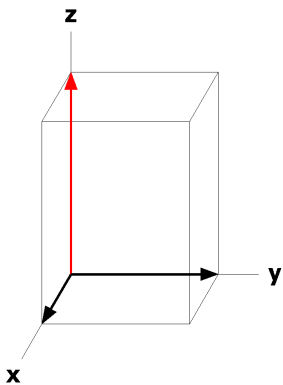
		Coordinates					
Multiplicity, Wyckoff letter, Site Symmetry.							
8 g 1							
(1)	x,y,z [u,v,w]	(2)	$\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3)	$\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4)	$x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
(5)	$\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6)	$x+1/2,y+1/2,\bar{z}$ [ $u,v,\bar{w}$ ]	(7)	$x,\bar{y},z$ [ $u,\bar{v},w$ ]	(8)	$\bar{x},y,z$ [ $\bar{u},v,w$ ]
4	f .m'. x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$\bar{x}+1/2,1/2,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	$x+1/2,1/2,\bar{z}$ [ $u,0,\bar{w}$ ]			
4	e m'.. 0,y,z [0,v,w]	$0,\bar{y},z$ [ $0,\bar{v},w$ ]	$1/2,y+1/2,\bar{z}$ [ $0,v,\bar{w}$ ]	$1/2,\bar{y}+1/2,\bar{z}$ [ $0,\bar{v},\bar{w}$ ]			
4	d $\bar{1}'$ 1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]			
4	c $\bar{1}'$ 1/4,1/4,0 [0,0,0]	3/4,3/4,0 [0,0,0]	1/4,3/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]			
2	b m'm'2 0,1/2,z [0,0,w]	$1/2,0,\bar{z}$ [ $0,0,\bar{w}$ ]					
2	a m'm'2 0,0,z [0,0,w]	$1/2,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]					

**Symmetry of Special Projections**

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



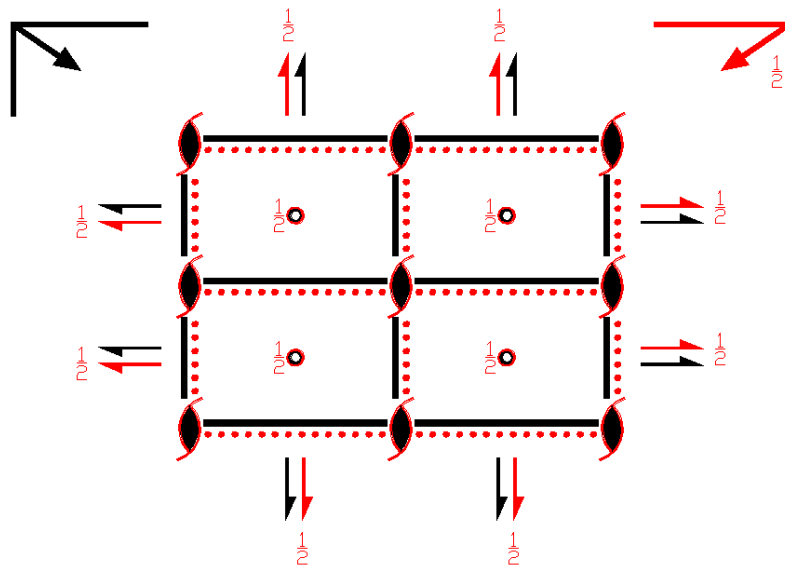
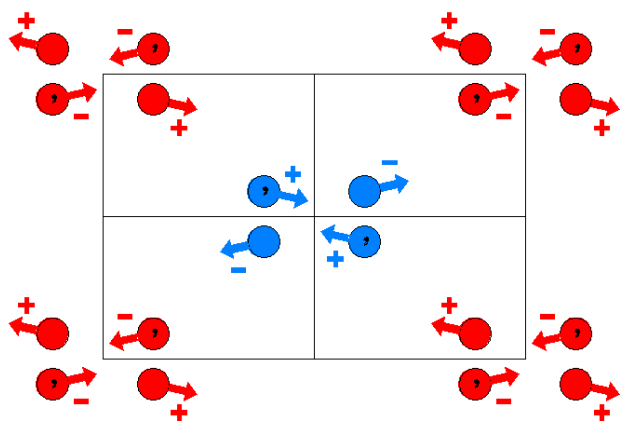
$P_{2c}$  mmm

59.8.485

mmm1'

$P_{2c} 2_1/m2_1/m2/n$

Orthorhombic



Origin at  $mm2/n$  at  $1/4, 1/4, 0$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $1$<br>( $1 0,0,0$ )                             | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                   | (3) $2$ $(0,1/2,0)$ $1/4,y,0$<br>( $2_y 1/2,1/2,0$ ) | (4) $2$ $(1/2,0,0)$ $x,1/4,0$<br>( $2_x 1/2,1/2,0$ ) |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1} 1/2,1/2,0$ ) | (6) $n$ $(1/2,1/2,0)$ $x,y,0$<br>( $m_z 1/2,1/2,0$ ) | (7) $m$ $x,0,z$<br>( $m_y 0,0,0$ )                   | (8) $m$ $0,y,z$<br>( $m_x 0,0,0$ )                   |

For  $(0,0,1)$ ' + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t'$ $(0,0,1)$<br>( $1 0,0,1$ )'                      | (2) $2'$ $(0,0,1)$ $0,0,z$<br>( $2_z 0,0,1$ )'           | (3) $2'$ $(0,1/2,0)$ $1/4,y,1/2$<br>( $2_y 1/2,1/2,1$ )' | (4) $2'$ $(1/2,0,0)$ $x,1/4,1/2$<br>( $2_x 1/2,1/2,1$ )' |
| (5) $\bar{1}'$ $1/4,1/4,1/2$<br>( $\bar{1}' 1/2,1/2,1$ )' | (6) $n'$ $(1/2,1/2,0)$ $x,y,1/2$<br>( $m_z 1/2,1/2,1$ )' | (7) $c'$ $(0,0,1)$ $x,0,z$<br>( $m_y 0,0,1$ )'           | (8) $c'$ $(0,0,1)$ $0,y,z$<br>( $m_x 0,0,1$ )'           |



**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

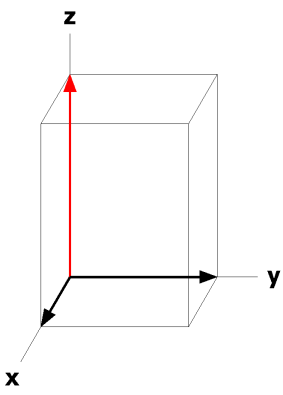
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
16 g 1				
(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	
(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [u,v,w]	(6) $x+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	
8 f .m. x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]	$\bar{x}+1/2,1/2,\bar{z}$ [0,v,0]	$x+1/2,1/2,\bar{z}$ [0, $\bar{v}$ ,0]	
8 e m.. 0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	1/2,y+1/2, $\bar{z}$ [ $\bar{u},0,0$ ]	1/2, $\bar{y}+1/2,\bar{z}$ [u,0,0]	
8 d $\bar{1}'$ 1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	
8 c $\bar{1}$ 1/4,1/4,0 [u,v,w]	3/4,3/4,0 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,0 [ $\bar{u},v,\bar{w}$ ]	3/4,1/4,0 [u, $\bar{v},\bar{w}$ ]	
4 b mm2 0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]			
4 a mm2 0,0,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



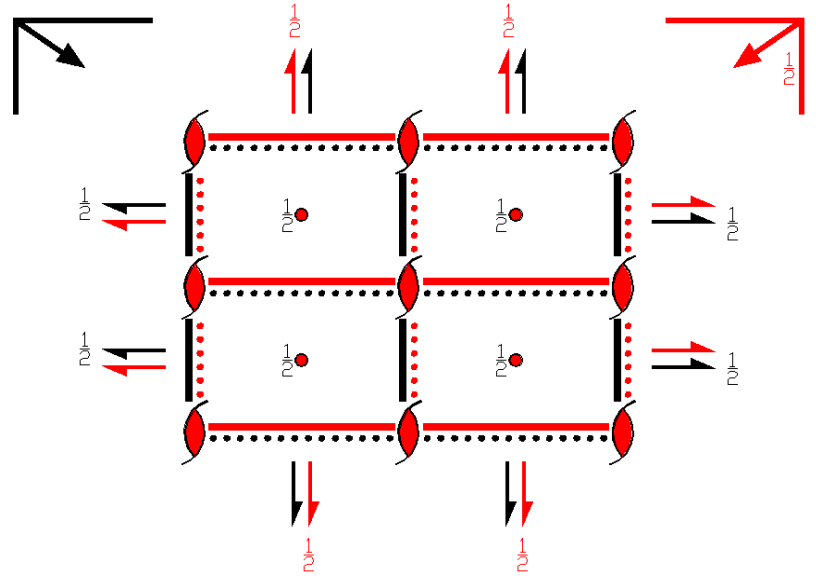
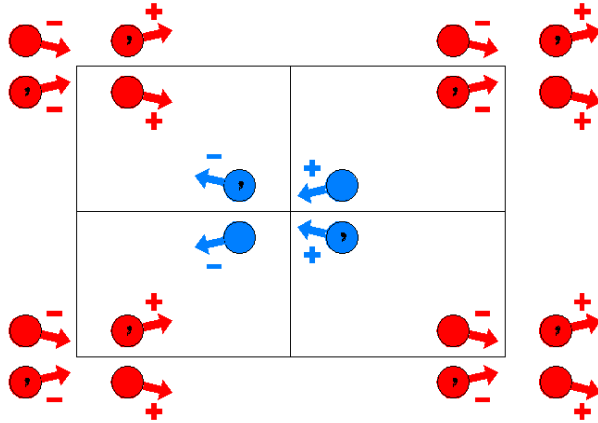
$P_{2c} m'mn$

59.9.486

$mmm1'$

$P_{2c} 2_1/m'2_1'/m2'/n$

Orthorhombic



Origin at  $m'm2'/n$  at  $1/4, 1/4, 0$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |  |  |   |
|---|--|--|---|
| (1) 1<br>(1 0,0,0)                                    | (2) $2'_z$ 0,0,z<br>( $2_z$  0,0,0)'               | (3) $2'_y$ (0,1/2,0) $1/4,y,0$<br>( $2_y$  1/2,1/2,0)' | (4) $2'_x$ (1/2,0,0) $x,1/4,0$<br>( $2_x$  1/2,1/2,0) |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$  1/2,1/2,0)' | (6) $n$ (1/2,1/2,0) $x,y,0$<br>( $m_z$  1/2,1/2,0) | (7) $m$ $x,0,z$<br>( $m_y$  0,0,0)                     | (8) $m'$ 0,y,z<br>( $m_x$  0,0,0)'                    |

For  $(0,0,1)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'                         | (2) $2$ (0,0,1) 0,0,z<br>( $2_z$  0,0,1)               | (3) $2$ (0,1/2,0) $1/4,y,1/2$<br>( $2_y$  1/2,1/2,1) | (4) $2'$ (1/2,0,0) $x,1/4,1/2$<br>( $2_x$  1/2,1/2,1)' |
| (5) $\bar{1}$ $1/4,1/4,1/2$<br>( $\bar{1}$  1/2,1/2,1) | (6) $n'$ (1/2,1/2,0) $x,y,1/2$<br>( $m_z$  1/2,1/2,1)' | (7) $c'$ (0,0,1) $x,0,z$<br>( $m_y$  0,0,1)'         | (8) $c$ (0,0,1) 0,y,z<br>( $m_x$  0,0,1)               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

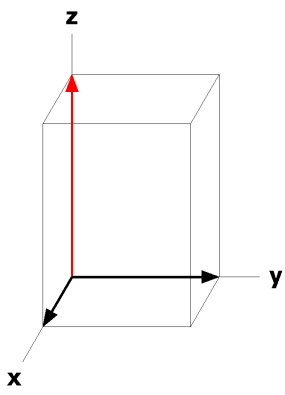
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
16 g 1				
(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [u, $\bar{v}$ ,w]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [u, $\bar{v},\bar{w}$ ]	
(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	
8 f .m. x,0,z [0,v,0]	$\bar{x},0,z$ [0,v,0]	$\bar{x}+1/2,1/2,\bar{z}$ [0, $\bar{v}$ ,0]	$x+1/2,1/2,\bar{z}$ [0, $\bar{v}$ ,0]	
8 e m'. 0,y,z [0,v,w]	$0,\bar{y},z$ [0,v, $\bar{w}$ ]	$1/2,y+1/2,\bar{z}$ [0, $\bar{v}$ ,w]	$1/2,\bar{y}+1/2,\bar{z}$ [0, $\bar{v},\bar{w}$ ]	
8 d $\bar{1}$ 1/4,1/4,1/2 [u,v,w]	$3/4,3/4,1/2$ [u,v, $\bar{w}$ ]	$1/4,3/4,1/2$ [ $\bar{u},v,\bar{w}$ ]	$3/4,1/4,1/2$ [ $\bar{u},v,w$ ]	
8 c $\bar{1}'$ 1/4,1/4,0 [0,0,0]	$3/4,3/4,0$ [0,0,0]	$1/4,3/4,0$ [0,0,0]	$3/4,1/4,0$ [0,0,0]	
4 b m'm2' 0,1/2,z [0,v,0]	$1/2,0,\bar{z}$ [0, $\bar{v}$ ,0]			
4 a m'm2' 0,0,z [0,v,0]	$1/2,1/2,\bar{z}$ [0, $\bar{v}$ ,0]			

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



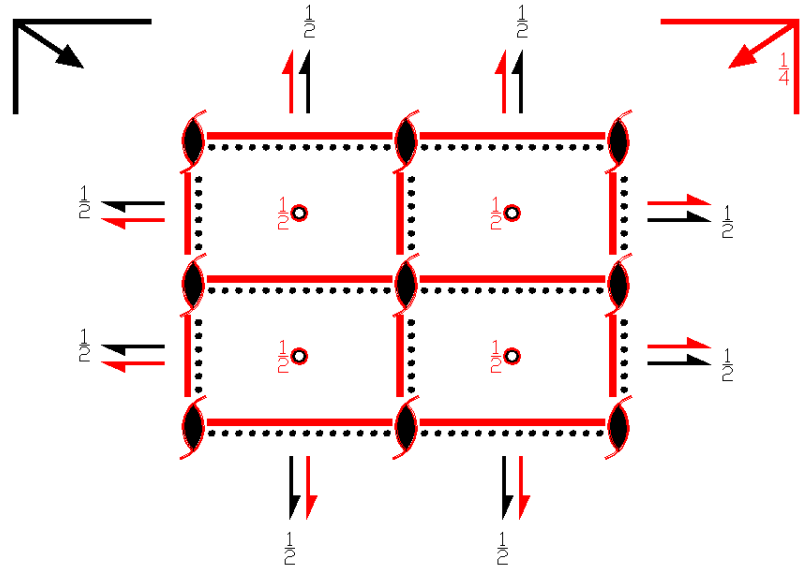
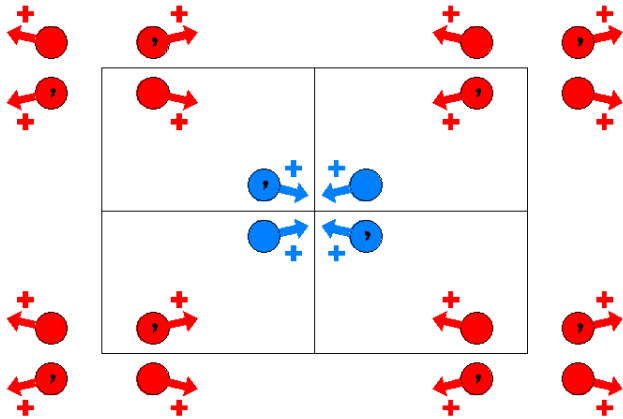
$P_{2c} m'm'n$

59.10.487

$mmm1'$

$P_{2c} 2_1'/m'2_1'/m'2/n$

Orthorhombic



Origin at  $m'm'2/n$  at  $1/4, 1/4, 0$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $1$<br>( $1 0,0,0$ )                             | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                   | (3) $2'$ $(0,1/2,0)$ $1/4,y,0$<br>( $2_y 1/2,1/2,0'$ ) | (4) $2'$ $(1/2,0,0)$ $x,1/4,0$<br>( $2_x 1/2,1/2,0'$ ) |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1} 1/2,1/2,0$ ) | (6) $n$ $(1/2,1/2,0)$ $x,y,0$<br>( $m_z 1/2,1/2,0$ ) | (7) $m'$ $x,0,z$<br>( $m_y 0,0,0'$ )                   | (8) $m'$ $0,y,z$<br>( $m_x 0,0,0'$ )                   |

For  $(0,0,1)$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t'$ $(0,0,1)$<br>( $1 0,0,1'$ )                      | (2) $2'$ $(0,0,1)$ $0,0,z$<br>( $2_z 0,0,1'$ )           | (3) $2$ $(0,1/2,0)$ $1/4,y,1/2$<br>( $2_y 1/2,1/2,1$ ) | (4) $2$ $(1/2,0,0)$ $x,1/4,1/2$<br>( $2_x 1/2,1/2,1$ ) |
| (5) $\bar{1}'$ $1/4,1/4,1/2$<br>( $\bar{1}' 1/2,1/2,1'$ ) | (6) $n'$ $(1/2,1/2,0)$ $x,y,1/2$<br>( $m_z 1/2,1/2,1'$ ) | (7) $c$ $(0,0,1)$ $x,0,z$<br>( $m_y 0,0,1$ )           | (8) $c$ $(0,0,1)$ $0,y,z$<br>( $m_x 0,0,1$ )           |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

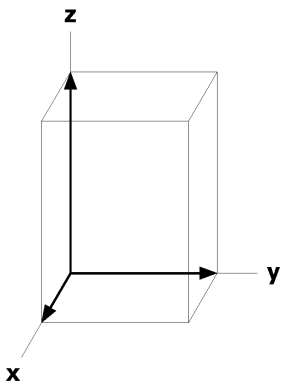
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
16 g 1				
(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $u,\bar{v},w$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]	
(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [u,v,w]	(6) $x+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y},z$ [ $u,\bar{v},w$ ]	(8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	
8 f .m'. x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$\bar{x}+1/2,1/2,\bar{z}$ [u,0,w]	$x+1/2,1/2,\bar{z}$ [ $\bar{u},0,w$ ]	
8 e m'.. 0,y,z [0,v,w]	$0,\bar{y},z$ [0, $\bar{v},w$ ]	$1/2,y+1/2,\bar{z}$ [0, $\bar{v},w$ ]	$1/2,\bar{y}+1/2,\bar{z}$ [0,v,w]	
8 d $\bar{1}'$ 1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	
8 c $\bar{1}$ 1/4,1/4,0 [u,v,w]	3/4,3/4,0 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,0 [u, $\bar{v},w$ ]	3/4,1/4,0 [ $\bar{u},v,w$ ]	
4 b m'm'2 0,1/2,z [0,0,w]	$1/2,0,\bar{z}$ [0,0,w]			
4 a m'm'2 0,0,z [0,0,w]	$1/2,1/2,\bar{z}$ [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

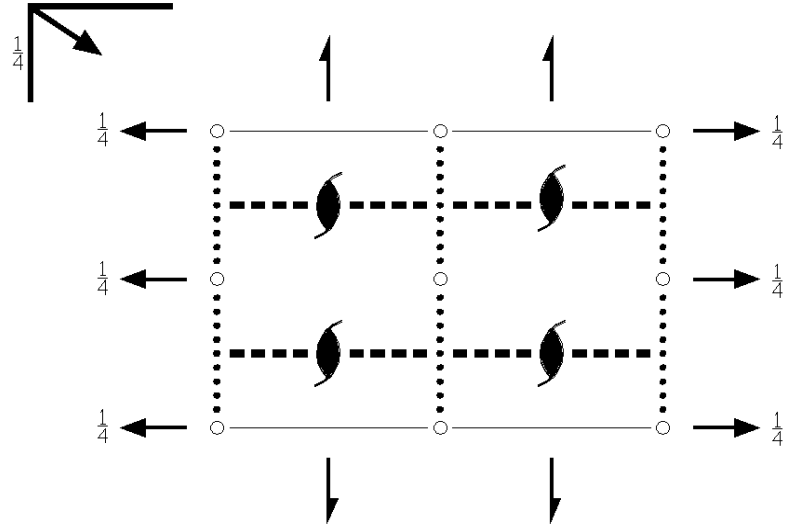
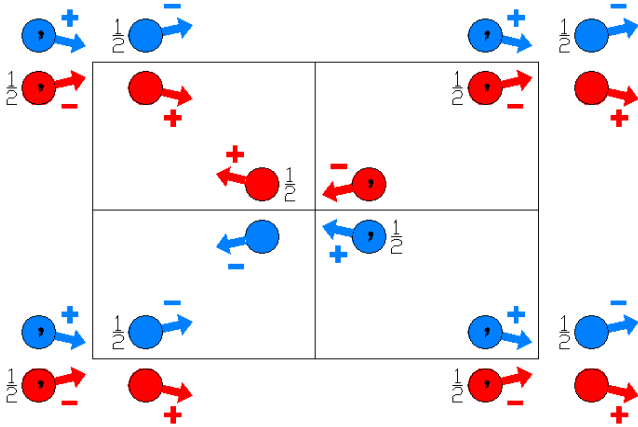
Along [0,1,0] p<sub>2b</sub>'-2m'g'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



Pbcn  
60.1.488

mmm  
 $P2_1/b2/c2_1/n$

Orthorhombic



Origin at  $\bar{1}$  on  $1c1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) $1/4, 1/4, z$<br>( $2_z$  1/2, 1/2, 1/2)   | (3) 2 $0, y, 1/4$<br>( $2_y$  0,0,1/2)         | (4) 2 (1/2,0,0) $x, 1/4, 0$<br>( $2_x$  1/2, 1/2, 0)   |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) n (1/2, 1/2, 0) $x, y, 1/4$<br>( $m_z$  1/2, 1/2, 1/2) | (7) c (0,0,1/2) $x, 0, z$<br>( $m_y$  0,0,1/2) | (8) b (0, 1/2, 0) $1/4, y, z$<br>( $m_x$  1/2, 1/2, 0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

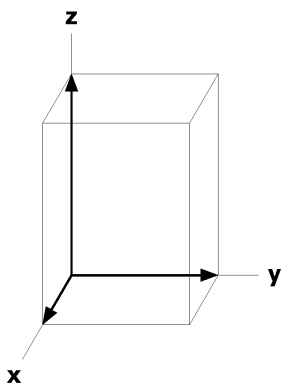
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}+1/2, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
		(3) $\bar{x}, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]		
		(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y+1/2, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
		(7) $x, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(8) $\bar{x}+1/2, y+1/2, z$ [ $u, \bar{v}, \bar{w}$ ]		
4	c .2.	0,y,1/4 [0,v,0]	$1/2, \bar{y}+1/2, 3/4$ [0, $\bar{v}$ ,0]	$0, \bar{y}, 3/4$ [0,v,0]	$1/2, y+1/2, 1/4$ [0, $\bar{v}$ ,0]
4	b $\bar{1}$	0,1/2,0 [u,v,w]	$1/2, 0, 1/2$ [ $\bar{u}, \bar{v}, w$ ]	$0, 1/2, 1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	$1/2, 0, 0$ [ $u, \bar{v}, \bar{w}$ ]
4	a $\bar{1}$	0,0,0 [u,v,w]	$1/2, 1/2, 1/2$ [ $\bar{u}, \bar{v}, w$ ]	$0, 0, 1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	$1/2, 1/2, 0$ [ $u, \bar{v}, \bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1]  $c_p, 2'mm'$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b}, 2m'g'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,1/4,0

Along [0,1,0]  $p_{2b}, 2m'g'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0

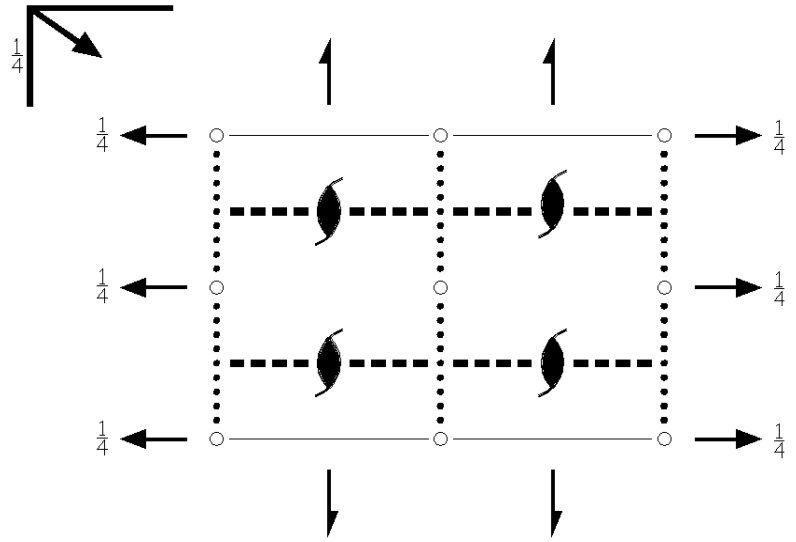
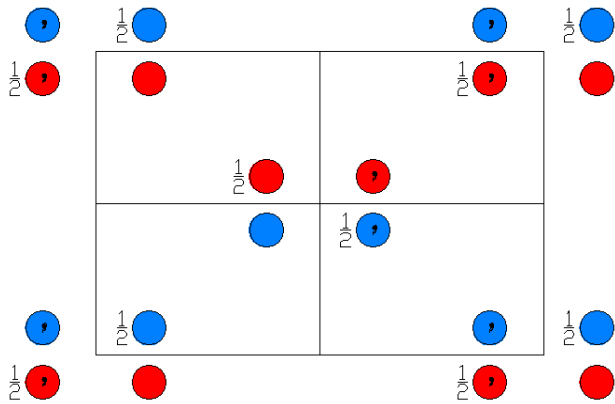


Pbcn1'  
60.2.489

mmm1'  
P2<sub>1</sub>/b2/c2<sub>1</sub>/n1'

Orthorhombic

1'



Origin at  $\bar{1}1'$  on  $1c11'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For 1 + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)         | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (7) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |

For 1' + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1'<br>(1 0,0,0)'                         | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'         | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (7) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

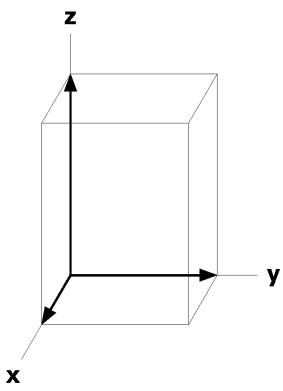
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +		1' +
8 d 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}+1/2, \bar{y}+1/2, z+1/2$ [0,0,0]		
	(3) $\bar{x}, y, \bar{z}+1/2$ [0,0,0]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [0,0,0]		
	(5) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]	(6) $x+1/2, y+1/2, \bar{z}+1/2$ [0,0,0]		
	(7) $x, \bar{y}, z+1/2$ [0,0,0]	(8) $\bar{x}+1/2, y+1/2, z$ [0,0,0]		
4 c .2.1'	0,y,1/4 [0,0,0]	$1/2, \bar{y}+1/2, 3/4$ [0,0,0]	$0, \bar{y}, 3/4$ [0,0,0]	$1/2, y+1/2, 1/4$ [0,0,0]
4 b $\bar{1}1'$	0,1/2,0 [0,0,0]	$1/2, 0, 1/2$ [0,0,0]	0,1/2,1/2 [0,0,0]	$1/2, 0, 0$ [0,0,0]
4 a $\bar{1}1'$	0,0,0 [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]	0,0,1/2 [0,0,0]	$1/2, 1/2, 0$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

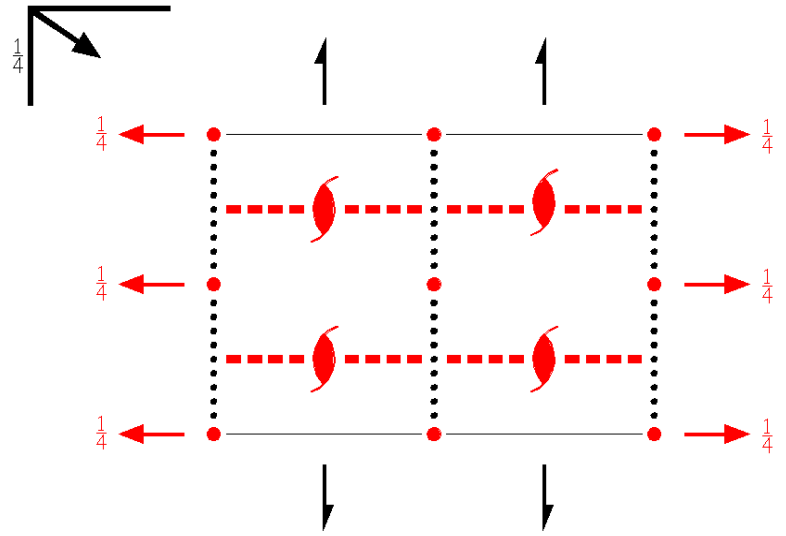
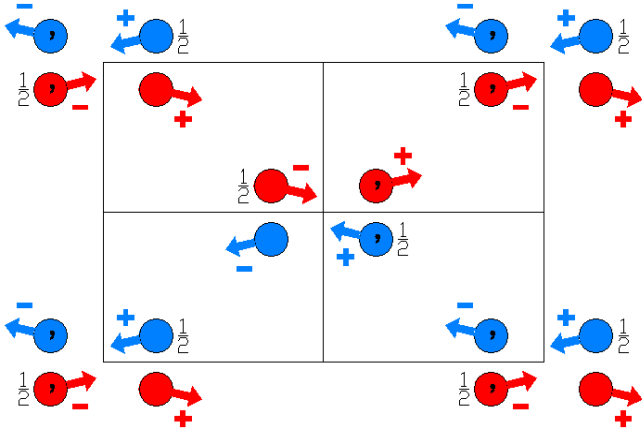
Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pb'cn  
60.3.490

m'mm  
P2<sub>1</sub>/b'2'/c2<sub>1</sub>'/n

Orthorhombic



Origin at  $\bar{1}$ ' on 1c1

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'       | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)   | (7) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

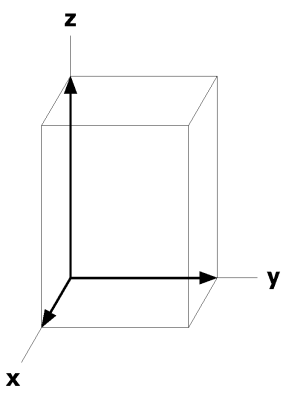
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}+1/2, z+1/2$ [u,v, $\bar{w}$ ]		
		(3) $\bar{x}, \bar{y}, \bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [u,v, $\bar{w}$ ]		
		(5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(6) $x+1/2, y+1/2, \bar{z}+1/2$ [ $\bar{u}$ , $\bar{v}$ ,w]		
		(7) $x, \bar{y}, z+1/2$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(8) $\bar{x}+1/2, y+1/2, z$ [ $\bar{u}$ ,v,w]		
4	c .2'	0,y,1/4 [u,0,w]	$1/2, \bar{y}+1/2, 3/4$ [u,0, $\bar{w}$ ]	$0, \bar{y}, 3/4$ [ $\bar{u}$ ,0, $\bar{w}$ ]	$1/2, y+1/2, 1/4$ [ $\bar{u}$ ,0,w]
4	b $\bar{1}'$	0,1/2,0 [0,0,0]	$1/2, 0, 1/2$ [0,0,0]	$0, 1/2, 1/2$ [0,0,0]	$1/2, 0, 0$ [0,0,0]
4	a $\bar{1}'$	0,0,0 [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]	$0, 0, 1/2$ [0,0,0]	$1/2, 1/2, 0$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $c_p$ -2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p$ 2mg  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

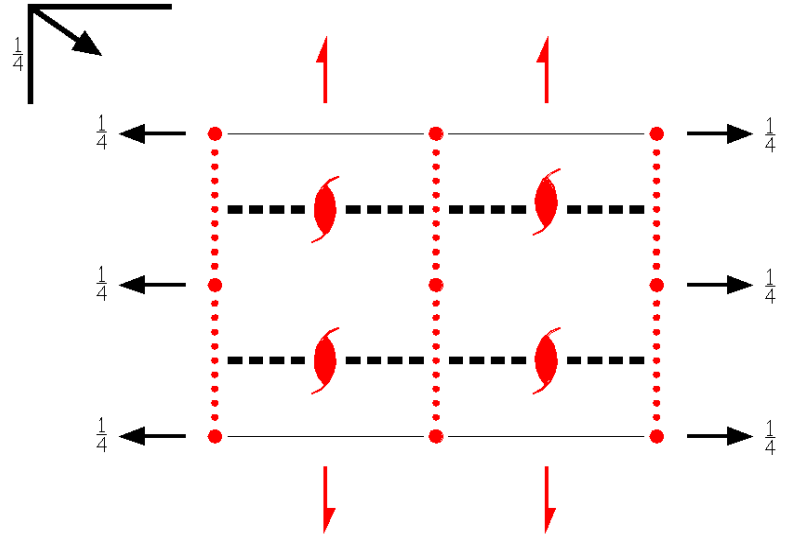
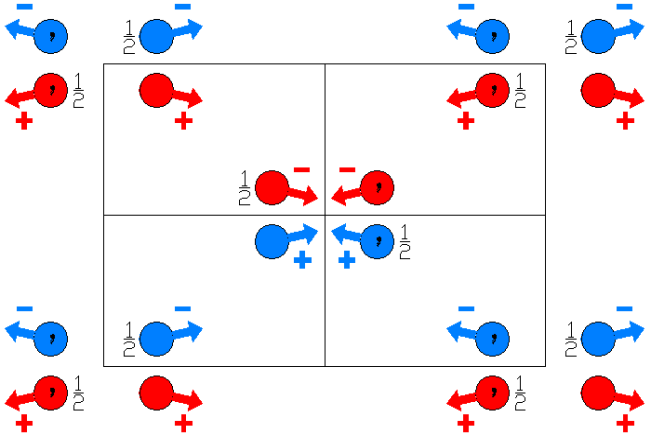
Along [0,1,0]  $p_{2b}$ -2m'g'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pbc'n  
60.4.491

mm'm  
P2<sub>1</sub>'/b2/c'2<sub>1</sub>'/n

Orthorhombic



Origin at  $\bar{1}'$  on  $1c'1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)           | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)   | (7) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

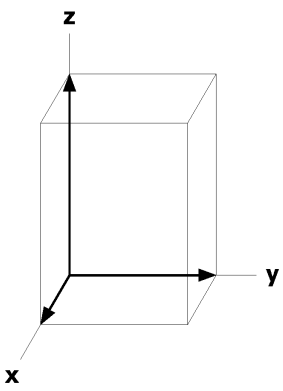
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}+1/2, z+1/2$ [u,v, $\bar{w}$ ]		
		(3) $\bar{x}, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $\bar{u}, v, w$ ]		
		(5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(6) $x+1/2, y+1/2, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
		(7) $x, \bar{y}, z+1/2$ [ $u, \bar{v}, w$ ]	(8) $\bar{x}+1/2, y+1/2, z$ [ $u, \bar{v}, \bar{w}$ ]		
4	c .2.	0,y,1/4 [0,v,0]	1/2, $\bar{y}+1/2, 3/4$ [0,v,0]	0, $\bar{y}, 3/4$ [0, $\bar{v}, 0$ ]	1/2,y+1/2,1/4 [0, $\bar{v}, 0$ ]
4	b $\bar{1}'$	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]
4	a $\bar{1}'$	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $c_p, 2m'm'$   
 $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b}, 2m'g'$   
 $\mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

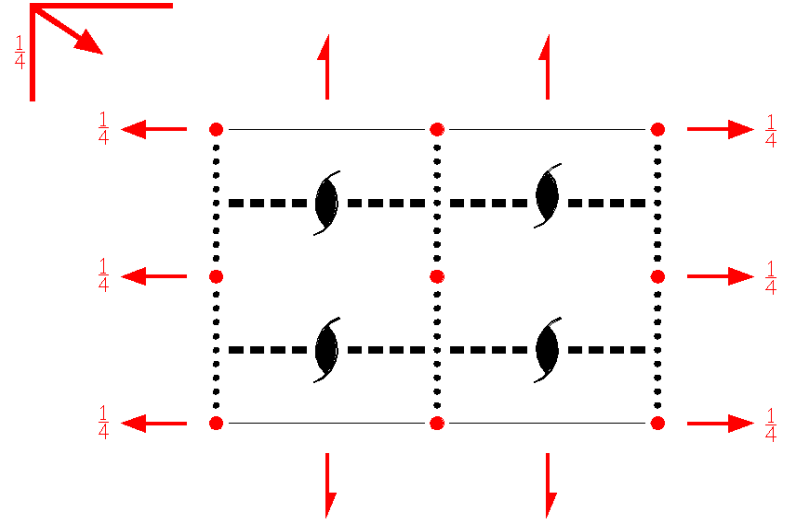
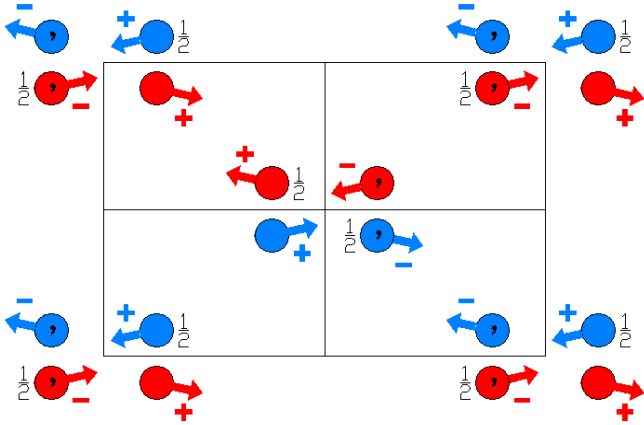
Along [0,1,0]  $p 2mg$   
 $\mathbf{a}^* = -\mathbf{a} \quad \mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pbcn'  
60.5.492

mmm'  
P2<sub>1</sub>'/b2'/c2<sub>1</sub>/n'

Orthorhombic



Origin at  $\bar{1}'$  on 1c1

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)   | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'       | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (7) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

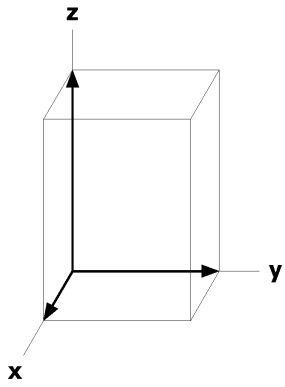
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}+1/2, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
		(3) $\bar{x}, y, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $\bar{u}, v, w$ ]		
		(5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(6) $x+1/2, y+1/2, \bar{z}+1/2$ [ $u, v, \bar{w}$ ]		
		(7) $x, \bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(8) $\bar{x}+1/2, y+1/2, z$ [ $u, \bar{v}, \bar{w}$ ]		
4	c .2'	0,y,1/4 [u,0,w]	$1/2, \bar{y}+1/2, 3/4$ [ $\bar{u}, 0, w$ ]	$0, \bar{y}, 3/4$ [ $\bar{u}, 0, \bar{w}$ ]	$1/2, y+1/2, 1/4$ [ $u, 0, \bar{w}$ ]
4	b $\bar{1}'$	0,1/2,0 [0,0,0]	$1/2, 0, 1/2$ [0,0,0]	0,1/2,1/2 [0,0,0]	$1/2, 0, 0$ [0,0,0]
4	a $\bar{1}'$	0,0,0 [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]	0,0,1/2 [0,0,0]	$1/2, 1/2, 0$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b^*} 2mg$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

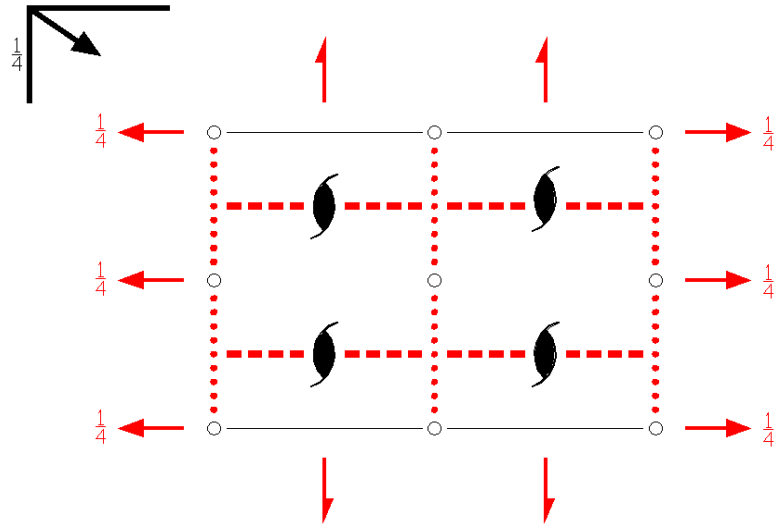
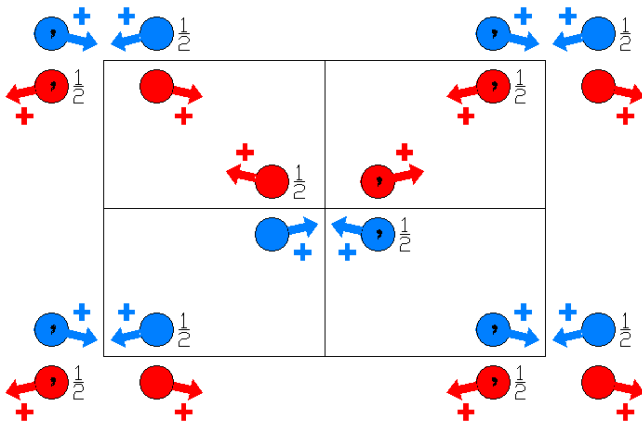
Along [0,1,0]  $p_{2b^*} 2mg$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pb'c'n  
60.6.493

m'm'm  
P2<sub>1</sub>'/b'2'/c'2<sub>1</sub>/n

Orthorhombic



Origin at  $\bar{1}$  on  $1c'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'         | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (7) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

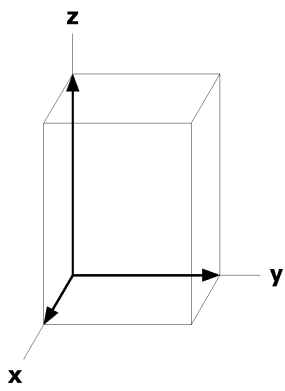
		Coordinates			
		Multiplicity, Wyckoff letter, Site Symmetry.			
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}+1/2, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
		(3) $\bar{x}, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $\bar{u}, v, w$ ]		
		(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y+1/2, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
		(7) $x, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(8) $\bar{x}+1/2, y+1/2, z$ [ $\bar{u}, v, w$ ]		
4	c .2'	0,y,1/4 [u,0,w]	$1/2, \bar{y}+1/2, 3/4$ [ $\bar{u}, 0, w$ ]	$0, \bar{y}, 3/4$ [u,0,w]	$1/2, y+1/2, 1/4$ [ $\bar{u}, 0, w$ ]
4	b $\bar{1}$	0,1/2,0 [u,v,w]	$1/2, 0, 1/2$ [ $\bar{u}, \bar{v}, w$ ]	0,1/2,1/2 [u, $\bar{v}$ ,w]	$1/2, 0, 0$ [ $\bar{u}, v, w$ ]
4	a $\bar{1}$	0,0,0 [u,v,w]	$1/2, 1/2, 1/2$ [ $\bar{u}, \bar{v}, w$ ]	0,0,1/2 [u, $\bar{v}$ ,w]	$1/2, 1/2, 0$ [ $\bar{u}, v, w$ ]

**Symmetry of Special Projections**

Along [0,0,1]  $c_p-2'mm'$   
 $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2'mg'$   
 $\mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

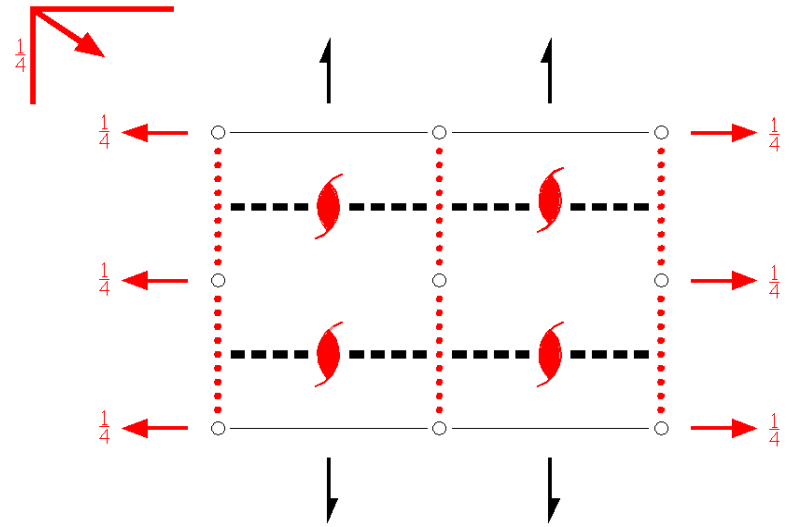
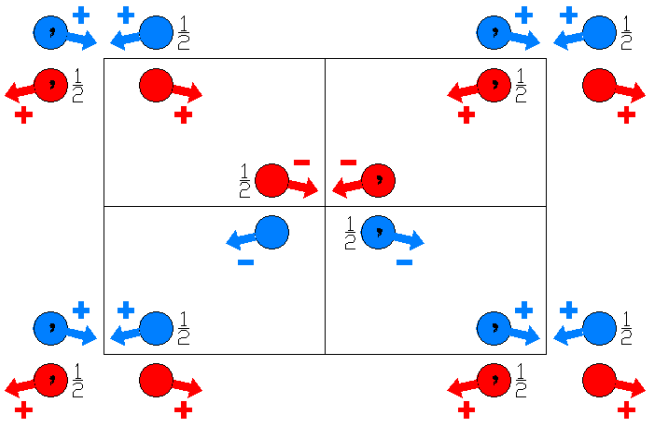
Along [0,1,0]  $p2'm'g$   
 $\mathbf{a}^* = -\mathbf{a} \quad \mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pbc'n'  
60.7.494

mm'm'  
P2<sub>1</sub>/b2'/c'2<sub>1</sub>'/n'

Orthorhombic



Origin at  $\bar{1}$  on  $1c'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'         | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (7) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

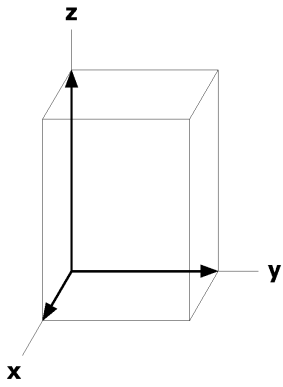
		Coordinates			
		Multiplicity, Wyckoff letter, Site Symmetry.			
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}+1/2, z+1/2$ [u,v, $\bar{w}$ ]		
		(3) $\bar{x}, \bar{y}, \bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [u, $\bar{v}$ , $\bar{w}$ ]		
		(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y+1/2, \bar{z}+1/2$ [u,v, $\bar{w}$ ]		
		(7) $x, \bar{y}, z+1/2$ [u, $\bar{v}$ ,w]	(8) $\bar{x}+1/2, y+1/2, z$ [u, $\bar{v}$ , $\bar{w}$ ]		
4	c .2'	0,y,1/4 [u,0,w]	$1/2, \bar{y}+1/2, 3/4$ [u,0, $\bar{w}$ ]	$0, \bar{y}, 3/4$ [u,0,w]	$1/2, y+1/2, 1/4$ [u,0, $\bar{w}$ ]
4	b $\bar{1}$	0,1/2,0 [u,v,w]	$1/2, 0, 1/2$ [u,v, $\bar{w}$ ]	$0, 1/2, 1/2$ [u, $\bar{v}$ ,w]	$1/2, 0, 0$ [u, $\bar{v}$ , $\bar{w}$ ]
4	a $\bar{1}$	0,0,0 [u,v,w]	$1/2, 1/2, 1/2$ [u,v, $\bar{w}$ ]	$0, 0, 1/2$ [u, $\bar{v}$ ,w]	$1/2, 1/2, 0$ [u, $\bar{v}$ , $\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b} 2mg$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,1/4,0

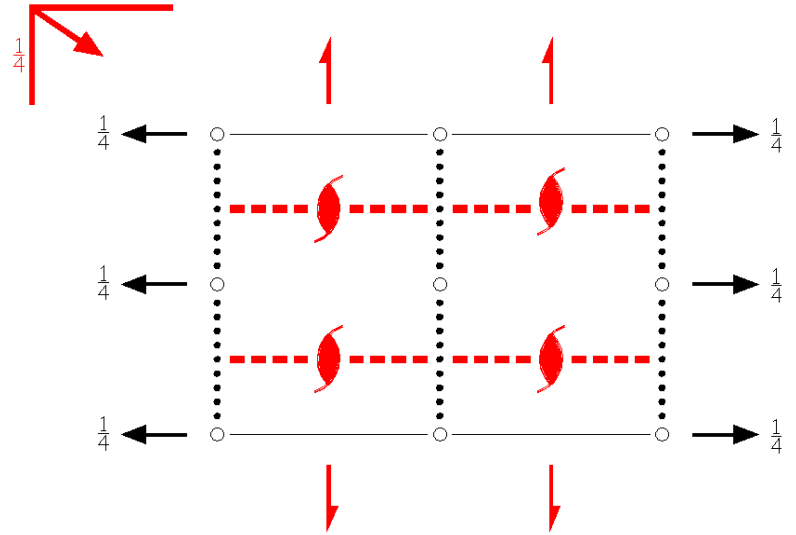
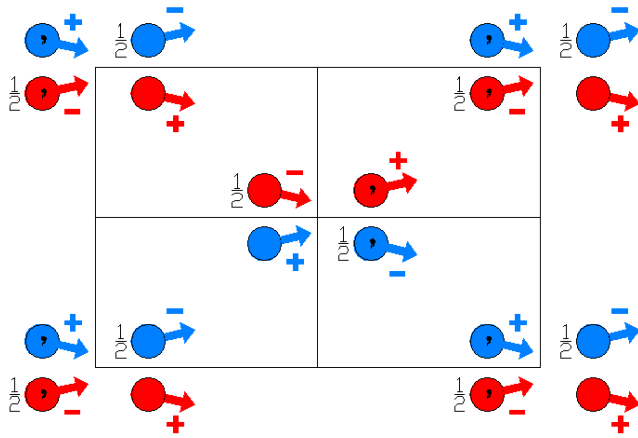
Along [0,1,0]  $p 2' mg'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pb'cn'  
60.8.495

m'mm'  
P2<sub>1</sub>'/b'2/c2<sub>1</sub>'/n'

Orthorhombic



Origin at  $\bar{1}$  on 1c1

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)         | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (7) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

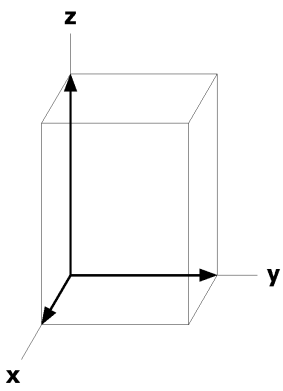
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}+1/2, z+1/2$ [u,v, $\bar{w}$ ]		
		(3) $\bar{x}, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $\bar{u}, v, w$ ]		
		(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y+1/2, \bar{z}+1/2$ [u,v, $\bar{w}$ ]		
		(7) $x, \bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(8) $\bar{x}+1/2, y+1/2, z$ [ $\bar{u}, v, w$ ]		
4	c .2.	0,y,1/4 [0,v,0]	$1/2, \bar{y}+1/2, 3/4$ [0,v,0]	$0, \bar{y}, 3/4$ [0,v,0]	$1/2, y+1/2, 1/4$ [0,v,0]
4	b $\bar{1}$	0,1/2,0 [u,v,w]	$1/2, 0, 1/2$ [u,v, $\bar{w}$ ]	$0, 1/2, 1/2$ [ $\bar{u}, v, \bar{w}$ ]	$1/2, 0, 0$ [ $\bar{u}, v, w$ ]
4	a $\bar{1}$	0,0,0 [u,v,w]	$1/2, 1/2, 1/2$ [u,v, $\bar{w}$ ]	$0, 0, 1/2$ [ $\bar{u}, v, \bar{w}$ ]	$1/2, 1/2, 0$ [ $\bar{u}, v, w$ ]

**Symmetry of Special Projections**

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

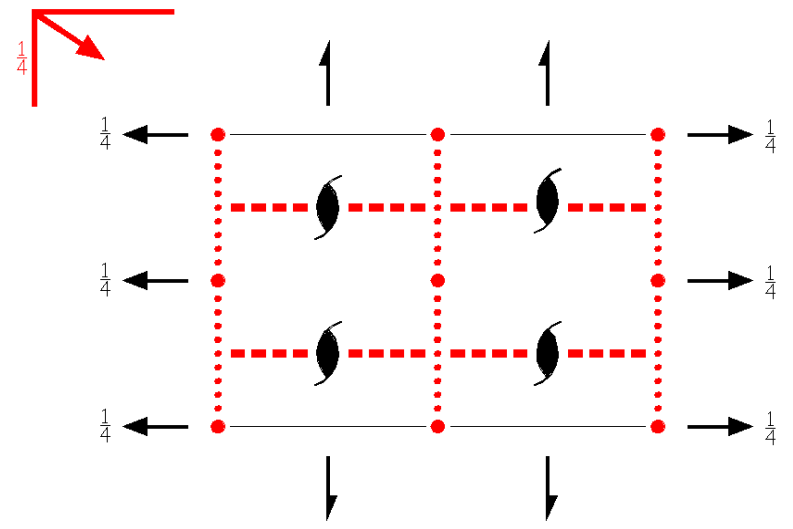
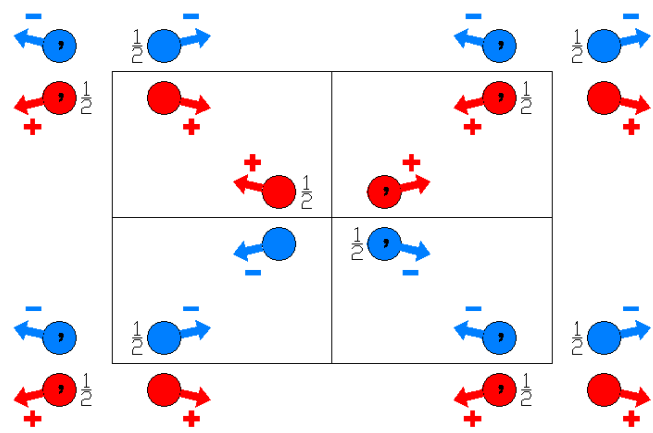
Along [0,1,0] p<sub>2b</sub>'2m'g'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pb'c'n'  
60.9.496

m'm'm'  
P2<sub>1</sub>/b'2/c'2<sub>1</sub>/n'

Orthorhombic



Origin at  $\bar{1}$ ' on 1c'1

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)   | (3) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)           | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (7) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

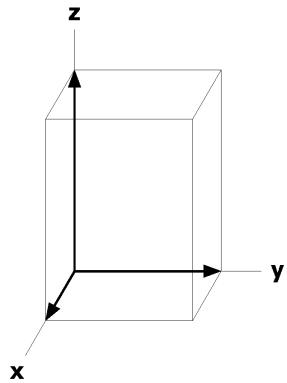
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}+1/2, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
		(3) $\bar{x}, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]		
		(5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(6) $x+1/2, y+1/2, \bar{z}+1/2$ [ $u, v, \bar{w}$ ]		
		(7) $x, \bar{y}, z+1/2$ [ $u, \bar{v}, w$ ]	(8) $\bar{x}+1/2, y+1/2, z$ [ $\bar{u}, v, w$ ]		
4	c .2.	0,y,1/4 [0,v,0]	$1/2, \bar{y}+1/2, 3/4$ [ $0, \bar{v}, 0$ ]	$0, \bar{y}, 3/4$ [ $0, \bar{v}, 0$ ]	$1/2, y+1/2, 1/4$ [0,v,0]
4	b $\bar{1}'$	0,1/2,0 [0,0,0]	$1/2, 0, 1/2$ [0,0,0]	0,1/2,1/2 [0,0,0]	$1/2, 0, 0$ [0,0,0]
4	a $\bar{1}'$	0,0,0 [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]	0,0,1/2 [0,0,0]	$1/2, 1/2, 0$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

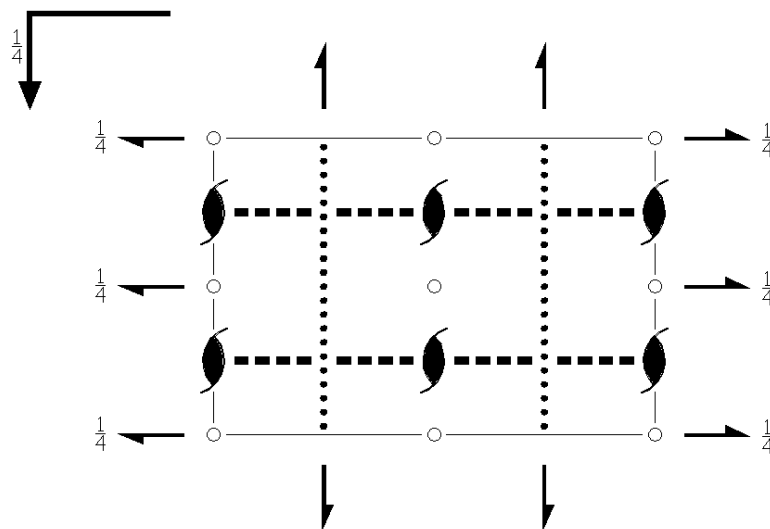
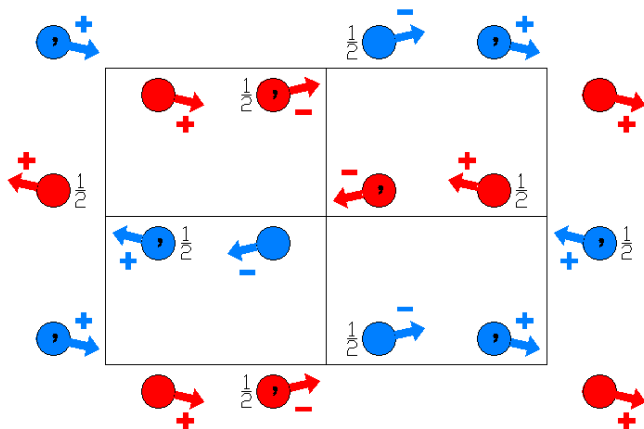
Along [0,1,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pbca  
61.1.497

mmm  
P2<sub>1</sub>/b2<sub>1</sub>/c2<sub>1</sub>/a

Orthorhombic



Origin at  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2) | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

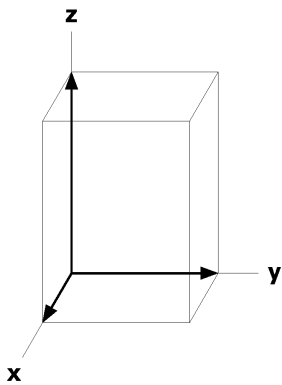
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
		(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]		
		(5) $\bar{x}, \bar{y}, z$ [u,v,w]	(6) $x+1/2, y, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
		(7) $x, \bar{y}+1/2, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(8) $\bar{x}+1/2, y+1/2, z$ [ $u, \bar{v}, \bar{w}$ ]		
4	b $\bar{1}$	0,0,1/2 [u,v,w]	1/2,0,0 [ $\bar{u}, \bar{v}, w$ ]	0,1/2,0 [ $\bar{u}, v, \bar{w}$ ]	1/2,1/2,1/2 [ $u, \bar{v}, \bar{w}$ ]
4	a $\bar{1}$	0,0,0 [u,v,w]	1/2,0,1/2 [ $\bar{u}, \bar{v}, w$ ]	0,1/2,1/2 [ $\bar{u}, v, \bar{w}$ ]	1/2,1/2,0 [ $u, \bar{v}, \bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2b} \cdot 2mg$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,0,z

Along [1,0,0]  $p_{2b} \cdot 2mg$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,1/4,0

Along [0,1,0]  $p_{2b} \cdot 2mg$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,1/4

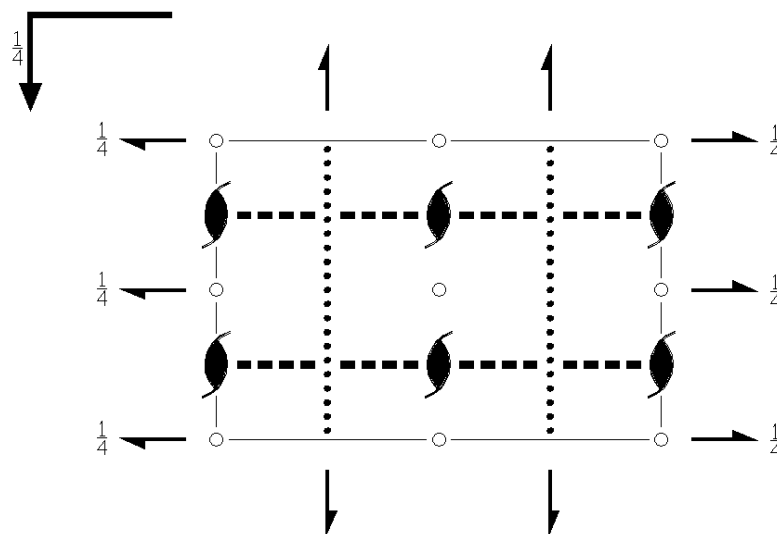
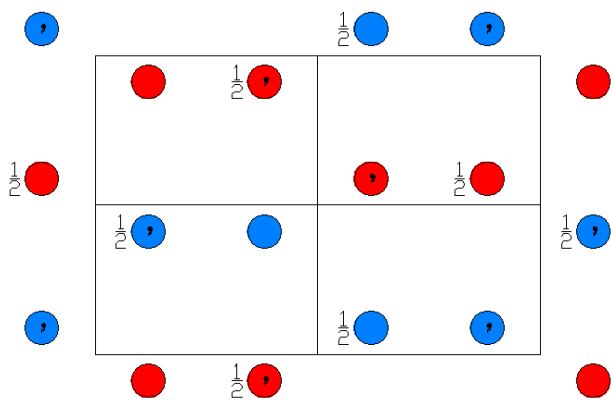


Pbca1'  
61.2.498

mmm1'  
P2<sub>1</sub>/b2<sub>1</sub>/c2<sub>1</sub>/a1'

Orthorhombic

1'



Origin at  $\bar{1}1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

For 1 + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2) | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |

For 1' + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1'<br>(1 0,0,0)'                         | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

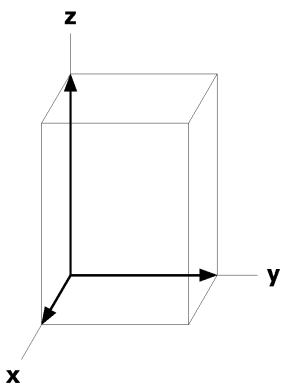
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
8 c 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [0,0,0]		
	(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [0,0,0]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [0,0,0]		
	(5) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]	(6) $x+1/2, y, \bar{z}+1/2$ [0,0,0]		
	(7) $x, \bar{y}+1/2, z+1/2$ [0,0,0]	(8) $\bar{x}+1/2, y+1/2, z$ [0,0,0]		
4 b $\bar{1}1'$	0,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]
4 a $\bar{1}1'$	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p2mg1'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

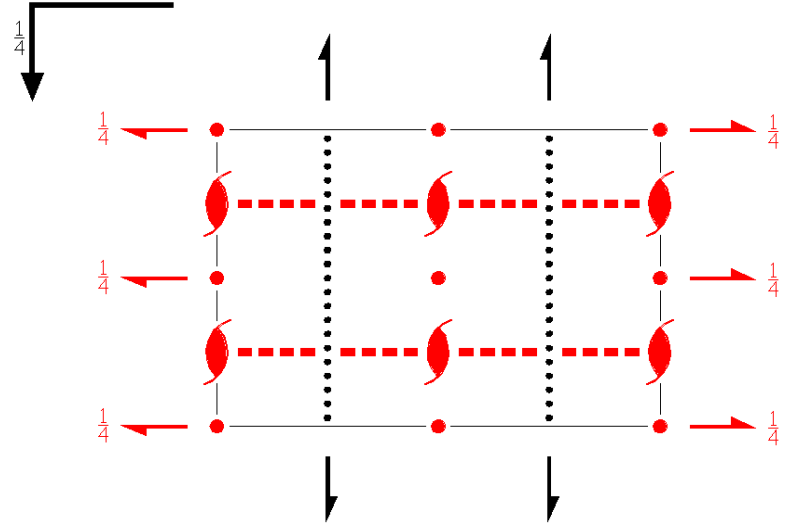
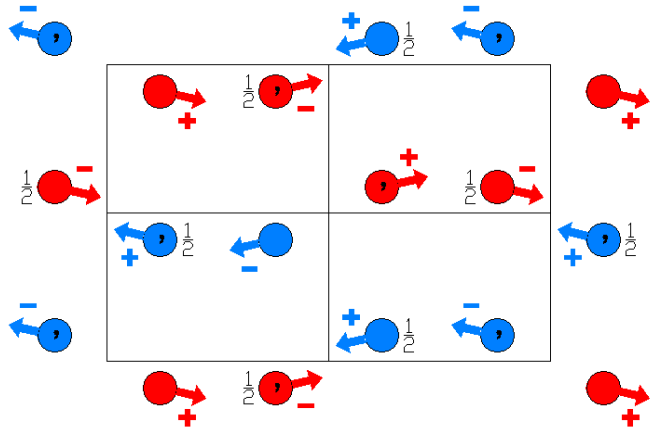
Along [0,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pb'ca  
61.3.499

m'mm  
P2<sub>1</sub>/b'2<sub>1</sub>'/c2<sub>1</sub>'/a

Orthorhombic



Origin at  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)   | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)   | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

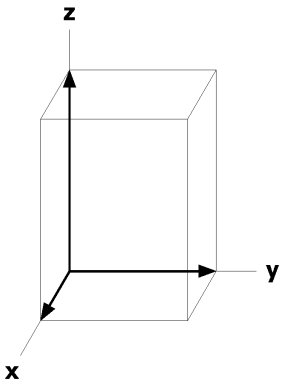
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [u,v, $\bar{w}$ ]		
		(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [u, $\bar{v}$ , $\bar{w}$ ]		
		(5) $\bar{x}, \bar{y}, z$ [ $\bar{u}$ , $\bar{v}$ ,w]	(6) $x+1/2, y, \bar{z}+1/2$ [ $\bar{u}$ , $\bar{v}$ ,w]		
		(7) $x, \bar{y}+1/2, z+1/2$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(8) $\bar{x}+1/2, y+1/2, z$ [ $\bar{u}$ ,v,w]		
4	b $\bar{1}'$	0,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]
4	a $\bar{1}'$	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2b} \cdot 2m_g$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2m_g}$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

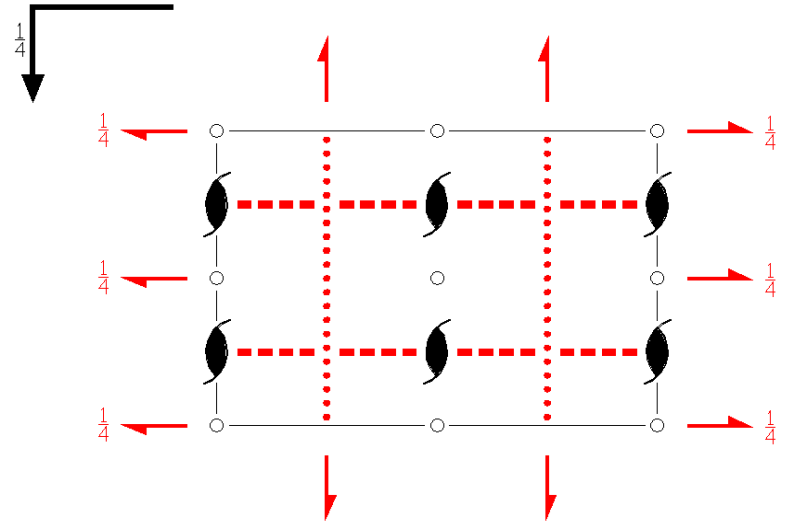
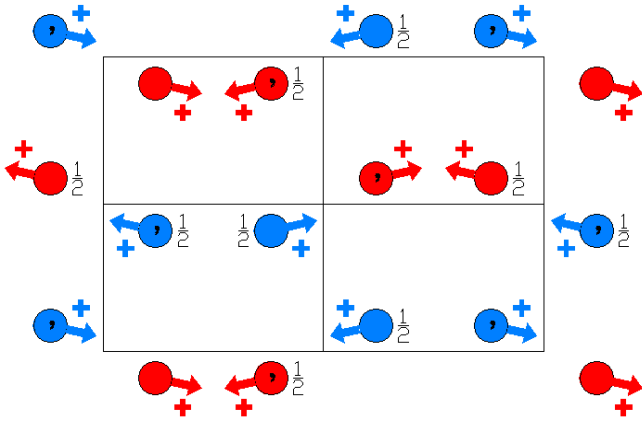
Along [0,1,0]  $p_{2b} \cdot 2m'_g$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pb'c'a  
61.4.500

m'm'm  
P2<sub>1</sub>'/b'2<sub>1</sub>'/c'2<sub>1</sub>/a

Orthorhombic



Origin at  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2) | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

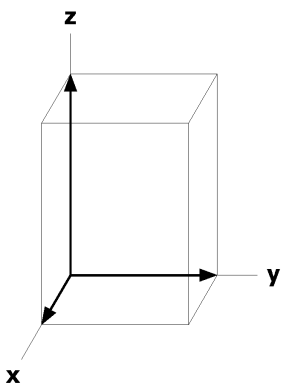
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
		(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]		
		(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
		(7) $x, \bar{y}+1/2, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(8) $\bar{x}+1/2, y+1/2, z$ [ $\bar{u}, \bar{v}, w$ ]		
4	b $\bar{1}$	0,0,1/2 [u,v,w]	1/2,0,0 [ $\bar{u}, \bar{v}, w$ ]	0,1/2,0 [ $\bar{u}, \bar{v}, w$ ]	1/2,1/2,1/2 [ $\bar{u}, \bar{v}, w$ ]
4	a $\bar{1}$	0,0,0 [u,v,w]	1/2,0,1/2 [ $\bar{u}, \bar{v}, w$ ]	0,1/2,1/2 [ $\bar{u}, \bar{v}, w$ ]	1/2,1/2,0 [ $\bar{u}, \bar{v}, w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p2m'g'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

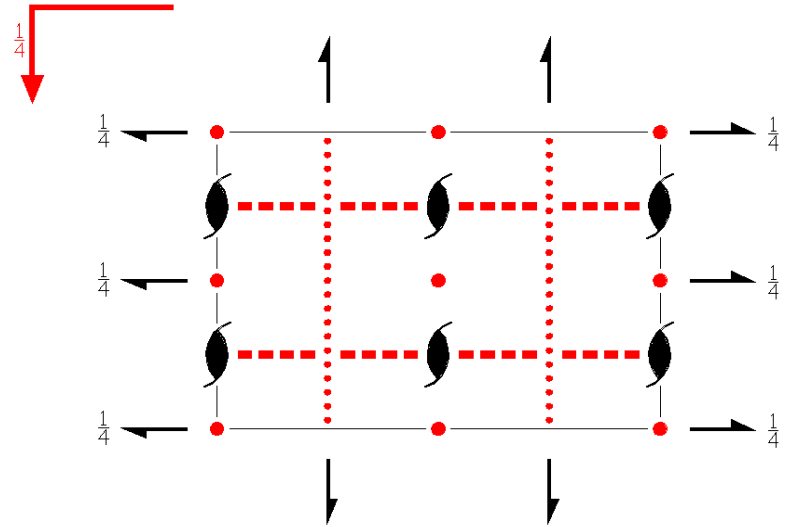
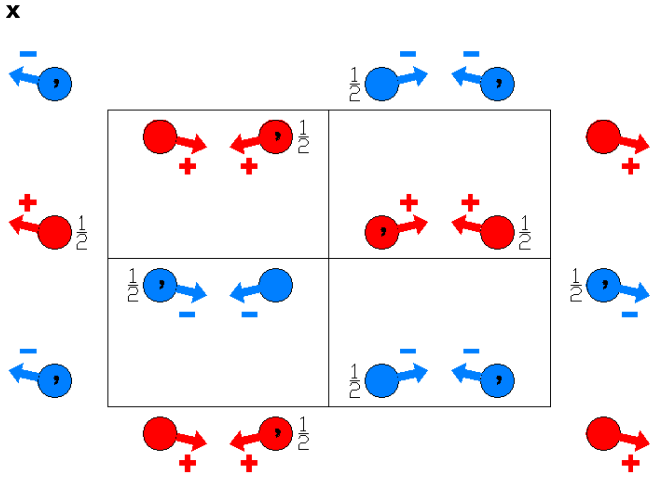
Along [0,1,0] p2'm'g  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pb'c'a'  
61.5.501

m'm'm'  
P2<sub>1</sub>/b'2<sub>1</sub>/c'2<sub>1</sub>/a'

Orthorhombic



Origin at  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

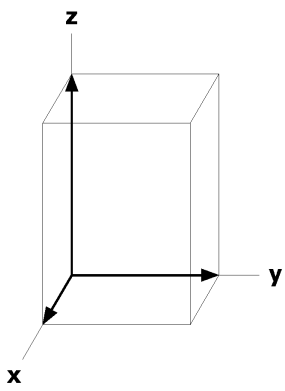
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	c 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
		(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]		
		(5) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(6) $x+1/2, y, \bar{z}+1/2$ [ $u, v, \bar{w}$ ]		
		(7) $x, \bar{y}+1/2, z+1/2$ [ $u, \bar{v}, w$ ]	(8) $\bar{x}+1/2, y+1/2, z$ [ $\bar{u}, v, w$ ]		
4	b $\bar{1}'$	0,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]
4	a $\bar{1}'$	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $p2m'g'$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0]  $p2m'g'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

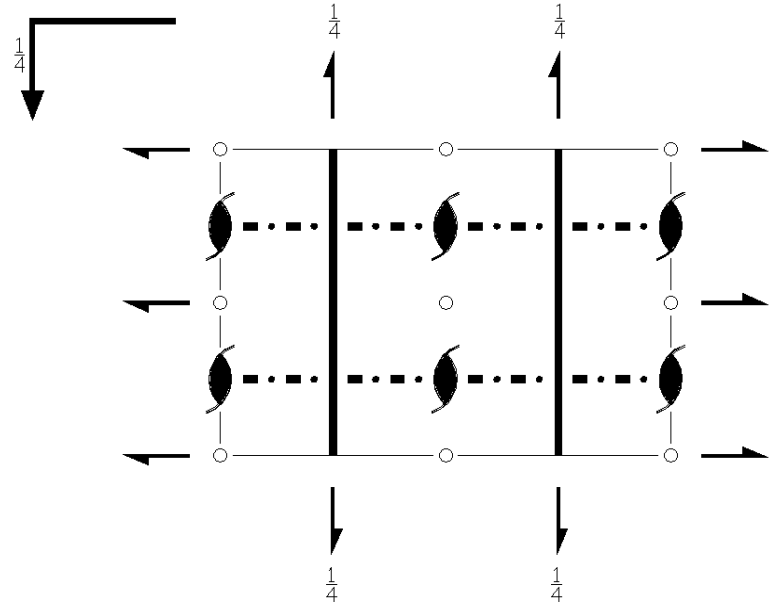
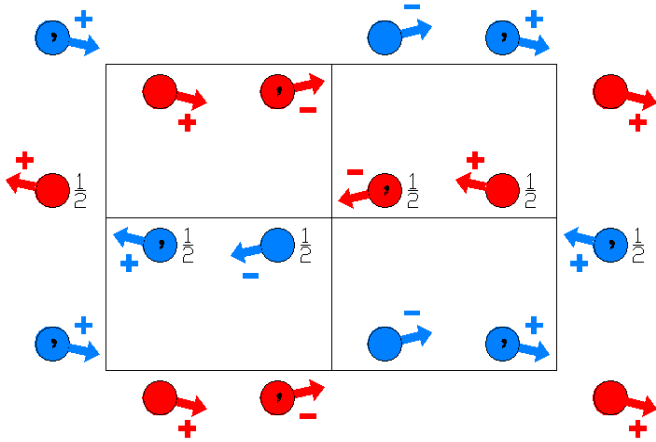
Along [0,1,0]  $p2m'g'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Pnma  
62.1.502

mmm  
P2<sub>1</sub>/n2<sub>1</sub>/m2<sub>1</sub>/a

Orthorhombic



Origin at  $\bar{1}$  on 12<sub>1</sub>1

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) 2 (0,1/2,0) 0,y,0<br>(2 <sub>y</sub>  0,1/2,0) | (4) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2) | (7) m x,1/4,z<br>(m <sub>y</sub>  0,1/2,0)         | (8) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

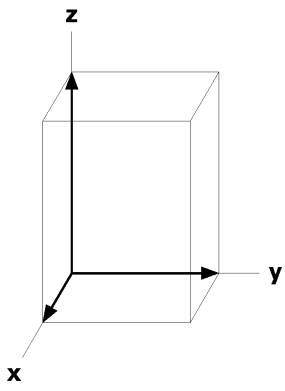
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) $x+1/2,y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
4	c .m.	x,1/4,z [0,v,0]	$\bar{x}+1/2,3/4,z+1/2$ [0, $\bar{v}$ ,0]	$\bar{x},3/4,\bar{z}$ [0,v,0]	$x+1/2,1/4,\bar{z}+1/2$ [0, $\bar{v}$ ,0]
4	b $\bar{1}$	0,0,1/2 [u,v,w]	1/2,0,0 [ $\bar{u},\bar{v},w$ ]	0,1/2,1/2 [ $\bar{u},v,\bar{w}$ ]	1/2,1/2,0 [u, $\bar{v},\bar{w}$ ]
4	a $\bar{1}$	0,0,0 [u,v,w]	1/2,0,1/2 [ $\bar{u},\bar{v},w$ ]	0,1/2,0 [ $\bar{u},v,\bar{w}$ ]	1/2,1/2,1/2 [u, $\bar{v},\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2b}2mg$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,0,z

Along [1,0,0]  $c_p2mm$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [0,1,0]  $p2gg1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pnma1'

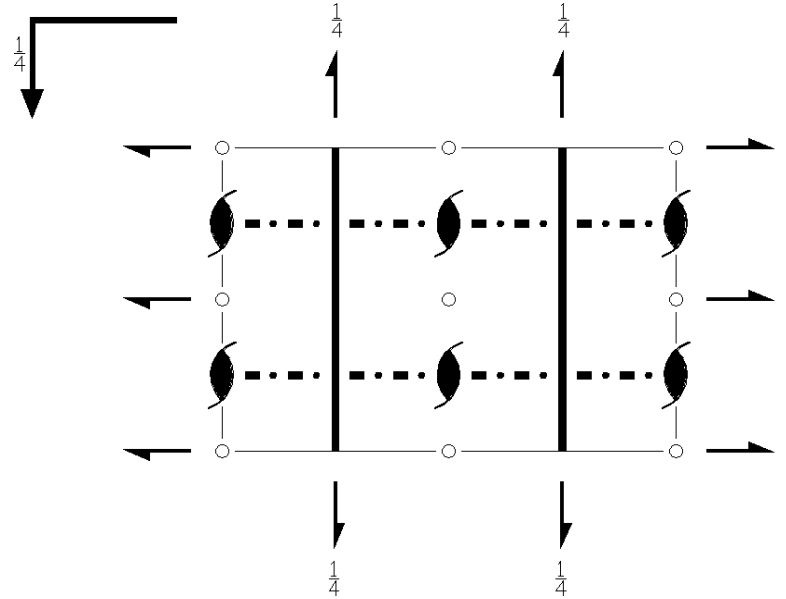
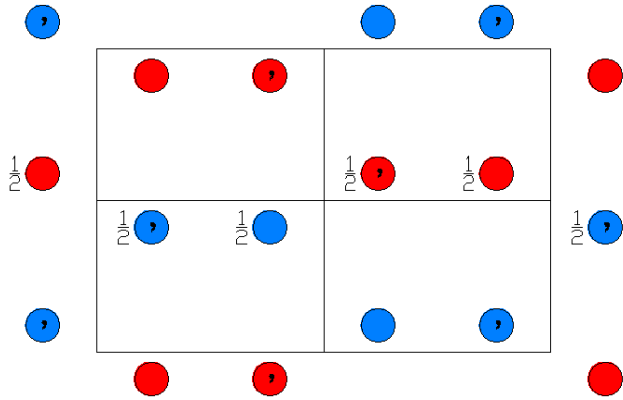
62.2.503

mmm1'

P2<sub>1</sub>/n2<sub>1</sub>/m2<sub>1</sub>/a1'

Orthorhombic

1'



Origin at  $\bar{1}1'$  on 12,11'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

Symmetry Operations

For 1 + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) 2 (0,1/2,0) 0,y,0<br>(2 <sub>y</sub>  0,1/2,0) | (4) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2) | (7) m x,1/4,z<br>(m <sub>y</sub>  0,1/2,0)         | (8) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) |

For 1' + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1'<br>(1 0,0,0)'                         | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) 2' (0,1/2,0) 0,y,0<br>(2 <sub>y</sub>  0,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) m' x,1/4,z<br>(m <sub>y</sub>  0,1/2,0)'         | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

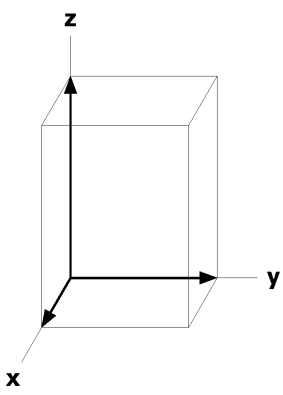
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +	1' +		
8 d 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [0,0,0]	(3) $\bar{x},y+1/2,\bar{z}$ [0,0,0]	(4) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [0,0,0]
	(5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(6) $x+1/2,y,\bar{z}+1/2$ [0,0,0]	(7) $x,\bar{y}+1/2,z$ [0,0,0]	(8) $\bar{x}+1/2,y+1/2,z+1/2$ [0,0,0]
4 c .m.1'	x,1/4,z [0,0,0]	$\bar{x}+1/2,3/4,z+1/2$ [0,0,0]	$\bar{x},3/4,\bar{z}$ [0,0,0]	$x+1/2,1/4,\bar{z}+1/2$ [0,0,0]
4 b $\bar{1}1'$	0,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
4 a $\bar{1}1'$	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p2mg1'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

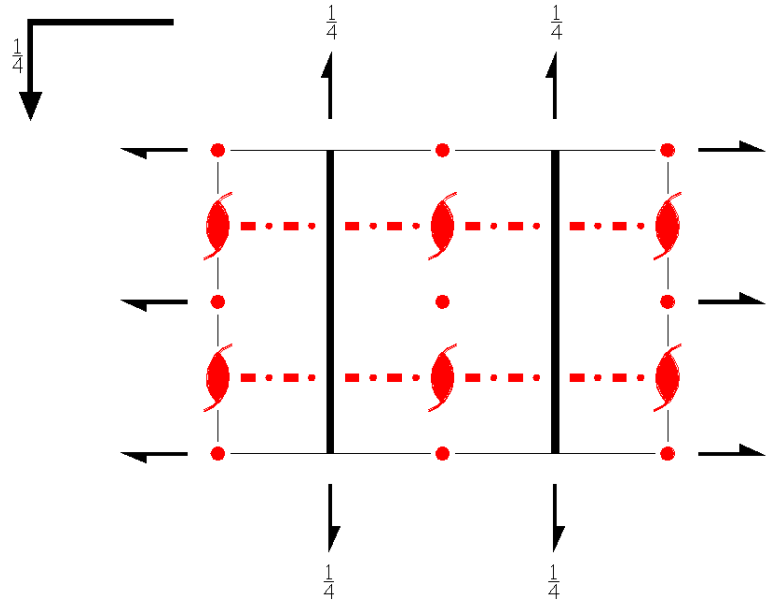
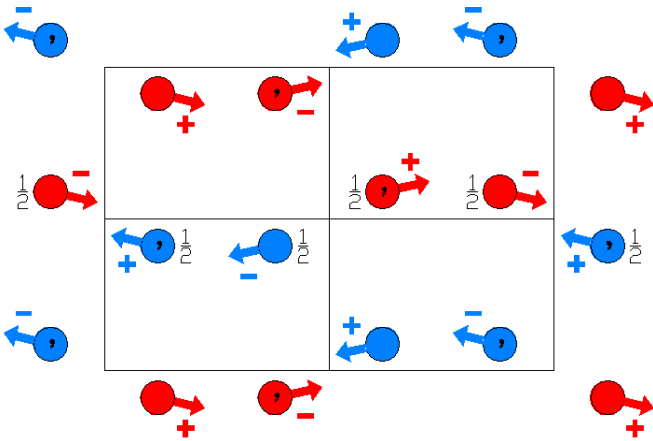
Along [0,1,0] p2gg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pn'ma  
62.3.504

m'mm  
P2<sub>1</sub>/n2<sub>1</sub>'/m2<sub>1</sub>'/a

Orthorhombic



Origin at  $\bar{1}$ ' on 12,1'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

### Symmetry Operations

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) 2' (0,1/2,0) 0,y,0<br>(2 <sub>y</sub>  0,1/2,0)' | (4) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)   |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)   | (7) m x,1/4,z<br>(m <sub>y</sub>  0,1/2,0)           | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

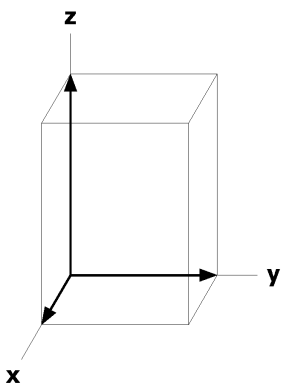
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}$ [u, $\bar{v}$ ,w]	(4) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]
4	c .m.	x,1/4,z [0,v,0]	$\bar{x}+1/2,3/4,z+1/2$ [0,v,0]	$\bar{x},3/4,\bar{z}$ [0, $\bar{v}$ ,0]	$x+1/2,1/4,\bar{z}+1/2$ [0, $\bar{v}$ ,0]
4	b $\bar{1}'$	0,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
4	a $\bar{1}'$	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2b}2mg$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2mm$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

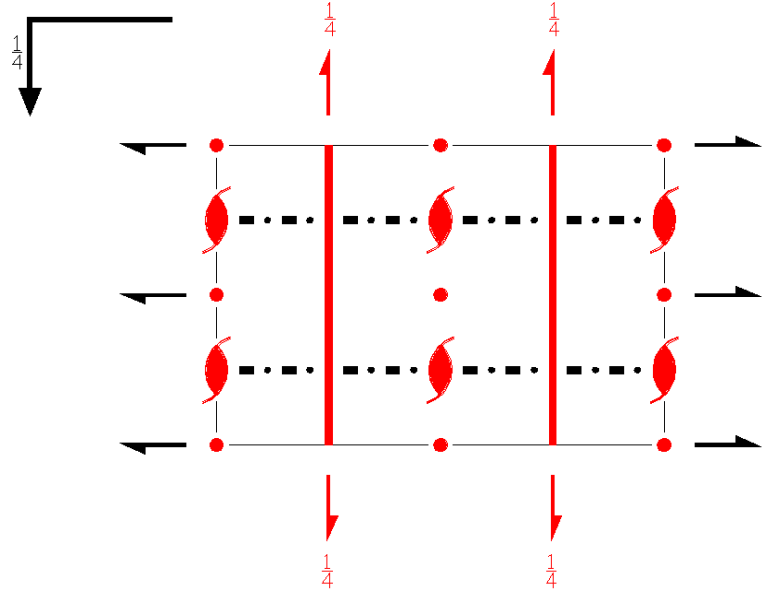
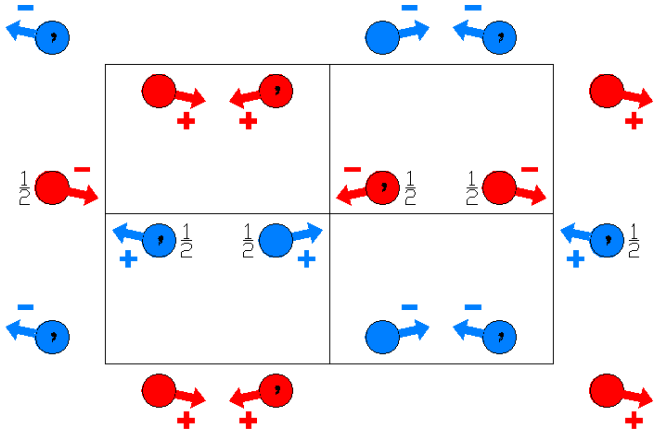
Along [0,1,0]  $p2gg1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pnm'a  
62.4.505

mm'm  
P2<sub>1</sub>'/n2<sub>1</sub>/m'2<sub>1</sub>'/a

Orthorhombic



Origin at  $\bar{1}'$  on 12,1

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) 2 (0,1/2,0) 0,y,0<br>(2 <sub>y</sub>  0,1/2,0) | (4) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)   | (7) m' x,1/4,z<br>(m <sub>y</sub>  0,1/2,0)'       | (8) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)   |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

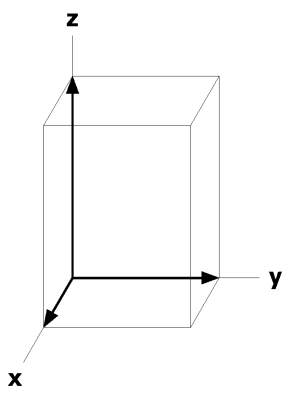
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y}+1/2,z$ [u, $\bar{v},w$ ]	(8) $\bar{x}+1/2,y+1/2,z+1/2$ [u, $\bar{v},\bar{w}$ ]
4	c .m'	x,1/4,z [u,0,w]	$\bar{x}+1/2,3/4,z+1/2$ [u,0, $\bar{w}$ ]	$\bar{x},3/4,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	$x+1/2,1/4,\bar{z}+1/2$ [ $\bar{u},0,w$ ]
4	b $\bar{1}'$	0,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
4	a $\bar{1}'$	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2b} \cdot 2m'g'$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,1/4,1/4

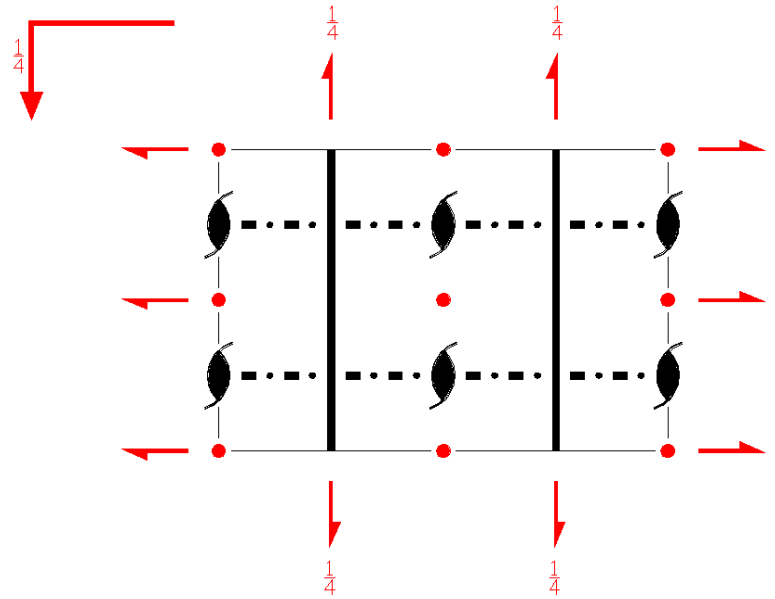
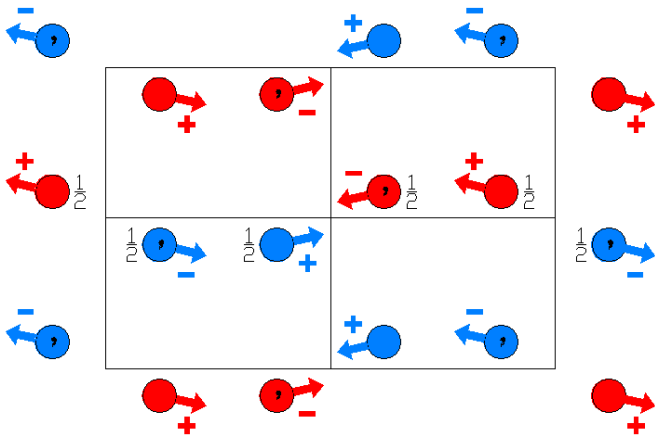
Along [0,1,0]  $p2gg$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pnma'  
62.5.506

mmm'  
P2<sub>1</sub>'/n2<sub>1</sub>'/m2<sub>1</sub>'/a'

Orthorhombic



Origin at  $\bar{1}$ ' on 12,1'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

### Symmetry Operations

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2' (0,1/2,0) 0,y,0<br>(2 <sub>y</sub>  0,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) m x,1/4,z<br>(m <sub>y</sub>  0,1/2,0)           | (8) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

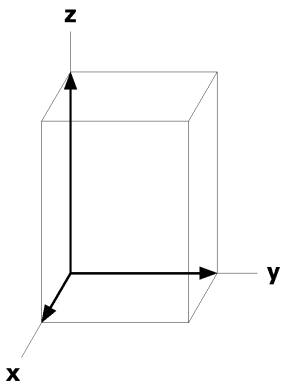
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y+1/2, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(4) $x+1/2, \bar{y}+1/2, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]
		(5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(6) $x+1/2, y, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(7) $x, \bar{y}+1/2, z$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(8) $\bar{x}+1/2, y+1/2, z+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]
4	c .m.	x,1/4,z [0,v,0]	$\bar{x}+1/2, 3/4, z+1/2$ [0, $\bar{v}$ ,0]	$\bar{x}, 3/4, \bar{z}$ [0, $\bar{v}$ ,0]	$x+1/2, 1/4, \bar{z}+1/2$ [0,v,0]
4	b $\bar{1}'$	0,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
4	a $\bar{1}'$	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p2mg  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0]  $c_p, 2'mm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

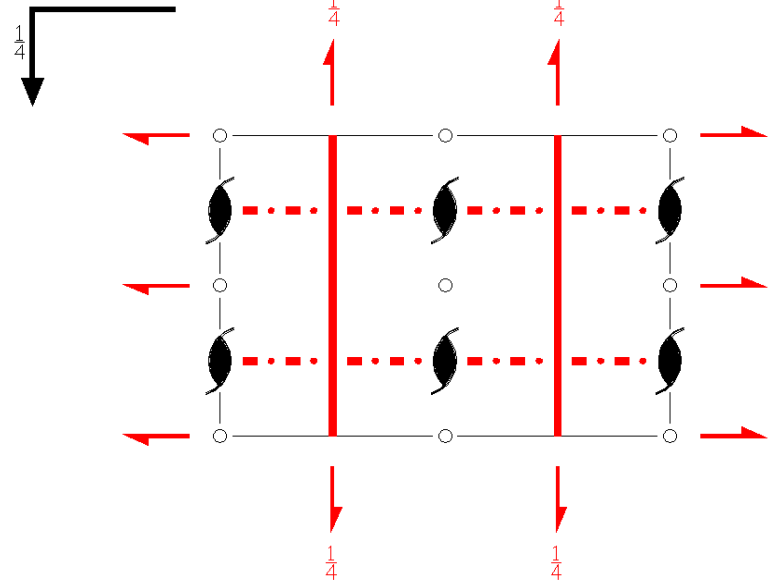
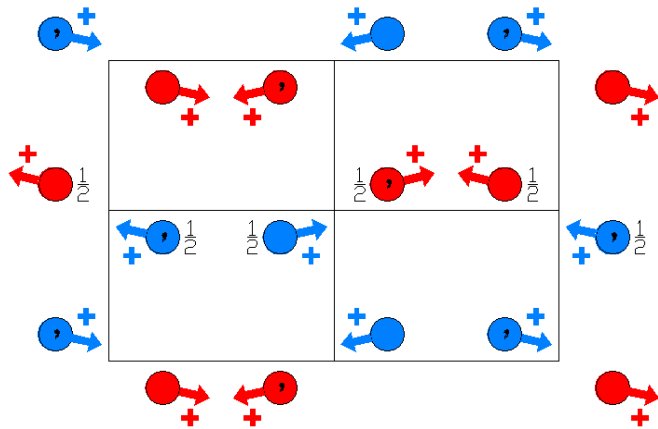
Along [0,1,0] p2gg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pn'm'a  
62.6.507

m'm'm  
P2<sub>1</sub>'n'2<sub>1</sub>'m'2<sub>1</sub>/a

Orthorhombic



Origin at  $\bar{1}$  on 12<sub>1</sub>'1

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) 2' (0,1/2,0) 0,y,0<br>(2 <sub>y</sub>  0,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2) | (7) m' x,1/4,z<br>(m <sub>y</sub>  0,1/2,0)'         | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

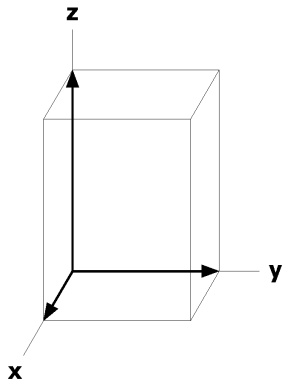
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y+1/2, \bar{z}$ [u, $\bar{v}, w$ ]	(4) $x+1/2, \bar{y}+1/2, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]
		(5) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(6) $x+1/2, y, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(7) $x, \bar{y}+1/2, z$ [u, $\bar{v}, w$ ]	(8) $\bar{x}+1/2, y+1/2, z+1/2$ [ $\bar{u}, v, w$ ]
4	c .m'	x, 1/4, z [u, 0, w]	$\bar{x}+1/2, 3/4, z+1/2$ [ $\bar{u}, 0, w$ ]	$\bar{x}, 3/4, \bar{z}$ [u, 0, w]	$x+1/2, 1/4, \bar{z}+1/2$ [ $\bar{u}, 0, w$ ]
4	b $\bar{1}$	0, 0, 1/2 [u, v, w]	1/2, 0, 0 [ $\bar{u}, \bar{v}, w$ ]	0, 1/2, 1/2 [u, $\bar{v}, w$ ]	1/2, 1/2, 0 [ $\bar{u}, v, w$ ]
4	a $\bar{1}$	0, 0, 0 [u, v, w]	1/2, 0, 1/2 [ $\bar{u}, \bar{v}, w$ ]	0, 1/2, 0 [u, $\bar{v}, w$ ]	1/2, 1/2, 1/2 [ $\bar{u}, v, w$ ]

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2b} \cdot 2m'g'$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x, 1/4, 1/4

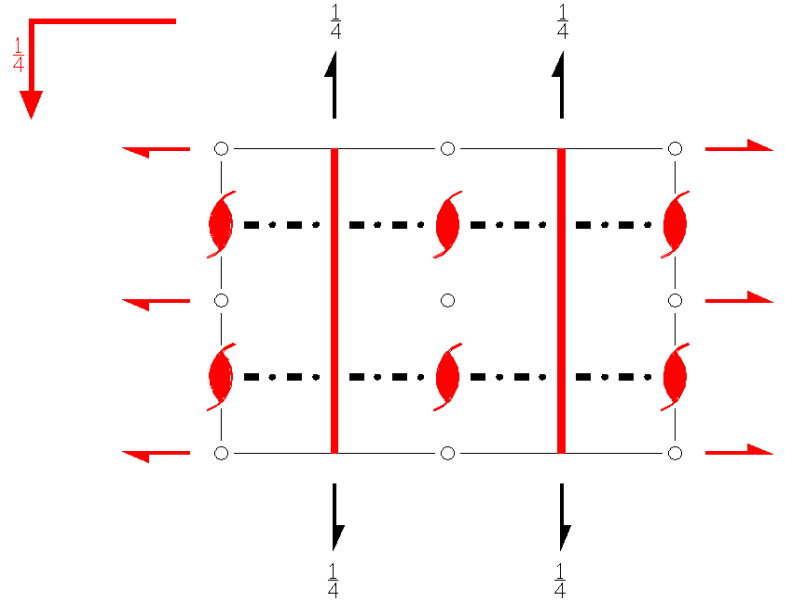
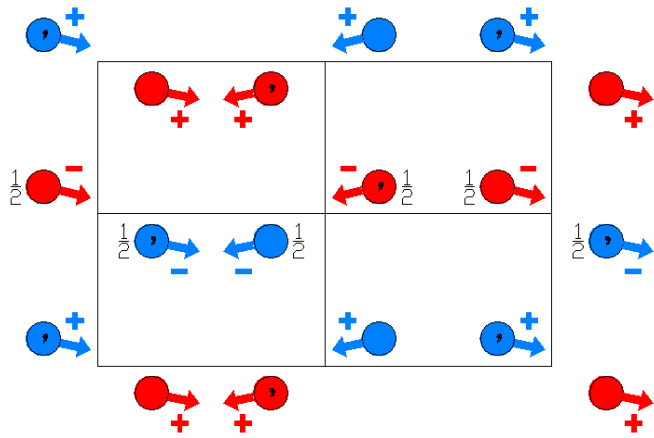
Along [0,1,0]  $p2'gg'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pnm'a'  
62.7.508

mm'm'  
P2<sub>1</sub>/n2<sub>1</sub>'/m'2<sub>1</sub>'/a'

Orthorhombic



Origin at  $\bar{1}$  on 12<sub>1</sub>'1

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) 2' (0,1/2,0) 0,y,0<br>(2 <sub>y</sub>  0,1/2,0)' | (4) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) m' x,1/4,z<br>(m <sub>y</sub>  0,1/2,0)'         | (8) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

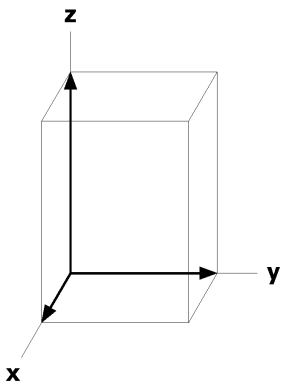
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	d 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}$ [u, $\bar{v}$ ,w]	(4) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) $x+1/2,y,\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(7) $x,\bar{y}+1/2,z$ [u, $\bar{v}$ ,w]	(8) $\bar{x}+1/2,y+1/2,z+1/2$ [u, $\bar{v},\bar{w}$ ]
4	c .m'	$x,1/4,z$ [u,0,w]	$\bar{x}+1/2,3/4,z+1/2$ [u,0, $\bar{w}$ ]	$\bar{x},3/4,\bar{z}$ [u,0,w]	$x+1/2,1/4,\bar{z}+1/2$ [u,0, $\bar{w}$ ]
4	b $\bar{1}$	$0,0,1/2$ [u,v,w]	$1/2,0,0$ [u,v, $\bar{w}$ ]	$0,1/2,1/2$ [u, $\bar{v}$ ,w]	$1/2,1/2,0$ [u, $\bar{v},\bar{w}$ ]
4	a $\bar{1}$	$0,0,0$ [u,v,w]	$1/2,0,1/2$ [u,v, $\bar{w}$ ]	$0,1/2,0$ [u, $\bar{v}$ ,w]	$1/2,1/2,1/2$ [u, $\bar{v},\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1]  $p2'm'g$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0]  $c_p, 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,1/4,1/4$

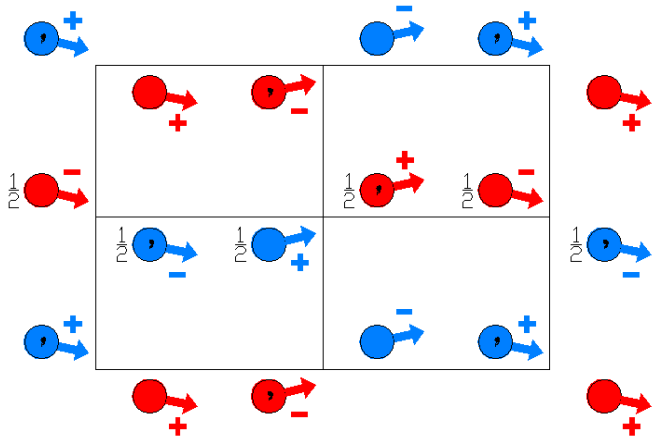
Along [0,1,0]  $p2'gg'$   
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Pn'ma'  
62.8.509

m'mm'  
P2<sub>1</sub>'/n'2<sub>1</sub>/m2<sub>1</sub>'/a'

Orthorhombic

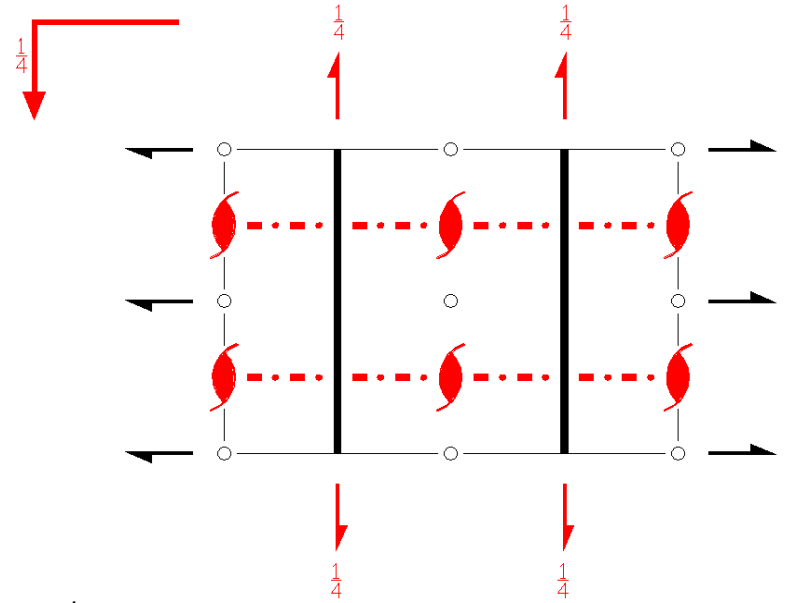


Origin at  $\bar{1}$  on 12<sub>1</sub>1

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) 2 (0,1/2,0) 0,y,0<br>(2 <sub>y</sub>  0,1/2,0) | (4) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) m x,1/4,z<br>(m <sub>y</sub>  0,1/2,0)         | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

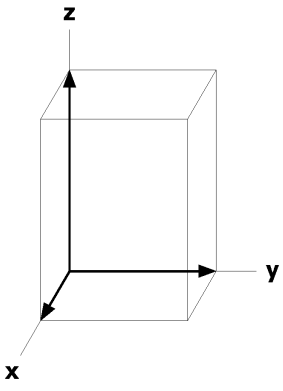
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) $x+1/2,y,\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(7) $x,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]
4	c .m.	x,1/4,z [0,v,0]	$\bar{x}+1/2,3/4,z+1/2$ [0,v,0]	$\bar{x},3/4,\bar{z}$ [0,v,0]	$x+1/2,1/4,\bar{z}+1/2$ [0,v,0]
4	b $\bar{1}$	0,0,1/2 [u,v,w]	1/2,0,0 [u,v, $\bar{w}$ ]	0,1/2,1/2 [ $\bar{u},v,\bar{w}$ ]	1/2,1/2,0 [ $\bar{u},v,w$ ]
4	a $\bar{1}$	0,0,0 [u,v,w]	1/2,0,1/2 [u,v, $\bar{w}$ ]	0,1/2,0 [ $\bar{u},v,\bar{w}$ ]	1/2,1/2,1/2 [ $\bar{u},v,w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p2'mg'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

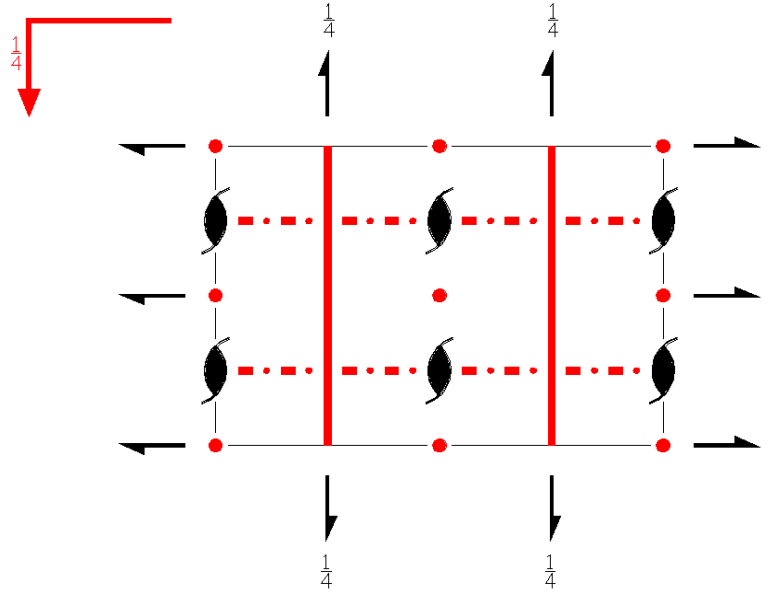
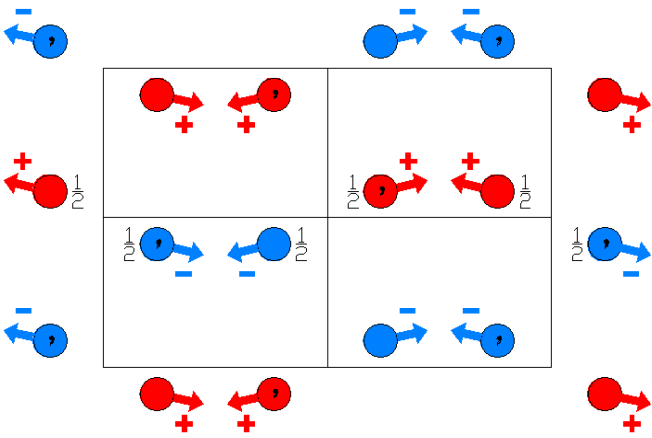
Along [0,1,0] p2gg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Pn'm'a'  
62.9.510

m'm'm'  
P2<sub>1</sub>/n'2<sub>1</sub>/m'2<sub>1</sub>/a'

Orthorhombic



Origin at  $\bar{1}$ ' on 12,1

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 (0,1/2,0) 0,y,0<br>(2 <sub>y</sub>  0,1/2,0) | (4) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)   |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) m' x,1/4,z<br>(m <sub>y</sub>  0,1/2,0)'       | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

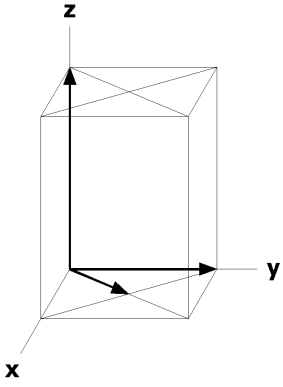
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y+1/2, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x+1/2, \bar{y}+1/2, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]
		(5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(6) $x+1/2, y, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(7) $x, \bar{y}+1/2, z$ [ $\bar{u}, \bar{v}, w$ ]	(8) $\bar{x}+1/2, y+1/2, z+1/2$ [ $\bar{u}, v, w$ ]
4	c .m'	x,1/4,z [u,0,w]	$\bar{x}+1/2, 3/4, z+1/2$ [ $\bar{u}, 0, w$ ]	$\bar{x}, 3/4, \bar{z}$ [ $\bar{u}, 0, \bar{w}$ ]	$x+1/2, 1/4, \bar{z}+1/2$ [ $\bar{u}, 0, \bar{w}$ ]
4	b $\bar{1}'$	0,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
4	a $\bar{1}'$	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p2m'g'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0]  $c_p$ .2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

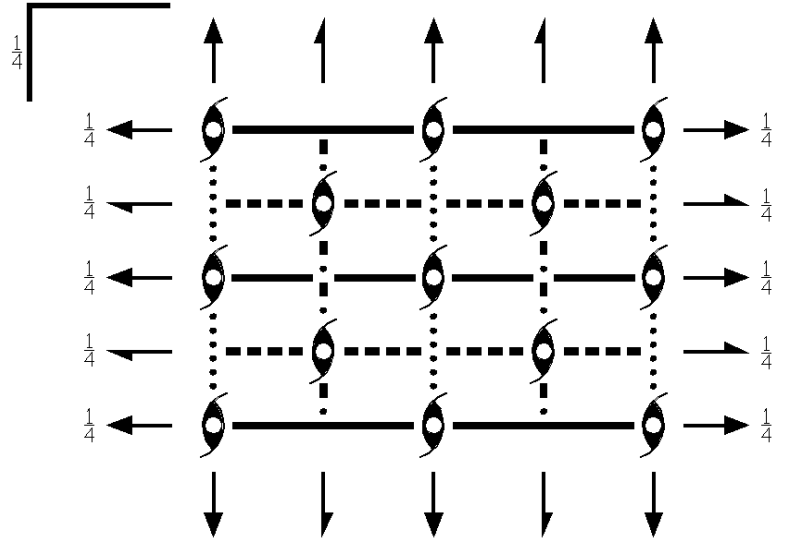
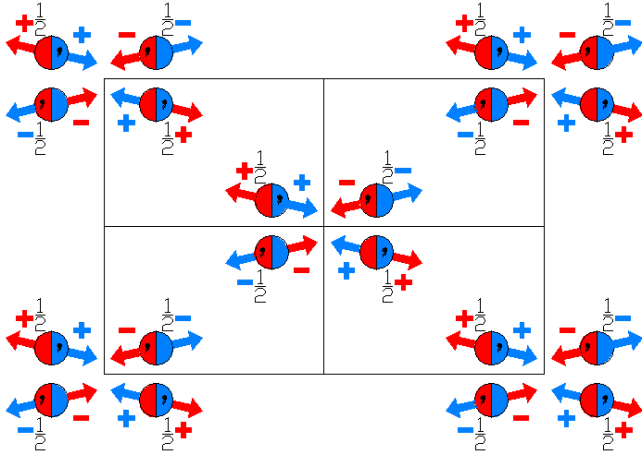
Along [0,1,0] p2g'g'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Cmcm  
63.1.511

mmm  
C2/m2/c2<sub>1</sub>/m

Orthorhombic



Origin at  $(\frac{1}{2}, \frac{1}{2}, 0)$  at  $2/mc2_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $(0,0,1/2)$ $0,0,z$<br>(2 <sub>z</sub>  0,0,1/2) | (3) 2 $0,y,1/4$<br>(2 <sub>y</sub>  0,0,1/2)           | (4) 2 $x,0,0$<br>(2 <sub>x</sub>  0,0,0) |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0) | (6) m $x,y,1/4$<br>(m <sub>z</sub>  0,0,1/2)           | (7) c $(0,0,1/2)$ $x,0,z$<br>(m <sub>y</sub>  0,0,1/2) | (8) m $0,y,z$<br>(m <sub>x</sub>  0,0,0) |

For  $(1/2,1/2,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) t $(1/2,1/2,0)$<br>(1 1/2,1/2,0)                 | (2) 2 $(0,0,1/2)$ $1/4,1/4,z$<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 2 $(0,1/2,0)$ $1/4,y,1/4$<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (4) 2 $(1/2,0,0)$ $x,1/4,0$<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$  1/2,1/2,0) | (6) n $(1/2,1/2,0)$ $x,y,1/4$<br>(m <sub>z</sub>  1/2,1/2,1/2) | (7) n $(1/2,0,1/2)$ $x,1/4,z$<br>(m <sub>y</sub>  1/2,1/2,1/2) | (8) b $(0,1/2,0)$ $1/4,y,z$<br>(m <sub>x</sub>  1/2,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5).

**Positions**

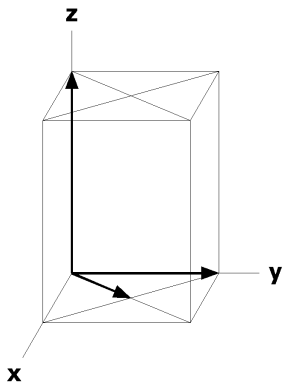
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 h 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},\bar{v},\bar{w}$ ]
8 g ..m	x,y,1/4 [0,0,w]	$\bar{x},\bar{y},3/4$ [0,0,w]	$\bar{x},y,1/4$ [0,0, $\bar{w}$ ]	x, $\bar{y},3/4$ [0,0, $\bar{w}$ ]
8 f m..	0,y,z [u,0,0]	0, $\bar{y},z+1/2$ [ $\bar{u},0,0$ ]	0,y, $\bar{z}+1/2$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]
8 e 2..	x,0,0 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},0,0$ [u,0,0]	x,0,1/2 [ $\bar{u},0,0$ ]
8 d $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,1/2 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,1/2 [ $\bar{u},v,\bar{w}$ ]	1/4,3/4,0 [ $\bar{u},\bar{v},\bar{w}$ ]
4 c m2m	0,y,1/4 [0,0,0]	0, $\bar{y},3/4$ [0,0,0]		
4 b 2/m..	0,1/2,0 [u,0,0]	0,1/2,1/2 [ $\bar{u},0,0$ ]		
4 a 2/m..	0,0,0 [u,0,0]	0,0,1/2 [ $\bar{u},0,0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



Cmc21'

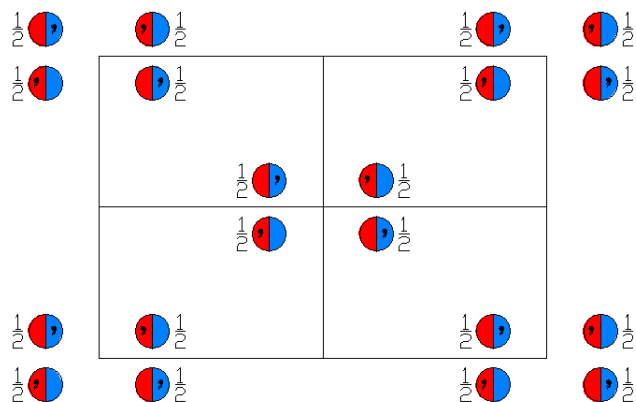
63.2.512

mmm1'

C2/m2/c2<sub>1</sub>/m1'

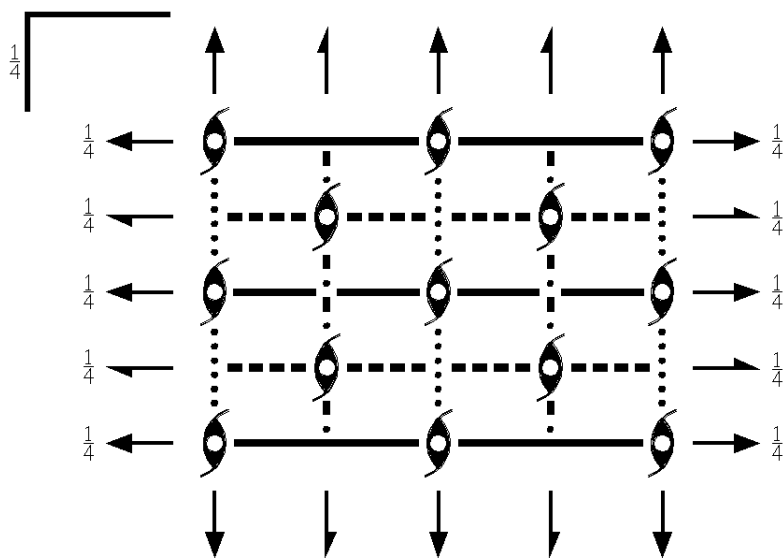
Orthorhombic

1'



Origin at  $(\frac{1}{2}, \frac{1}{2}, 0)$  at  $2/mc2_1, 1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$



**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                          | (2) 2 $(0,0,1/2)$ $0,0,z$<br>(2 <sub>z</sub>   0,0,1/2) | (3) 2 $0,y,1/4$<br>(2 <sub>y</sub>   0,0,1/2)           | (4) 2 $x,0,0$<br>(2 <sub>x</sub>   0,0,0) |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   0,0,0) | (6) m $x,y,1/4$<br>(m <sub>z</sub>   0,0,1/2)           | (7) c $(0,0,1/2)$ $x,0,z$<br>(m <sub>y</sub>   0,0,1/2) | (8) m $0,y,z$<br>(m <sub>x</sub>   0,0,0) |

For  $(1/2,1/2,0)$  + set

- |   |   |   |   |
|---|---|---|---|
| (1) t $(1/2,1/2,0)$<br>(1   1/2,1/2,0)                | (2) 2 $(0,0,1/2)$ $1/4,1/4,z$<br>(2 <sub>z</sub>   1/2,1/2,1/2) | (3) 2 $(0,1/2,0)$ $1/4,y,1/4$<br>(2 <sub>y</sub>   1/2,1/2,1/2) | (4) 2 $(1/2,0,0)$ $x,1/4,0$<br>(2 <sub>x</sub>   1/2,1/2,0) |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   1/2,1/2,0) | (6) n $(1/2,1/2,0)$ $x,y,1/4$<br>(m <sub>z</sub>   1/2,1/2,1/2) | (7) n $(1/2,0,1/2)$ $x,1/4,z$<br>(m <sub>y</sub>   1/2,1/2,1/2) | (8) b $(0,1/2,0)$ $1/4,y,z$<br>(m <sub>x</sub>   1/2,1/2,0) |

For  $(0,0,0)'$  + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1'<br>(1   0,0,0)'                           | (2) 2' $(0,0,1/2)$ $0,0,z$<br>(2 <sub>z</sub> '   0,0,1/2)' | (3) 2' $0,y,1/4$<br>(2 <sub>y</sub> '   0,0,1/2)'           | (4) 2' $x,0,0$<br>(2 <sub>x</sub> '   0,0,0)' |
| (5) $\bar{1}'$ $0,0,0$<br>( $\bar{1}'$   0,0,0)' | (6) m' $x,y,1/4$<br>(m <sub>z</sub> '   0,0,1/2)'           | (7) c' $(0,0,1/2)$ $x,0,z$<br>(m <sub>y</sub> '   0,0,1/2)' | (8) m' $0,y,z$<br>(m <sub>x</sub> '   0,0,0)' |

For  $(1/2,1/2,0)'$  + set

- |  |   |   |   |
|--|---|---|---|
| (1) t' $(1/2,1/2,0)$<br>(1   1/2,1/2,0)'                 | (2) 2' $(0,0,1/2)$ $1/4,1/4,z$<br>(2 <sub>z</sub> '   1/2,1/2,1/2)' | (3) 2' $(0,1/2,0)$ $1/4,y,1/4$<br>(2 <sub>y</sub> '   1/2,1/2,1/2)' | (4) 2' $(1/2,0,0)$ $x,1/4,0$<br>(2 <sub>x</sub> '   1/2,1/2,0)' |
| (5) $\bar{1}'$ $1/4,1/4,0$<br>( $\bar{1}'$   1/2,1/2,0)' | (6) n' $(1/2,1/2,0)$ $x,y,1/4$<br>(m <sub>z</sub> '   1/2,1/2,1/2)' | (7) n' $(1/2,0,1/2)$ $x,1/4,z$<br>(m <sub>y</sub> '   1/2,1/2,1/2)' | (8) b' $(0,1/2,0)$ $1/4,y,z$<br>(m <sub>x</sub> '   1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5);1'.

**Positions**

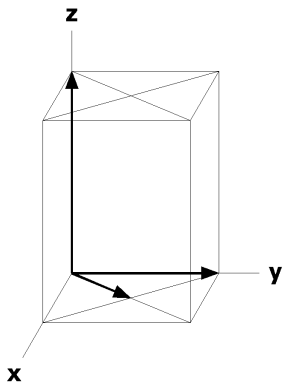
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) + (0,0,0)'	(1/2,1/2,0) + (1/2,1/2,0)'	(0,0,0) + (0,0,0)'	(1/2,1/2,0) + (1/2,1/2,0)'
16 h 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z+1/2$ [0,0,0]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [0,0,0]	(4) $x,\bar{y},\bar{z}$ [0,0,0]
	(5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(6) $x,y,\bar{z}+1/2$ [0,0,0]	(7) $x,\bar{y},z+1/2$ [0,0,0]	(8) $\bar{x},y,z$ [0,0,0]
8 g ..m1'	x,y,1/4 [0,0,0]	$\bar{x},\bar{y},3/4$ [0,0,0]	$\bar{x},y,1/4$ [0,0,0]	$x,\bar{y},3/4$ [0,0,0]
8 f m..1'	0,y,z [0,0,0]	$0,\bar{y},z+1/2$ [0,0,0]	$0,y,\bar{z}+1/2$ [0,0,0]	$0,\bar{y},\bar{z}$ [0,0,0]
8 e 2..1'	x,0,0 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]	$\bar{x},0,0$ [0,0,0]	$x,0,1/2$ [0,0,0]
8 d $\bar{1}1'$	1/4,1/4,0 [0,0,0]	3/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,3/4,0 [0,0,0]
4 c m2m1'	0,y,1/4 [0,0,0]	$0,\bar{y},3/4$ [0,0,0]		
4 b 2/m..1'	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 a 2/m..1'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

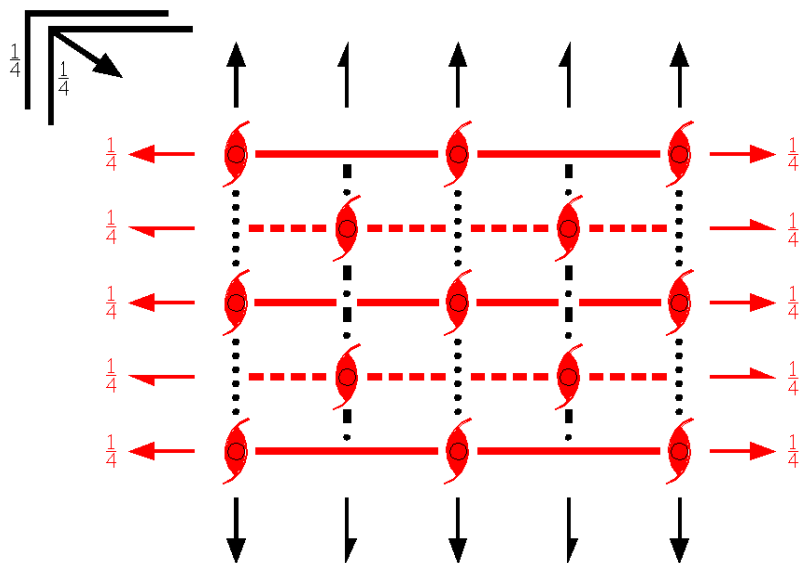
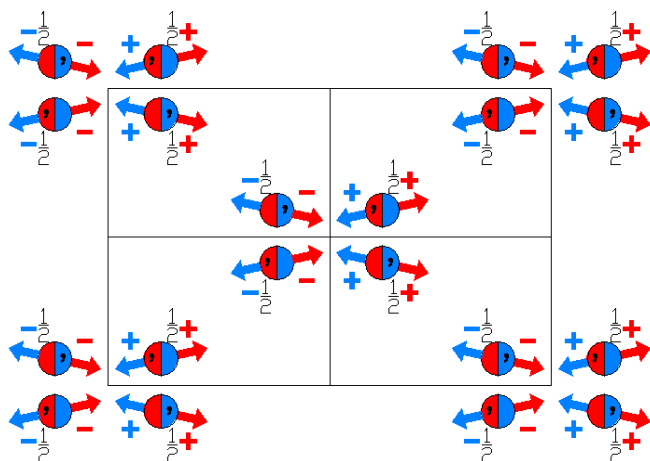
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Cm'cm  
63.3.513

m'mm  
C2/m'2'/c2<sub>1</sub>'/m

Orthorhombic



Origin at  $(\frac{1}{2}, \frac{1}{2}, 0)$  at  $2/m'c2_1'$

Asymmetric unit  $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

### Symmetry Operations

For  $(0,0,0)$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)' | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'       | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m x,y,1/4<br>(m <sub>z</sub>  0,0,1/2)           | (7) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

For  $(\frac{1}{2}, \frac{1}{2}, 0)$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2, 1/2, 0)<br>(1 1/2, 1/2, 0)                    | (2) 2' (0,0,1/2) 1/4, 1/4, z<br>(2 <sub>z</sub>  1/2, 1/2, 1/2)' | (3) 2' (0,1/2,0) 1/4, y, 1/4<br>(2 <sub>y</sub>  1/2, 1/2, 1/2)' | (4) 2 (1/2, 0, 0) x, 1/4, 0<br>(2 <sub>x</sub>  1/2, 1/2, 0)   |
| (5) $\bar{1}$ ' 1/4, 1/4, 0<br>( $\bar{1}$  1/2, 1/2, 0)' | (6) n (1/2, 1/2, 0) x, y, 1/4<br>(m <sub>z</sub>  1/2, 1/2, 1/2) | (7) n (1/2, 0, 1/2) x, 1/4, z<br>(m <sub>y</sub>  1/2, 1/2, 1/2) | (8) b' (0, 1/2, 0) 1/4, y, z<br>(m <sub>x</sub>  1/2, 1/2, 0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5).

**Positions**

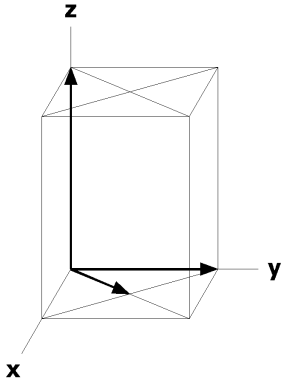
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 h 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 g ..m	x,y,1/4 [0,0,w]	$\bar{x},\bar{y},3/4$ [0,0, $\bar{w}$ ]	$\bar{x},y,1/4$ [0,0,w]	x, $\bar{y},3/4$ [0,0, $\bar{w}$ ]
8 f m'..	0,y,z [0,v,w]	0, $\bar{y},z+1/2$ [0,v, $\bar{w}$ ]	0,y, $\bar{z}+1/2$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 e 2..	x,0,0 [u,0,0]	$\bar{x},0,1/2$ [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	x,0,1/2 [ $\bar{u},0,0$ ]
8 d $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,3/4,0 [0,0,0]
4 c m'2'm	0,y,1/4 [0,0,w]	0, $\bar{y},3/4$ [0,0, $\bar{w}$ ]		
4 b 2/m'..	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 a 2/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

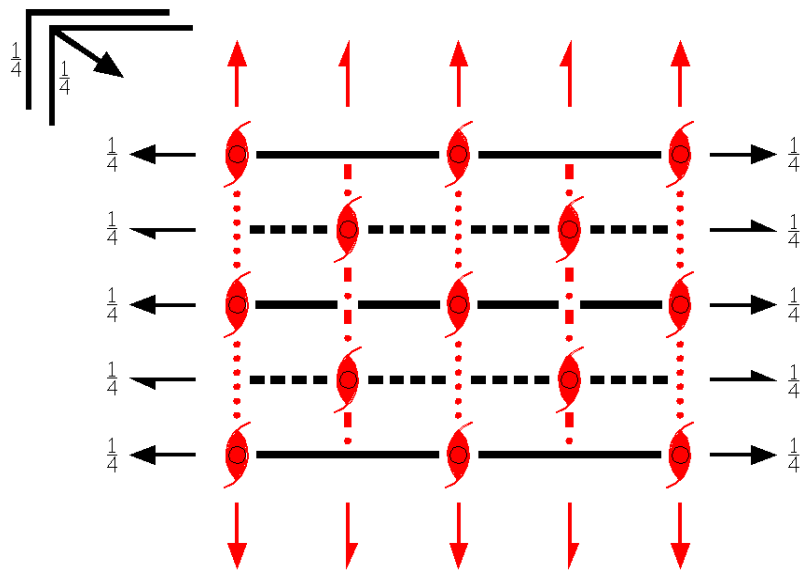
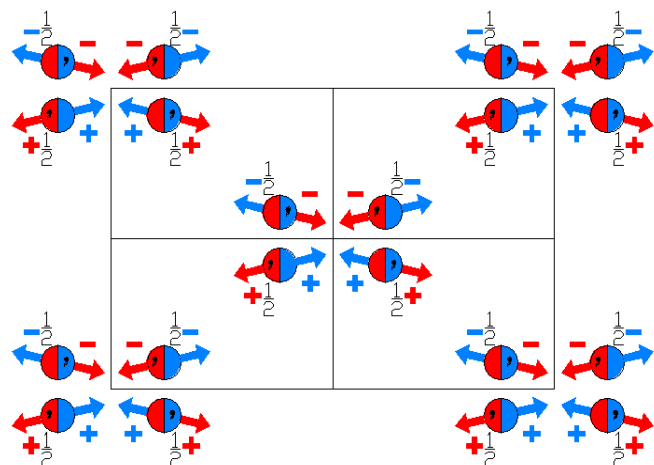
Along [0,1,0]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Cmc'm  
63.4.514

mm'm  
C2'/m2/c'2, '1/m

Orthorhombic



Origin at  $(\frac{1}{2}, \frac{1}{2}, 0)$  at  $2'/mc'2, '1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

For  $(0,0,0)$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)' | (3) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)           | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m x,y,1/4<br>(m <sub>z</sub>  0,0,1/2)           | (7) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   |

For  $(1/2,1/2,0)$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                    | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)   | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)   | (7) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5).

**Positions**

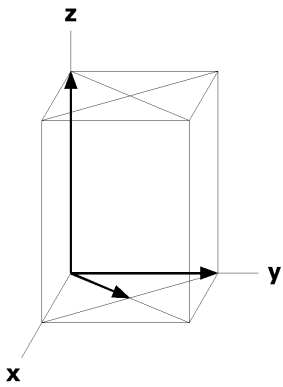
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 h 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 g ..m	x,y,1/4 [0,0,w]	$\bar{x},\bar{y},3/4$ [0,0, $\bar{w}$ ]	$\bar{x},y,1/4$ [0,0, $\bar{w}$ ]	x, $\bar{y},3/4$ [0,0,w]
8 f m..	0,y,z [u,0,0]	0, $\bar{y},z+1/2$ [u,0,0]	0,y, $\bar{z}+1/2$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
8 e 2'..	x,0,0 [0,v,w]	$\bar{x},0,1/2$ [0,v, $\bar{w}$ ]	$\bar{x},0,0$ [0, $\bar{v},\bar{w}$ ]	x,0,1/2 [0, $\bar{v},w$ ]
8 d $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,3/4,0 [0,0,0]
4 c m2m	0,y,1/4 [0,0,0]	0, $\bar{y},3/4$ [0,0,0]		
4 b 2'/m..	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 a 2'/m..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



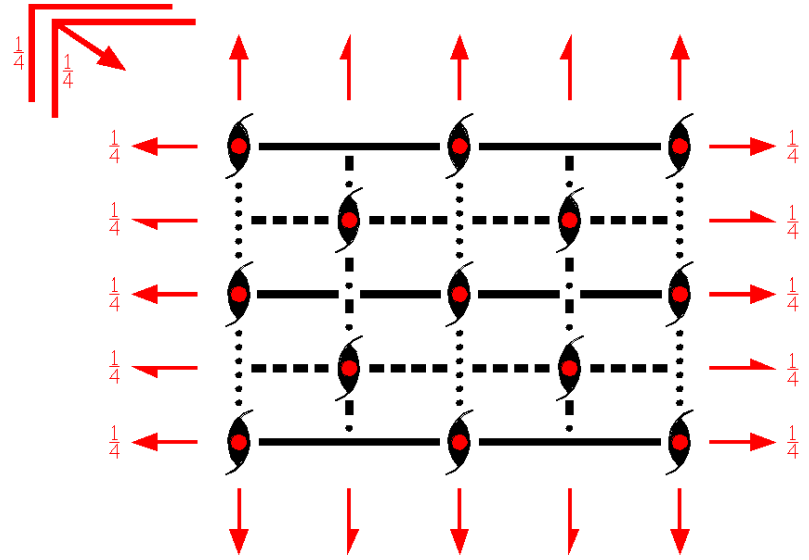
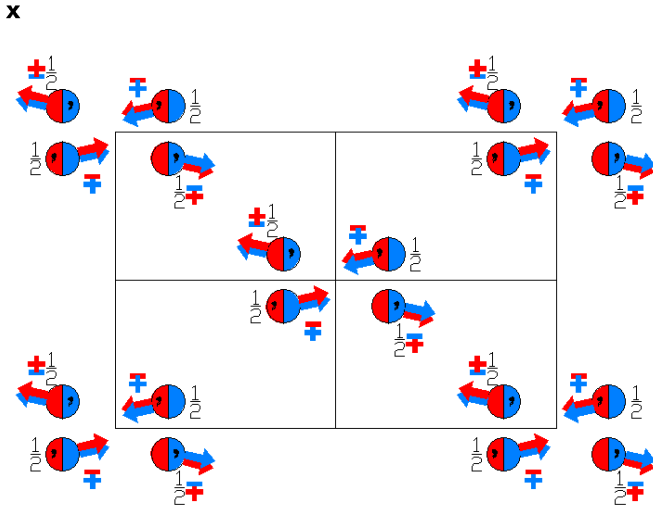
Cmcm'

63.5.515

mmm'

C2'/m2'/c2<sub>1</sub>/m'

Orthorhombic



Origin at  $(\frac{1}{2}, \frac{1}{2}, 0)$  at  $2'/mc2_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

For  $(0,0,0)$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $(0,0,1/2)$ $0,0,z$<br>(2 <sub>z</sub>  0,0,1/2) | (3) 2' $0,y,1/4$<br>(2 <sub>y</sub>  0,0,1/2)'         | (4) 2' $x,0,0$<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)' | (6) m' $x,y,1/4$<br>(m <sub>z</sub>  0,0,1/2)'         | (7) c $(0,0,1/2)$ $x,0,z$<br>(m <sub>y</sub>  0,0,1/2) | (8) m $0,y,z$<br>(m <sub>x</sub>  0,0,0)   |

For  $(1/2,1/2,0)$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) t $(1/2,1/2,0)$<br>(1 1/2,1/2,0)                  | (2) 2 $(0,0,1/2)$ $1/4,1/4,z$<br>(2 <sub>z</sub>  1/2,1/2,1/2)   | (3) 2' $(0,1/2,0)$ $1/4,y,1/4$<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (4) 2' $(1/2,0,0)$ $x,1/4,0$<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$  1/2,1/2,0)' | (6) n' $(1/2,1/2,0)$ $x,y,1/4$<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (7) n $(1/2,0,1/2)$ $x,1/4,z$<br>(m <sub>y</sub>  1/2,1/2,1/2)   | (8) b $(0,1/2,0)$ $1/4,y,z$<br>(m <sub>x</sub>  1/2,1/2,0)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5).

**Positions**

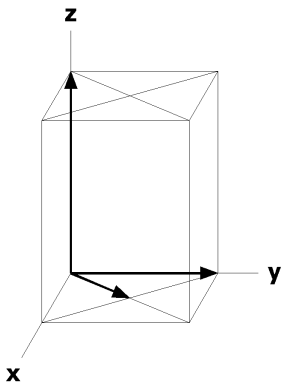
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 h 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 g ..m'	x,y,1/4 [u,v,0]	$\bar{x},\bar{y},3/4$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/4$ [u, $\bar{v},0$ ]	x, $\bar{y},3/4$ [ $\bar{u},v,0$ ]
8 f m..	0,y,z [u,0,0]	0, $\bar{y},z+1/2$ [ $\bar{u},0,0$ ]	0,y, $\bar{z}+1/2$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
8 e 2'..	x,0,0 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0, $\bar{v},\bar{w}$ ]	x,0,1/2 [0,v, $\bar{w}$ ]
8 d $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,3/4,0 [0,0,0]
4 c m2'm'	0,y,1/4 [u,0,0]	0, $\bar{y},3/4$ [ $\bar{u},0,0$ ]		
4 b 2'/m..	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 a 2'/m..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a'}2mm$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



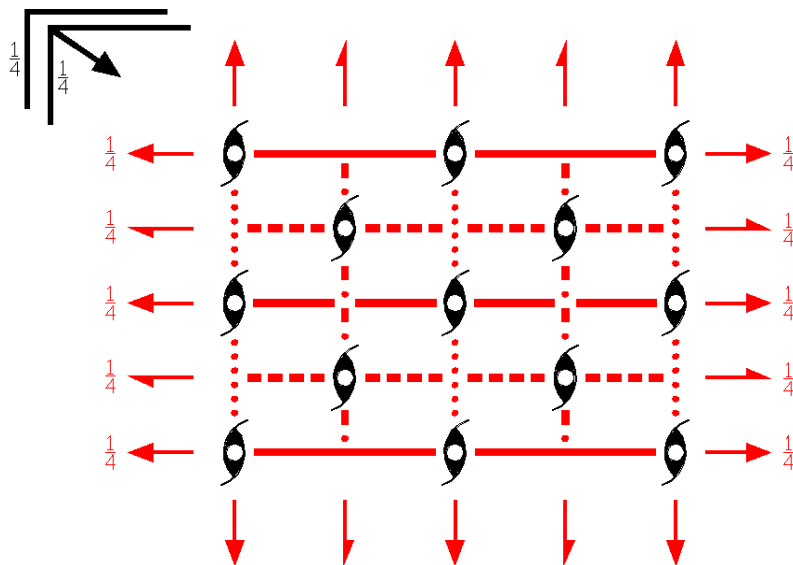
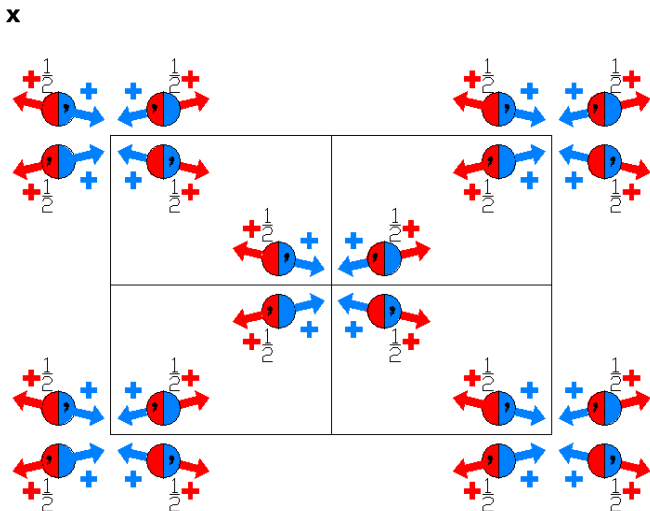
Cm'c'm

63.6.516

m'm'm

C2'/m'2'/c'2<sub>1</sub>/m

Orthorhombic



Origin at ( 2'/m' ) at 2'/m'c'2<sub>1</sub>

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                        | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>   0,0,1/2) | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>   0,0,1/2)'         | (4) 2' x,0,0<br>(2 <sub>x</sub>   0,0,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0) | (6) m x,y,1/4<br>(m <sub>z</sub>   0,0,1/2)         | (7) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>   0,0,1/2)' | (8) m' 0,y,z<br>(m <sub>x</sub>   0,0,0)' |

For (1/2,1/2,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2) | (3) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,1/2,1/2)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)' |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>   1/2,1/2,1/2) | (7) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,1/2)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5).

**Positions**

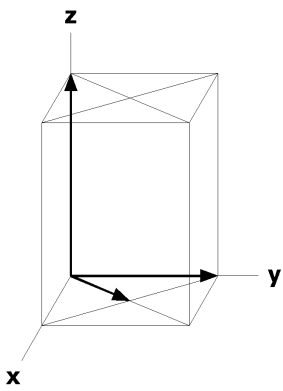
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 h 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(4) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) $x,y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 g ..m	x,y,1/4 [0,0,w]	$\bar{x},\bar{y},3/4$ [0,0,w]	$\bar{x},y,1/4$ [0,0,w]	x, $\bar{y},3/4$ [0,0,w]
8 f m'..	0,y,z [0,v,w]	0, $\bar{y},z+1/2$ [0, $\bar{v},w$ ]	0,y, $\bar{z}+1/2$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
8 e 2'..	x,0,0 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0,v,w]	x,0,1/2 [0, $\bar{v},w$ ]
8 d $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,1/2 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,1/2 [ $u,\bar{v},w$ ]	1/4,3/4,0 [ $\bar{u},v,w$ ]
4 c m'2'm	0,y,1/4 [0,0,w]	0, $\bar{y},3/4$ [0,0,w]		
4 b 2'/m'..	0,1/2,0 [0,v,w]	0,1/2,1/2 [0, $\bar{v},w$ ]		
4 a 2'/m'..	0,0,0 [0,v,w]	0,0,1/2 [0, $\bar{v},w$ ]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p 2'mm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



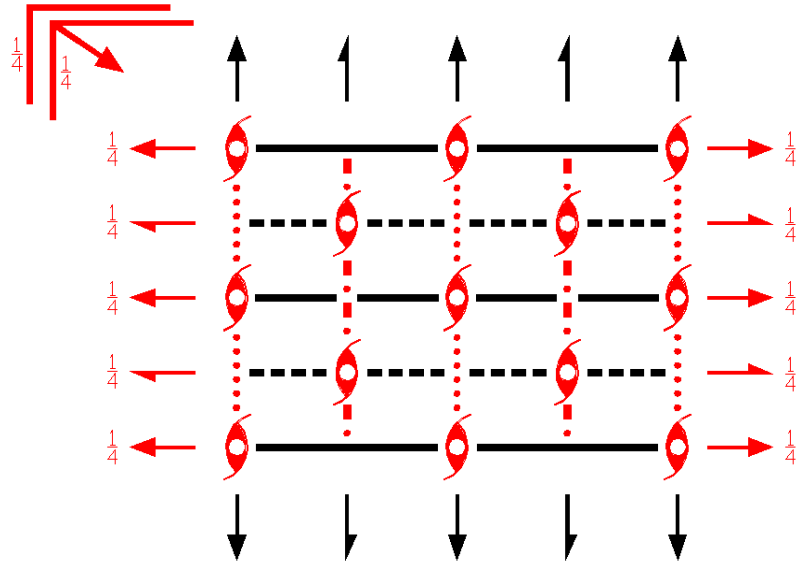
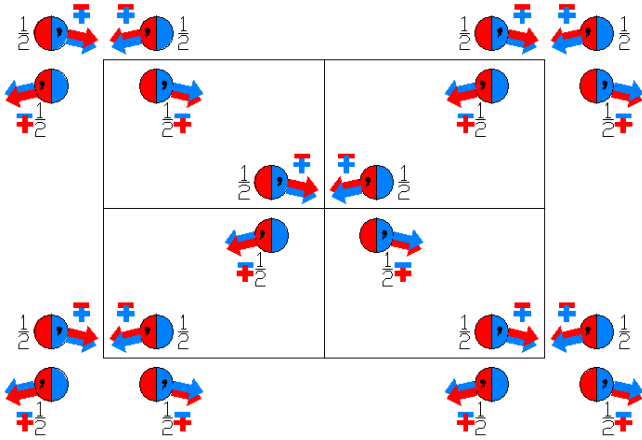
Cmc'm'

63.7.517

mm'm'

C2/m2'/c'2<sub>1</sub>'/m'

Orthorhombic



Origin at  $(\frac{1}{2}, \frac{1}{2}, 0)$  at  $2/mc'2_1'$

Asymmetric unit  $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                        | (2) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>   0,0,1/2)' | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>   0,0,1/2)'         | (4) 2 x,0,0<br>(2 <sub>x</sub>   0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0) | (6) m' x,y,1/4<br>(m <sub>z</sub>   0,0,1/2)'         | (7) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>   0,0,1/2)' | (8) m 0,y,z<br>(m <sub>x</sub>   0,0,0) |

For  $(\frac{1}{2}, \frac{1}{2}, 0)$  + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2)' | (3) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,1/2,1/2)' | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0) | (6) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>   1/2,1/2,1/2)' | (7) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,1/2)' | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5).

**Positions**

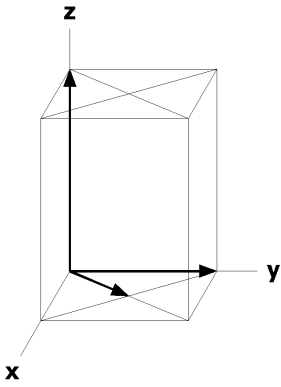
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 h 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(7) x, $\bar{y},z+1/2$ [u, $\bar{v}$ ,w]	(8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 g ..m'	x,y,1/4 [u,v,0]	$\bar{x},\bar{y},3/4$ [u,v,0]	$\bar{x},y,1/4$ [u, $\bar{v}$ ,0]	x, $\bar{y},3/4$ [u, $\bar{v}$ ,0]
8 f m..	0,y,z [u,0,0]	0, $\bar{y},z+1/2$ [u,0,0]	0,y, $\bar{z}+1/2$ [u,0,0]	0, $\bar{y},\bar{z}$ [u,0,0]
8 e 2..	x,0,0 [u,0,0]	$\bar{x},0,1/2$ [u,0,0]	$\bar{x},0,0$ [u,0,0]	x,0,1/2 [u,0,0]
8 d $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,1/2 [u,v, $\bar{w}$ ]	3/4,1/4,1/2 [u, $\bar{v}$ ,w]	1/4,3/4,0 [u, $\bar{v},\bar{w}$ ]
4 c m2'm'	0,y,1/4 [u,0,0]	0, $\bar{y},3/4$ [u,0,0]		
4 b 2/m..	0,1/2,0 [u,0,0]	0,1/2,1/2 [u,0,0]		
4 a 2/m..	0,0,0 [u,0,0]	0,0,1/2 [u,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,1/4



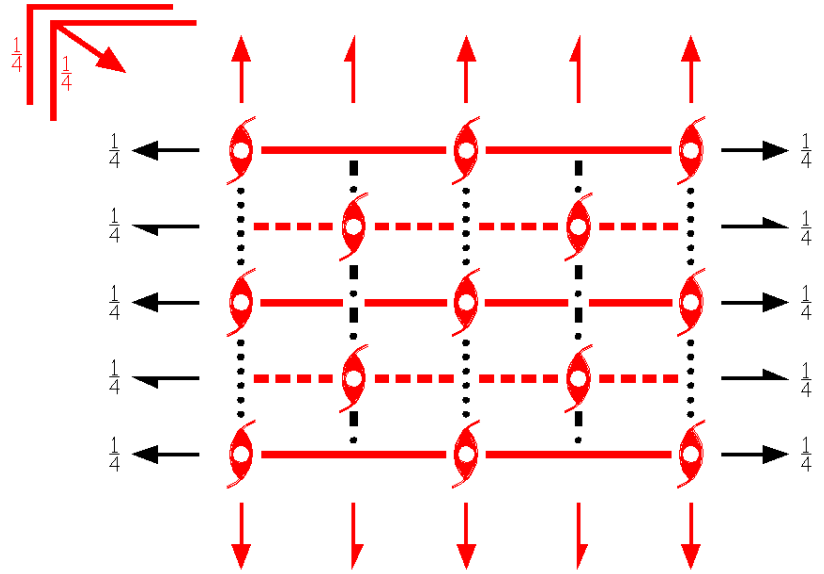
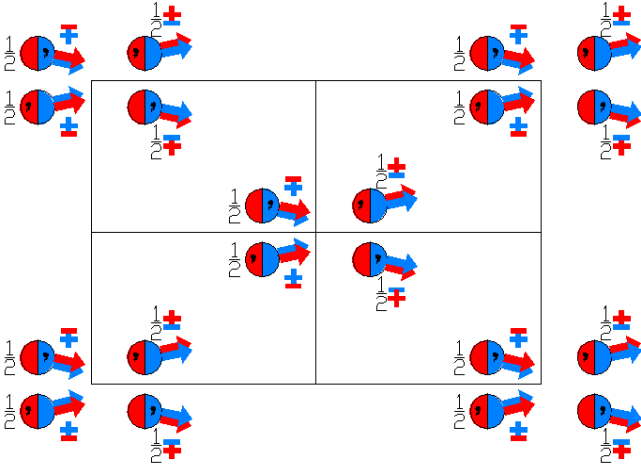
Cm'cm'

63.8.518

m'mm'

C2'/m'2/c2<sub>1</sub>'/m'

Orthorhombic



Origin at ( 2'/m' ) at 2'/m'c2<sub>1</sub>'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2' (0,0,1/2)<br>(2 <sub>z</sub>  0,0,1/2)' | (3) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)         | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m' x,y,1/4<br>(m <sub>z</sub>  0,0,1/2)'   | (7) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                 | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (7) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5).

**Positions**

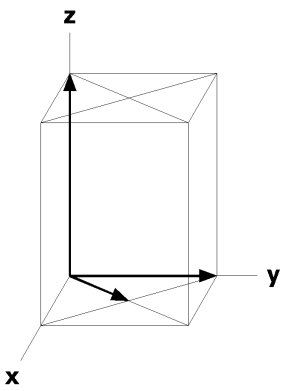
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 h 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u}$ ,v,w]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(7) x, $\bar{y},z+1/2$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(8) $\bar{x},y,z$ [ $\bar{u}$ ,v,w]
8 g ..m'	x,y,1/4 [u,v,0]	$\bar{x},\bar{y},3/4$ [u,v,0]	$\bar{x},y,1/4$ [ $\bar{u}$ ,v,0]	x, $\bar{y},3/4$ [ $\bar{u}$ ,v,0]
8 f m'..	0,y,z [0,v,w]	0, $\bar{y},z+1/2$ [0,v, $\bar{w}$ ]	0,y, $\bar{z}+1/2$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
8 e 2'..	x,0,0 [0,v,w]	$\bar{x},0,1/2$ [0,v, $\bar{w}$ ]	$\bar{x},0,0$ [0,v,w]	x,0,1/2 [0,v, $\bar{w}$ ]
8 d $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,1/2 [u,v, $\bar{w}$ ]	3/4,1/4,1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	1/4,3/4,0 [ $\bar{u}$ ,v,w]
4 c m'2m'	0,y,1/4 [0,v,0]	0, $\bar{y},3/4$ [0,v,0]		
4 b 2'/m'..	0,1/2,0 [0,v,w]	0,1/2,1/2 [0,v, $\bar{w}$ ]		
4 a 2'/m'..	0,0,0 [0,v,w]	0,0,1/2 [0,v, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a'</sub>2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



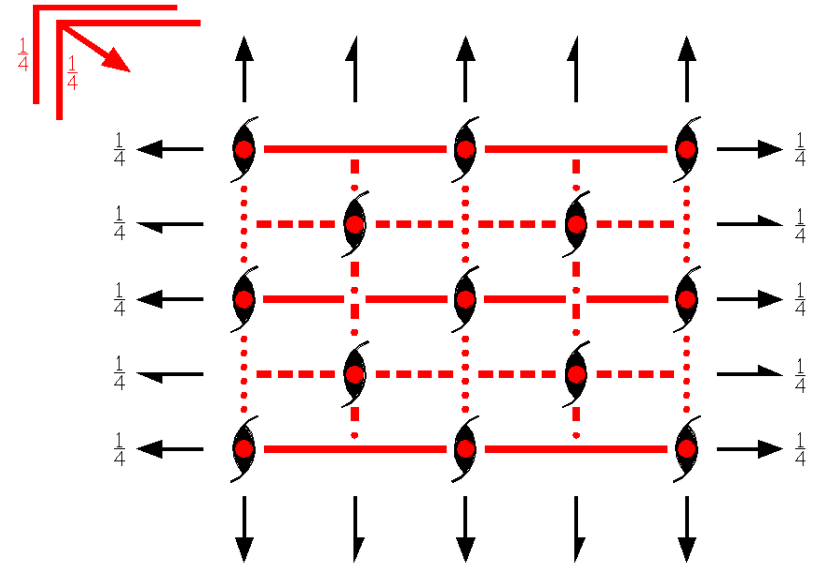
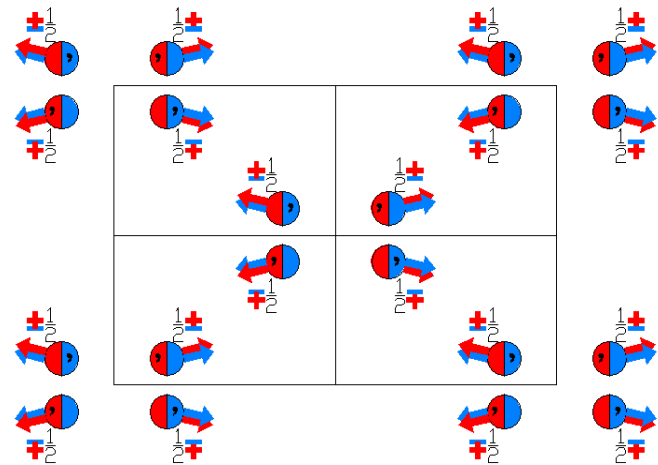
Cm'c'm'

63.9.519

m'm'm'

C2/m'2/c'2<sub>1</sub>/m'

Orthorhombic



Origin at (0,0,0) at 2/m'c'2<sub>1</sub>

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                          | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)           | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,1/4<br>(m <sub>z</sub>  0,0,1/2)'       | (7) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

For (1/2,1/2,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                  | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)   | (3) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (7) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5).

**Positions**

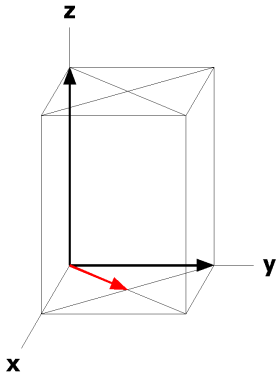
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 h 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 g ..m'	x,y,1/4 [u,v,0]	$\bar{x},\bar{y},3/4$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/4$ [ $\bar{u},v,0$ ]	x, $\bar{y},3/4$ [u, $\bar{v},0$ ]
8 f m'..	0,y,z [0,v,w]	0, $\bar{y},z+1/2$ [0, $\bar{v},w$ ]	0,y, $\bar{z}+1/2$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 e 2..	x,0,0 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	x,0,1/2 [u,0,0]
8 d $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,3/4,0 [0,0,0]
4 c m'2m'	0,y,1/4 [0,v,0]	0, $\bar{y},3/4$ [0, $\bar{v},0$ ]		
4 b 2/m'..	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 a 2/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

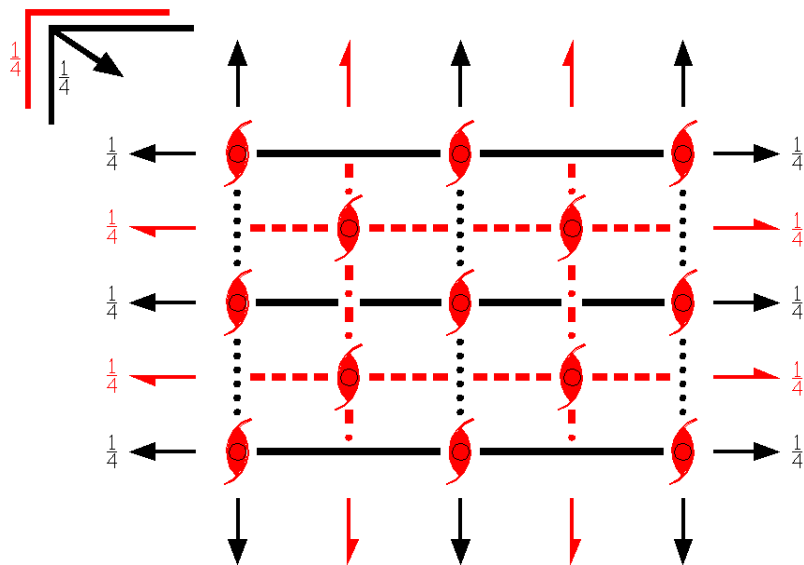
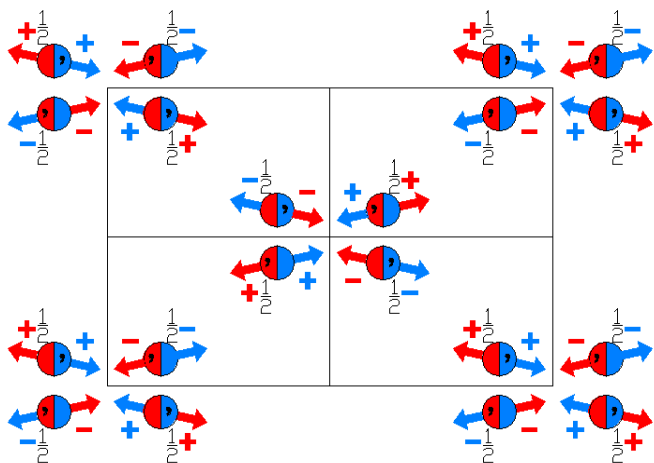
Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



$C_{p2}mcm$   
63.10.520

$mmm1'$   
 $C_{p2}2/m2/c2_1/m$

Orthorhombic



Origin at  $(\frac{1}{2}, \frac{1}{2}, 0)$  at  $2/mc2_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

For  $(0,0,0)$  + set

- |   |   |   |                                   |
|---|---|---|-----------------------------------|
| (1) 1<br>(1   0,0,0)                          | (2) 2 $(0,0,1/2)$ $0,0,z$<br>( $2_z$   0,0,1/2) | (3) 2 $0,y,1/4$<br>( $2_y$   0,0,1/2)           | (4) 2 $x,0,0$<br>( $2_x$   0,0,0) |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   0,0,0) | (6) m $x,y,1/4$<br>( $m_z$   0,0,1/2)           | (7) c $(0,0,1/2)$ $x,0,z$<br>( $m_y$   0,0,1/2) | (8) m $0,y,z$<br>( $m_x$   0,0,0) |

For  $(1/2,1/2,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,0)$<br>(1   $1/2,1/2,0$ )'              | (2) $2'$ $(0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1/2$ )' | (3) $2'$ $(0,1/2,0)$ $1/4,y,1/4$<br>( $2_y$   $1/2,1/2,1/2$ )' | (4) $2'$ $(1/2,0,0)$ $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )' |
| (5) $\bar{1}'$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ )' | (6) $n'$ $(1/2,1/2,0)$ $x,y,1/4$<br>( $m_z$   $1/2,1/2,1/2$ )' | (7) $n'$ $(1/2,0,1/2)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,1/2$ )' | (8) $b'$ $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0);(2); (3); (5).

**Positions**

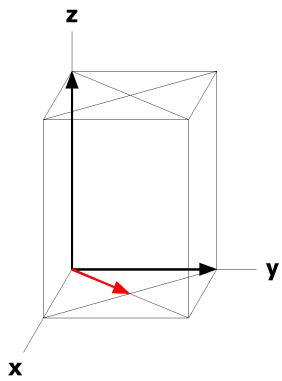
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 h 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(6) $x,y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y},z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(8) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
8 g ..m	x,y,1/4 [0,0,w]	$\bar{x},\bar{y},3/4$ [0,0,w]	$\bar{x},y,1/4$ [0,0, $\bar{w}$ ]	$x,\bar{y},3/4$ [0,0, $\bar{w}$ ]
8 f m..	0,y,z [u,0,0]	0, $\bar{y},z+1/2$ [ $\bar{u},0,0$ ]	0,y, $\bar{z}+1/2$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]
8 e 2..	x,0,0 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},0,0$ [u,0,0]	x,0,1/2 [ $\bar{u},0,0$ ]
8 d $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,3/4,0 [0,0,0]
4 c m2m	0,y,1/4 [0,0,0]	0, $\bar{y},3/4$ [0,0,0]		
4 b 2/m..	0,1/2,0 [u,0,0]	0,1/2,1/2 [ $\bar{u},0,0$ ]		
4 a 2/m..	0,0,0 [u,0,0]	0,0,1/2 [ $\bar{u},0,0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

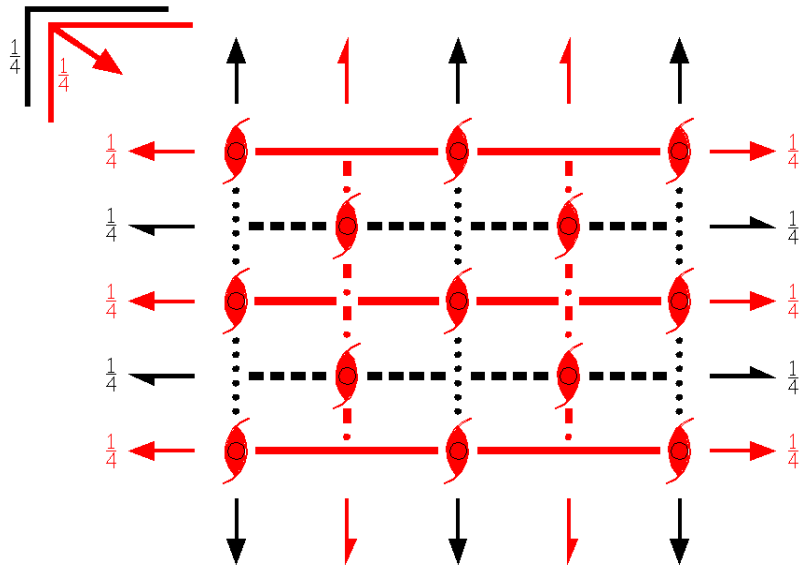
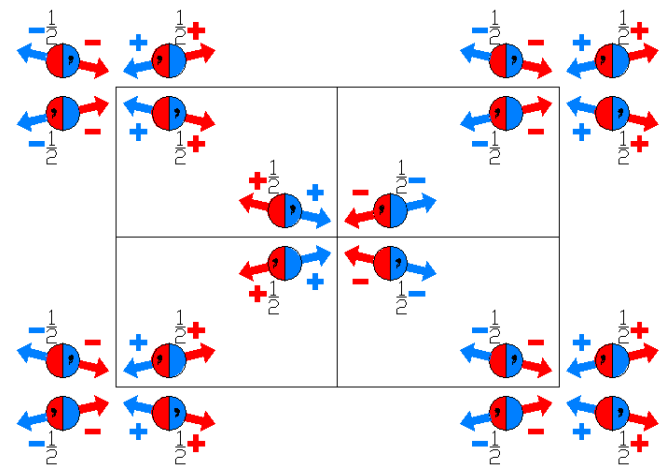
Along [0,1,0] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



$C_{2v}m'$   
63.11.521

$mmm1'$   
 $C_{2v}m'2'/c2_1'/m$

Orthorhombic



Origin at  $(\frac{1}{2}, 0, 0)$  at  $2/m'c2_1'$

Asymmetric unit  $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |  |  |                                      |
|---|--|--|--------------------------------------|
| (1) 1<br>(1 0,0,0)                            | (2) $2' (0,0,1/2)$<br>( $2_z$  0,0,1/2)' | (3) $2' (0,y,1/4)$<br>( $2_y$  0,0,1/2)' | (4) $2 (x,0,0)$<br>( $2_x$  0,0,0)   |
| (5) $\bar{1} (0,0,0)$<br>( $\bar{1}$  0,0,0)' | (6) $m (x,y,1/4)$<br>( $m_z$  0,0,1/2)   | (7) $c (0,0,1/2)$<br>( $m_y$  0,0,1/2)   | (8) $m' (0,y,z)$<br>( $m_x$  0,0,0)' |

For  $(1/2,1/2,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t' (1/2,1/2,0)$<br>(1 1/2,1/2,0)'               | (2) $2 (0,0,1/2)$<br>( $2_z$  1/2,1/2,1/2)     | (3) $2 (0,1/2,0)$<br>( $2_y$  1/2,1/2,1/2)     | (4) $2' (1/2,0,0)$<br>( $2_x$  1/2,1/2,0)' |
| (5) $\bar{1} (1/4,1/4,0)$<br>( $\bar{1}$  1/2,1/2,0) | (6) $n' (1/2,1/2,0)$<br>( $m_z$  1/2,1/2,1/2)' | (7) $n' (1/2,0,1/2)$<br>( $m_y$  1/2,1/2,1/2)' | (8) $b (0,1/2,0)$<br>( $m_x$  1/2,1/2,0)   |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0);(2); (3); (5).

**Positions**

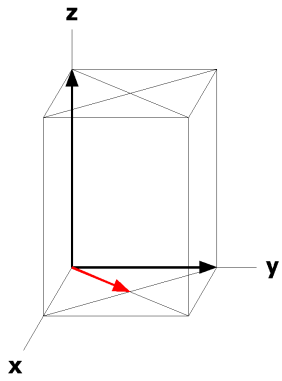
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 h 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 g ..m	x,y,1/4 [0,0,w]	$\bar{x},\bar{y},3/4$ [0,0, $\bar{w}$ ]	$\bar{x},y,1/4$ [0,0,w]	x, $\bar{y},3/4$ [0,0, $\bar{w}$ ]
8 f m'..	0,y,z [0,v,w]	0, $\bar{y},z+1/2$ [0,v, $\bar{w}$ ]	0,y, $\bar{z}+1/2$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 e 2..	x,0,0 [u,0,0]	$\bar{x},0,1/2$ [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	x,0,1/2 [ $\bar{u},0,0$ ]
8 d $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,1/2 [u,v, $\bar{w}$ ]	3/4,1/4,1/2 [u, $\bar{v},w$ ]	1/4,3/4,0 [u, $\bar{v},\bar{w}$ ]
4 c m'2'm	0,y,1/4 [0,0,w]	0, $\bar{y},3/4$ [0,0, $\bar{w}$ ]		
4 b 2/m'..	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 a 2/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>2mg  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>c</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,1/4



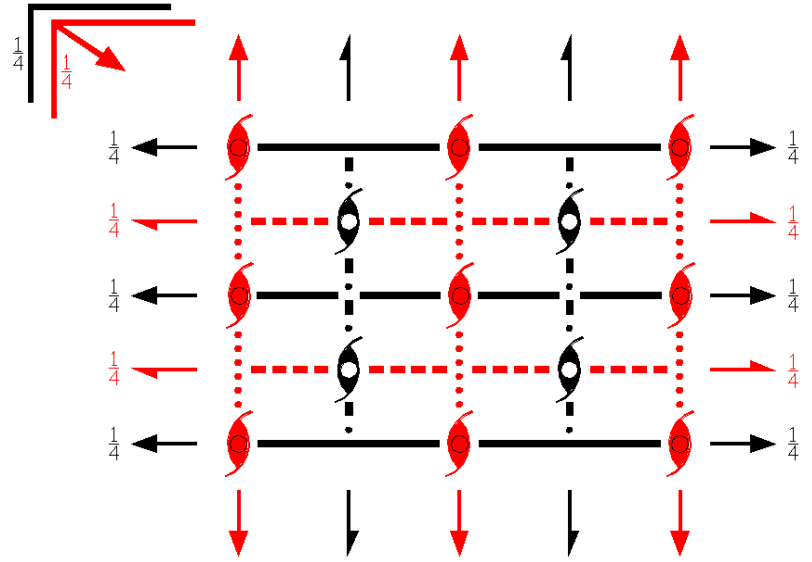
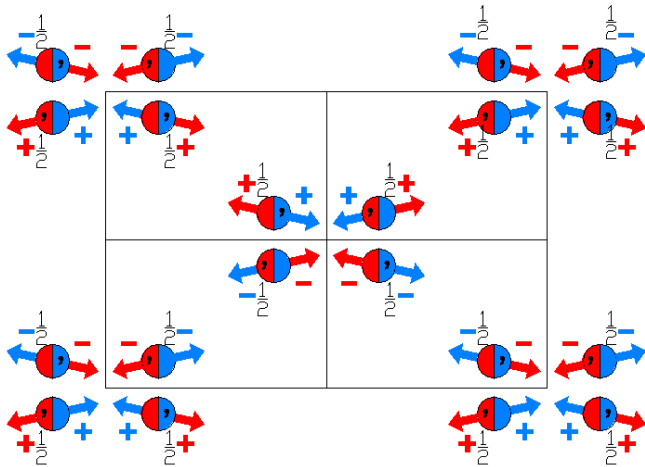
$C_{2v}mc'm$

63.12.522

$mmm1'$

$C_{2v}2'/m2/c'2_1'/m$

Orthorhombic



Origin at  $(\frac{1}{2}, \frac{1}{2}, 0)$  at  $2'/mc'2_1'$

Asymmetric unit  $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |   |   |                                       |
|--|---|---|---------------------------------------|
| (1) 1<br>(1   0,0,0)                             | (2) $2' (0,0,1/2)$<br>( $2_z$   0,0,1/2)' | (3) $2' (0,y,1/4)$<br>( $2_y$   0,0,1/2)  | (4) $2' (x,0,0)$<br>( $2_x$   0,0,0)' |
| (5) $\bar{1}' (0,0,0)$<br>( $\bar{1}'$   0,0,0)' | (6) $m (x,y,1/4)$<br>( $m_z$   0,0,1/2)   | (7) $c' (0,0,1/2)$<br>( $m_y$   0,0,1/2)' | (8) $m (0,y,z)$<br>( $m_x$   0,0,0)   |

For  $(1/2,1/2,0)$ ' + set

- |   |   |   |   |
|---|---|---|---|
| (1) $t' (1/2,1/2,0)$<br>(1   1/2,1/2,0)'                | (2) $2 (0,0,1/2)$<br>( $2_z$   1/2,1/2,1/2)     | (3) $2' (0,1/2,0)$<br>( $2_y$   1/2,1/2,1/2)' | (4) $2 (1/2,0,0)$<br>( $2_x$   1/2,1/2,0)   |
| (5) $\bar{1}' (1/4,1/4,0)$<br>( $\bar{1}'$   1/2,1/2,0) | (6) $n' (1/2,1/2,0)$<br>( $m_z$   1/2,1/2,1/2)' | (7) $n (1/2,0,1/2)$<br>( $m_y$   1/2,1/2,1/2) | (8) $b' (0,1/2,0)$<br>( $m_x$   1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0);(2); (3); (5).

**Positions**

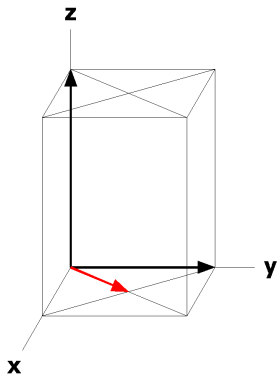
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 h 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ] (7) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ] (8) $\bar{x},\bar{y},z$ [u, $\bar{v},\bar{w}$ ]
8 g ..m	x,y,1/4 [0,0,w]	$\bar{x},\bar{y},3/4$ [0,0, $\bar{w}$ ]	$\bar{x},y,1/4$ [0,0, $\bar{w}$ ]	x, $\bar{y},3/4$ [0,0,w]
8 f m..	0,y,z [u,0,0]	0, $\bar{y},z+1/2$ [u,0,0]	0,y, $\bar{z}+1/2$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
8 e 2'..	x,0,0 [0,v,w]	$\bar{x},0,1/2$ [0,v, $\bar{w}$ ]	$\bar{x},0,0$ [0, $\bar{v},\bar{w}$ ]	x,0,1/2 [0, $\bar{v},w$ ]
8 d $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,1/2 [u,v, $\bar{w}$ ]	3/4,1/4,1/2 [ $\bar{u},\bar{v},\bar{w}$ ]	1/4,3/4,0 [ $\bar{u},\bar{v},w$ ]
4 c m2m	0,y,1/4 [0,0,0]	0, $\bar{y},3/4$ [0,0,0]		
4 b 2'/m..	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 a 2'/m..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

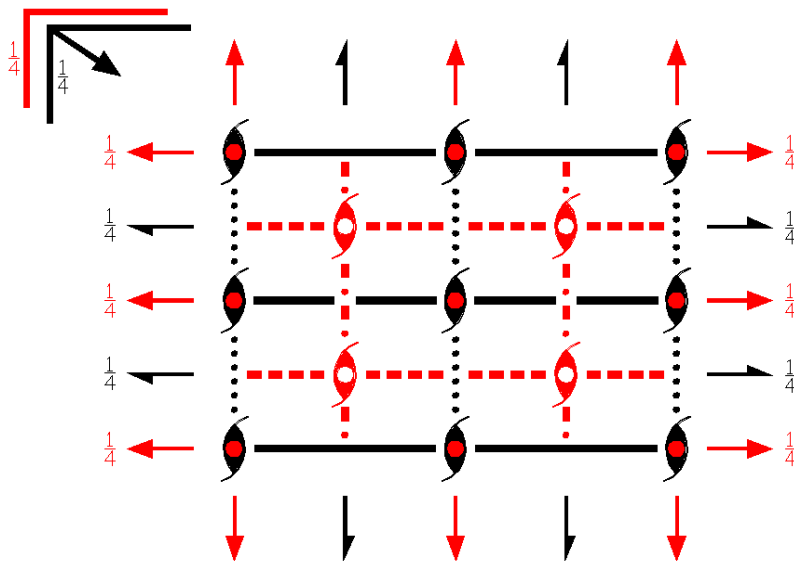
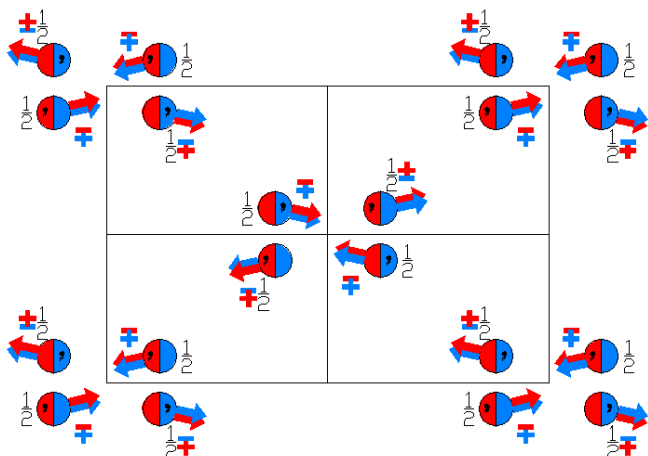
Along [0,1,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



$C_{p}mcm'$   
63.13.523

$mmm1'$   
 $C_{p}2'/m2'/c2_1/m'$

Orthorhombic



Origin at  $(\frac{1}{2}, \frac{1}{2}, 0)$  at  $2'/mc2_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |   |   |                                     |
|--|---|---|-------------------------------------|
| (1) 1<br>(1   0,0,0)                           | (2) 2 $(0,0,1/2)$ $0,0,z$<br>( $2_z$   0,0,1/2) | (3) 2' $0,y,1/4$<br>( $2_y$   0,0,1/2)'           | (4) 2' $x,0,0$<br>( $2_x$   0,0,0)' |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   0,0,0)' | (6) $m'$ $x,y,1/4$<br>( $m_z$   0,0,1/2)'       | (7) $c$ $(0,0,1/2)$ $x,0,z$<br>( $m_y$   0,0,1/2) | (8) $m$ $0,y,z$<br>( $m_x$   0,0,0) |

For  $(1/2,1/2,0)$ ' + set

- |   |   |   |   |
|---|---|---|---|
| (1) $t'$ $(1/2,1/2,0)$<br>(1   1/2,1/2,0)'            | (2) 2' $(0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$   1/2,1/2,1/2)' | (3) 2 $(0,1/2,0)$ $1/4,y,1/4$<br>( $2_y$   1/2,1/2,1/2)     | (4) 2 $(1/2,0,0)$ $x,1/4,0$<br>( $2_x$   1/2,1/2,0)     |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   1/2,1/2,0) | (6) $n$ $(1/2,1/2,0)$ $x,y,1/4$<br>( $m_z$   1/2,1/2,1/2) | (7) $n'$ $(1/2,0,1/2)$ $x,1/4,z$<br>( $m_y$   1/2,1/2,1/2)' | (8) $b'$ $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$   1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0);(2); (3); (5).

**Positions**

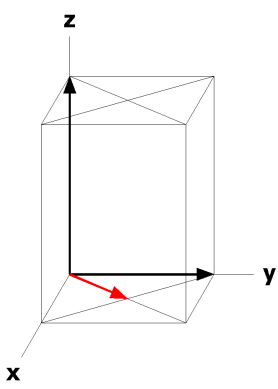
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 h 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 g ..m'	x,y,1/4 [u,v,0]	$\bar{x},\bar{y},3/4$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/4$ [u, $\bar{v},0$ ]	x, $\bar{y},3/4$ [ $\bar{u},v,0$ ]
8 f m..	0,y,z [u,0,0]	0, $\bar{y},z+1/2$ [ $\bar{u},0,0$ ]	0,y, $\bar{z}+1/2$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
8 e 2'..	x,0,0 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0, $\bar{v},\bar{w}$ ]	x,0,1/2 [0,v, $\bar{w}$ ]
8 d $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,1/2 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,1/2 [u, $\bar{v},w$ ]	1/4,3/4,0 [ $\bar{u},v,w$ ]
4 c m2'm'	0,y,1/4 [u,0,0]	0, $\bar{y},3/4$ [ $\bar{u},0,0$ ]		
4 b 2'/m..	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 a 2'/m..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



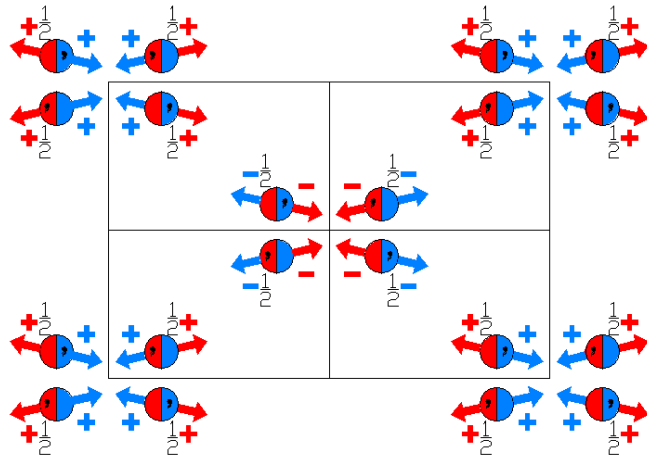
$C_{2v}m'c'm$

63.14.524

$mmm1'$

$C_{2v}2'/m'2'/c'2_1/m$

Orthorhombic



Origin at  $(2'/m')$  at  $2'/m'c'2_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |  |                                    |
|--|--|--|------------------------------------|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $(0,0,1/2)$ $0,0,z$<br>( $2_z$  0,0,1/2) | (3) 2' $0,y,1/4$<br>( $2_y$  0,0,1/2)'           | (4) 2' $x,0,0$<br>( $2_x$  0,0,0)' |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0) | (6) m $x,y,1/4$<br>( $m_z$  0,0,1/2)           | (7) c' $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2)' | (8) m' $0,y,z$<br>( $m_x$  0,0,0)' |

For  $(1/2,1/2,0)'$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' $(1/2,1/2,0)$<br>(1 1/2,1/2,0)'                  | (2) 2' $(0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2)' | (3) 2 $(0,1/2,0)$ $1/4,y,1/4$<br>( $2_y$  1/2,1/2,1/2) | (4) 2 $(1/2,0,0)$ $x,1/4,0$<br>( $2_x$  1/2,1/2,0) |
| (5) $\bar{1}'$ $1/4,1/4,0$<br>( $\bar{1}'$  1/2,1/2,0)' | (6) n' $(1/2,1/2,0)$ $x,y,1/4$<br>( $m_z$  1/2,1/2,1/2)' | (7) n $(1/2,0,1/2)$ $x,1/4,z$<br>( $m_y$  1/2,1/2,1/2) | (8) b $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$  1/2,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0);(2); (3); (5).

**Positions**

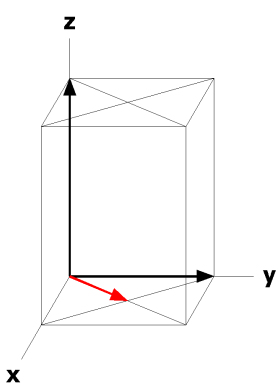
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 h 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(4) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) $x,y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 g ..m	x,y,1/4 [0,0,w]	$\bar{x},\bar{y},3/4$ [0,0,w]	$\bar{x},y,1/4$ [0,0,w]	x, $\bar{y},3/4$ [0,0,w]
8 f m'..	0,y,z [0,v,w]	0, $\bar{y},z+1/2$ [0, $\bar{v},w$ ]	0,y, $\bar{z}+1/2$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
8 e 2'..	x,0,0 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0,v,w]	x,0,1/2 [0, $\bar{v},w$ ]
8 d $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,3/4,0 [0,0,0]
4 c m'2'm	0,y,1/4 [0,0,w]	0, $\bar{y},3/4$ [0,0,w]		
4 b 2'/m'..	0,1/2,0 [0,v,w]	0,1/2,1/2 [0, $\bar{v},w$ ]		
4 a 2'/m'..	0,0,0 [0,v,w]	0,0,1/2 [0, $\bar{v},w$ ]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>2mg  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,1/4,0

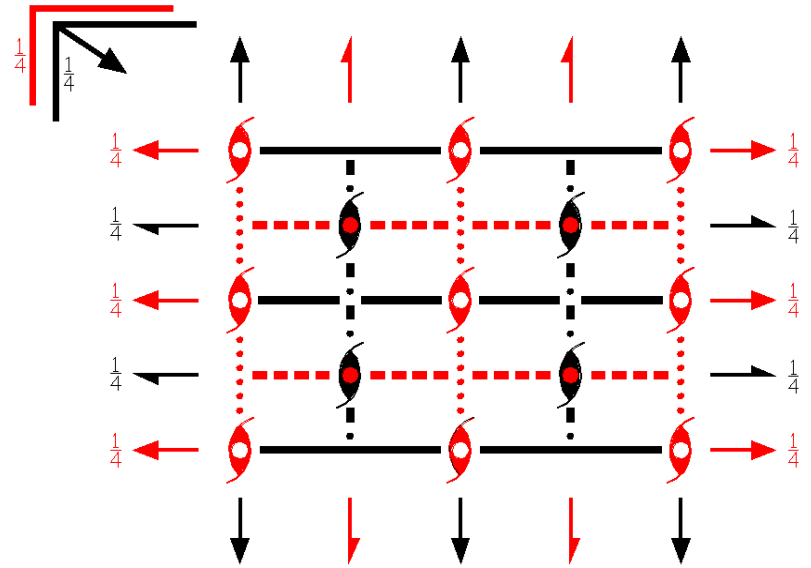
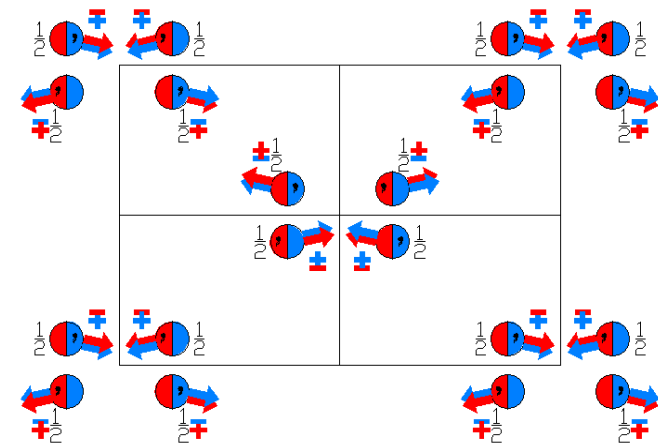
Along [0,1,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 1/4,y,1/4



$C_pmc'm'$   
63.15.525

$mmm1'$   
 $C_p2/m2'/c'2_1'/m'$

Orthorhombic



Origin at  $(2/m)$  at  $2/mc'2_1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |  |                                    |
|--|--|--|------------------------------------|
| (1) 1<br>(1 0,0,0)                           | (2) $2'$ $(0,0,1/2)$ $0,0,z$<br>( $2_z$  0,0,1/2)' | (3) $2'$ $0,y,1/4$<br>( $2_y$  0,0,1/2)'           | (4) $2$ $x,0,0$<br>( $2_x$  0,0,0) |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0) | (6) $m'$ $x,y,1/4$<br>( $m_z$  0,0,1/2)'           | (7) $c'$ $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2)' | (8) $m$ $0,y,z$<br>( $m_x$  0,0,0) |

For  $(1/2,1/2,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,0)$<br>(1 1/2,1/2,0)'               | (2) $2$ $(0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2) | (3) $2$ $(0,1/2,0)$ $1/4,y,1/4$<br>( $2_y$  1/2,1/2,1/2) | (4) $2'$ $(1/2,0,0)$ $x,1/4,0$<br>( $2_x$  1/2,1/2,0)' |
| (5) $\bar{1}'$ $1/4,1/4,0$<br>( $\bar{1}$  1/2,1/2,0)' | (6) $n$ $(1/2,1/2,0)$ $x,y,1/4$<br>( $m_z$  1/2,1/2,1/2) | (7) $n$ $(1/2,0,1/2)$ $x,1/4,z$<br>( $m_y$  1/2,1/2,1/2) | (8) $b'$ $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$  1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0);(2); (3); (5).

**Positions**

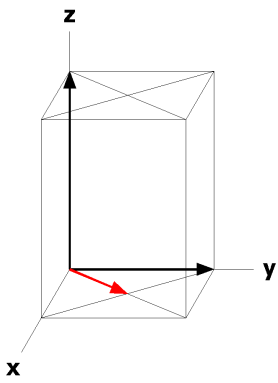
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 h 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(7) x, $\bar{y},z+1/2$ [u, $\bar{v}$ ,w]	(8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 g ..m'	x,y,1/4 [u,v,0]	$\bar{x},\bar{y},3/4$ [u,v,0]	$\bar{x},y,1/4$ [u, $\bar{v}$ ,0]	x, $\bar{y},3/4$ [u, $\bar{v}$ ,0]
8 f m..	0,y,z [u,0,0]	0, $\bar{y},z+1/2$ [u,0,0]	0,y, $\bar{z}+1/2$ [u,0,0]	0, $\bar{y},\bar{z}$ [u,0,0]
8 e 2..	x,0,0 [u,0,0]	$\bar{x},0,1/2$ [u,0,0]	$\bar{x},0,0$ [u,0,0]	x,0,1/2 [u,0,0]
8 d $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,3/4,0 [0,0,0]
4 c m2'm'	0,y,1/4 [u,0,0]	0, $\bar{y},3/4$ [u,0,0]		
4 b 2/m..	0,1/2,0 [u,0,0]	0,1/2,1/2 [u,0,0]		
4 a 2/m..	0,0,0 [u,0,0]	0,0,1/2 [u,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>'2m'm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



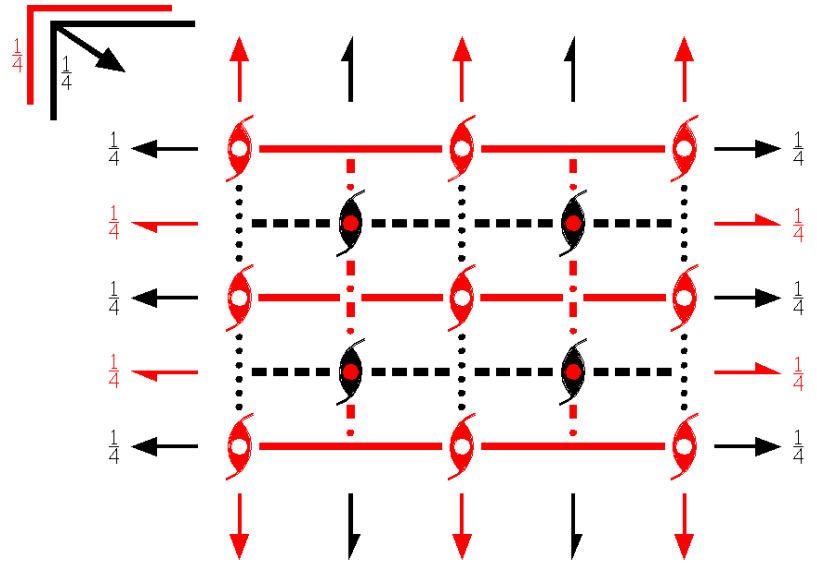
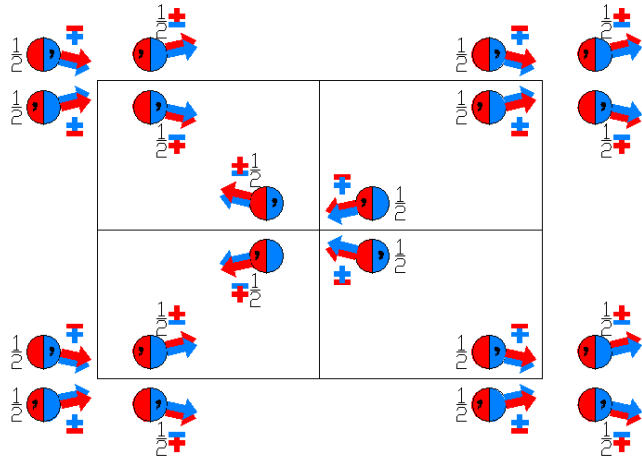
$C_{pm}'cm'$

63.16.526

$mmm1'$

$C_{p2}'/m'2/c2_1'/m'$

Orthorhombic



Origin at  $(\frac{1}{2}, \frac{1}{2}, 0)$  at  $2'/m'c2_1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                                      |  |   |                                      |
|--------------------------------------|--|---|--------------------------------------|
| (1) 1<br>(1 0,0,0)                   | (2) $2' (0,0,1/2)$<br>( $2_z$  0,0,1/2)' | (3) $2' (0,y,1/4)$<br>( $2_y$  0,0,1/2) | (4) $2' (x,0,0)$<br>( $2_x$  0,0,0)' |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) $m' (x,y,1/4)$<br>( $m_z$  0,0,1/2)' | (7) $c (0,0,1/2)$<br>( $m_y$  0,0,1/2)  | (8) $m' (0,y,z)$<br>( $m_x$  0,0,0)' |

For  $(1/2,1/2,0)$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t' (1/2,1/2,0)$<br>(1 1/2,1/2,0)'                  | (2) $2 (0,0,1/2)$<br>( $2_z$  1/2,1/2,1/2)   | (3) $2' (0,1/2,0)$<br>( $2_y$  1/2,1/2,1/2)'   | (4) $2 (1/2,0,0)$<br>( $2_x$  1/2,1/2,0) |
| (5) $\bar{1}' (1/4,1/4,0)$<br>( $\bar{1}'$  1/2,1/2,0)' | (6) $n (1/2,1/2,0)$<br>( $m_z$  1/2,1/2,1/2) | (7) $n' (1/2,0,1/2)$<br>( $m_y$  1/2,1/2,1/2)' | (8) $b (0,1/2,0)$<br>( $m_x$  1/2,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0);(2); (3); (5).

### Positions

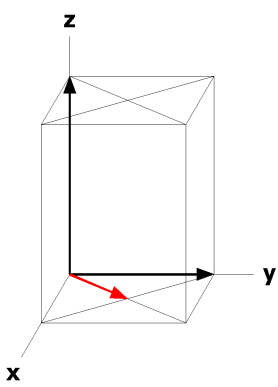
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 h 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 g ..m'	x,y,1/4 [u,v,0]	$\bar{x},\bar{y},3/4$ [u,v,0]	$\bar{x},y,1/4$ [ $\bar{u},v,0$ ]	x, $\bar{y},3/4$ [ $\bar{u},v,0$ ]
8 f m'..	0,y,z [0,v,w]	0, $\bar{y},z+1/2$ [0,v, $\bar{w}$ ]	0,y, $\bar{z}+1/2$ [0,v,w]	0, $\bar{y},\bar{z}$ [0,v, $\bar{w}$ ]
8 e 2'..	x,0,0 [0,v,w]	$\bar{x},0,1/2$ [0,v, $\bar{w}$ ]	$\bar{x},0,0$ [0,v,w]	x,0,1/2 [0,v, $\bar{w}$ ]
8 d $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,3/4,0 [0,0,0]
4 c m'2m'	0,y,1/4 [0,v,0]	0, $\bar{y},3/4$ [0,v,0]		
4 b 2'/m'..	0,1/2,0 [0,v,w]	0,1/2,1/2 [0,v, $\bar{w}$ ]		
4 a 2'/m'..	0,0,0 [0,v,w]	0,0,1/2 [0,v, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>'2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,1/4,0

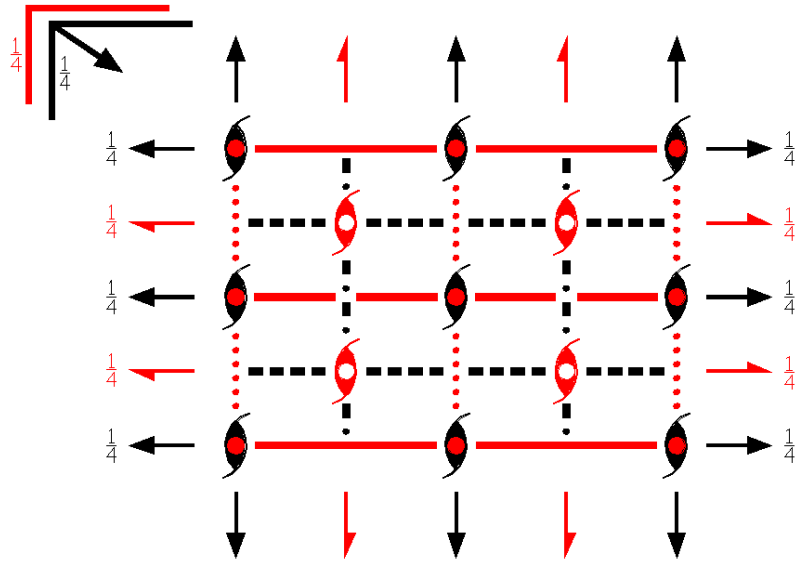
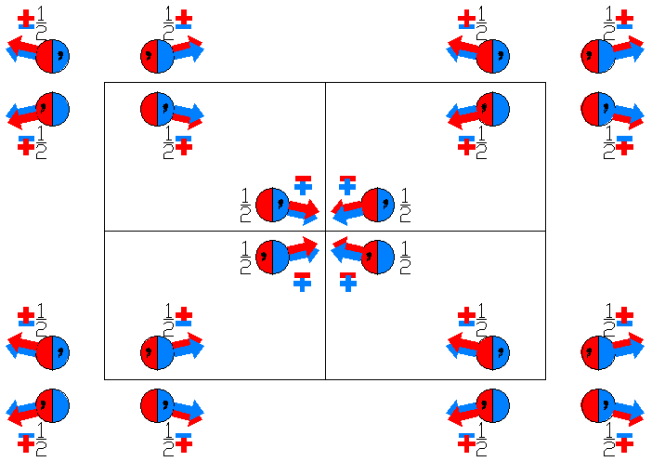
Along [0,1,0] p<sub>c</sub>'2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,0



$C_{pm}'c'm'$   
63.17.527

$mmm1'$   
 $C_{2/m}2/c'2_1/m'$

Orthorhombic



Origin at  $(\frac{1}{2}, \frac{1}{2}, 0)$  at  $2/m'c'2_1$

Asymmetric unit  $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |   |   |                                       |
|--|---|---|---------------------------------------|
| (1) 1<br>(1   0,0,0)                           | (2) 2 $(0,0,1/2)$ $0,0,z$<br>( $2_z$   0,0,1/2) | (3) 2 $0,y,1/4$<br>( $2_y$   0,0,1/2)               | (4) 2 $x,0,0$<br>( $2_x$   0,0,0)     |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   0,0,0)' | (6) $m'$ $x,y,1/4$<br>( $m_z$   0,0,1/2)'       | (7) $c'$ $(0,0,1/2)$ $x,0,z$<br>( $m_y$   0,0,1/2)' | (8) $m'$ $0,y,z$<br>( $m_x$   0,0,0)' |

For  $(1/2,1/2,0)$ ' + set

- |   |   |   |   |
|---|---|---|---|
| (1) $t'$ $(1/2,1/2,0)$<br>(1   1/2,1/2,0)'            | (2) 2' $(0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$   1/2,1/2,1/2)' | (3) 2' $(0,1/2,0)$ $1/4,y,1/4$<br>( $2_y$   1/2,1/2,1/2)' | (4) 2' $(1/2,0,0)$ $x,1/4,0$<br>( $2_x$   1/2,1/2,0)' |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   1/2,1/2,0) | (6) $n$ $(1/2,1/2,0)$ $x,y,1/4$<br>( $m_z$   1/2,1/2,1/2) | (7) $n$ $(1/2,0,1/2)$ $x,1/4,z$<br>( $m_y$   1/2,1/2,1/2) | (8) $b$ $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$   1/2,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0);(2); (3); (5).

**Positions**

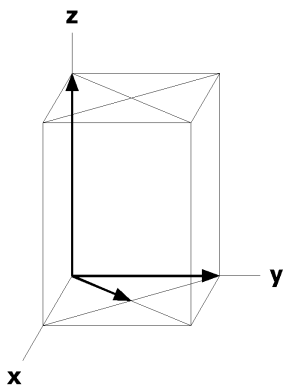
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 h 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ] (7) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 g ..m'	x,y,1/4 [u,v,0]	$\bar{x},\bar{y},3/4$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/4$ [ $\bar{u},v,0$ ]	x, $\bar{y},3/4$ [u, $\bar{v},0$ ]
8 f m'..	0,y,z [0,v,w]	0, $\bar{y},z+1/2$ [0, $\bar{v},w$ ]	0,y, $\bar{z}+1/2$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 e 2..	x,0,0 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	x,0,1/2 [u,0,0]
8 d $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,1/2 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,1/2 [ $\bar{u},v,\bar{w}$ ]	1/4,3/4,0 [u, $\bar{v},\bar{w}$ ]
4 c m'2m'	0,y,1/4 [0,v,0]	0, $\bar{y},3/4$ [0, $\bar{v},0$ ]		
4 b 2/m'..	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 a 2/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

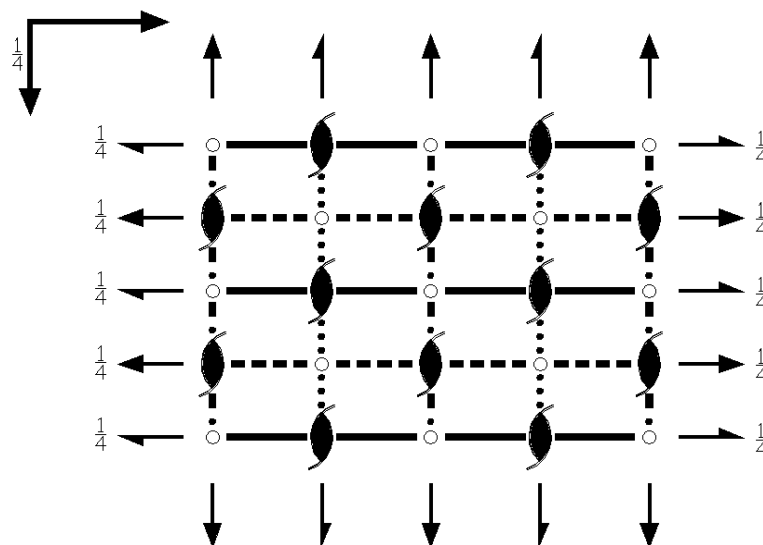
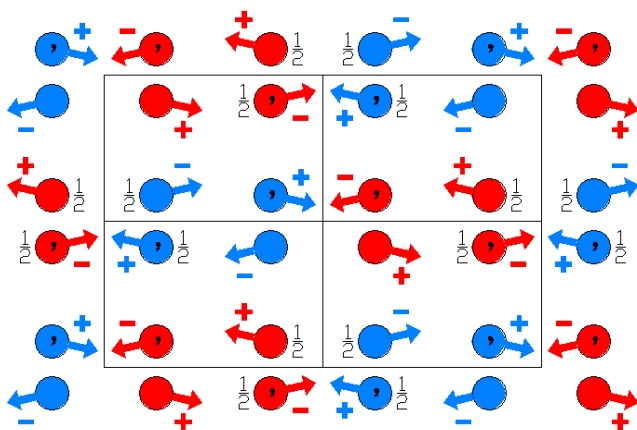
Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Cmca  
64.1.528

mmm  
C2/m2/c2<sub>1</sub>/a

Orthorhombic



Origin at center ( $2/m$ ) at  $2/mn1$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2) | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2) | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) b (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>  0,1/2,1/2) | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2) | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0) |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                 | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)         | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2) | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5).

**Positions**

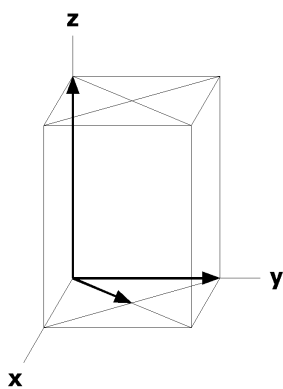
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 g 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y}+1/2,z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) x,y+1/2, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},\bar{v},\bar{w}$ ]
8 f m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z+1/2$ [ $\bar{u},0,0$ ]	0,y+1/2, $\bar{z}+1/2$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]
8 e .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y}+1/2,3/4$ [0, $\bar{v},0$ ]	3/4, $\bar{y},3/4$ [0,v,0]	1/4,y+1/2,1/4 [0, $\bar{v},0$ ]
8 d 2..	x,0,0 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},0,0$ [u,0,0]	x,1/2,1/2 [ $\bar{u},0,0$ ]
8 c $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,1/4,1/2 [ $\bar{u},\bar{v},w$ ]	3/4,3/4,1/2 [ $\bar{u},v,\bar{w}$ ]	1/4,3/4,0 [u, $\bar{v},\bar{w}$ ]
4 b 2/m..	1/2,0,0 [u,0,0]	1/2,1/2,1/2 [ $\bar{u},0,0$ ]		
4 a 2/m..	0,0,0 [u,0,0]	0,1/2,1/2 [ $\bar{u},0,0$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_c$ -2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,1/4,z

Along [1,0,0]  $p_{2mg}1'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a}$ -2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Cmca1'

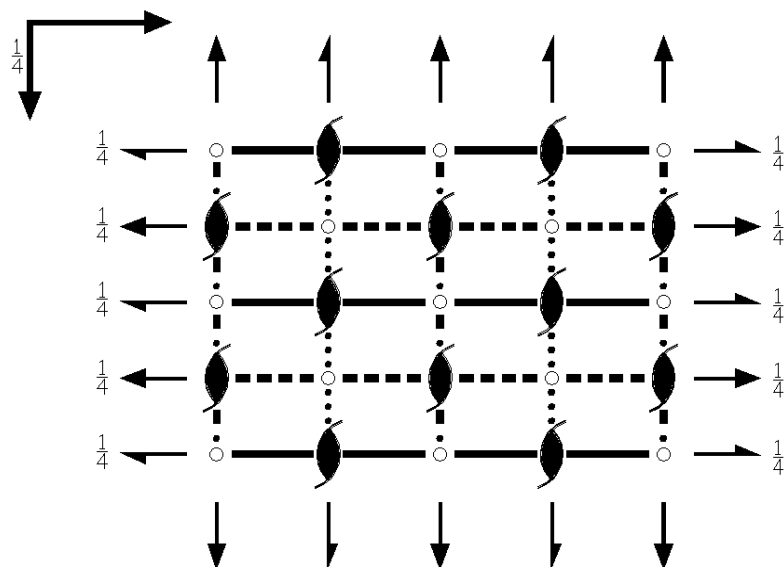
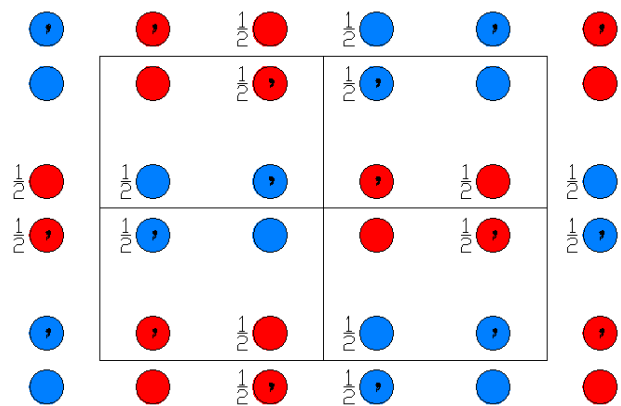
64.2.529

mmm1'

C2/m2/c2<sub>1</sub>/a1'

Orthorhombic

1'



Origin at center ( 2/m1' ) at 2/mn11'

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- (1) 1 (1 | 0,0,0)
- (2) 2 (0,0,1/2) 0,1/4,z (2<sub>z</sub> | 0,1/2,1/2)
- (3) 2 (0,1/2,0) 0,y,1/4 (2<sub>y</sub> | 0,1/2,1/2)
- (4) 2 x,0,0 (2<sub>x</sub> | 0,0,0)
- (5)  $\bar{1}$  0,0,0 ( $\bar{1}$  | 0,0,0)
- (6) b (0,1/2,0) x,y,1/4 (m<sub>z</sub> | 0,1/2,1/2)
- (7) c (0,0,1/2) x,1/4,z (m<sub>y</sub> | 0,1/2,1/2)
- (8) m 0,y,z (m<sub>x</sub> | 0,0,0)

For (1/2,1/2,0) + set

- (1) t (1/2,1/2,0) (1 | 1/2,1/2,0)
- (2) 2 (0,0,1/2) 1/4,0,z (2<sub>z</sub> | 1/2,0,1/2)
- (3) 2 1/4,y,1/4 (2<sub>y</sub> | 1/2,0,1/2)
- (4) 2 (1/2,0,0) x,1/4,0 (2<sub>x</sub> | 1/2,1/2,0)
- (5)  $\bar{1}$  1/4,1/4,0 ( $\bar{1}$  | 1/2,1/2,0)
- (6) a (1/2,0,0) x,y,1/4 (m<sub>z</sub> | 1/2,0,1/2)
- (7) n (1/2,0,1/2) x,0,z (m<sub>y</sub> | 1/2,0,1/2)
- (8) b (0,1/2,0) 1/4,y,z (m<sub>x</sub> | 1/2,1/2,0)

For (0,0,0)' + set

- (1) 1' (1 | 0,0,0)'
- (2) 2' (0,0,1/2) 0,1/4,z (2<sub>z</sub> | 0,1/2,1/2)'
- (3) 2' (0,1/2,0) 0,y,1/4 (2<sub>y</sub> | 0,1/2,1/2)'
- (4) 2' x,0,0 (2<sub>x</sub> | 0,0,0)'
- (5)  $\bar{1}$ ' 0,0,0 ( $\bar{1}$  | 0,0,0)'
- (6) b' (0,1/2,0) x,y,1/4 (m<sub>z</sub> | 0,1/2,1/2)'
- (7) c' (0,0,1/2) x,1/4,z (m<sub>y</sub> | 0,1/2,1/2)'
- (8) m' 0,y,z (m<sub>x</sub> | 0,0,0)'

For (1/2,1/2,0)' + set

- (1) t' (1/2,1/2,0) (1 | 1/2,1/2,0)'
- (2) 2' (0,0,1/2) 1/4,0,z (2<sub>z</sub> | 1/2,0,1/2)'
- (3) 2' 1/4,y,1/4 (2<sub>y</sub> | 1/2,0,1/2)'
- (4) 2' (1/2,0,0) x,1/4,0 (2<sub>x</sub> | 1/2,1/2,0)'
- (5)  $\bar{1}$ ' 1/4,1/4,0 ( $\bar{1}$  | 1/2,1/2,0)'
- (6) a' (1/2,0,0) x,y,1/4 (m<sub>z</sub> | 1/2,0,1/2)'
- (7) n' (1/2,0,1/2) x,0,z (m<sub>y</sub> | 1/2,0,1/2)'
- (8) b' (0,1/2,0) 1/4,y,z (m<sub>x</sub> | 1/2,1/2,0)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5); 1'.

**Positions**

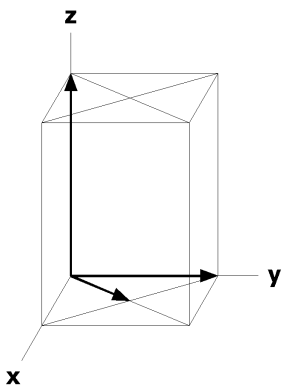
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) + (0,0,0)' +	(1/2,1/2,0) + (1/2,1/2,0)' +		
16	g 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y}+1/2,z+1/2$ [0,0,0]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [0,0,0]	(4) $x,\bar{y},\bar{z}$ [0,0,0]
		(5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(6) $x,y+1/2,\bar{z}+1/2$ [0,0,0]	(7) $x,\bar{y}+1/2,z+1/2$ [0,0,0]	(8) $\bar{x},y,z$ [0,0,0]
8	f m..1'	0,y,z [0,0,0]	$0,\bar{y}+1/2,z+1/2$ [0,0,0]	$0,y+1/2,\bar{z}+1/2$ [0,0,0]	$0,\bar{y},\bar{z}$ [0,0,0]
8	e .2.1'	1/4,y,1/4 [0,0,0]	$3/4,\bar{y}+1/2,3/4$ [0,0,0]	$3/4,\bar{y},3/4$ [0,0,0]	$1/4,y+1/2,1/4$ [0,0,0]
8	d 2..1'	x,0,0 [0,0,0]	$\bar{x},1/2,1/2$ [0,0,0]	$\bar{x},0,0$ [0,0,0]	$x,1/2,1/2$ [0,0,0]
8	c $\bar{1}1'$	1/4,1/4,0 [0,0,0]	$3/4,1/4,1/2$ [0,0,0]	$3/4,3/4,1/2$ [0,0,0]	$1/4,3/4,0$ [0,0,0]
4	b 2/m..1'	1/2,0,0 [0,0,0]	$1/2,1/2,1/2$ [0,0,0]		
4	a 2/m..1'	0,0,0 [0,0,0]	$0,1/2,1/2$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

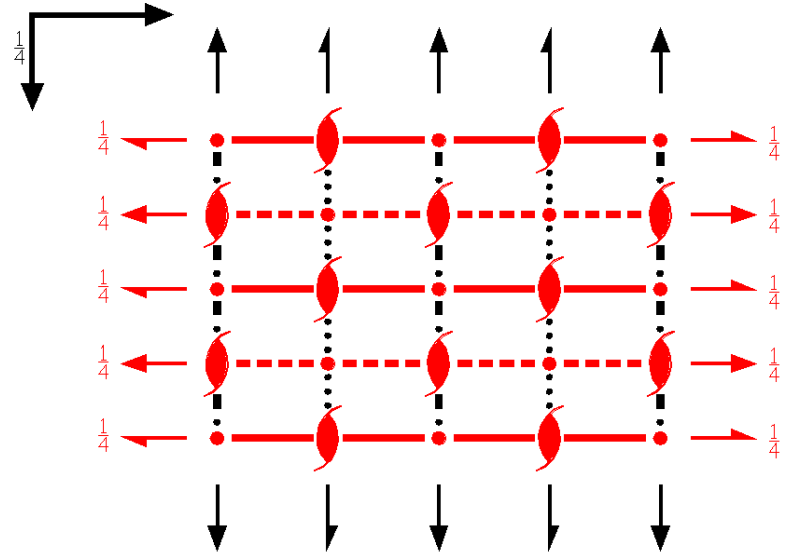
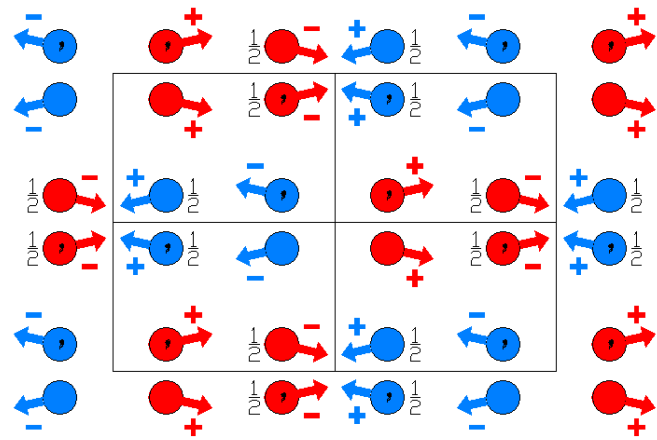
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Cm'ca  
64.3.530

m'mm  
C2/m'2'/c2, '1/a

Orthorhombic



Origin at center ( $2/m'$ ) at  $2/m'n1$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |                                    |
|--|--|--|------------------------------------|
| (1) 1<br>(1 0,0,0)                           | (2) $2'$ (0,0,1/2) $0,1/4,z$<br>( $2_z$  0,1/2,1/2)' | (3) $2'$ (0,1/2,0) $0,y,1/4$<br>( $2_y$  0,1/2,1/2)' | (4) $2$ x,0,0<br>( $2_x$  0,0,0)   |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) b (0,1/2,0) x,y,1/4<br>( $m_z$  0,1/2,1/2)       | (7) c (0,0,1/2) x,1/4,z<br>( $m_y$  0,1/2,1/2)       | (8) $m'$ 0,y,z<br>( $m_x$  0,0,0)' |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                   | (2) $2'$ (0,0,1/2) $1/4,0,z$<br>( $2_z$  1/2,0,1/2)' | (3) $2'$ $1/4,y,1/4$<br>( $2_y$  1/2,0,1/2)'   | (4) $2$ (1/2,0,0) x,1/4,0<br>( $2_x$  1/2,1/2,0)   |
| (5) $\bar{1}'$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) a (1/2,0,0) x,y,1/4<br>( $m_z$  1/2,0,1/2)       | (7) n (1/2,0,1/2) x,0,z<br>( $m_y$  1/2,0,1/2) | (8) b' (0,1/2,0) $1/4,y,z$<br>( $m_x$  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5).

**Positions**

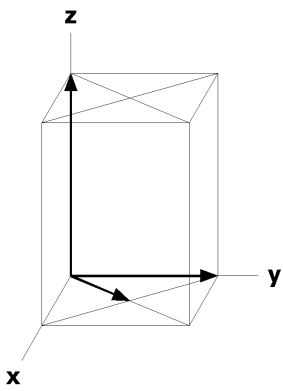
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 g 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y}+1/2,z+1/2$ [u,v, $\bar{w}$ ] (6) x,y+1/2, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 f m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z+1/2$ [0,v, $\bar{w}$ ]	0,y+1/2, $\bar{z}+1/2$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 e .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,3/4$ [u,0, $\bar{w}$ ]	3/4, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,1/4 [ $\bar{u},0,w$ ]
8 d 2..	x,0,0 [u,0,0]	$\bar{x},1/2,1/2$ [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	x,1/2,1/2 [ $\bar{u},0,0$ ]
8 c $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,0 [0,0,0]
4 b 2/m'..	1/2,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a 2/m'..	0,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

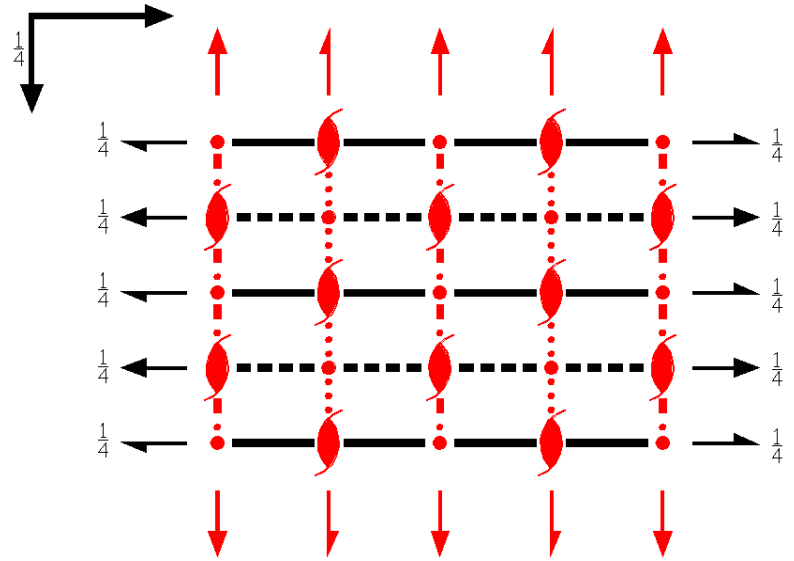
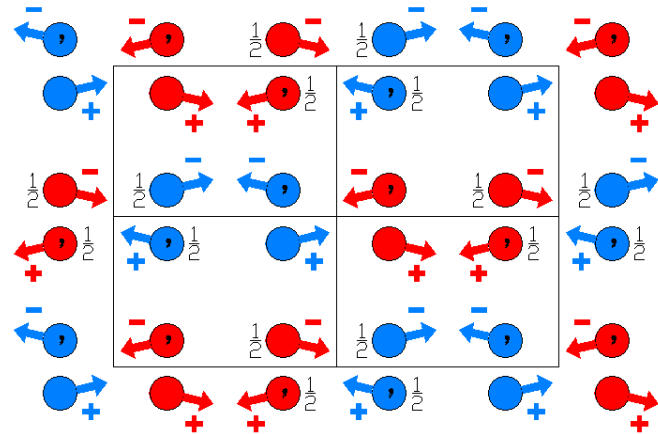
Along [0,1,0] p<sub>2a</sub>·2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Cmc'a  
64.4.531

mm'm  
C2'/m2/c'2, '1/a

Orthorhombic



Origin at center ( $2'/m$ ) at  $2'/mn'1$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |                                    |
|--|--|--|------------------------------------|
| (1) 1<br>(1 0,0,0)                           | (2) $2' (0,0,1/2)$<br>( $2_z$  0,1/2,1/2)' | (3) $2 (0,1/2,0)$<br>( $2_y$  0,1/2,1/2)   | (4) $2' x,0,0$<br>( $2_x$  0,0,0)' |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) $b (0,1/2,0)$<br>( $m_z$  0,1/2,1/2)   | (7) $c' (0,0,1/2)$<br>( $m_y$  0,1/2,1/2)' | (8) $m$ 0,y,z<br>( $m_x$  0,0,0)   |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t (1/2,1/2,0)$<br>(1 1/2,1/2,0)                 | (2) $2' (0,0,1/2)$<br>( $2_z$  1/2,0,1/2)' | (3) $2$ 1/4,y,1/4<br>( $2_y$  1/2,0,1/2)     | (4) $2' (1/2,0,0)$<br>( $2_x$  1/2,1/2,0)' |
| (5) $\bar{1}'$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) $a (1/2,0,0)$<br>( $m_z$  1/2,0,1/2)   | (7) $n' (1/2,0,1/2)$<br>( $m_y$  1/2,0,1/2)' | (8) $b (0,1/2,0)$<br>( $m_x$  1/2,1/2,0)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5).

**Positions**

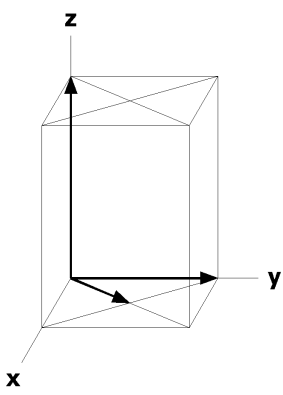
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 g 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y}+1/2,z+1/2$ [u,v, $\bar{w}$ ] (6) x,y+1/2, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y}+1/2,z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 f m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z+1/2$ [u,0,0]	0,y+1/2, $\bar{z}+1/2$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
8 e .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y}+1/2,3/4$ [0,v,0]	3/4, $\bar{y},3/4$ [0, $\bar{v},0$ ]	1/4,y+1/2,1/4 [0, $\bar{v},0$ ]
8 d 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,1/2$ [0,v, $\bar{w}$ ]	$\bar{x},0,0$ [0, $\bar{v},\bar{w}$ ]	x,1/2,1/2 [0, $\bar{v},w$ ]
8 c $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,0 [0,0,0]
4 b 2'/m..	1/2,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a 2'/m..	0,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,1/4,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

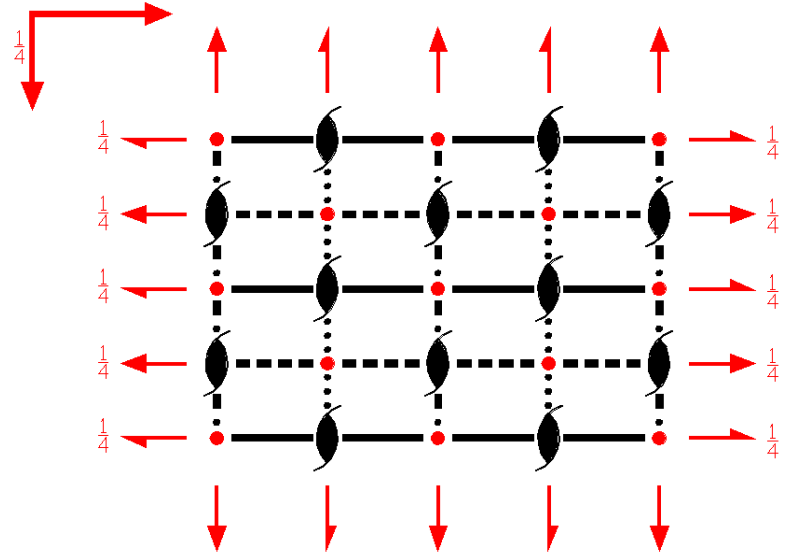
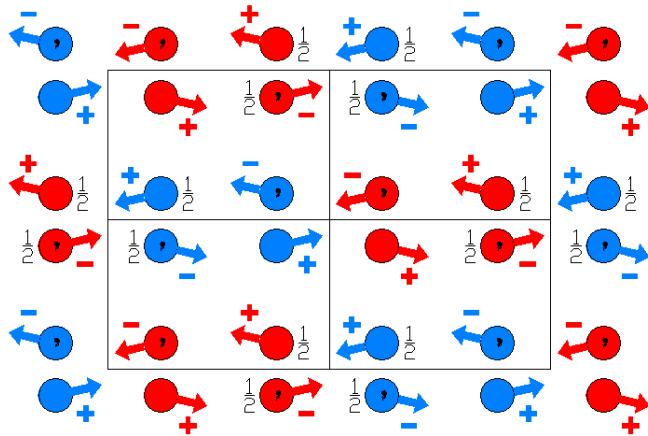
Along [0,1,0] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Cmca'  
64.5.532

mmm'  
C2'/m2'/c2<sub>1</sub>/a'

Orthorhombic



Origin at center ( $2'/m$ ) at  $2'/mn1$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)   | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) b' (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>  0,1/2,1/2)' | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)   | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   |

For (1/2,1/2,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                    | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2' 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)'       | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5).

**Positions**

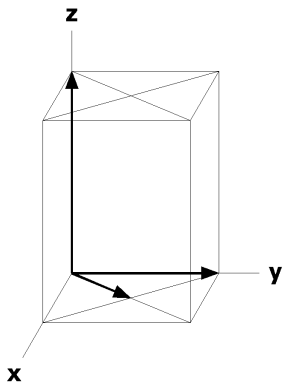
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 g 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y}+1/2,z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) x,y+1/2, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 f m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z+1/2$ [ $\bar{u},0,0$ ]	0,y+1/2, $\bar{z}+1/2$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
8 e .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,3/4$ [ $\bar{u},0,w$ ]	3/4, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,1/4 [u,0, $\bar{w}$ ]
8 d 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,1/2$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0, $\bar{v},\bar{w}$ ]	x,1/2,1/2 [0,v, $\bar{w}$ ]
8 c $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,0 [0,0,0]
4 b 2'/m..	1/2,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a 2'/m..	0,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

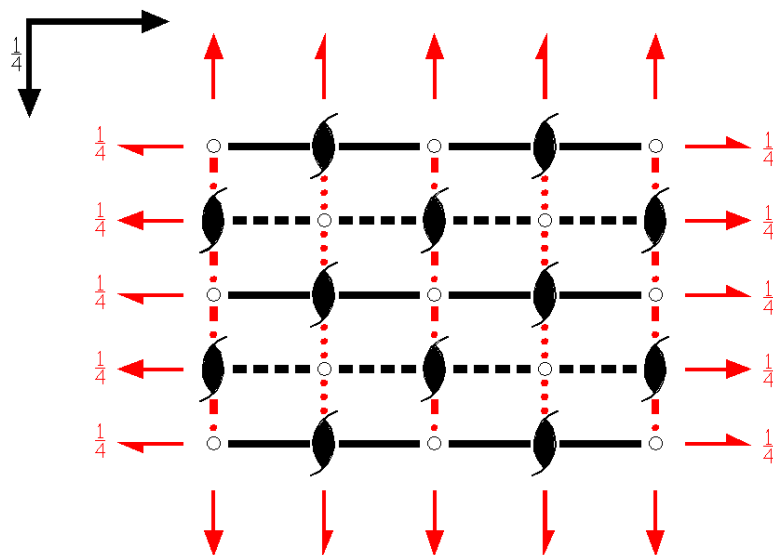
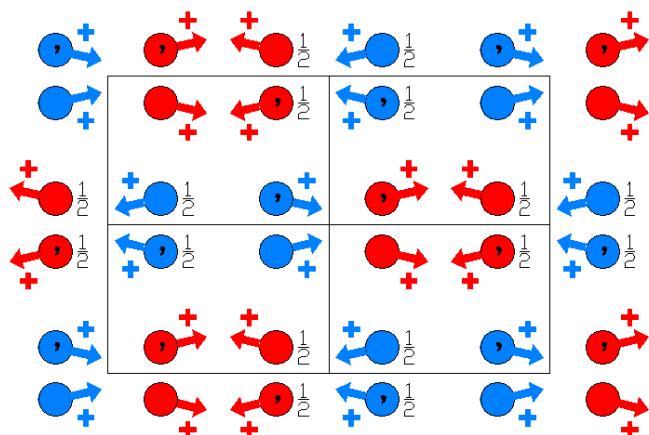
Along [0,1,0] p<sub>2a</sub>·2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Cm'c'a  
64.6.533

m'm'm  
C2'/m'2'/c' 2<sub>1</sub>/a

Orthorhombic



Origin at center ( $2'/m'$ ) at  $2'/m'n'1$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2) | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) b (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>  0,1/2,1/2) | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                 | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) 2' 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)'         | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2) | (7) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5).

**Positions**

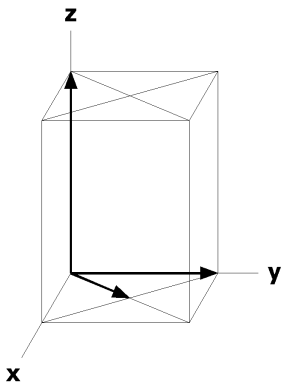
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1/2,1/2,0) +	
16 g 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y}+1/2,z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) x,y+1/2, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y}+1/2,z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 f m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z+1/2$ [0, $\bar{v},w$ ]	0,y+1/2, $\bar{z}+1/2$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
8 e .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,3/4$ [ $\bar{u},0,w$ ]	3/4, $\bar{y},3/4$ [u,0,w]	1/4,y+1/2,1/4 [ $\bar{u},0,w$ ]
8 d 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,1/2$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0,v,w]	x,1/2,1/2 [0, $\bar{v},w$ ]
8 c $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,1/4,1/2 [ $\bar{u},\bar{v},w$ ]	3/4,3/4,1/2 [u, $\bar{v},w$ ]	1/4,3/4,0 [ $\bar{u},v,w$ ]
4 b 2'/m'..	1/2,0,0 [0,v,w]	1/2,1/2,1/2 [0, $\bar{v},w$ ]		
4 a 2'/m'..	0,0,0 [0,v,w]	0,1/2,1/2 [0, $\bar{v},w$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

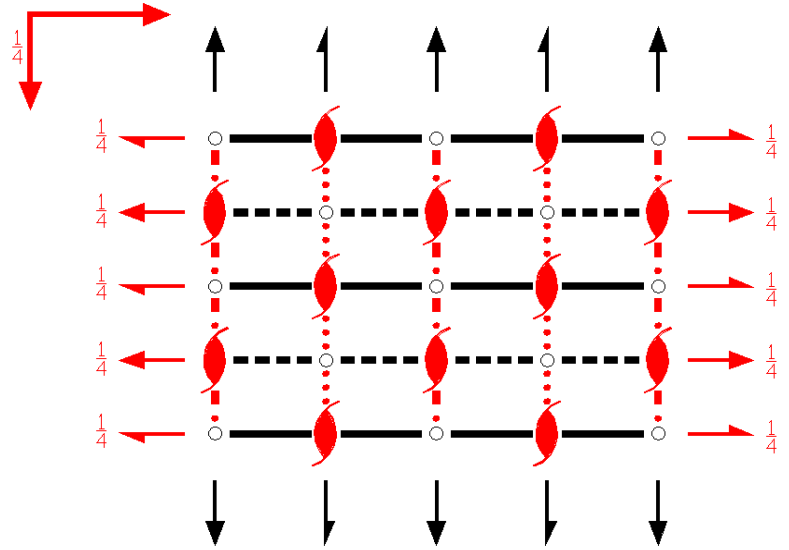
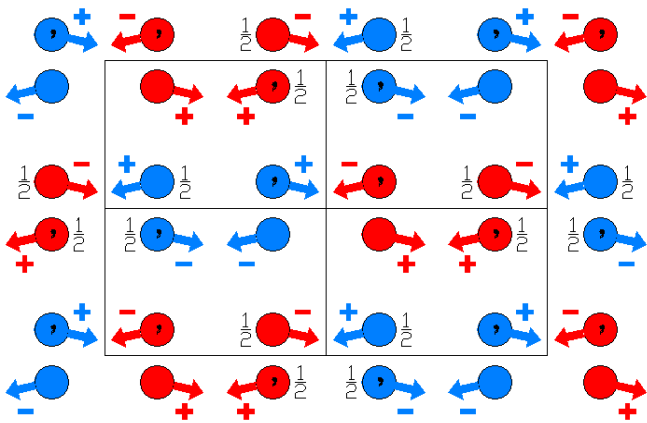
Along [0,1,0] p2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,1/4



Cmc'a'  
64.7.534

mm'm'  
C2/m2'/c2, 'a'

Orthorhombic



Origin at center ( $2/m$ ) at  $2/mn'1$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |                                |
|--|--|--|--------------------------------|
| (1) 1<br>(1 0,0,0)                         | (2) $2'$ (0,0,1/2) 0,1/4,z<br>( $2_z$  0,1/2,1/2)' | (3) $2'$ (0,1/2,0) 0,y,1/4<br>( $2_y$  0,1/2,1/2)' | (4) 2 x,0,0<br>( $2_x$  0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) $b'$ (0,1/2,0) x,y,1/4<br>( $m_z$  0,1/2,1/2)' | (7) $c'$ (0,0,1/2) x,1/4,z<br>( $m_y$  0,1/2,1/2)' | (8) m 0,y,z<br>( $m_x$  0,0,0) |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                 | (2) $2'$ (0,0,1/2) 1/4,0,z<br>( $2_z$  1/2,0,1/2)' | (3) $2'$ 1/4,y,1/4<br>( $2_y$  1/2,0,1/2)'         | (4) 2 (1/2,0,0) x,1/4,0<br>( $2_x$  1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) $a'$ (1/2,0,0) x,y,1/4<br>( $m_z$  1/2,0,1/2)' | (7) $n'$ (1/2,0,1/2) x,0,z<br>( $m_y$  1/2,0,1/2)' | (8) b (0,1/2,0) 1/4,y,z<br>( $m_x$  1/2,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5).

**Positions**

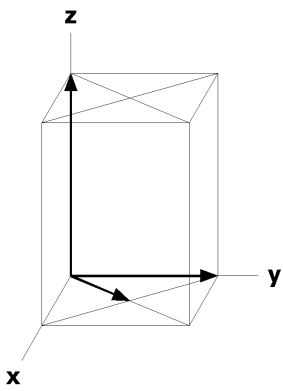
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 g 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y}+1/2,z+1/2$ [u,v, $\bar{w}$ ] (6) x,y+1/2, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [u, $\bar{v}$ ,w] (7) x, $\bar{y}+1/2,z+1/2$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 f m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z+1/2$ [u,0,0]	0,y+1/2, $\bar{z}+1/2$ [u,0,0]	0, $\bar{y},\bar{z}$ [u,0,0]
8 e .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,3/4$ [u,0, $\bar{w}$ ]	3/4, $\bar{y},3/4$ [u,0,w]	1/4,y+1/2,1/4 [u,0, $\bar{w}$ ]
8 d 2..	x,0,0 [u,0,0]	$\bar{x},1/2,1/2$ [u,0,0]	$\bar{x},0,0$ [u,0,0]	x,1/2,1/2 [u,0,0]
8 c $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,1/4,1/2 [u,v, $\bar{w}$ ]	3/4,3/4,1/2 [u, $\bar{v}$ ,w]	1/4,3/4,0 [u, $\bar{v},\bar{w}$ ]
4 b 2/m..	1/2,0,0 [u,0,0]	1/2,1/2,1/2 [u,0,0]		
4 a 2/m..	0,0,0 [u,0,0]	0,1/2,1/2 [u,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

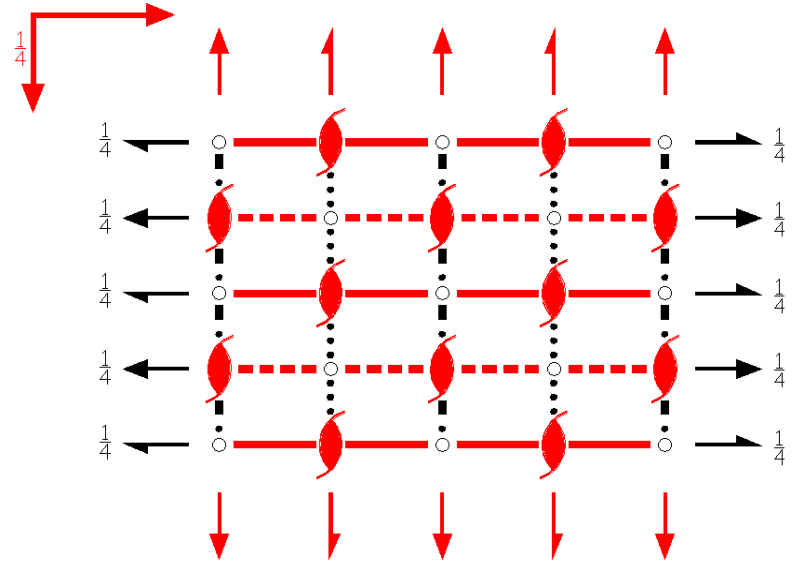
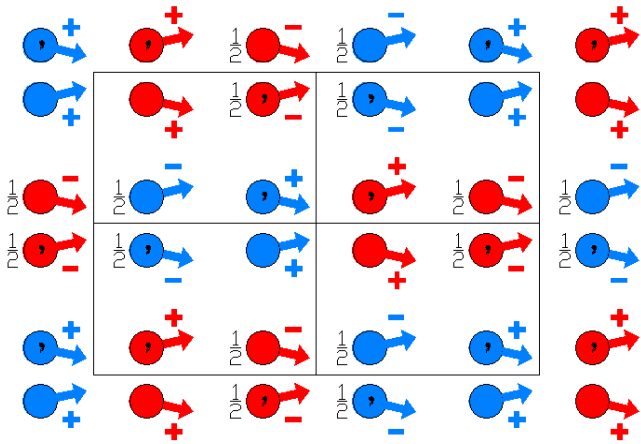
Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



$Cm'ca'$   
64.8.535

$m'mm'$   
 $C2'/m'2/c2_1/a'$

Orthorhombic



Origin at center ( $2'/m'$ ) at  $2'/m'n1$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |                                      |
|--|--|--|--------------------------------------|
| (1) $1$<br>( $1 0,0,0$ )                     | (2) $2'$ (0,0,1/2) $0,1/4,z$<br>( $2_z 0,1/2,1/2$ )' | (3) $2$ (0,1/2,0) $0,y,1/4$<br>( $2_y 0,1/2,1/2$ ) | (4) $2'$ $x,0,0$<br>( $2_x 0,0,0$ )' |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1} 0,0,0$ ) | (6) $b'$ (0,1/2,0) $x,y,1/4$<br>( $m_z 0,1/2,1/2$ )' | (7) $c$ (0,0,1/2) $x,1/4,z$<br>( $m_y 0,1/2,1/2$ ) | (8) $m'$ $0,y,z$<br>( $m_x 0,0,0$ )' |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t$ (1/2,1/2,0)<br>( $1 1/2,1/2,0$ )             | (2) $2'$ (0,0,1/2) $1/4,0,z$<br>( $2_z 1/2,0,1/2$ )' | (3) $2$ $1/4,y,1/4$<br>( $2_y 1/2,0,1/2$ )         | (4) $2'$ (1/2,0,0) $x,1/4,0$<br>( $2_x 1/2,1/2,0$ )' |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1} 1/2,1/2,0$ ) | (6) $a'$ (1/2,0,0) $x,y,1/4$<br>( $m_z 1/2,0,1/2$ )' | (7) $n$ (1/2,0,1/2) $x,0,z$<br>( $m_y 1/2,0,1/2$ ) | (8) $b'$ (0,1/2,0) $1/4,y,z$<br>( $m_x 1/2,1/2,0$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5).

**Positions**

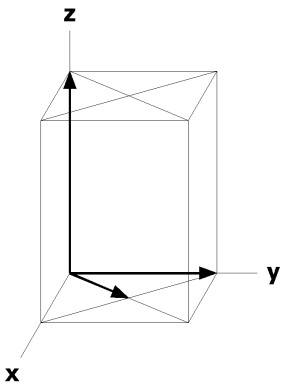
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 g 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y}+1/2,z+1/2$ [u,v, $\bar{w}$ ] (6) x,y+1/2, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u}$ ,v, $\bar{w}$ ] (7) x, $\bar{y}+1/2,z+1/2$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u}$ ,v,w] (8) $\bar{x},y,z$ [ $\bar{u}$ ,v,w]
8 f m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z+1/2$ [0,v, $\bar{w}$ ]	0,y+1/2, $\bar{z}+1/2$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
8 e .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y}+1/2,3/4$ [0,v,0]	3/4, $\bar{y},3/4$ [0,v,0]	1/4,y+1/2,1/4 [0,v,0]
8 d 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,1/2$ [0,v, $\bar{w}$ ]	$\bar{x},0,0$ [0,v,w]	x,1/2,1/2 [0,v, $\bar{w}$ ]
8 c $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,1/4,1/2 [u,v, $\bar{w}$ ]	3/4,3/4,1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	1/4,3/4,0 [ $\bar{u}$ ,v,w]
4 b 2'/m'..	1/2,0,0 [0,v,w]	1/2,1/2,1/2 [0,v, $\bar{w}$ ]		
4 a 2'/m'..	0,0,0 [0,v,w]	0,1/2,1/2 [0,v, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

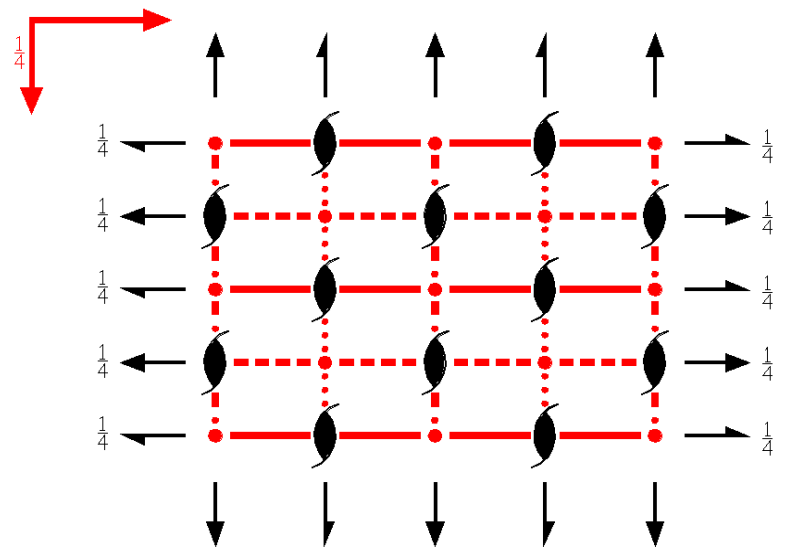
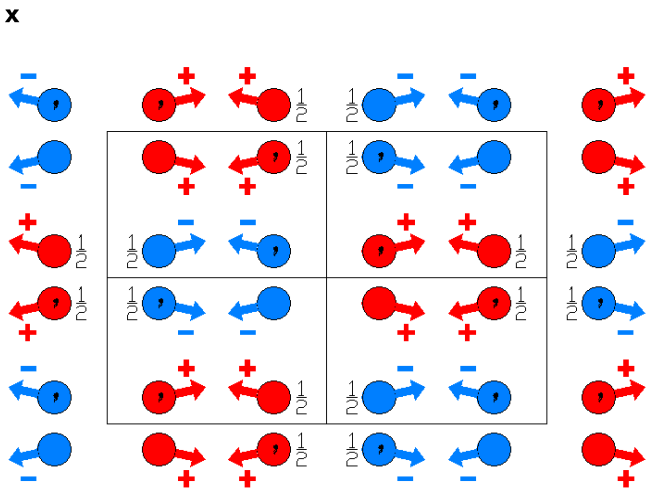
Along [0,1,0] p<sub>2a</sub>·2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



Cm'c'a'  
64.9.536

m'm'm'  
C2/m'2/c'2<sub>1</sub>/a'

Orthorhombic



Origin at center ( $\frac{1}{2}m'$ ) at  $2/m'n'1$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}'$  0,0,0)' | (6) b' (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>  0,1/2,1/2)' | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

For (1/2,1/2,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                    | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)           | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) $\bar{1}'$ 1/4,1/4,0<br>( $\bar{1}'$  1/2,1/2,0)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0);(2); (3); (5).

**Positions**

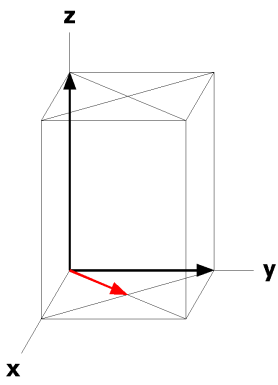
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 g 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y}+1/2,z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) x,y+1/2, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y}+1/2,z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 f m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z+1/2$ [0, $\bar{v},w$ ]	0,y+1/2, $\bar{z}+1/2$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 e .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y}+1/2,3/4$ [0, $\bar{v},0$ ]	3/4, $\bar{y},3/4$ [0, $\bar{v},0$ ]	1/4,y+1/2,1/4 [0,v,0]
8 d 2..	x,0,0 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	x,1/2,1/2 [u,0,0]
8 c $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,0 [0,0,0]
4 b 2/m'..	1/2,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a 2/m'..	0,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

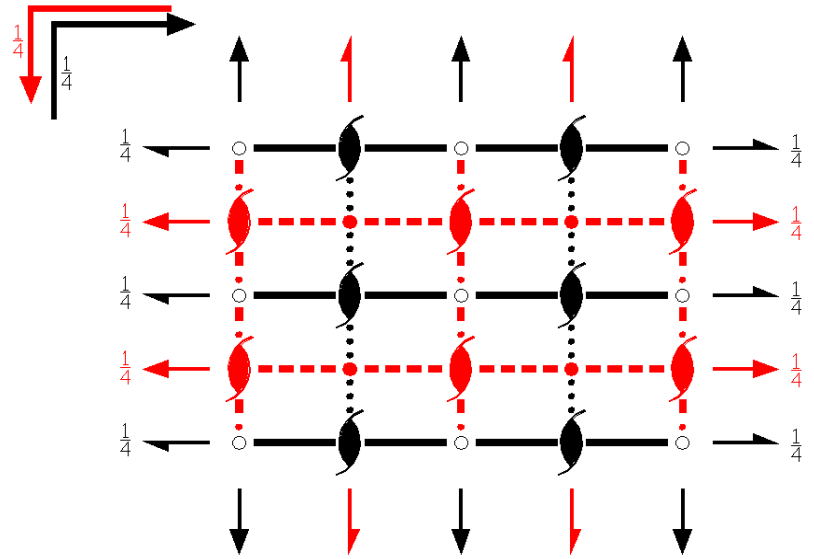
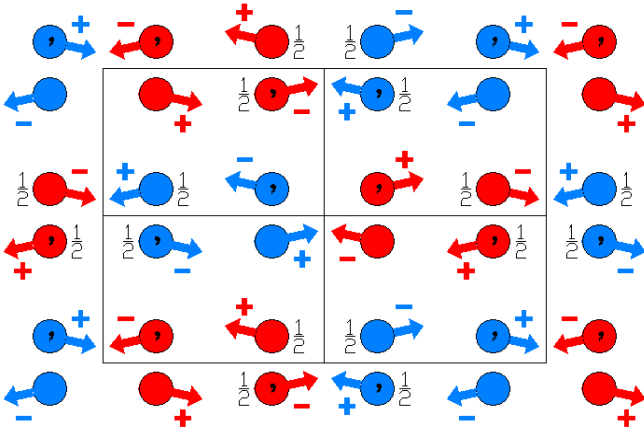
Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



$C_{pmca}$   
64.10.537

$mmm1'$   
 $C_{p2/m2/c2_1/a}$

Orthorhombic



Origin at center ( $2/m$ ) at  $2/mn'1$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2) | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2) | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) b (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>  0,1/2,1/2) | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2) | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0) |

For  $(1/2,1/2,0)'$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' (1/2,1/2,0)<br>(1 1/2,1/2,0)'                  | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) 2' 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)'         | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}'$ 1/4,1/4,0<br>( $\bar{1}'$  1/2,1/2,0)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0);(2); (3); (5).

### Positions

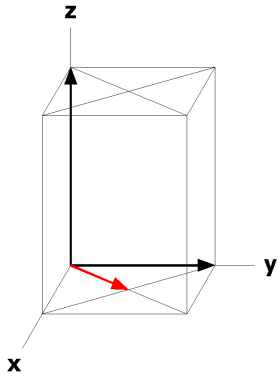
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 g 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y}+1/2,z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) x,y+1/2, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 f m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z+1/2$ [ $\bar{u},0,0$ ]	0,y+1/2, $\bar{z}+1/2$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]
8 e .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y}+1/2,3/4$ [0, $\bar{v},0$ ]	3/4, $\bar{y},3/4$ [0,v,0]	1/4,y+1/2,1/4 [0, $\bar{v},0$ ]
8 d 2..	x,0,0 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},0,0$ [u,0,0]	x,1/2,1/2 [ $\bar{u},0,0$ ]
8 c $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,0 [0,0,0]
4 b 2/m..	1/2,0,0 [u,0,0]	1/2,1/2,1/2 [ $\bar{u},0,0$ ]		
4 a 2/m..	0,0,0 [u,0,0]	0,1/2,1/2 [ $\bar{u},0,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,1/4,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

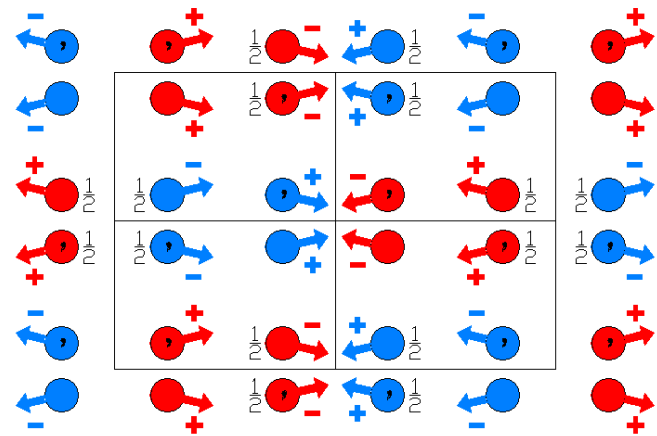
Along [0,1,0] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,0



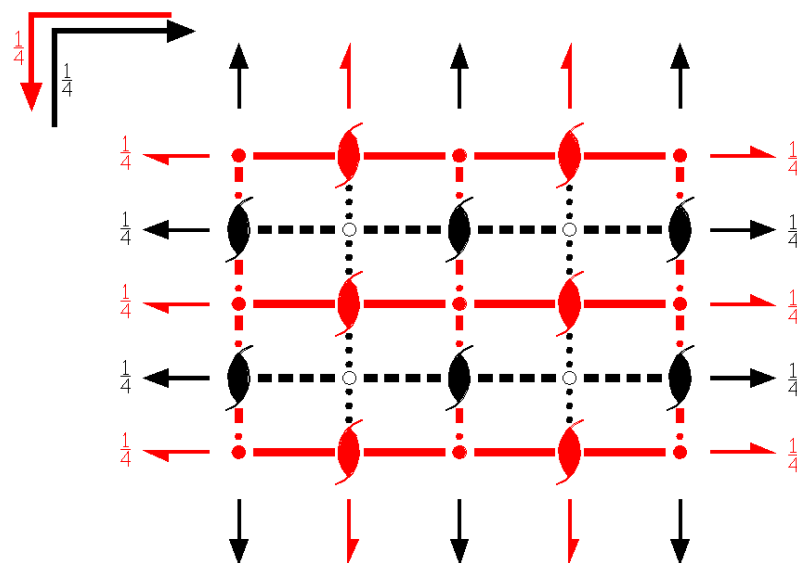
$C_p m'ca$   
64.11.538

$mmm1'$   
 $C_p 2/m'2'/c2_1'/a$

Orthorhombic



Origin at center ( $2/m'$ ) at  $2/m'n'1$



Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |  |   |   |                                     |
|--|---|---|-------------------------------------|
| (1) 1<br>(1   0,0,0)                           | (2) $2'$ (0,0,1/2) 0,1/4,z<br>( $2_z$   0,1/2,1/2)' | (3) $2'$ (0,1/2,0) 0,y,1/4<br>( $2_y$   0,1/2,1/2)' | (4) 2 x,0,0<br>( $2_x$   0,0,0)     |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$   0,0,0)' | (6) b (0,1/2,0) x,y,1/4<br>( $m_z$   0,1/2,1/2)     | (7) c (0,0,1/2) x,1/4,z<br>( $m_y$   0,1/2,1/2)     | (8) $m'$ 0,y,z<br>( $m_x$   0,0,0)' |

For (1/2,1/2,0)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) $t'$ (1/2,1/2,0)<br>(1   1/2,1/2,0)'              | (2) 2 (0,0,1/2) 1/4,0,z<br>( $2_z$   1/2,0,1/2)     | (3) 2 1/4,y,1/4<br>( $2_y$   1/2,0,1/2)             | (4) $2'$ (1/2,0,0) x,1/4,0<br>( $2_x$   1/2,1/2,0)' |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0) | (6) $a'$ (1/2,0,0) x,y,1/4<br>( $m_z$   1/2,0,1/2)' | (7) $n'$ (1/2,0,1/2) x,0,z<br>( $m_y$   1/2,0,1/2)' | (8) b (0,1/2,0) 1/4,y,z<br>( $m_x$   1/2,1/2,0)     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0);(2); (3); (5).

**Positions**

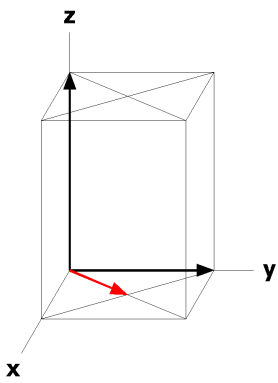
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 g 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y}+1/2,z+1/2$ [u,v, $\bar{w}$ ] (6) x,y+1/2, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 f m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z+1/2$ [0,v, $\bar{w}$ ]	0,y+1/2, $\bar{z}+1/2$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 e .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,3/4$ [u,0, $\bar{w}$ ]	3/4, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,1/4 [ $\bar{u},0,w$ ]
8 d 2..	x,0,0 [u,0,0]	$\bar{x},1/2,1/2$ [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	x,1/2,1/2 [ $\bar{u},0,0$ ]
8 c $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,1/4,1/2 [u,v, $\bar{w}$ ]	3/4,3/4,1/2 [u, $\bar{v},w$ ]	1/4,3/4,0 [u, $\bar{v},\bar{w}$ ]
4 b 2/m'..	1/2,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a 2/m'..	0,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

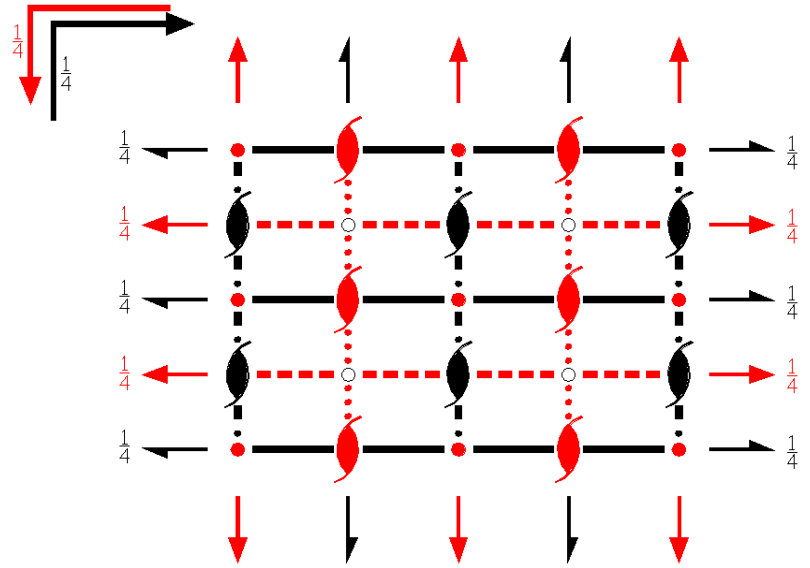
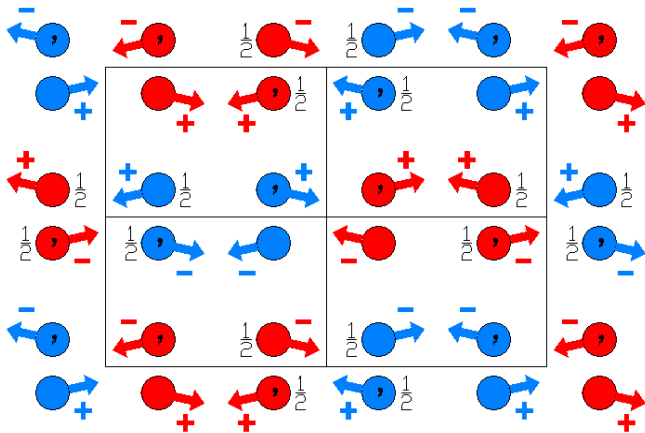
Along [0,1,0] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,1/4



$C_{2v}mc'a$   
64.12.539

$mmm1'$   
 $C_{2v}2'/m2/c'2_1'/a$

Orthorhombic



Origin at center ( $2'/m$ ) at  $2'/mn1$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |                                    |
|--|--|--|------------------------------------|
| (1) 1<br>(1 0,0,0)                           | (2) $2' (0,0,1/2)$<br>( $2_z$  0,1/2,1/2)' | (3) $2 (0,1/2,0)$<br>( $2_y$  0,1/2,1/2)   | (4) $2' x,0,0$<br>( $2_x$  0,0,0)' |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) $b (0,1/2,0)$<br>( $m_z$  0,1/2,1/2)   | (7) $c' (0,0,1/2)$<br>( $m_y$  0,1/2,1/2)' | (8) $m$ 0,y,z<br>( $m_x$  0,0,0)   |

For (1/2,1/2,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t' (1/2,1/2,0)$<br>(1 1/2,1/2,0)'             | (2) $2 (0,0,1/2)$<br>( $2_z$  1/2,0,1/2)   | (3) $2' 1/4,y,1/4$<br>( $2_y$  1/2,0,1/2)' | (4) $2 (1/2,0,0)$<br>( $2_x$  1/2,1/2,0)   |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) $a' (1/2,0,0)$<br>( $m_z$  1/2,0,1/2)' | (7) $n (1/2,0,1/2)$<br>( $m_y$  1/2,0,1/2) | (8) $b' (0,1/2,0)$<br>( $m_x$  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0);(2); (3); (5).

**Positions**

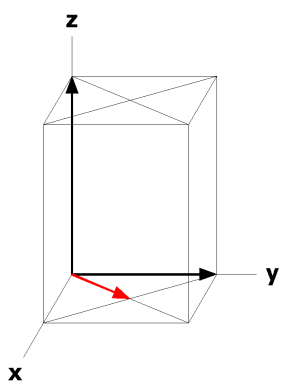
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 g 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y}+1/2,z+1/2$ [u,v, $\bar{w}$ ] (6) x,y+1/2, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y}+1/2,z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 f m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z+1/2$ [u,0,0]	0,y+1/2, $\bar{z}+1/2$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
8 e .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y}+1/2,3/4$ [0,v,0]	3/4, $\bar{y},3/4$ [0, $\bar{v},0$ ]	1/4,y+1/2,1/4 [0, $\bar{v},0$ ]
8 d 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,1/2$ [0,v, $\bar{w}$ ]	$\bar{x},0,0$ [0, $\bar{v},\bar{w}$ ]	x,1/2,1/2 [0, $\bar{v},w$ ]
8 c $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,1/4,1/2 [u,v, $\bar{w}$ ]	3/4,3/4,1/2 [ $\bar{u},v,\bar{w}$ ]	1/4,3/4,0 [ $\bar{u},v,w$ ]
4 b 2'/m..	1/2,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a 2'/m..	0,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>·2mm  
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

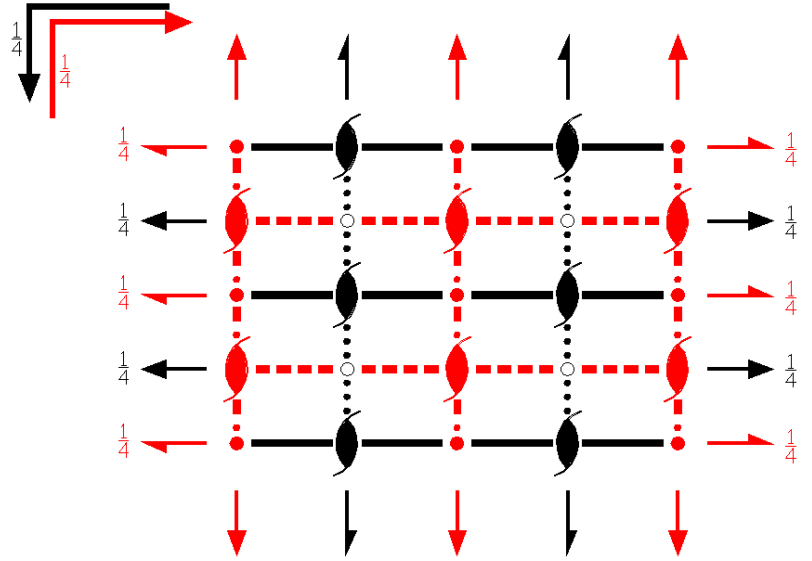
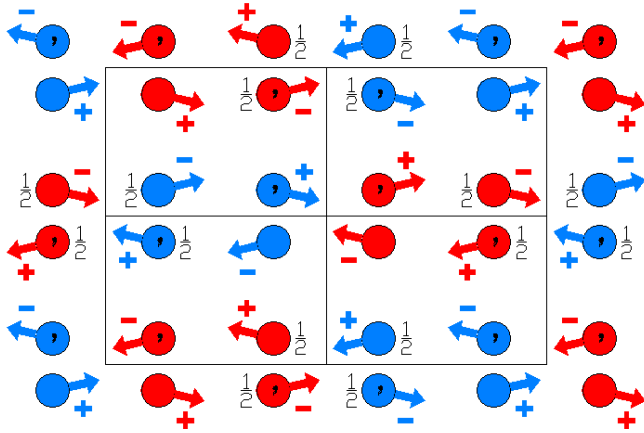
Along [0,1,0] p<sub>2a</sub>·2mm  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$C_{pmca}'$   
64.13.540

$mmm1'$   
 $C_{p2}'/m2'/c2_1/a'$

Orthorhombic



Origin at center ( $2'/m$ ) at  $2'/mn1'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1   0,0,0)                           | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>   0,1/2,1/2)   | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>   0,1/2,1/2)' | (4) 2' x,0,0<br>(2 <sub>x</sub>   0,0,0)' |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$   0,0,0)' | (6) b' (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>   0,1/2,1/2)' | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>   0,1/2,1/2)   | (8) m 0,y,z<br>(m <sub>x</sub>   0,0,0)   |

For (1/2,1/2,0)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) t' (1/2,1/2,0)<br>(1   1/2,1/2,0)'                | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>   1/2,0,1/2)' | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,0,1/2)           | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)   |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>   1/2,0,1/2)   | (7) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>   1/2,0,1/2)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0);(2); (3); (5).

**Positions**

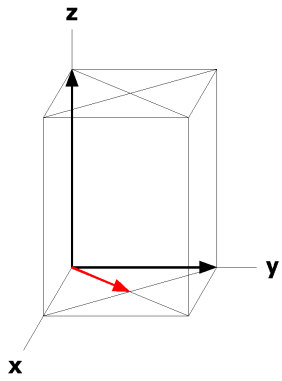
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 g 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y}+1/2,z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) x,y+1/2, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 f m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z+1/2$ [ $\bar{u},0,0$ ]	0,y+1/2, $\bar{z}+1/2$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
8 e .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,3/4$ [ $\bar{u},0,w$ ]	3/4, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,1/4 [u,0, $\bar{w}$ ]
8 d 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,1/2$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0, $\bar{v},\bar{w}$ ]	x,1/2,1/2 [0, $\bar{v},w$ ]
8 c $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,1/4,1/2 [ $\bar{u},\bar{v},w$ ]	3/4,3/4,1/2 [u, $\bar{v},w$ ]	1/4,3/4,0 [ $\bar{u},v,w$ ]
4 b 2'/m..	1/2,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a 2'/m..	0,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

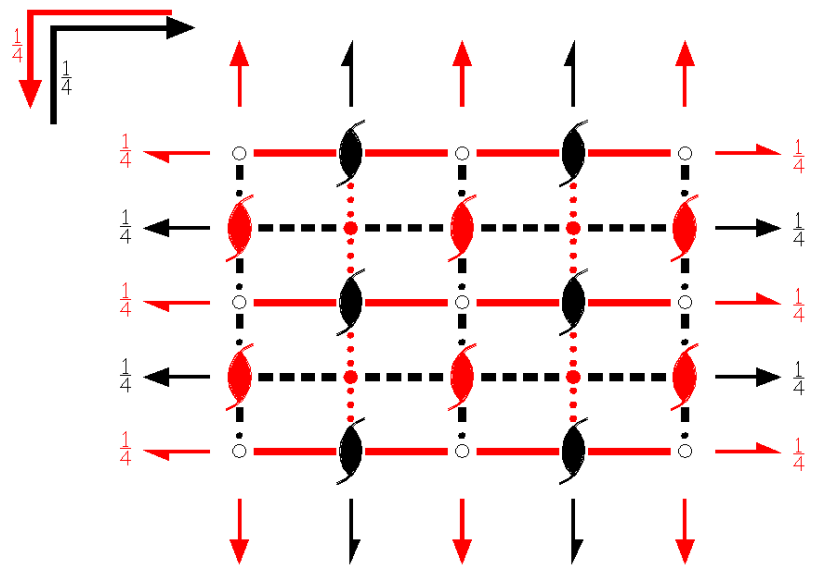
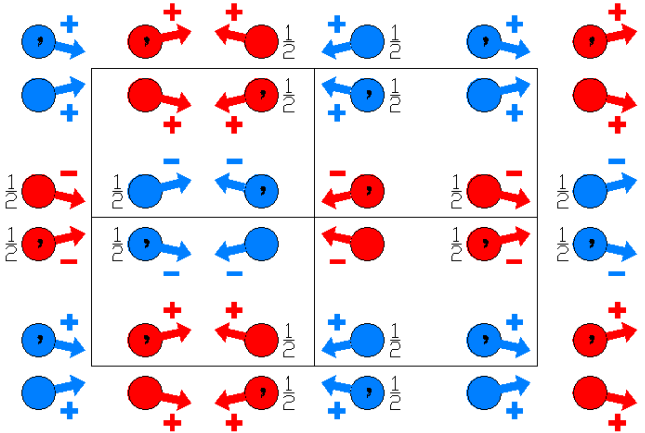
Along [0,1,0] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



$C_{pm}'c'a$   
64.14.541

$mmm1'$   
 $C_{p2}'/m'2'/c'2_1/a$

Orthorhombic



Origin at center ( $2'/m'$ ) at  $2'/m'n1$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2) | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) b (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>  0,1/2,1/2) | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

For (1/2,1/2,0)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' (1/2,1/2,0)<br>(1 1/2,1/2,0)'                  | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)         | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0);(2); (3); (5).

**Positions**

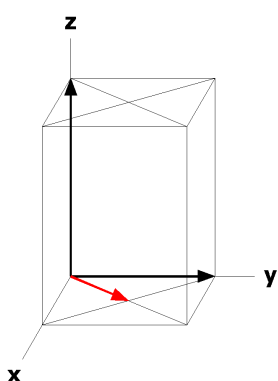
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 g 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y}+1/2,z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) x,y+1/2, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y}+1/2,z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 f m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z+1/2$ [0, $\bar{v},w$ ]	0,y+1/2, $\bar{z}+1/2$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
8 e .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,3/4$ [ $\bar{u},0,w$ ]	3/4, $\bar{y},3/4$ [u,0,w]	1/4,y+1/2,1/4 [ $\bar{u},0,w$ ]
8 d 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,1/2$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0,v,w]	x,1/2,1/2 [0, $\bar{v},w$ ]
8 c $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,0 [0,0,0]
4 b 2'/m'..	1/2,0,0 [0,v,w]	1/2,1/2,1/2 [0, $\bar{v},w$ ]		
4 a 2'/m'..	0,0,0 [0,v,w]	0,1/2,1/2 [0, $\bar{v},w$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,1/4,z

Along [1,0,0] p<sub>2b</sub>-2mg  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,1/4,0

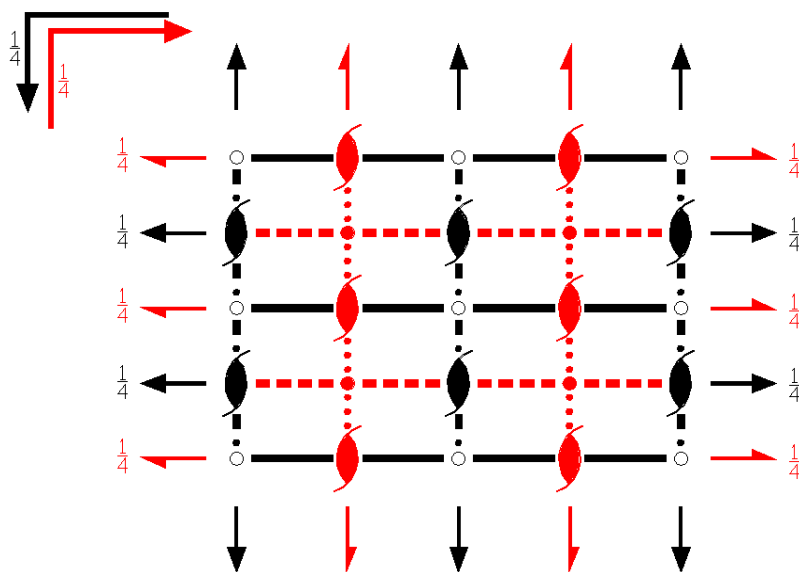
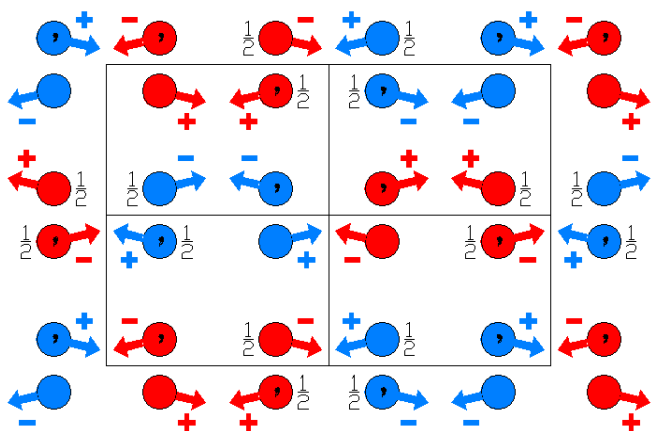
Along [0,1,0] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 1/4,y,1/4



$C_pmc'a'$   
64.15.542

$mmm1'$   
 $C_p2/m2'/c'2_1'/a'$

Orthorhombic



Origin at center ( $2/m$ ) at  $2/mn1$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                               | (2) $2' (0,0,1/2) \quad 0,1/4,z$<br>( $2_z$  0,1/2,1/2)' | (3) $2' (0,1/2,0) \quad 0,y,1/4$<br>( $2_y$  0,1/2,1/2)' | (4) $2 \quad x,0,0$<br>( $2_x$  0,0,0) |
| (5) $\bar{1} \quad 0,0,0$<br>( $\bar{1}$  0,0,0) | (6) $b' (0,1/2,0) \quad x,y,1/4$<br>( $m_z$  0,1/2,1/2)' | (7) $c' (0,0,1/2) \quad x,1/4,z$<br>( $m_y$  0,1/2,1/2)' | (8) $m \quad 0,y,z$<br>( $m_x$  0,0,0) |

For (1/2,1/2,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t' (1/2,1/2,0)$<br>(1 1/2,1/2,0)'                     | (2) $2 (0,0,1/2) \quad 1/4,0,z$<br>( $2_z$  1/2,0,1/2) | (3) $2 \quad 1/4,y,1/4$<br>( $2_y$  1/2,0,1/2)         | (4) $2' (1/2,0,0) \quad x,1/4,0$<br>( $2_x$  1/2,1/2,0)' |
| (5) $\bar{1}' \quad 1/4,1/4,0$<br>( $\bar{1}$  1/2,1/2,0)' | (6) $a (1/2,0,0) \quad x,y,1/4$<br>( $m_z$  1/2,0,1/2) | (7) $n (1/2,0,1/2) \quad x,0,z$<br>( $m_y$  1/2,0,1/2) | (8) $b' (0,1/2,0) \quad 1/4,y,z$<br>( $m_x$  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0);(2); (3); (5).

**Positions**

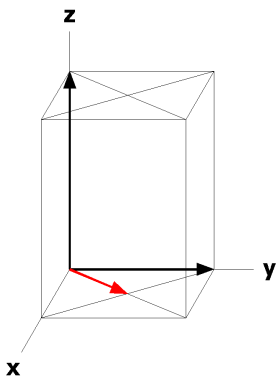
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y}+1/2,z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y+1/2, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(7) x, $\bar{y}+1/2,z+1/2$ [u, $\bar{v}$ ,w]	(8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 f m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z+1/2$ [u,0,0]	0,y+1/2, $\bar{z}+1/2$ [u,0,0]	0, $\bar{y},\bar{z}$ [u,0,0]
8 e .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,3/4$ [u,0, $\bar{w}$ ]	3/4, $\bar{y},3/4$ [u,0,w]	1/4,y+1/2,1/4 [u,0, $\bar{w}$ ]
8 d 2..	x,0,0 [u,0,0]	$\bar{x},1/2,1/2$ [u,0,0]	$\bar{x},0,0$ [u,0,0]	x,1/2,1/2 [u,0,0]
8 c $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,0 [0,0,0]
4 b 2/m..	1/2,0,0 [u,0,0]	1/2,1/2,1/2 [u,0,0]		
4 a 2/m..	0,0,0 [u,0,0]	0,1/2,1/2 [u,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>·2m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

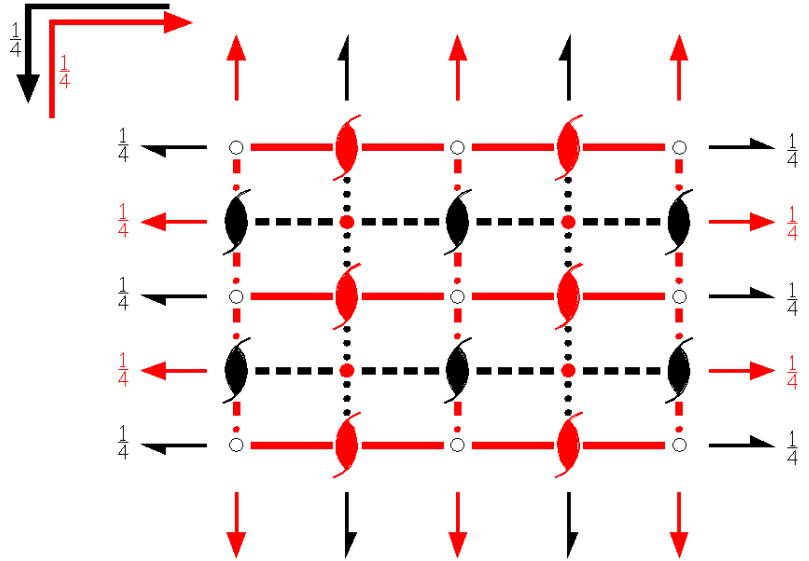
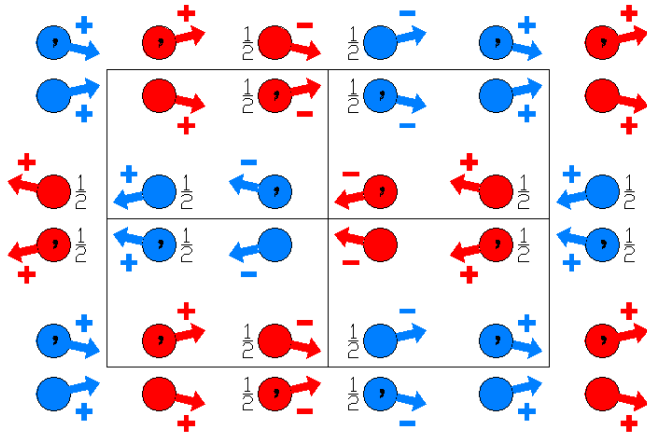
Along [0,1,0] p<sub>2a</sub>·2m'm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$C_p m' c a'$   
64.16.543

$m m m 1'$   
 $C_p 2'/m'2/c_2'1'/a'$

Orthorhombic



Origin at center ( $2'/m'$ ) at  $2'/m'n'1$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |                                      |  |  |                                    |
|--------------------------------------|--|--|------------------------------------|
| (1) 1<br>(1 0,0,0)                   | (2) $2' (0,0,1/2)$<br>( $2_z$  0,1/2,1/2)' | (3) $2 (0,1/2,0)$<br>( $2_y$  0,1/2,1/2) | (4) $2' x,0,0$<br>( $2_x$  0,0,0)' |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) $b' (0,1/2,0)$<br>( $m_z$  0,1/2,1/2)' | (7) $c (0,0,1/2)$<br>( $m_y$  0,1/2,1/2) | (8) $m'$<br>( $m_x$  0,0,0)'       |

For (1/2,1/2,0)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t' (1/2,1/2,0)$<br>(1 1/2,1/2,0)'                | (2) $2 (0,0,1/2)$<br>( $2_z$  1/2,0,1/2) | (3) $2' 1/4,y,1/4$<br>( $2_y$  1/2,0,1/2)'   | (4) $2 (1/2,0,0)$<br>( $2_x$  1/2,1/2,0) |
| (5) $\bar{1}' 1/4,1/4,0$<br>( $\bar{1}'$  1/2,1/2,0)' | (6) $a (1/2,0,0)$<br>( $m_z$  1/2,0,1/2) | (7) $n' (1/2,0,1/2)$<br>( $m_y$  1/2,0,1/2)' | (8) $b (0,1/2,0)$<br>( $m_x$  1/2,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0);(2); (3); (5).

### Positions

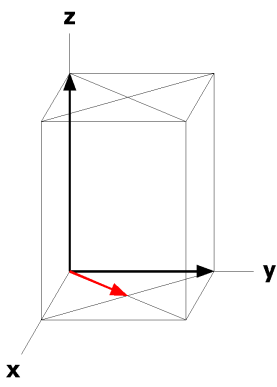
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y}+1/2,z+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y+1/2, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(7) x, $\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 f m..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z+1/2$ [0,v, $\bar{w}$ ]	0,y+1/2, $\bar{z}+1/2$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
8 e .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y}+1/2,3/4$ [0,v,0]	3/4, $\bar{y},3/4$ [0,v,0]	1/4,y+1/2,1/4 [0,v,0]
8 d 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,1/2$ [0,v, $\bar{w}$ ]	$\bar{x},0,0$ [0,v,w]	x,1/2,1/2 [0,v, $\bar{w}$ ]
8 c $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,0 [0,0,0]
4 b 2'/m'..	1/2,0,0 [0,v,w]	1/2,1/2,1/2 [0,v, $\bar{w}$ ]		
4 a 2'/m'..	0,0,0 [0,v,w]	0,1/2,1/2 [0,v, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,0,z

Along [1,0,0] p<sub>2b</sub>-2mg  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,1/4,0

Along [0,1,0] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,0



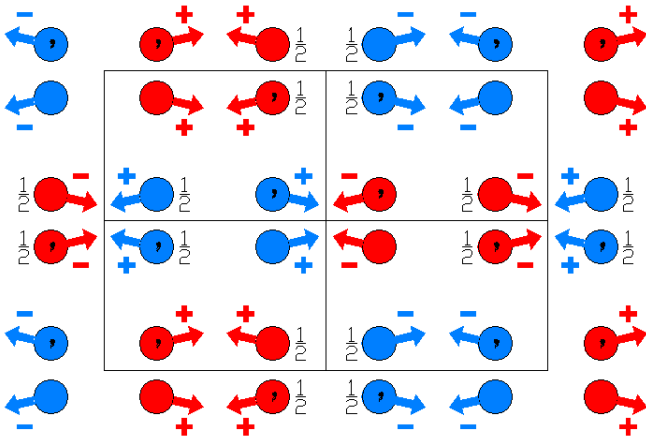
$C_{pm}'c'a'$

64.17.544

$mmm1'$

$C_{p2/m'2/c'2_1/a'}$

Orthorhombic



Origin at center ( $2/m'$ ) at  $2/m'n1$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

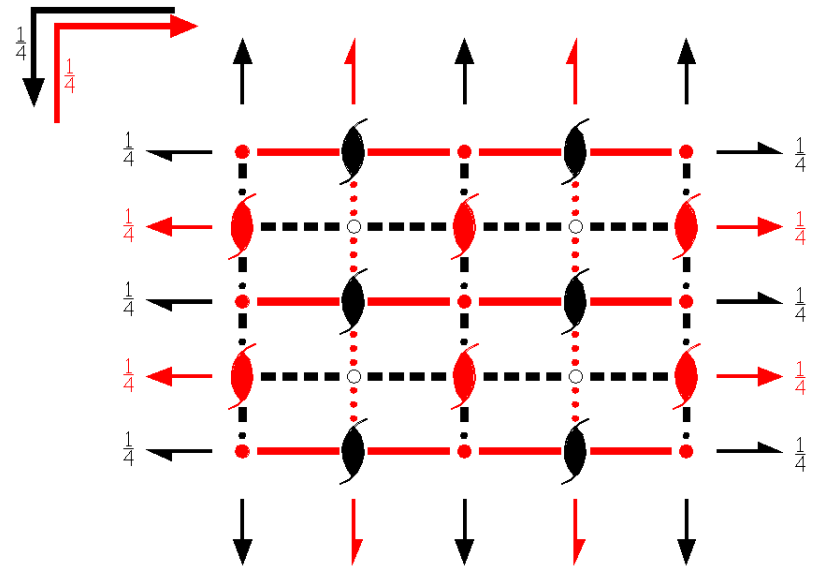
**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) b' (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>  0,1/2,1/2)' | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

For (1/2,1/2,0)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' (1/2,1/2,0)<br>(1 1/2,1/2,0)'                  | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) 2' 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)'       | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)   | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)   |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0);(2); (3); (5).

**Positions**

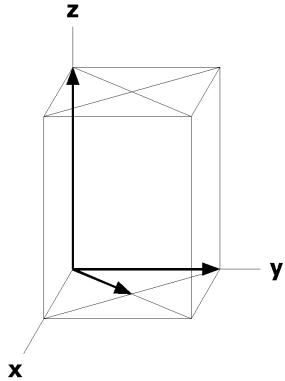
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 g 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y}+1/2,z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) x,y+1/2, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y}+1/2,z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 f m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z+1/2$ [0, $\bar{v},w$ ]	0,y+1/2, $\bar{z}+1/2$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 e .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y}+1/2,3/4$ [0, $\bar{v},0$ ]	3/4, $\bar{y},3/4$ [0, $\bar{v},0$ ]	1/4,y+1/2,1/4 [0,v,0]
8 d 2..	x,0,0 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	x,1/2,1/2 [u,0,0]
8 c $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,1/4,1/2 [ $\bar{u},\bar{v},w$ ]	3/4,3/4,1/2 [ $\bar{u},v,\bar{w}$ ]	1/4,3/4,0 [u, $\bar{v},\bar{w}$ ]
4 b 2/m'..	1/2,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a 2/m'..	0,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b} \cdot 2mg$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



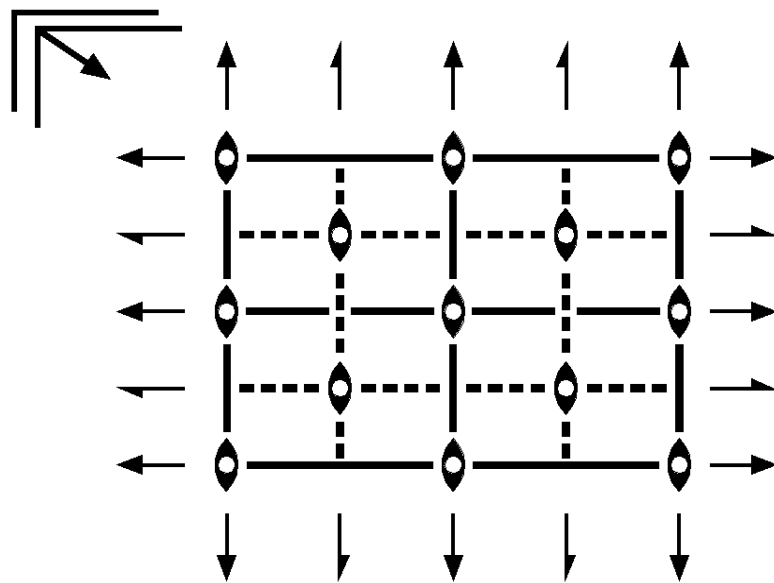
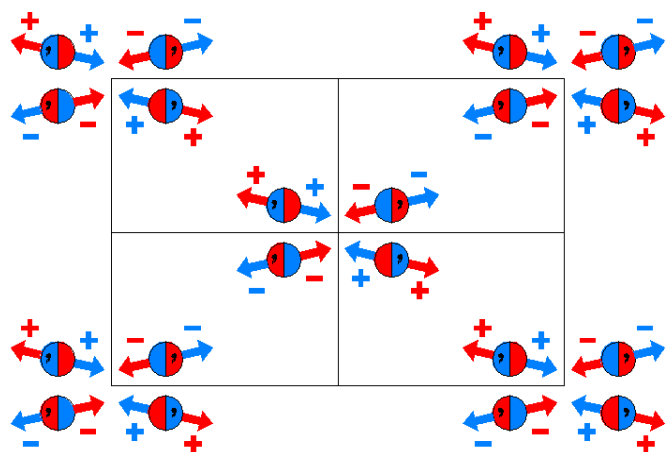
Cmmm

65.1.545

mmm

C2/m2/m2/m

Orthorhombic



Origin at center (mmm)

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0) | (3) 2 0,y,0<br>(2 <sub>y</sub>   0,0,0) | (4) 2 x,0,0<br>(2 <sub>x</sub>   0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>   0,0,0) | (7) m x,0,z<br>(m <sub>y</sub>   0,0,0) | (8) m 0,y,z<br>(m <sub>x</sub>   0,0,0) |

For (1/2,1/2,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)         | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>   1/2,1/2,0) | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

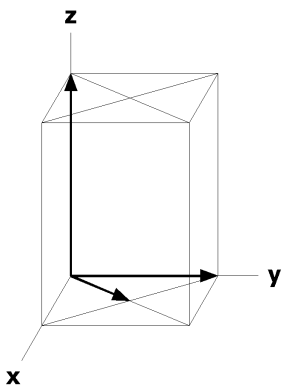
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 q ..m	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0,w]	$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
8 p ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0, $\bar{w}$ ]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
8 o .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]	$\bar{x},0,\bar{z}$ [0,v,0]	x,0, $\bar{z}$ [0, $\bar{v}$ ,0]
8 n m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u}$ ,0,0]	0,y, $\bar{z}$ [ $\bar{u}$ ,0,0]	0, $\bar{y},\bar{z}$ [u,0,0]
8 m ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0, $\bar{w}$ ]	3/4,3/4, $\bar{z}$ [0,0,w]	1/4,3/4,z [0,0, $\bar{w}$ ]
4 l mm2	0,1/2,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]		
4 k mm2	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 j m2m	0,y,1/2 [0,0,0]	0, $\bar{y},1/2$ [0,0,0]		
4 i m2m	0,y,0 [0,0,0]	0, $\bar{y},0$ [0,0,0]		
4 h 2mm	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]		
4 g 2mm	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
4 f ..2/m	1/4,1/4,1/2 [0,0,w]	3/4,1/4,1/2 [0,0, $\bar{w}$ ]		
4 e ..2/m	1/4,1/4,0 [0,0,w]	3/4,1/4,0 [0,0, $\bar{w}$ ]		
2 d mmm	0,0,1/2 [0,0,0]			
2 c mmm	1/2,0,1/2 [0,0,0]			
2 b mmm	1/2,0,0 [0,0,0]			
2 a mmm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Cmmm1'

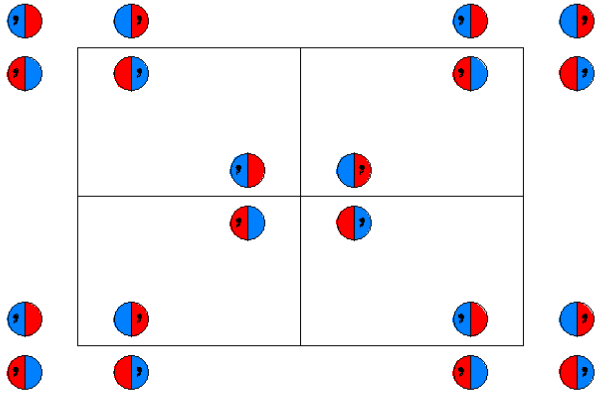
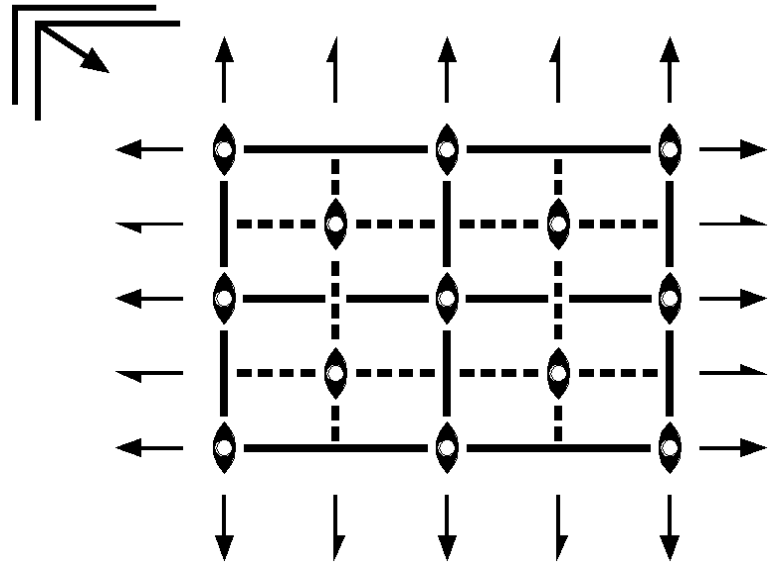
65.2.546

mmm1'

C2/m2/m2/m1'

Orthorhombic

1'



Origin at center (mmm1')

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0) | (3) 2 0,y,0<br>(2 <sub>y</sub>   0,0,0) | (4) 2 x,0,0<br>(2 <sub>x</sub>   0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>   0,0,0) | (7) m x,0,z<br>(m <sub>y</sub>   0,0,0) | (8) m 0,y,z<br>(m <sub>x</sub>   0,0,0) |

For (1/2,1/2,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)         | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>   1/2,1/2,0) | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0) |

For (0,0,0)' + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1'<br>(1   0,0,0)'                         | (2) 2' 0,0,z<br>(2 <sub>z</sub>   0,0,0)' | (3) 2' 0,y,0<br>(2 <sub>y</sub>   0,0,0)' | (4) 2' x,0,0<br>(2 <sub>x</sub>   0,0,0)' |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$   0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>   0,0,0)' | (7) m' x,0,z<br>(m <sub>y</sub>   0,0,0)' | (8) m' 0,y,z<br>(m <sub>x</sub>   0,0,0)' |

For (1/2,1/2,0)' + set

- |  |   |   |   |
|--|---|---|---|
| (1) t' (1/2,1/2,0)<br>(1   1/2,1/2,0)'                 | (2) 2' 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)'         | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)' |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>   1/2,1/2,0)' | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5);1'.

### Positions

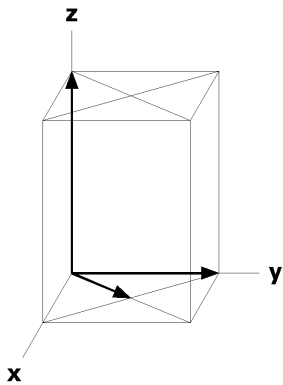
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) + (0,0,0)'	(1/2,1/2,0) + (1/2,1/2,0)'		
16 r 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{x},y,\bar{z}$ [0,0,0]	(4) $x,\bar{y},\bar{z}$ [0,0,0]
	(5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(6) $x,y,\bar{z}$ [0,0,0]	(7) $x,\bar{y},z$ [0,0,0]	(8) $\bar{x},y,z$ [0,0,0]
8 q ..m1'	x,y,1/2 [0,0,0]	$\bar{x},\bar{y},1/2$ [0,0,0]	$\bar{x},y,1/2$ [0,0,0]	$x,\bar{y},1/2$ [0,0,0]
8 p ..m1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{x},y,0$ [0,0,0]	$x,\bar{y},0$ [0,0,0]
8 o .m.1'	x,0,z [0,0,0]	$\bar{x},0,z$ [0,0,0]	$\bar{x},0,\bar{z}$ [0,0,0]	$x,0,\bar{z}$ [0,0,0]
8 n m..1'	0,y,z [0,0,0]	$0,\bar{y},z$ [0,0,0]	$0,y,\bar{z}$ [0,0,0]	$0,\bar{y},\bar{z}$ [0,0,0]
8 m ..21'	1/4,1/4,z [0,0,0]	3/4,1/4, $\bar{z}$ [0,0,0]	3/4,3/4, $\bar{z}$ [0,0,0]	1/4,3/4,z [0,0,0]
4 l mm21'	0,1/2,z [0,0,0]	$0,1/2,\bar{z}$ [0,0,0]		
4 k mm21'	0,0,z [0,0,0]	$0,0,\bar{z}$ [0,0,0]		
4 j m2m1'	0,y,1/2 [0,0,0]	$0,\bar{y},1/2$ [0,0,0]		
4 i m2m1'	0,y,0 [0,0,0]	$0,\bar{y},0$ [0,0,0]		
4 h 2mm1'	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]		
4 g 2mm1'	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
4 f ..2/m1'	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 e ..2/m1'	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
2 d mmm1'	0,0,1/2 [0,0,0]			
2 c mmm1'	1/2,0,1/2 [0,0,0]			
2 b mmm1'	1/2,0,0 [0,0,0]			
2 a mmm1'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



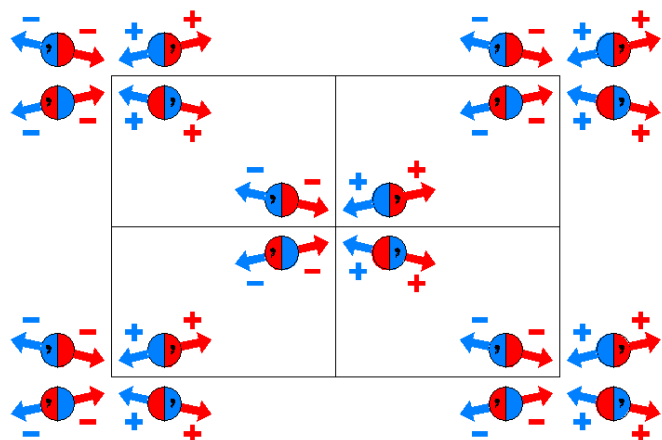
Cm'mm

65.3.547

m'mm

C2/m'2'/m2'/m

Orthorhombic



Origin at center (m'mm)

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

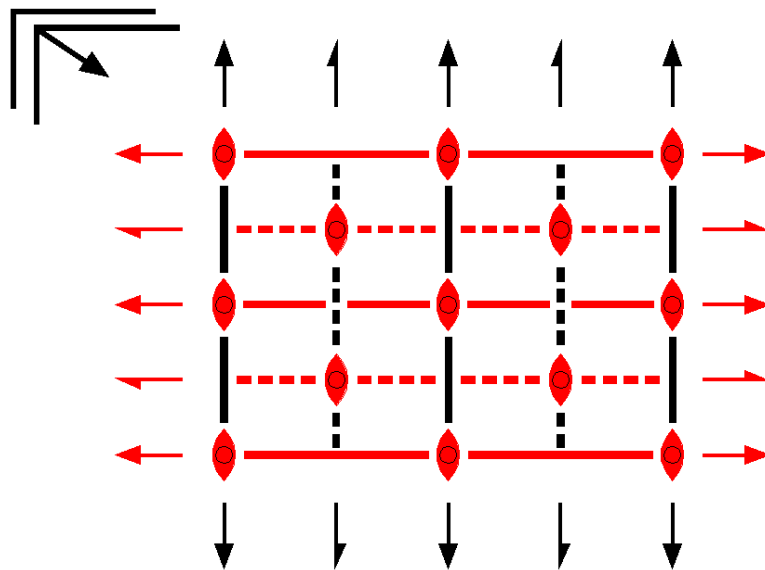
### Symmetry Operations

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0)   | (7) m x,0,z<br>(m <sub>y</sub>  0,0,0)   | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

For (1/2,1/2,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                    | (2) 2' 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)'       | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)   | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

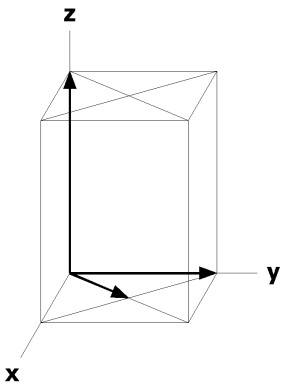
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 q ..m	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0, $\bar{w}$ ]	$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
8 p ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
8 o .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0,v,0]	$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	x,0, $\bar{z}$ [0, $\bar{v},0$ ]
8 n m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0,v, $\bar{w}$ ]	0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 m ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	3/4,3/4, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,3/4,z [ $\bar{u},v,0$ ]
4 l m'm2'	0,1/2,z [0,v,0]	0,1/2, $\bar{z}$ [0, $\bar{v},0$ ]		
4 k m'm2'	0,0,z [0,v,0]	0,0, $\bar{z}$ [0, $\bar{v},0$ ]		
4 j m'2'm	0,y,1/2 [0,0,w]	0, $\bar{y},1/2$ [0,0, $\bar{w}$ ]		
4 i m'2'm	0,y,0 [0,0,w]	0, $\bar{y},0$ [0,0, $\bar{w}$ ]		
4 h 2mm	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]		
4 g 2mm	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
4 f ..2'/m	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 e ..2'/m	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
2 d m'mm	0,0,1/2 [0,0,0]			
2 c m'mm	1/2,0,1/2 [0,0,0]			
2 b m'mm	1/2,0,0 [0,0,0]			
2 a m'mm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



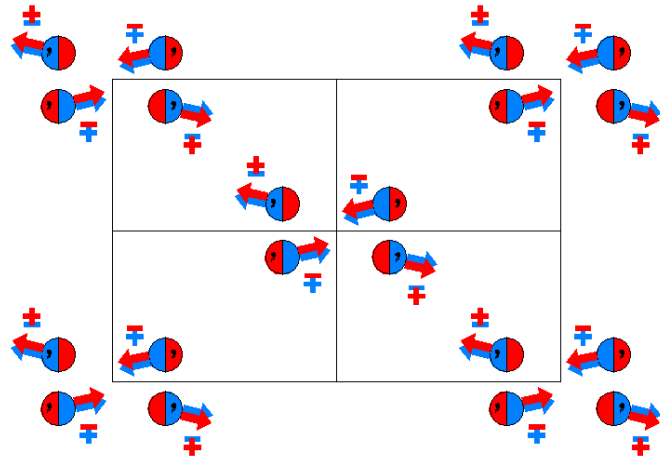
Cmmm'

65.4.548

mmm'

C2'/m2'/m2/m'

Orthorhombic



Origin at center (mmm')

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

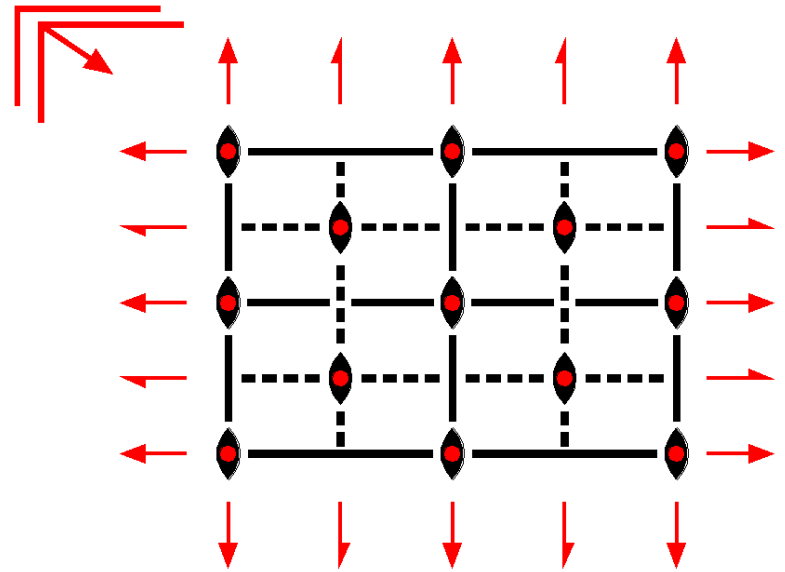
**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) m x,0,z<br>(m <sub>y</sub>  0,0,0)   | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   |

For (1/2,1/2,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                    | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)           | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)   | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)   |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

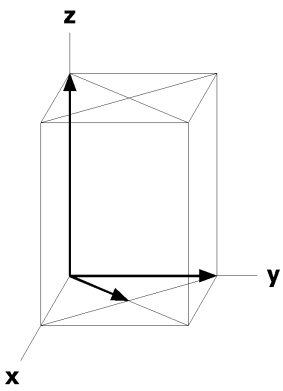
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 q ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [u, $\bar{v},0$ ]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]
8 p ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,0$ [u, $\bar{v},0$ ]	x, $\bar{y},0$ [ $\bar{u},v,0$ ]
8 o .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	x,0, $\bar{z}$ [0,v,0]
8 n m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	0,y, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
8 m ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0,w]	3/4,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,3/4,z [0,0, $\bar{w}$ ]
4 l mm2	0,1/2,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]		
4 k mm2	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 j m2'm'	0,y,1/2 [u,0,0]	0, $\bar{y},1/2$ [ $\bar{u},0,0$ ]		
4 i m2'm'	0,y,0 [u,0,0]	0, $\bar{y},0$ [ $\bar{u},0,0$ ]		
4 h 2'mm'	x,0,1/2 [0,v,0]	$\bar{x},0,1/2$ [0, $\bar{v},0$ ]		
4 g 2'mm'	x,0,0 [0,v,0]	$\bar{x},0,0$ [0, $\bar{v},0$ ]		
4 f ..2/m'	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 e ..2/m'	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
2 d mmm'	0,0,1/2 [0,0,0]			
2 c mmm'	1/2,0,1/2 [0,0,0]			
2 b mmm'	1/2,0,0 [0,0,0]			
2 a mmm'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



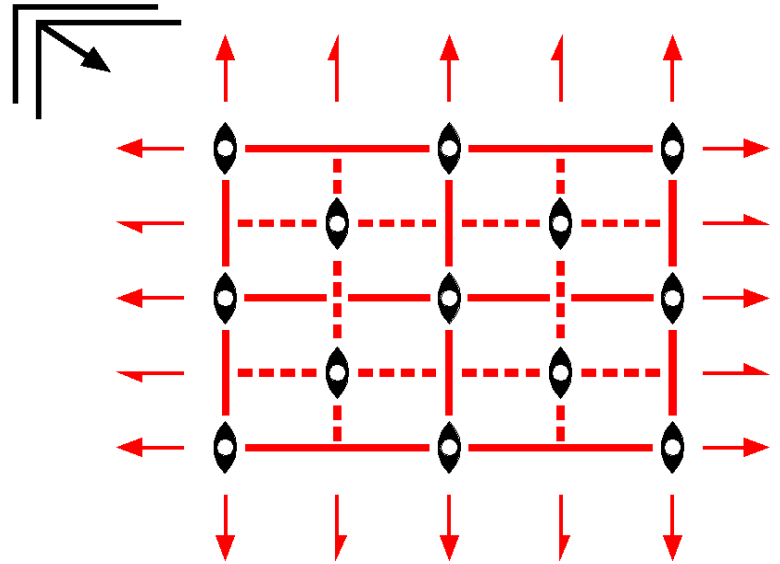
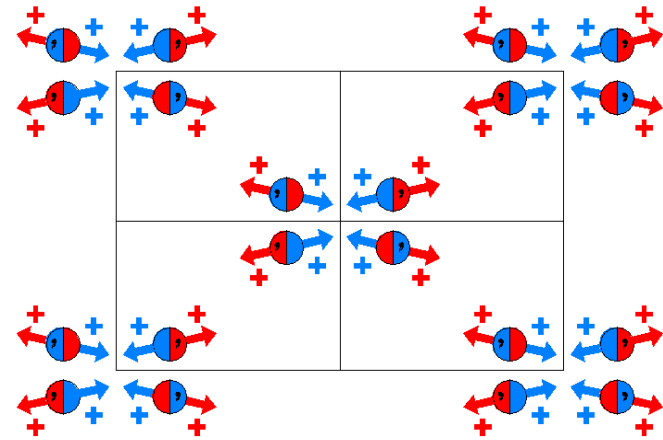
Cm'm'm

65.5.549

m'm'm

C2'/m'2'/m'2/m

Orthorhombic



**Origin** at center (m'm'm)

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                 | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)         | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

### Positions

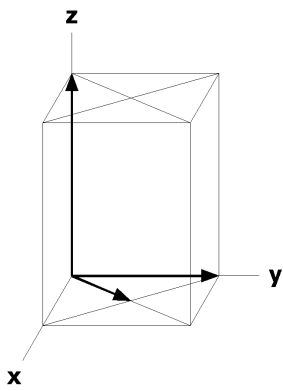
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 q ..m	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0,w]	$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0,w]
8 p ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0,w]
8 o .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$\bar{x},0,\bar{z}$ [u,0,w]	x,0, $\bar{z}$ [ $\bar{u},0,w$ ]
8 n m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
8 m ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0,w]	3/4,3/4, $\bar{z}$ [0,0,w]	1/4,3/4,z [0,0,w]
4 l m'm'2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]		
4 k m'm'2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
4 j m'2'm	0,y,1/2 [0,0,w]	0, $\bar{y},1/2$ [0,0,w]		
4 i m'2'm	0,y,0 [0,0,w]	0, $\bar{y},0$ [0,0,w]		
4 h 2'm'm	x,0,1/2 [0,0,w]	$\bar{x},0,1/2$ [0,0,w]		
4 g 2'm'm	x,0,0 [0,0,w]	$\bar{x},0,0$ [0,0,w]		
4 f ..2/m	1/4,1/4,1/2 [0,0,w]	3/4,1/4,1/2 [0,0,w]		
4 e ..2/m	1/4,1/4,0 [0,0,w]	3/4,1/4,0 [0,0,w]		
2 d m'm'm	0,0,1/2 [0,0,w]			
2 c m'm'm	1/2,0,1/2 [0,0,w]			
2 b m'm'm	1/2,0,0 [0,0,w]			
2 a m'm'm	0,0,0 [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



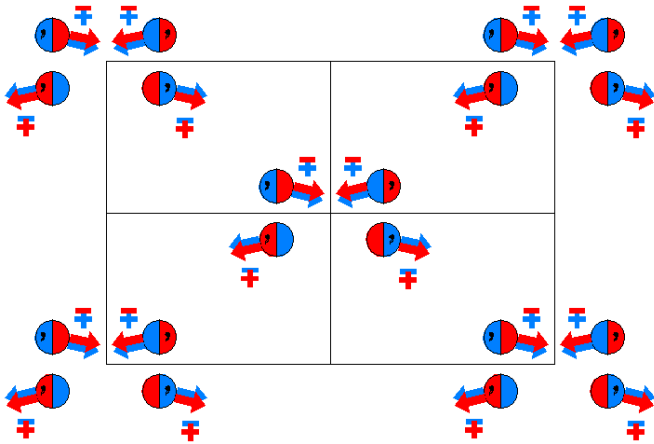
Cmm'm'

65.6.550

mm'm'

C2/m2'/m'2'/m'

Orthorhombic



Origin at center (mm'm')

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

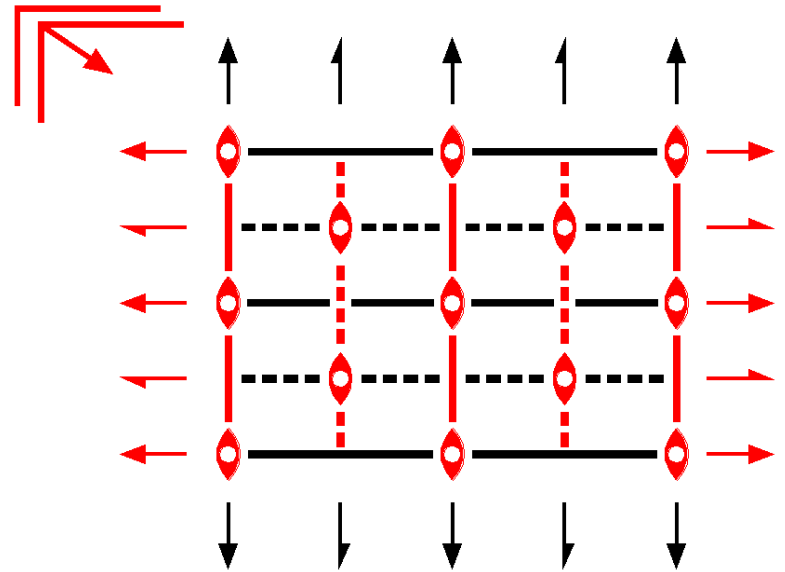
**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0) |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                 | (2) 2' 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)'         | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

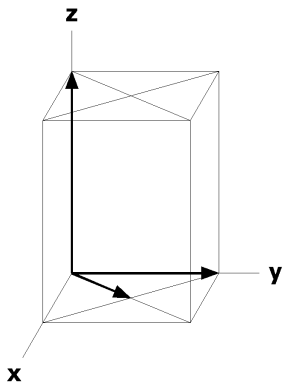
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v}$ ,w] (7) x, $\bar{y},z$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 q ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [u,v,0]	$\bar{x},y,1/2$ [u, $\bar{v}$ ,0]	x, $\bar{y},1/2$ [u, $\bar{v}$ ,0]
8 p ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [u,v,0]	$\bar{x},y,0$ [u, $\bar{v}$ ,0]	x, $\bar{y},0$ [u, $\bar{v}$ ,0]
8 o .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [u,0, $\bar{w}$ ]	$\bar{x},0,\bar{z}$ [u,0,w]	x,0, $\bar{z}$ [u,0, $\bar{w}$ ]
8 n m..	0,y,z [u,0,0]	0, $\bar{y},z$ [u,0,0]	0,y, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [u,0,0]
8 m ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [u, $\bar{v}$ ,0]	3/4,3/4, $\bar{z}$ [u,v,0]	1/4,3/4,z [u, $\bar{v}$ ,0]
4 l mm'2'	0,1/2,z [u,0,0]	0,1/2, $\bar{z}$ [u,0,0]		
4 k mm'2'	0,0,z [u,0,0]	0,0, $\bar{z}$ [u,0,0]		
4 j m2'm'	0,y,1/2 [u,0,0]	0, $\bar{y},1/2$ [u,0,0]		
4 i m2'm'	0,y,0 [u,0,0]	0, $\bar{y},0$ [u,0,0]		
4 h 2m'm'	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [u,0,0]		
4 g 2m'm'	x,0,0 [u,0,0]	$\bar{x},0,0$ [u,0,0]		
4 f ..2'/m'	1/4,1/4,1/2 [u,v,0]	3/4,1/4,1/2 [u, $\bar{v}$ ,0]		
4 e ..2'/m'	1/4,1/4,0 [u,v,0]	3/4,1/4,0 [u, $\bar{v}$ ,0]		
2 d mm'm'	0,0,1/2 [u,0,0]			
2 c mm'm'	1/2,0,1/2 [u,0,0]			
2 b mm'm'	1/2,0,0 [u,0,0]			
2 a mm'm'	0,0,0 [u,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



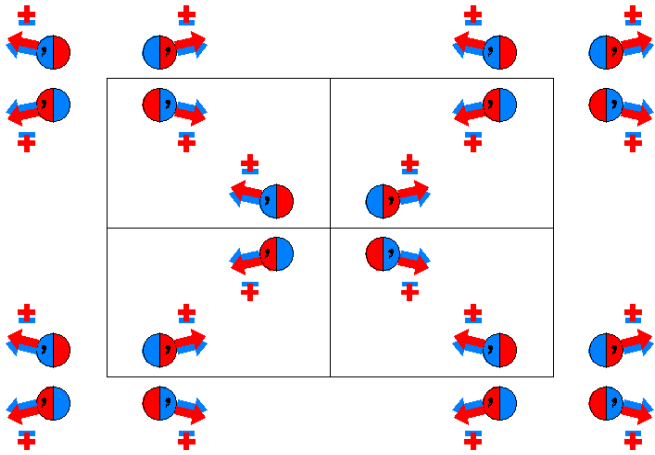
$Cm'm'm'$

65.7.551

$m'm'm'$

$C2/m'2/m'2/m'$

Orthorhombic



**Origin** at center ( $m'm'm'$ )

**Asymmetric unit**  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

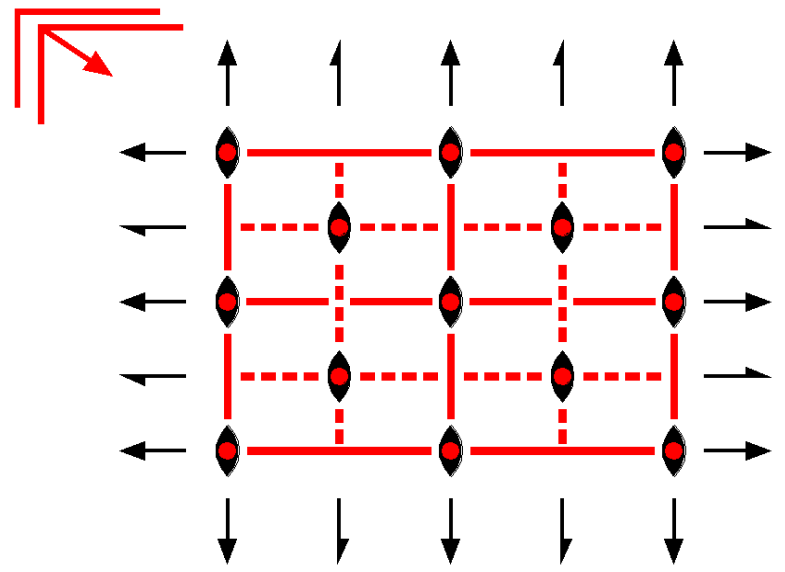
**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                          | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

For (1/2,1/2,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                  | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)           | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

### Positions

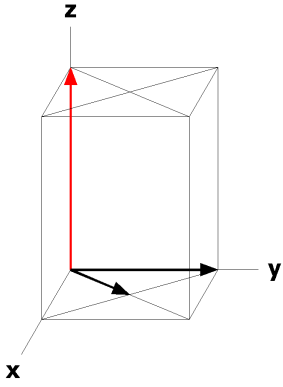
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 q ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	x, $\bar{y},1/2$ [u, $\bar{v},0$ ]
8 p ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,0$ [ $\bar{u},v,0$ ]	x, $\bar{y},0$ [u, $\bar{v},0$ ]
8 o .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$\bar{x},0,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	x,0, $\bar{z}$ [u,0, $\bar{w}$ ]
8 n m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	0,y, $\bar{z}$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 m ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0, $\bar{w}$ ]	3/4,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,3/4,z [0,0,w]
4 l m'm'2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 k m'm'2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 j m'2m'	0,y,1/2 [0,v,0]	0, $\bar{y},1/2$ [0, $\bar{v},0$ ]		
4 i m'2m'	0,y,0 [0,v,0]	0, $\bar{y},0$ [0, $\bar{v},0$ ]		
4 h 2m'm'	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]		
4 g 2m'm'	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]		
4 f ..2/m'	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 e ..2/m'	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
2 d m'm'm'	0,0,1/2 [0,0,0]			
2 c m'm'm'	1/2,0,1/2 [0,0,0]			
2 b m'm'm'	1/2,0,0 [0,0,0]			
2 a m'm'm'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



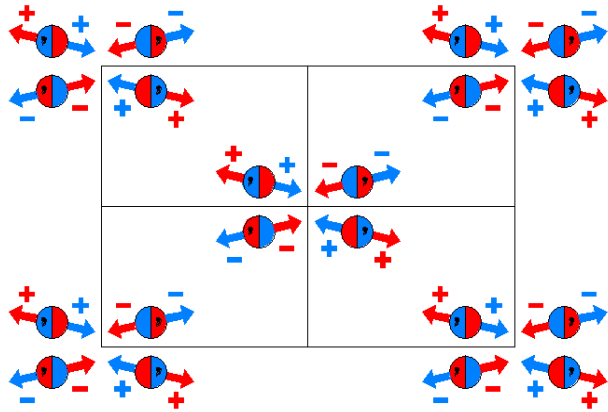
$C_{2c}mmm$

65.8.552

$mmm1'$

$C_{2c}2/m2/m2/m$

Orthorhombic



Origin at center (mmm)

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0) | (3) 2 0,y,0<br>(2 <sub>y</sub>   0,0,0) | (4) 2 x,0,0<br>(2 <sub>x</sub>   0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>   0,0,0) | (7) m x,0,z<br>(m <sub>y</sub>   0,0,0) | (8) m 0,y,z<br>(m <sub>x</sub>   0,0,0) |

For (1/2,1/2,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)         | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>   1/2,1/2,0) | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0) |

For (0,0,1)' + set

- |  |   |   |   |
|--|---|---|---|
| (1) t' (0,0,1)<br>(1   0,0,1)'                   | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>   0,0,1)' | (3) 2' 0,y,1/2<br>(2 <sub>y</sub>   0,0,1)'       | (4) 2' x,0,1/2<br>(2 <sub>x</sub>   0,0,1)'       |
| (5) $\bar{1}$ ' 0,0,1/2<br>( $\bar{1}$   0,0,1)' | (6) m' x,y,1/2<br>(m <sub>z</sub>   0,0,1)'       | (7) c' (0,0,1) x,0,z<br>(m <sub>y</sub>   0,0,1)' | (8) c' (0,0,1) 0,y,z<br>(m <sub>x</sub>   0,0,1)' |

For (1/2,1/2,1)' + set

- |  |   |   |   |
|--|---|---|---|
| (1) t' (1/2,1/2,1)<br>(1   1/2,1/2,1)'                   | (2) 2' (0,0,1) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1)'   | (3) 2' (0,1/2,0) 1/4,y,1/2<br>(2 <sub>y</sub>   1/2,1/2,1)' | (4) 2' (1/2,0,0) x,1/4,1/2<br>(2 <sub>x</sub>   1/2,1/2,1)' |
| (5) $\bar{1}$ ' 1/4,1/4,1/2<br>( $\bar{1}$   1/2,1/2,1)' | (6) n' (1/2,1/2,0) x,y,1/2<br>(m <sub>z</sub>   1/2,1/2,1)' | (7) n' (1/2,0,1) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,1)'   | (8) n' (0,1/2,1) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,1)'   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

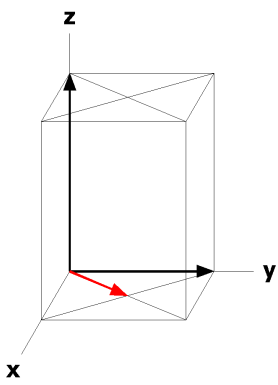
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,1)' +	(1/2,1/2,0) + (1/2,1/2,1)' +	
32 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
16 q ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [u, $\bar{v},0$ ]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]
16 p ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0, $\bar{w}$ ]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
16 o .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	$\bar{x},0,\bar{z}$ [0,v,0]	x,0, $\bar{z}$ [0, $\bar{v},0$ ]
16 n m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	0,y, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
16 m ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0, $\bar{w}$ ]	3/4,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,3/4,z [0,0,w]
8 l mm2	0,1/2,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]		
8 k mm2	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
8 j m2'm'	0,y,1/2 [u,0,0]	0, $\bar{y},1/2$ [ $\bar{u},0,0$ ]		
8 i m2m	0,y,0 [0,0,0]	0, $\bar{y},0$ [0,0,0]		
8 h 2'mm'	x,0,1/2 [0,v,0]	$\bar{x},0,1/2$ [0, $\bar{v},0$ ]		
8 g 2mm	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
8 f ..2/m'	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
8 e ..2/m	1/4,1/4,0 [0,0,w]	3/4,1/4,0 [0,0, $\bar{w}$ ]		
4 d mmm'	0,0,1/2 [0,0,0]			
4 c mmm'	1/2,0,1/2 [0,0,0]			
4 b mmm	1/2,0,0 [0,0,0]			
4 a mmm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



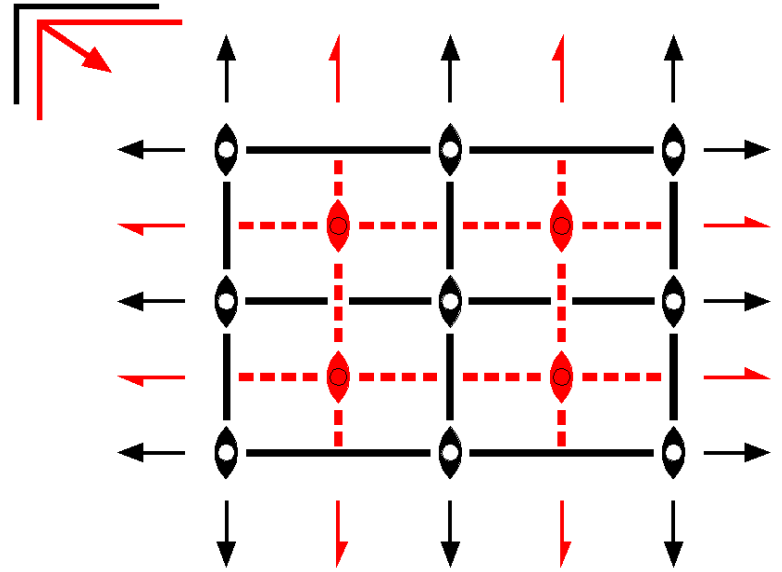
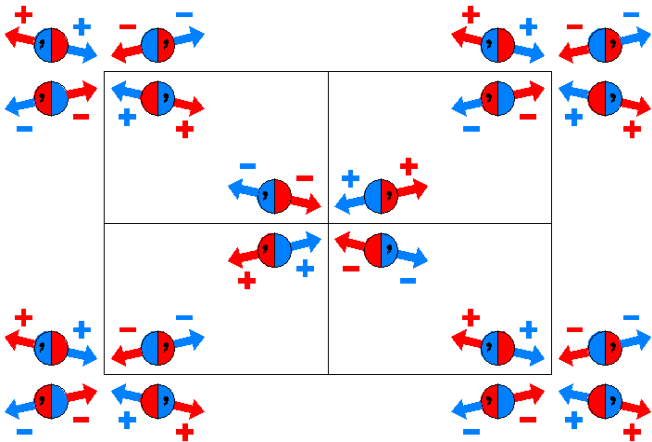
$C_{pmmm}$

65.9.553

$mmm1'$

$C_{p2/m2/m2/m}$

Orthorhombic



**Origin** at center (mmm)

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0) |

For (1/2,1/2,0)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' (1/2,1/2,0)<br>(1 1/2,1/2,0)'                  | (2) 2' 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)'         | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

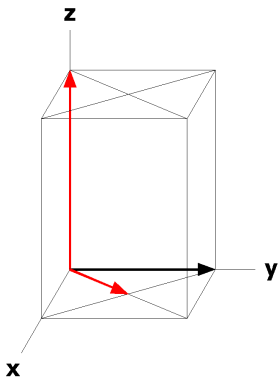
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},\bar{v},\bar{w}$ ]
8 q ..m	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0,w]	$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
8 p ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0, $\bar{w}$ ]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
8 o .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]	$\bar{x},0,\bar{z}$ [0,v,0]	x,0, $\bar{z}$ [0, $\bar{v}$ ,0]
8 n m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u}$ ,0,0]	0,y, $\bar{z}$ [ $\bar{u}$ ,0,0]	0, $\bar{y},\bar{z}$ [u,0,0]
8 m ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [ $\bar{u},v,0$ ]	3/4,3/4, $\bar{z}$ [u,v,0]	1/4,3/4,z [ $\bar{u},v,0$ ]
4 l mm2	0,1/2,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]		
4 k mm2	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 j m2m	0,y,1/2 [0,0,0]	0, $\bar{y},1/2$ [0,0,0]		
4 i m2m	0,y,0 [0,0,0]	0, $\bar{y},0$ [0,0,0]		
4 h 2mm	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]		
4 g 2mm	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
4 f ..2'/m	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 e ..2'/m	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
2 d mmm	0,0,1/2 [0,0,0]			
2 c mmm	1/2,0,1/2 [0,0,0]			
2 b mmm	1/2,0,0 [0,0,0]			
2 a mmm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

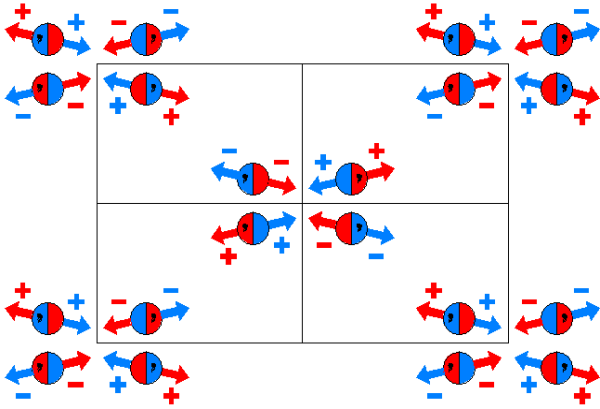
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



$C_{1h}$   
65.10.554

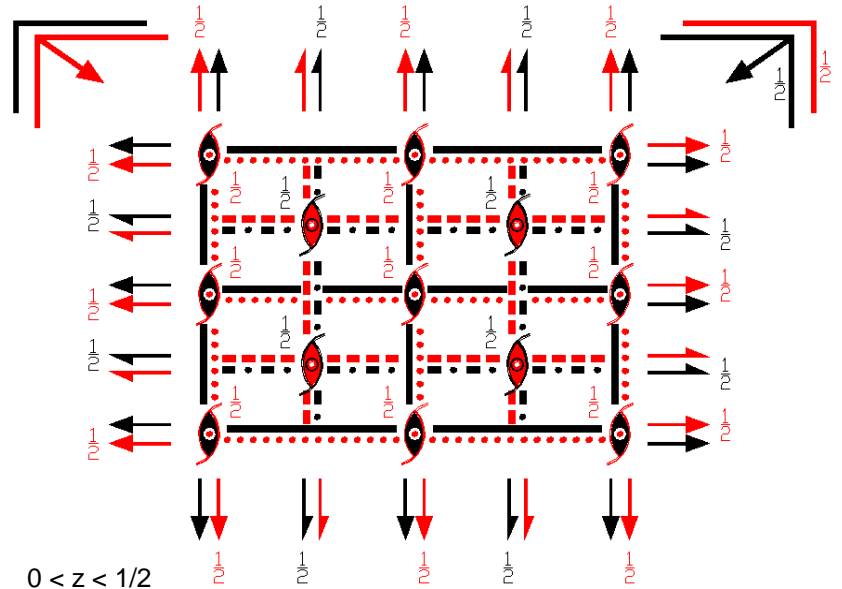
$mmm1'$   
 $C_{2h}/m2/m2/m$

Orthorhombic



Origin at center ( $mmm$ )

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$



### Symmetry Operations

For  $(0,0,0)$  + set

- |   |                                   |                                   |                                   |
|---|-----------------------------------|-----------------------------------|-----------------------------------|
| (1) 1<br>(1   0,0,0)                          | (2) 2 $0,0,z$<br>( $2_z$   0,0,0) | (3) 2 $0,y,0$<br>( $2_y$   0,0,0) | (4) 2 $x,0,0$<br>( $2_x$   0,0,0) |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   0,0,0) | (6) m $x,y,0$<br>( $m_z$   0,0,0) | (7) m $x,0,z$<br>( $m_y$   0,0,0) | (8) m $0,y,z$<br>( $m_x$   0,0,0) |

For  $(1/2,1/2,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,0)$<br>(1   $1/2,1/2,0$ )'              | (2) $2'$ $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,0$ )'           | (3) $2'$ $(0,1/2,0)$ $1/4,y,0$<br>( $2_y$   $1/2,1/2,0$ )' | (4) $2'$ $(1/2,0,0)$ $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )' |
| (5) $\bar{1}'$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ )' | (6) $n'$ $(1/2,1/2,0)$ $x,y,0$<br>( $m_z$   $1/2,1/2,0$ )' | (7) $a'$ $(1/2,0,0)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,0$ )' | (8) $b'$ $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |

For  $(0,0,1)'$  + set

- |   |   |   |   |
|---|---|---|---|
| (1) $t'$ $(0,0,1)$<br>(1   0,0,1)'                | (2) $2'$ $(0,0,1)$ $0,0,z$<br>( $2_z$   0,0,1)' | (3) $2'$ $0,y,1/2$<br>( $2_y$   0,0,1)'         | (4) $2'$ $x,0,1/2$<br>( $2_x$   0,0,1)'         |
| (5) $\bar{1}'$ $0,0,1/2$<br>( $\bar{1}$   0,0,1)' | (6) $m'$ $x,y,1/2$<br>( $m_z$   0,0,1)'         | (7) $c'$ $(0,0,1)$ $x,0,z$<br>( $m_y$   0,0,1)' | (8) $c'$ $(0,0,1)$ $0,y,z$<br>( $m_x$   0,0,1)' |

For  $(1/2,1/2,1)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t$ $(1/2,1/2,1)$<br>(1   $1/2,1/2,1$ )                | (2) 2 $(0,0,1)$ $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1$ )   | (3) 2 $(0,1/2,0)$ $1/4,y,1/2$<br>( $2_y$   $1/2,1/2,1$ ) | (4) 2 $(1/2,0,0)$ $x,1/4,1/2$<br>( $2_x$   $1/2,1/2,1$ ) |
| (5) $\bar{1}$ $1/4,1/4,1/2$<br>( $\bar{1}$   $1/2,1/2,1$ ) | (6) n $(1/2,1/2,0)$ $x,y,1/2$<br>( $m_z$   $1/2,1/2,1$ ) | (7) n $(1/2,0,1)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,1$ )   | (8) n $(0,1/2,1)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,1$ )   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

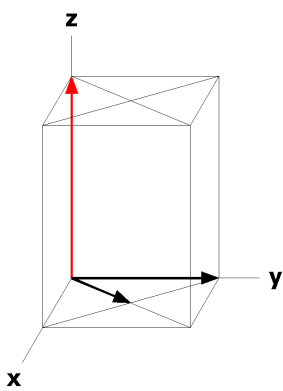
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,1)' +	(1/2,1/2,0)' + (1/2,1/2,1) +	
32 r 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
16 q ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [u, $\bar{v},0$ ]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]
16 p ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0, $\bar{w}$ ]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
16 o .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	$\bar{x},0,\bar{z}$ [0,v,0]	x,0, $\bar{z}$ [0, $\bar{v},0$ ]
16 n m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	0,y, $\bar{z}$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]
16 m ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [ $\bar{u},v,0$ ]	3/4,3/4, $\bar{z}$ [u,v,0]	1/4,3/4,z [ $\bar{u},v,0$ ]
8 l mm2	0,1/2,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]		
8 k mm2	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
8 j m2'm'	0,y,1/2 [u,0,0]	0, $\bar{y},1/2$ [ $\bar{u},0,0$ ]		
8 i m2m	0,y,0 [0,0,0]	0, $\bar{y},0$ [0,0,0]		
8 h 2'mm'	x,0,1/2 [0,v,0]	$\bar{x},0,1/2$ [0, $\bar{v},0$ ]		
8 g 2mm	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
8 f ..2'/m'	1/4,1/4,1/2 [u,v,0]	3/4,1/4,1/2 [u, $\bar{v},0$ ]		
8 e ..2'/m	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
4 d mmm'	0,0,1/2 [0,0,0]			
4 c mmm'	1/2,0,1/2 [0,0,0]			
4 b mmm	1/2,0,0 [0,0,0]			
4 a mmm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



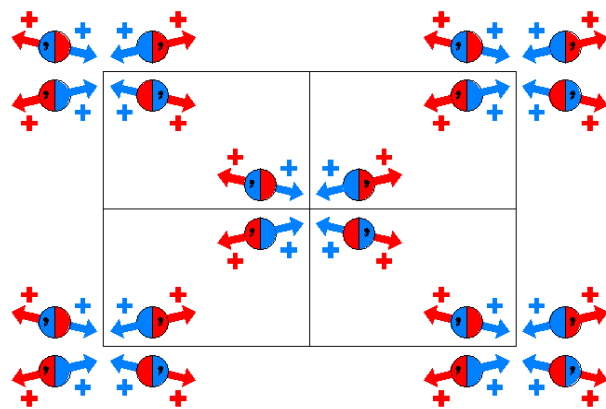
$C_{2c}m'm'm$

65.11.555

$mmm1'$

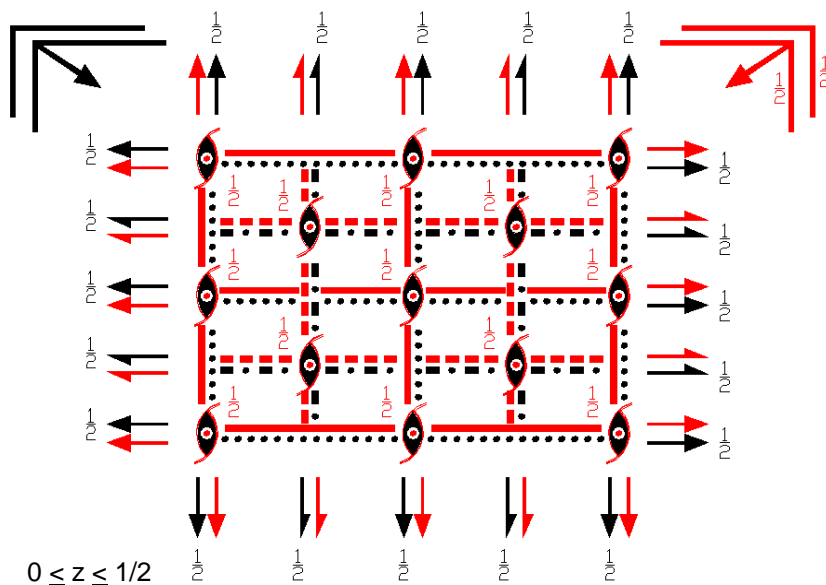
$C_{2c}2'/m'2'/m'2/m$

Orthorhombic



Origin at center ( $m'm'm'$ )

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$



### Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                 | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)         | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

For (0,0,1)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' (0,0,1)<br>(1 0,0,1)'                    | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)' | (3) 2 0,y,1/2<br>(2 <sub>y</sub>  0,0,1)       | (4) 2 x,0,1/2<br>(2 <sub>x</sub>  0,0,1)       |
| (5) $\bar{1}$ ' 0,0,1/2<br>( $\bar{1}$  0,0,1)' | (6) m' x,y,1/2<br>(m <sub>z</sub>  0,0,1)'       | (7) c (0,0,1) x,0,z<br>(m <sub>y</sub>  0,0,1) | (8) c (0,0,1) 0,y,z<br>(m <sub>x</sub>  0,0,1) |

For (1/2,1/2,1)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' (1/2,1/2,1)<br>(1 1/2,1/2,1)'                    | (2) 2' (0,0,1) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1)'   | (3) 2 (0,1/2,0) 1/4,y,1/2<br>(2 <sub>y</sub>  1/2,1/2,1) | (4) 2 (1/2,0,0) x,1/4,1/2<br>(2 <sub>x</sub>  1/2,1/2,1) |
| (5) $\bar{1}$ ' 1/4,1/4,1/2<br>( $\bar{1}$  1/2,1/2,1)' | (6) n' (1/2,1/2,0) x,y,1/2<br>(m <sub>z</sub>  1/2,1/2,1)' | (7) n (1/2,0,1) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1)   | (8) n (0,1/2,1) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

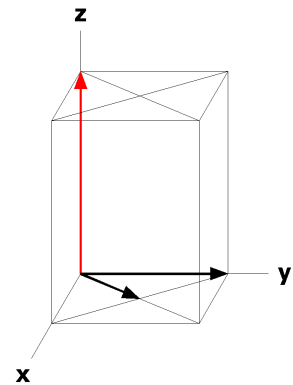
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,1)' +	(1/2,1/2,0) + (1/2,1/2,1)' +	
32 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
16 q ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	x, $\bar{y},1/2$ [u, $\bar{v},0$ ]
16 p ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0,w]
16 o ..m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$\bar{x},0,\bar{z}$ [u,0,w]	x,0, $\bar{z}$ [ $\bar{u},0,w$ ]
16 n m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
16 m ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0, $\bar{w}$ ]	3/4,3/4, $\bar{z}$ [0,0,w]	1/4,3/4,z [0,0, $\bar{w}$ ]
8 l m'm'2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]		
8 k m'm'2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
8 j m'2m'	0,y,1/2 [0,v,0]	0, $\bar{y},1/2$ [0, $\bar{v},0$ ]		
8 i m'2'm	0,y,0 [0,0,w]	0, $\bar{y},0$ [0,0,w]		
8 h 2m'm'	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]		
8 g 2'm'm	x,0,0 [0,0,w]	$\bar{x},0,0$ [0,0,w]		
8 f ..2'/m'	1/4,1/4,1/2 [u,v,0]	3/4,1/4,1/2 [ $\bar{u},v,0$ ]		
8 e ..2/m	1/4,1/4,0 [0,0,w]	3/4,1/4,0 [0,0,w]		
4 d mmm'	0,0,1/2 [0,0,0]			
4 c mmm'	1/2,0,1/2 [0,0,0]			
4 b m'm'm	1/2,0,0 [0,0,w]			
4 a m'm'm	0,0,0 [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,1/4

Along [0,1,0] p<sub>2a</sub>'2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



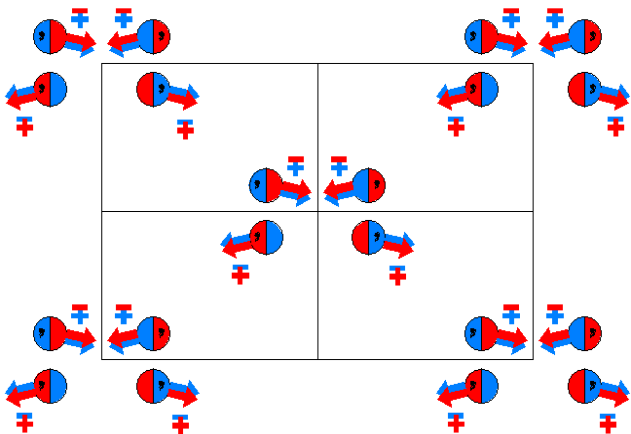
$C_{2c}mm'm'$

65.12.556

$mmm1'$

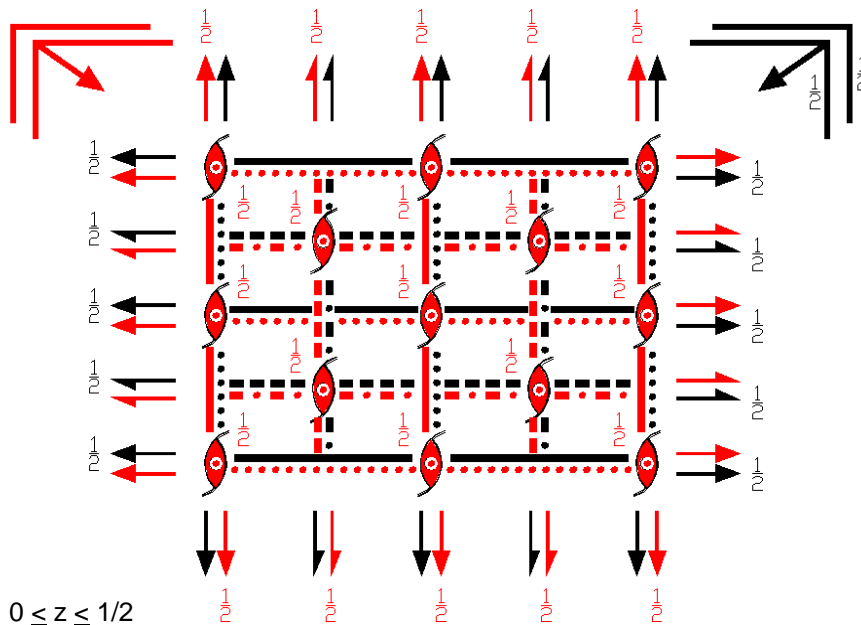
$C_{2c}2/m2'/m2'/m'$

Orthorhombic



Origin at center ( $mm'm'$ )

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$



### Symmetry Operations

For (0,0,0) + set

- |  |                                      |                                      |                                     |
|--|--------------------------------------|--------------------------------------|-------------------------------------|
| (1) 1<br>(1 0,0,0)                         | (2) $2'_z$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $2'_y$ 0,y,0<br>( $2_y$  0,0,0)' | (4) $2'_x$ x,0,0<br>( $2_x$  0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) $m'_z$ x,y,0<br>( $m_z$  0,0,0)' | (7) $m'_y$ x,0,z<br>( $m_y$  0,0,0)' | (8) $m'_x$ 0,y,z<br>( $m_x$  0,0,0) |

For (1/2,1/2,0) + set

- |  |  |  |   |
|--|--|--|---|
| (1) $t$ (1/2,1/2,0)<br>(1 1/2,1/2,0)               | (2) $2'_z$ 1/4,1/4,z<br>( $2_z$  1/2,1/2,0)'         | (3) $2'_y$ (0,1/2,0) 1/4,y,0<br>( $2_y$  1/2,1/2,0)' | (4) $2'_x$ (1/2,0,0) x,1/4,0<br>( $2_x$  1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) $n'_z$ (1/2,1/2,0) x,y,0<br>( $m_z$  1/2,1/2,0)' | (7) $a'_y$ (1/2,0,0) x,1/4,z<br>( $m_y$  1/2,1/2,0)' | (8) $b'_x$ (0,1/2,0) 1/4,y,z<br>( $m_x$  1/2,1/2,0) |

For (0,0,1/2) + set

- |  |   |   |  |
|--|---|---|--|
| (1) $t'$ (0,0,1/2)<br>(1 0,0,1/2)'               | (2) $2'_z$ (0,0,1) 0,0,z<br>( $2_z$  0,0,1) | (3) $2'_y$ 0,y,1/2<br>( $2_y$  0,0,1)       | (4) $2'_x$ x,0,1/2<br>( $2_x$  0,0,1)'       |
| (5) $\bar{1}'$ 0,0,1/2<br>( $\bar{1}$  0,0,1/2)' | (6) $m'_z$ x,y,1/2<br>( $m_z$  0,0,1)       | (7) $c'_y$ (0,0,1) x,0,z<br>( $m_y$  0,0,1) | (8) $c'_x$ (0,0,1) 0,y,z<br>( $m_x$  0,0,1)' |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'               | (2) $2'_z$ (0,0,1) 1/4,1/4,z<br>( $2_z$  1/2,1/2,1/2)'   | (3) $2'_y$ (0,1/2,0) 1/4,y,1/2<br>( $2_y$  1/2,1/2,1/2)' | (4) $2'_x$ (1/2,0,0) x,1/4,1/2<br>( $2_x$  1/2,1/2,1/2)' |
| (5) $\bar{1}'$ 1/4,1/4,1/2<br>( $\bar{1}$  1/2,1/2,1/2)' | (6) $n'_z$ (1/2,1/2,0) x,y,1/2<br>( $m_z$  1/2,1/2,1/2)' | (7) $n'_y$ (1/2,0,1) x,1/4,z<br>( $m_y$  1/2,1/2,1/2)'   | (8) $n'_x$ (0,1/2,1) 1/4,y,z<br>( $m_x$  1/2,1/2,1/2)'   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

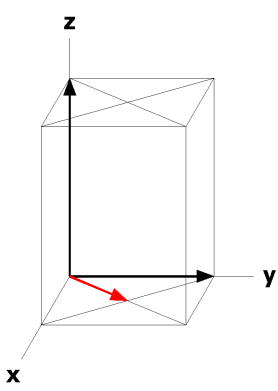
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,1)' +	(1/2,1/2,0) + (1/2,1/2,1)' +	
32 r 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) x, $\bar{y},z$ [u, $\bar{v}$ ,w]	(8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
16 q ..m	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0, $\bar{w}$ ]	$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	x, $\bar{y},1/2$ [0,0,w]
16 p ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [u,v,0]	$\bar{x},y,0$ [u, $\bar{v}$ ,0]	x, $\bar{y},0$ [u, $\bar{v}$ ,0]
16 o ..m'	x,0,z [u,0,w]	$\bar{x},0,z$ [u,0, $\bar{w}$ ]	$\bar{x},0,\bar{z}$ [u,0,w]	x,0, $\bar{z}$ [u,0, $\bar{w}$ ]
16 n m..	0,y,z [u,0,0]	0, $\bar{y},z$ [u,0,0]	0,y, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [u,0,0]
16 m ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [u, $\bar{v}$ ,0]	3/4,3/4, $\bar{z}$ [u,v,0]	1/4,3/4,z [u, $\bar{v}$ ,0]
8 l mm'2'	0,1/2,z [u,0,0]	0,1/2, $\bar{z}$ [u,0,0]		
8 k mm'2'	0,0,z [u,0,0]	0,0, $\bar{z}$ [u,0,0]		
8 j m2m	0,y,1/2 [0,0,0]	0, $\bar{y},1/2$ [0,0,0]		
8 i m2'm'	0,y,0 [u,0,0]	0, $\bar{y},0$ [u,0,0]		
8 h 2'm'm	x,0,1/2 [0,0,w]	$\bar{x},0,1/2$ [0,0, $\bar{w}$ ]		
8 g 2m'm'	x,0,0 [u,0,0]	$\bar{x},0,0$ [u,0,0]		
8 f ..2'/m	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
8 e ..2'/m'	1/4,1/4,0 [u,v,0]	3/4,1/4,0 [u, $\bar{v}$ ,0]		
4 d mm'm	0,0,1/2 [0,0,0]			
4 c mm'm	1/2,0,1/2 [0,0,0]			
4 b mm'm'	1/2,0,0 [u,0,0]			
4 a mm'm'	0,0,0 [u,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

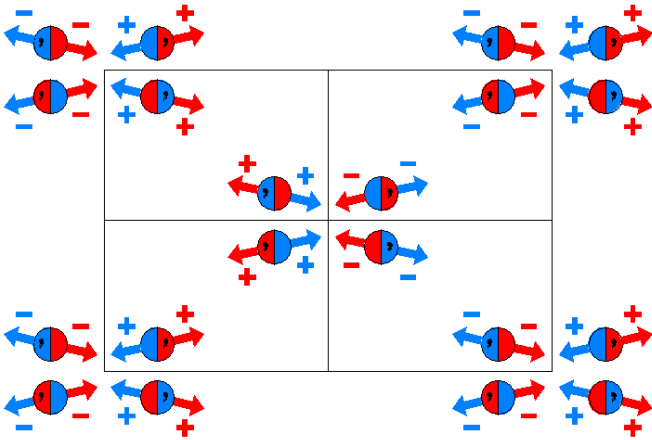
Along [0,1,0] p<sub>2a'</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/2,y,0



$C_p m' m m$   
65.13.557

$m m m 1'$   
 $C_p 2/m' 2'/m 2'/m$

Orthorhombic



**Origin** at center ( $m' m m$ )

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

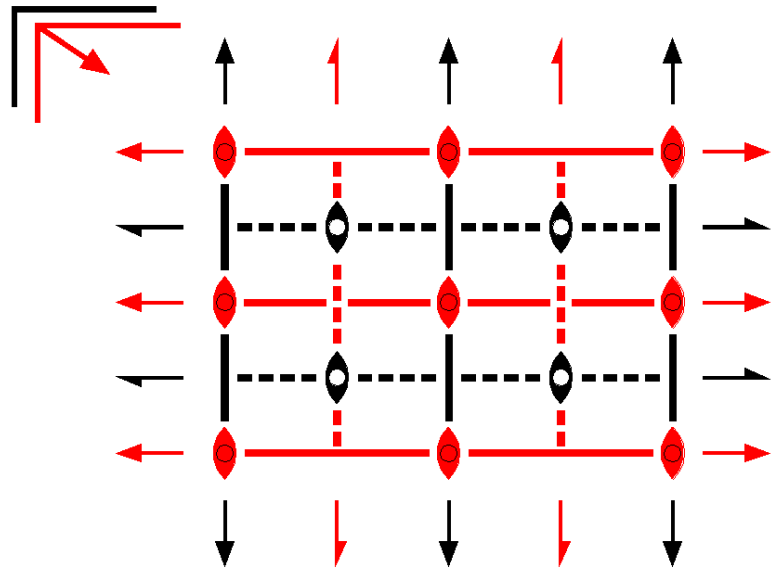
**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |                                    |                                    |                                    |
|---|------------------------------------|------------------------------------|------------------------------------|
| (1) 1<br>(1 0,0,0)                          | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $2'$ 0,y,0<br>( $2_y$  0,0,0)' | (4) $2$ x,0,0<br>( $2_x$  0,0,0)   |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m x,y,0<br>( $m_z$  0,0,0)     | (7) m x,0,z<br>( $m_y$  0,0,0)     | (8) $m'$ 0,y,z<br>( $m_x$  0,0,0)' |

For  $(1/2,1/2,0)$ ' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (1/2,1/2,0)<br>(1 1/2,1/2,0)'             | (2) $2$ 1/4,1/4,z<br>( $2_z$  1/2,1/2,0)           | (3) $2$ (0,1/2,0) 1/4,y,0<br>( $2_y$  1/2,1/2,0)   | (4) $2'$ (1/2,0,0) x,1/4,0<br>( $2_x$  1/2,1/2,0)' |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) $n'$ (1/2,1/2,0) x,y,0<br>( $m_z$  1/2,1/2,0)' | (7) $a'$ (1/2,0,0) x,1/4,z<br>( $m_y$  1/2,1/2,0)' | (8) $b$ (0,1/2,0) 1/4,y,z<br>( $m_x$  1/2,1/2,0)   |





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t'(1/2,1/2,0); (2); (3); (5).

### Positions

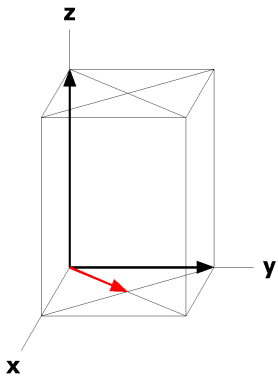
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 q ..m	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0, $\bar{w}$ ]	$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
8 p ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
8 o .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0,v,0]	$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	x,0, $\bar{z}$ [0, $\bar{v},0$ ]
8 n m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0,v, $\bar{w}$ ]	0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 m ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0,w]	3/4,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,3/4,z [0,0, $\bar{w}$ ]
4 l m'm2'	0,1/2,z [0,v,0]	0,1/2, $\bar{z}$ [0, $\bar{v},0$ ]		
4 k m'm2'	0,0,z [0,v,0]	0,0, $\bar{z}$ [0, $\bar{v},0$ ]		
4 j m'2'm	0,y,1/2 [0,0,w]	0, $\bar{y},1/2$ [0,0, $\bar{w}$ ]		
4 i m'2'm	0,y,0 [0,0,w]	0, $\bar{y},0$ [0,0, $\bar{w}$ ]		
4 h 2mm	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]		
4 g 2mm	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
4 f ..2/m	1/4,1/4,1/2 [0,0,w]	3/4,1/4,1/2 [0,0,w]		
4 e ..2/m	1/4,1/4,0 [0,0,w]	3/4,1/4,0 [0,0,w]		
2 d m'mm	0,0,1/2 [0,0,0]			
2 c m'mm	1/2,0,1/2 [0,0,0]			
2 b m'mm	1/2,0,0 [0,0,0]			
2 a m'mm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

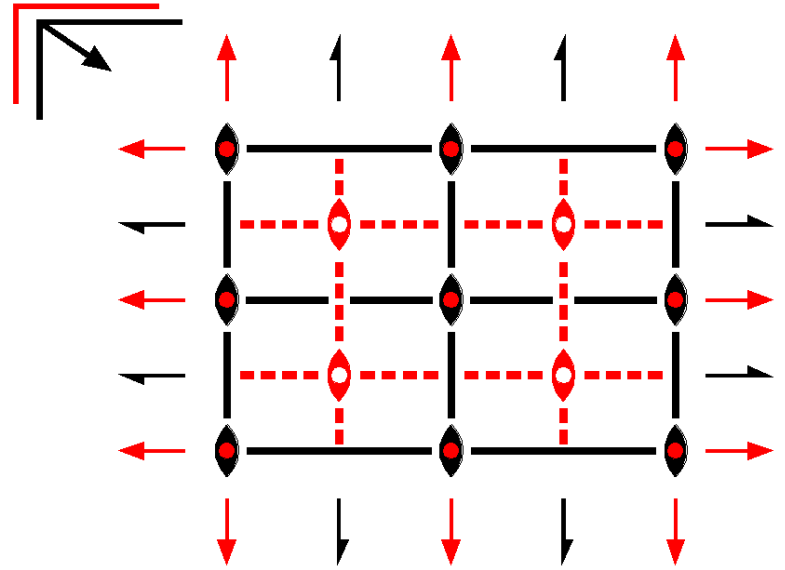
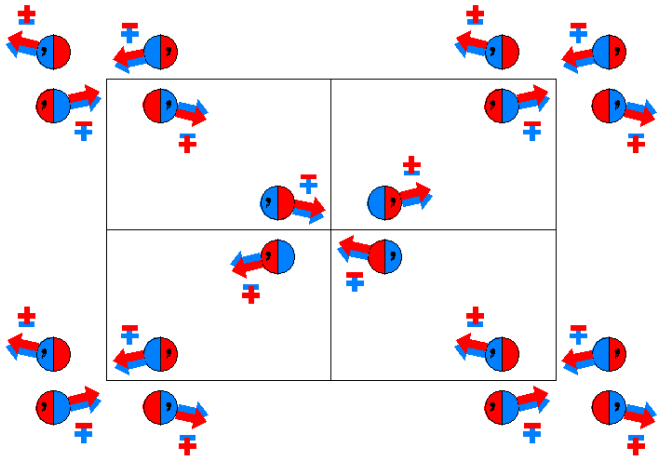
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



$C_{pmmm}'$   
65.14.558

$mmm1'$   
 $C_{p2'}/m2'/m2/m'$

Orthorhombic



**Origin** at center ( $mmm'$ )

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) 2' $0,y,0$<br>(2 <sub>y</sub>  0,0,0)' | (4) 2' $x,0,0$<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)' | (6) $m'$ $x,y,0$<br>( $m_z$  0,0,0)'     | (7) $m$ $x,0,z$<br>( $m_y$  0,0,0)         | (8) $m$ $0,y,z$<br>( $m_x$  0,0,0)         |

For  $(1/2,1/2,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,0)$<br>(1 1/2,1/2,0)'             | (2) 2' $1/4,1/4,z$<br>(2 <sub>z</sub>  1/2,1/2,0)'   | (3) 2 $(0,1/2,0)$ $1/4,y,0$<br>(2 <sub>y</sub>  1/2,1/2,0) | (4) 2 $(1/2,0,0)$ $x,1/4,0$<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$  1/2,1/2,0) | (6) $n$ $(1/2,1/2,0)$ $x,y,0$<br>( $m_z$  1/2,1/2,0) | (7) $a'$ $(1/2,0,0)$ $x,1/4,z$<br>( $m_y$  1/2,1/2,0)'     | (8) $b'$ $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$  1/2,1/2,0)      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

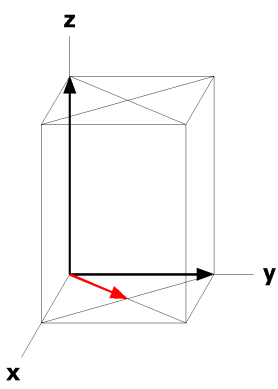
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},\bar{v},w$ ] (7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 q ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [u, $\bar{v},0$ ]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]
8 p ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,0$ [u, $\bar{v},0$ ]	x, $\bar{y},0$ [ $\bar{u},v,0$ ]
8 o .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	x,0, $\bar{z}$ [0,v,0]
8 n m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	0,y, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
8 m ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	3/4,3/4, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,3/4,z [ $\bar{u},v,0$ ]
4 l mm2	0,1/2,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]		
4 k mm2	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 j m2'm'	0,y,1/2 [u,0,0]	0, $\bar{y},1/2$ [ $\bar{u},0,0$ ]		
4 i m2'm'	0,y,0 [u,0,0]	0, $\bar{y},0$ [ $\bar{u},0,0$ ]		
4 h 2'mm'	x,0,1/2 [0,v,0]	$\bar{x},0,1/2$ [0, $\bar{v},0$ ]		
4 g 2'mm'	x,0,0 [0,v,0]	$\bar{x},0,0$ [0, $\bar{v},0$ ]		
4 f ..2'/m'	1/4,1/4,1/2 [u,v,0]	3/4,1/4,1/2 [u, $\bar{v},0$ ]		
4 e ..2'/m'	1/4,1/4,0 [u,v,0]	3/4,1/4,0 [u, $\bar{v},0$ ]		
2 d mmm'	0,0,1/2 [0,0,0]			
2 c mmm'	1/2,0,1/2 [0,0,0]			
2 b mmm'	1/2,0,0 [0,0,0]			
2 a mmm'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c<sub>p</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

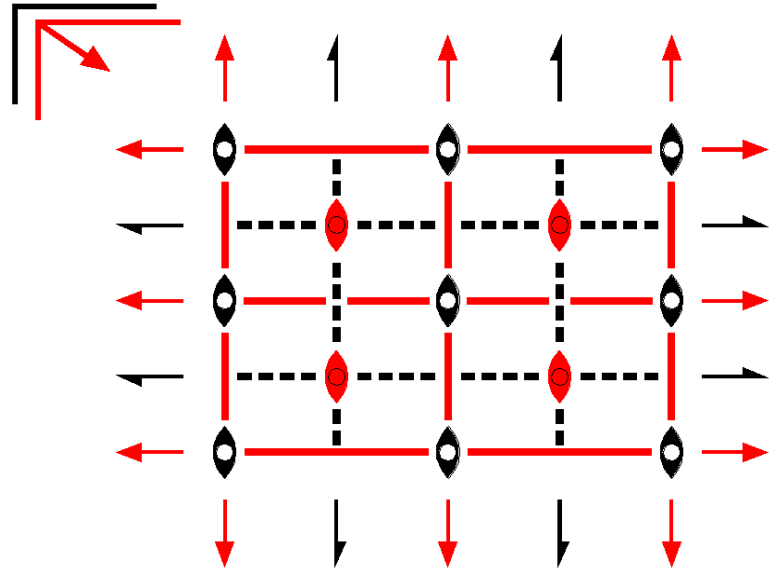
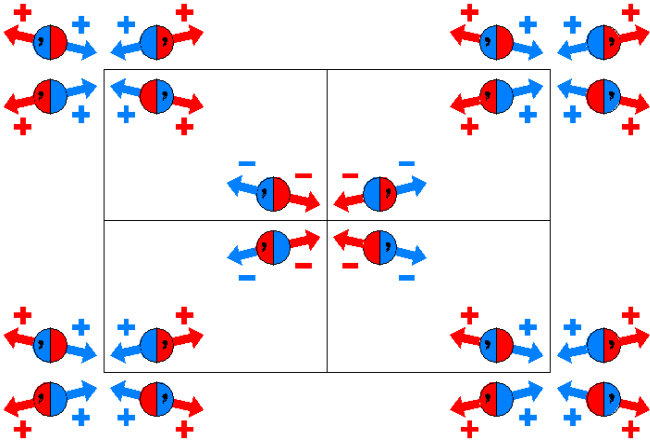
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



$C_{pm}'m'm'$   
65.15.559

$mmm1'$   
 $C_{p2}'/m'2'/m'2'/m$

Orthorhombic



**Origin** at center ( $m'm'm'$ )

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

For (1/2,1/2,0)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' (1/2,1/2,0)<br>(1 1/2,1/2,0)'                  | (2) 2' 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)'         | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

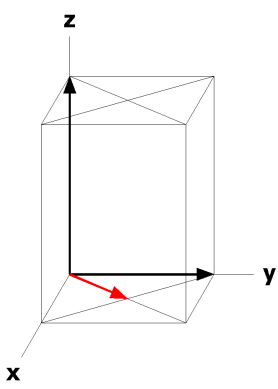
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 q ..m	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0,w]	$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0,w]
8 p ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0,w]
8 o .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$\bar{x},0,\bar{z}$ [u,0,w]	x,0, $\bar{z}$ [ $\bar{u},0,w$ ]
8 n m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
8 m ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [u, $\bar{v},0$ ]	3/4,3/4, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,3/4,z [ $\bar{u},v,0$ ]
4 l m'm'2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]		
4 k m'm'2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
4 j m'2'm	0,y,1/2 [0,0,w]	0, $\bar{y},1/2$ [0,0,w]		
4 i m'2'm	0,y,0 [0,0,w]	0, $\bar{y},0$ [0,0,w]		
4 h 2'm'm	x,0,1/2 [0,0,w]	$\bar{x},0,1/2$ [0,0,w]		
4 g 2'm'm	x,0,0 [0,0,w]	$\bar{x},0,0$ [0,0,w]		
4 f ..2'/m	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 e ..2'/m	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
2 d m'm'm	0,0,1/2 [0,0,w]			
2 c m'm'm	1/2,0,1/2 [0,0,w]			
2 b m'm'm	1/2,0,0 [0,0,w]			
2 a m'm'm	0,0,0 [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

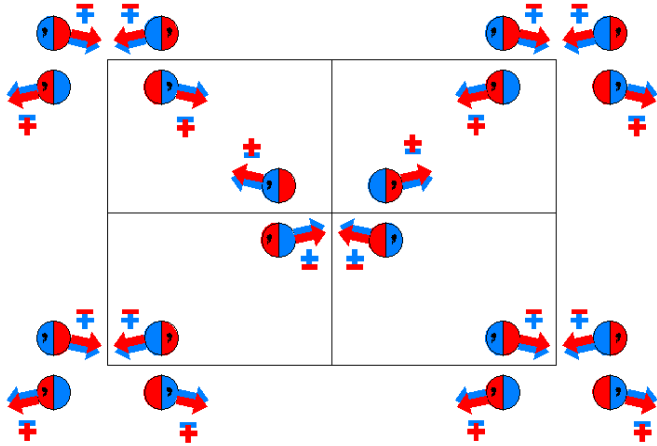
Along [0,1,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,1/4



$C_pmm'm'$   
65.16.560

$mmm1'$   
 $C_p2/m2'/m2'/m'$

Orthorhombic



**Origin** at center ( $mm'm'$ )

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

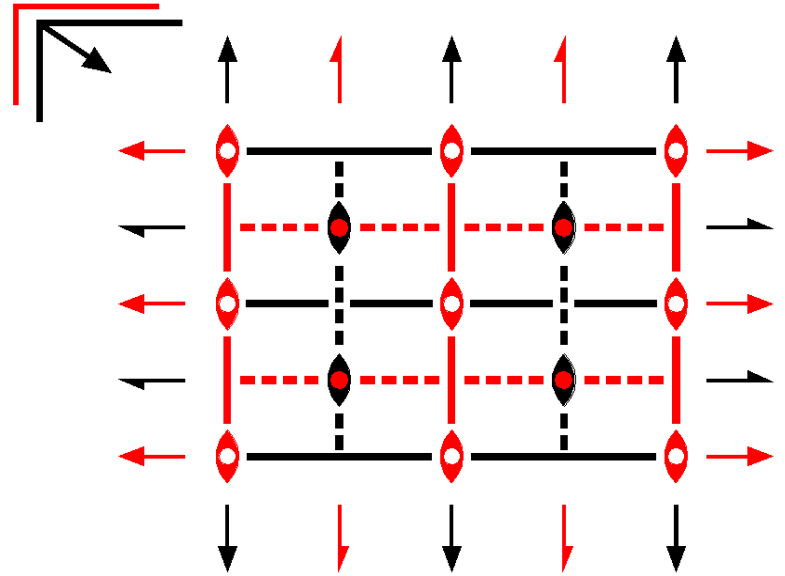
**Symmetry Operations**

For (0,0,0) + set

- |  |                                      |                                      |                                     |
|--|--------------------------------------|--------------------------------------|-------------------------------------|
| (1) 1<br>(1 0,0,0)                         | (2) $2'_z$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $2'_y$ 0,y,0<br>( $2_y$  0,0,0)' | (4) $2'_x$ x,0,0<br>( $2_x$  0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) $m'_z$ x,y,0<br>( $m_z$  0,0,0)' | (7) $m'_y$ x,0,z<br>( $m_y$  0,0,0)' | (8) $m'_x$ 0,y,z<br>( $m_x$  0,0,0) |

For (1/2,1/2,0)' + set

- |   |  |   |  |
|---|--|---|--|
| (1) $t'$ (1/2,1/2,0)<br>(1 1/2,1/2,0)'              | (2) $2'_z$ 1/4,1/4,z<br>( $2_z$  1/2,1/2,0)      | (3) $2'_y$ (0,1/2,0) 1/4,y,0<br>( $2_y$  1/2,1/2,0) | (4) $2'_x$ (1/2,0,0) x,1/4,0<br>( $2_x$  1/2,1/2,0)' |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) $n$ (1/2,1/2,0) x,y,0<br>( $m_z$  1/2,1/2,0) | (7) $a$ (1/2,0,0) x,1/4,z<br>( $m_y$  1/2,1/2,0)    | (8) $b'$ (0,1/2,0) 1/4,y,z<br>( $m_x$  1/2,1/2,0)'   |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

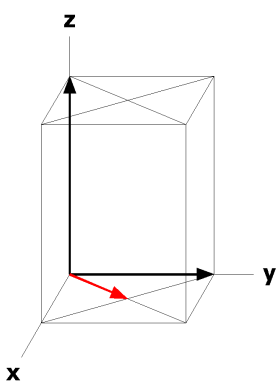
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(1/2,1/2,0)' +		
16	r 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
		(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) x, $\bar{y},z$ [u, $\bar{v}$ ,w]	(8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8	q ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [u,v,0]	$\bar{x},y,1/2$ [u, $\bar{v}$ ,0]	x, $\bar{y},1/2$ [u, $\bar{v}$ ,0]
8	p ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [u,v,0]	$\bar{x},y,0$ [u, $\bar{v}$ ,0]	x, $\bar{y},0$ [u, $\bar{v}$ ,0]
8	o .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [u,0, $\bar{w}$ ]	$\bar{x},0,\bar{z}$ [u,0,w]	x,0, $\bar{z}$ [u,0, $\bar{w}$ ]
8	n m..	0,y,z [u,0,0]	0, $\bar{y},z$ [u,0,0]	0,y, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [u,0,0]
8	m ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0,w]	3/4,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,3/4,z [0,0, $\bar{w}$ ]
4	l mm'2'	0,1/2,z [u,0,0]	0,1/2, $\bar{z}$ [u,0,0]		
4	k mm'2'	0,0,z [u,0,0]	0,0, $\bar{z}$ [u,0,0]		
4	j m2'm'	0,y,1/2 [u,0,0]	0, $\bar{y},1/2$ [u,0,0]		
4	i m2'm'	0,y,0 [u,0,0]	0, $\bar{y},0$ [u,0,0]		
4	h 2m'm'	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [u,0,0]		
4	g 2m'm'	x,0,0 [u,0,0]	$\bar{x},0,0$ [u,0,0]		
4	f ..2/m'	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4	e ..2/m'	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
2	d mm'm'	0,0,1/2 [u,0,0]			
2	c mm'm'	1/2,0,1/2 [u,0,0]			
2	b mm'm'	1/2,0,0 [u,0,0]			
2	a mm'm'	0,0,0 [u,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c<sub>p</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>-2'mm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



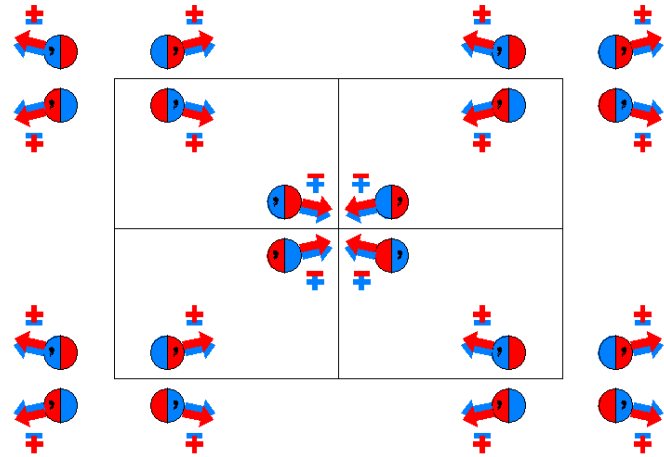
$C_p m' m' m'$

65.17.561

$mmm1'$

$C_p 2/m' 2/m' 2/m'$

Orthorhombic



**Origin** at center ( $m' m' m'$ )

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

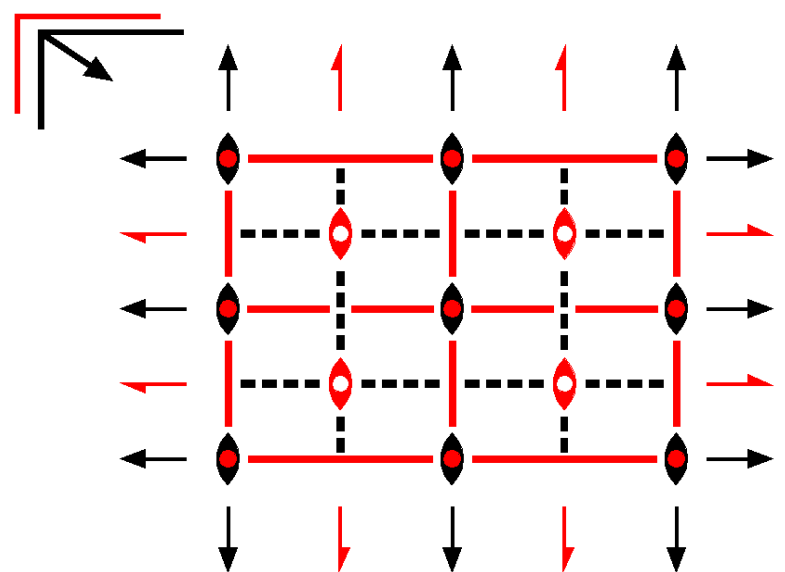
**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1   0,0,0)                           | (2) 2 $0,0,z$<br>(2 <sub>z</sub>   0,0,0) | (3) 2 $0,y,0$<br>(2 <sub>y</sub>   0,0,0) | (4) 2 $x,0,0$<br>(2 <sub>x</sub>   0,0,0) |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   0,0,0)' | (6) $m'$ $x,y,0$<br>( $m_z$   0,0,0)'     | (7) $m'$ $x,0,z$<br>( $m_y$   0,0,0)'     | (8) $m'$ $0,y,z$<br>( $m_x$   0,0,0)'     |

For  $(1/2,1/2,0)$ ' + set

- |   |   |  |  |
|---|---|--|--|
| (1) $t'$ $(1/2,1/2,0)$<br>(1   $1/2,1/2,0$ )'             | (2) 2' $1/4,1/4,z$<br>(2 <sub>z</sub> '   $1/2,1/2,0$ )'    | (3) 2' $(0,1/2,0)$ $1/4,y,0$<br>(2 <sub>y</sub> '   $1/2,1/2,0$ )' | (4) 2' $(1/2,0,0)$ $x,1/4,0$<br>(2 <sub>x</sub> '   $1/2,1/2,0$ )' |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ )' | (6) $n$ $(1/2,1/2,0)$ $x,y,0$<br>( $m_z$ '   $1/2,1/2,0$ )' | (7) $a$ $(1/2,0,0)$ $x,1/4,z$<br>( $m_y$ '   $1/2,1/2,0$ )'        | (8) $b$ $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$ '   $1/2,1/2,0$ )'        |





**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(1/2,1/2,0)$ ; (2); (3); (5).

### Positions

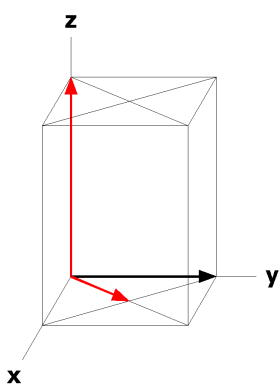
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 r 1	(1) $x,y,z [u,v,w]$ (5) $\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$ (6) $x,y,\bar{z} [u,v,\bar{w}]$	(3) $\bar{x},y,\bar{z} [\bar{u},v,\bar{w}]$ (7) $x,\bar{y},z [u,\bar{v},w]$	(4) $x,\bar{y},\bar{z} [u,\bar{v},\bar{w}]$ (8) $\bar{x},y,z [\bar{u},v,w]$
8 q ..m'	$x,y,1/2 [u,v,0]$	$\bar{x},\bar{y},1/2 [\bar{u},\bar{v},0]$	$\bar{x},y,1/2 [\bar{u},v,0]$	$x,\bar{y},1/2 [u,\bar{v},0]$
8 p ..m'	$x,y,0 [u,v,0]$	$\bar{x},\bar{y},0 [\bar{u},\bar{v},0]$	$\bar{x},y,0 [\bar{u},v,0]$	$x,\bar{y},0 [u,\bar{v},0]$
8 o .m'	$x,0,z [u,0,w]$	$\bar{x},0,z [\bar{u},0,w]$	$\bar{x},0,\bar{z} [\bar{u},0,\bar{w}]$	$x,0,\bar{z} [u,0,\bar{w}]$
8 n m'..	$0,y,z [0,v,w]$	$0,\bar{y},z [0,\bar{v},w]$	$0,y,\bar{z} [0,v,\bar{w}]$	$0,\bar{y},\bar{z} [0,\bar{v},\bar{w}]$
8 m ..2'	$1/4,1/4,z [u,v,0]$	$3/4,1/4,\bar{z} [\bar{u},\bar{v},0]$	$3/4,3/4,\bar{z} [\bar{u},\bar{v},0]$	$1/4,3/4,z [u,\bar{v},0]$
4 l m'm'2	$0,1/2,z [0,0,w]$	$0,1/2,\bar{z} [0,0,\bar{w}]$		
4 k m'm'2	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,\bar{w}]$		
4 j m'2m'	$0,y,1/2 [0,v,0]$	$0,\bar{y},1/2 [0,\bar{v},0]$		
4 i m'2m'	$0,y,0 [0,v,0]$	$0,\bar{y},0 [0,\bar{v},0]$		
4 h 2m'm'	$x,0,1/2 [u,0,0]$	$\bar{x},0,1/2 [\bar{u},0,0]$		
4 g 2m'm'	$x,0,0 [u,0,0]$	$\bar{x},0,0 [\bar{u},0,0]$		
4 f ..2'/m'	$1/4,1/4,1/2 [u,v,0]$	$3/4,1/4,1/2 [\bar{u},\bar{v},0]$		
4 e ..2'/m'	$1/4,1/4,0 [u,v,0]$	$3/4,1/4,0 [\bar{u},\bar{v},0]$		
2 d m'm'm'	$0,0,1/2 [0,0,0]$			
2 c m'm'm'	$1/2,0,1/2 [0,0,0]$			
2 b m'm'm'	$1/2,0,0 [0,0,0]$			
2 a m'm'm'	$0,0,0 [0,0,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

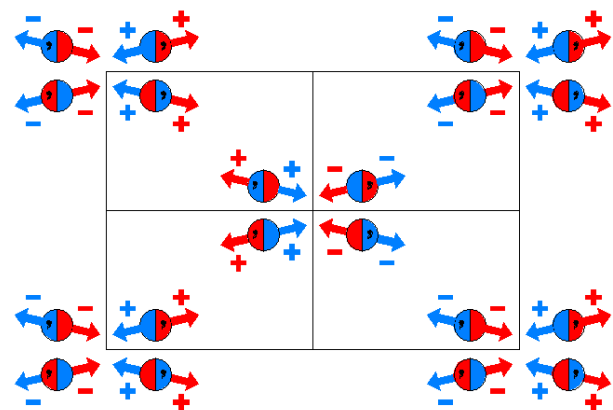
Along  $[0,1,0]$   $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $0,y,0$



$C_1m'mm$   
65.18.562

$mmm1'$   
 $C_2/m'2'/m2'/m$

Orthorhombic



Origin at center ( $m'mm$ )

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |  |                                       |                                       |                                       |
|--|---------------------------------------|---------------------------------------|---------------------------------------|
| (1) 1<br>(1   0,0,0)                         | (2) $2'_z$ 0,0,z<br>( $2_z$   0,0,0)' | (3) $2'_y$ 0,y,0<br>( $2_y$   0,0,0)' | (4) $2'_x$ x,0,0<br>( $2_x$   0,0,0)  |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0)' | (6) m x,y,0<br>( $m_z$   0,0,0)       | (7) m x,0,z<br>( $m_y$   0,0,0)       | (8) $m'_x$ 0,y,z<br>( $m_x$   0,0,0)' |

For (1/2,1/2,0)' + set

- |   |  |   |   |
|---|--|---|---|
| (1) $t$ (1/2,1/2,0)<br>(1   1/2,1/2,0)'             | (2) $2$ 1/4,1/4,z<br>( $2_z$   1/2,1/2,0)          | (3) $2$ (0,1/2,0) 1/4,y,0<br>( $2_y$   1/2,1/2,0)   | (4) $2'_x$ (1/2,0,0) x,1/4,0<br>( $2_x$   1/2,1/2,0)' |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0) | (6) $n$ (1/2,1/2,0) x,y,0<br>( $m_z$   1/2,1/2,0)' | (7) $a'$ (1/2,0,0) x,1/4,z<br>( $m_y$   1/2,1/2,0)' | (8) b (0,1/2,0) 1/4,y,z<br>( $m_x$   1/2,1/2,0)       |

For (0,0,1)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) $t$ (0,0,1)<br>(1   0,0,1)'               | (2) $2$ (0,0,1) 0,0,z<br>( $2_z$   0,0,1) | (3) $2$ 0,y,1/2<br>( $2_y$   0,0,1)         | (4) $2'_x$ x,0,1/2<br>( $2_x$   0,0,1)' |
| (5) $\bar{1}$ 0,0,1/2<br>( $\bar{1}$   0,0,1) | (6) $m'_z$ x,y,1/2<br>( $m_z$   0,0,1)'   | (7) $c'$ (0,0,1) x,0,z<br>( $m_y$   0,0,1)' | (8) c (0,0,1) 0,y,z<br>( $m_x$   0,0,1) |

For (1/2,1/2,1) + set

- |  |   |   |  |
|--|---|---|--|
| (1) $t$ (1/2,1/2,1)<br>(1   1/2,1/2,1)                 | (2) $2'_z$ (0,0,1) 1/4,1/4,z<br>( $2_z$   1/2,1/2,1)' | (3) $2'_y$ (0,1/2,0) 1/4,y,1/2<br>( $2_y$   1/2,1/2,1)' | (4) $2'_x$ (1/2,0,0) x,1/4,1/2<br>( $2_x$   1/2,1/2,1) |
| (5) $\bar{1}$ 1/4,1/4,1/2<br>( $\bar{1}$   1/2,1/2,1)' | (6) n (1/2,1/2,0) x,y,1/2<br>( $m_z$   1/2,1/2,1)     | (7) n (1/2,0,1) x,1/4,z<br>( $m_y$   1/2,1/2,1)         | (8) $n'_x$ (0,1/2,1) 1/4,y,z<br>( $m_x$   1/2,1/2,1)'  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

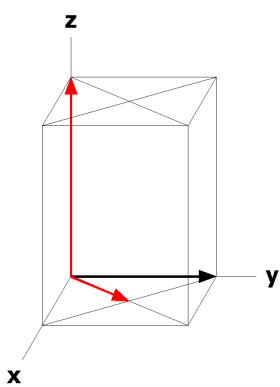
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) + (0,0,1)' +	(1/2,1/2,0)' + (1/2,1/2,1) +		
32 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
16 q ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [u,v,0]	$\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]
16 p ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
16 o .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0,v,0]	$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	x,0, $\bar{z}$ [0, $\bar{v},0$ ]
16 n m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0,v, $\bar{w}$ ]	0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
16 m ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0,w]	3/4,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,3/4,z [0,0, $\bar{w}$ ]
8 l m'm2'	0,1/2,z [0,v,0]	0,1/2, $\bar{z}$ [0, $\bar{v},0$ ]		
8 k m'm2'	0,0,z [0,v,0]	0,0, $\bar{z}$ [0, $\bar{v},0$ ]		
8 j m'2m'	0,y,1/2 [0,v,0]	0, $\bar{y},1/2$ [0,v,0]		
8 i m'2'm	0,y,0 [0,0,w]	0, $\bar{y},0$ [0,0, $\bar{w}$ ]		
8 h 2'mm'	x,0,1/2 [0,v,0]	$\bar{x},0,1/2$ [0,v,0]		
8 g 2mm	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
8 f ..2'/m	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
8 e ..2'/m	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]	mm	
4 d m'mm'	0,0,1/2 [0,v,0]			
4 c m'mm'	1/2,0,1/2 [0,v,0]			
4 b m'mm	1/2,0,0 [0,0,0]			
4 a m'mm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>c</sub>2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

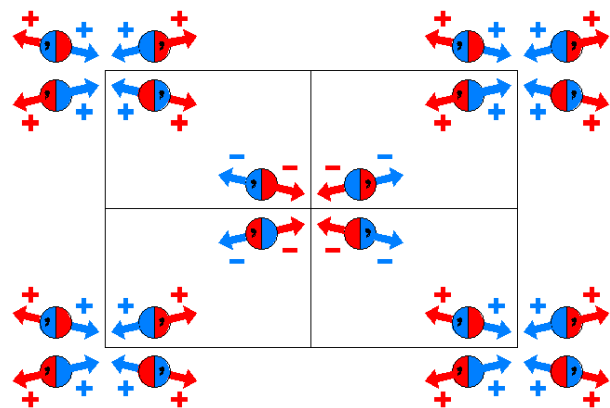
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



$C_1m'm'm$   
65.19.563

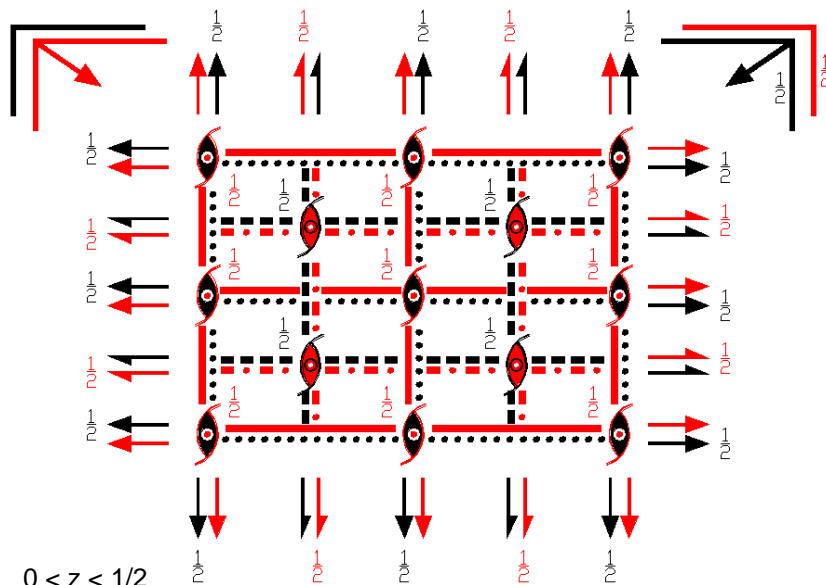
$mmm1'$   
 $C_2/m'2'/m'2/m$

Orthorhombic



Origin at center ( $m'm'm$ )

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$



### Symmetry Operations

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0) | (3) 2' 0,y,0<br>(2 <sub>y</sub>   0,0,0)' | (4) 2' x,0,0<br>(2 <sub>x</sub>   0,0,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>   0,0,0) | (7) m' x,0,z<br>(m <sub>y</sub>   0,0,0)' | (8) m' 0,y,z<br>(m <sub>x</sub>   0,0,0)' |

For (1/2,1/2,0)' + set

- |  |   |   |   |
|--|---|---|---|
| (1) t' (1/2,1/2,0)<br>(1   1/2,1/2,0)'                 | (2) 2' 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)'         | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0) |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>   1/2,1/2,0)' | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0) |

For (0,0,1)' + set

- |  |   |   |   |
|--|---|---|---|
| (1) t' (0,0,1)<br>(1   0,0,1)'                   | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>   0,0,1)' | (3) 2 0,y,1/2<br>(2 <sub>y</sub>   0,0,1)       | (4) 2 x,0,1/2<br>(2 <sub>x</sub>   0,0,1)       |
| (5) $\bar{1}$ ' 0,0,1/2<br>( $\bar{1}$   0,0,1)' | (6) m' x,y,1/2<br>(m <sub>z</sub>   0,0,1)'       | (7) c (0,0,1) x,0,z<br>(m <sub>y</sub>   0,0,1) | (8) c (0,0,1) 0,y,z<br>(m <sub>x</sub>   0,0,1) |

For (1/2,1/2,1) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,1)<br>(1   1/2,1/2,1)                  | (2) 2 (0,0,1) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1)   | (3) 2' (0,1/2,0) 1/4,y,1/2<br>(2 <sub>y</sub>   1/2,1/2,1)' | (4) 2' (1/2,0,0) x,1/4,1/2<br>(2 <sub>x</sub>   1/2,1/2,1)' |
| (5) $\bar{1}$ 1/4,1/4,1/2<br>( $\bar{1}$   1/2,1/2,1) | (6) n (1/2,1/2,0) x,y,1/2<br>(m <sub>z</sub>   1/2,1/2,1) | (7) n' (1/2,0,1) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,1)'   | (8) n' (0,1/2,1) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,1)'   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

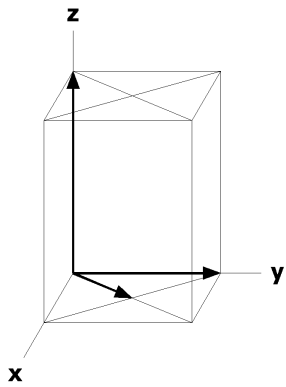
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,1)' +	(1/2,1/2,0)' + (1/2,1/2,1) +	
32 r 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
16 q ..m'	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	x, $\bar{y},1/2$ [u, $\bar{v},0$ ]
16 p ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0,w]
16 o ..m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$\bar{x},0,\bar{z}$ [u,0,w]	x,0, $\bar{z}$ [ $\bar{u},0,w$ ]
16 n m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
16 m ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [u, $\bar{v},0$ ]	3/4,3/4, $\bar{z}$ [u,v,0]	1/4,3/4,z [u, $\bar{v},0$ ]
8 l m'm'2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]		
8 k m'm'2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
8 j m'2m'	0,y,1/2 [0,v,0]	0, $\bar{y},1/2$ [0, $\bar{v},0$ ]		
8 i m'2'm	0,y,0 [0,0,w]	0, $\bar{y},0$ [0,0,w]		
8 h 2m'm'	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]		
8 g 2'm'm	x,0,0 [0,0,w]	$\bar{x},0,0$ [0,0,w]		
8 f ..2'/m'	1/4,1/4,1/2 [u,v,0]	3/4,1/4,1/2 [ $\bar{u},v,0$ ]		
8 e ..2'/m	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
4 d m'm'm'	0,0,1/2 [0,0,0]			
4 c m'm'm'	1/2,0,1/2 [0,0,0]			
4 b m'm'm	1/2,0,0 [0,0,w]			
4 a m'm'm	0,0,0 [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

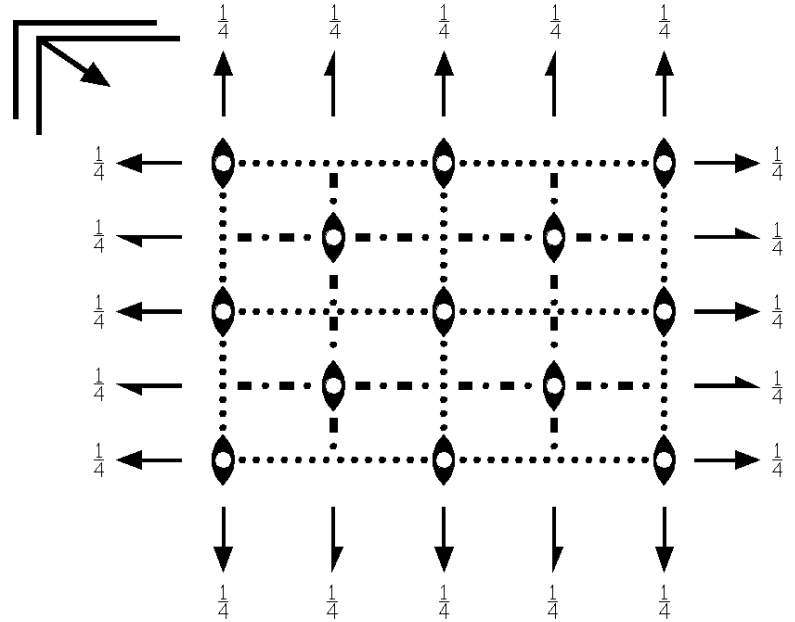
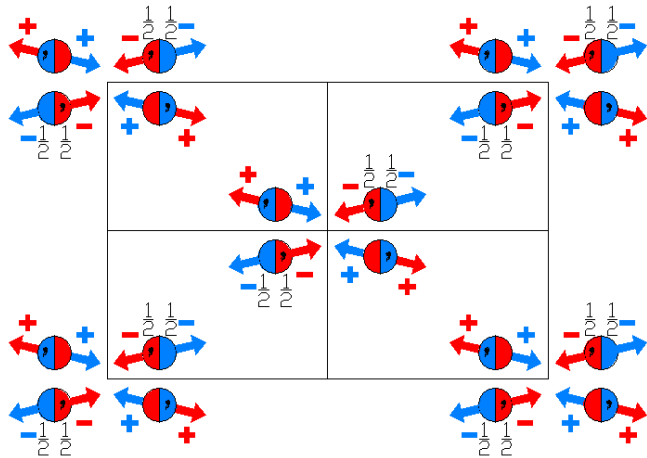
Along [0,1,0] p<sub>2a</sub>'2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,0



Cccm  
66.1.564

mmm  
C2/c2/c2/m

Orthorhombic



**Origin** at center ( $2/m$ ) at  $cc2/m$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)         | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (8) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                 | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)         | (3) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (4) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (7) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (8) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

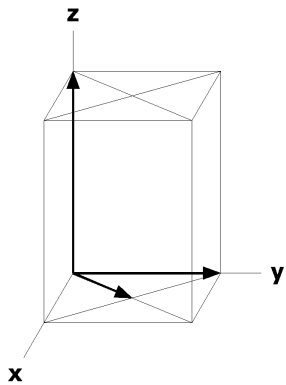
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1/2,1/2,0) +	
16 m 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]
8 l ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
8 k ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	3/4,3/4, $\bar{z}$ [0,0,w]	1/4,3/4,z+1/2 [0,0, $\bar{w}$ ]
8 j ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
8 i ..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]
8 h .2.	0,y,1/4 [0,v,0]	0, $\bar{y},1/4$ [0, $\bar{v},0$ ]	0, $\bar{y},3/4$ [0,v,0]	0,y,3/4 [0, $\bar{v},0$ ]
8 g 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [u,0,0]
4 f ..2/m	1/4,3/4,0 [0,0,w]	3/4,3/4,1/2 [0,0, $\bar{w}$ ]		
4 e ..2/m	1/4,1/4,0 [0,0,w]	3/4,1/4,1/2 [0,0, $\bar{w}$ ]		
4 d ..2/m	0,1/2,0 [0,0,w]	0,1/2,1/2 [0,0, $\bar{w}$ ]		
4 c ..2/m	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		
4 b 222	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]		
4 a 222	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Cccm1'

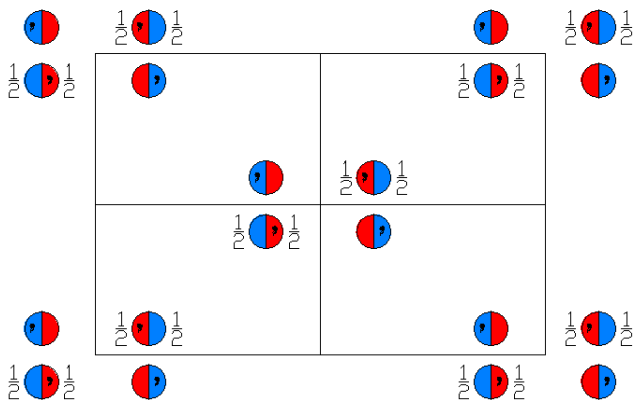
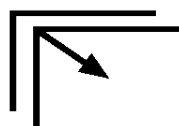
66.2.565

mmm1'

C2/c2/c2/m1'

Orthorhombic

1'



Origin at center ( $2/m1'$ ) at  $cc2/m1'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)         | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (8) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                 | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)         | (3) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (4) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (7) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (8) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) |

For (0,0,0)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1'<br>(1 0,0,0)'                          | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'         | (4) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'         |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (8) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |

For (1/2,1/2,0)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' (1/2,1/2,0)<br>(1 1/2,1/2,0)'                  | (2) 2' 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)'         | (3) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (4) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (7) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5);1'.

### Positions

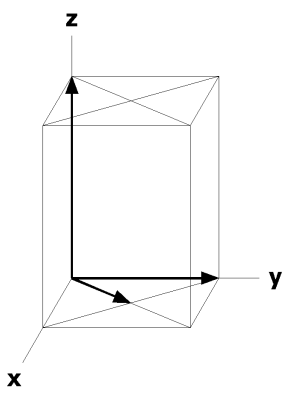
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) + (0,0,0)'	(1/2,1/2,0) + (1/2,1/2,0)'		
16 m 11'	(1) x,y,z [0,0,0] (5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0] (6) x,y, $\bar{z}$ [0,0,0]	(3) $\bar{x},y,\bar{z}+1/2$ [0,0,0] (7) x, $\bar{y},z+1/2$ [0,0,0]	(4) x, $\bar{y},\bar{z}+1/2$ [0,0,0] (8) $\bar{x},y,z+1/2$ [0,0,0]
8 l ..m1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{x},y,1/2$ [0,0,0]	x, $\bar{y},1/2$ [0,0,0]
8 k ..21'	1/4,1/4,z [0,0,0]	3/4,1/4, $\bar{z}+1/2$ [0,0,0]	3/4,3/4, $\bar{z}$ [0,0,0]	1/4,3/4,z+1/2 [0,0,0]
8 j ..21'	0,1/2,z [0,0,0]	0,1/2, $\bar{z}+1/2$ [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	0,1/2,z+1/2 [0,0,0]
8 i ..21'	0,0,z [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0,z+1/2 [0,0,0]
8 h .2.1'	0,y,1/4 [0,0,0]	0, $\bar{y},1/4$ [0,0,0]	0, $\bar{y},3/4$ [0,0,0]	0,y,3/4 [0,0,0]
8 g 2..1'	x,0,1/4 [0,0,0]	$\bar{x},0,1/4$ [0,0,0]	$\bar{x},0,3/4$ [0,0,0]	x,0,3/4 [0,0,0]
4 f ..2/m1'	1/4,3/4,0 [0,0,0]	3/4,3/4,1/2 [0,0,0]		
4 e ..2/m1'	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 d ..2/m1'	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 c ..2/m1'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
4 b 2221'	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]		
4 a 2221'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



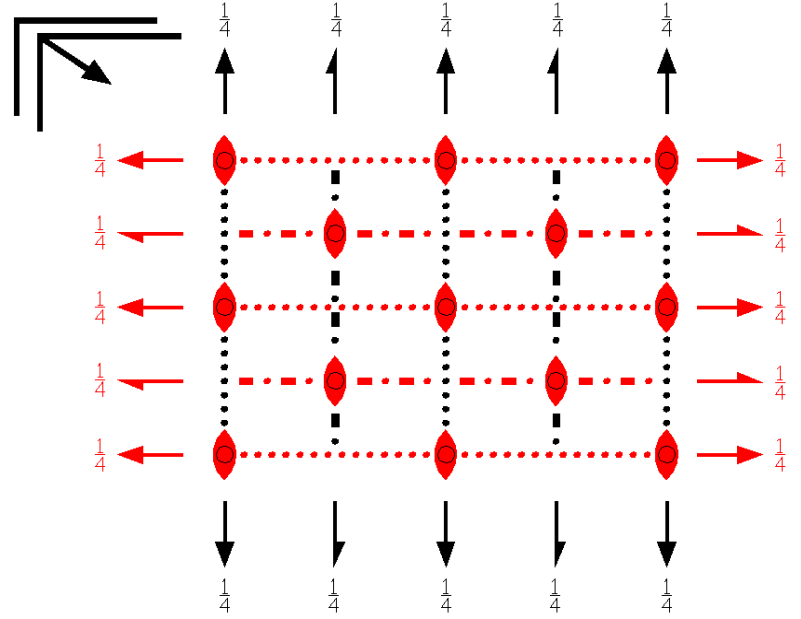
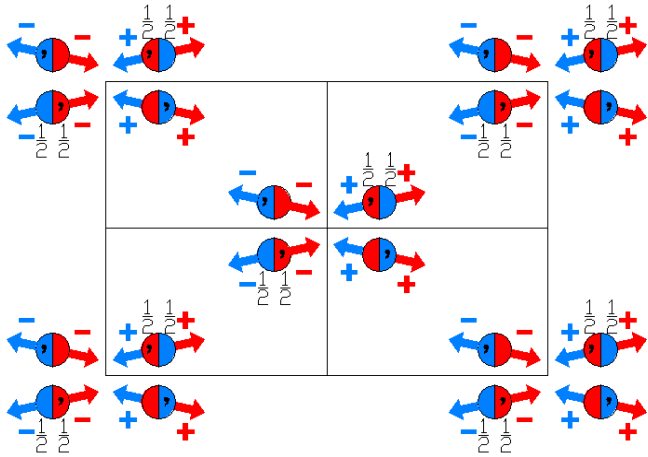
Cc'cm

66.3.566

m'mm

C2/c'2'/c2'/m

Orthorhombic



**Origin** at center ( $2'/m$ ) at  $c'c2'/m$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |                                    |  |  |
|--|------------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $2'$ 0,y,1/4<br>( $2_y$  0,0,1/2)'     | (4) $2$ x,0,1/4<br>( $2_x$  0,0,1/2)           |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m x,y,0<br>( $m_z$  0,0,0)     | (7) c (0,0,1/2) x,0,z<br>( $m_y$  0,0,1/2) | (8) $c'$ (0,0,1/2) 0,y,z<br>( $m_x$  0,0,1/2)' |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                   | (2) $2'$ 1/4,1/4,z<br>( $2_z$  1/2,1/2,0)'     | (3) $2'$ (0,1/2,0) 1/4,y,1/4<br>( $2_y$  1/2,1/2,1/2)' | (4) $2$ (1/2,0,0) x,1/4,1/4<br>( $2_x$  1/2,1/2,1/2) |
| (5) $\bar{1}'$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) n (1/2,1/2,0) x,y,0<br>( $m_z$  1/2,1/2,0) | (7) n (1/2,0,1/2) x,1/4,z<br>( $m_y$  1/2,1/2,1/2)     | (8) n' (0,1/2,1/2) 1/4,y,z<br>( $m_x$  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

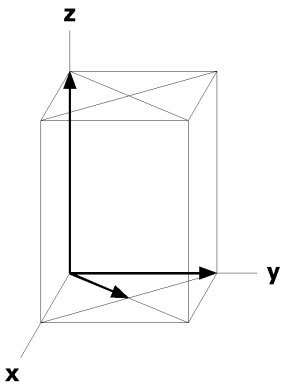
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 m 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
8 l ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
8 k ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	3/4,3/4, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,3/4,z+1/2 [ $\bar{u},v,0$ ]
8 j ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	0,1/2, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	0,1/2,z+1/2 [ $\bar{u},v,0$ ]
8 i ..2'	0,0,z [u,v,0]	0,0, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	0,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	0,0,z+1/2 [ $\bar{u},v,0$ ]
8 h .2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [u,0, $\bar{w}$ ]	0, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	0,y,3/4 [ $\bar{u},0,w$ ]
8 g 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [u,0,0]	$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [ $\bar{u},0,0$ ]
4 f ..2'/m	1/4,3/4,0 [0,0,0]	3/4,3/4,1/2 [0,0,0]		
4 e ..2'/m	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 d ..2'/m	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 c ..2'/m	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
4 b 22'2'	0,1/2,1/4 [u,0,0]	0,1/2,3/4 [ $\bar{u},0,0$ ]		
4 a 22'2'	0,0,1/4 [u,0,0]	0,0,3/4 [ $\bar{u},0,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

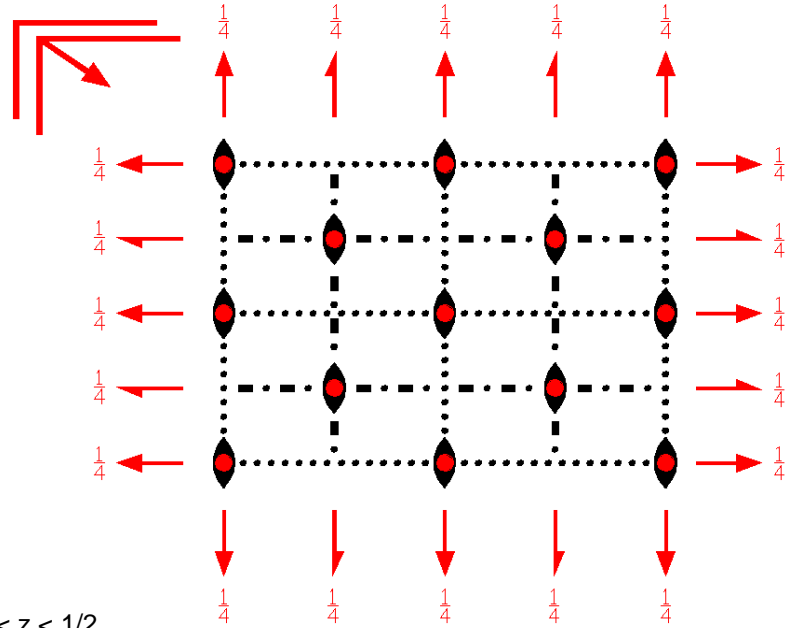
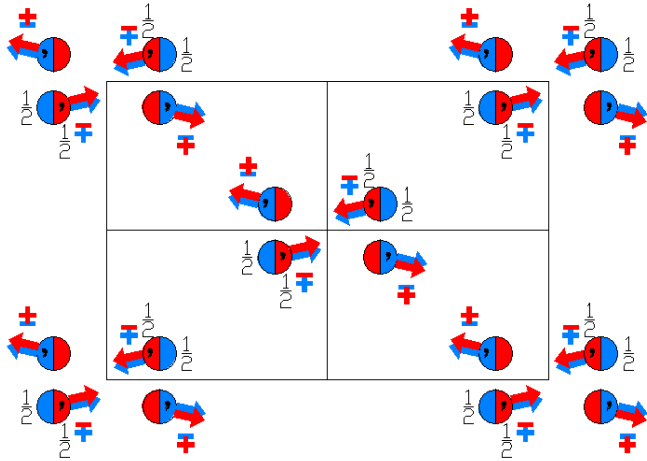
Along [0,1,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



Cccm'  
66.4.567

mmm'  
C2'/c2'/c2/m'

Orthorhombic



**Origin** at center ( $2/m'$ ) at  $cc2/m'$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |                                      |  |  |
|---|--------------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)     | (3) 2' $0,y,1/4$<br>( $2_y$  0,0,1/2)'         | (4) 2' $x,0,1/4$<br>( $2_x$  0,0,1/2)'         |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)' | (6) $m'$ $x,y,0$<br>( $m_z$  0,0,0)' | (7) c $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2) | (8) c $(0,0,1/2)$ $0,y,z$<br>( $m_x$  0,0,1/2) |

For (1/2,1/2,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t $(1/2,1/2,0)$<br>(1 1/2,1/2,0)                  | (2) 2 $1/4,1/4,z$<br>( $2_z$  1/2,1/2,0)               | (3) 2' $(0,1/2,0)$ $1/4,y,1/4$<br>( $2_y$  1/2,1/2,1/2)' | (4) 2' $(1/2,0,0)$ $x,1/4,1/4$<br>( $2_x$  1/2,1/2,1/2)' |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$  1/2,1/2,0)' | (6) $n'$ $(1/2,1/2,0)$ $x,y,0$<br>( $m_z$  1/2,1/2,0)' | (7) n $(1/2,0,1/2)$ $x,1/4,z$<br>( $m_y$  1/2,1/2,1/2)   | (8) n $(0,1/2,1/2)$ $1/4,y,z$<br>( $m_x$  1/2,1/2,1/2)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

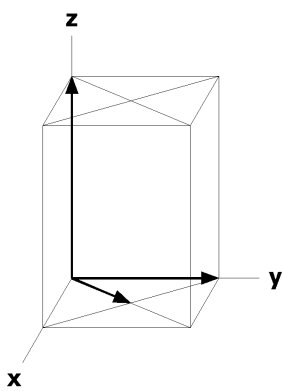
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 m 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z+1/2$ [u, $\bar{v},\bar{w}$ ]
8 l ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [u, $\bar{v},0$ ]]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]
8 k ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}+1/2$ [0,0,w]	3/4,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,3/4,z+1/2 [0,0, $\bar{w}$ ]
8 j ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
8 i ..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]
8 h .2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	0, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	0,y,3/4 [u,0, $\bar{w}$ ]
8 g 2'..	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	$\bar{x},0,3/4$ [0, $\bar{v},\bar{w}$ ]	x,0,3/4 [0,v, $\bar{w}$ ]
4 f ..2/m'	1/4,3/4,0 [0,0,0]	3/4,3/4,1/2 [0,0,0]		
4 e ..2/m'	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 d ..2/m'	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 c ..2/m'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
4 b 2'2'2	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0, $\bar{w}$ ]		
4 a 2'2'2	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a'}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,1/4

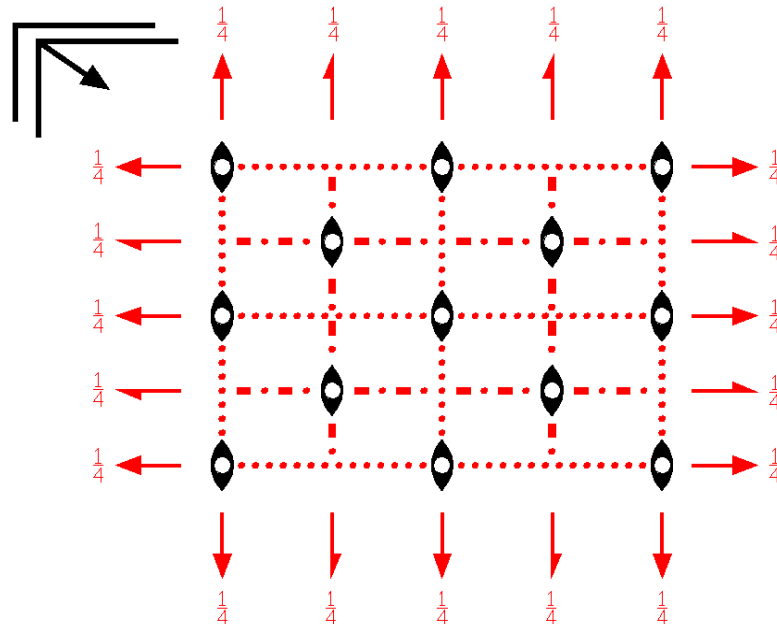
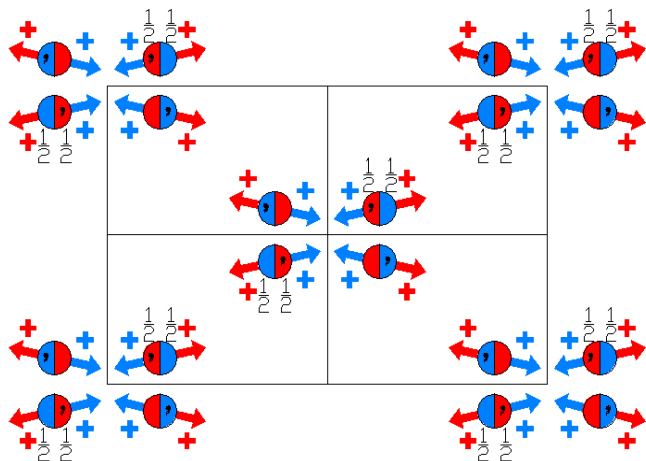
Along [0,1,0]  $p_{2a'}2m'm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



Cc'c'm  
66.5.568

m'm'm  
C2'/c'2'/c'2'/m

Orthorhombic



**Origin** at center ( $2/m$ ) at  $c'c'2'/m$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'         | (4) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (8) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                 | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)         | (3) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (4) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (7) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

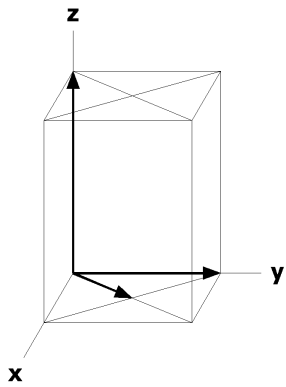
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 m 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
8 l ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0,w]
8 k ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}+1/2$ [0,0,w]	3/4,3/4, $\bar{z}$ [0,0,w]	1/4,3/4,z+1/2 [0,0,w]
8 j ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	0,1/2,z+1/2 [0,0,w]
8 i ..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0,w]
8 h .2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	0, $\bar{y},3/4$ [u,0,w]	0,y,3/4 [ $\bar{u},0,w$ ]
8 g 2'..	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	$\bar{x},0,3/4$ [0,v,w]	x,0,3/4 [0, $\bar{v},w$ ]
4 f ..2/m	1/4,3/4,0 [0,0,w]	3/4,3/4,1/2 [0,0,w]		
4 e ..2/m	1/4,1/4,0 [0,0,w]	3/4,1/4,1/2 [0,0,w]		
4 d ..2/m	0,1/2,0 [0,0,w]	0,1/2,1/2 [0,0,w]		
4 c ..2/m	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]		
4 b 2'2'2	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0,w]		
4 a 2'2'2	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

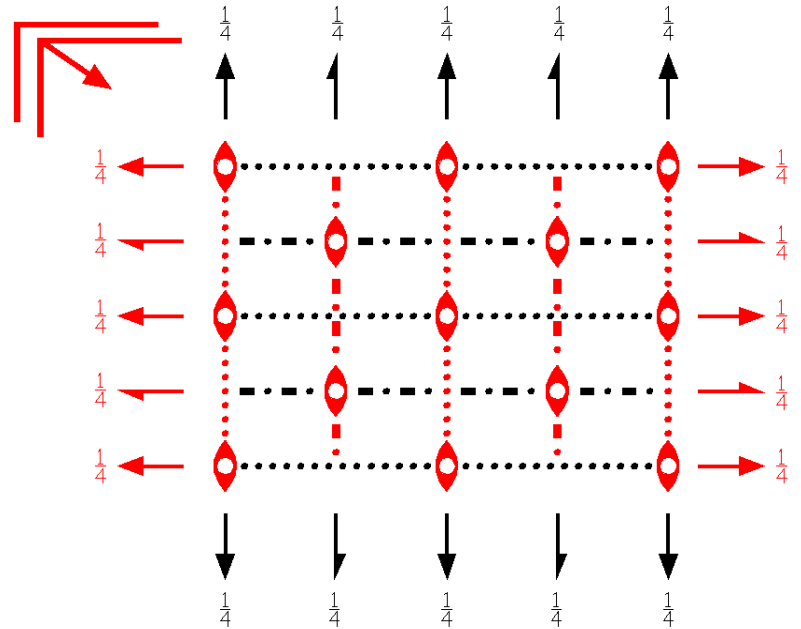
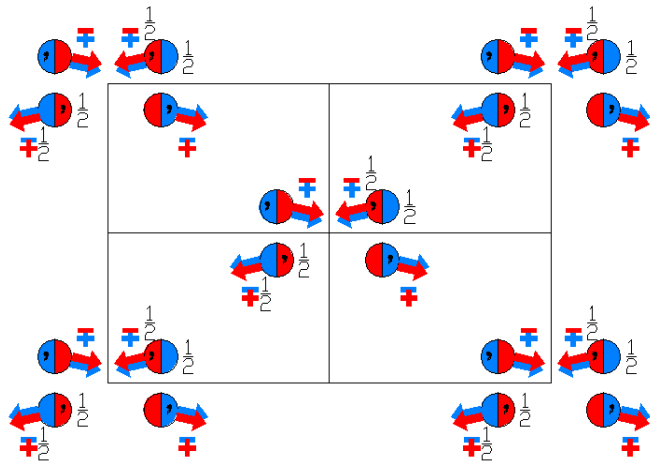
Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Ccc'm'  
66.6.569

mm'm'  
C2/c2'/c'2'/m'

Orthorhombic



**Origin** at center ( $2'/m'$ ) at  $cc'2'/m'$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |                                    |  |  |
|--|------------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $2'$ 0,y,1/4<br>( $2_y$  0,0,1/2)'         | (4) $2$ x,0,1/4<br>( $2_x$  0,0,1/2)         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) $m'$ x,y,0<br>( $m_z$  0,0,0)' | (7) $c'$ (0,0,1/2) x,0,z<br>( $m_y$  0,0,1/2)' | (8) $c$ (0,0,1/2) 0,y,z<br>( $m_x$  0,0,1/2) |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t$ (1/2,1/2,0)<br>(1 1/2,1/2,0)               | (2) $2'$ 1/4,1/4,z<br>( $2_z$  1/2,1/2,0)'         | (3) $2'$ (0,1/2,0) 1/4,y,1/4<br>( $2_y$  1/2,1/2,1/2)' | (4) $2$ (1/2,0,0) x,1/4,1/4<br>( $2_x$  1/2,1/2,1/2) |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) $n'$ (1/2,1/2,0) x,y,0<br>( $m_z$  1/2,1/2,0)' | (7) $n'$ (1/2,0,1/2) x,1/4,z<br>( $m_y$  1/2,1/2,1/2)' | (8) $n$ (0,1/2,1/2) 1/4,y,z<br>( $m_x$  1/2,1/2,1/2) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

### Positions

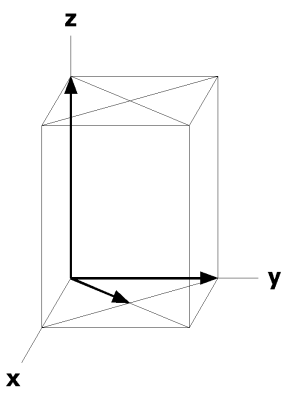
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 m 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v}$ ,w] (7) x, $\bar{y},z+1/2$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z+1/2$ [u, $\bar{v},\bar{w}$ ]
8 l ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,1/2$ [u,v,0]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
8 k ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}+1/2$ [u, $\bar{v}$ ,0]	3/4,3/4, $\bar{z}$ [u,v,0]	1/4,3/4,z+1/2 [u, $\bar{v}$ ,0]
8 j ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}+1/2$ [u, $\bar{v}$ ,0]	0,1/2, $\bar{z}$ [u,v,0]	0,1/2,z+1/2 [u, $\bar{v}$ ,0]
8 i ..2'	0,0,z [u,v,0]	0,0, $\bar{z}+1/2$ [u, $\bar{v}$ ,0]	0,0, $\bar{z}$ [u,v,0]	0,0,z+1/2 [u, $\bar{v}$ ,0]
8 h .2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [u,0, $\bar{w}$ ]	0, $\bar{y},3/4$ [u,0,w]	0,y,3/4 [u,0, $\bar{w}$ ]
8 g 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [u,0,0]	$\bar{x},0,3/4$ [u,0,0]	x,0,3/4 [u,0,0]
4 f ..2'/m'	1/4,3/4,0 [u,v,0]	3/4,3/4,1/2 [u, $\bar{v}$ ,0]		
4 e ..2'/m'	1/4,1/4,0 [u,v,0]	3/4,1/4,1/2 [u, $\bar{v}$ ,0]		
4 d ..2'/m'	0,1/2,0 [u,v,0]	0,1/2,1/2 [u, $\bar{v}$ ,0]		
4 c ..2'/m'	0,0,0 [u,v,0]	0,0,1/2 [u, $\bar{v}$ ,0]		
4 b 22'2'	0,1/2,1/4 [u,0,0]	0,1/2,3/4 [u,0,0]		
4 a 22'2'	0,0,1/4 [u,0,0]	0,0,3/4 [u,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'2mm  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



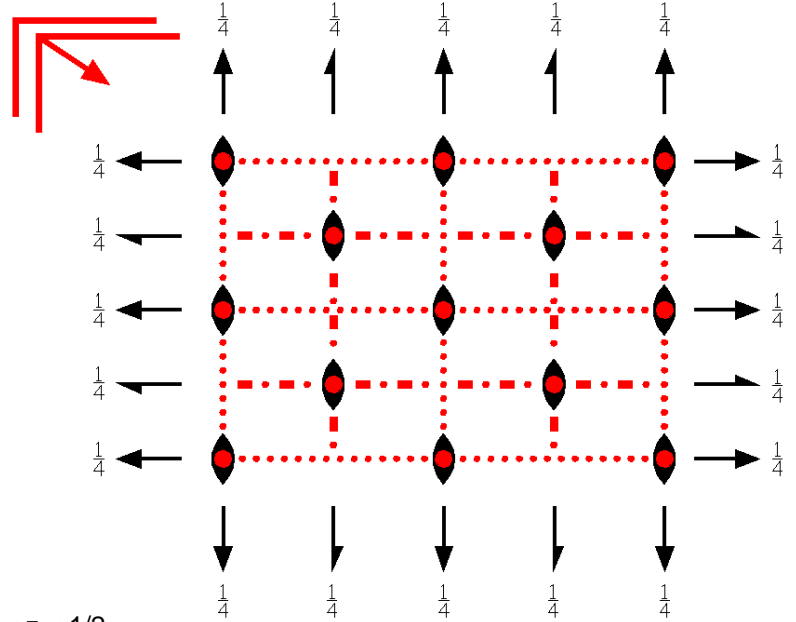
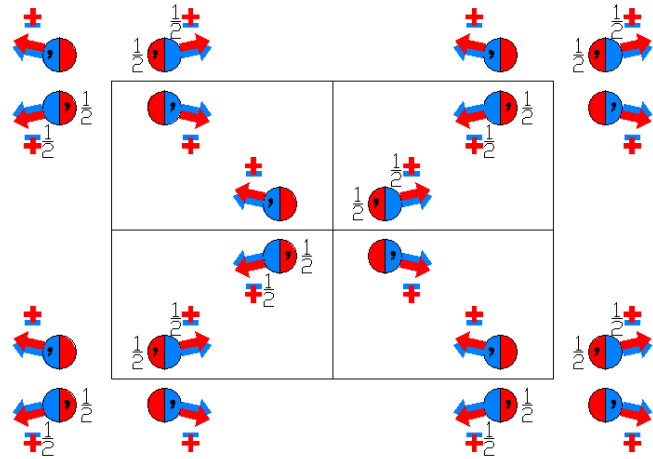
Cc'c'm'

66.7.570

m'm'm'

C2/c'2/c'2/m'

Orthorhombic



Origin at center ( $2/m'$ ) at  $c'c'2/m'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                          | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)           | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)           |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (8) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |

For (1/2,1/2,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                  | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)           | (3) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)   | (4) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)   |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (7) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

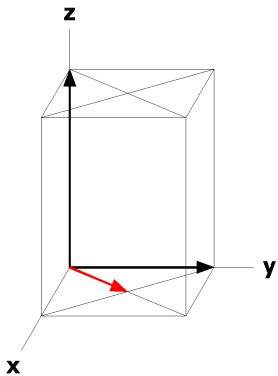
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 m 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
8 l ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	x, $\bar{y},1/2$ [u, $\bar{v},0$ ]
8 k ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	3/4,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,3/4,z+1/2 [0,0,w]
8 j ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0,w]
8 i ..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]
8 h .2.	0,y,1/4 [0,v,0]	0, $\bar{y},1/4$ [0, $\bar{v},0$ ]	0, $\bar{y},3/4$ [0, $\bar{v},0$ ]	0,y,3/4 [0,v,0]
8 g 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [u,0,0]
4 f ..2/m'	1/4,3/4,0 [0,0,0]	3/4,3/4,1/2 [0,0,0]		
4 e ..2/m'	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 d ..2/m'	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 c ..2/m'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
4 b 222	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]		
4 a 222	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

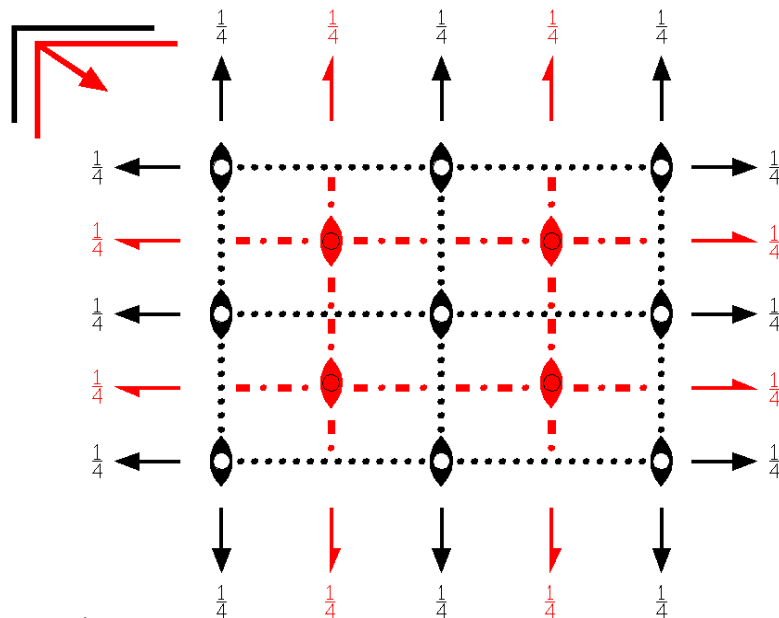
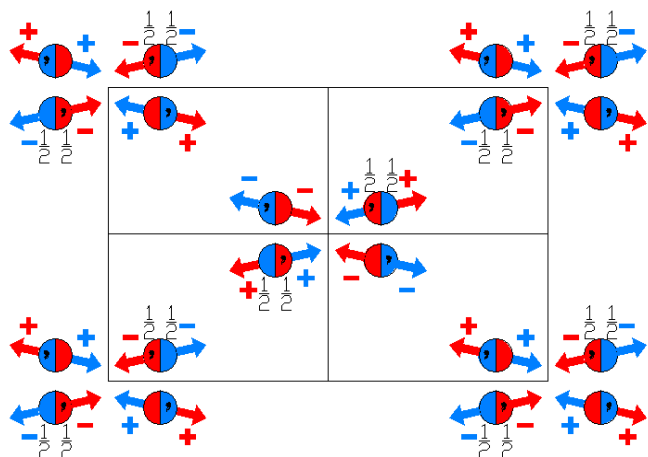
Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



$C_{pccm}$   
66.8.571

$mmm1'$   
 $C_{p2/c2/c2/m}$

Orthorhombic



**Origin** at center ( $2/m$ ) at  $cc2/m$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |                                  |  |  |
|--|----------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) 2 $0,y,1/4$<br>( $2_y$  0,0,1/2)           | (4) 2 $x,0,1/4$<br>( $2_x$  0,0,1/2)           |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0) | (6) m $x,y,0$<br>( $m_z$  0,0,0) | (7) c $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2) | (8) c $(0,0,1/2)$ $0,y,z$<br>( $m_x$  0,0,1/2) |

For  $(1/2,1/2,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,0)$<br>(1  $1/2,1/2,0$ )'               | (2) $2'$ $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,0$ )'           | (3) $2'$ $(0,1/2,0)$ $1/4,y,1/4$<br>( $2_y$   $1/2,1/2,1/2$ )' | (4) $2'$ $(1/2,0,0)$ $x,1/4,1/4$<br>( $2_x$   $1/2,1/2,1/2$ )' |
| (5) $\bar{1}'$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ )' | (6) $n'$ $(1/2,1/2,0)$ $x,y,0$<br>( $m_z$   $1/2,1/2,0$ )' | (7) $n'$ $(1/2,0,1/2)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,1/2$ )' | (8) $n'$ $(0,1/2,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,1/2$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

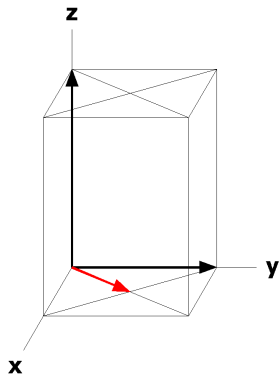
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 m 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]
8 l ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
8 k ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	3/4,3/4, $\bar{z}$ [u,v,0]	1/4,3/4,z+1/2 [ $\bar{u},v,0$ ]
8 j ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
8 i ..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]
8 h .2.	0,y,1/4 [0,v,0]	0, $\bar{y},1/4$ [0, $\bar{v},0$ ]	0, $\bar{y},3/4$ [0,v,0]	0,y,3/4 [0, $\bar{v},0$ ]
8 g 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [u,0,0]
4 f ..2'/m	1/4,3/4,0 [0,0,0]	3/4,3/4,1/2 [0,0,0]		
4 e ..2'/m	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 d ..2/m	0,1/2,0 [0,0,w]	0,1/2,1/2 [0,0, $\bar{w}$ ]		
4 c ..2/m	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		
4 b 222	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]		
4 a 222	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



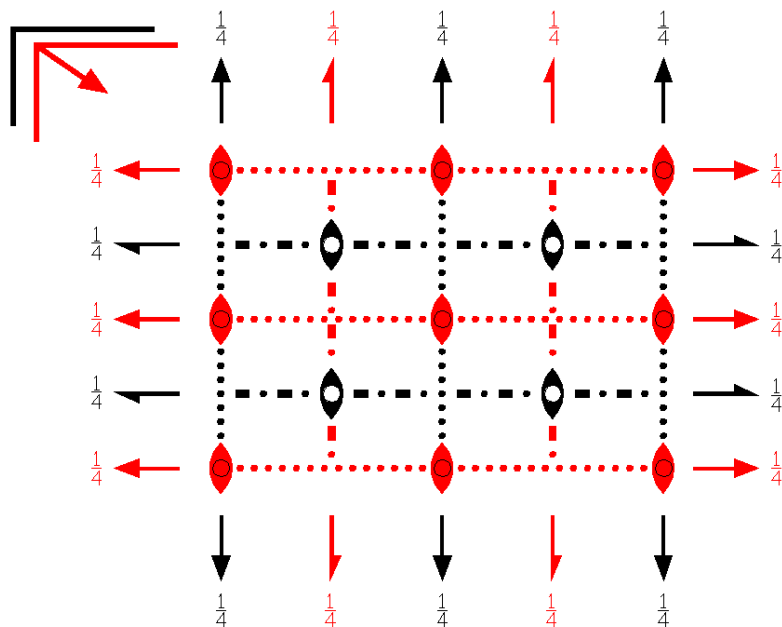
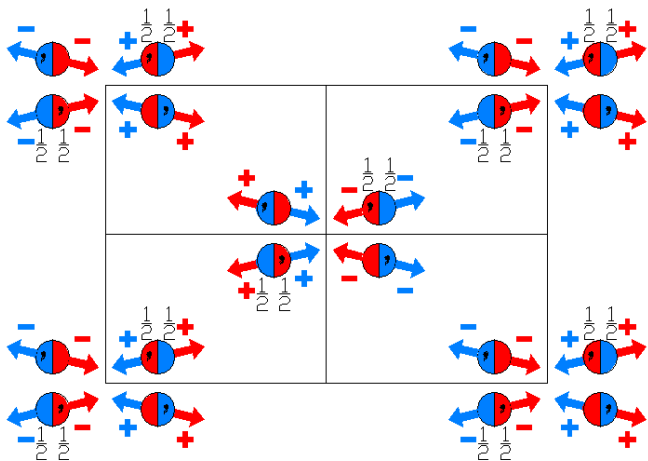
$C_{2v}cm$

66.9.572

$mmm1'$

$C_{2v}c2'/c2'/m$

Orthorhombic



**Origin** at center ( $2/m$ ) at  $c'c2'/m$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |   |                                    |  |  |
|---|------------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                          | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $2'$ 0,y,1/4<br>( $2_y$  0,0,1/2)'     | (4) $2$ x,0,1/4<br>( $2_x$  0,0,1/2)           |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m x,y,0<br>( $m_z$  0,0,0)     | (7) c (0,0,1/2) x,0,z<br>( $m_y$  0,0,1/2) | (8) $c'$ (0,0,1/2) 0,y,z<br>( $m_x$  0,0,1/2)' |

For (1/2,1/2,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (1/2,1/2,0)<br>(1 1/2,1/2,0)'             | (2) $2$ 1/4,1/4,z<br>( $2_z$  1/2,1/2,0)           | (3) $2$ (0,1/2,0) 1/4,y,1/4<br>( $2_y$  1/2,1/2,1/2)   | (4) $2'$ (1/2,0,0) x,1/4,1/4<br>( $2_x$  1/2,1/2,1/2)' |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) $n'$ (1/2,1/2,0) x,y,0<br>( $m_z$  1/2,1/2,0)' | (7) $n'$ (1/2,0,1/2) x,1/4,z<br>( $m_y$  1/2,1/2,1/2)' | (8) n (0,1/2,1/2) 1/4,y,z<br>( $m_x$  1/2,1/2,1/2)     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

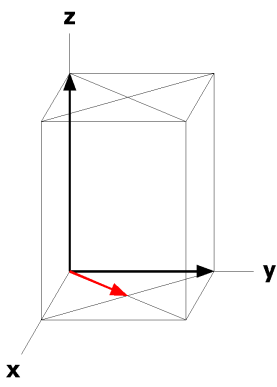
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 m 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
8 l ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
8 k ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}+1/2$ [0,0,w]	3/4,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,3/4,z+1/2 [0,0, $\bar{w}$ ]
8 j ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
8 i ..2'	0,0,z [u,v,0]	0,0, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	0,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	0,0,z+1/2 [ $\bar{u},v,0$ ]
8 h .2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [u,0, $\bar{w}$ ]	0, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	0,y,3/4 [ $\bar{u},0,w$ ]
8 g 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [u,0,0]	$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [ $\bar{u},0,0$ ]
4 f ..2/m'	1/4,3/4,0 [0,0,0]	3/4,3/4,1/2 [0,0,0]		
4 e ..2/m'	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 d ..2'/m	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 c ..2'/m	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
4 b 22'2'	0,1/2,1/4 [u,0,0]	0,1/2,3/4 [ $\bar{u},0,0$ ]		
4 a 22'2'	0,0,1/4 [u,0,0]	0,0,3/4 [ $\bar{u},0,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

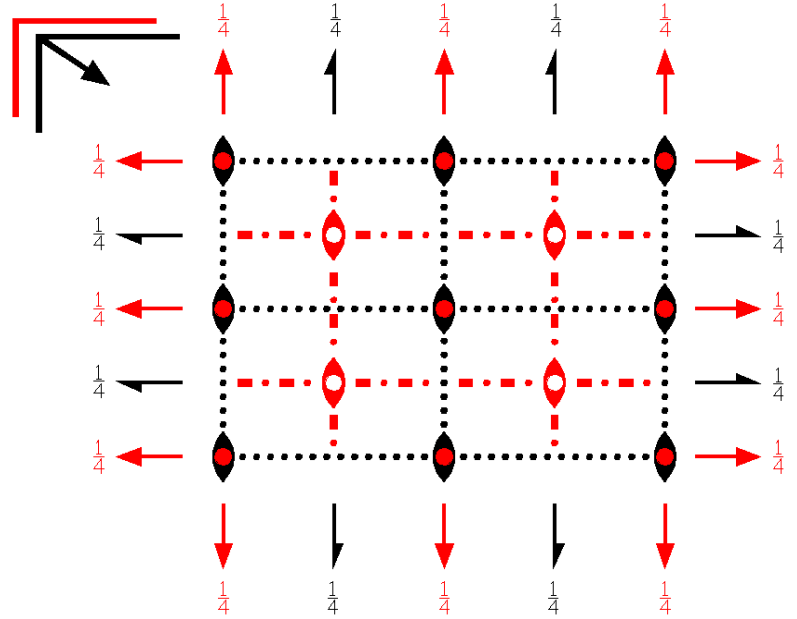
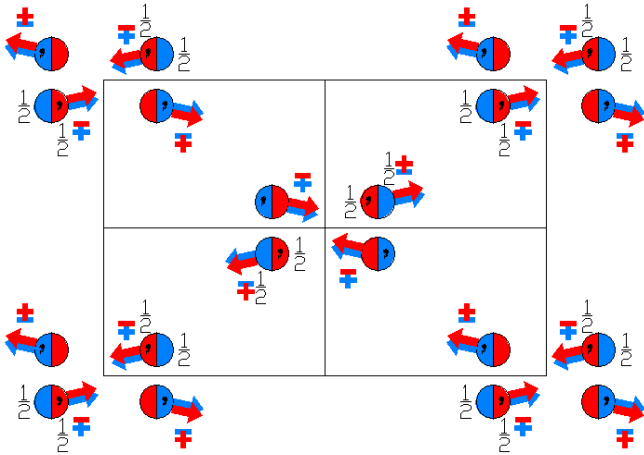
Along [0,1,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



$C_{pccm}'$   
66.10.573

$mmm1'$   
 $C_{p2'}'/c2'/c2'/m'$

Orthorhombic



**Origin** at center ( $2/m'$ ) at  $cc2/m'$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                          | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'       | (4) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'       |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (8) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) |

For (1/2,1/2,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1/2,1/2,0)<br>(1 1/2,1/2,0)'               | (2) 2' 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)'       | (3) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)   | (4) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)   |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (7) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

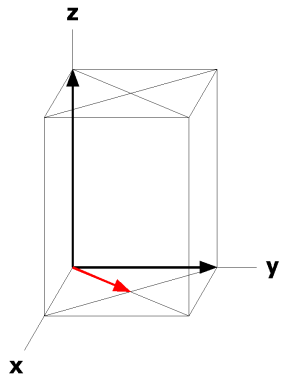
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1/2,1/2,0)' +	
16 m 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z+1/2$ [u, $\bar{v},\bar{w}$ ]
8 l ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [u, $\bar{v},0$ ]]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]
8 k ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	3/4,3/4, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,3/4,z+1/2 [ $\bar{u},v,0$ ]
8 j ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
8 i ..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]
8 h .2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	0, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	0,y,3/4 [u,0, $\bar{w}$ ]
8 g 2'..	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	$\bar{x},0,3/4$ [0, $\bar{v},\bar{w}$ ]	x,0,3/4 [0,v, $\bar{w}$ ]
4 f ..2'/m'	1/4,3/4,0 [u,v,0]	3/4,3/4,1/2 [u, $\bar{v},0$ ]		
4 e ..2'/m'	1/4,1/4,0 [u,v,0]	3/4,1/4,1/2 [u, $\bar{v},0$ ]		
4 d ..2'/m'	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 c ..2'/m'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
4 b 2'2'2	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0, $\bar{w}$ ]		
4 a 2'2'2	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a'</sub>2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,1/4

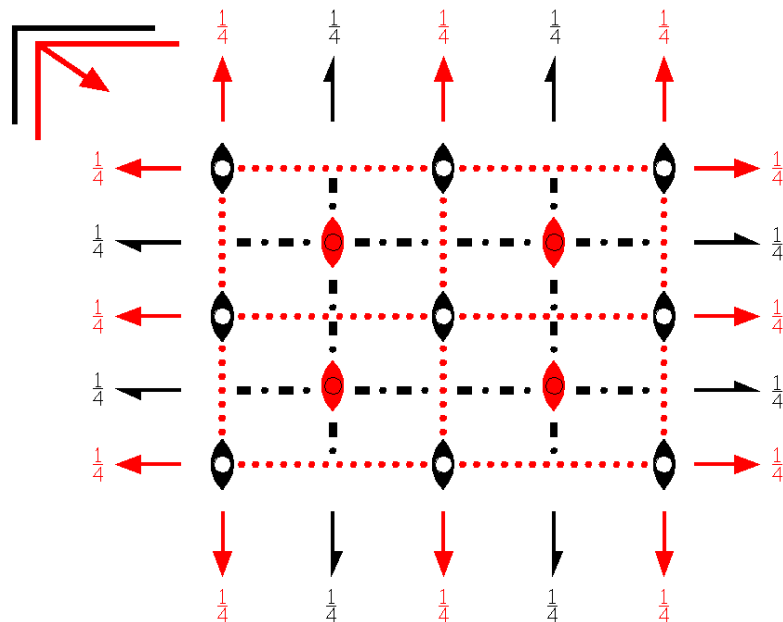
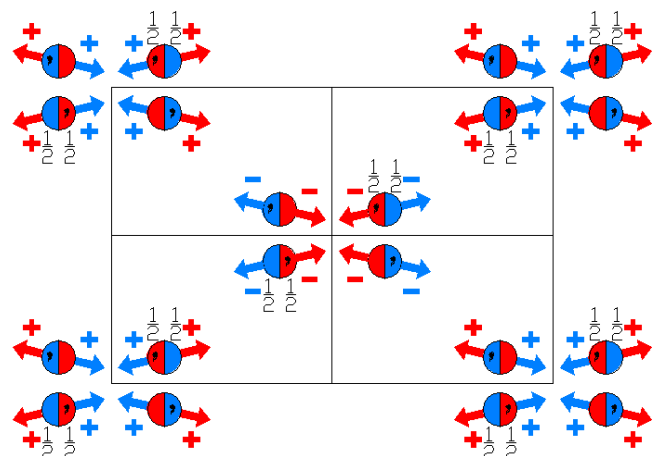
Along [0,1,0] p<sub>2a'</sub>2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



$C_p c' c' m$   
66.11.574

$m m m 1'$   
 $C_p 2' / c' 2' / c' 2' / m$

Orthorhombic



**Origin** at center ( $2/m$ ) at  $c'c'2'/m$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |                                      |   |   |   |
|--------------------------------------|---|---|---|
| (1) 1<br>(1 0,0,0)                   | (2) 2 <sub>0,0,z</sub><br>(2 <sub>z</sub>  0,0,0) | (3) 2' <sub>0,y,1/4</sub><br>(2 <sub>y</sub>  0,0,1/2)'   | (4) 2' <sub>x,0,1/4</sub><br>(2 <sub>x</sub>  0,0,1/2)'   |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) m <sub>x,y,0</sub><br>(m <sub>z</sub>  0,0,0) | (7) c' <sub>(0,0,1/2)</sub><br>(m <sub>y</sub>  0,0,1/2)' | (8) c' <sub>(0,0,1/2)</sub><br>(m <sub>x</sub>  0,0,1/2)' |

For (1/2,1/2,0)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) t' <sub>(1/2,1/2,0)</sub><br>(1 1/2,1/2,0)' | (2) 2' <sub>1/4,1/4,z</sub><br>(2 <sub>z</sub>  1/2,1/2,0)'   | (3) 2 <sub>(0,1/2,0)</sub><br>(2 <sub>y</sub>  1/2,1/2,1/2)   | (4) 2 <sub>(1/2,0,0)</sub><br>(2 <sub>x</sub>  1/2,1/2,1/2)   |
| (5) $\bar{1}$ '<br>( $\bar{1}$  1/2,1/2,0)'     | (6) n' <sub>(1/2,1/2,0)</sub><br>(m <sub>z</sub>  1/2,1/2,0)' | (7) n <sub>(1/2,0,1/2)</sub><br>(m <sub>y</sub>  1/2,1/2,1/2) | (8) n <sub>(0,1/2,1/2)</sub><br>(m <sub>x</sub>  1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

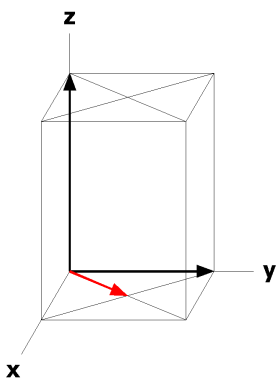
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1/2,1/2,0)' +	
16 m 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ] (8) $\bar{x},y,z+1/2$ [ $\bar{u},\bar{v},w$ ]
8 l ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0,w]
8 k ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}+1/2$ [ $\bar{u},\bar{v},0$ ]	3/4,3/4, $\bar{z}$ [u,v,0]	1/4,3/4,z+1/2 [ $\bar{u},\bar{v},0$ ]
8 j ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	0,1/2,z+1/2 [0,0,w]
8 i ..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0,w]
8 h .2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	0, $\bar{y},3/4$ [u,0,w]	0,y,3/4 [ $\bar{u},0,w$ ]
8 g 2'..	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	$\bar{x},0,3/4$ [0,v,w]	x,0,3/4 [0, $\bar{v},w$ ]
4 f ..2'/m	1/4,3/4,0 [0,0,0]	3/4,3/4,1/2 [0,0,0]		
4 e ..2'/m	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 d ..2/m	0,1/2,0 [0,0,w]	0,1/2,1/2 [0,0,w]		
4 c ..2/m	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]		
4 b 2'2'2	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0,w]		
4 a 2'2'2	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



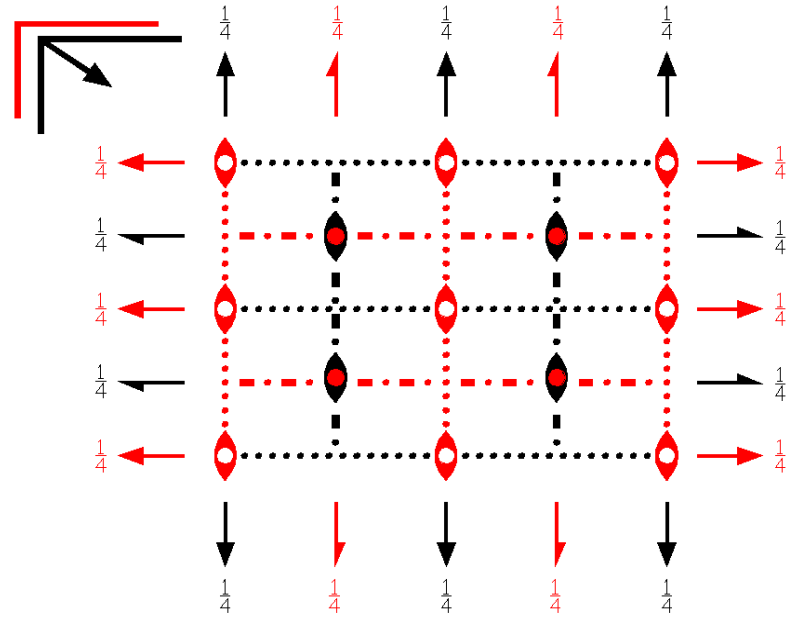
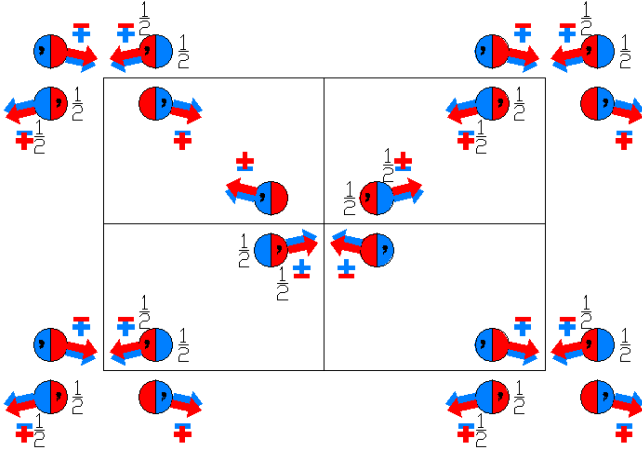
$C_{pcc}m'$

66.12.575

$mmm1'$

$C_{p2/c2'/c'2'/m'}$

Orthorhombic



**Origin** at center ( $2'/m'$ ) at  $cc'2'/m'$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |                                    |  |  |
|--|------------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $2'$ 0,y,1/4<br>( $2_y$  0,0,1/2)'         | (4) $2$ x,0,1/4<br>( $2_x$  0,0,1/2)         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) $m'$ x,y,0<br>( $m_z$  0,0,0)' | (7) $c'$ (0,0,1/2) x,0,z<br>( $m_y$  0,0,1/2)' | (8) $c$ (0,0,1/2) 0,y,z<br>( $m_x$  0,0,1/2) |

For (1/2,1/2,0)' + set

- |  |  |   |  |
|--|--|---|--|
| (1) $t'$ (1/2,1/2,0)<br>(1 1/2,1/2,0)'               | (2) $2$ 1/4,1/4,z<br>( $2_z$  1/2,1/2,0)         | (3) $2$ (0,1/2,0) 1/4,y,1/4<br>( $2_y$  1/2,1/2,1/2)' | (4) $2'$ (1/2,0,0) x,1/4,1/4<br>( $2_x$  1/2,1/2,1/2)' |
| (5) $\bar{1}'$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)' | (6) $n$ (1/2,1/2,0) x,y,0<br>( $m_z$  1/2,1/2,0) | (7) $n$ (1/2,0,1/2) x,1/4,z<br>( $m_y$  1/2,1/2,1/2)' | (8) $n'$ (0,1/2,1/2) 1/4,y,z<br>( $m_x$  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

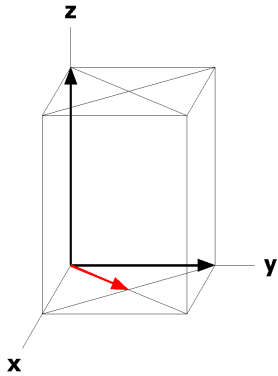
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1/2,1/2,0)' +	
16 m 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v}$ ,w] (7) x, $\bar{y},z+1/2$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z+1/2$ [u, $\bar{v},\bar{w}$ ]
8 l ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,1/2$ [u,v,0]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
8 k ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}+1/2$ [0,0,w]	3/4,3/4, $\bar{z}$ [0,0,w]	1/4,3/4,z+1/2 [0,0,w]
8 j ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}+1/2$ [u, $\bar{v}$ ,0]	0,1/2, $\bar{z}$ [u,v,0]	0,1/2,z+1/2 [u, $\bar{v}$ ,0]
8 i ..2'	0,0,z [u,v,0]	0,0, $\bar{z}+1/2$ [u, $\bar{v}$ ,0]	0,0, $\bar{z}$ [u,v,0]	0,0,z+1/2 [u, $\bar{v}$ ,0]
8 h .2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [u,0, $\bar{w}$ ]	0, $\bar{y},3/4$ [u,0,w]	0,y,3/4 [u,0, $\bar{w}$ ]
8 g 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [u,0,0]	$\bar{x},0,3/4$ [u,0,0]	x,0,3/4 [u,0,0]
4 f ..2/m'	1/4,3/4,0 [0,0,0]	3/4,3/4,1/2 [0,0,0]		
4 e ..2/m'	1/4,1/4,0 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 d ..2'/m'	0,1/2,0 [u,v,0]	0,1/2,1/2 [u, $\bar{v}$ ,0]		
4 c ..2'/m'	0,0,0 [u,v,0]	0,0,1/2 [u, $\bar{v}$ ,0]		
4 b 22'2'	0,1/2,1/4 [u,0,0]	0,1/2,3/4 [u,0,0]		
4 a 22'2'	0,0,1/4 [u,0,0]	0,0,3/4 [u,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'2mm  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

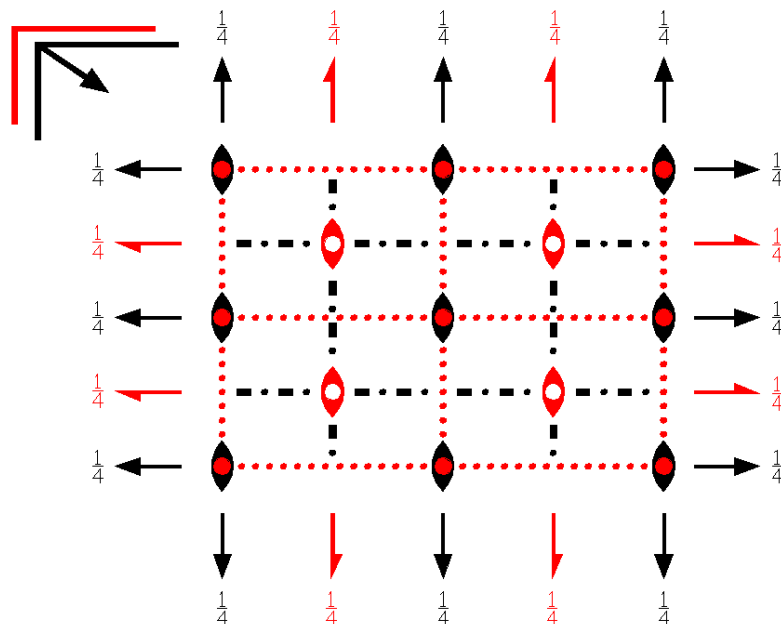
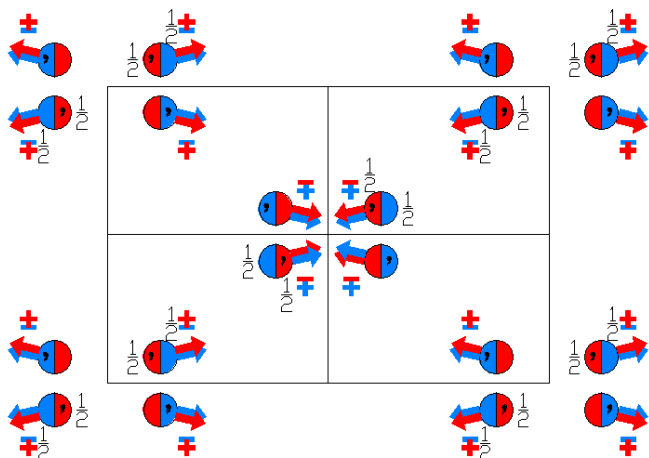
Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$C_{2v}c'c'm'$   
66.13.576

$mmm1'$   
 $C_{2v}c'c'2'/m'$

Orthorhombic



**Origin** at center ( $2/m$ ) at  $c'c'2'/m'$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |                                       |   |   |
|--|---------------------------------------|---|---|
| (1) 1<br>(1   0,0,0)                           | (2) 2 $0,0,z$<br>( $2_z$   0,0,0)     | (3) 2 $0,y,1/4$<br>( $2_y$   0,0,1/2)             | (4) 2 $x,0,1/4$<br>( $2_x$   0,0,1/2)             |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   0,0,0)' | (6) $m'$ $x,y,0$<br>( $m_z$   0,0,0)' | (7) $c'$ (0,0,1/2) $x,0,z$<br>( $m_y$   0,0,1/2)' | (8) $c'$ (0,0,1/2) $0,y,z$<br>( $m_x$   0,0,1/2)' |

For (1/2,1/2,0)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) $t'$ (1/2,1/2,0)<br>(1   1/2,1/2,0)'              | (2) $2'$ $1/4,1/4,z$<br>( $2_z$   1/2,1/2,0)'       | (3) $2'$ (0,1/2,0) $1/4,y,1/4$<br>( $2_y$   1/2,1/2,1/2)' | (4) $2'$ (1/2,0,0) $x,1/4,1/4$<br>( $2_x$   1/2,1/2,1/2)' |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   1/2,1/2,0) | (6) $n$ (1/2,1/2,0) $x,y,0$<br>( $m_z$   1/2,1/2,0) | (7) $n$ (1/2,0,1/2) $x,1/4,z$<br>( $m_y$   1/2,1/2,1/2)   | (8) $n$ (0,1/2,1/2) $1/4,y,z$<br>( $m_x$   1/2,1/2,1/2)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

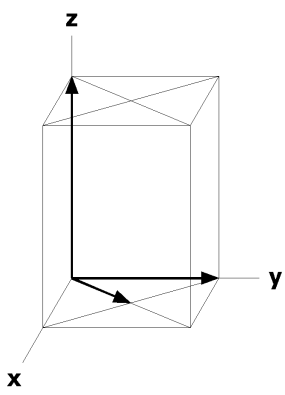
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 m 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ] (7) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
8 l ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	x, $\bar{y},1/2$ [u, $\bar{v},0$ ]
8 k ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	3/4,3/4, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,3/4,z+1/2 [u, $\bar{v},0$ ]
8 j ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0,w]
8 i ..2	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]
8 h .2.	0,y,1/4 [0,v,0]	0, $\bar{y},1/4$ [0, $\bar{v},0$ ]	0, $\bar{y},3/4$ [0, $\bar{v},0$ ]	0,y,3/4 [0,v,0]
8 g 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [u,0,0]
4 f ..2'/m'	1/4,3/4,0 [u,v,0]	3/4,3/4,1/2 [ $\bar{u},v,0$ ]		
4 e ..2'/m'	1/4,1/4,0 [u,v,0]	3/4,1/4,1/2 [ $\bar{u},v,0$ ]		
4 d ..2/m'	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 c ..2/m'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
4 b 222	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]		
4 a 222	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

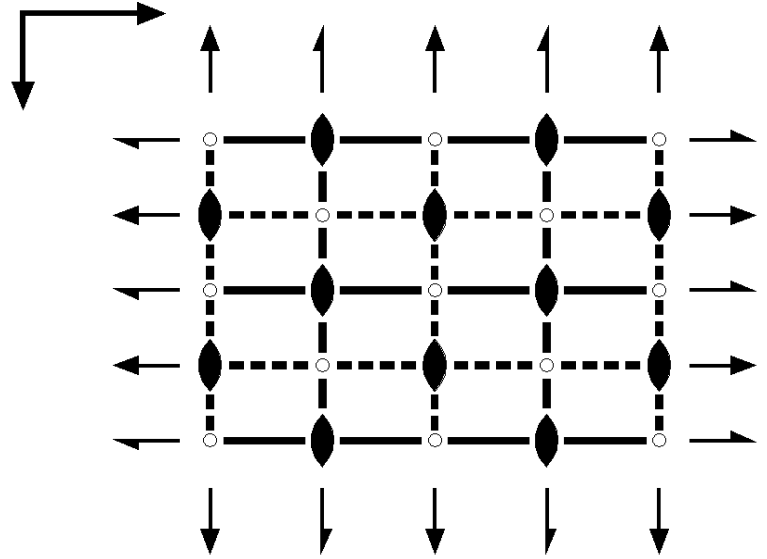
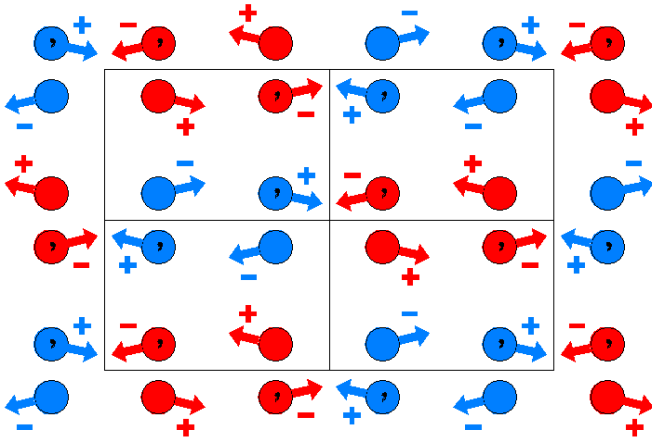
Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Cmma  
67.1.577

mmm  
C2/m2/m2/a

Orthorhombic



Origin at center ( 2/m ) at  $2/m2_1/a$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                        | (2) 2 $1/4,0,z$<br>(2 <sub>z</sub>   1/2,0,0)         | (3) 2 $1/4,y,0$<br>(2 <sub>y</sub>   1/2,0,0)         | (4) 2 $x,0,0$<br>(2 <sub>x</sub>   0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0) | (6) a (1/2,0,0) $x,y,0$<br>(m <sub>z</sub>   1/2,0,0) | (7) a (1/2,0,0) $x,0,z$<br>(m <sub>y</sub>   1/2,0,0) | (8) m 0,y,z<br>(m <sub>x</sub>   0,0,0)   |

For (1/2,1/2,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                  | (2) 2 $0,1/4,z$<br>(2 <sub>z</sub>   0,1/2,0)         | (3) 2 (0,1/2,0) $0,y,0$<br>(2 <sub>y</sub>   0,1/2,0) | (4) 2 (1/2,0,0) $x,1/4,0$<br>(2 <sub>x</sub>   1/2,1/2,0) |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   1/2,1/2,0) | (6) b (0,1/2,0) $x,y,0$<br>(m <sub>z</sub>   0,1/2,0) | (7) m $x,1/4,z$<br>(m <sub>y</sub>   0,1/2,0)         | (8) b (0,1/2,0) $1/4,y,z$<br>(m <sub>x</sub>   1/2,1/2,0) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

### Positions

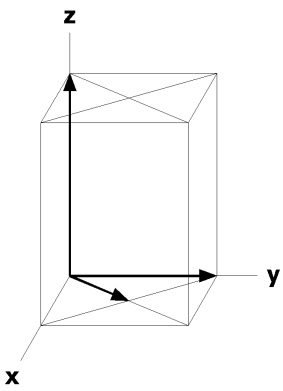
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1/2,1/2,0) +	
16 o 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) $x+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x+1/2,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
8 n .m.	x,1/4,z [0,v,0]	$\bar{x},1/4,z$ [0, $\bar{v}$ ,0]	$\bar{x},3/4,\bar{z}$ [0,v,0]	x,3/4, $\bar{z}$ [0, $\bar{v}$ ,0]
8 m m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z$ [ $\bar{u},0,0$ ]	0,y+1/2, $\bar{z}$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]
8 l ..2	1/4,0,z [0,0,w]	3/4,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	3/4,0, $\bar{z}$ [0,0,w]	1/4,1/2,z [0,0, $\bar{w}$ ]
8 k .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y}+1/2,1/2$ [0, $\bar{v}$ ,0]	3/4, $\bar{y},1/2$ [0,v,0]	1/4,y+1/2,1/2 [0, $\bar{v}$ ,0]
8 j .2.	1/4,y,0 [0,v,0]	3/4, $\bar{y}+1/2,0$ [0, $\bar{v}$ ,0]	3/4, $\bar{y},0$ [0,v,0]	1/4,y+1/2,0 [0, $\bar{v}$ ,0]
8 i 2..	x,0,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},0,1/2$ [u,0,0]	x,1/2,1/2 [ $\bar{u},0,0$ ]
8 h 2..	x,0,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	$\bar{x},0,0$ [u,0,0]	x,1/2,0 [ $\bar{u},0,0$ ]
4 g mm2	0,1/4,z [0,0,0]	0,3/4, $\bar{z}$ [0,0,0]		
4 f .2/m.	1/4,1/4,1/2 [0,v,0]	3/4,1/4,1/2 [0, $\bar{v}$ ,0]		
4 e .2/m.	1/4,1/4,0 [0,v,0]	3/4,1/4,0 [0, $\bar{v}$ ,0]		
4 d 2/m..	0,0,1/2 [u,0,0]	0,1/2,1/2 [ $\bar{u},0,0$ ]		
4 c 2/m..	0,0,0 [u,0,0]	0,1/2,0 [ $\bar{u},0,0$ ]		
4 b 222	1/4,0,1/2 [0,0,0]	3/4,0,1/2 [0,0,0]		
4 a 222	1/4,0,0 [0,0,0]	3/4,0,0 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1]  $p_c-2mm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,1/4,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a}-2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,0



Cmma1'

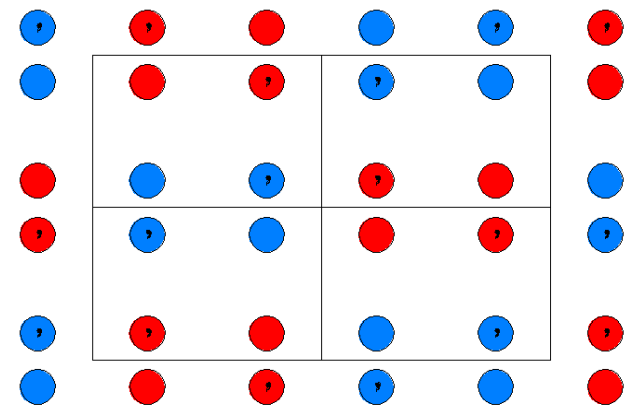
67.2.578

mmm1'

C2/m2/m2/a1'

Orthorhombic

1'



Origin at center ( $2/m1'$ ) at  $2/m2_1/aa1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |                                      |
|--|--|--|--------------------------------------|
| (1) 1<br>(1 0,0,0)                               | (2) 2 $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )             | (3) 2 $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )             | (4) 2 $x,0,0$<br>( $2_x$   $0,0,0$ ) |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ ) | (6) a ( $1/2,0,0$ ) $x,y,0$<br>( $m_z$   $1/2,0,0$ ) | (7) a ( $1/2,0,0$ ) $x,0,z$<br>( $m_y$   $1/2,0,0$ ) | (8) m $0,y,z$<br>( $m_x$   $0,0,0$ ) |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t ( $1/2,1/2,0$ )<br>(1  $1/2,1/2,0$ )               | (2) 2 $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )             | (3) 2 ( $0,1/2,0$ ) $0,y,0$<br>( $2_y$   $0,1/2,0$ ) | (4) 2 ( $1/2,0,0$ ) $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ ) |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ ) | (6) b ( $0,1/2,0$ ) $x,y,0$<br>( $m_z$   $0,1/2,0$ ) | (7) m $x,1/4,z$<br>( $m_y$   $0,1/2,0$ )             | (8) b ( $0,1/2,0$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ ) |

For (0,0,0)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1'<br>(1  $0,0,0$ )'                            | (2) 2' $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )'             | (3) 2' $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )'             | (4) 2' $x,0,0$<br>( $2_x$   $0,0,0$ )' |
| (5) $\bar{1}$ ' $0,0,0$<br>( $\bar{1}$   $0,0,0$ )' | (6) a' ( $1/2,0,0$ ) $x,y,0$<br>( $m_z$   $1/2,0,0$ )' | (7) a' ( $1/2,0,0$ ) $x,0,z$<br>( $m_y$   $1/2,0,0$ )' | (8) m' $0,y,z$<br>( $m_x$   $0,0,0$ )' |

For (1/2,1/2,0)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' ( $1/2,1/2,0$ )<br>(1  $1/2,1/2,0$ )'                | (2) 2' $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )'             | (3) 2' ( $0,1/2,0$ ) $0,y,0$<br>( $2_y$   $0,1/2,0$ )' | (4) 2' ( $1/2,0,0$ ) $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )' |
| (5) $\bar{1}$ ' $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ )' | (6) b' ( $0,1/2,0$ ) $x,y,0$<br>( $m_z$   $0,1/2,0$ )' | (7) m' $x,1/4,z$<br>( $m_y$   $0,1/2,0$ )'             | (8) b' ( $0,1/2,0$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5);1'.

**Positions**

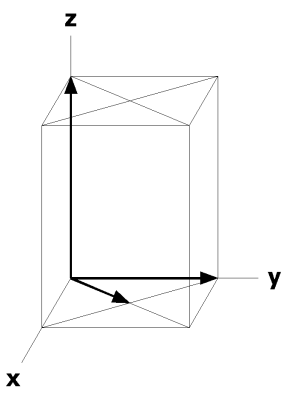
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) + (0,0,0)' +	(1/2,1/2,0) + (1/2,1/2,0)' +		
16 o 11'	(1) x,y,z [0,0,0] (5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(2) $\bar{x}+1/2,\bar{y},z$ [0,0,0] (6) $x+1/2,y,\bar{z}$ [0,0,0]	(3) $\bar{x}+1/2,y,\bar{z}$ [0,0,0] (7) $x+1/2,\bar{y},z$ [0,0,0]	(4) $x,\bar{y},\bar{z}$ [0,0,0] (8) $\bar{x},y,z$ [0,0,0]
8 n .m.1'	x,1/4,z [0,0,0]	$\bar{x},1/4,z$ [0,0,0]	$\bar{x},3/4,\bar{z}$ [0,0,0]	x,3/4, $\bar{z}$ [0,0,0]
8 m m..1'	0,y,z [0,0,0]	$0,\bar{y}+1/2,z$ [0,0,0]	0,y+1/2, $\bar{z}$ [0,0,0]	$0,\bar{y},\bar{z}$ [0,0,0]
8 l ..21'	1/4,0,z [0,0,0]	3/4,1/2, $\bar{z}$ [0,0,0]	3/4,0, $\bar{z}$ [0,0,0]	1/4,1/2,z [0,0,0]
8 k .2.1'	1/4,y,1/4 [0,0,0]	3/4, $\bar{y}+1/2,1/2$ [0,0,0]	3/4, $\bar{y},1/2$ [0,0,0]	1/4,y+1/2,1/2 [0,0,0]
8 j .2.1'	1/4,y,0 [0,0,0]	3/4, $\bar{y}+1/2,0$ [0,0,0]	3/4, $\bar{y},0$ [0,0,0]	1/4,y+1/2,0 [0,0,0]
8 i 2..1'	x,0,1/2 [0,0,0]	$\bar{x},1/2,1/2$ [0,0,0]	$\bar{x},0,1/2$ [0,0,0]	x,1/2,1/2 [0,0,0]
8 h 2..1'	x,0,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]	$\bar{x},0,0$ [0,0,0]	x,1/2,0 [0,0,0]
4 g mm21'	0,1/4,z [0,0,0]	0,3/4, $\bar{z}$ [0,0,0]		
4 f .2/m.1'	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 e .2/m.1'	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
4 d 2/m..1'	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 c 2/m..1'	0,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
4 b 2221'	1/4,0,1/2 [0,0,0]	3/4,0,1/2 [0,0,0]		
4 a 2221'	1/4,0,0 [0,0,0]	3/4,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

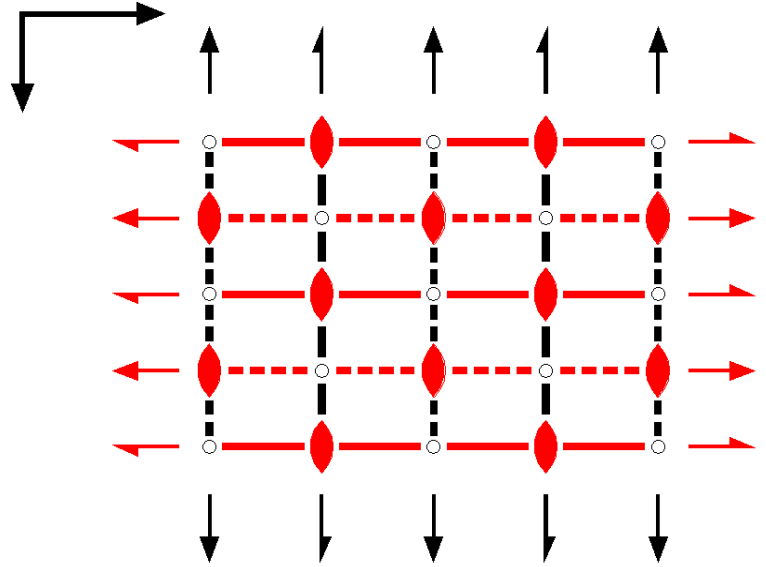
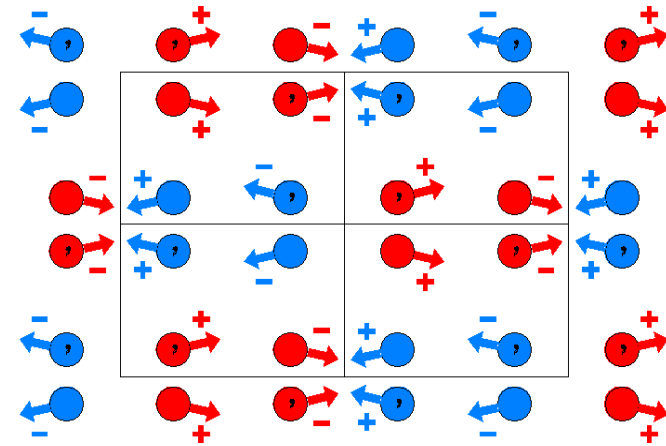
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Cm'ma  
67.3.579

m'mm  
C2/m'2'/m2'/a

Orthorhombic



Origin at center ( $2/m'$ ) at  $2/m'2_1/a$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) $2'_z$ $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )'       | (3) $2'_y$ $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )'       | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)       |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)' | (6) a ( $1/2,0,0$ ) $x,y,0$<br>( $m_z$   $1/2,0,0$ ) | (7) a ( $1/2,0,0$ ) $x,0,z$<br>( $m_y$   $1/2,0,0$ ) | (8) $m'_x$ $0,y,z$<br>( $m_x$  0,0,0)' |

For (1/2,1/2,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t$ ( $1/2,1/2,0$ )<br>(1  $1/2,1/2,0$ )              | (2) $2'_z$ $0,1/4,z$<br>( $2_z$  0,1/2,0)'       | (3) $2'_y$ ( $0,1/2,0$ ) $0,y,0$<br>( $2_y$  0,1/2,0)' | (4) 2 ( $1/2,0,0$ ) $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )   |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ )' | (6) b ( $0,1/2,0$ ) $x,y,0$<br>( $m_z$  0,1/2,0) | (7) m $x,1/4,z$<br>( $m_y$  0,1/2,0)                   | (8) b' ( $0,1/2,0$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

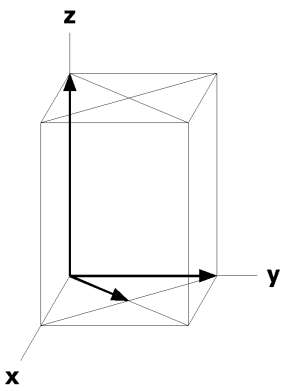
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1/2,1/2,0) +	
16 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [ $u,v,\bar{w}$ ] (6) $x+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y,\bar{z}$ [ $u,\bar{v},w$ ] (7) $x+1/2,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 n .m.	x,1/4,z [0,v,0]	$\bar{x},1/4,z$ [0,v,0]	$\bar{x},3/4,\bar{z}$ [0, $\bar{v}$ ,0]	x,3/4, $\bar{z}$ [0, $\bar{v}$ ,0]
8 m m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z$ [0,v, $\bar{w}$ ]	0,y+1/2, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 l ..2'	1/4,0,z [u,v,0]	3/4,1/2, $\bar{z}$ [ $u,\bar{v},0$ ]	3/4,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,1/2,z [ $\bar{u},v,0$ ]
8 k .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,1/2$ [ $u,0,\bar{w}$ ]	3/4, $\bar{y},1/2$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,1/2 [ $\bar{u},0,w$ ]
8 j .2'	1/4,y,0 [u,0,w]	3/4, $\bar{y}+1/2,0$ [ $u,0,\bar{w}$ ]	3/4, $\bar{y},0$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,0 [ $\bar{u},0,w$ ]
8 i 2..	x,0,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	x,1/2,1/2 [ $\bar{u},0,0$ ]
8 h 2..	x,0,0 [u,0,0]	$\bar{x},1/2,0$ [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	x,1/2,0 [ $\bar{u},0,0$ ]
4 g m'm2'	0,1/4,z [0,v,0]	0,3/4, $\bar{z}$ [0, $\bar{v},0$ ]		
4 f .2'/m.	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 e .2'/m.	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
4 d 2/m'..	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 c 2/m'..	0,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
4 b 22'2'	1/4,0,1/2 [u,0,0]	3/4,0,1/2 [ $\bar{u},0,0$ ]		
4 a 22'2'	1/4,0,0 [u,0,0]	3/4,0,0 [ $\bar{u},0,0$ ]		

### Symmetry of Special Projections

Along [0,0,1]  $p_c$ -2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

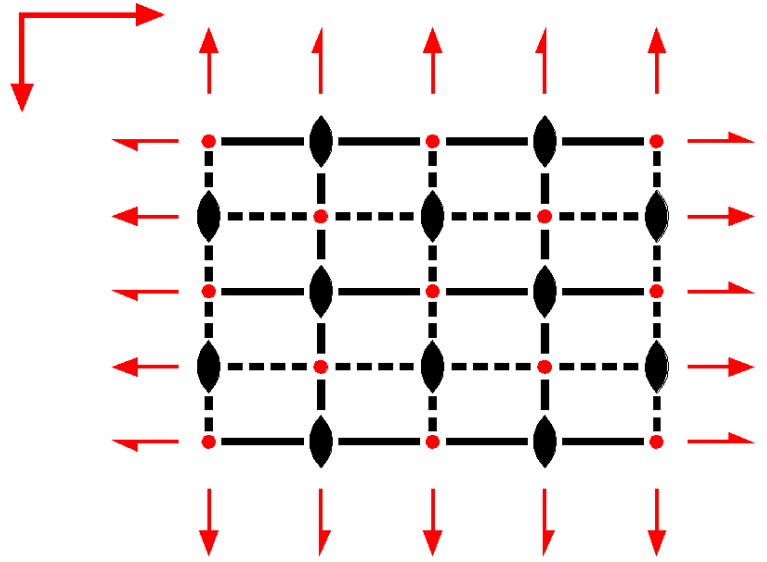
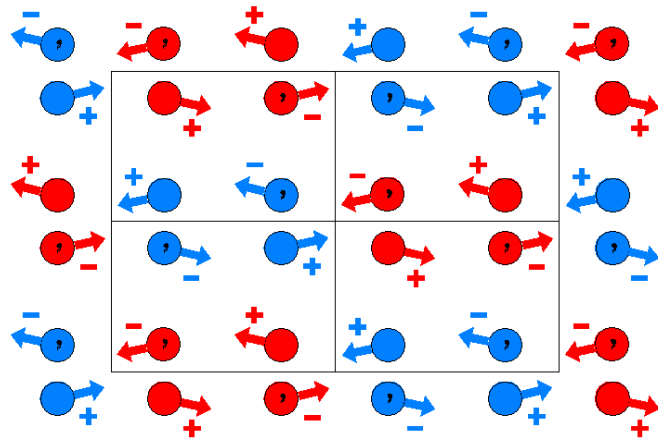
Along [0,1,0]  $p_{2a}$ -2m'm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Cmma'  
67.4.580

mmm'  
C2'/m2'/m2/a'

Orthorhombic



Origin at center ( $2/m$ ) at  $2'/m2, 1/aa'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                                | (2) 2 $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )               | (3) 2' $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )'           | (4) 2' $x,0,0$<br>( $2_x$   $0,0,0$ )' |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ )' | (6) a' ( $1/2,0,0$ ) $x,y,0$<br>( $m_z$   $1/2,0,0$ )' | (7) a ( $1/2,0,0$ ) $x,0,z$<br>( $m_y$   $1/2,0,0$ ) | (8) m $0,y,z$<br>( $m_x$   $0,0,0$ )   |

For (1/2,1/2,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t ( $1/2,1/2,0$ )<br>(1  $1/2,1/2,0$ )                | (2) 2 $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )               | (3) 2' ( $0,1/2,0$ ) $0,y,0$<br>( $2_y$   $0,1/2,0$ )' | (4) 2' ( $1/2,0,0$ ) $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )' |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ )' | (6) b' ( $0,1/2,0$ ) $x,y,0$<br>( $m_z$   $0,1/2,0$ )' | (7) m $x,1/4,z$<br>( $m_y$   $0,1/2,0$ )               | (8) b ( $0,1/2,0$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

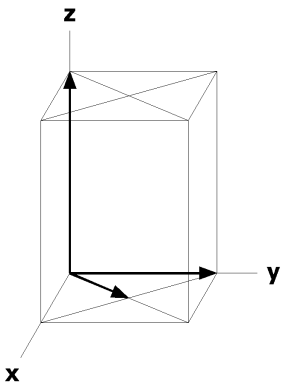
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1/2,1/2,0) +	
16 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(3) $\bar{x}+1/2,y,\bar{z}$ [ $u,\bar{v},w$ ] (7) $x+1/2,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
8 n .m.	x,1/4,z [0,v,0]	$\bar{x},1/4,z$ [0, $\bar{v}$ ,0]	$\bar{x},3/4,\bar{z}$ [0, $\bar{v}$ ,0]	x,3/4, $\bar{z}$ [0,v,0]
8 m m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z$ [ $\bar{u},0,0$ ]	0,y+1/2, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
8 l ..2	1/4,0,z [0,0,w]	3/4,1/2, $\bar{z}$ [0,0,w]	3/4,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,1/2,z [0,0, $\bar{w}$ ]
8 k .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,1/2$ [ $\bar{u},0,w$ ]	3/4, $\bar{y},1/2$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,1/2 [u,0, $\bar{w}$ ]
8 j .2'	1/4,y,0 [u,0,w]	3/4, $\bar{y}+1/2,0$ [ $\bar{u},0,w$ ]	3/4, $\bar{y},0$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,0 [u,0, $\bar{w}$ ]
8 i 2'..	x,0,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0, $\bar{v},w$ ]	$\bar{x},0,1/2$ [0, $\bar{v},\bar{w}$ ]	x,1/2,1/2 [0,v, $\bar{w}$ ]
8 h 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,0$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0, $\bar{v},\bar{w}$ ]	x,1/2,0 [0,v, $\bar{w}$ ]
4 g mm2	0,1/4,z [0,0,0]	0,3/4, $\bar{z}$ [0,0,0]		
4 f .2'/m.	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 e .2'/m.	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
4 d 2'/m..	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 c 2'/m..	0,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
4 b 2'2'2	1/4,0,1/2 [0,0,w]	3/4,0,1/2 [0,0, $\bar{w}$ ]		
4 a 2'2'2	1/4,0,0 [0,0,w]	3/4,0,0 [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

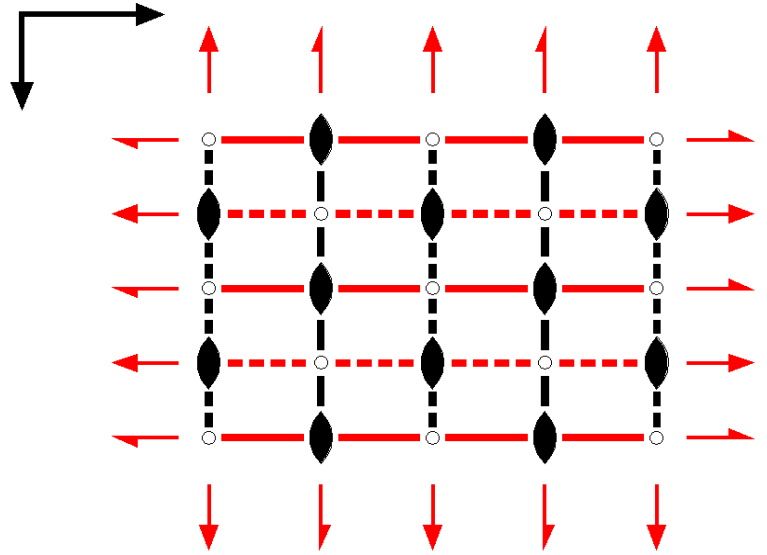
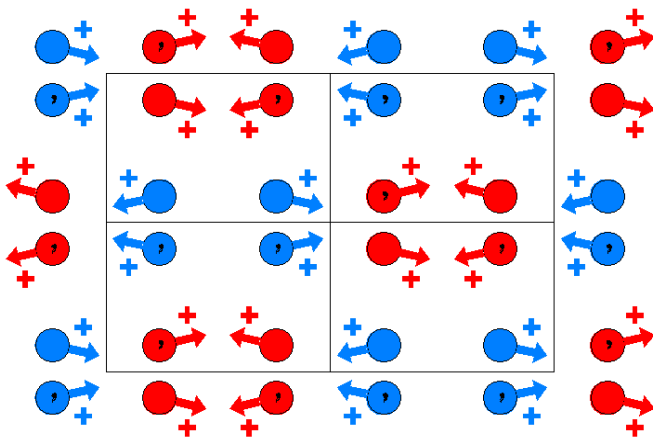
Along [0,1,0] p<sub>2a</sub>'2mm  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



Cm'm'a  
67.5.581

m'm'm  
C2'/m'2'/m'2'/a

Orthorhombic



**Origin** at center ( $2'/m'$ ) at  $2'/m'2',/a'a$

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )             | (3) 2' $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )'             | (4) 2' $x,0,0$<br>( $2_x$   $0,0,0$ )' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a ( $1/2,0,0$ ) $x,y,0$<br>( $m_z$   $1/2,0,0$ ) | (7) a' ( $1/2,0,0$ ) $x,0,z$<br>( $m_y$   $1/2,0,0$ )' | (8) m' $0,y,z$<br>( $m_x$   $0,0,0$ )' |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t ( $1/2,1/2,0$ )<br>(1  $1/2,1/2,0$ )               | (2) 2 $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )             | (3) 2' ( $0,1/2,0$ ) $0,y,0$<br>( $2_y$   $0,1/2,0$ )' | (4) 2' ( $1/2,0,0$ ) $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )' |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ ) | (6) b ( $0,1/2,0$ ) $x,y,0$<br>( $m_z$   $0,1/2,0$ ) | (7) m' $x,1/4,z$<br>( $m_y$   $0,1/2,0$ )'             | (8) b' ( $0,1/2,0$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

### Positions

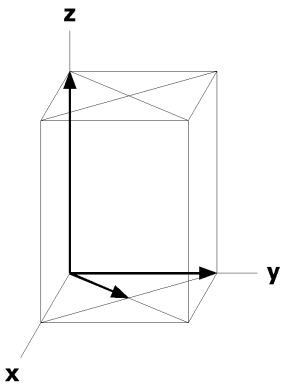
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ] (7) $x+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(4) $x,\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ] (8) $\bar{x},y,z$ [ $\bar{u},\bar{v},w$ ]
8 n .m'	x,1/4,z [u,0,w]	$\bar{x},1/4,z$ [ $\bar{u},0,w$ ]	$\bar{x},3/4,\bar{z}$ [u,0,w]	x,3/4, $\bar{z}$ [ $\bar{u},0,w$ ]
8 m m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z$ [0, $\bar{v},w$ ]	0,y+1/2, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
8 l ..2	1/4,0,z [0,0,w]	3/4,1/2, $\bar{z}$ [0,0,w]	3/4,0, $\bar{z}$ [0,0,w]	1/4,1/2,z [0,0,w]
8 k .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,1/2$ [ $\bar{u},0,w$ ]	3/4, $\bar{y},1/2$ [u,0,w]	1/4,y+1/2,1/2 [ $\bar{u},0,w$ ]
8 j .2'	1/4,y,0 [u,0,w]	3/4, $\bar{y}+1/2,0$ [ $\bar{u},0,w$ ]	3/4, $\bar{y},0$ [u,0,w]	1/4,y+1/2,0 [ $\bar{u},0,w$ ]
8 i 2'..	x,0,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0, $\bar{v},w$ ]	$\bar{x},0,1/2$ [0,v,w]	x,1/2,1/2 [0, $\bar{v},w$ ]
8 h 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,0$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0,v,w]	x,1/2,0 [0, $\bar{v},w$ ]
4 g m'm'2	0,1/4,z [0,0,w]	0,3/4, $\bar{z}$ [0,0,w]		
4 f .2'/m'	1/4,1/4,1/2 [u,0,w]	3/4,1/4,1/2 [ $\bar{u},0,w$ ]		
4 e .2'/m'	1/4,1/4,0 [u,0,w]	3/4,1/4,0 [ $\bar{u},0,w$ ]		
4 d 2'/m'..	0,0,1/2 [0,v,w]	0,1/2,1/2 [0, $\bar{v},w$ ]		
4 c 2'/m'..	0,0,0 [0,v,w]	0,1/2,0 [0, $\bar{v},w$ ]		
4 b 2'2'2	1/4,0,1/2 [0,0,w]	3/4,0,1/2 [0,0,w]		
4 a 2'2'2	1/4,0,0 [0,0,w]	3/4,0,0 [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1]  $p_c-2mm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,0,z

Along [1,0,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

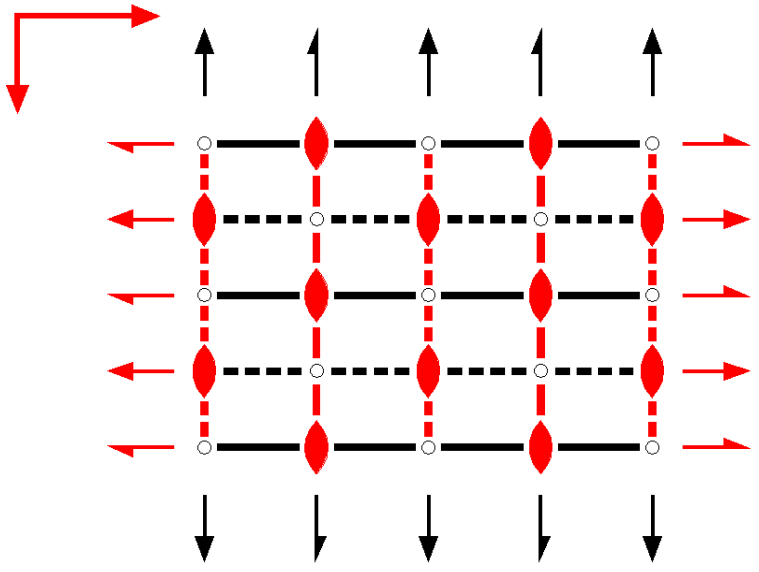
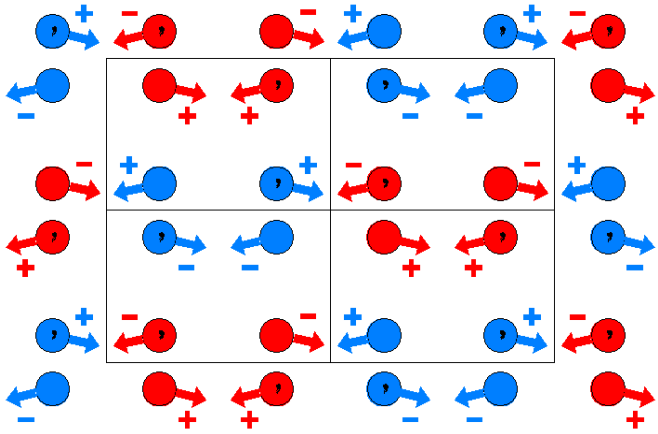
Along [0,1,0]  $p2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Cmm'a'  
67.6.582

mm'm'  
C2/m2'/m'2'/a'

Orthorhombic



Origin at center ( 2/m ) at  $2/m2_1/a'a'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |                                      |                                      |                                      |                                  |
|--------------------------------------|--------------------------------------|--------------------------------------|----------------------------------|
| (1) 1<br>(1 0,0,0)                   | (2) 2'<br>(2 <sub>z</sub>  1/2,0,0)' | (3) 2'<br>(2 <sub>y</sub>  1/2,0,0)' | (4) 2<br>(2 <sub>x</sub>  0,0,0) |
| (5) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (6) a'<br>(m <sub>z</sub>  1/2,0,0)' | (7) a'<br>(m <sub>y</sub>  1/2,0,0)' | (8) m<br>(m <sub>x</sub>  0,0,0) |

For (1/2,1/2,0) + set

- |  |                                      |                                      |                                      |
|--|--------------------------------------|--------------------------------------|--------------------------------------|
| (1) t<br>(1 1/2,1/2,0)                   | (2) 2'<br>(2 <sub>z</sub>  0,1/2,0)' | (3) 2'<br>(2 <sub>y</sub>  0,1/2,0)' | (4) 2<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$<br>( $\bar{1}$  1/2,1/2,0) | (6) b'<br>(m <sub>z</sub>  0,1/2,0)' | (7) m'<br>(m <sub>y</sub>  0,1/2,0)' | (8) b<br>(m <sub>x</sub>  1/2,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

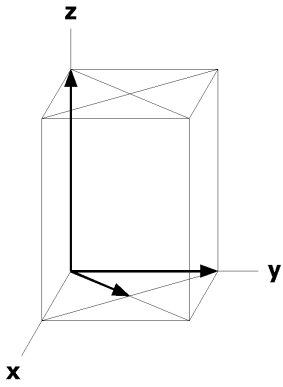
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1/2,1/2,0) +	
16 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [u,v, $\bar{w}$ ] (6) $x+1/2,y,\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x}+1/2,y,\bar{z}$ [u, $\bar{v}$ ,w] (7) $x+1/2,\bar{y},z$ [u, $\bar{v}$ ,w]	(4) $x,\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 n .m'	x,1/4,z [u,0,w]	$\bar{x},1/4,z$ [u,0, $\bar{w}$ ]	$\bar{x},3/4,\bar{z}$ [u,0,w]	x,3/4, $\bar{z}$ [u,0, $\bar{w}$ ]
8 m m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z$ [u,0,0]	0,y+1/2, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [u,0,0]
8 l ..2'	1/4,0,z [u,v,0]	3/4,1/2, $\bar{z}$ [u, $\bar{v}$ ,0]	3/4,0, $\bar{z}$ [u,v,0]	1/4,1/2,z [u, $\bar{v}$ ,0]
8 k .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,1/2$ [u,0, $\bar{w}$ ]	3/4, $\bar{y},1/2$ [u,0,w]	1/4,y+1/2,1/2 [u,0, $\bar{w}$ ]
8 j .2'	1/4,y,0 [u,0,w]	3/4, $\bar{y}+1/2,0$ [u,0, $\bar{w}$ ]	3/4, $\bar{y},0$ [u,0,w]	1/4,y+1/2,0 [u,0, $\bar{w}$ ]
8 i 2..	x,0,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [u,0,0]	$\bar{x},0,1/2$ [u,0,0]	x,1/2,1/2 [u,0,0]
8 h 2..	x,0,0 [u,0,0]	$\bar{x},1/2,0$ [u,0,0]	$\bar{x},0,0$ [u,0,0]	x,1/2,0 [u,0,0]
4 g mm'2'	0,1/4,z [u,0,0]	0,3/4, $\bar{z}$ [u,0,0]		
4 f .2'/m'	1/4,1/4,1/2 [u,0,w]	3/4,1/4,1/2 [u,0, $\bar{w}$ ]		
4 e .2'/m'	1/4,1/4,0 [u,0,w]	3/4,1/4,0 [u,0, $\bar{w}$ ]		
4 d 2/m..	0,0,1/2 [u,0,0]	0,1/2,1/2 [u,0,0]		
4 c 2/m..	0,0,0 [u,0,0]	0,1/2,0 [u,0,0]		
4 b 22'2'	1/4,0,1/2 [u,0,0]	3/4,0,1/2 [u,0,0]		
4 a 22'2'	1/4,0,0 [u,0,0]	3/4,0,0 [u,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



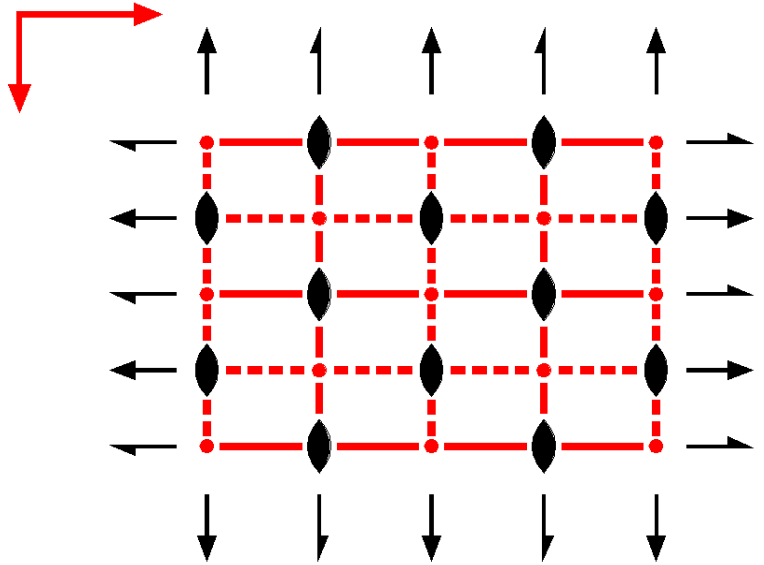
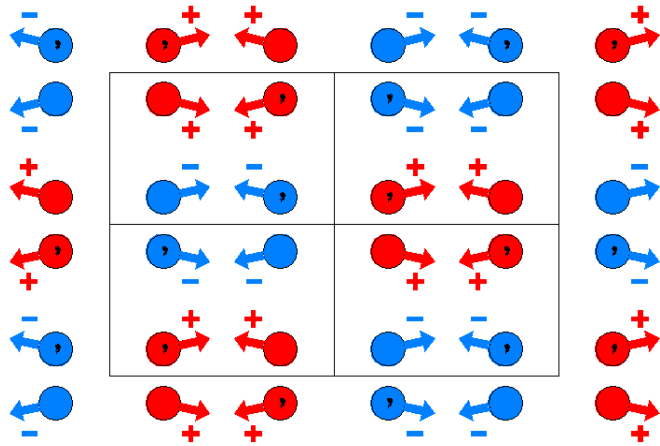
Cm'm'a'

67.7.583

m'm'm'

C2/m'2/m'2/a'

Orthorhombic



Origin at center ( $2/m'$ ) at  $2/m'2_1/a'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                                | (2) 2 $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )                 | (3) 2 $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )                 | (4) 2 $x,0,0$<br>( $2_x$   $0,0,0$ )     |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ )' | (6) $a'$ ( $1/2,0,0$ ) $x,y,0$<br>( $m_z$   $1/2,0,0$ )' | (7) $a'$ ( $1/2,0,0$ ) $x,0,z$<br>( $m_y$   $1/2,0,0$ )' | (8) $m'$ $0,y,z$<br>( $m_x$   $0,0,0$ )' |

For (1/2,1/2,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t$ ( $1/2,1/2,0$ )<br>(1  $1/2,1/2,0$ )              | (2) 2 $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )                 | (3) 2 ( $0,1/2,0$ ) $0,y,0$<br>( $2_y$   $0,1/2,0$ ) | (4) 2 ( $1/2,0,0$ ) $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )     |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ )' | (6) $b'$ ( $0,1/2,0$ ) $x,y,0$<br>( $m_z$   $0,1/2,0$ )' | (7) $m'$ $x,1/4,z$<br>( $m_y$   $0,1/2,0$ )'         | (8) $b'$ ( $0,1/2,0$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

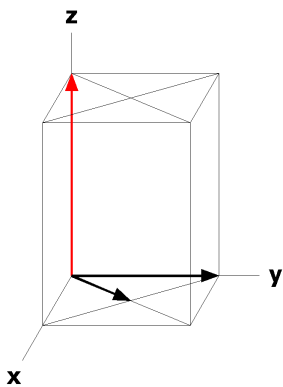
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1/2,1/2,0) +	
16 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(3) $\bar{x}+1/2,y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) $x+1/2,\bar{y},z$ [ $u,\bar{v},w$ ]	(4) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 n .m'	x,1/4,z [u,0,w]	$\bar{x},1/4,z$ [ $\bar{u},0,w$ ]	$\bar{x},3/4,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	x,3/4, $\bar{z}$ [u,0, $\bar{w}$ ]
8 m m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z$ [0, $\bar{v},w$ ]	0,y+1/2, $\bar{z}$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 l ..2	1/4,0,z [0,0,w]	3/4,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	3/4,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,1/2,z [0,0,w]
8 k .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y}+1/2,1/2$ [0, $\bar{v},0$ ]	3/4, $\bar{y},1/2$ [0, $\bar{v},0$ ]	1/4,y+1/2,1/2 [0,v,0]
8 j .2.	1/4,y,0 [0,v,0]	3/4, $\bar{y}+1/2,0$ [0, $\bar{v},0$ ]	3/4, $\bar{y},0$ [0, $\bar{v},0$ ]	1/4,y+1/2,0 [0,v,0]
8 i 2..	x,0,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	x,1/2,1/2 [u,0,0]
8 h 2..	x,0,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	x,1/2,0 [u,0,0]
4 g m'm'2	0,1/4,z [0,0,w]	0,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 f .2/m'	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 e .2/m'	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
4 d 2/m'..	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 c 2/m'..	0,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
4 b 222	1/4,0,1/2 [0,0,0]	3/4,0,1/2 [0,0,0]		
4 a 222	1/4,0,0 [0,0,0]	3/4,0,0 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



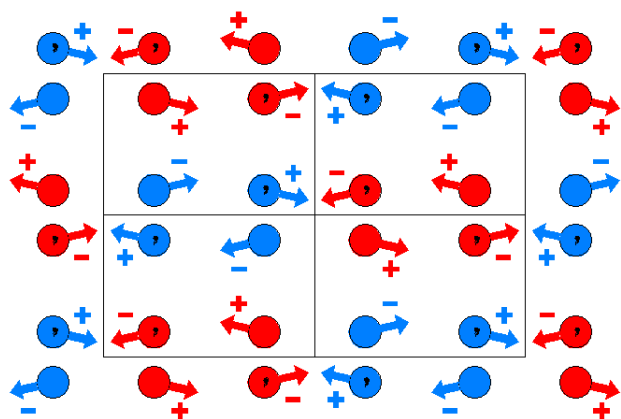
$C_{2c} mma$

67.8.584

$mmm1'$

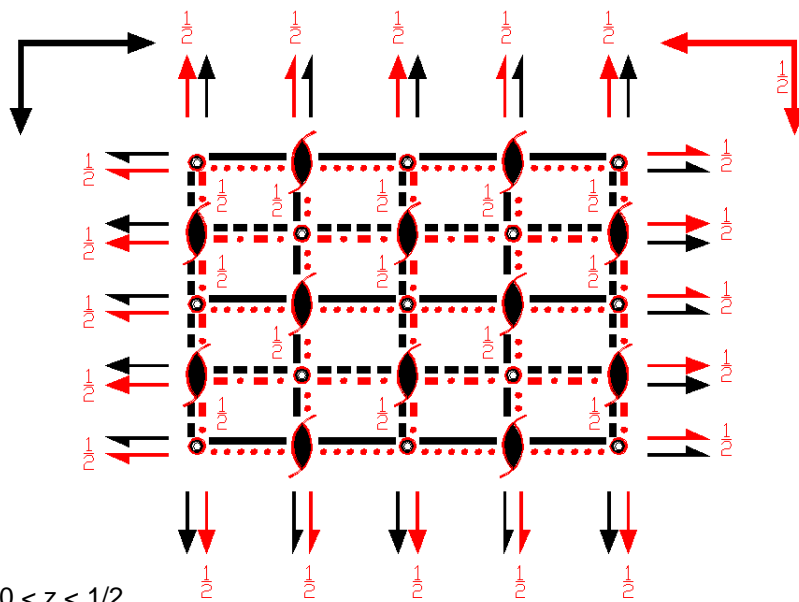
$C_{2c} 2/m2/m2/a$

Orthorhombic



Origin at center ( $2/m$ ) at  $2/m2_1/a$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$



### Symmetry Operations

For (0,0,0) + set

- |  |  |  |                                      |
|--|--|--|--------------------------------------|
| (1) 1<br>(1   0,0,0)                             | (2) 2 $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )             | (3) 2 $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )             | (4) 2 $x,0,0$<br>( $2_x$   $0,0,0$ ) |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ ) | (6) a ( $1/2,0,0$ ) $x,y,0$<br>( $m_z$   $1/2,0,0$ ) | (7) a ( $1/2,0,0$ ) $x,0,z$<br>( $m_y$   $1/2,0,0$ ) | (8) m $0,y,z$<br>( $m_x$   $0,0,0$ ) |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t ( $1/2,1/2,0$ )<br>(1   $1/2,1/2,0$ )              | (2) 2 $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )             | (3) 2 ( $0,1/2,0$ ) $0,y,0$<br>( $2_y$   $0,1/2,0$ ) | (4) 2 ( $1/2,0,0$ ) $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ ) |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ ) | (6) b ( $0,1/2,0$ ) $x,y,0$<br>( $m_z$   $0,1/2,0$ ) | (7) m $x,1/4,z$<br>( $m_y$   $0,1/2,0$ )             | (8) b ( $0,1/2,0$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ ) |

For (0,0,1)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' ( $0,0,1$ )<br>(1   $0,0,1$ )'                 | (2) 2' ( $0,0,1$ ) $1/4,0,z$<br>( $2_z$   $1/2,0,1$ )'   | (3) 2' $1/4,y,1/2$<br>( $2_y$   $1/2,0,1$ )'           | (4) 2' $x,0,1/2$<br>( $2_x$   $0,0,1$ )'           |
| (5) $\bar{1}$ ' $0,0,1/2$<br>( $\bar{1}$   $0,0,1$ )' | (6) a' ( $1/2,0,0$ ) $x,y,1/2$<br>( $m_z$   $1/2,0,1$ )' | (7) n' ( $1/2,0,1$ ) $x,0,z$<br>( $m_y$   $1/2,0,1$ )' | (8) c' ( $0,0,1$ ) $0,y,z$<br>( $m_x$   $0,0,1$ )' |

For (1/2,1/2,1)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' ( $1/2,1/2,1$ )<br>(1   $1/2,1/2,1$ )'                 | (2) 2' ( $0,0,1$ ) $0,1/4,z$<br>( $2_z$   $0,1/2,1$ )'   | (3) 2' ( $0,1/2,0$ ) $0,y,1/2$<br>( $2_y$   $0,1/2,1$ )' | (4) 2' ( $1/2,0,0$ ) $x,1/4,1/2$<br>( $2_x$   $1/2,1/2,1$ )' |
| (5) $\bar{1}$ ' $1/4,1/4,1/2$<br>( $\bar{1}$   $1/2,1/2,1$ )' | (6) b' ( $0,1/2,0$ ) $x,y,1/2$<br>( $m_z$   $0,1/2,1$ )' | (7) c' ( $0,0,1$ ) $x,1/4,z$<br>( $m_y$   $0,1/2,1$ )'   | (8) n' ( $0,1/2,1$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,1$ )'   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); t(1/2,1/2,0); (2); (3); (5).

**Positions**

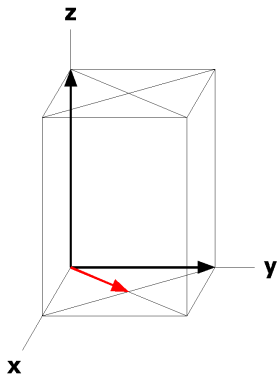
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,1)' +	(1/2,1/2,0) + (1/2,1/2,1)' +	
32 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) $x+1/2,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
16 n .m.	x,1/4,z [0,v,0]	$\bar{x},1/4,z$ [0, $\bar{v}$ ,0]	$\bar{x},3/4,\bar{z}$ [0,v,0]	x,3/4, $\bar{z}$ [0, $\bar{v}$ ,0]
16 m m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z$ [ $\bar{u},0,0$ ]	0,y+1/2, $\bar{z}$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]
16 l ..2	1/4,0,z [0,0,w]	3/4,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	3/4,0, $\bar{z}$ [0,0,w]	1/4,1/2,z [0,0, $\bar{w}$ ]
16 k .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,1/2$ [ $\bar{u},0,w$ ]	3/4, $\bar{y},1/2$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,1/2 [u,0, $\bar{w}$ ]
16 j .2.	1/4,y,0 [0,v,0]	3/4, $\bar{y}+1/2,0$ [0, $\bar{v},0$ ]	3/4, $\bar{y},0$ [0,v,0]	1/4,y+1/2,0 [0, $\bar{v},0$ ]
16 i 2'..	x,0,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0, $\bar{v},w$ ]	$\bar{x},0,1/2$ [0, $\bar{v},\bar{w}$ ]	x,1/2,1/2 [0,v, $\bar{w}$ ]
16 h 2..	x,0,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	$\bar{x},0,0$ [u,0,0]	x,1/2,0 [ $\bar{u},0,0$ ]
8 g mm2	0,1/4,z [0,0,0]	0,3/4, $\bar{z}$ [0,0,0]		
8 f .2'/m.	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
8 e .2/m.	1/4,1/4,0 [0,v,0]	3/4,1/4,0 [0, $\bar{v},0$ ]		
8 d 2'/m..	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
8 c 2/m..	0,0,0 [u,0,0]	0,1/2,0 [ $\bar{u},0,0$ ]		
8 b 2'2'2	1/4,0,1/2 [0,0,w]	3/4,0,1/2 [0,0, $\bar{w}$ ]		
8 a 222	1/4,0,0 [0,0,0]	3/4,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/2,y,0



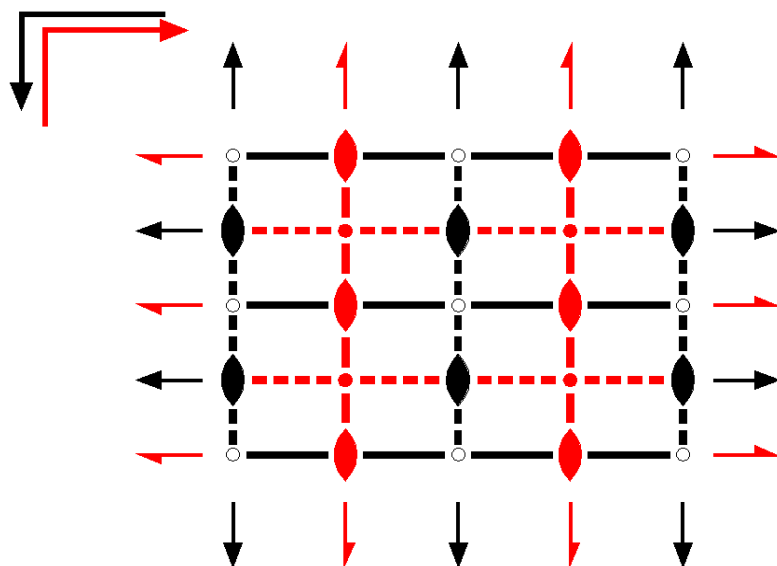
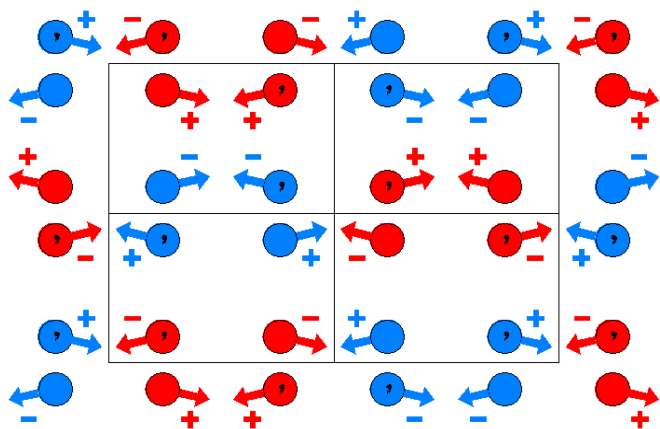
$C_{p}mma$

67.9.585

$mmm1'$

$C_{p}2/m2/m2/a$

Orthorhombic



**Origin** at center ( $2/m$ ) at  $2/m2_1/a$

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |                                      |
|--|--|--|--------------------------------------|
| (1) 1<br>(1 0,0,0)                         | (2) 2 $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )             | (3) 2 $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )             | (4) 2 $x,0,0$<br>( $2_x$   $0,0,0$ ) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a ( $1/2,0,0$ ) $x,y,0$<br>( $m_z$   $1/2,0,0$ ) | (7) a ( $1/2,0,0$ ) $x,0,z$<br>( $m_y$   $1/2,0,0$ ) | (8) m $0,y,z$<br>( $m_x$   $0,0,0$ ) |

For (1/2,1/2,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ ( $1/2,1/2,0$ )<br>(1  $1/2,1/2,0$ )'             | (2) 2' $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )'             | (3) 2' ( $0,1/2,0$ ) $0,y,0$<br>( $2_y$   $0,1/2,0$ )' | (4) 2' ( $1/2,0,0$ ) $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )' |
| (5) $\bar{1}'$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ )' | (6) b' ( $0,1/2,0$ ) $x,y,0$<br>( $m_z$   $0,1/2,0$ )' | (7) m' $x,1/4,z$<br>( $m_y$   $0,1/2,0$ )'             | (8) b' ( $0,1/2,0$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

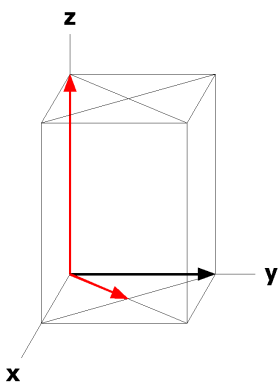
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) $x+1/2,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},\bar{v},\bar{w}$ ]
8 n .m'	x,1/4,z [u,0,w]	$\bar{x},1/4,z$ [u,0, $\bar{w}$ ]	$\bar{x},3/4,\bar{z}$ [u,0,w]	x,3/4, $\bar{z}$ [u,0, $\bar{w}$ ]
8 m m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z$ [u,0,0]	0,y+1/2, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [u,0,0]
8 l ..2	1/4,0,z [0,0,w]	3/4,1/2, $\bar{z}$ [0,0,w]	3/4,0, $\bar{z}$ [0,0,w]	1/4,1/2,z [0,0,w]
8 k .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y}+1/2,1/2$ [0,v,0]	3/4, $\bar{y},1/2$ [0,v,0]	1/4,y+1/2,1/2 [0,v,0]
8 j .2.	1/4,y,0 [0,v,0]	3/4, $\bar{y}+1/2,0$ [0,v,0]	3/4, $\bar{y},0$ [0,v,0]	1/4,y+1/2,0 [0,v,0]
8 i 2..	x,0,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [u,0,0]	$\bar{x},0,1/2$ [u,0,0]	x,1/2,1/2 [u,0,0]
8 h 2..	x,0,0 [u,0,0]	$\bar{x},1/2,0$ [u,0,0]	$\bar{x},0,0$ [u,0,0]	x,1/2,0 [u,0,0]
4 g m'm'2	0,1/4,z [0,0,w]	0,3/4, $\bar{z}$ [0,0,w]		
4 f .2/m'	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
4 e .2/m'	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
4 d 2/m..	0,0,1/2 [u,0,0]	0,1/2,1/2 [u,0,0]		
4 c 2/m..	0,0,0 [u,0,0]	0,1/2,0 [u,0,0]		
4 b 222	1/4,0,1/2 [0,0,0]	3/4,0,1/2 [0,0,0]		
4 a 222	1/4,0,0 [0,0,0]	3/4,0,0 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,0,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

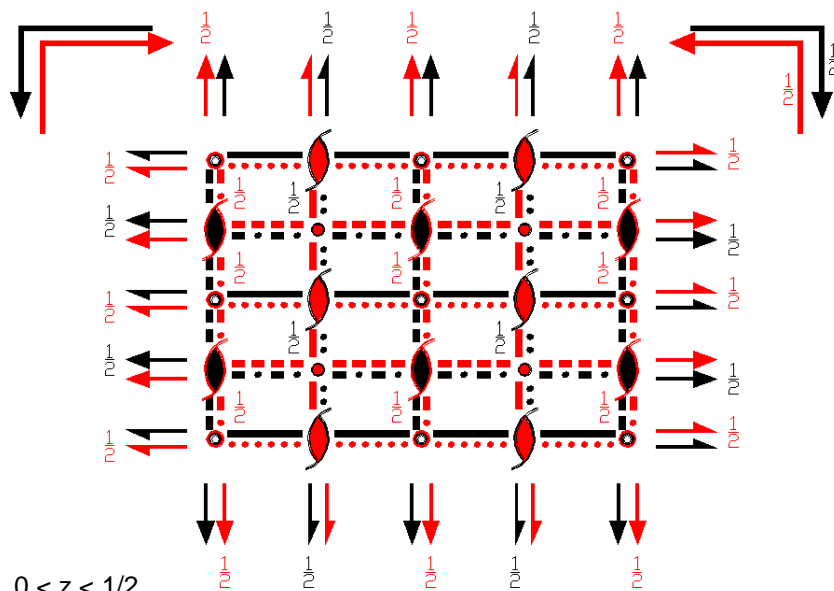
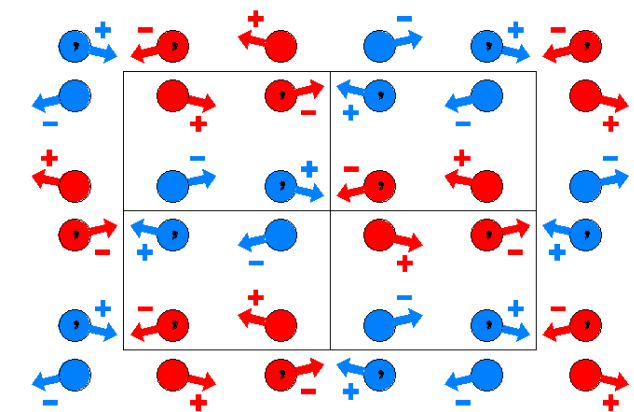
Along [0,1,0]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



$C_1 m m a$   
67.10.586

$m m m 1'$   
 $C_1 2/m 2/m 2/a$

Orthorhombic



**Origin** at center ( $2/m$ ) at  $2/m 2_1/a a$

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 $1/4, 0, z$<br>( $2_z$   $1/2, 0, 0$ )               | (3) 2 $1/4, y, 0$<br>( $2_y$   $1/2, 0, 0$ )               | (4) 2 $x, 0, 0$<br>( $2_x$   $0, 0, 0$ ) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a ( $1/2, 0, 0$ ) $x, y, 0$<br>( $m_z$   $1/2, 0, 0$ ) | (7) a ( $1/2, 0, 0$ ) $x, 0, z$<br>( $m_y$   $1/2, 0, 0$ ) | (8) m $0, y, z$<br>( $m_x$   $0, 0, 0$ ) |

For (1/2,1/2,0)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' ( $1/2, 1/2, 0$ )<br>(1  $1/2, 1/2, 0$ )'                | (2) 2' $0, 1/4, z$<br>( $2_z$   $0, 1/2, 0$ )'               | (3) 2' ( $0, 1/2, 0$ ) $0, y, 0$<br>( $2_y$   $0, 1/2, 0$ )' | (4) 2' ( $1/2, 0, 0$ ) $x, 1/4, 0$<br>( $2_x$   $1/2, 1/2, 0$ )' |
| (5) $\bar{1}$ ' $1/4, 1/4, 0$<br>( $\bar{1}$   $1/2, 1/2, 0$ )' | (6) b' ( $0, 1/2, 0$ ) $x, y, 0$<br>( $m_z$   $0, 1/2, 0$ )' | (7) m' $x, 1/4, z$<br>( $m_y$   $0, 1/2, 0$ )'               | (8) b' ( $0, 1/2, 0$ ) $1/4, y, z$<br>( $m_x$   $1/2, 1/2, 0$ )' |

For (0,0,1)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' (0,0,1)<br>(1 0,0,1)'                    | (2) 2' (0,0,1) $1/4, 0, z$<br>( $2_z$   $1/2, 0, 1$ )'         | (3) 2' $1/4, y, 1/2$<br>( $2_y$   $1/2, 0, 1$ )'             | (4) 2' $x, 0, 1/2$<br>( $2_x$   $0, 0, 1$ )'       |
| (5) $\bar{1}$ ' 0,0,1/2<br>( $\bar{1}$  0,0,1)' | (6) a' ( $1/2, 0, 0$ ) $x, y, 1/2$<br>( $m_z$   $1/2, 0, 1$ )' | (7) n' ( $1/2, 0, 1$ ) $x, 0, z$<br>( $m_y$   $1/2, 0, 1$ )' | (8) c' (0,0,1) $0, y, z$<br>( $m_x$   $0, 0, 1$ )' |

For (1/2,1/2,1) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t ( $1/2, 1/2, 1$ )<br>(1  $1/2, 1/2, 1$ )                 | (2) 2 (0,0,1) $0, 1/4, z$<br>( $2_z$   $0, 1/2, 1$ )   | (3) 2 (0,1/2,0) $0, y, 1/2$<br>( $2_y$   $0, 1/2, 1$ ) | (4) 2 ( $1/2, 0, 0$ ) $x, 1/4, 1/2$<br>( $2_x$   $1/2, 1/2, 1$ ) |
| (5) $\bar{1}$ $1/4, 1/4, 1/2$<br>( $\bar{1}$   $1/2, 1/2, 1$ ) | (6) b (0,1/2,0) $x, y, 1/2$<br>( $m_z$   $0, 1/2, 1$ ) | (7) c (0,0,1) $x, 1/4, z$<br>( $m_y$   $0, 1/2, 1$ )   | (8) n (0,1/2,1) $1/4, y, z$<br>( $m_x$   $1/2, 1/2, 1$ )         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

**Positions**

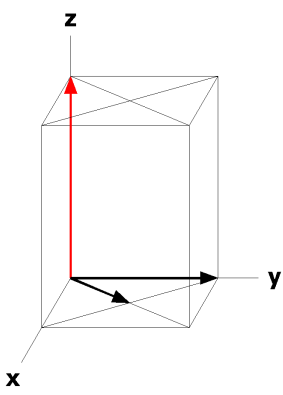
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) + (0,0,1)'	(1/2,1/2,0)' + (1/2,1/2,1) +		
32 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (7) $x+1/2,\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},\bar{v},\bar{w}$ ]
16 n .m'	x,1/4,z [u,0,w]	$\bar{x},1/4,z$ [u,0, $\bar{w}$ ]	$\bar{x},3/4,\bar{z}$ [u,0,w]	x,3/4, $\bar{z}$ [u,0, $\bar{w}$ ]
16 m m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z$ [u,0,0]	0,y+1/2, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [u,0,0]
16 l ..2	1/4,0,z [0,0,w]	3/4,1/2, $\bar{z}$ [0,0,w]	3/4,0, $\bar{z}$ [0,0,w]	1/4,1/2,z [0,0,w]
16 k .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,1/2$ [u,0, $\bar{w}$ ]	3/4, $\bar{y},1/2$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,1/2 [ $\bar{u},0,w$ ]
16 j .2.	1/4,y,0 [0,v,0]	3/4, $\bar{y}+1/2,0$ [0,v,0]	3/4, $\bar{y},0$ [0,v,0]	1/4,y+1/2,0 [0,v,0]
16 i 2'..	x,0,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0,v, $\bar{w}$ ]	$\bar{x},0,1/2$ [0, $\bar{v},\bar{w}$ ]	x,1/2,1/2 [0, $\bar{v},w$ ]
16 h 2..	x,0,0 [u,0,0]	$\bar{x},1/2,0$ [u,0,0]	$\bar{x},0,0$ [u,0,0]	x,1/2,0 [u,0,0]
8 g m'm'2	0,1/4,z [0,0,w]	0,3/4, $\bar{z}$ [0,0,w]		
8 f .2'/m'	1/4,1/4,1/2 [u,0,w]	3/4,1/4,1/2 [u,0, $\bar{w}$ ]		
8 e .2/m'	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
8 d 2'/m..	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
8 c 2/m..	0,0,0 [u,0,0]	0,1/2,0 [u,0,0]		
8 b 2'2'2	1/4,0,1/2 [0,0,w]	3/4,0,1/2 [0,0, $\bar{w}$ ]		
8 a 222	1/4,0,0 [0,0,0]	3/4,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/2,y,0



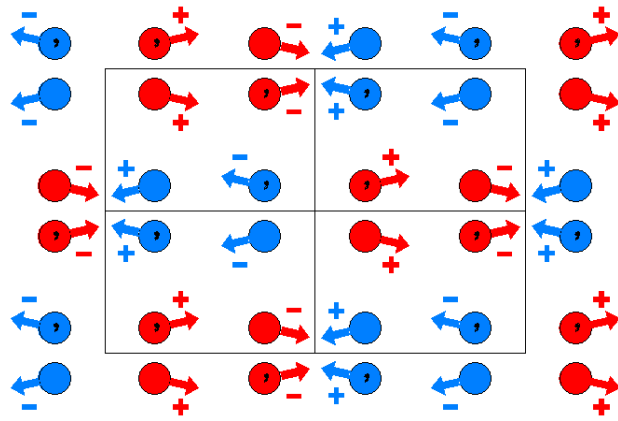
$C_{2c} m'ma$

67.11.587

$mmm1'$

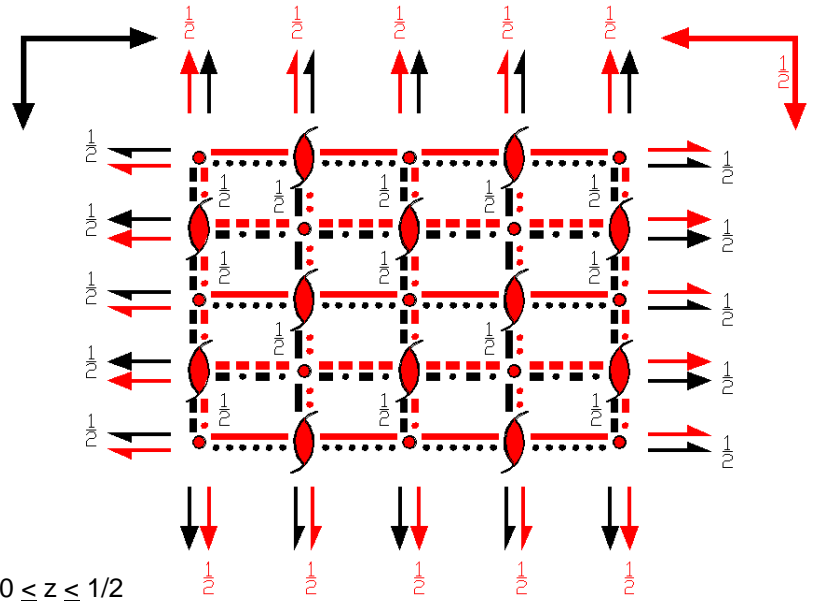
$C_{2c} 2/m'2'/m2'/a$

Orthorhombic



**Origin** at center ( $2/m'$ ) at  $2/m'2'/a$

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$



**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2' $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,0)'         | (3) 2' $1/4,y,0$<br>(2 <sub>y</sub>  1/2,0,0)'         | (4) 2 $x,0,0$<br>(2 <sub>x</sub>  0,0,0)   |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)' | (6) a $(1/2,0,0)$ $x,y,0$<br>(m <sub>z</sub>  1/2,0,0) | (7) a $(1/2,0,0)$ $x,0,z$<br>(m <sub>y</sub>  1/2,0,0) | (8) m' $0,y,z$<br>(m <sub>x</sub>  0,0,0)' |

For (1/2,1/2,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t $(1/2,1/2,0)$<br>(1 1/2,1/2,0)                  | (2) 2' $0,1/4,z$<br>(2 <sub>z</sub>  0,1/2,0)'         | (3) 2' $(0,1/2,0)$ $0,y,0$<br>(2 <sub>y</sub>  0,1/2,0)' | (4) 2 $(1/2,0,0)$ $x,1/4,0$<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$  1/2,1/2,0)' | (6) b $(0,1/2,0)$ $x,y,0$<br>(m <sub>z</sub>  0,1/2,0) | (7) m $x,1/4,z$<br>(m <sub>y</sub>  0,1/2,0)             | (8) b' $(0,1/2,0)$ $1/4,y,z$<br>(m <sub>x</sub>  1/2,1/2,0)' |

For (0,0,1)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' $(0,0,1)$<br>(1 0,0,1)'                 | (2) 2 $(0,0,1)$ $1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,1)'    | (3) 2 $1/4,y,1/2$<br>(2 <sub>y</sub>  1/2,0,1)           | (4) 2' $x,0,1/2$<br>(2 <sub>x</sub>  0,0,1)'       |
| (5) $\bar{1}$ $0,0,1/2$<br>( $\bar{1}$  0,0,1) | (6) a' $(1/2,0,0)$ $x,y,1/2$<br>(m <sub>z</sub>  1/2,0,1)' | (7) n' $(1/2,0,1)$ $x,0,z$<br>(m <sub>y</sub>  1/2,0,1)' | (8) c $(0,0,1)$ $0,y,z$<br>(m <sub>x</sub>  0,0,1) |

For (1/2,1/2,1)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' $(1/2,1/2,1)$<br>(1 1/2,1/2,1)'                 | (2) 2 $(0,0,1)$ $0,1/4,z$<br>(2 <sub>z</sub>  0,1/2,1)     | (3) 2 $(0,1/2,0)$ $0,y,1/2$<br>(2 <sub>y</sub>  0,1/2,1) | (4) 2' $(1/2,0,0)$ $x,1/4,1/2$<br>(2 <sub>x</sub>  1/2,1/2,1)' |
| (5) $\bar{1}$ $1/4,1/4,1/2$<br>( $\bar{1}$  1/2,1/2,1) | (6) b' $(0,1/2,0)$ $x,y,1/2$<br>(m <sub>z</sub>  0,1/2,1)' | (7) c' $(0,0,1)$ $x,1/4,z$<br>(m <sub>y</sub>  0,1/2,1)' | (8) n $(0,1/2,1)$ $1/4,y,z$<br>(m <sub>x</sub>  1/2,1/2,1)     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1);t(1/2,1/2,0); (2); (3); (5).

**Positions**

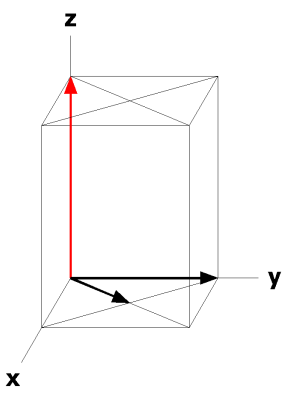
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) + (0,0,1)' +	(1/2,1/2,0) + (1/2,1/2,1)' +		
32 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [u,v, $\bar{w}$ ] (6) x+1/2,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y,\bar{z}$ [u, $\bar{v},w$ ] (7) x+1/2, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
16 n .m.	x,1/4,z [0,v,0]	$\bar{x},1/4,z$ [0,v,0]	$\bar{x},3/4,\bar{z}$ [0, $\bar{v},0$ ]	x,3/4, $\bar{z}$ [0, $\bar{v},0$ ]
16 m m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z$ [0,v, $\bar{w}$ ]	0,y+1/2, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
16 l ..2'	1/4,0,z [u,v,0]	3/4,1/2, $\bar{z}$ [u, $\bar{v},0$ ]	3/4,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,1/2,z [ $\bar{u},v,0$ ]
16 k .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y}+1/2,1/2$ [0,v,0]	3/4, $\bar{y},1/2$ [0, $\bar{v},0$ ]	1/4,y+1/2,1/2 [0, $\bar{v},0$ ]
16 j .2'.	1/4,y,0 [u,0,w]	3/4, $\bar{y}+1/2,0$ [u,0, $\bar{w}$ ]	3/4, $\bar{y},0$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,0 [ $\bar{u},0,w$ ]
16 i 2'..	x,0,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0,v, $\bar{w}$ ]	$\bar{x},0,1/2$ [0, $\bar{v},\bar{w}$ ]	x,1/2,1/2 [0, $\bar{v},w$ ]
16 h 2..	x,0,0 [u,0,0]	$\bar{x},1/2,0$ [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	x,1/2,0 [ $\bar{u},0,0$ ]
8 g m'm2'	0,1/4,z [0,v,0]	0,3/4, $\bar{z}$ [0, $\bar{v},0$ ]		
8 f .2/m.	1/4,1/4,1/2 [u,0,w]	3/4,1/4,1/2 [ $\bar{u},0,w$ ]		
8 e .2'/m.	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
8 d 2'/m..	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
8 c 2/m'..	0,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
8 b 2'22'	1/4,0,1/2 [0,v,0]	3/4,0,1/2 [0, $\bar{v},0$ ]		
8 a 22'2'	1/4,0,0 [u,0,0]	3/4,0,0 [ $\bar{u},0,0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>c</sub>2mm  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 1/4,y,0



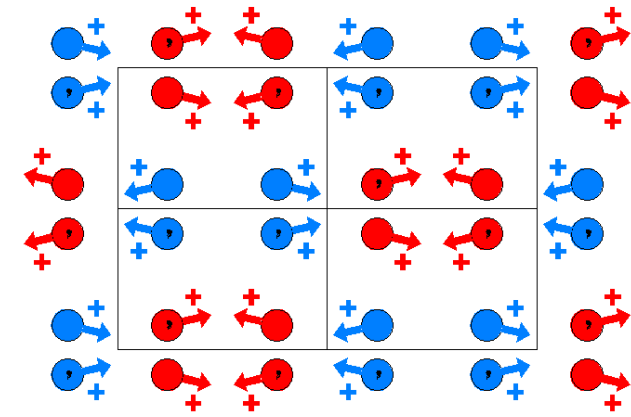
$C_{2c} m'm'a$

67.12.588

$mmm1'$

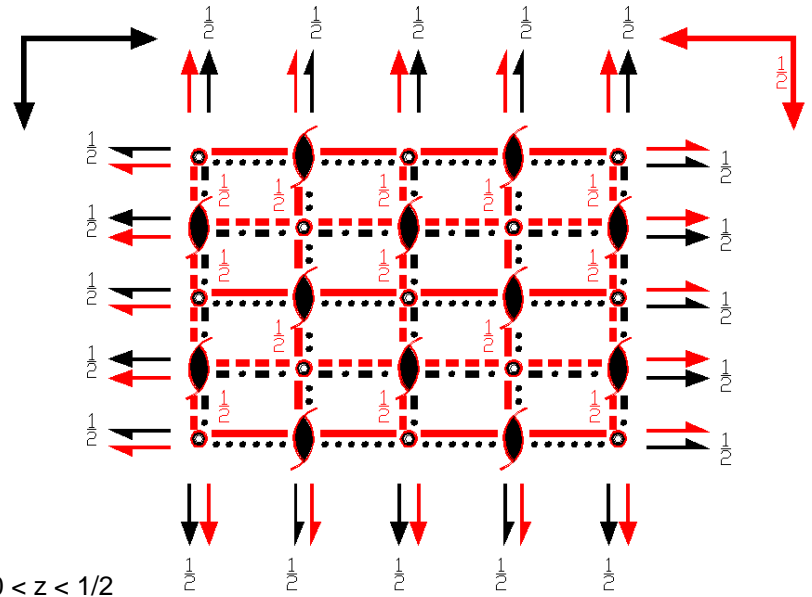
$C_{2c} 2'/m'2'/m'2/a$

Orthorhombic



Origin at center ( $2/m'$ ) at  $2/m'2_1/a'a$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$



**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                               | (2) 2 $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )             | (3) 2' $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )'             | (4) 2' $x,0,0$<br>( $2_x$   $0,0,0$ )' |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ ) | (6) a ( $1/2,0,0$ ) $x,y,0$<br>( $m_z$   $1/2,0,0$ ) | (7) a' ( $1/2,0,0$ ) $x,0,z$<br>( $m_y$   $1/2,0,0$ )' | (8) m' $0,y,z$<br>( $m_x$   $0,0,0$ )' |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t ( $1/2,1/2,0$ )<br>(1  $1/2,1/2,0$ )               | (2) 2 $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )             | (3) 2' ( $0,1/2,0$ ) $0,y,0$<br>( $2_y$   $0,1/2,0$ )' | (4) 2' ( $1/2,0,0$ ) $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )' |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ ) | (6) b ( $0,1/2,0$ ) $x,y,0$<br>( $m_z$   $0,1/2,0$ ) | (7) m' $x,1/4,z$<br>( $m_y$   $0,1/2,0$ )'             | (8) b' ( $0,1/2,0$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |

For (0,0,1)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' ( $0,0,1$ )<br>(1  $0,0,1$ )'                  | (2) 2' ( $0,0,1$ ) $1/4,0,z$<br>( $2_z$   $1/2,0,1$ )'   | (3) 2 $1/4,y,1/2$<br>( $2_y$   $1/2,0,1$ )           | (4) 2 $x,0,1/2$<br>( $2_x$   $0,0,1$ )           |
| (5) $\bar{1}$ ' $0,0,1/2$<br>( $\bar{1}$   $0,0,1$ )' | (6) a' ( $1/2,0,0$ ) $x,y,1/2$<br>( $m_z$   $1/2,0,1$ )' | (7) n ( $1/2,0,1$ ) $x,0,z$<br>( $m_y$   $1/2,0,1$ ) | (8) c ( $0,0,1$ ) $0,y,z$<br>( $m_x$   $0,0,1$ ) |

For (1/2,1/2,1)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' ( $1/2,1/2,1$ )<br>(1  $1/2,1/2,1$ )'                  | (2) 2' ( $0,0,1$ ) $0,1/4,z$<br>( $2_z$   $0,1/2,1$ )'   | (3) 2 ( $0,1/2,0$ ) $0,y,1/2$<br>( $2_y$   $0,1/2,1$ ) | (4) 2 ( $1/2,0,0$ ) $x,1/4,1/2$<br>( $2_x$   $1/2,1/2,1$ ) |
| (5) $\bar{1}$ ' $1/4,1/4,1/2$<br>( $\bar{1}$   $1/2,1/2,1$ )' | (6) b' ( $0,1/2,0$ ) $x,y,1/2$<br>( $m_z$   $0,1/2,1$ )' | (7) c ( $0,0,1$ ) $x,1/4,z$<br>( $m_y$   $0,1/2,1$ )   | (8) n ( $0,1/2,1$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,1$ )   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); t(1/2,1/2,0); (2); (3); (5).

**Positions**

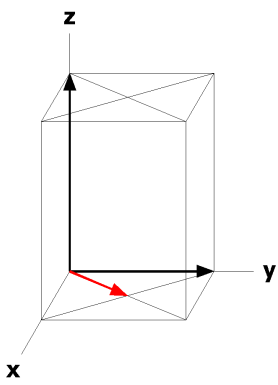
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) + (0,0,1)' +	(1/2,1/2,0) + (1/2,1/2,1)' +		
32 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x+1/2,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y,\bar{z}$ [u, $\bar{v},w$ ] (7) x+1/2, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
16 n .m'	x,1/4,z [u,0,w]	$\bar{x},1/4,z$ [ $\bar{u},0,w$ ]	$\bar{x},3/4,\bar{z}$ [u,0,w]	x,3/4, $\bar{z}$ [ $\bar{u},0,w$ ]
16 m m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z$ [0, $\bar{v},w$ ]	0,y+1/2, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
16 l ..2	1/4,0,z [0,0,w]	3/4,1/2, $\bar{z}$ [0,0,w]	3/4,0, $\bar{z}$ [0,0,w]	1/4,1/2,z [0,0,w]
16 k .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y}+1/2,1/2$ [0, $\bar{v},0$ ]	3/4, $\bar{y},1/2$ [0, $\bar{v},0$ ]	1/4,y+1/2,1/2 [0,v,0]
16 j .2'	1/4,y,0 [u,0,w]	3/4, $\bar{y}+1/2,0$ [ $\bar{u},0,w$ ]	3/4, $\bar{y},0$ [u,0,w]	1/4,y+1/2,0 [ $\bar{u},0,w$ ]
16 i 2..	x,0,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	x,1/2,1/2 [u,0,0]
16 h 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,0$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0,v,w]	x,1/2,0 [0, $\bar{v},w$ ]
8 g m'm'2	0,1/4,z [0,0,w]	0,3/4, $\bar{z}$ [0,0,w]		
8 f .2/m'	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
8 e .2'/m'	1/4,1/4,0 [u,0,w]	3/4,1/4,0 [ $\bar{u},0,w$ ]		
8 d 2/m'..	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
8 c 2'/m'..	0,0,0 [0,v,w]	0,1/2,0 [0, $\bar{v},w$ ]		
8 b 222	1/4,0,1/2 [0,0,0]	3/4,0,1/2 [0,0,0]		
8 a 2'2'2	1/4,0,0 [0,0,w]	3/4,0,0 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,1/2

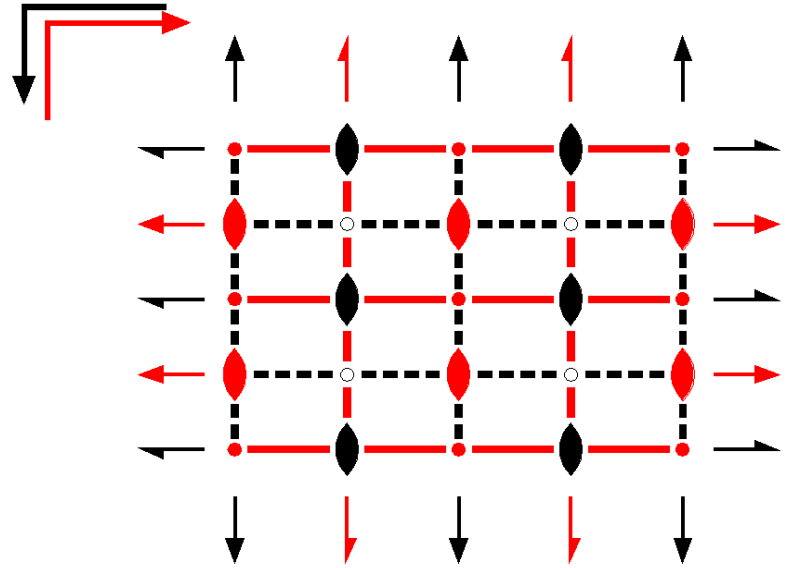
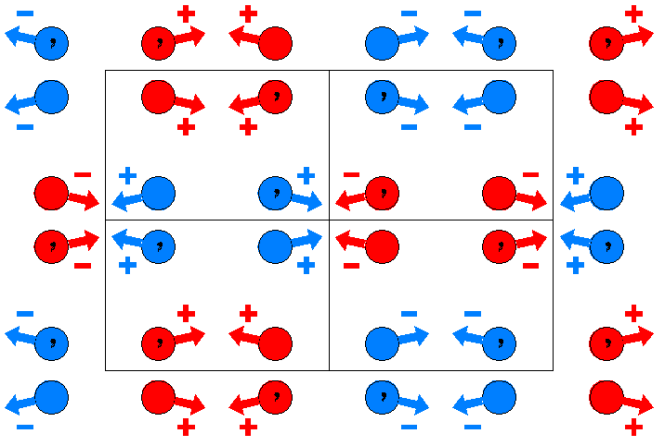
Along [0,1,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/2



$C_{2v}m'ma$   
67.13.589

$mmm1'$   
 $C_{2v}2/m'2'/m2'/a$

Orthorhombic



**Origin** at center ( $2/m'$ ) at  $2/m'2'/1/aa$

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                                | (2) $2'$ $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )'           | (3) $2'$ $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )'           | (4) $2$ $x,0,0$<br>( $2_x$   $0,0,0$ )   |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ )' | (6) $a$ ( $1/2,0,0$ ) $x,y,0$<br>( $m_z$   $1/2,0,0$ ) | (7) $a$ ( $1/2,0,0$ ) $x,0,z$<br>( $m_y$   $1/2,0,0$ ) | (8) $m'$ $0,y,z$<br>( $m_x$   $0,0,0$ )' |

For (1/2,1/2,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ ( $1/2,1/2,0$ )<br>(1  $1/2,1/2,0$ )'           | (2) $2$ $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )               | (3) $2$ ( $0,1/2,0$ ) $0,y,0$<br>( $2_y$   $0,1/2,0$ ) | (4) $2'$ ( $1/2,0,0$ ) $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )' |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ ) | (6) $b'$ ( $0,1/2,0$ ) $x,y,0$<br>( $m_z$   $0,1/2,0$ )' | (7) $m'$ $x,1/4,z$<br>( $m_y$   $0,1/2,0$ )'           | (8) $b$ ( $0,1/2,0$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )   |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

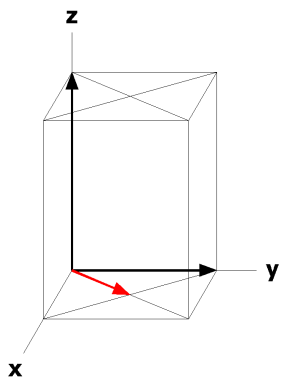
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1/2,1/2,0)' +	
16 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [u,v, $\bar{w}$ ] (6) x+1/2,y, $\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{x}+1/2,\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (7) x+1/2, $\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 n .m'	x,1/4,z [u,0,w]	$\bar{x},1/4,z$ [u,0, $\bar{w}$ ]	$\bar{x},3/4,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	x,3/4, $\bar{z}$ [ $\bar{u},0,\bar{w}$ ]
8 m m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z$ [0, $\bar{v},\bar{w}$ ]	0,y+1/2, $\bar{z}$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 l ..2'	1/4,0,z [u,v,0]	3/4,1/2, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	3/4,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,1/2,z [u, $\bar{v},0$ ]
8 k .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,1/2$ [ $\bar{u},0,\bar{w}$ ]	3/4, $\bar{y},1/2$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,1/2 [u,0, $\bar{w}$ ]
8 j .2	1/4,y,0 [0,v,0]	3/4, $\bar{y}+1/2,0$ [0, $\bar{v},0$ ]	3/4, $\bar{y},0$ [0, $\bar{v},0$ ]	1/4,y+1/2,0 [0,v,0]
8 i 2..	x,0,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	x,1/2,1/2 [u,0,0]
8 h 2..	x,0,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	x,1/2,0 [u,0,0]
4 g m'm'2	0,1/4,z [0,0,w]	0,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 f .2'/m'	1/4,1/4,1/2 [u,0,w]	3/4,1/4,1/2 [ $\bar{u},0,\bar{w}$ ]		
4 e .2'/m'	1/4,1/4,0 [u,0,w]	3/4,1/4,0 [ $\bar{u},0,\bar{w}$ ]		
4 d 2/m'..	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 c 2/m'..	0,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
4 b 22'2'	1/4,0,1/2 [u,0,0]	3/4,0,1/2 [ $\bar{u},0,0$ ]		
4 a 22'2'	1/4,0,0 [u,0,0]	3/4,0,0 [ $\bar{u},0,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

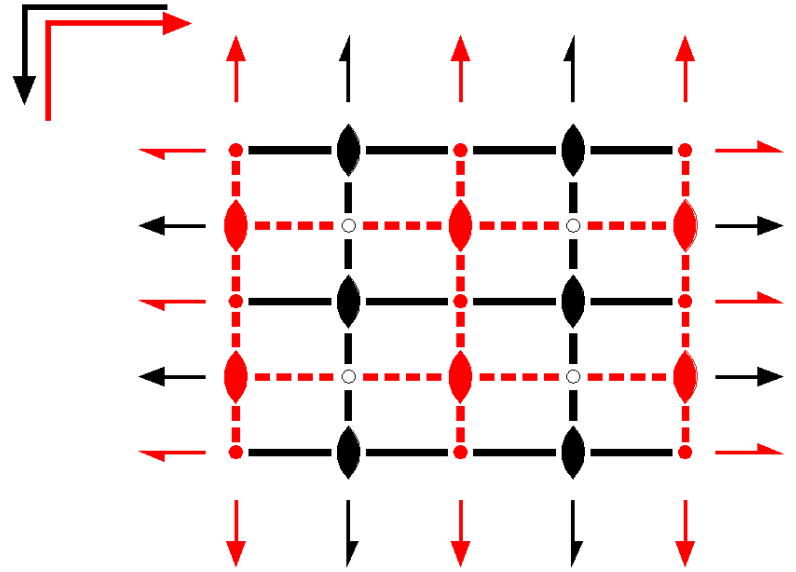
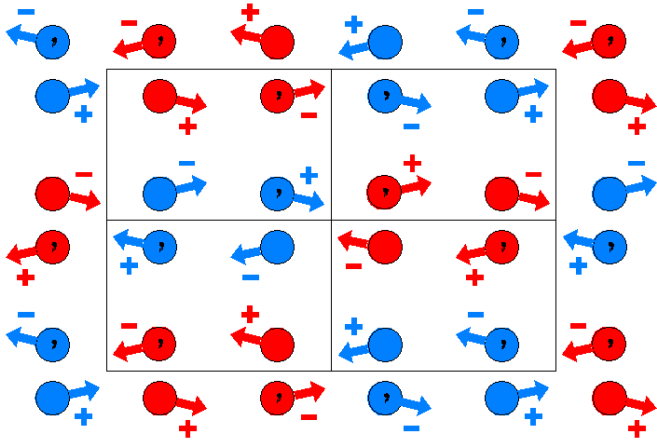
Along [0,1,0] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



$C_{2v}mm'a$   
67.14.590

$mmm1'$   
 $C_{2v}2'/m2/m'2'/a$

Orthorhombic



**Origin** at center ( $2'/m$ ) at  $2'/m2, /a'a$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                                | (2) $2'$ $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )'         | (3) $2$ $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )             | (4) $2'$ $x,0,0$<br>( $2_x$   $0,0,0$ )' |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ )' | (6) a ( $1/2,0,0$ ) $x,y,0$<br>( $m_z$   $1/2,0,0$ ) | (7) a' ( $1/2,0,0$ ) $x,0,z$<br>( $m_y$   $1/2,0,0$ )' | (8) m $0,y,z$<br>( $m_x$   $0,0,0$ )     |

For (1/2,1/2,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ ( $1/2,1/2,0$ )<br>(1  $1/2,1/2,0$ )'           | (2) $2$ $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )             | (3) $2'$ ( $0,1/2,0$ ) $0,y,0$<br>( $2_y$   $0,1/2,0$ )' | (4) $2$ ( $1/2,0,0$ ) $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ ) |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ ) | (6) b' ( $0,1/2,0$ ) $x,y,0$<br>( $m_z$   $0,1/2,0$ )' | (7) m $x,1/4,z$<br>( $m_y$   $0,1/2,0$ )                 | (8) b' ( $0,1/2,0$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

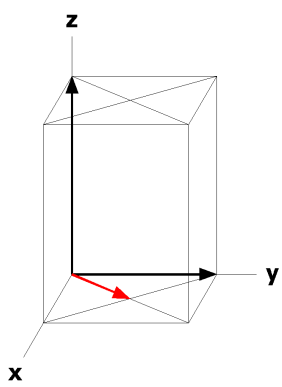
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [u,v, $\bar{w}$ ] (6) x+1/2,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) x+1/2, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 n .m.	x,1/4,z [0,v,0]	$\bar{x},1/4,z$ [0, $\bar{v},0$ ]	$\bar{x},3/4,\bar{z}$ [0, $\bar{v},0$ ]	x,3/4, $\bar{z}$ [0,v,0]
8 m m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z$ [ $\bar{u},0,0$ ]	0,y+1/2, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
8 l ..2'	1/4,0,z [u,v,0]	3/4,1/2, $\bar{z}$ [u, $\bar{v},0$ ]	3/4,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,1/2,z [ $\bar{u},v,0$ ]
8 k .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y}+1/2,1/2$ [0, $\bar{v},0$ ]	3/4, $\bar{y},1/2$ [0, $\bar{v},0$ ]	1/4,y+1/2,1/2 [0,v,0]
8 j .2.	1/4,y,0 [0,v,0]	3/4, $\bar{y}+1/2,0$ [0, $\bar{v},0$ ]	3/4, $\bar{y},0$ [0, $\bar{v},0$ ]	1/4,y+1/2,0 [0,v,0]
8 i 2'..	x,0,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0, $\bar{v},w$ ]	$\bar{x},0,1/2$ [0, $\bar{v},\bar{w}$ ]	x,1/2,1/2 [0,v, $\bar{w}$ ]
8 h 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,0$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0, $\bar{v},\bar{w}$ ]	x,1/2,0 [0,v, $\bar{w}$ ]
4 g mm2	0,1/4,z [0,0,0]	0,3/4, $\bar{z}$ [0,0,0]		
4 f .2/m.	1/4,1/4,1/2 [0,v,0]	3/4,1/4,1/2 [0,v,0]		
4 e .2/m.	1/4,1/4,0 [0,v,0]	3/4,1/4,0 [0,v,0]		
4 d 2'/m..	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 c 2'/m..	0,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
4 b 2'22'	1/4,0,1/2 [0,v,0]	3/4,0,1/2 [0, $\bar{v},0$ ]		
4 a 2'22'	1/4,0,0 [0,v,0]	3/4,0,0 [0, $\bar{v},0$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

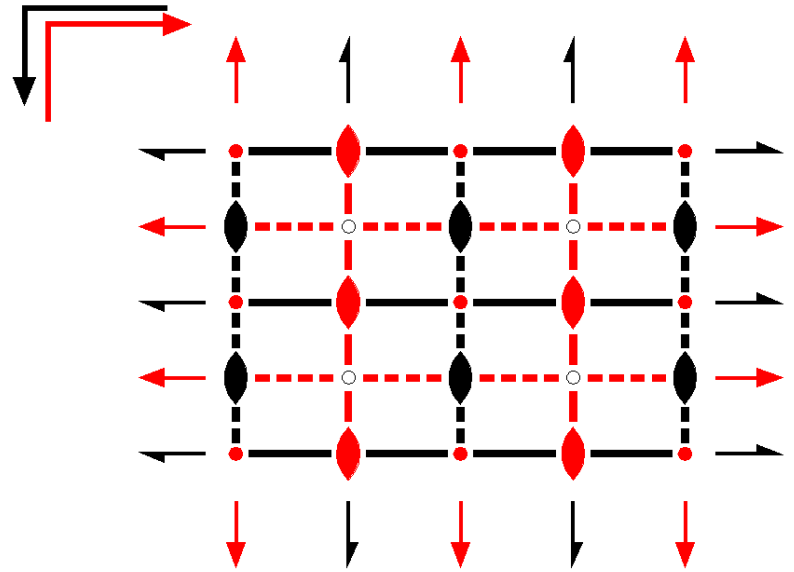
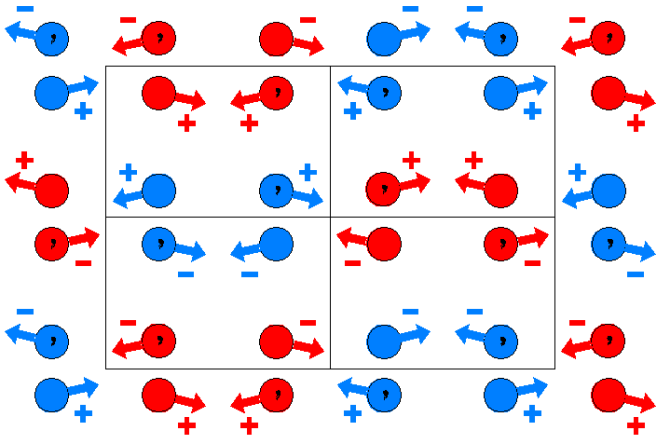
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



$C_{p}mma'$   
67.15.591

$mmm1'$   
 $C_{p}2'/m2'/m2/a'$

Orthorhombic



**Origin** at center ( $2'/m$ ) at  $2'/m2, /aa'$

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                                | (2) 2 $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )'              | (3) 2' $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )'           | (4) 2' $x,0,0$<br>( $2_x$   $0,0,0$ )' |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ )' | (6) a' ( $1/2,0,0$ ) $x,y,0$<br>( $m_z$   $1/2,0,0$ )' | (7) a ( $1/2,0,0$ ) $x,0,z$<br>( $m_y$   $1/2,0,0$ ) | (8) m $0,y,z$<br>( $m_x$   $0,0,0$ )   |

For (1/2,1/2,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' ( $1/2,1/2,0$ )<br>(1  $1/2,1/2,0$ )'             | (2) 2' $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )'           | (3) 2 ( $0,1/2,0$ ) $0,y,0$<br>( $2_y$   $0,1/2,0$ ) | (4) 2 ( $1/2,0,0$ ) $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )   |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ ) | (6) b ( $0,1/2,0$ ) $x,y,0$<br>( $m_z$   $0,1/2,0$ ) | (7) m' $x,1/4,z$<br>( $m_y$   $0,1/2,0$ )'           | (8) b' ( $0,1/2,0$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

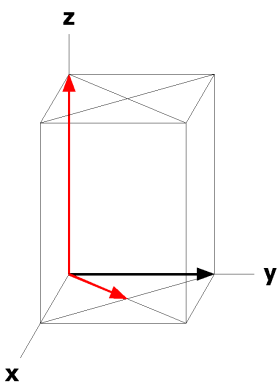
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(3) $\bar{x}+1/2,y,\bar{z}$ [ $u,\bar{v},w$ ] (7) $x+1/2,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
8 n .m'	x,1/4,z [u,0,w]	$\bar{x},1/4,z$ [ $u,0,\bar{w}$ ]	$\bar{x},3/4,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	x,3/4, $\bar{z}$ [ $\bar{u},0,w$ ]
8 m m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z$ [ $u,0,0$ ]	0,y+1/2, $\bar{z}$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
8 l ..2	1/4,0,z [0,0,w]	3/4,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	3/4,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,1/2,z [0,0,w]
8 k .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,1/2$ [ $u,0,\bar{w}$ ]	3/4, $\bar{y},1/2$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,1/2 [ $\bar{u},0,w$ ]
8 j .2'	1/4,y,0 [u,0,w]	3/4, $\bar{y}+1/2,0$ [ $u,0,\bar{w}$ ]	3/4, $\bar{y},0$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,0 [ $\bar{u},0,w$ ]
8 i 2'..	x,0,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0, $\bar{v},w$ ]	$\bar{x},0,1/2$ [0, $\bar{v},\bar{w}$ ]	x,1/2,1/2 [0,v, $\bar{w}$ ]
8 h 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,0$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0, $\bar{v},\bar{w}$ ]	x,1/2,0 [0,v, $\bar{w}$ ]
4 g mm'2'	0,1/4,z [u,0,0]	0,3/4, $\bar{z}$ [ $\bar{u},0,0$ ]		
4 f .2'/m'	1/4,1/4,1/2 [u,0,w]	3/4,1/4,1/2 [u,0, $\bar{w}$ ]		
4 e .2'/m'	1/4,1/4,0 [u,0,w]	3/4,1/4,0 [u,0, $\bar{w}$ ]		
4 d 2'/m..	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 c 2'/m..	0,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
4 b 2'2'2	1/4,0,1/2 [0,0,w]	3/4,0,1/2 [0,0, $\bar{w}$ ]		
4 a 2'2'2	1/4,0,0 [0,0,w]	3/4,0,0 [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

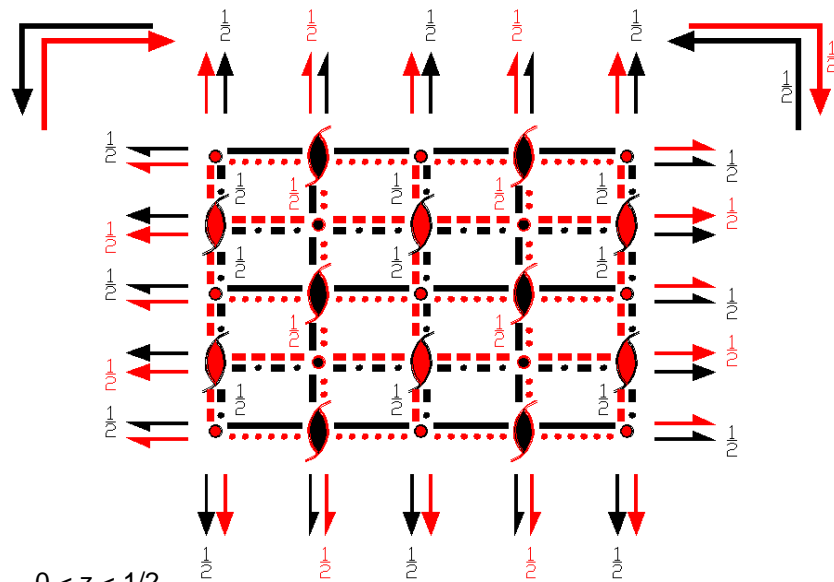
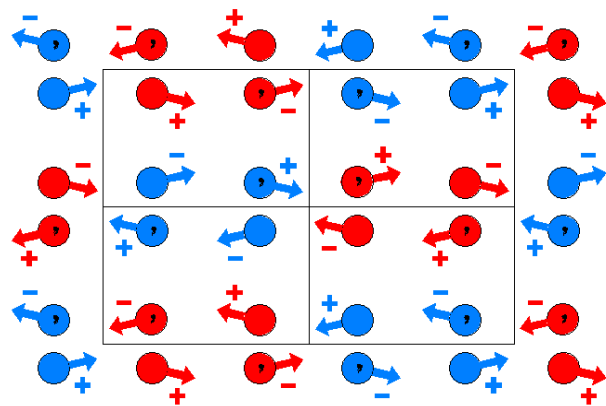
Along [0,1,0] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



$C_1mm'a$   
67.16.592

$mmm1'$   
 $C_12'/m2/m'2'/a$

Orthorhombic



**Origin** at center ( $2'/m$ ) at  $2'/m2_1/a$

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) $2'_1$ $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )'         | (3) $2$ $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )               | (4) $2'_1$ $x,0,0$<br>( $2_x$   $0,0,0$ )' |
| (5) $\bar{1}'$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ )' | (6) $a$ ( $1/2,0,0$ ) $x,y,0$<br>( $m_z$   $1/2,0,0$ ) | (7) $a'$ ( $1/2,0,0$ ) $x,0,z$<br>( $m_y$   $1/2,0,0$ )' | (8) $m$ $0,y,z$<br>( $m_x$   $0,0,0$ )     |

For (1/2,1/2,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ ( $1/2,1/2,0$ )<br>(1  $1/2,1/2,0$ )'           | (2) $2$ $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )               | (3) $2'_1$ ( $0,1/2,0$ ) $0,y,0$<br>( $2_y$   $0,1/2,0$ )' | (4) $2$ ( $1/2,0,0$ ) $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )   |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ ) | (6) $b'$ ( $0,1/2,0$ ) $x,y,0$<br>( $m_z$   $0,1/2,0$ )' | (7) $m$ $x,1/4,z$<br>( $m_y$   $0,1/2,0$ )                 | (8) $b'$ ( $0,1/2,0$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |

For (0,0,1)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ ( $0,0,1$ )<br>(1  $0,0,1$ )'             | (2) $2$ ( $0,0,1$ ) $1/4,0,z$<br>( $2_z$   $1/2,0,1$ )     | (3) $2'_1$ $1/4,y,1/2$<br>( $2_y$   $1/2,0,1$ )'       | (4) $2$ $x,0,1/2$<br>( $2_x$   $0,0,1$ )             |
| (5) $\bar{1}$ $0,0,1/2$<br>( $\bar{1}$   $0,0,1$ ) | (6) $a'$ ( $1/2,0,0$ ) $x,y,1/2$<br>( $m_z$   $1/2,0,1$ )' | (7) $n$ ( $1/2,0,1$ ) $x,0,z$<br>( $m_y$   $1/2,0,1$ ) | (8) $c'$ ( $0,0,1$ ) $0,y,z$<br>( $m_x$   $0,0,1$ )' |

For (1/2,1/2,1) + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t$ ( $1/2,1/2,1$ )<br>(1  $1/2,1/2,1$ )                 | (2) $2'_1$ ( $0,0,1$ ) $0,1/4,z$<br>( $2_z$   $0,1/2,1$ )' | (3) $2$ ( $0,1/2,0$ ) $0,y,1/2$<br>( $2_y$   $0,1/2,1$ ) | (4) $2'_1$ ( $1/2,0,0$ ) $x,1/4,1/2$<br>( $2_x$   $1/2,1/2,1$ )' |
| (5) $\bar{1}'$ $1/4,1/4,1/2$<br>( $\bar{1}$   $1/2,1/2,1$ )' | (6) $b$ ( $0,1/2,0$ ) $x,y,1/2$<br>( $m_z$   $0,1/2,1$ )   | (7) $c'$ ( $0,0,1$ ) $x,1/4,z$<br>( $m_y$   $0,1/2,1$ )' | (8) $n$ ( $0,1/2,1$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,1$ )       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

**Positions**

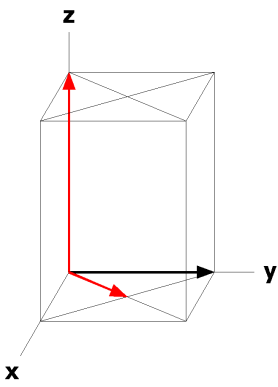
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) + (0,0,1)' +	(1/2,1/2,0)' + (1/2,1/2,1) +		
32 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z$ [ $u,v,\bar{w}$ ] (6) $x+1/2,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x}+1/2,y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) $x+1/2,\bar{y},z$ [ $u,\bar{v},w$ ]	(4) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
16 n .m.	x,1/4,z [0,v,0]	$\bar{x},1/4,z$ [0, $\bar{v}$ ,0]	$\bar{x},3/4,\bar{z}$ [0,v,0]	x,3/4, $\bar{z}$ [0,v,0]
16 m m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z$ [ $\bar{u},0,0$ ]	0,y+1/2, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
16 l ..2'	1/4,0,z [u,v,0]	3/4,1/2, $\bar{z}$ [ $u,\bar{v},0$ ]	3/4,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,1/2,z [ $\bar{u},v,0$ ]
16 k .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,1/2$ [ $\bar{u},0,w$ ]	3/4, $\bar{y},1/2$ [u,0,w]	1/4,y+1/2,1/2 [ $\bar{u},0,w$ ]
16 j .2.	1/4,y,0 [0,v,0]	3/4, $\bar{y}+1/2,0$ [0, $\bar{v},0$ ]	3/4, $\bar{y},0$ [0, $\bar{v},0$ ]	1/4,y+1/2,0 [0,v,0]
16 i 2..	x,0,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},0,1/2$ [u,0,0]	x,1/2,1/2 [ $\bar{u},0,0$ ]
16 h 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,0$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0, $\bar{v},\bar{w}$ ]	x,1/2,0 [0,v, $\bar{w}$ ]
8 g mm2	0,1/4,z [0,0,0]	0,3/4, $\bar{z}$ [0,0,0]		
8 f .2'/m.	1/4,1/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]		
8 e .2/m.	1/4,1/4,0 [0,v,0]	3/4,1/4,0 [0, $\bar{v},0$ ]		
8 d 2/m..	0,0,1/2 [u,0,0]	0,1/2,1/2 [ $\bar{u},0,0$ ]		
8 c 2'/m..	0,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
8 b 22'2'	1/4,0,1/2 [u,0,0]	3/4,0,1/2 [u,0,0]		
8 a 2'22'	1/4,0,0 [0,v,0]	3/4,0,0 [0, $\bar{v},0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

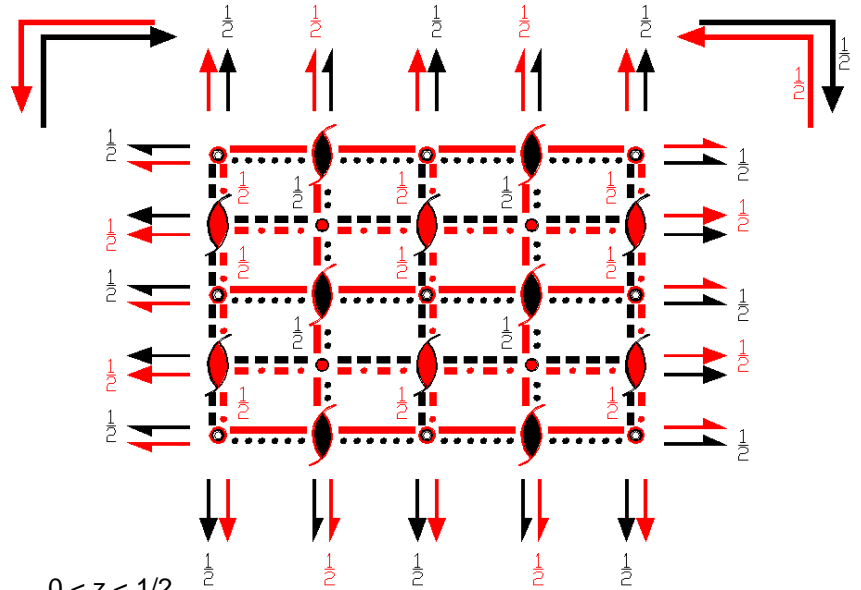
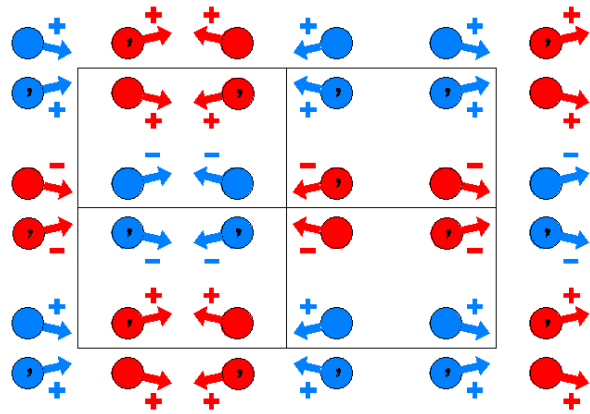
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



$C_1 m' m a'$   
67.17.593

$mmm1'$   
 $C_1 2'/m'2/m2'/a'$

Orthorhombic



**Origin** at center ( $2'/m'$ ) at  $2'/m'2_1'/aa'$

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                               | (2) $2'$ $1/4,0,z$<br>( $2_z$   $1/2,0,0$ )'             | (3) $2$ $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )             | (4) $2'$ $x,0,0$<br>( $2_x$   $0,0,0$ )' |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ ) | (6) $a'$ ( $1/2,0,0$ ) $x,y,0$<br>( $m_z$   $1/2,0,0$ )' | (7) $a$ ( $1/2,0,0$ ) $x,0,z$<br>( $m_y$   $1/2,0,0$ ) | (8) $m'$ $0,y,z$<br>( $m_x$   $0,0,0$ )' |

For (1/2,1/2,0)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t'$ ( $1/2,1/2,0$ )<br>(1  $1/2,1/2,0$ )'              | (2) $2$ $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )             | (3) $2'$ ( $0,1/2,0$ ) $0,y,0$<br>( $2_y$   $0,1/2,0$ )' | (4) $2$ ( $1/2,0,0$ ) $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ ) |
| (5) $\bar{1}'$ $1/4,1/4,0$<br>( $\bar{1}'$   $1/2,1/2,0$ )' | (6) $b$ ( $0,1/2,0$ ) $x,y,0$<br>( $m_z$   $0,1/2,0$ ) | (7) $m'$ $x,1/4,z$<br>( $m_y$   $0,1/2,0$ )'             | (8) $b$ ( $0,1/2,0$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ ) |

For (0,0,1)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t'$ ( $0,0,1$ )<br>(1  $0,0,1$ )'                | (2) $2$ ( $0,0,1$ ) $1/4,0,z$<br>( $2_z$   $1/2,0,1$ )   | (3) $2'$ $1/4,y,1/2$<br>( $2_y$   $1/2,0,1$ )'           | (4) $2$ $x,0,1/2$<br>( $2_x$   $0,0,1$ )           |
| (5) $\bar{1}'$ $0,0,1/2$<br>( $\bar{1}'$   $0,0,1$ )' | (6) $a$ ( $1/2,0,0$ ) $x,y,1/2$<br>( $m_z$   $1/2,0,1$ ) | (7) $n'$ ( $1/2,0,1$ ) $x,0,z$<br>( $m_y$   $1/2,0,1$ )' | (8) $c$ ( $0,0,1$ ) $0,y,z$<br>( $m_x$   $0,0,1$ ) |

For (1/2,1/2,1) + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t$ ( $1/2,1/2,1$ )<br>(1  $1/2,1/2,1$ )               | (2) $2'$ ( $0,0,1$ ) $0,1/4,z$<br>( $2_z$   $0,1/2,1$ )'   | (3) $2$ ( $0,1/2,0$ ) $0,y,1/2$<br>( $2_y$   $0,1/2,1$ ) | (4) $2'$ ( $1/2,0,0$ ) $x,1/4,1/2$<br>( $2_x$   $1/2,1/2,1$ )' |
| (5) $\bar{1}$ $1/4,1/4,1/2$<br>( $\bar{1}$   $1/2,1/2,1$ ) | (6) $b'$ ( $0,1/2,0$ ) $x,y,1/2$<br>( $m_z$   $0,1/2,1$ )' | (7) $c$ ( $0,0,1$ ) $x,1/4,z$<br>( $m_y$   $0,1/2,1$ )   | (8) $n'$ ( $0,1/2,1$ ) $1/4,y,z$<br>( $m_x$   $1/2,1/2,1$ )'   |



**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

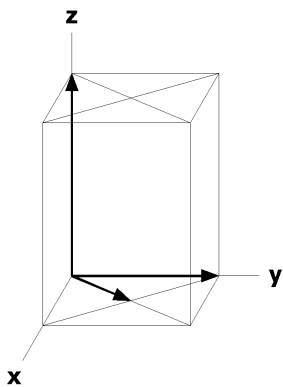
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) + (0,0,1)' +	(1/2,1/2,0)' + (1/2,1/2,1) +		
32 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z$ [u,v, $\bar{w}$ ] (6) $x+1/2,y,\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x}+1/2,y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) $x+1/2,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
16 n .m'	x,1/4,z [u,0,w]	$\bar{x},1/4,z$ [ $\bar{u},0,w$ ]	$\bar{x},3/4,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	x,3/4, $\bar{z}$ [u,0, $\bar{w}$ ]
16 m m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z$ [0, $\bar{v},w$ ]	0,y+1/2, $\bar{z}$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
16 l ..2'	1/4,0,z [u,v,0]	3/4,1/2, $\bar{z}$ [u, $\bar{v},0$ ]	3/4,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,1/2,z [ $\bar{u},v,0$ ]
16 k .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,1/2$ [ $\bar{u},0,w$ ]	3/4, $\bar{y},1/2$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,1/2 [u,0, $\bar{w}$ ]
16 j .2.	1/4,y,0 [0,v,0]	3/4, $\bar{y}+1/2,0$ [0, $\bar{v},0$ ]	3/4, $\bar{y},0$ [0,v,0]	1/4,y+1/2,0 [0, $\bar{v},0$ ]
16 i 2..	x,0,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	x,1/2,1/2 [u,0,0]
16 h 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,0$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0,v,w]	x,1/2,0 [0, $\bar{v},w$ ]
8 g m'm'2	0,1/4,z [0,0,w]	0,3/4, $\bar{z}$ [0,0,w]		
8 f .2'/m'	1/4,1/4,1/2 [u,0,w]	3/4,1/4,1/2 [ $\bar{u},0,w$ ]		
8 e .2/m'	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
8 d 2/m'..	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
8 c 2'/m'..	0,0,0 [0,v,w]	0,1/2,0 [0, $\bar{v},w$ ]		
8 b 2'2'2'	1/4,0,1/2 [u,0,0]	3/4,0,1/2 [ $\bar{u},0,0$ ]		
8 a 2'2'2'	1/4,0,0 [0,v,0]	3/4,0,0 [0,v,0]		

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>c</sub>-2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,1/2

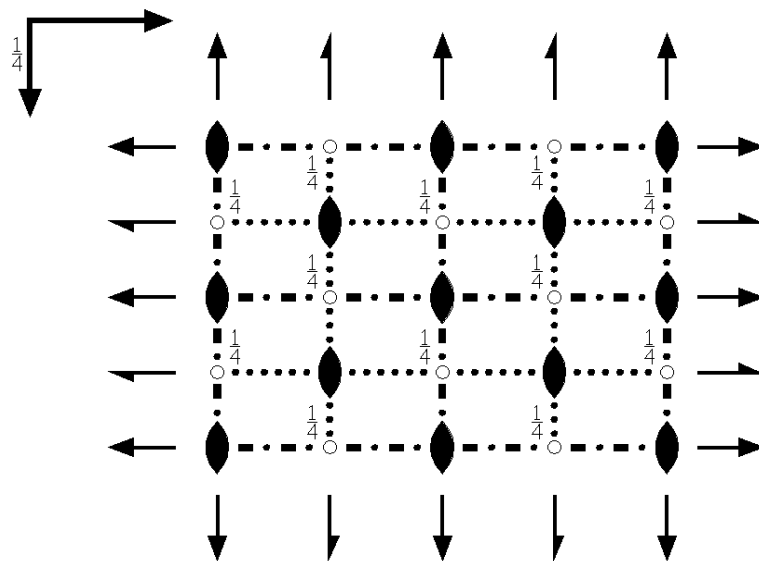
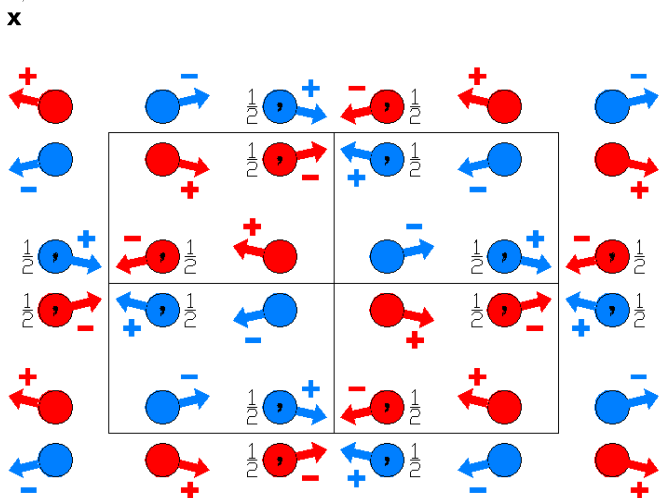
Along [0,1,0] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,0



Ccca  
68.1.594

mmm  
C2/c2/c2/a

Orthorhombic



**Origin** at 222 at  $2/n2/n2$  at  $0, 1/4, 1/4$  from  $\bar{1}$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                 | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                 |
| (5) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$  0,1/2,1/2) | (6) b (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>  0,1/2,1/2) | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2) | (8) n (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>  0,1/2,1/2) |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                 | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)         | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$  1/2,0,1/2) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2) | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2) | (8) c (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,0,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

**Positions**

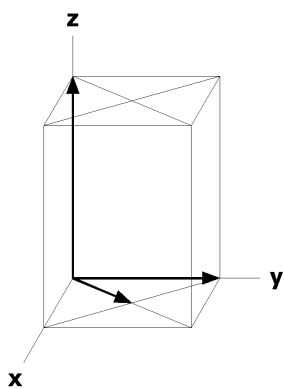
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 i 1	(1) x,y,z [u,v,w] (5) $\bar{x}, \bar{y} + 1/2, \bar{z} + 1/2$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ] (6) x,y+1/2, $\bar{z} + 1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ] (7) x, $\bar{y} + 1/2, z + 1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ] (8) $\bar{x}, y + 1/2, z + 1/2$ [u, $\bar{v}, \bar{w}$ ]
8 h ..2	1/4, 1/4, z [0,0,w]	3/4, 1/4, $\bar{z}$ [0,0, $\bar{w}$ ]	3/4, 1/4, $\bar{z} + 1/2$ [0,0,w]	1/4, 1/4, z+1/2 [0,0, $\bar{w}$ ]
8 g ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z} + 1/2$ [0,0,w]	0,1/2, z+1/2 [0,0, $\bar{w}$ ]
8 f .2.	0,y,0 [0,v,0]	1/2, $\bar{y} + 1/2, 0$ [0, $\bar{v}, 0$ ]	0, $\bar{y} + 1/2, 1/2$ [0,v,0]	1/2, y, 1/2 [0, $\bar{v}, 0$ ]
8 e 2..	x,0,0 [u,0,0]	$\bar{x} + 1/2, 1/2, 0$ [ $\bar{u}, 0, 0$ ]	$\bar{x}, 1/2, 1/2$ [u,0,0]	x+1/2, 0, 1/2 [ $\bar{u}, 0, 0$ ]
8 d $\bar{1}$	0,1/4,1/4 [u,v,w]	1/2, 1/4, 1/4 [ $\bar{u}, \bar{v}, w$ ]	0, 1/4, 3/4 [ $\bar{u}, v, \bar{w}$ ]	1/2, 1/4, 3/4 [u, $\bar{v}, \bar{w}$ ]
8 c $\bar{1}$	1/4, 0, 1/4 [u,v,w]	1/4, 1/2, 1/4 [ $\bar{u}, \bar{v}, w$ ]	3/4, 0, 3/4 [ $\bar{u}, v, \bar{w}$ ]	3/4, 1/2, 3/4 [u, $\bar{v}, \bar{w}$ ]
4 b 222	0,0,1/2 [0,0,0]	0,1/2,0 [0,0,0]		
4 a 222	0,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_c$ -2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,1/4,z

Along [1,0,0]  $p_{2a}$ -2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a}$ -2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0

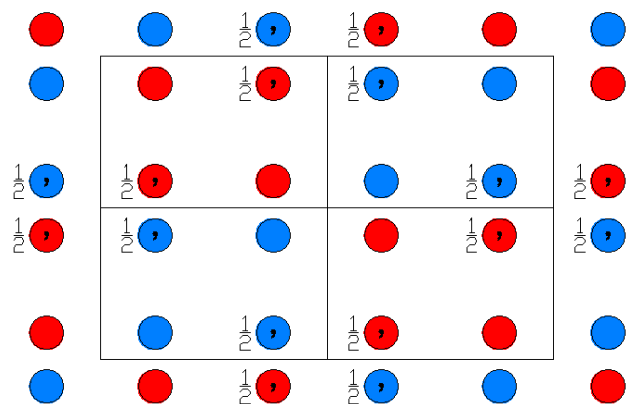


Ccca1'  
68.2.595

mmm1'  
C2/c2/c2/a1'

Orthorhombic

1'



Origin at 2221' at  $2/n2/n21'$  at  $0, 1/4, 1/4$  from  $\bar{1}1'$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                 | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                 |
| (5) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$  0,1/2,1/2) | (6) b (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>  0,1/2,1/2) | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2) | (8) n (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>  0,1/2,1/2) |

For (1/2,1/2,0) + set

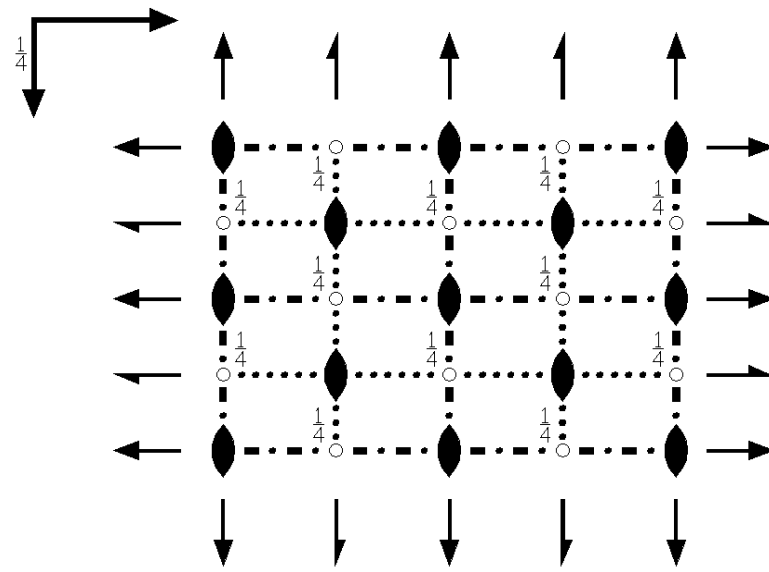
- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                 | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)         | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$  1/2,0,1/2) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2) | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2) | (8) c (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,0,1/2) |

For (0,0,0)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1'<br>(1 0,0,0)'                                  | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                 | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                 | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                 |
| (5) $\bar{1}'$ 0,1/4,1/4<br>( $\bar{1}'$  0,1/2,1/2)' | (6) b' (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>  0,1/2,1/2)' | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) n' (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>  0,1/2,1/2)' |

For (1/2,1/2,0)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' (1/2,1/2,0)<br>(1 1/2,1/2,0)'                  | (2) 2' 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)'         | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}'$ 1/4,0,1/4<br>( $\bar{1}'$  1/2,0,1/2)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2)' | (8) c' (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,0,1/2)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5);1'.

**Positions**

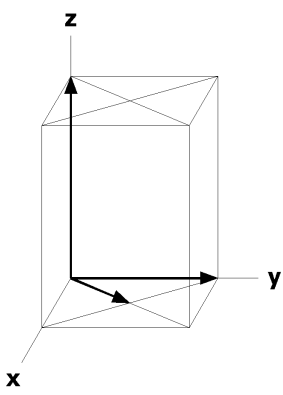
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) + (0,0,0)'	(1/2,1/2,0) + (1/2,1/2,0)'		
16	i 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{x},y,\bar{z}$ [0,0,0]	(4) $x,\bar{y},\bar{z}$ [0,0,0]
		(5) $\bar{x},\bar{y}+1/2,\bar{z}+1/2$ [0,0,0]	(6) $x,y+1/2,\bar{z}+1/2$ [0,0,0]	(7) $x,\bar{y}+1/2,z+1/2$ [0,0,0]	(8) $\bar{x},y+1/2,z+1/2$ [0,0,0]
8	h ..21'	1/4,1/4,z [0,0,0]	3/4,1/4, $\bar{z}$ [0,0,0]	3/4,1/4, $\bar{z}+1/2$ [0,0,0]	1/4,1/4,z+1/2 [0,0,0]
8	g ..21'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,1/2, $\bar{z}+1/2$ [0,0,0]	0,1/2,z+1/2 [0,0,0]
8	f .2.1'	0,y,0 [0,0,0]	1/2, $\bar{y}+1/2,0$ [0,0,0]	0, $\bar{y}+1/2,1/2$ [0,0,0]	1/2,y,1/2 [0,0,0]
8	e 2..1'	x,0,0 [0,0,0]	$\bar{x}+1/2,1/2,0$ [0,0,0]	$\bar{x},1/2,1/2$ [0,0,0]	x+1/2,0,1/2 [0,0,0]
8	d $\bar{1}1'$	0,1/4,1/4 [0,0,0]	1/2,1/4,1/4 [0,0,0]	0,1/4,3/4 [0,0,0]	1/2,1/4,3/4 [0,0,0]
8	c $\bar{1}1'$	1/4,0,1/4 [0,0,0]	1/4,1/2,1/4 [0,0,0]	3/4,0,3/4 [0,0,0]	3/4,1/2,3/4 [0,0,0]
4	b 2221'	0,0,1/2 [0,0,0]	0,1/2,0 [0,0,0]		
4	a 2221'	0,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

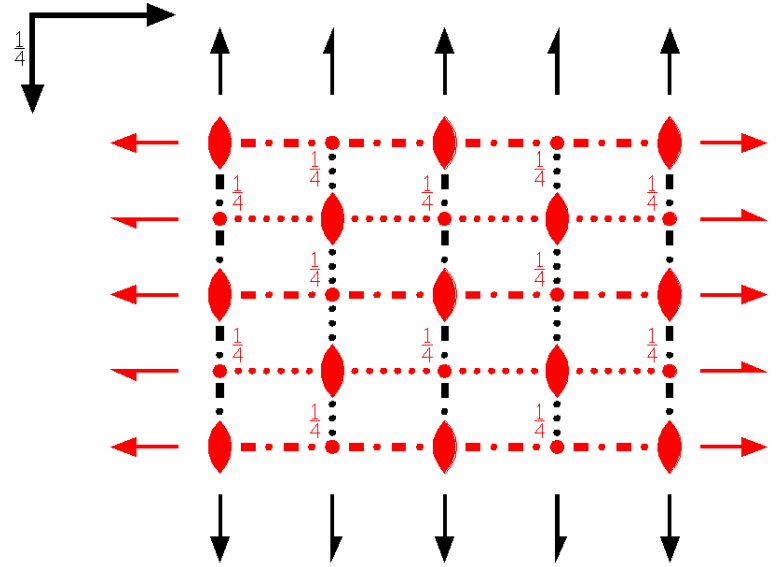
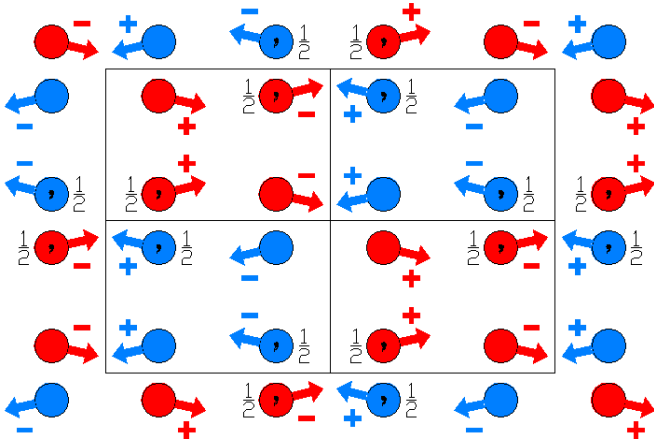
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Cc'ca  
68.3.596

m'mm  
C2/c'2'/c2'/a

Orthorhombic



Origin at  $22'2'$  at  $2/n'2'/n2'$  at  $0, 1/4, 1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |   |
|---|--|--|---|
| (1) 1<br>(1 0,0,0)                                  | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)'             | (3) $2'$ 0,y,0<br>( $2_y$  0,0,0)'             | (4) 2 x,0,0<br>( $2_x$  0,0,0)                  |
| (5) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$  0,1/2,1/2)' | (6) b (0,1/2,0) x,y,1/4<br>( $m_z$  0,1/2,1/2) | (7) c (0,0,1/2) x,1/4,z<br>( $m_y$  0,1/2,1/2) | (8) n (0,1/2,1/2) 0,y,z<br>( $m_x$  0,1/2,1/2)' |

For (1/2,1/2,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                  | (2) $2'$ 1/4,1/4,z<br>( $2_z$  1/2,1/2,0)'     | (3) $2'$ (0,1/2,0) 1/4,y,0<br>( $2_y$  1/2,1/2,0)' | (4) 2 (1/2,0,0) x,1/4,0<br>( $2_x$  1/2,1/2,0)   |
| (5) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$  1/2,0,1/2)' | (6) a (1/2,0,0) x,y,1/4<br>( $m_z$  1/2,0,1/2) | (7) n (1/2,0,1/2) x,0,z<br>( $m_y$  1/2,0,1/2)     | (8) c' (0,0,1/2) 1/4,y,z<br>( $m_x$  1/2,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

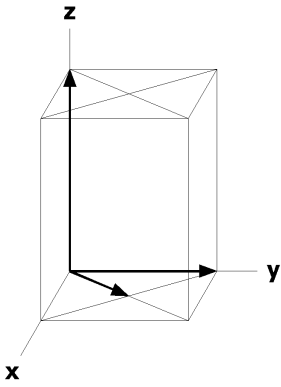
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v}$ ,w]	(4) $x,\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y+1/2,z+1/2$ [ $\bar{u},v,w$ ]
8 h ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [u, $\bar{v}$ ,0]	3/4,1/4, $\bar{z}+1/2$ [ $\bar{u},\bar{v}$ ,0]	1/4,1/4,z+1/2 [ $\bar{u},v,0$ ]
8 g ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [u, $\bar{v}$ ,0]	0,1/2, $\bar{z}+1/2$ [ $\bar{u},\bar{v}$ ,0]	0,1/2,z+1/2 [ $\bar{u},v,0$ ]
8 f .2'	0,y,0 [u,0,w]	1/2, $\bar{y}+1/2,0$ [u,0, $\bar{w}$ ]	0, $\bar{y}+1/2,1/2$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,1/2 [ $\bar{u},0,w$ ]
8 e 2..	x,0,0 [u,0,0]	$\bar{x}+1/2,1/2,0$ [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	x+1/2,0,1/2 [ $\bar{u},0,0$ ]
8 d $\bar{1}'$	0,1/4,1/4 [0,0,0]	1/2,1/4,1/4 [0,0,0]	0,1/4,3/4 [0,0,0]	1/2,1/4,3/4 [0,0,0]
8 c $\bar{1}'$	1/4,0,1/4 [0,0,0]	1/4,1/2,1/4 [0,0,0]	3/4,0,3/4 [0,0,0]	3/4,1/2,3/4 [0,0,0]
4 b 22'2'	0,0,1/2 [u,0,0]	0,1/2,0 [ $\bar{u},0,0$ ]		
4 a 22'2'	0,0,0 [u,0,0]	0,1/2,1/2 [ $\bar{u},0,0$ ]		

### Symmetry of Special Projections

Along [0,0,1]  $p_c$ -2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,1/4,z

Along [1,0,0]  $p_2$ mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

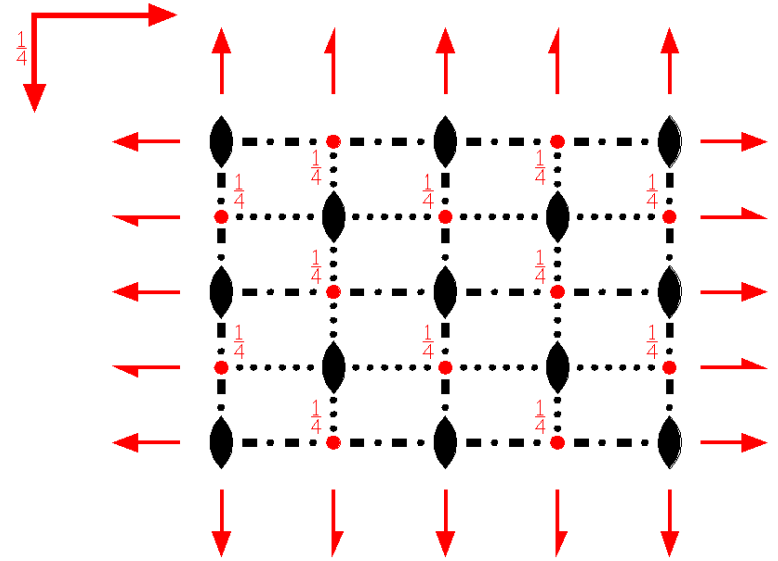
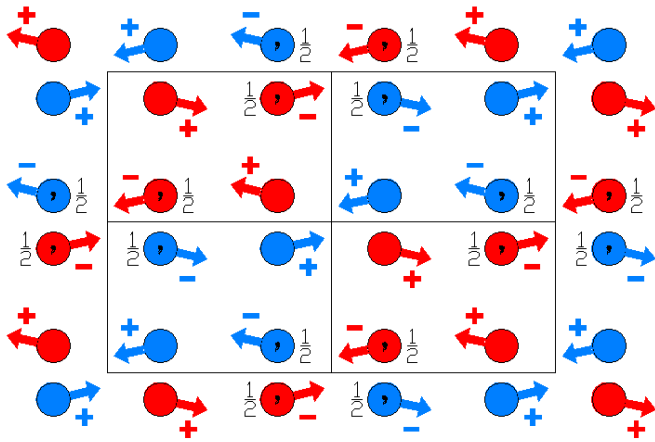
Along [0,1,0]  $p_{2a}$ -2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



Ccca'  
68.4.597

mmm'  
C2'/c2'/c2/a'

Orthorhombic



Origin at 2'2'2 at 2'/n2'/n2 at 0,1/4,1/4 from  $\bar{1}$ '

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                  | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'               | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'               |
| (5) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$  0,1/2,1/2)' | (6) b (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>  0,1/2,1/2)' | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2) | (8) n (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>  0,1/2,1/2) |

For (1/2,1/2,0) + set

- |  |   |  |  |
|--|---|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                     | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)            | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ ' 1/4,0,1/4<br>( $\bar{1}$ ' 1/2,0,1/2)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub> ' 1/2,0,1/2)' | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub> ' 1/2,0,1/2)  | (8) c (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub> ' 1/2,0,1/2)  |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

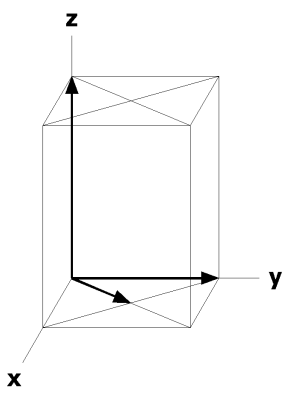
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 i 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $\bar{x},y,\bar{z} [u,\bar{v},w]$	(4) $x,\bar{y},\bar{z} [\bar{u},v,w]$
	(5) $\bar{x},\bar{y}+1/2,\bar{z}+1/2 [\bar{u},\bar{v},\bar{w}]$	(6) $x,y+1/2,\bar{z}+1/2 [u,v,\bar{w}]$	(7) $x,\bar{y}+1/2,z+1/2 [\bar{u},v,\bar{w}]$	(8) $\bar{x},y+1/2,z+1/2 [u,\bar{v},\bar{w}]$
8 h ..2	$1/4,1/4,z [0,0,w]$	$3/4,1/4,\bar{z} [0,0,w]$	$3/4,1/4,\bar{z}+1/2 [0,0,\bar{w}]$	$1/4,1/4,z+1/2 [0,0,\bar{w}]$
8 g ..2	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,w]$	$0,1/2,\bar{z}+1/2 [0,0,\bar{w}]$	$0,1/2,z+1/2 [0,0,\bar{w}]$
8 f .2'	$0,y,0 [u,0,w]$	$1/2,\bar{y}+1/2,0 [\bar{u},0,w]$	$0,\bar{y}+1/2,1/2 [\bar{u},0,\bar{w}]$	$1/2,y,1/2 [u,0,\bar{w}]$
8 e 2'..	$x,0,0 [0,v,w]$	$\bar{x}+1/2,1/2,0 [0,\bar{v},w]$	$\bar{x},1/2,1/2 [0,\bar{v},\bar{w}]$	$x+1/2,0,1/2 [0,v,\bar{w}]$
8 d $\bar{1}'$	$0,1/4,1/4 [0,0,0]$	$1/2,1/4,1/4 [0,0,0]$	$0,1/4,3/4 [0,0,0]$	$1/2,1/4,3/4 [0,0,0]$
8 c $\bar{1}'$	$1/4,0,1/4 [0,0,0]$	$1/4,1/2,1/4 [0,0,0]$	$3/4,0,3/4 [0,0,0]$	$3/4,1/2,3/4 [0,0,0]$
4 b 2'2'2	$0,0,1/2 [0,0,w]$	$0,1/2,0 [0,0,\bar{w}]$		
4 a 2'2'2	$0,0,0 [0,0,w]$	$0,1/2,1/2 [0,0,\bar{w}]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p2mm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,0,1/4$

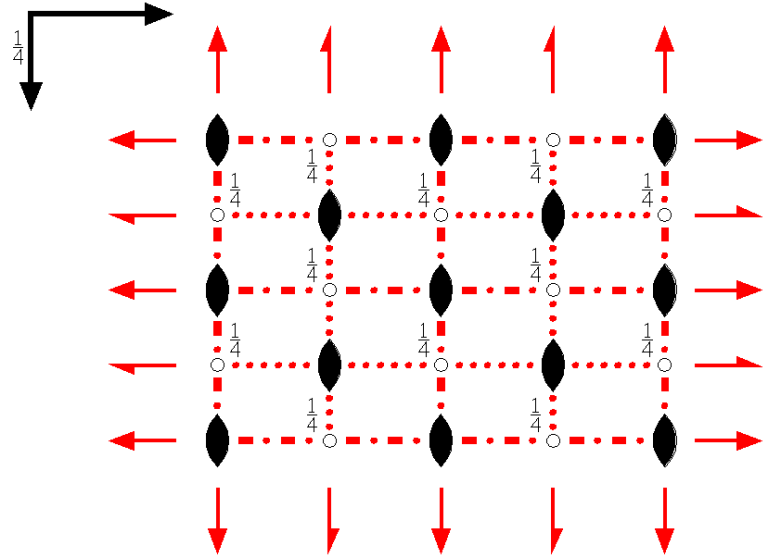
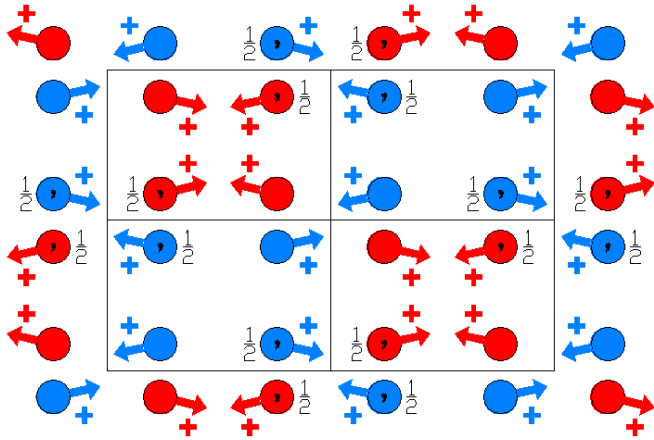
Along  $[0,1,0]$   $p_{2a}2m'm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at  $0,y,0$



Cc'c'a  
68.5.598

m'm'm  
C2'/c'2'/c'2'/a

Orthorhombic



**Origin** at 2'2'2 at 2'/n'2'/n'2 at 0,1/4,1/4 from  $\bar{1}$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                |
| (5) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$  0,1/2,1/2) | (6) b (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>  0,1/2,1/2) | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) n (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>  0,1/2,1/2)' |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                 | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)         | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$  1/2,0,1/2) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2) | (7) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2)' | (8) c' (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

### Positions

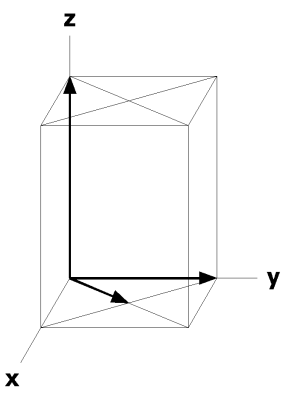
Multiplicity, Wyckoff letter, Site Symmetry.		Coordinates						
		(0,0,0) +	(1/2,1/2,0) +					
16 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(4) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(5) $\bar{x},\bar{y}+1/2,\bar{z}+1/2$ [ $u,v,w$ ]	(6) $x,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(8) $\bar{x},y+1/2,z+1/2$ [ $\bar{u},v,w$ ]
8 h ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0,w]	3/4,1/4, $\bar{z}+1/2$ [0,0,w]	1/4,1/4,z+1/2 [0,0,w]				
8 g ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	0,1/2,z+1/2 [0,0,w]				
8 f .2'	0,y,0 [u,0,w]	1/2, $\bar{y}+1/2,0$ [ $\bar{u},0,w$ ]	0, $\bar{y}+1/2,1/2$ [u,0,w]	1/2,y,1/2 [ $\bar{u},0,w$ ]				
8 e 2'..	x,0,0 [0,v,w]	$\bar{x}+1/2,1/2,0$ [ $0,\bar{v},w$ ]	$\bar{x},1/2,1/2$ [0,v,w]	x+1/2,0,1/2 [ $0,\bar{v},w$ ]				
8 d $\bar{1}$	0,1/4,1/4 [u,v,w]	1/2,1/4,1/4 [ $\bar{u},\bar{v},w$ ]	0,1/4,3/4 [u, $\bar{v},w$ ]	1/2,1/4,3/4 [ $\bar{u},v,w$ ]				
8 c $\bar{1}$	1/4,0,1/4 [u,v,w]	1/4,1/2,1/4 [ $\bar{u},\bar{v},w$ ]	3/4,0,3/4 [u, $\bar{v},w$ ]	3/4,1/2,3/4 [ $\bar{u},v,w$ ]				
4 b 2'2'2	0,0,1/2 [0,0,w]	0,1/2,0 [0,0,w]						
4 a 2'2'2	0,0,0 [0,0,w]	0,1/2,1/2 [0,0,w]						

### Symmetry of Special Projections

Along [0,0,1]  $p_c2mm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

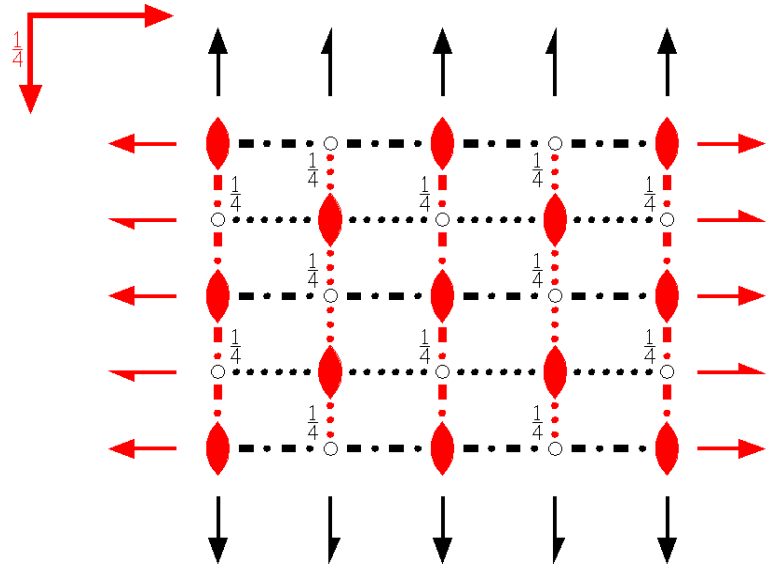
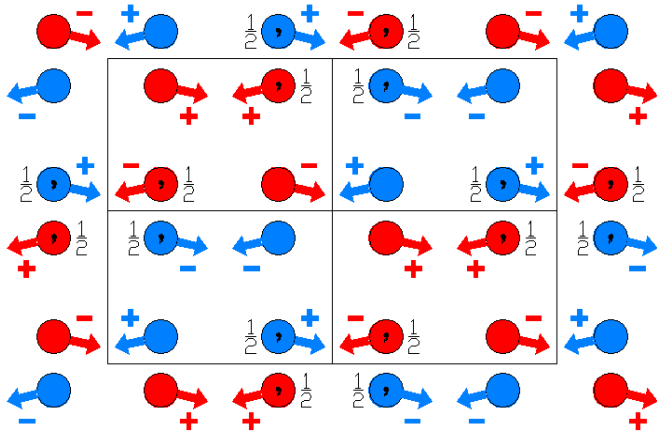
Along [0,1,0]  $p2'mm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Ccc'a'  
68.6.599

mm'm'  
C2/c2'/c'2'/a'

Orthorhombic



Origin at  $22'2'$  at  $2/n2'/n'2'$  at  $0, 1/4, 1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |  |   |   |  |
|--|---|---|--|
| (1) 1<br>(1 0,0,0)                                 | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)'              | (3) $2'$ 0,y,0<br>( $2_y$  0,0,0)'              | (4) 2 x,0,0<br>( $2_x$  0,0,0)                 |
| (5) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$  0,1/2,1/2) | (6) b (0,1/2,0) x,y,1/4<br>( $m_z$  0,1/2,1/2)' | (7) c (0,0,1/2) x,1/4,z<br>( $m_y$  0,1/2,1/2)' | (8) n (0,1/2,1/2) 0,y,z<br>( $m_x$  0,1/2,1/2) |

For (1/2,1/2,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                 | (2) $2'$ 1/4,1/4,z<br>( $2_z$  1/2,1/2,0)'       | (3) $2'$ (0,1/2,0) 1/4,y,0<br>( $2_y$  1/2,1/2,0)' | (4) 2 (1/2,0,0) x,1/4,0<br>( $2_x$  1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$  1/2,0,1/2) | (6) a' (1/2,0,0) x,y,1/4<br>( $m_z$  1/2,0,1/2)' | (7) n' (1/2,0,1/2) x,0,z<br>( $m_y$  1/2,0,1/2)'   | (8) c (0,0,1/2) 1/4,y,z<br>( $m_x$  1/2,0,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

**Positions**

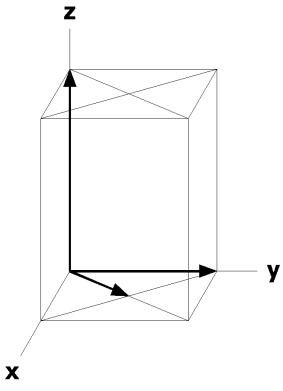
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y}+1/2,\bar{z}+1/2$ [u,v,w]	(6) x,y+1/2, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(7) x, $\bar{y}+1/2,z+1/2$ [u, $\bar{v}$ ,w]	(8) $\bar{x},y+1/2,z+1/2$ [u, $\bar{v},\bar{w}$ ]
8 h ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [u, $\bar{v}$ ,0]	3/4,1/4, $\bar{z}+1/2$ [u,v,0]	1/4,1/4,z+1/2 [u, $\bar{v}$ ,0]
8 g ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [u, $\bar{v}$ ,0]	0,1/2, $\bar{z}+1/2$ [u,v,0]	0,1/2,z+1/2 [u, $\bar{v}$ ,0]
8 f .2'	0,y,0 [u,0,w]	1/2, $\bar{y}+1/2,0$ [u,0, $\bar{w}$ ]	0, $\bar{y}+1/2,1/2$ [u,0,w]	1/2,y,1/2 [u,0, $\bar{w}$ ]
8 e 2..	x,0,0 [u,0,0]	$\bar{x}+1/2,1/2,0$ [u,0,0]	$\bar{x},1/2,1/2$ [u,0,0]	x+1/2,0,1/2 [u,0,0]
8 d $\bar{1}$	0,1/4,1/4 [u,v,w]	1/2,1/4,1/4 [u,v, $\bar{w}$ ]	0,1/4,3/4 [u, $\bar{v}$ ,w]	1/2,1/4,3/4 [u, $\bar{v},\bar{w}$ ]
8 c $\bar{1}$	1/4,0,1/4 [u,v,w]	1/4,1/2,1/4 [u,v, $\bar{w}$ ]	3/4,0,3/4 [u, $\bar{v}$ ,w]	3/4,1/2,3/4 [u, $\bar{v},\bar{w}$ ]
4 b 22'2'	0,0,1/2 [u,0,0]	0,1/2,0 [u,0,0]		
4 a 22'2'	0,0,0 [u,0,0]	0,1/2,1/2 [u,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] p<sub>2a</sub>'2mm  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

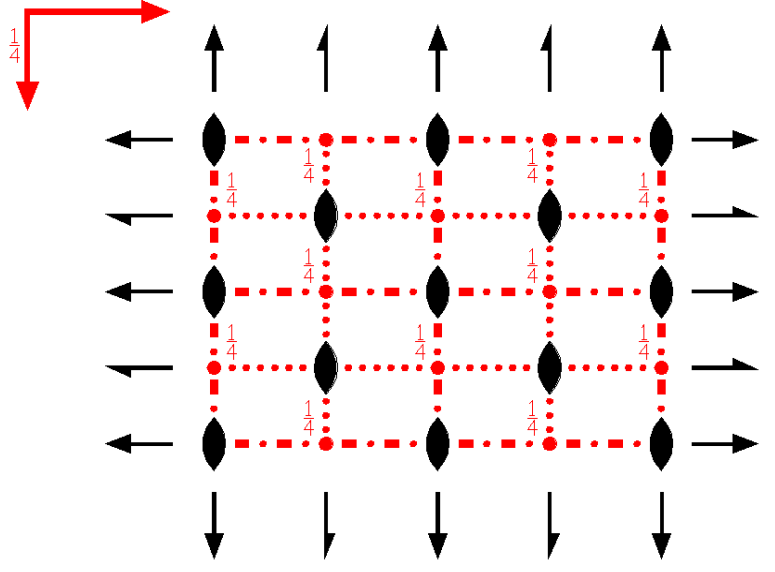
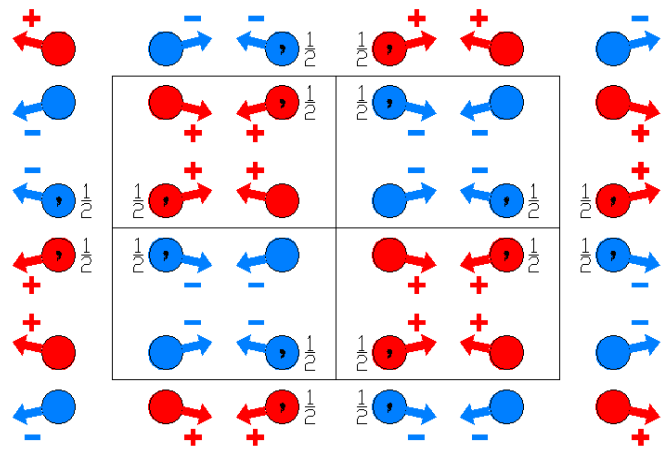
Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



Cc'c'a'  
68.7.600

m'm'm'  
C2/c'2/c'2/a'

Orthorhombic



Origin at 222 at  $2/n'2/n'2$  at  $0, 1/4, 1/4$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                                    | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                  |
| (5) $\bar{1}'$ 0,1/4,1/4<br>( $\bar{1}'$  0,1/2,1/2)' | (6) b (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>  0,1/2,1/2)' | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) n (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>  0,1/2,1/2)' |

For (1/2,1/2,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)                    | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)           | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) $\bar{1}'$ 1/4,0,1/4<br>( $\bar{1}'$  1/2,0,1/2)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2)' | (8) c' (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

**Positions**

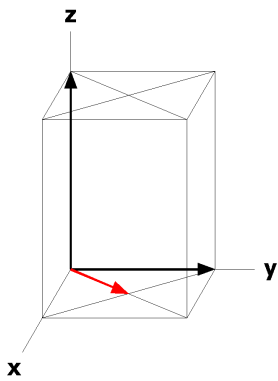
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0) +		
16 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x, \bar{y}, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]
	(5) $\bar{x}, \bar{y}+1/2, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(6) $x, y+1/2, \bar{z}+1/2$ [ $u, v, \bar{w}$ ]	(7) $x, \bar{y}+1/2, z+1/2$ [ $u, \bar{v}, w$ ]	(8) $\bar{x}, y+1/2, z+1/2$ [ $\bar{u}, v, w$ ]
8 h ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0, $\bar{w}$ ]	3/4,1/4, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/4,1/4,z+1/2 [0,0,w]
8 g ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0,w]
8 f .2.	0,y,0 [0,v,0]	1/2, $\bar{y}+1/2,0$ [0, $\bar{v},0$ ]	0, $\bar{y}+1/2,1/2$ [0, $\bar{v},0$ ]	1/2,y,1/2 [0,v,0]
8 e 2..	x,0,0 [u,0,0]	$\bar{x}+1/2,1/2,0$ [ $\bar{u},0,0$ ]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	x+1/2,0,1/2 [u,0,0]
8 d $\bar{1}'$	0,1/4,1/4 [0,0,0]	1/2,1/4,1/4 [0,0,0]	0,1/4,3/4 [0,0,0]	1/2,1/4,3/4 [0,0,0]
8 c $\bar{1}'$	1/4,0,1/4 [0,0,0]	1/4,1/2,1/4 [0,0,0]	3/4,0,3/4 [0,0,0]	3/4,1/2,3/4 [0,0,0]
4 b 222	0,0,1/2 [0,0,0]	0,1/2,0 [0,0,0]		
4 a 222	0,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at x,0,0

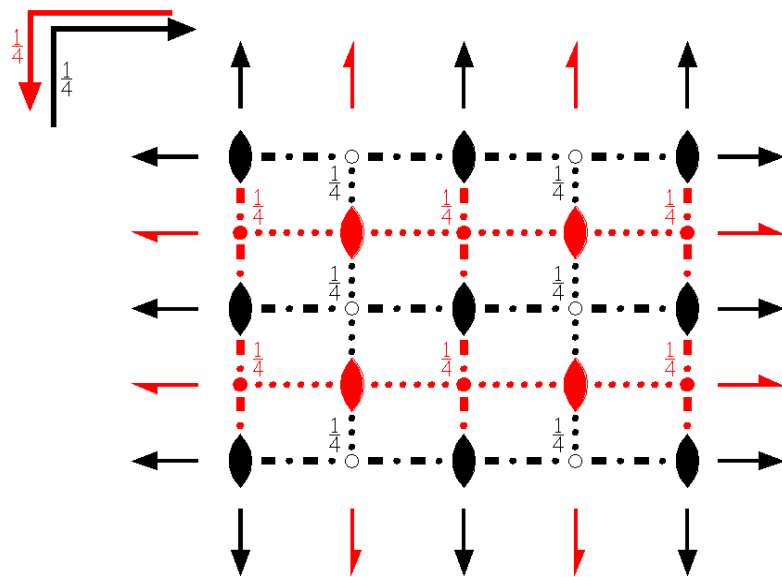
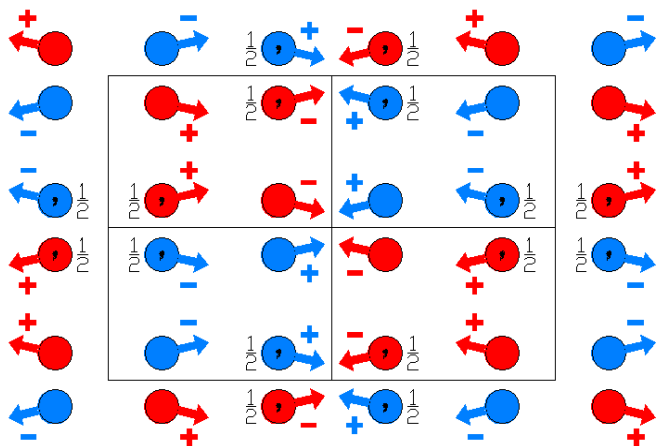
Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



$C_{pcca}$   
68.8.601

$mmm1'$   
 $C_{p2/c2/c2/a}$

Orthorhombic



**Origin** at 222 at  $2/n2/n2$  at  $0, 1/4, 1/4$  from  $\bar{1}$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                       | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                       | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                       |
| (5) $\bar{1}$ $0,1/4,1/4$<br>( $\bar{1}$   $0,1/2,1/2$ ) | (6) b $(0,1/2,0)$ $x,y,1/4$<br>( $m_z$   $0,1/2,1/2$ ) | (7) c $(0,0,1/2)$ $x,1/4,z$<br>( $m_y$   $0,1/2,1/2$ ) | (8) n $(0,1/2,1/2)$ $0,y,z$<br>( $m_x$   $0,1/2,1/2$ ) |

For  $(1/2,1/2,0)'$  + set

- |   |   |   |   |
|---|---|---|---|
| (1) $t'$ $(1/2,1/2,0)$<br>(1  $1/2,1/2,0$ )'                | (2) $2'$ $1/4,1/4,z$<br>( $2'_z$   $1/2,1/2,0$ )'           | (3) $2'$ $(0,1/2,0)$ $1/4,y,0$<br>( $2'_y$   $1/2,1/2,0$ )' | (4) $2'$ $(1/2,0,0)$ $x,1/4,0$<br>( $2'_x$   $1/2,1/2,0$ )' |
| (5) $\bar{1}'$ $1/4,0,1/4$<br>( $\bar{1}'$   $1/2,0,1/2$ )' | (6) $a'$ $(1/2,0,0)$ $x,y,1/4$<br>( $m'_z$   $1/2,0,1/2$ )' | (7) $n'$ $(1/2,0,1/2)$ $x,0,z$<br>( $m'_y$   $1/2,0,1/2$ )' | (8) $c'$ $(0,0,1/2)$ $1/4,y,z$<br>( $m'_x$   $1/2,0,1/2$ )' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

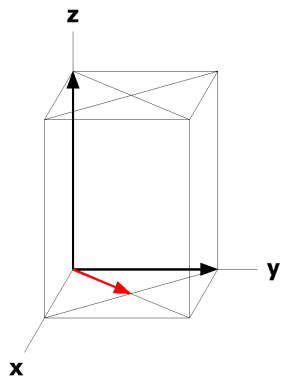
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x, \bar{y}, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]
	(5) $\bar{x}, \bar{y}+1/2, \bar{z}+1/2$ [u,v,w]	(6) $x, y+1/2, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(7) $x, \bar{y}+1/2, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(8) $\bar{x}, y+1/2, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]
8 h ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [ $\bar{u}, v, 0$ ]	3/4,1/4, $\bar{z}+1/2$ [ $\bar{u}, \bar{v}, 0$ ]	1/4,1/4,z+1/2 [u, $\bar{v}, 0$ ]
8 g ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
8 f .2.	0,y,0 [0,v,0]	1/2, $\bar{y}+1/2, 0$ [0,v,0]	0, $\bar{y}+1/2, 1/2$ [0, $\bar{v}, 0$ ]	1/2,y,1/2 [0, $\bar{v}, 0$ ]
8 e 2..	x,0,0 [u,0,0]	$\bar{x}+1/2, 1/2, 0$ [u,0,0]	$\bar{x}, 1/2, 1/2$ [ $\bar{u}, 0, 0$ ]	x+1/2,0,1/2 [ $\bar{u}, 0, 0$ ]
8 d $\bar{1}$	0,1/4,1/4 [u,v,w]	1/2,1/4,1/4 [u,v, $\bar{w}$ ]	0,1/4,3/4 [ $\bar{u}, v, \bar{w}$ ]	1/2,1/4,3/4 [ $\bar{u}, v, w$ ]
8 c $\bar{1}'$	1/4,0,1/4 [0,0,0]	1/4,1/2,1/4 [0,0,0]	3/4,0,3/4 [0,0,0]	3/4,1/2,3/4 [0,0,0]
4 b 222	0,0,1/2 [0,0,0]	0,1/2,0 [0,0,0]		
4 a 222	0,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

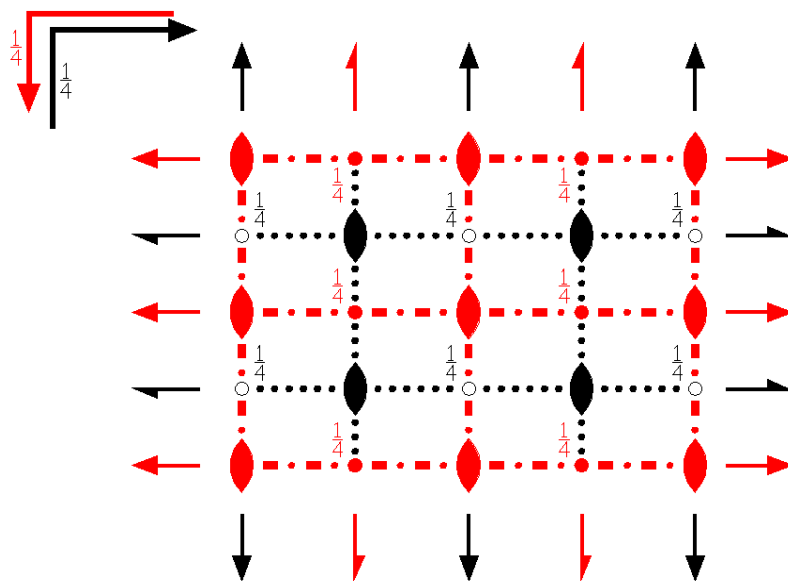
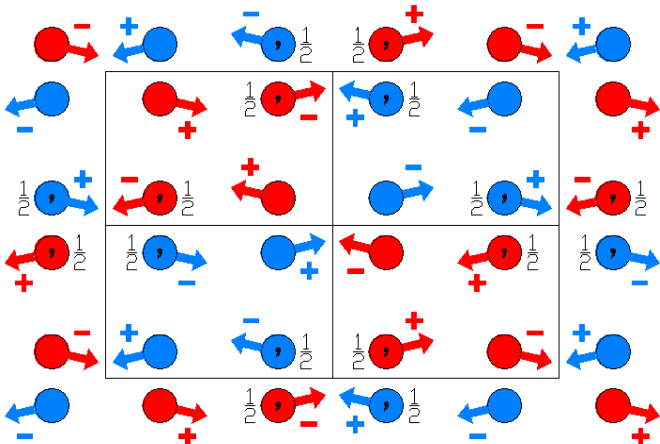
Along [0,1,0]  $p2mm$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



$C_p c'ca$   
68.9.602

$mmm1'$   
 $C_p 2/c'2'/c2'/a$

Orthorhombic



**Origin** at  $22'2'$  at  $2/n'2'/n'2'$  at  $0, 1/4, 1/4$  from  $\bar{1}'$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |  |  |   |
|---|--|--|---|
| (1) 1<br>(1 0,0,0)                                  | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)'             | (3) $2'$ 0,y,0<br>( $2_y$  0,0,0)'             | (4) $2$ x,0,0<br>( $2_x$  0,0,0)                |
| (5) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$  0,1/2,1/2)' | (6) b (0,1/2,0) x,y,1/4<br>( $m_z$  0,1/2,1/2) | (7) c (0,0,1/2) x,1/4,z<br>( $m_y$  0,1/2,1/2) | (8) n (0,1/2,1/2) 0,y,z<br>( $m_x$  0,1/2,1/2)' |

For  $(1/2,1/2,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (1/2,1/2,0)<br>(1 1/2,1/2,0)'             | (2) $2$ 1/4,1/4,z<br>( $2_z$  1/2,1/2,0)           | (3) $2$ (0,1/2,0) 1/4,y,0<br>( $2_y$  1/2,1/2,0)   | (4) $2'$ (1/2,0,0) x,1/4,0<br>( $2_x$  1/2,1/2,0)' |
| (5) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$  1/2,0,1/2) | (6) $a'$ (1/2,0,0) x,y,1/4<br>( $m_z$  1/2,0,1/2)' | (7) $n'$ (1/2,0,1/2) x,0,z<br>( $m_y$  1/2,0,1/2)' | (8) c (0,0,1/2) 1/4,y,z<br>( $m_x$  1/2,0,1/2)     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

**Positions**

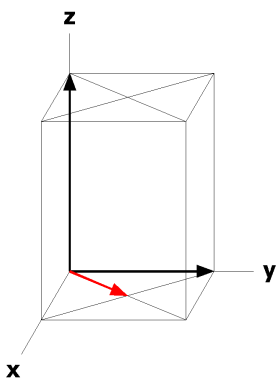
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x,y+1/2, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) x, $\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y+1/2,z+1/2$ [ $\bar{u},v,w$ ]
8 h ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0,w]	3/4,1/4, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/4,1/4,z+1/2 [0,0, $\bar{w}$ ]
8 g ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [u, $\bar{v}$ ,0]	0,1/2, $\bar{z}+1/2$ [ $\bar{u},\bar{v}$ ,0]	0,1/2,z+1/2 [ $\bar{u},v,0$ ]
8 f .2'	0,y,0 [u,0,w]	1/2, $\bar{y}+1/2,0$ [ $\bar{u},0,w$ ]	0, $\bar{y}+1/2,1/2$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,1/2 [u,0, $\bar{w}$ ]
8 e 2..	x,0,0 [u,0,0]	$\bar{x}+1/2,1/2,0$ [ $\bar{u},0,0$ ]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	x+1/2,0,1/2 [u,0,0]
8 d $\bar{1}'$	0,1/4,1/4 [0,0,0]	1/2,1/4,1/4 [0,0,0]	0,1/4,3/4 [0,0,0]	1/2,1/4,3/4 [0,0,0]
8 c $\bar{1}$	1/4,0,1/4 [u,v,w]	1/4,1/2,1/4 [ $\bar{u},\bar{v},w$ ]	3/4,0,3/4 [u, $\bar{v},w$ ]	3/4,1/2,3/4 [ $\bar{u},v,w$ ]
4 b 22'2'	0,0,1/2 [u,0,0]	0,1/2,0 [ $\bar{u},0,0$ ]		
4 a 22'2'	0,0,0 [u,0,0]	0,1/2,1/2 [ $\bar{u},0,0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>.2mm  
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,1/4,z

Along [1,0,0] p<sub>c</sub>.2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

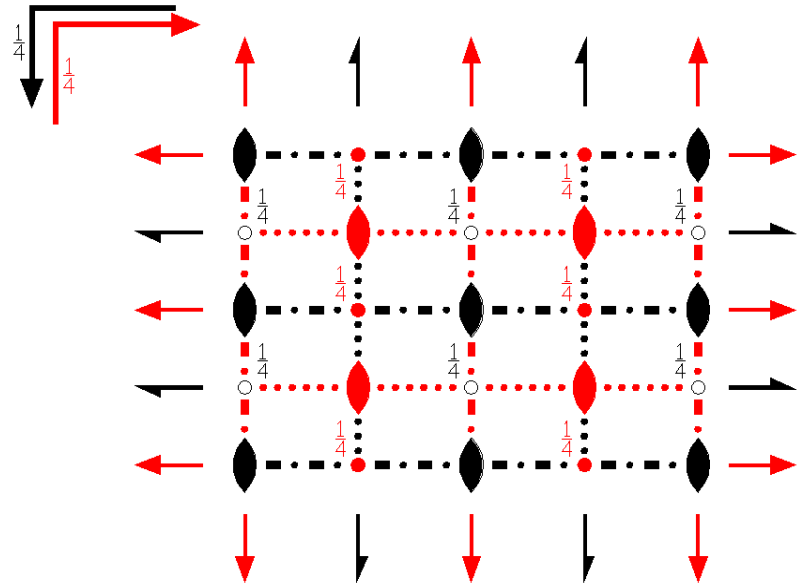
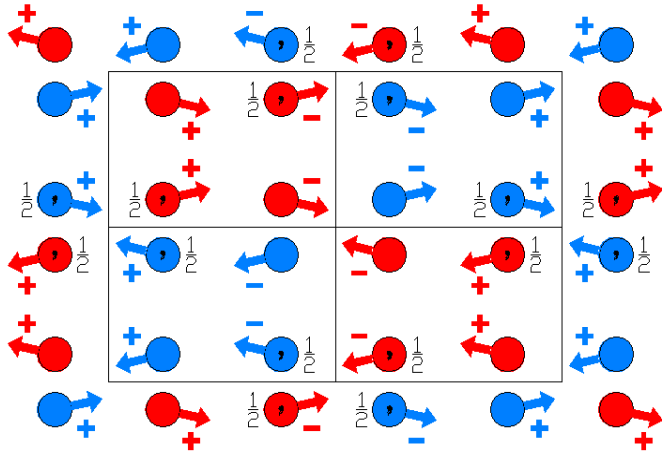
Along [0,1,0] p<sub>c</sub>.2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



$C_pcca'$   
68.10.603

$mmm1'$   
 $C_p2'/c2'/c2/a'$

Orthorhombic



**Origin** at  $2'2'2$  at  $2'/n2'/n'2$  at  $0, 1/4, 1/4$  from  $\bar{1}$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                  | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'               | (4) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'               |
| (5) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$  0,1/2,1/2)' | (6) b (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>  0,1/2,1/2)' | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2) | (8) n (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>  0,1/2,1/2) |

For  $(1/2,1/2,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1/2,1/2,0)<br>(1 1/2,1/2,0)'               | (2) 2' 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)'       | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$  1/2,0,1/2) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2) | (7) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2)' | (8) c' (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

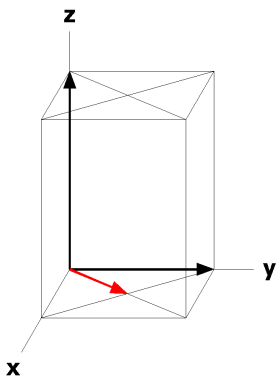
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,0)' +		
16 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(4) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]
	(5) $\bar{x},\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]	(7) $x,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
8 h ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [ $u,\bar{v},0$ ]	3/4,1/4, $\bar{z}+1/2$ [ $\bar{u},\bar{v},0$ ]	1/4,1/4,z+1/2 [ $\bar{u},v,0$ ]
8 g ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
8 f .2'	0,y,0 [u,0,w]	1/2, $\bar{y}+1/2,0$ [ $u,0,\bar{w}$ ]	0, $\bar{y}+1/2,1/2$ [ $\bar{u},0,\bar{w}$ ]	1/2,y,1/2 [ $\bar{u},0,w$ ]
8 e 2'..	x,0,0 [0,v,w]	$\bar{x}+1/2,1/2,0$ [0,v, $\bar{w}$ ]	$\bar{x},1/2,1/2$ [0, $\bar{v},\bar{w}$ ]	x+1/2,0,1/2 [0, $\bar{v},w$ ]
8 d $\bar{1}'$	0,1/4,1/4 [0,0,0]	1/2,1/4,1/4 [0,0,0]	0,1/4,3/4 [0,0,0]	1/2,1/4,3/4 [0,0,0]
8 c $\bar{1}$	1/4,0,1/4 [u,v,w]	1/4,1/2,1/4 [u,v, $\bar{w}$ ]	3/4,0,3/4 [u, $\bar{v},w$ ]	3/4,1/2,3/4 [u, $\bar{v},\bar{w}$ ]
4 b 2'2'2	0,0,1/2 [0,0,w]	0,1/2,0 [0,0, $\bar{w}$ ]		
4 a 2'2'2	0,0,0 [0,0,w]	0,1/2,1/2 [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,1/4

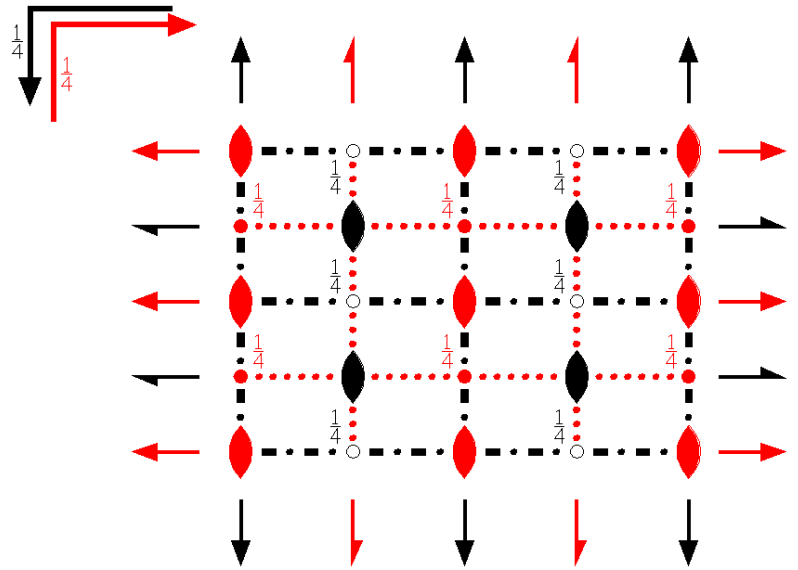
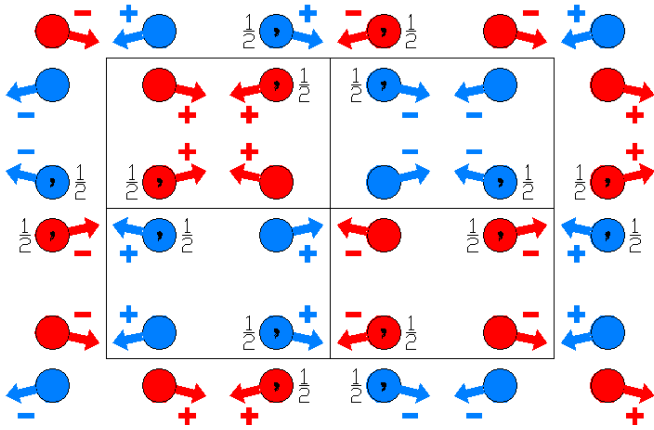
Along [0,1,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 1/4,y,1/4



$C_{pcc'a'}$   
68.11.604

$mmm1'$   
 $C_{p2/c2'/c'2'/a'}$

Orthorhombic



**Origin** at  $22'2'$  at  $2/n2'/n2'$  at  $0,1/4,1/4$  from  $\bar{1}$

**Asymmetric unit**  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |   |   |  |
|--|---|---|--|
| (1) 1<br>(1 0,0,0)                                 | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)'                | (3) $2'$ 0,y,0<br>( $2_y$  0,0,0)'                | (4) $2$ x,0,0<br>( $2_x$  0,0,0)                 |
| (5) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$  0,1/2,1/2) | (6) b $(0,1/2,0)$ x,y,1/4<br>( $m_z$  0,1/2,1/2)' | (7) c $(0,0,1/2)$ x,1/4,z<br>( $m_y$  0,1/2,1/2)' | (8) n $(0,1/2,1/2)$ 0,y,z<br>( $m_x$  0,1/2,1/2) |

For  $(1/2,1/2,0)$ ' + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t'$ $(1/2,1/2,0)$<br>(1 1/2,1/2,0)'              | (2) $2$ 1/4,1/4,z<br>( $2_z$  1/2,1/2,0)         | (3) $2$ $(0,1/2,0)$ 1/4,y,0<br>( $2_y$  1/2,1/2,0) | (4) $2'$ $(1/2,0,0)$ x,1/4,0<br>( $2_x$  1/2,1/2,0)' |
| (5) $\bar{1}'$ 1/4,0,1/4<br>( $\bar{1}'$  1/2,0,1/2)' | (6) a $(1/2,0,0)$ x,y,1/4<br>( $m_z$  1/2,0,1/2) | (7) n $(1/2,0,1/2)$ x,0,z<br>( $m_y$  1/2,0,1/2)   | (8) $c'$ $(0,0,1/2)$ 1/4,y,z<br>( $m_x$  1/2,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

**Positions**

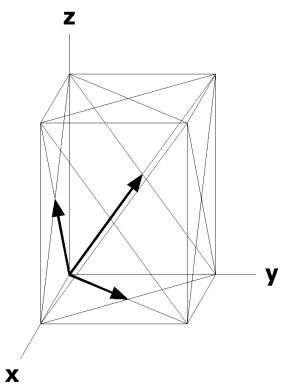
Multiplicity, Wyckoff letter, Site Symmetry.		Coordinates						
		(0,0,0) +	(1/2,1/2,0)' +					
16 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	(3) $\bar{x}, y, \bar{z}$ [u, $\bar{v}$ ,w]	(4) $x, \bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]	(5) $\bar{x}, \bar{y}+1/2, \bar{z}+1/2$ [u,v,w]	(6) $x, y+1/2, \bar{z}+1/2$ [u,v, $\bar{w}$ ]	(7) $x, \bar{y}+1/2, z+1/2$ [u, $\bar{v}$ ,w]	(8) $\bar{x}, y+1/2, z+1/2$ [u, $\bar{v}, \bar{w}$ ]
8 h ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0,w]	3/4,1/4, $\bar{z}+1/2$ [0,0,w]	1/4,1/4,z+1/2 [0,0,w]				
8 g ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [u, $\bar{v}$ ,0]	0,1/2, $\bar{z}+1/2$ [u,v,0]	0,1/2,z+1/2 [u, $\bar{v}$ ,0]				
8 f .2'	0,y,0 [u,0,w]	1/2, $\bar{y}+1/2,0$ [ $\bar{u}$ ,0,w]	0, $\bar{y}+1/2,1/2$ [u,0,w]	1/2,y,1/2 [ $\bar{u}$ ,0,w]				
8 e 2..	x,0,0 [u,0,0]	$\bar{x}+1/2,1/2,0$ [ $\bar{u}$ ,0,0]	$\bar{x},1/2,1/2$ [u,0,0]	x+1/2,0,1/2 [ $\bar{u}$ ,0,0]				
8 d $\bar{1}$	0,1/4,1/4 [u,v,w]	1/2,1/4,1/4 [ $\bar{u}, \bar{v}, w$ ]	0,1/4,3/4 [u, $\bar{v}, w$ ]	1/2,1/4,3/4 [ $\bar{u}, v, w$ ]				
8 c $\bar{1}'$	1/4,0,1/4 [0,0,0]	1/4,1/2,1/4 [0,0,0]	3/4,0,3/4 [0,0,0]	3/4,1/2,3/4 [0,0,0]				
4 b 22'2'	0,0,1/2 [u,0,0]	0,1/2,0 [u,0,0]						
4 a 22'2'	0,0,0 [u,0,0]	0,1/2,1/2 [u,0,0]						

**Symmetry of Special Projections**

Along [0,0,1] p<sub>2a</sub>.2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] p<sub>c</sub>.2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>.2m'm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,1/4



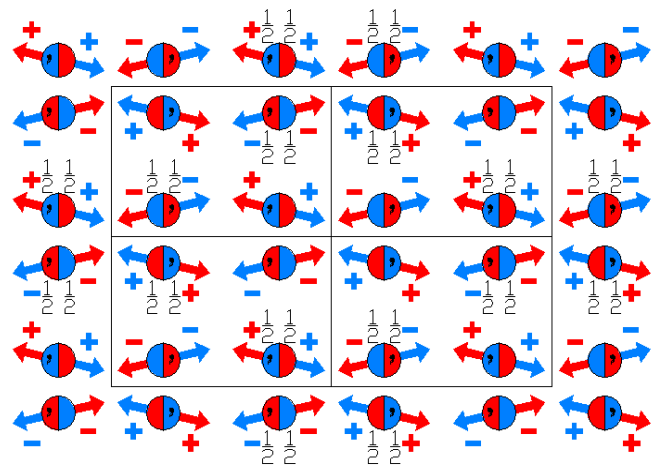
Fmmm

69.1.605

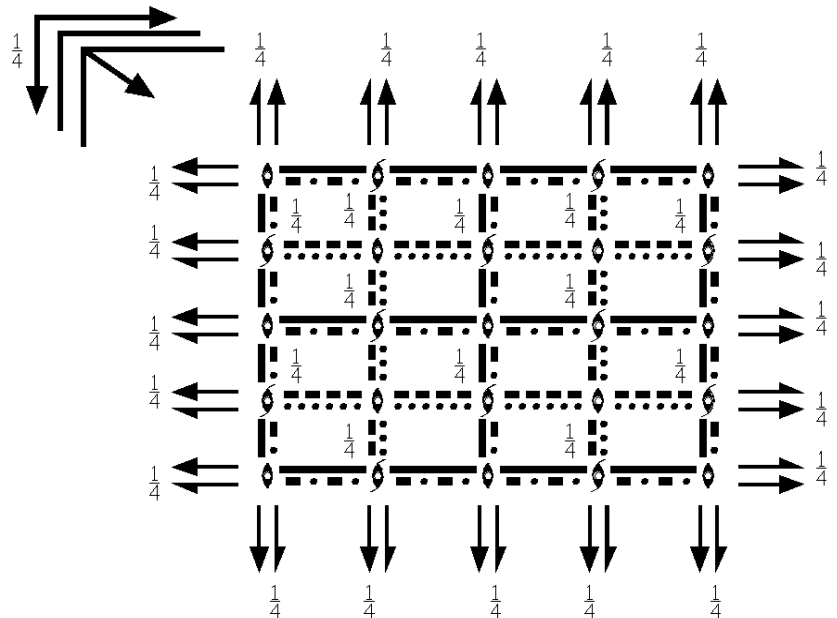
mmm

F2/m2/m2/m

Orthorhombic



Origin at center (mmm)



Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0) | (3) 2 0,y,0<br>(2 <sub>y</sub>   0,0,0) | (4) 2 x,0,0<br>(2 <sub>x</sub>   0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>   0,0,0) | (7) m x,0,z<br>(m <sub>y</sub>   0,0,0) | (8) m 0,y,z<br>(m <sub>x</sub>   0,0,0) |

For (0,1/2,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (0,1/2,1/2)<br>(1   0,1/2,1/2)                | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>   0,1/2,1/2) | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>   0,1/2,1/2) | (4) 2 x,1/4,1/4<br>(2 <sub>x</sub>   0,1/2,1/2)         |
| (5) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$   0,1/2,1/2) | (6) b (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>   0,1/2,1/2) | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>   0,1/2,1/2) | (8) n (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>   0,1/2,1/2) |

For (1/2,0,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,0,1/2)<br>(1   1/2,0,1/2)                | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>   1/2,0,1/2) | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,0,1/2)         | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>   1/2,0,1/2) |
| (5) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$   1/2,0,1/2) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>   1/2,0,1/2) | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>   1/2,0,1/2) | (8) c (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>   1/2,0,1/2) |

For (1/2,1/2,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)         | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>   1/2,1/2,0) | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5).

### Positions

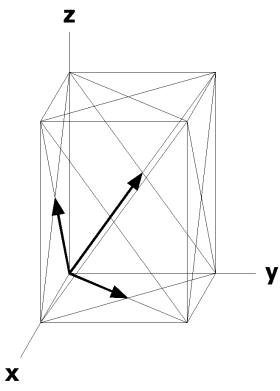
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
32 p 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},\bar{v},\bar{w}$ ]
16 o ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0, $\bar{w}$ ]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
16 n .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]	$\bar{x},0,\bar{z}$ [0,v,0]	x,0, $\bar{z}$ [0, $\bar{v}$ ,0]
16 m m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	0,y, $\bar{z}$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]
16 l 2..	x,1/4,1/4 [u,0,0]	$\bar{x},3/4,1/4$ [ $\bar{u},0,0$ ]	$\bar{x},3/4,3/4$ [u,0,0]	x,1/4,3/4 [ $\bar{u},0,0$ ]
16 k .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y},1/4$ [0, $\bar{v}$ ,0]	3/4, $\bar{y},3/4$ [0,v,0]	1/4,y,3/4 [0, $\bar{v}$ ,0]
16 j ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0, $\bar{w}$ ]	3/4,3/4, $\bar{z}$ [0,0,w]	1/4,3/4,z [0,0, $\bar{w}$ ]
8 i mm2	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
8 h m2m	0,y,0 [0,0,0]	0, $\bar{y},0$ [0,0,0]		
8 g 2mm	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
8 f 222	1/4,1/4,1/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]		
8 e ..2/m	1/4,1/4,0 [0,0,w]	3/4,1/4,0 [0,0, $\bar{w}$ ]		
8 d .2/m.	1/4,0,1/4 [0,v,0]	3/4,0,1/4 [0, $\bar{v}$ ,0]		
8 c 2/m..	0,1/4,1/4 [u,0,0]	0,3/4,1/4 [ $\bar{u},0,0$ ]		
4 b mmm	0,0,1/2 [0,0,0]			
4 a mmm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Fmmm1'

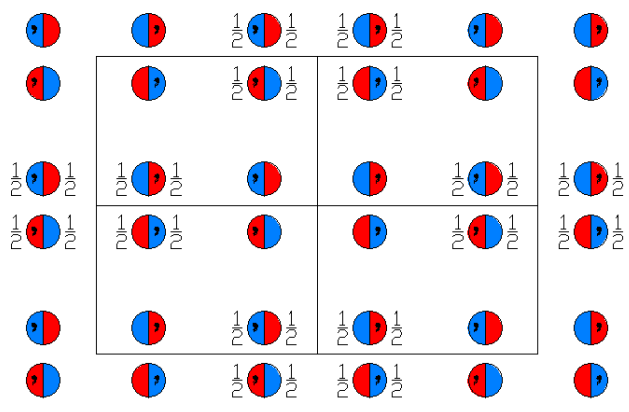
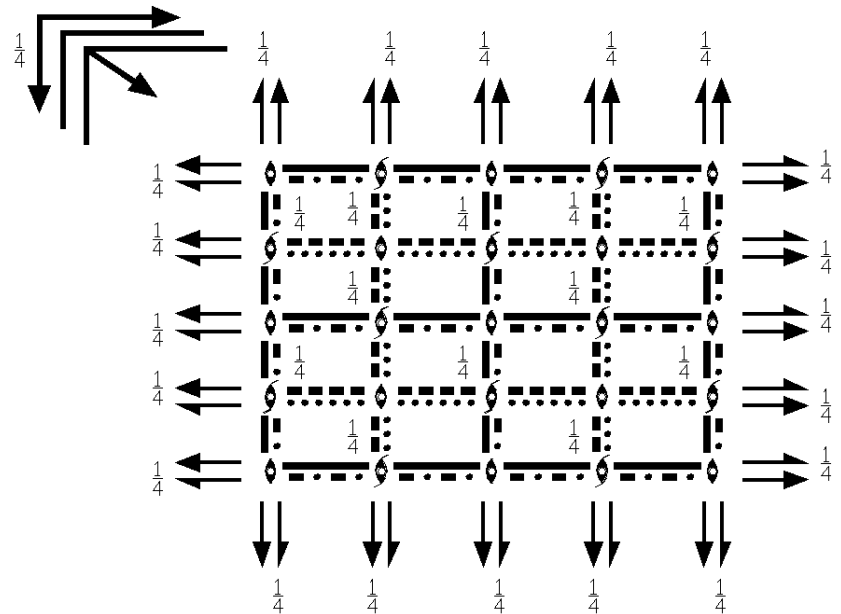
69.2.606

mmm1'

F2/m2/m2/m1'

Orthorhombic

1'



Origin at center (mmm1')

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0) | (3) 2 0,y,0<br>(2 <sub>y</sub>   0,0,0) | (4) 2 x,0,0<br>(2 <sub>x</sub>   0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>   0,0,0) | (7) m x,0,z<br>(m <sub>y</sub>   0,0,0) | (8) m 0,y,z<br>(m <sub>x</sub>   0,0,0) |

For (0,1/2,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (0,1/2,1/2)<br>(1   0,1/2,1/2)                | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>   0,1/2,1/2) | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>   0,1/2,1/2) | (4) 2 x,1/4,1/4<br>(2 <sub>x</sub>   0,1/2,1/2)         |
| (5) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$   0,1/2,1/2) | (6) b (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>   0,1/2,1/2) | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>   0,1/2,1/2) | (8) n (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>   0,1/2,1/2) |

For (1/2,0,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,0,1/2)<br>(1   1/2,0,1/2)                | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>   1/2,0,1/2) | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,0,1/2)         | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>   1/2,0,1/2) |
| (5) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$   1/2,0,1/2) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>   1/2,0,1/2) | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>   1/2,0,1/2) | (8) c (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>   1/2,0,1/2) |

For (1/2,1/2,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)         | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>   1/2,1/2,0) | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0) |

## For (0,0,0)' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(4) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'
(5) $\bar{1}$ ' 0,0,0 ( $\bar{1}$  0,0,0)'	(6) m' x,y,0 (m <sub>z</sub>  0,0,0)'	(7) m' x,0,z (m <sub>y</sub>  0,0,0)'	(8) m' 0,y,z (m <sub>x</sub>  0,0,0)'

## For (0,1/2,1/2)' + set

(1) t' (0,1/2,1/2) (1 0,1/2,1/2)'	(2) 2' (0,0,1/2) 0,1/4,z (2 <sub>z</sub>  0,1/2,1/2)'	(3) 2' (0,1/2,0) 0,y,1/4 (2 <sub>y</sub>  0,1/2,1/2)'	(4) 2' x,1/4,1/4 (2 <sub>x</sub>  0,1/2,1/2)'
(5) $\bar{1}$ ' 0,1/4,1/4 ( $\bar{1}$  0,1/2,1/2)'	(6) b' (0,1/2,0) x,y,1/4 (m <sub>z</sub>  0,1/2,1/2)'	(7) c' (0,0,1/2) x,1/4,z (m <sub>y</sub>  0,1/2,1/2)'	(8) n' (0,1/2,1/2) 0,y,z (m <sub>x</sub>  0,1/2,1/2)'

## For (1/2,0,1/2)' + set

(1) t' (1/2,0,1/2) (1 1/2,0,1/2)'	(2) 2' (0,0,1/2) 1/4,0,z (2 <sub>z</sub>  1/2,0,1/2)'	(3) 2' 1/4,y,1/4 (2 <sub>y</sub>  1/2,0,1/2)'	(4) 2' (1/2,0,0) x,0,1/4 (2 <sub>x</sub>  1/2,0,1/2)'
(5) $\bar{1}$ ' 1/4,0,1/4 ( $\bar{1}$  1/2,0,1/2)'	(6) a' (1/2,0,0) x,y,1/4 (m <sub>z</sub>  1/2,0,1/2)'	(7) n' (1/2,0,1/2) x,0,z (m <sub>y</sub>  1/2,0,1/2)'	(8) c' (0,0,1/2) 1/4,y,z (m <sub>x</sub>  1/2,0,1/2)'

## For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0) (1 1/2,1/2,0)'	(2) 2' 1/4,1/4,z (2 <sub>z</sub>  1/2,1/2,0)'	(3) 2' (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>  1/2,1/2,0)'	(4) 2' (1/2,0,0) x,1/4,0 (2 <sub>x</sub>  1/2,1/2,0)'
(5) $\bar{1}$ ' 1/4,1/4,0 ( $\bar{1}$  1/2,1/2,0)'	(6) n' (1/2,1/2,0) x,y,0 (m <sub>z</sub>  1/2,1/2,0)'	(7) a' (1/2,0,0) x,1/4,z (m <sub>y</sub>  1/2,1/2,0)'	(8) b' (0,1/2,0) 1/4,y,z (m <sub>x</sub>  1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); 1'.

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

		(0,0,0) + (0,0,0)'	(0,1/2,1/2) + (0,1/2,1/2)'	(1/2,0,1/2) + (1/2,0,1/2)'	(1/2,1/2,0) + (1/2,1/2,0)'
32 p 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{x},y,\bar{z}$ [0,0,0]	(4) x, $\bar{y},\bar{z}$ [0,0,0]	
	(5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(6) x,y, $\bar{z}$ [0,0,0]	(7) x, $\bar{y},z$ [0,0,0]	(8) $\bar{x},y,z$ [0,0,0]	
16 o ..m1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{x},y,0$ [0,0,0]	x, $\bar{y},0$ [0,0,0]	
16 n .m.1'	x,0,z [0,0,0]	$\bar{x},0,z$ [0,0,0]	$\bar{x},0,\bar{z}$ [0,0,0]	x,0, $\bar{z}$ [0,0,0]	
16 m m..1'	0,y,z [0,0,0]	0, $\bar{y},z$ [0,0,0]	0,y, $\bar{z}$ [0,0,0]	0, $\bar{y},\bar{z}$ [0,0,0]	
16 l 2..1'	x,1/4,1/4 [0,0,0]	$\bar{x},3/4,1/4$ [0,0,0]	$\bar{x},3/4,3/4$ [0,0,0]	x,1/4,3/4 [0,0,0]	

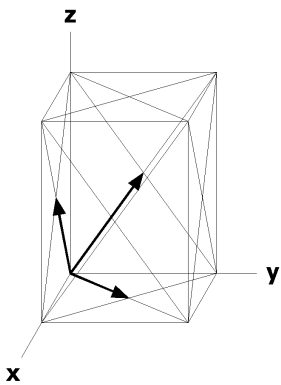
16	k	.2.1'	1/4,y,1/4 [0,0,0]	3/4, $\bar{y}$ ,1/4 [0,0,0]	3/4, $\bar{y}$ ,3/4 [0,0,0]	1/4,y,3/4 [0,0,0]
16	j	..21'	1/4,1/4,z [0,0,0]	3/4,1/4, $\bar{z}$ [0,0,0]	3/4,3/4, $\bar{z}$ [0,0,0]	1/4,3/4,z [0,0,0]
8	i	mm21'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
8	h	m2m1'	0,y,0 [0,0,0]	0, $\bar{y}$ ,0 [0,0,0]		
8	g	2mm1'	x,0,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0]		
8	f	2221'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]		
8	e	..2/m1'	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
8	d	.2/m.1'	1/4,0,1/4 [0,0,0]	3/4,0,1/4 [0,0,0]		
8	c	2/m..1'	0,1/4,1/4 [0,0,0]	0,3/4,1/4 [0,0,0]		
4	b	mmm1'	0,0,1/2 [0,0,0]			
4	a	mmm1'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



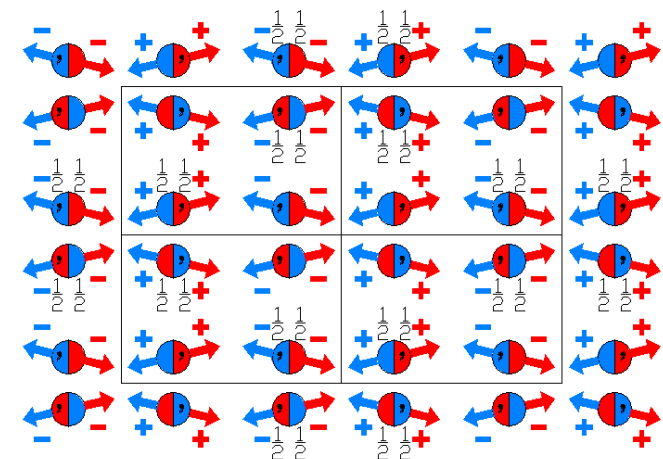
Fm'mm

69.3.607

m'mm

F2/m'2'/m2'/m

Orthorhombic



Origin at center (m'mm)

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1   0,0,0)                           | (2) 2' 0,0,z<br>(2 <sub>z</sub>   0,0,0)' | (3) 2' 0,y,0<br>(2 <sub>y</sub>   0,0,0)' | (4) 2 x,0,0<br>(2 <sub>x</sub>   0,0,0)   |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$   0,0,0)' | (6) m x,y,0<br>(m <sub>z</sub>   0,0,0)   | (7) m x,0,z<br>(m <sub>y</sub>   0,0,0)   | (8) m' 0,y,z<br>(m <sub>x</sub>   0,0,0)' |

For (0,1/2,1/2) + set

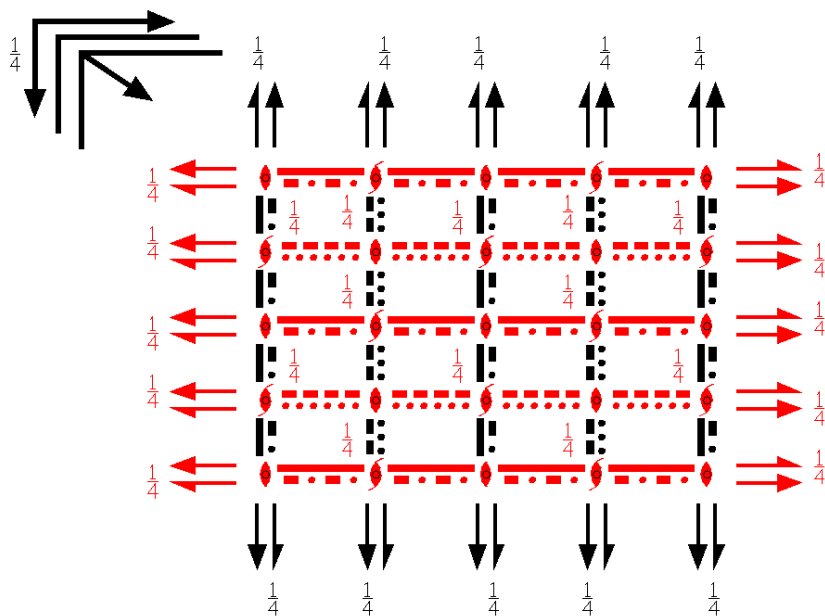
- |  |   |   |   |
|--|---|---|---|
| (1) t (0,1/2,1/2)<br>(1   0,1/2,1/2)                   | (2) 2' (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>   0,1/2,1/2)' | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>   0,1/2,1/2)' | (4) 2 x,1/4,1/4<br>(2 <sub>x</sub>   0,1/2,1/2)           |
| (5) $\bar{1}$ ' 0,1/4,1/4<br>( $\bar{1}$   0,1/2,1/2)' | (6) b (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>   0,1/2,1/2)   | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>   0,1/2,1/2)   | (8) n' (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>   0,1/2,1/2)' |

For (1/2,0,1/2) + set

- |  |   |   |   |
|--|---|---|---|
| (1) t (1/2,0,1/2)<br>(1   1/2,0,1/2)                   | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>   1/2,0,1/2)' | (3) 2' 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,0,1/2)'       | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>   1/2,0,1/2)   |
| (5) $\bar{1}$ ' 1/4,0,1/4<br>( $\bar{1}$   1/2,0,1/2)' | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>   1/2,0,1/2)   | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>   1/2,0,1/2) | (8) c' (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>   1/2,0,1/2)' |

For (1/2,1/2,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                   | (2) 2' 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)'       | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)' | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)   |
| (5) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0)' | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>   1/2,1/2,0) | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0)   | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5).

### Positions

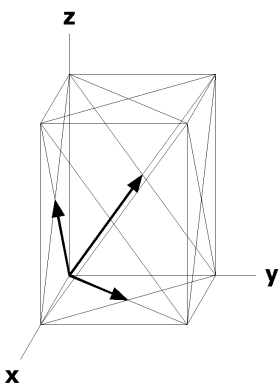
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
32 p 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
16 o ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
16 n .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0,v,0]	$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	x,0, $\bar{z}$ [0, $\bar{v},0$ ]
16 m m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0,v, $\bar{w}$ ]	0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
16 l 2..	x,1/4,1/4 [u,0,0]	$\bar{x},3/4,1/4$ [u,0,0]	$\bar{x},3/4,3/4$ [ $\bar{u},0,0$ ]	x,1/4,3/4 [ $\bar{u},0,0$ ]
16 k .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y},1/4$ [u,0, $\bar{w}$ ]	3/4, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	1/4,y,3/4 [ $\bar{u},0,w$ ]
16 j ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [u, $\bar{v},0$ ]	3/4,3/4, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,3/4,z [ $\bar{u},v,0$ ]
8 i m'm2'	0,0,z [0,v,0]	0,0, $\bar{z}$ [0, $\bar{v},0$ ]		
8 h m'2'm	0,y,0 [0,0,w]	0, $\bar{y},0$ [0,0, $\bar{w}$ ]		
8 g 2mm	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
8 f 22'2'	1/4,1/4,1/4 [u,0,0]	3/4,3/4,3/4 [ $\bar{u},0,0$ ]		
8 e ..2'/m	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
8 d .2'/m.	1/4,0,1/4 [0,0,0]	3/4,0,1/4 [0,0,0]		
8 c 2/m'..	0,1/4,1/4 [0,0,0]	0,3/4,1/4 [0,0,0]		
4 b m'mm	0,0,1/2 [0,0,0]			
4 a m'mm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



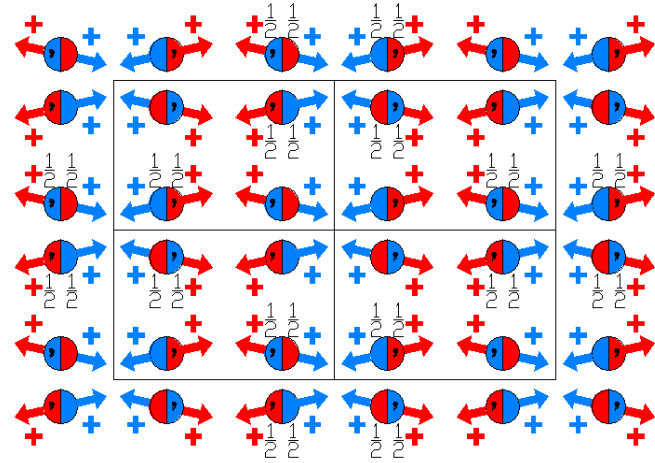
Fm'm'm

69.4.608

m'm'm

F2'/m'2'/m'2'/m

Orthorhombic



Origin at center (m'm'm)

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0) | (3) 2' 0,y,0<br>(2 <sub>y</sub>   0,0,0)' | (4) 2' x,0,0<br>(2 <sub>x</sub>   0,0,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>   0,0,0) | (7) m' x,0,z<br>(m <sub>y</sub>   0,0,0)' | (8) m' 0,y,z<br>(m <sub>x</sub>   0,0,0)' |

For (0,1/2,1/2) + set

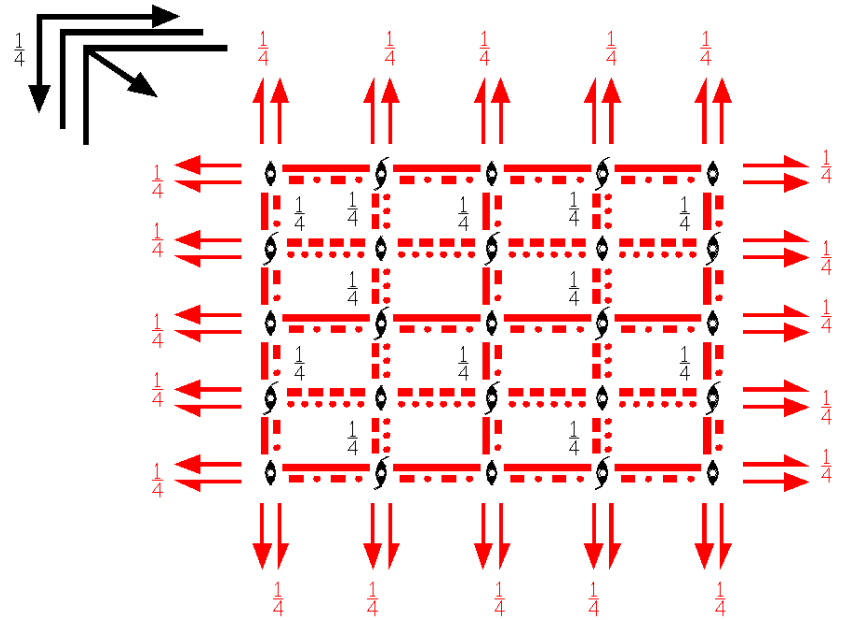
- |   |   |   |   |
|---|---|---|---|
| (1) t (0,1/2,1/2)<br>(1   0,1/2,1/2)                | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>   0,1/2,1/2) | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>   0,1/2,1/2)' | (4) 2' x,1/4,1/4<br>(2 <sub>x</sub>   0,1/2,1/2)'         |
| (5) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$   0,1/2,1/2) | (6) b (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>   0,1/2,1/2) | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>   0,1/2,1/2)' | (8) n' (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>   0,1/2,1/2)' |

For (1/2,0,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,0,1/2)<br>(1   1/2,0,1/2)                | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>   1/2,0,1/2) | (3) 2' 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,0,1/2)'         | (4) 2' (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>   1/2,0,1/2)' |
| (5) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$   1/2,0,1/2) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>   1/2,0,1/2) | (7) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>   1/2,0,1/2)' | (8) c' (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>   1/2,0,1/2)' |

For (1/2,1/2,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)         | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)' |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>   1/2,1/2,0) | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
32 p 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
16 o ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0,w]
16 n .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$\bar{x},0,\bar{z}$ [u,0,w]	x,0, $\bar{z}$ [ $\bar{u},0,w$ ]
16 m m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
16 l 2'..	x,1/4,1/4 [0,v,w]	$\bar{x},3/4,1/4$ [0, $\bar{v},w$ ]	$\bar{x},3/4,3/4$ [0,v,w]	x,1/4,3/4 [0, $\bar{v},w$ ]
16 k .2'	1/4,y,1/4 [u,0,w]3/4, $\bar{y},1/4$ [ $\bar{u},0,w$ ]3/4, $\bar{y},3/4$ [u,0,w]1/4,y,3/4 [ $\bar{u},0,w$ ]			
16 j ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0,w]	3/4,3/4, $\bar{z}$ [0,0,w]	1/4,3/4,z [0,0,w]
8 i m'm'2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
8 h m'2'm	0,y,0 [0,0,w]	0, $\bar{y},0$ [0,0,w]		
8 g 2'm'm	x,0,0 [0,0,w]	$\bar{x},0,0$ [0,0,w]		
8 f 2'2'2	1/4,1/4,1/4 [0,0,w]	3/4,3/4,3/4 [0,0,w]		
8 e ..2/m	1/4,1/4,0 [0,0,w]	3/4,1/4,0 [0,0,w]		
8 d .2'/m'	1/4,0,1/4 [u,0,w]	3/4,0,1/4 [ $\bar{u},0,w$ ]		
8 c 2'/m'..	0,1/4,1/4 [0,v,w]	0,3/4,1/4 [0, $\bar{v},w$ ]		
4 b m'm'm	0,0,1/2 [0,0,w]			
4 a m'm'm	0,0,0 [0,0,w]			

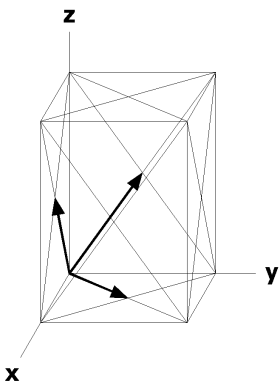
### Symmetry of Special Projections

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0





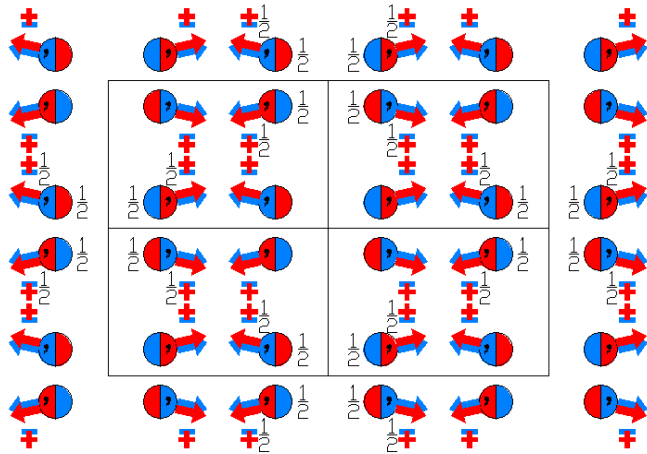
Fm'm'm'

69.5.609

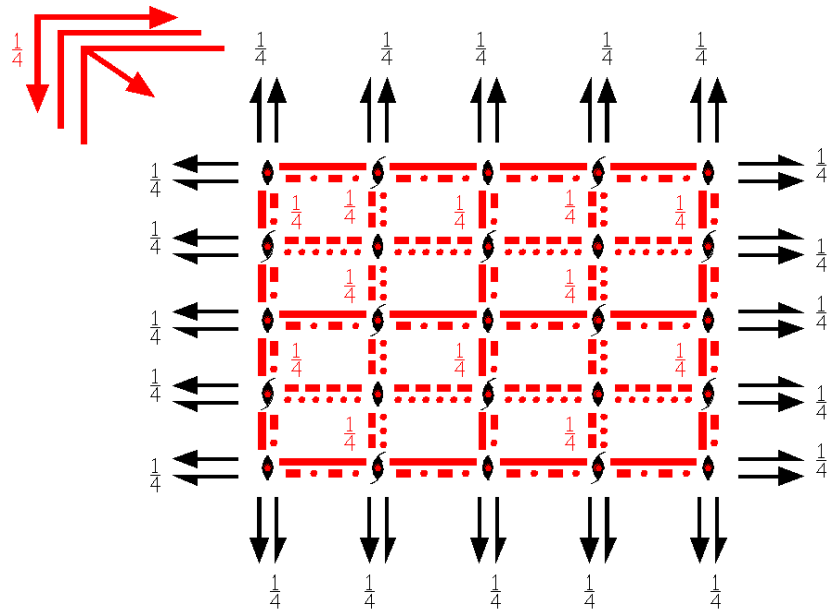
m'm'm'

F2/m'2/m'2/m'

Orthorhombic



Origin at center (m'm'm')



Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1   0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>   0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>   0,0,0)   |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>   0,0,0)' | (7) m' x,0,z<br>(m <sub>y</sub>   0,0,0)' | (8) m' 0,y,z<br>(m <sub>x</sub>   0,0,0)' |

For (0,1/2,1/2) + set

- |  |   |   |   |
|--|---|---|---|
| (1) t (0,1/2,1/2)<br>(1   0,1/2,1/2)                 | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>   0,1/2,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>   0,1/2,1/2)   | (4) 2 x,1/4,1/4<br>(2 <sub>x</sub>   0,1/2,1/2)           |
| (5) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$   0,1/2,1/2)' | (6) b' (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>   0,1/2,1/2)' | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>   0,1/2,1/2)' | (8) n' (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>   0,1/2,1/2)' |

For (1/2,0,1/2) + set

- |  |   |   |   |
|--|---|---|---|
| (1) t (1/2,0,1/2)<br>(1   1/2,0,1/2)                 | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>   1/2,0,1/2)   | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,0,1/2)           | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>   1/2,0,1/2)   |
| (5) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$   1/2,0,1/2)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>   1/2,0,1/2)' | (7) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>   1/2,0,1/2)' | (8) c' (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>   1/2,0,1/2)' |

For (1/2,1/2,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                 | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)           | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)   |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>   1/2,1/2,0)' | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5).

### Positions

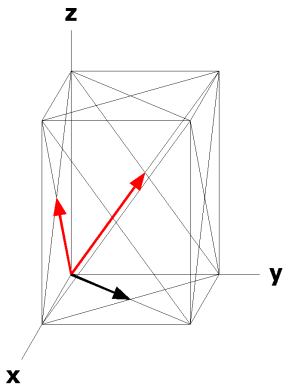
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
32 p 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
16 o ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,0$ [ $\bar{u},v,0$ ]	x, $\bar{y},0$ [u, $\bar{v},0$ ]
16 n .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$\bar{x},0,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	x,0, $\bar{z}$ [u,0, $\bar{w}$ ]
16 m m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	0,y, $\bar{z}$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
16 l 2..	x,1/4,1/4 [u,0,0]	$\bar{x},3/4,1/4$ [ $\bar{u},0,0$ ]	$\bar{x},3/4,3/4$ [ $\bar{u},0,0$ ]	x,1/4,3/4 [u,0,0]
16 k .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y},1/4$ [0, $\bar{v},0$ ]	3/4, $\bar{y},3/4$ [0, $\bar{v},0$ ]	1/4,y,3/4 [0,v,0]
16 j ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0, $\bar{w}$ ]	3/4,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,3/4,z [0,0,w]
8 i m'm'2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
8 h m'2m'	0,y,0 [0,v,0]	0, $\bar{y},0$ [0, $\bar{v},0$ ]		
8 g 2m'm'	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]		
8 f 222	1/4,1/4,1/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]		
8 e ..2/m'	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
8 d .2/m'	1/4,0,1/4 [0,0,0]	3/4,0,1/4 [0,0,0]		
8 c 2/m'..	0,1/4,1/4 [0,0,0]	0,3/4,1/4 [0,0,0]		
4 b m'm'm'	0,0,1/2 [0,0,0]			
4 a m'm'm'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



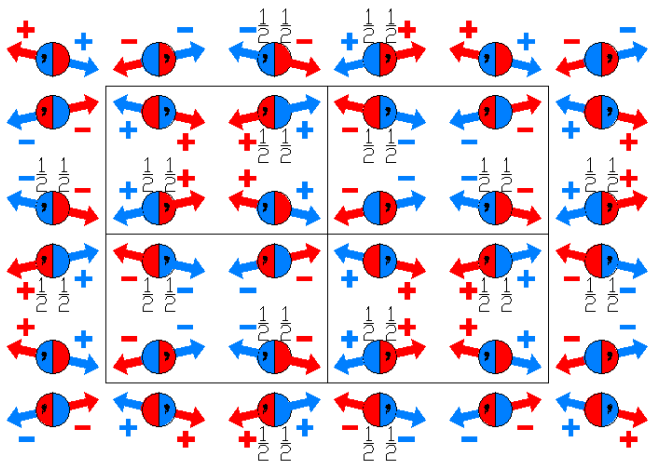
$F_C mmm$

69.6.610

$mmm1'$

$F_C 2/m2/m2/m$

Orthorhombic



Origin at center ( $mmm$ )

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |                                   |                                   |                                   |
|---|-----------------------------------|-----------------------------------|-----------------------------------|
| (1) 1<br>(1   0,0,0)                          | (2) 2 $0,0,z$<br>( $2_z$   0,0,0) | (3) 2 $0,y,0$<br>( $2_y$   0,0,0) | (4) 2 $x,0,0$<br>( $2_x$   0,0,0) |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   0,0,0) | (6) m $x,y,0$<br>( $m_z$   0,0,0) | (7) m $x,0,z$<br>( $m_y$   0,0,0) | (8) m $0,y,z$<br>( $m_x$   0,0,0) |

For  $(0,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(0,1/2,1/2)$<br>(1   $0,1/2,1/2$ )'              | (2) 2 $(0,0,1/2)'$ $0,1/4,z$<br>( $2_z$   $0,1/2,1/2$ )'   | (3) 2' $(0,1/2,0)$ $0,y,1/4$<br>( $2_y$   $0,1/2,1/2$ )'   | (4) 2' $x,1/4,1/4$<br>( $2_x$   $0,1/2,1/2$ )'             |
| (5) $\bar{1}'$ $0,1/4,1/4$<br>( $\bar{1}$   $0,1/2,1/2$ )' | (6) $b'$ $(0,1/2,0)$ $x,y,1/4$<br>( $m_z$   $0,1/2,1/2$ )' | (7) $c'$ $(0,0,1/2)$ $x,1/4,z$<br>( $m_y$   $0,1/2,1/2$ )' | (8) $n'$ $(0,1/2,1/2)$ $0,y,z$<br>( $m_x$   $0,1/2,1/2$ )' |

For  $(1/2,0,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,0,1/2)$<br>(1   $1/2,0,1/2$ )'              | (2) 2' $(0,0,1/2)$ $1/4,0,z$<br>( $2_z$   $1/2,0,1/2$ )'   | (3) 2' $1/4,y,1/4$<br>( $2_y$   $1/2,0,1/2$ )'             | (4) 2' $(1/2,0,0)$ $x,0,1/4$<br>( $2_x$   $1/2,0,1/2$ )'   |
| (5) $\bar{1}'$ $1/4,0,1/4$<br>( $\bar{1}$   $1/2,0,1/2$ )' | (6) $a'$ $(1/2,0,0)$ $x,y,1/4$<br>( $m_z$   $1/2,0,1/2$ )' | (7) $n'$ $(1/2,0,1/2)$ $x,0,z$<br>( $m_y$   $1/2,0,1/2$ )' | (8) $c'$ $(0,0,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,0,1/2$ )' |

For  $(1/2,1/2,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t$ $(1/2,1/2,0)$<br>(1   $1/2,1/2,0$ )              | (2) 2 $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,0$ )           | (3) 2 $(0,1/2,0)$ $1/4,y,0$<br>( $2_y$   $1/2,1/2,0$ ) | (4) 2 $(1/2,0,0)$ $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ ) |
| (5) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1}$   $1/2,1/2,0$ ) | (6) n $(1/2,1/2,0)$ $x,y,0$<br>( $m_z$   $1/2,1/2,0$ ) | (7) a $(1/2,0,0)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,0$ ) | (8) b $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ ) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); t'(1/2,0,1/2); (2); (3); (5).

### Positions

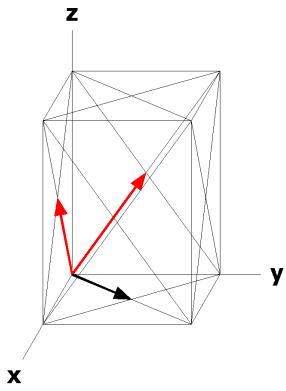
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2)' +	(1/2,0,1/2)' +	(1/2,1/2,0) +
32 p 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},\bar{v},\bar{w}$ ]
16 o ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0, $\bar{w}$ ]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
16 n .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]	$\bar{x},0,\bar{z}$ [0,v,0]	x,0, $\bar{z}$ [0, $\bar{v}$ ,0]
16 m m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	0,y, $\bar{z}$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]
16 l 2'..	x,1/4,1/4 [0,v,w]	$\bar{x},3/4,1/4$ [0, $\bar{v},w$ ]	$\bar{x},3/4,3/4$ [0,v,w]	x,1/4,3/4 [0, $\bar{v},w$ ]
16 k .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	3/4, $\bar{y},3/4$ [u,0,w]	1/4,y,3/4 [ $\bar{u},0,w$ ]
16 j ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0, $\bar{w}$ ]	3/4,3/4, $\bar{z}$ [0,0,w]	1/4,3/4,z [0,0, $\bar{w}$ ]
8 i mm2	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
8 h m2m	0,y,0 [0,0,0]	0, $\bar{y},0$ [0,0,0]		
8 g 2mm	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
8 f 2'2'2	1/4,1/4,1/4 [0,0,w]	3/4,3/4,3/4 [0,0,w]		
8 e ..2/m	1/4,1/4,0 [0,0,w]	3/4,1/4,0 [0,0, $\bar{w}$ ]		
8 d .2'/m.	1/4,0,1/4 [0,0,0]	3/4,0,1/4 [0,0,0]		
8 c 2'/m..	0,1/4,1/4 [0,0,0]	0,3/4,1/4 [0,0,0]		
4 b mmm	0,0,1/2 [0,0,0]			
4 a mmm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



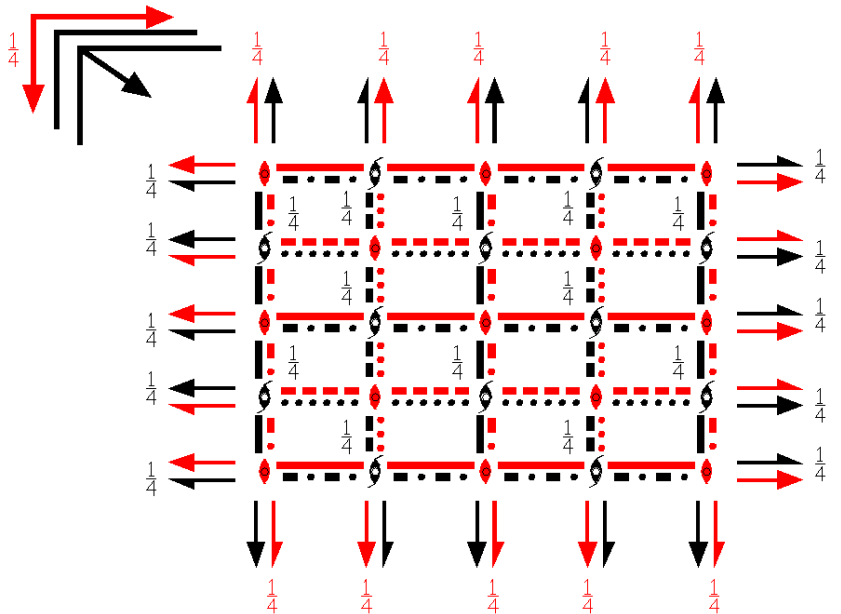
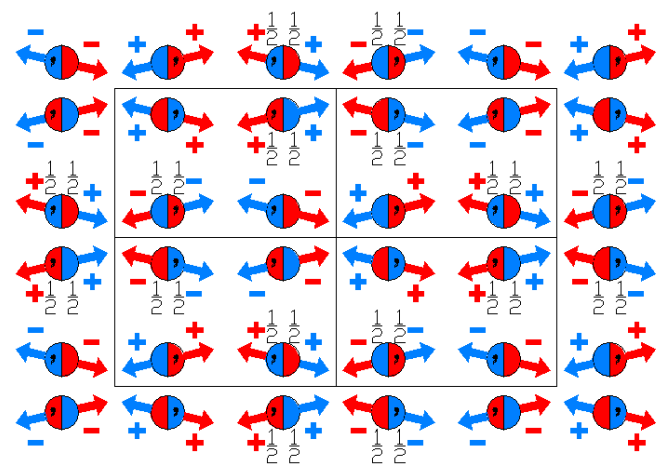
$F_C m'm'm$

69.7.611

$mmm1'$

$F_C 2/m'2'/m2'/m$

Orthorhombic



Origin at center ( $m'm'm$ )

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |                                       |                                       |                                      |
|--|---------------------------------------|---------------------------------------|--------------------------------------|
| (1) 1<br>(1   0,0,0)                         | (2) $2'_z$ 0,0,z<br>( $2_z$   0,0,0)' | (3) $2'_y$ 0,y,0<br>( $2_y$   0,0,0)' | (4) $2'_x$ x,0,0<br>( $2_x$   0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0)' | (6) m x,y,0<br>( $m_z$   0,0,0)       | (7) m x,0,z<br>( $m_y$   0,0,0)       | (8) m' 0,y,z<br>( $m_x$   0,0,0)'    |

For (0,1/2,1/2)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) $t'$ (0,1/2,1/2)<br>(1   0,1/2,1/2)'            | (2) $2'_z$ (0,0,1/2) 0,1/4,z<br>( $2_z$   0,1/2,1/2)  | (3) $2'_y$ (0,1/2,0) 0,y,1/4<br>( $2_y$   0,1/2,1/2)  | (4) $2'_x$ (x,1/4,1/4)<br>( $2_x$   0,1/2,1/2)' |
| (5) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$   0,1/2,1/2) | (6) $b'_z$ (0,1/2,0) x,y,1/4<br>( $m_z$   0,1/2,1/2)' | (7) $c'_y$ (0,0,1/2) x,1/4,z<br>( $m_y$   0,1/2,1/2)' | (8) n (0,1/2,1/2) 0,y,z<br>( $m_x$   0,1/2,1/2) |

For (1/2,0,1/2)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) $t'$ (1/2,0,1/2)<br>(1   1/2,0,1/2)'            | (2) $2'_z$ (0,0,1/2) 1/4,0,z<br>( $2_z$   1/2,0,1/2)  | (3) $2'_y$ (1/4,y,1/4)<br>( $2_y$   1/2,0,1/2)        | (4) $2'_x$ (1/2,0,0) x,0,1/4<br>( $2_x$   1/2,0,1/2)' |
| (5) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$   1/2,0,1/2) | (6) $a'_z$ (1/2,0,0) x,y,1/4<br>( $m_z$   1/2,0,1/2)' | (7) $n'_y$ (1/2,0,1/2) x,0,z<br>( $m_y$   1/2,0,1/2)' | (8) c (0,0,1/2) 1/4,y,z<br>( $m_x$   1/2,0,1/2)       |

For (1/2,1/2,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t$ (1/2,1/2,0)<br>(1   1/2,1/2,0)               | (2) $2'_z$ (1/4,1/4,z)<br>( $2_z$   1/2,1/2,0)' | (3) $2'_y$ (0,1/2,0) 1/4,y,0<br>( $2_y$   1/2,1/2,0)' | (4) $2'_x$ (1/2,0,0) x,1/4,0<br>( $2_x$   1/2,1/2,0)  |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0)' | (6) n (1/2,1/2,0) x,y,0<br>( $m_z$   1/2,1/2,0) | (7) a (1/2,0,0) x,1/4,z<br>( $m_y$   1/2,1/2,0)       | (8) $b'_x$ (0,1/2,0) 1/4,y,z<br>( $m_x$   1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); t'(1/2,0,1/2); (2); (3); (5).

### Positions

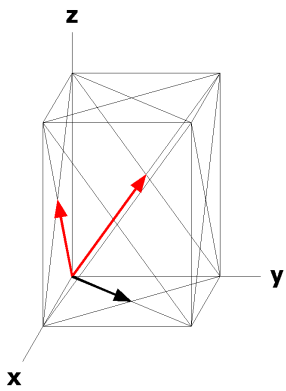
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2)' +	(1/2,0,1/2)' +	(1/2,1/2,0) +
32 p 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
16 o ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
16 n .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0,v,0]	$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	x,0, $\bar{z}$ [0, $\bar{v},0$ ]
16 m m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0,v, $\bar{w}$ ]	0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
16 l 2'..	x,1/4,1/4 [0,v,w]	$\bar{x},3/4,1/4$ [0,v, $\bar{w}$ ]	$\bar{x},3/4,3/4$ [0, $\bar{v},\bar{w}$ ]	x,1/4,3/4 [0, $\bar{v},w$ ]
16 k .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y},1/4$ [0,v,0]	3/4, $\bar{y},3/4$ [0, $\bar{v},0$ ]	1/4,y,3/4 [0, $\bar{v},0$ ]
16 j ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [u, $\bar{v},0$ ]	3/4,3/4, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/4,3/4,z [ $\bar{u},v,0$ ]
8 i m'm2'	0,0,z [0,v,0]	0,0, $\bar{z}$ [0,v,0]		
8 h m'2'm	0,y,0 [0,0,w]	0, $\bar{y},0$ [0,0, $\bar{w}$ ]		
8 g 2mm	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
8 f 2'22'	1/4,1/4,1/4 [0,v,0]	3/4,3/4,3/4 [0, $\bar{v},0$ ]		
8 e ..2'/m	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
8 d .2/m.	1/4,0,1/4 [0,v,0]	3/4,0,1/4 [0,v,0]		
8 c 2'/m'..	0,1/4,1/4 [0,v,w]	0,3/4,1/4 [0,v, $\bar{w}$ ]		
4 b m'mm	0,0,1/2 [0,0,0]			
4 a m'mm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



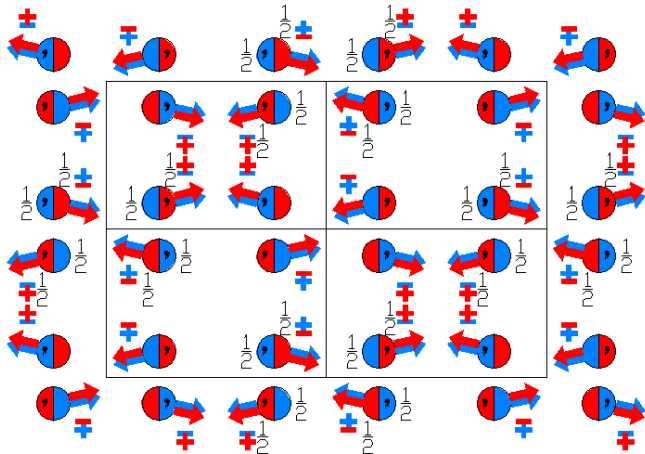
$F_C mmm'$

69.8.612

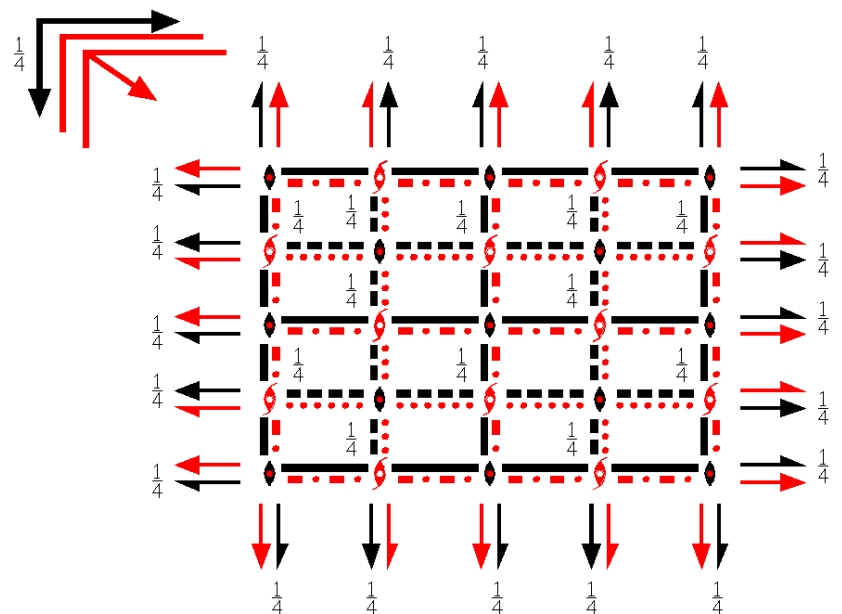
$mmm1'$

$F_C 2'/m2'/m2/m'$

Orthorhombic



Origin at center ( $mmm'$ )



Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1   0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0)   | (3) 2' 0,y,0<br>(2 <sub>y</sub>   0,0,0)' | (4) 2' x,0,0<br>(2 <sub>x</sub>   0,0,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>   0,0,0)' | (7) m x,0,z<br>(m <sub>y</sub>   0,0,0)   | (8) m 0,y,z<br>(m <sub>x</sub>   0,0,0)   |

For (0,1/2,1/2)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) t' (0,1/2,1/2)<br>(1   0,1/2,1/2)'              | (2) 2' (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>   0,1/2,1/2)' | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>   0,1/2,1/2)   | (4) 2 x,1/4,1/4<br>(2 <sub>x</sub>   0,1/2,1/2)           |
| (5) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$   0,1/2,1/2) | (6) b (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>   0,1/2,1/2)   | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>   0,1/2,1/2)' | (8) n' (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>   0,1/2,1/2)' |

For (1/2,0,1/2)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) t' (1/2,0,1/2)<br>(1   1/2,0,1/2)'              | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>   1/2,0,1/2)' | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,0,1/2)           | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>   1/2,0,1/2)   |
| (5) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$   1/2,0,1/2) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>   1/2,0,1/2)   | (7) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>   1/2,0,1/2)' | (8) c' (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>   1/2,0,1/2)' |

For (1/2,1/2,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                 | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)           | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)' |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>   1/2,1/2,0)' | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0)   | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); t'(1/2,0,1/2); (2); (3); (5).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2)' +	(1/2,0,1/2)' +	(1/2,1/2,0) +
32 p 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},\bar{v},w$ ] (7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
16 o ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,0$ [u, $\bar{v},0$ ]	x, $\bar{y},0$ [ $\bar{u},v,0$ ]
16 n .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	x,0, $\bar{z}$ [0,v,0]
16 m m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	0,y, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
16 l 2..	x,1/4,1/4 [u,0,0]	$\bar{x},3/4,1/4$ [ $\bar{u},0,0$ ]	$\bar{x},3/4,3/4$ [ $\bar{u},0,0$ ]	x,1/4,3/4 [u,0,0]
16 k .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y},1/4$ [0, $\bar{v},0$ ]	3/4, $\bar{y},3/4$ [0, $\bar{v},0$ ]	1/4,y,3/4 [0,v,0]
16 j ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0,w]	3/4,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,3/4,z [0,0, $\bar{w}$ ]
8 i mm2	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
8 h m2'm'	0,y,0 [u,0,0]	0, $\bar{y},0$ [ $\bar{u},0,0$ ]		
8 g 2'mm'	x,0,0 [0,v,0]	$\bar{x},0,0$ [0, $\bar{v},0$ ]		
8 f 222	1/4,1/4,1/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]		
8 e ..2/m'	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
8 d .2/m.	1/4,0,1/4 [0,v,0]	3/4,0,1/4 [0, $\bar{v},0$ ]		
8 c 2/m..	0,1/4,1/4 [u,0,0]	0,3/4,1/4 [ $\bar{u},0,0$ ]		
4 b mmm'	0,0,1/2 [0,0,0]			
4 a mmm'	0,0,0 [0,0,0]			

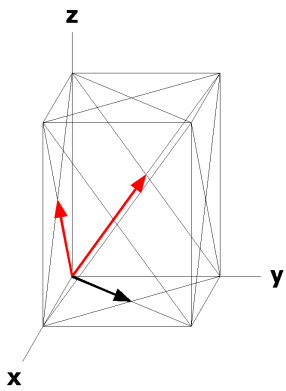
### Symmetry of Special Projections

Along [0,0,1] p<sub>c</sub>2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0





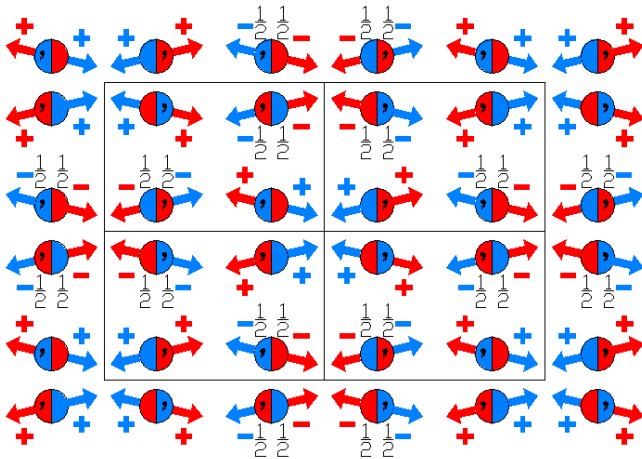
$F_C m'm'm$

69.9.613

$mmm1'$

$F_C 2'/m'2'/m'2'/m$

Orthorhombic



Origin at center ( $m'm'm$ )

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0) | (3) 2' 0,y,0<br>(2 <sub>y</sub>   0,0,0)' | (4) 2' x,0,0<br>(2 <sub>x</sub>   0,0,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>   0,0,0) | (7) m' x,0,z<br>(m <sub>y</sub>   0,0,0)' | (8) m' 0,y,z<br>(m <sub>x</sub>   0,0,0)' |

For (0,1/2,1/2)' + set

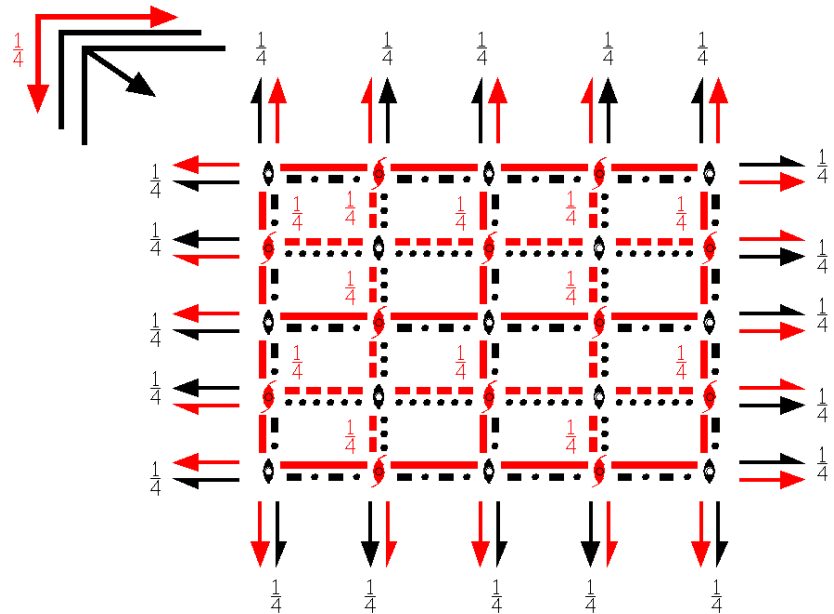
- |  |   |   |   |
|--|---|---|---|
| (1) t' (0,1/2,1/2)<br>(1   0,1/2,1/2)'                 | (2) 2' (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>   0,1/2,1/2)' | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>   0,1/2,1/2) | (4) 2 x,1/4,1/4<br>(2 <sub>x</sub>   0,1/2,1/2)         |
| (5) $\bar{1}$ ' 0,1/4,1/4<br>( $\bar{1}$   0,1/2,1/2)' | (6) b' (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>   0,1/2,1/2)' | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>   0,1/2,1/2) | (8) n (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>   0,1/2,1/2) |

For (1/2,0,1/2)' + set

- |  |   |   |   |
|--|---|---|---|
| (1) t' (1/2,0,1/2)<br>(1   1/2,0,1/2)'                 | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>   1/2,0,1/2)' | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,0,1/2)         | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>   1/2,0,1/2) |
| (5) $\bar{1}$ ' 1/4,0,1/4<br>( $\bar{1}$   1/2,0,1/2)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>   1/2,0,1/2)' | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>   1/2,0,1/2) | (8) c (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>   1/2,0,1/2) |

For (1/2,1/2,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)         | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)' |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>   1/2,1/2,0) | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); t'(1/2,0,1/2); (2); (3); (5).

### Positions

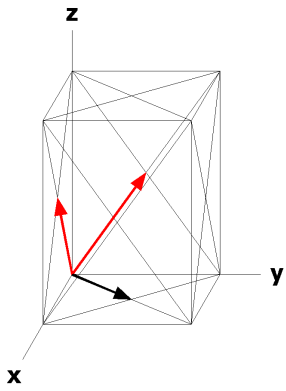
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2)' +	(1/2,0,1/2)' +	(1/2,1/2,0) +
32 p 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
16 o ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0,w]
16 n .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$\bar{x},0,\bar{z}$ [u,0,w]	x,0, $\bar{z}$ [ $\bar{u},0,w$ ]
16 m m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
16 l 2..	x,1/4,1/4 [u,0,0]	$\bar{x},3/4,1/4$ [ $\bar{u},0,0$ ]	$\bar{x},3/4,3/4$ [u,0,0]	x,1/4,3/4 [ $\bar{u},0,0$ ]
16 k .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y},1/4$ [0, $\bar{v},0$ ]	3/4, $\bar{y},3/4$ [0,v,0]	1/4,y,3/4 [0, $\bar{v},0$ ]
16 j ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0,w]	3/4,3/4, $\bar{z}$ [0,0,w]	1/4,3/4,z [0,0,w]
8 i m'm'2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
8 h m'2'm	0,y,0 [0,0,w]	0, $\bar{y},0$ [0,0,w]		
8 g 2'm'm	x,0,0 [0,0,w]	$\bar{x},0,0$ [0,0,w]		
8 f 222	1/4,1/4,1/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]		
8 e ..2/m	1/4,1/4,0 [0,0,w]	3/4,1/4,0 [0,0,w]		
8 d .2/m'	1/4,0,1/4 [0,0,0]	3/4,0,1/4 [0,0,0]		
8 c 2/m'..	0,1/4,1/4 [0,0,0]	0,3/4,1/4 [0,0,0]		
4 b m'm'm	0,0,1/2 [0,0,w]			
4 a m'm'm	0,0,0 [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,1/4

Along [0,1,0] p<sub>2a</sub>'2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



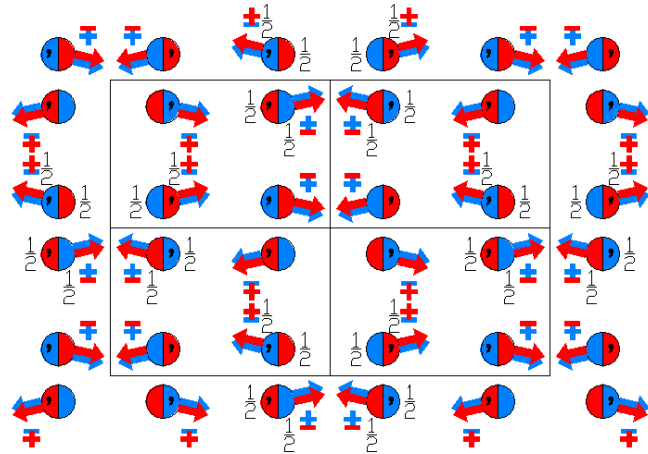
$F_C mm'm'$

69.10.614

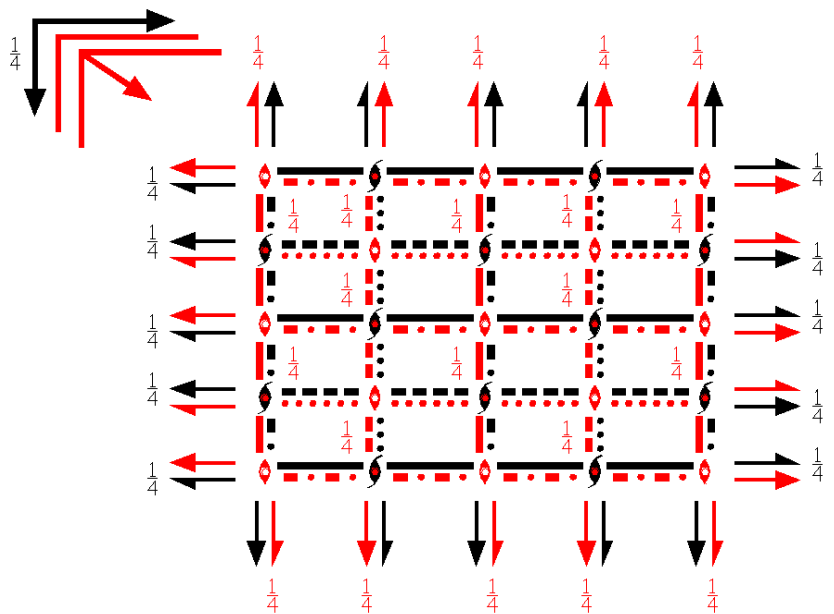
$mmm1'$

$F_C 2/m2'/m'2'/m'$

Orthorhombic



Origin at center ( $mm'm'$ )



Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |                                       |                                       |                                      |
|---|---------------------------------------|---------------------------------------|--------------------------------------|
| (1) 1<br>(1   0,0,0)                        | (2) $2'_z$ 0,0,z<br>( $2_z$   0,0,0)' | (3) $2'_y$ 0,y,0<br>( $2_y$   0,0,0)' | (4) $2'_x$ x,0,0<br>( $2_x$   0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0) | (6) $m'_x$ x,y,0<br>( $m_x$   0,0,0)' | (7) $m'_y$ x,0,z<br>( $m_y$   0,0,0)' | (8) $m'_z$ 0,y,z<br>( $m_z$   0,0,0) |

For (0,1/2,1/2)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) $t'$ (0,1/2,1/2)<br>(1   0,1/2,1/2)'               | (2) $2'_z$ (0,0,1/2) 0,1/4,z<br>( $2_z$   0,1/2,1/2) | (3) $2'_y$ (0,1/2,0) 0,y,1/4<br>( $2_y$   0,1/2,1/2) | (4) $2'_x$ (x,1/4,1/4)<br>( $2_x$   0,1/2,1/2)'     |
| (5) $\bar{1}'$ 0,1/4,1/4<br>( $\bar{1}'$   0,1/2,1/2)' | (6) $b$ (0,1/2,0) x,y,1/4<br>( $m_z$   0,1/2,1/2)    | (7) $c$ (0,0,1/2) x,1/4,z<br>( $m_y$   0,1/2,1/2)    | (8) $n'$ (0,1/2,1/2) 0,y,z<br>( $m_x$   0,1/2,1/2)' |

For (1/2,0,1/2)' + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t'$ (1/2,0,1/2)<br>(1   1/2,0,1/2)'               | (2) $2'_z$ (0,0,1/2) 1/4,0,z<br>( $2_z$   1/2,0,1/2) | (3) $2'_y$ (1/4,y,1/4)<br>( $2_y$   1/2,0,1/2)    | (4) $2'_x$ (1/2,0,0) x,0,1/4<br>( $2_x$   1/2,0,1/2)' |
| (5) $\bar{1}'$ 1/4,0,1/4<br>( $\bar{1}'$   1/2,0,1/2)' | (6) $a$ (1/2,0,0) x,y,1/4<br>( $m_z$   1/2,0,1/2)    | (7) $n$ (1/2,0,1/2) x,0,z<br>( $m_y$   1/2,0,1/2) | (8) $c'$ (0,0,1/2) 1/4,y,z<br>( $m_x$   1/2,0,1/2)'   |

For (1/2,1/2,0) + set

- |   |   |   |  |
|---|---|---|--|
| (1) $t$ (1/2,1/2,0)<br>(1   1/2,1/2,0)              | (2) $2'_z$ (1/4,1/4,z)<br>( $2_z$   1/2,1/2,0)'     | (3) $2'_y$ (0,1/2,0) 1/4,y,0<br>( $2_y$   1/2,1/2,0)' | (4) $2'_x$ (1/2,0,0) x,1/4,0<br>( $2_x$   1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0) | (6) $n'$ (1/2,1/2,0) x,y,0<br>( $m_z$   1/2,1/2,0)' | (7) $a'$ (1/2,0,0) x,1/4,z<br>( $m_y$   1/2,1/2,0)'   | (8) $b$ (0,1/2,0) 1/4,y,z<br>( $m_x$   1/2,1/2,0)    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); t'(1/2,0,1/2); (2); (3); (5).

### Positions

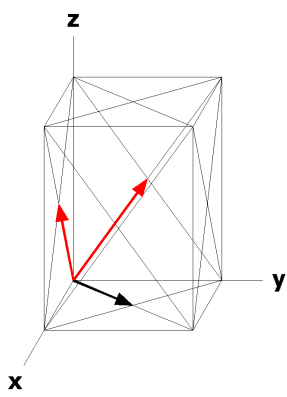
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2)' +	(1/2,0,1/2)' +	(1/2,1/2,0) +
32 p 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v}$ ,w] (7) x, $\bar{y},z$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
16 o ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [u,v,0]	$\bar{x},y,0$ [u, $\bar{v}$ ,0]	x, $\bar{y},0$ [u, $\bar{v}$ ,0]
16 n .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [u,0, $\bar{w}$ ]	$\bar{x},0,\bar{z}$ [u,0,w]	x,0, $\bar{z}$ [u,0, $\bar{w}$ ]
16 m m..	0,y,z [u,0,0]	0, $\bar{y},z$ [u,0,0]	0,y, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [u,0,0]
16 l 2'..	x,1/4,1/4 [0,v,w]	$\bar{x},3/4,1/4$ [0,v, $\bar{w}$ ]	$\bar{x},3/4,3/4$ [0,v,w]	x,1/4,3/4 [0,v, $\bar{w}$ ]
16 k .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y},1/4$ [0,v,0]	3/4, $\bar{y},3/4$ [0,v,0]	1/4,y,3/4 [0,v,0]
16 j ..2'	1/4,1/4,z [u,v,0]	3/4,1/4, $\bar{z}$ [u, $\bar{v}$ ,0]	3/4,3/4, $\bar{z}$ [u,v,0]	1/4,3/4,z [u, $\bar{v}$ ,0]
8 i mm'2'	0,0,z [u,0,0]	0,0, $\bar{z}$ [u,0,0]		
8 h m2'm'	0,y,0 [u,0,0]	0, $\bar{y},0$ [u,0,0]		
8 g 2m'm'	x,0,0 [u,0,0]	$\bar{x},0,0$ [u,0,0]		
8 f 2'22'	1/4,1/4,1/4 [0,v,0]	3/4,3/4,3/4 [0,v,0]		
8 e ..2'/m'	1/4,1/4,0 [u,v,w]	3/4,1/4,0 [u, $\bar{v}$ ,0]		
8 d .2/m.	1/4,0,1/4 [0,v,0]	3/4,0,1/4 [0, $\bar{v}$ ,0]		
8 c 2'/m..	0,1/4,1/4 [0,0,0]	0,3/4,1/4 [0,0,0]		
4 b mm'm'	0,0,1/2 [u,0,0]			
4 a mm'm'	0,0,0 [u,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p<sub>c</sub>2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,1/4,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



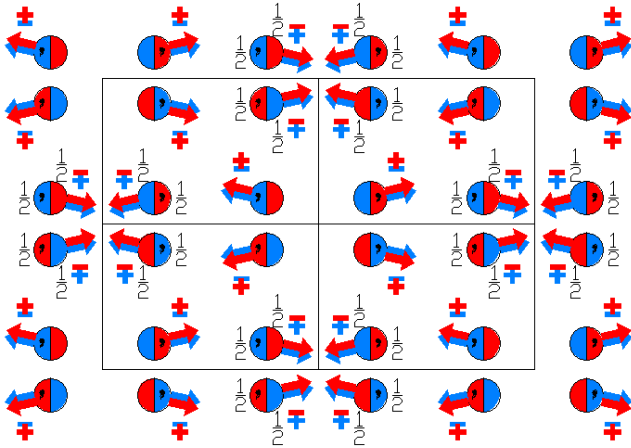
$F_C m'm'm'$

69.11.615

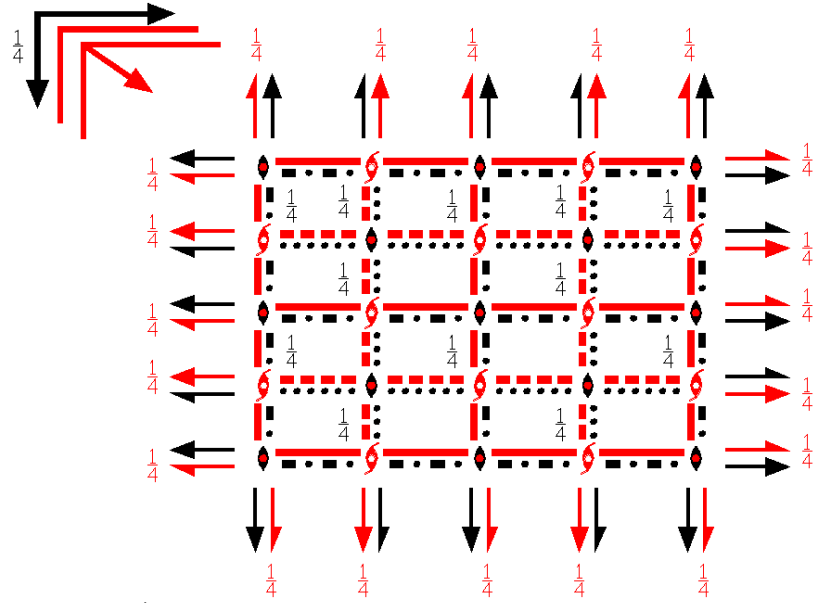
$mmm1'$

$F_C 2/m'2/m'2/m'$

Orthorhombic



Origin at center ( $m'm'm'$ )



Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1   0,0,0)                         | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>   0,0,0)    | (3) 2 <sub>y</sub> 0,y,0<br>(2 <sub>y</sub>   0,0,0)    | (4) 2 <sub>x</sub> x,0,0<br>(2 <sub>x</sub>   0,0,0)    |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0)' | (6) m' <sub>z</sub> x,y,0<br>(m' <sub>z</sub>   0,0,0)' | (7) m' <sub>y</sub> x,0,z<br>(m' <sub>y</sub>   0,0,0)' | (8) m' <sub>x</sub> 0,y,z<br>(m' <sub>x</sub>   0,0,0)' |

For (0,1/2,1/2)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) t' (0,1/2,1/2)<br>(1   0,1/2,1/2)'              | (2) 2' (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>   0,1/2,1/2)' | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>   0,1/2,1/2)' | (4) 2' x,1/4,1/4<br>(2 <sub>x</sub>   0,1/2,1/2)'       |
| (5) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$   0,1/2,1/2) | (6) b (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>   0,1/2,1/2)   | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>   0,1/2,1/2)   | (8) n (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>   0,1/2,1/2) |

For (1/2,0,1/2)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) t' (1/2,0,1/2)<br>(1   1/2,0,1/2)'              | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>   1/2,0,1/2)' | (3) 2' 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,0,1/2)'       | (4) 2' (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>   1/2,0,1/2)' |
| (5) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$   1/2,0,1/2) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>   1/2,0,1/2)   | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>   1/2,0,1/2) | (8) c (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>   1/2,0,1/2)   |

For (1/2,1/2,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                 | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)           | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)   |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>   1/2,1/2,0)' | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); t'(1/2,0,1/2); (2); (3); (5).

### Positions

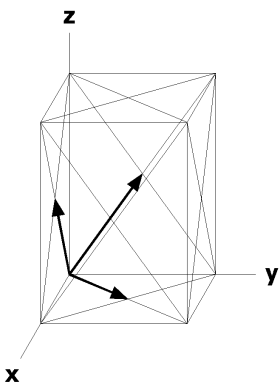
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2)' +	(1/2,0,1/2)' +	(1/2,1/2,0) +
32 p 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
16 o ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,0$ [ $\bar{u},v,0$ ]	x, $\bar{y},0$ [u, $\bar{v},0$ ]
16 n .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$\bar{x},0,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	x,0, $\bar{z}$ [u,0, $\bar{w}$ ]
16 m m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	0,y, $\bar{z}$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
16 l 2'..	x,1/4,1/4 [0,v,w]	$\bar{x},3/4,1/4$ [0, $\bar{v},w$ ]	$\bar{x},3/4,3/4$ [0, $\bar{v},\bar{w}$ ]	x,1/4,3/4 [0,v, $\bar{w}$ ]
16 k .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	3/4, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	1/4,y,3/4 [u,0, $\bar{w}$ ]
16 j ..2	1/4,1/4,z [0,0,w]	3/4,1/4, $\bar{z}$ [0,0, $\bar{w}$ ]	3/4,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,3/4,z [0,0,w]
8 i m'm'2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
8 h m'2m'	0,y,0 [0,v,0]	0, $\bar{y},0$ [0, $\bar{v},0$ ]		
8 g 2m'm'	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]		
8 f 2'2'2	1/4,1/4,1/4 [0,0,w]	3/4,3/4,3/4 [0,0, $\bar{w}$ ]		
8 e ..2/m'	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]		
8 d .2'/m'	1/4,0,1/4 [0,v,0]	3/4,0,1/4 [0,v,0]		
8 c 2'/m'..	0,1/4,1/4 [u,0,0]	0,3/4,1/4 [u,0,0]		
4 b m'm'm'	0,0,1/2 [0,0,0]			
4 a m'm'm'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p<sub>c</sub>2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



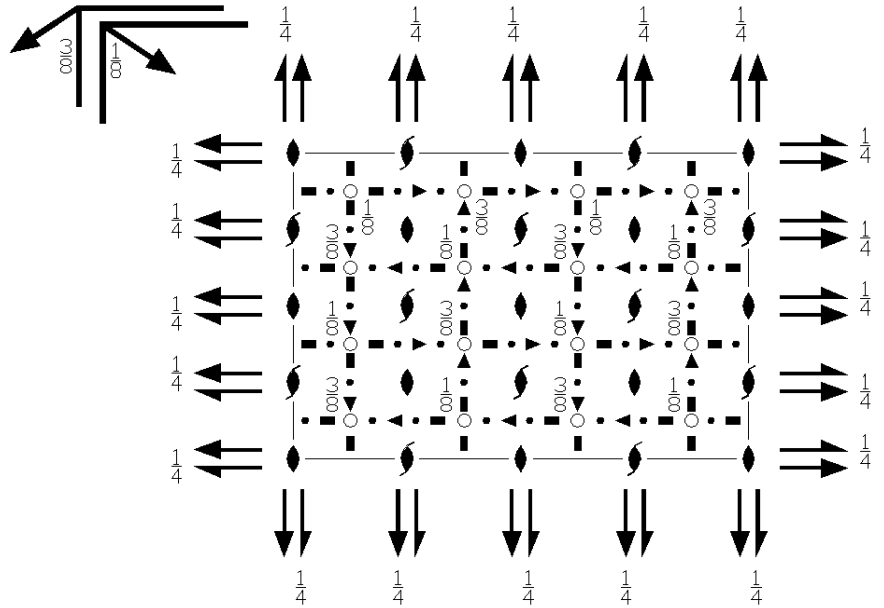
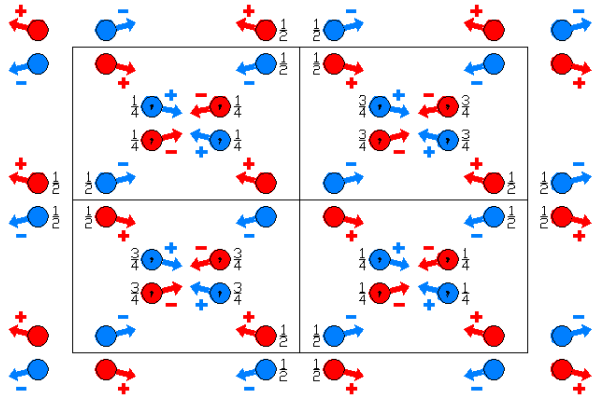
Fddd

70.1.616

mmm

F2/d2/d2/d

Orthorhombic



Origin at 222 at  $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq \frac{1}{8}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{4}$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                                    | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0)                     | (3) 2 0,y,0<br>(2 <sub>y</sub>   0,0,0)                     | (4) 2 x,0,0<br>(2 <sub>x</sub>   0,0,0)                     |
| (5) $\bar{1}$ 1/8,1/8,1/8<br>( $\bar{1}$   1/4,1/4,1/4) | (6) d (1/4,1/4,0) x,y,1/8<br>(m <sub>z</sub>   1/4,1/4,1/4) | (7) d (1/4,0,1/4) x,1/8,z<br>(m <sub>y</sub>   1/4,1/4,1/4) | (8) d (0,1/4,1/4) 1/8,y,z<br>(m <sub>x</sub>   1/4,1/4,1/4) |

For (0,1/2,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (0,1/2,1/2)<br>(1   0,1/2,1/2)                    | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>   0,1/2,1/2)     | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>   0,1/2,1/2)     | (4) 2 x,1/4,1/4<br>(2 <sub>x</sub>   0,1/2,1/2)             |
| (5) $\bar{1}$ 1/8,3/8,3/8<br>( $\bar{1}$   1/4,3/4,3/4) | (6) d (1/4,3/4,0) x,y,3/8<br>(m <sub>z</sub>   1/4,3/4,3/4) | (7) d (1/4,0,1/4) x,3/8,z<br>(m <sub>y</sub>   1/4,3/4,3/4) | (8) d (0,3/4,3/4) 1/8,y,z<br>(m <sub>x</sub>   1/4,3/4,3/4) |

For (1/2,0,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,0,1/2)<br>(1   1/2,0,1/2)                    | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>   1/2,0,1/2)     | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,0,1/2)             | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>   1/2,0,1/2)     |
| (5) $\bar{1}$ 3/8,1/8,3/8<br>( $\bar{1}$   3/4,1/4,3/4) | (6) d (3/4,1/4,0) x,y,3/8<br>(m <sub>z</sub>   3/4,1/4,3/4) | (7) d (3/4,0,3/4) x,1/8,z<br>(m <sub>y</sub>   3/4,1/4,3/4) | (8) d (0,1/4,3/4) 3/8,y,z<br>(m <sub>x</sub>   3/4,1/4,3/4) |

For (1/2,1/2,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                    | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)             | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)     | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)     |
| (5) $\bar{1}$ 3/8,3/8,1/8<br>( $\bar{1}$   3/4,3/4,1/4) | (6) d (3/4,3/4,0) x,y,1/8<br>(m <sub>z</sub>   3/4,3/4,1/4) | (7) d (3/4,0,1/4) x,3/8,z<br>(m <sub>y</sub>   3/4,3/4,1/4) | (8) d (0,3/4,1/4) 3/8,y,z<br>(m <sub>x</sub>   3/4,3/4,1/4) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
32 h 1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
	(5) $\bar{x}+1/4,\bar{y}+1/4,\bar{z}+1/4$ [ $u,v,w$ ]	(6) $x+1/4,y+1/4,\bar{z}+1/4$ [ $\bar{u},\bar{v},w$ ]	(7) $x+1/4,\bar{y}+1/4,z+1/4$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/4,y+1/4,z+1/4$ [ $u,\bar{v},\bar{w}$ ]
16 g ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,1/4, $\bar{z}+1/4$ [0,0,w]	1/4,1/4,z+1/4 [0,0, $\bar{w}$ ]
16 f .2.	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]	1/4, $\bar{y}+1/4$ ,1/4 [0,v,0]	1/4,y+1/4,1/4 [0, $\bar{v}$ ,0]
16 e 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0]	$\bar{x}+1/4$ ,1/4,1/4 [u,0,0]	x+1/4,1/4,1/4 [ $\bar{u}$ ,0,0]
16 d $\bar{1}$	5/8,5/8,5/8 [u,v,w]	3/8,3/8,5/8 [ $\bar{u},\bar{v},w$ ]	3/8,5/8,3/8 [ $\bar{u},v,\bar{w}$ ]	5/8,3/8,3/8 [u, $\bar{v},\bar{w}$ ]
16 c $\bar{1}$	1/8,1/8,1/8 [u,v,w]	7/8,7/8,1/8 [ $\bar{u},\bar{v},w$ ]	7/8,1/8,7/8 [ $\bar{u},v,\bar{w}$ ]	1/8,7/8,7/8 [u, $\bar{v},\bar{w}$ ]
8 b 222	0,0,1/2 [0,0,0]	1/4,1/4,3/4 [0,0,0]		
8 a 222	0,0,0 [0,0,0]	1/4,1/4,1/4 [0,0,0]		

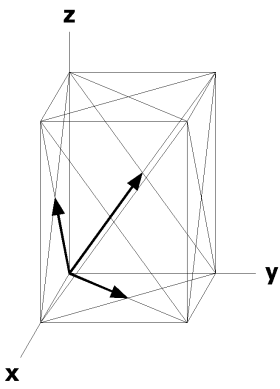
**Symmetry of Special Projections**

Along [0,0,1]  $c_p \cdot 2m'm'$   
 $a^* = a/2$   $b^* = b/2$   
 Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 2m'm'$   
 $a^* = b/2$   $b^* = c/2$   
 Origin at x,0,0

Along [0,1,0]  $c_p \cdot 2m'm'$   
 $a^* = c/2$   $b^* = a/2$   
 Origin at 0,y,0



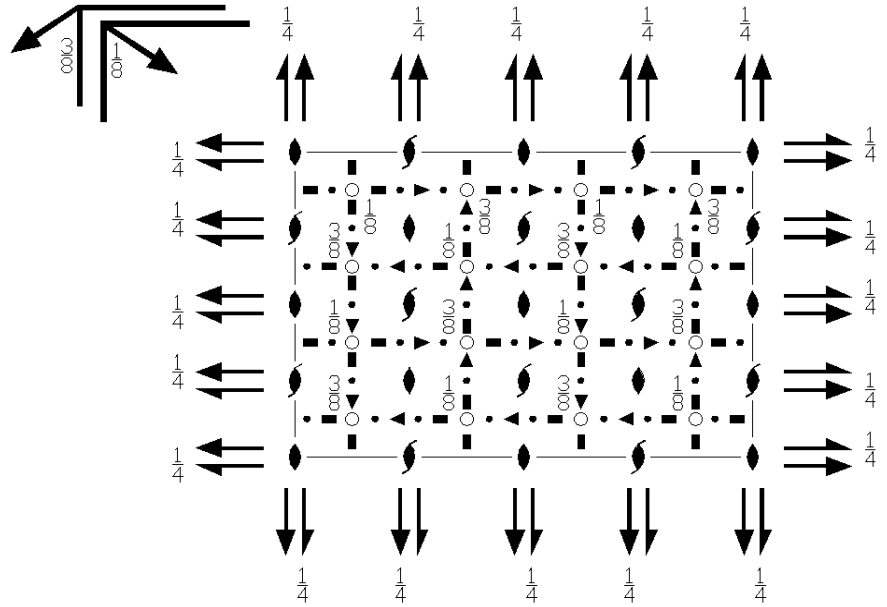


Fddd1'  
70.2.617

mmm1'  
F2/d2/d2/d1'

Orthorhombic

1'



Origin at 2221' at  $-1/8, -1/8, -1/8$  from  $\bar{1}1'$

Asymmetric unit  $0 \leq x \leq 1/8; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                                    | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0)                     | (3) 2 0,y,0<br>(2 <sub>y</sub>   0,0,0)                     | (4) 2 x,0,0<br>(2 <sub>x</sub>   0,0,0)                     |
| (5) $\bar{1}$ 1/8,1/8,1/8<br>( $\bar{1}$   1/4,1/4,1/4) | (6) d (1/4,1/4,0) x,y,1/8<br>(m <sub>z</sub>   1/4,1/4,1/4) | (7) d (1/4,0,1/4) x,1/8,z<br>(m <sub>y</sub>   1/4,1/4,1/4) | (8) d (0,1/4,1/4) 1/8,y,z<br>(m <sub>x</sub>   1/4,1/4,1/4) |

For (0,1/2,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (0,1/2,1/2)<br>(1   0,1/2,1/2)                    | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>   0,1/2,1/2)     | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>   0,1/2,1/2)     | (4) 2 x,1/4,1/4<br>(2 <sub>x</sub>   0,1/2,1/2)             |
| (5) $\bar{1}$ 1/8,3/8,3/8<br>( $\bar{1}$   1/4,3/4,3/4) | (6) d (1/4,3/4,0) x,y,3/8<br>(m <sub>z</sub>   1/4,3/4,3/4) | (7) d (1/4,0,1/4) x,3/8,z<br>(m <sub>y</sub>   1/4,3/4,3/4) | (8) d (0,3/4,3/4) 1/8,y,z<br>(m <sub>x</sub>   1/4,3/4,3/4) |

For (1/2,0,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,0,1/2)<br>(1   1/2,0,1/2)                    | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>   1/2,0,1/2)     | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,0,1/2)             | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>   1/2,0,1/2)     |
| (5) $\bar{1}$ 3/8,1/8,3/8<br>( $\bar{1}$   3/4,1/4,3/4) | (6) d (3/4,1/4,0) x,y,3/8<br>(m <sub>z</sub>   3/4,1/4,3/4) | (7) d (3/4,0,3/4) x,1/8,z<br>(m <sub>y</sub>   3/4,1/4,3/4) | (8) d (0,1/4,3/4) 3/8,y,z<br>(m <sub>x</sub>   3/4,1/4,3/4) |

For (1/2,1/2,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                    | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)             | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)     | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)     |
| (5) $\bar{1}$ 3/8,3/8,1/8<br>( $\bar{1}$   3/4,3/4,1/4) | (6) d (3/4,3/4,0) x,y,1/8<br>(m <sub>z</sub>   3/4,3/4,1/4) | (7) d (3/4,0,1/4) x,3/8,z<br>(m <sub>y</sub>   3/4,3/4,1/4) | (8) d (0,3/4,1/4) 3/8,y,z<br>(m <sub>x</sub>   3/4,3/4,1/4) |

## For (0,0,0)' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(4) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'
(5) $\bar{1}$ ' 1/8,1/8,1/8 ( $\bar{1}$  1/4,1/4,1/4)'	(6) d' (1/4,1/4,0) x,y,1/8 (m <sub>z</sub>  1/4,1/4,1/4)'	(7) d' (1/4,0,1/4) x,1/8,z (m <sub>y</sub>  1/4,1/4,1/4)'	(8) d' (0,1/4,1/4) 1/8,y,z (m <sub>x</sub>  1/4,1/4,1/4)'

## For (0,1/2,1/2)' + set

(1) t' (0,1/2,1/2) (1 0,1/2,1/2)'	(2) 2' (0,0,1/2) 0,1/4,z (2 <sub>z</sub>  0,1/2,1/2)'	(3) 2' (0,1/2,0) 0,y,1/4 (2 <sub>y</sub>  0,1/2,1/2)'	(4) 2' x,1/4,1/4 (2 <sub>x</sub>  0,1/2,1/2)'
(5) $\bar{1}$ ' 1/8,3/8,3/8 ( $\bar{1}$  1/4,3/4,3/4)'	(6) d' (1/4,3/4,0) x,y,3/8 (m <sub>z</sub>  1/4,3/4,3/4)'	(7) d' (1/4,0,1/4) x,3/8,z (m <sub>y</sub>  1/4,3/4,3/4)'	(8) d' (0,3/4,3/4) 1/8,y,z (m <sub>x</sub>  1/4,3/4,3/4)'

## For (1/2,0,1/2)' + set

(1) t' (1/2,0,1/2) (1 1/2,0,1/2)'	(2) 2' (0,0,1/2) 1/4,0,z (2 <sub>z</sub>  1/2,0,1/2)'	(3) 2' 1/4,y,1/4 (2 <sub>y</sub>  1/2,0,1/2)'	(4) 2' (1/2,0,0) x,0,1/4 (2 <sub>x</sub>  1/2,0,1/2)'
(5) $\bar{1}$ ' 3/8,1/8,3/8 ( $\bar{1}$  3/4,1/4,3/4)'	(6) d' (3/4,1/4,0) x,y,3/8 (m <sub>z</sub>  3/4,1/4,3/4)'	(7) d' (3/4,0,3/4) x,1/8,z (m <sub>y</sub>  3/4,1/4,3/4)'	(8) d' (0,1/4,3/4) 3/8,y,z (m <sub>x</sub>  3/4,1/4,3/4)'

## For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0) (1 1/2,1/2,0)'	(2) 2' 1/4,1/4,z (2 <sub>z</sub>  1/2,1/2,0)'	(3) 2' (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>  1/2,1/2,0)'	(4) 2' (1/2,0,0) x,1/4,0 (2 <sub>x</sub>  1/2,1/2,0)'
(5) $\bar{1}$ ' 3/8,3/8,1/8 ( $\bar{1}$  3/4,3/4,1/4)'	(6) d' (3/4,3/4,0) x,y,1/8 (m <sub>z</sub>  3/4,3/4,1/4)'	(7) d' (3/4,0,1/4) x,3/8,z (m <sub>y</sub>  3/4,3/4,1/4)'	(8) d' (0,3/4,1/4) 3/8,y,z (m <sub>x</sub>  3/4,3/4,1/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

	(0,0,0) + (0,0,0)'	(0,1/2,1/2) + (0,1/2,1/2)'	(1/2,0,1/2) + (1/2,0,1/2)'	(1/2,1/2,0) + (1/2,1/2,0)'
32 h 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{x},y,\bar{z}$ [0,0,0]	(4) $x,\bar{y},\bar{z}$ [0,0,0]
	(5) $\bar{x}+1/4,\bar{y}+1/4,\bar{z}+1/4$ [0,0,0]	(6) $x+1/4,y+1/4,\bar{z}+1/4$ [0,0,0]	(7) $x+1/4,\bar{y}+1/4,z+1/4$ [0,0,0]	(8) $\bar{x}+1/4,y+1/4,z+1/4$ [0,0,0]
16 g ..21'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/4,1/4, $\bar{z}+1/4$ [0,0,0]	1/4,1/4,z+1/4 [0,0,0]
16 f ..2.1'	0,y,0 [0,0,0]	0, $\bar{y}$ ,0 [0,0,0]	1/4, $\bar{y}+1/4$ ,1/4 [0,0,0]	1/4,y+1/4,1/4 [0,0,0]

Continued

70.2.617

Fddd1'

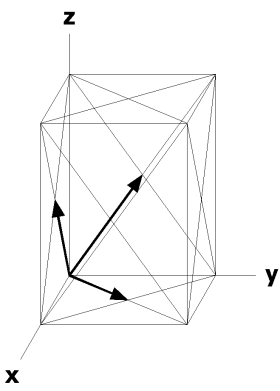
16 e	2..1'	x,0,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0]	$\bar{x}+1/4,1/4,1/4$ [0,0,0]	x+1/4,1/4,1/4 [0,0,0]
16 d	$\bar{1}1'$	5/8,5/8,5/8 [0,0,0]	3/8,3/8,5/8 [0,0,0]	3/8,5/8,3/8 [0,0,0]	5/8,3/8,3/8 [0,0,0]
16 c	$\bar{1}1'$	1/8,1/8,1/8 [0,0,0]	7/8,7/8,1/8 [0,0,0]	7/8,1/8,7/8 [0,0,0]	1/8,7/8,7/8 [0,0,0]
8 b	2221'	0,0,1/2 [0,0,0]	1/4,1/4,3/4 [0,0,0]		
8 a	2221'	0,0,0 [0,0,0]	1/4,1/4,1/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

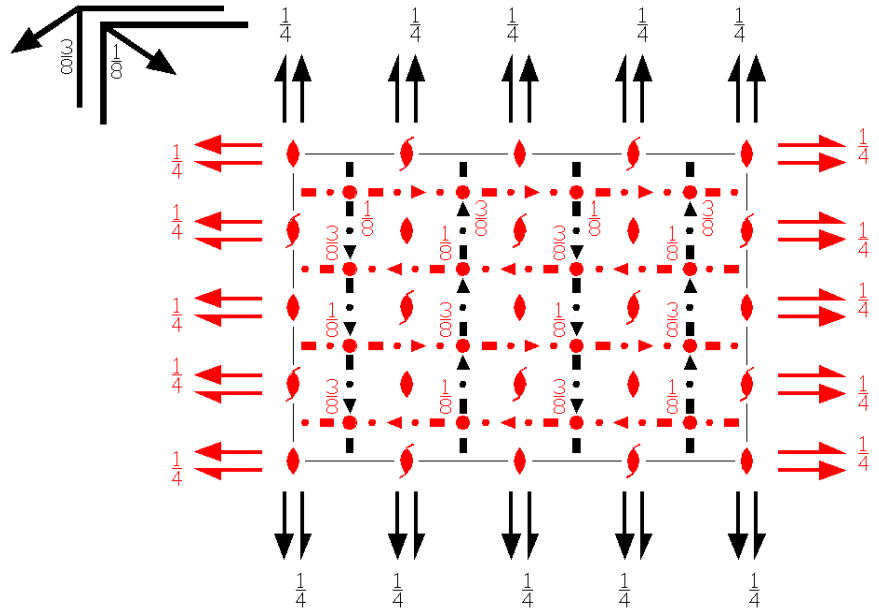
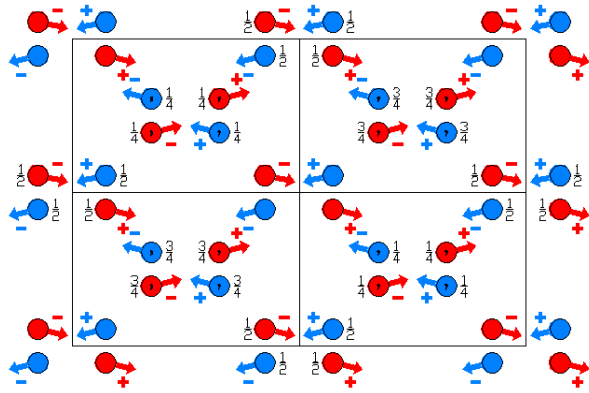
Along [0,1,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Fd'dd  
70.3.618

m'mm  
F2/d'2'/d2'/d

Orthorhombic



Origin at 22'2' at  $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}$  from  $\bar{1}$ '

Asymmetric unit  $0 \leq x \leq \frac{1}{8}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1   0,0,0)                                       | (2) 2' 0,0,z<br>(2 <sub>z</sub>   0,0,0)'                   | (3) 2' 0,y,0<br>(2 <sub>y</sub>   0,0,0)'                   | (4) 2 x,0,0<br>(2 <sub>x</sub>   0,0,0)                       |
| (5) $\bar{1}$ ' 1/8,1/8,1/8<br>( $\bar{1}$   1/4,1/4,1/4)' | (6) d (1/4,1/4,0) x,y,1/8<br>(m <sub>z</sub>   1/4,1/4,1/4) | (7) d (1/4,0,1/4) x,1/8,z<br>(m <sub>y</sub>   1/4,1/4,1/4) | (8) d' (0,1/4,1/4) 1/8,y,z<br>(m <sub>x</sub>   1/4,1/4,1/4)' |

For (0,1/2,1/2) + set

- |  |   |   |   |
|--|---|---|---|
| (1) t (0,1/2,1/2)<br>(1   0,1/2,1/2)                       | (2) 2' (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>   0,1/2,1/2)'   | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>   0,1/2,1/2)'   | (4) 2 x,1/4,1/4<br>(2 <sub>x</sub>   0,1/2,1/2)               |
| (5) $\bar{1}$ ' 1/8,3/8,3/8<br>( $\bar{1}$   1/4,3/4,3/4)' | (6) d (1/4,3/4,0) x,y,3/8<br>(m <sub>z</sub>   1/4,3/4,3/4) | (7) d (1/4,0,1/4) x,3/8,z<br>(m <sub>y</sub>   1/4,3/4,3/4) | (8) d' (0,3/4,3/4) 1/8,y,z<br>(m <sub>x</sub>   1/4,3/4,3/4)' |

For (1/2,0,1/2) + set

- |  |   |   |   |
|--|---|---|---|
| (1) t (1/2,0,1/2)<br>(1   1/2,0,1/2)                       | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>   1/2,0,1/2)'   | (3) 2' 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,0,1/2)'           | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>   1/2,0,1/2)       |
| (5) $\bar{1}$ ' 3/8,1/8,3/8<br>( $\bar{1}$   3/4,1/4,3/4)' | (6) d (3/4,1/4,0) x,y,3/8<br>(m <sub>z</sub>   3/4,1/4,3/4) | (7) d (3/4,0,3/4) x,1/8,z<br>(m <sub>y</sub>   3/4,1/4,3/4) | (8) d' (0,1/4,3/4) 3/8,y,z<br>(m <sub>x</sub>   3/4,1/4,3/4)' |

For (1/2,1/2,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                       | (2) 2' 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)'           | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)'   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)       |
| (5) $\bar{1}$ ' 3/8,3/8,1/8<br>( $\bar{1}$   3/4,3/4,1/4)' | (6) d (3/4,3/4,0) x,y,1/8<br>(m <sub>z</sub>   3/4,3/4,1/4) | (7) d (3/4,0,1/4) x,3/8,z<br>(m <sub>y</sub>   3/4,3/4,1/4) | (8) d' (0,3/4,1/4) 3/8,y,z<br>(m <sub>x</sub>   3/4,3/4,1/4)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5).

### Positions

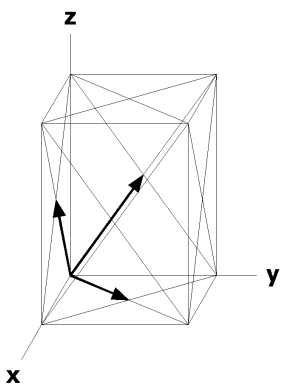
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
32 h 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
	(5) $\bar{x}+1/4,\bar{y}+1/4,\bar{z}+1/4$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x+1/4,y+1/4, $\bar{z}+1/4$ [ $\bar{u},\bar{v},w$ ]	(7) x+1/4, $\bar{y}+1/4,z+1/4$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x}+1/4,y+1/4,z+1/4$ [ $\bar{u},v,w$ ]
16 g ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [u, $\bar{v}$ ,0]	1/4,1/4, $\bar{z}+1/4$ [ $\bar{u},\bar{v},0$ ]	1/4,1/4,z+1/4 [ $\bar{u},v,0$ ]
16 f .2'	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [u,0, $\bar{w}$ ]	1/4, $\bar{y}+1/4,1/4$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/4,1/4 [ $\bar{u},0,w$ ]
16 e 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [u,0,0]	$\bar{x}+1/4,1/4,1/4$ [ $\bar{u},0,0$ ]	x+1/4,1/4,1/4 [ $\bar{u},0,0$ ]
16 d $\bar{1}$	5/8,5/8,5/8 [0,0,0]	3/8,3/8,5/8 [0,0,0]	3/8,5/8,3/8 [0,0,0]	5/8,3/8,3/8 [0,0,0]
16 c $\bar{1}$	1/8,1/8,1/8 [0,0,0]	7/8,7/8,1/8 [0,0,0]	7/8,1/8,7/8 [0,0,0]	1/8,7/8,7/8 [0,0,0]
8 b 22'2'	0,0,1/2 [u,0,0]	1/4,1/4,3/4 [ $\bar{u},0,0$ ]		
8 a 22'2'	0,0,0 [u,0,0]	1/4,1/4,1/4 [ $\bar{u},0,0$ ]		

### Symmetry of Special Projections

Along [0,0,1]  $c_p \cdot 2'mm'$   
 $a^* = a/2$   $b^* = b/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2mm$   
 $a^* = b/2$   $b^* = c/2$   
 Origin at x,0,0

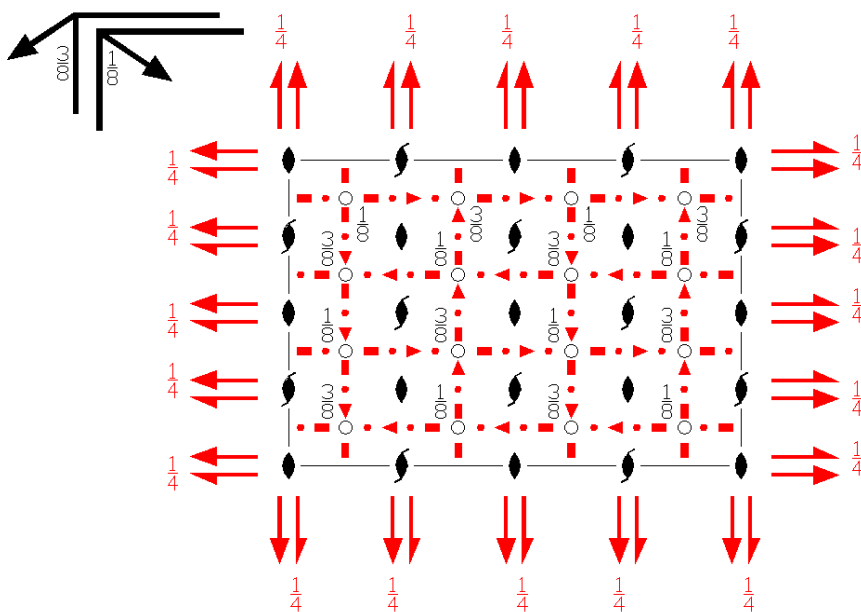
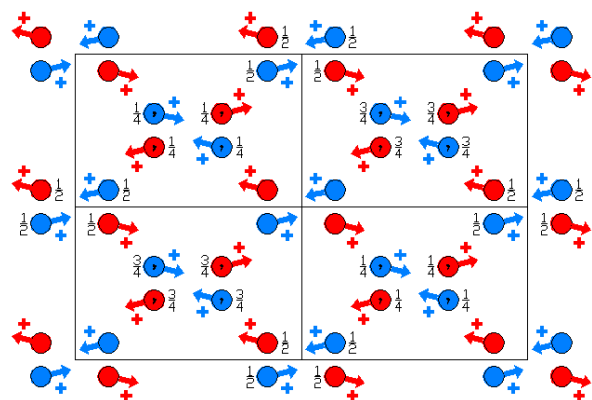
Along [0,1,0]  $c_p \cdot 2'mm'$   
 $a^* = -a/2$   $b^* = c/2$   
 Origin at 0,y,0



Fd'd'd  
70.4.619

m'm'm  
F2'd'2'/d'2'/d

Orthorhombic



Origin at 2'2'2 at  $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq \frac{1}{8}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                                    | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0)                     | (3) 2' 0,y,0<br>(2 <sub>y</sub>   0,0,0)'                     | (4) 2' x,0,0<br>(2 <sub>x</sub>   0,0,0)'                     |
| (5) $\bar{1}$ 1/8,1/8,1/8<br>( $\bar{1}$   1/4,1/4,1/4) | (6) d (1/4,1/4,0) x,y,1/8<br>(m <sub>z</sub>   1/4,1/4,1/4) | (7) d' (1/4,0,1/4) x,1/8,z<br>(m <sub>y</sub>   1/4,1/4,1/4)' | (8) d' (0,1/4,1/4) 1/8,y,z<br>(m <sub>x</sub>   1/4,1/4,1/4)' |

For (0,1/2,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (0,1/2,1/2)<br>(1   0,1/2,1/2)                    | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>   0,1/2,1/2)     | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>   0,1/2,1/2)'     | (4) 2' x,1/4,1/4<br>(2 <sub>x</sub>   0,1/2,1/2)'             |
| (5) $\bar{1}$ 1/8,3/8,3/8<br>( $\bar{1}$   1/4,3/4,3/4) | (6) d (1/4,3/4,0) x,y,3/8<br>(m <sub>z</sub>   1/4,3/4,3/4) | (7) d' (1/4,0,1/4) x,3/8,z<br>(m <sub>y</sub>   1/4,3/4,3/4)' | (8) d' (0,3/4,3/4) 1/8,y,z<br>(m <sub>x</sub>   1/4,3/4,3/4)' |

For (1/2,0,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,0,1/2)<br>(1   1/2,0,1/2)                    | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>   1/2,0,1/2)     | (3) 2' 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,0,1/2)'             | (4) 2' (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>   1/2,0,1/2)'     |
| (5) $\bar{1}$ 3/8,1/8,3/8<br>( $\bar{1}$   3/4,1/4,3/4) | (6) d (3/4,1/4,0) x,y,3/8<br>(m <sub>z</sub>   3/4,1/4,3/4) | (7) d' (3/4,0,3/4) x,1/8,z<br>(m <sub>y</sub>   3/4,1/4,3/4)' | (8) d' (0,1/4,3/4) 3/8,y,z<br>(m <sub>x</sub>   3/4,1/4,3/4)' |

For (1/2,1/2,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                    | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)             | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)'     | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)'     |
| (5) $\bar{1}$ 3/8,3/8,1/8<br>( $\bar{1}$   3/4,3/4,1/4) | (6) d (3/4,3/4,0) x,y,1/8<br>(m <sub>z</sub>   3/4,3/4,1/4) | (7) d' (3/4,0,1/4) x,3/8,z<br>(m <sub>y</sub>   3/4,3/4,1/4)' | (8) d' (0,3/4,1/4) 3/8,y,z<br>(m <sub>x</sub>   3/4,3/4,1/4)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5).

### Positions

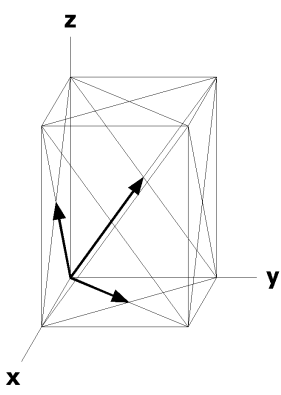
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
32 h 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,w$ ]	(4) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]
	(5) $\bar{x}+1/4,\bar{y}+1/4,\bar{z}+1/4$ [u,v,w]	(6) $x+1/4,y+1/4,\bar{z}+1/4$ [ $\bar{u},\bar{v},w$ ]	(7) $x+1/4,\bar{y}+1/4,z+1/4$ [ $\bar{u},\bar{v},w$ ]	(8) $\bar{x}+1/4,y+1/4,z+1/4$ [ $\bar{u},v,w$ ]
16 g ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	1/4,1/4, $\bar{z}+1/4$ [0,0,w]	1/4,1/4,z+1/4 [0,0,w]
16 f .2'	0,y,0 [u,0,w]	0, $\bar{y}$ ,0 [ $\bar{u},0,w$ ]	1/4, $\bar{y}+1/4$ ,1/4 [u,0,w]	1/4,y+1/4,1/4 [ $\bar{u},0,w$ ]
16 e 2'..	x,0,0 [0,v,w]	$\bar{x}$ ,0,0 [0, $\bar{v},w$ ]	$\bar{x}+1/4$ ,1/4,1/4 [0,v,w]	x+1/4,1/4,1/4 [0, $\bar{v},w$ ]
16 d $\bar{1}$	5/8,5/8,5/8 [u,v,w]	3/8,3/8,5/8 [ $\bar{u},\bar{v},w$ ]	3/8,5/8,3/8 [u, $\bar{v},w$ ]	5/8,3/8,3/8 [ $\bar{u},v,w$ ]
16 c $\bar{1}$	1/8,1/8,1/8 [u,v,w]	7/8,7/8,1/8 [ $\bar{u},\bar{v},w$ ]	7/8,1/8,7/8 [u, $\bar{v},w$ ]	1/8,7/8,7/8 [ $\bar{u},v,w$ ]
8 b 2'2'2	0,0,1/2 [0,0,w]	1/4,1/4,3/4 [0,0,w]		
8 a 2'2'2	0,0,0 [0,0,w]	1/4,1/4,1/4 [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1]  $c_p \cdot 2mm$   
 $a^* = a/2$   $b^* = b/2$   
 Origin at 0,0,z

Along [1,0,0]  $c 2'mm'$   
 $a^* = -c/2$   $b^* = b/2$   
 Origin at x,0,0

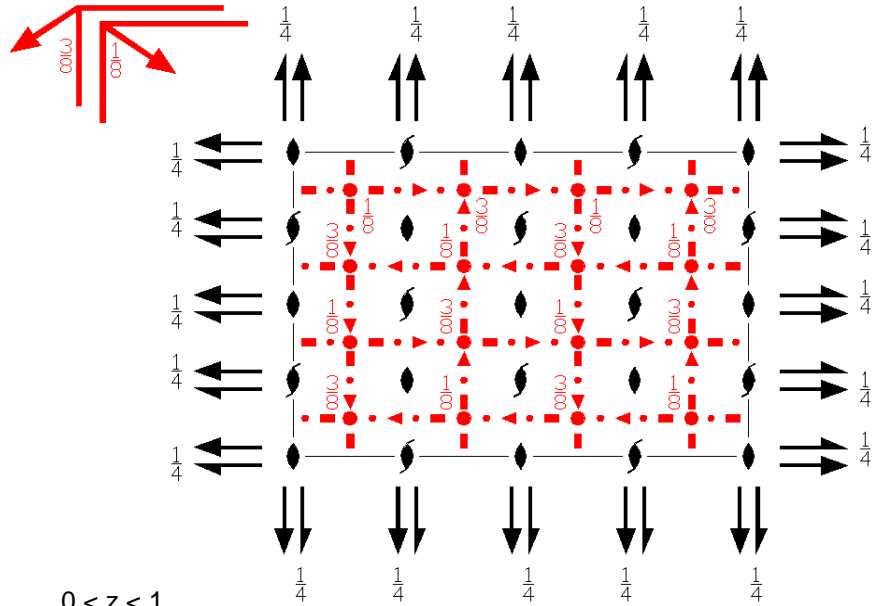
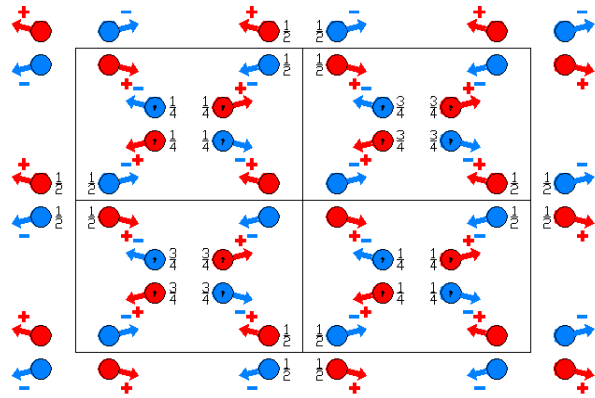
Along [0,1,0]  $c 2'mm'$   
 $a^* = c/2$   $b^* = a/2$   
 Origin at 0,y,0



Fd'd'd'  
70.5.620

m'm'm'  
F2/d'2/d'2/d'

Orthorhombic



Origin at 222 at  $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq \frac{1}{8}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1   0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0)                       | (3) 2 0,y,0<br>(2 <sub>y</sub>   0,0,0)                       | (4) 2 x,0,0<br>(2 <sub>x</sub>   0,0,0)                       |
| (5) $\bar{1}$ 1/8,1/8,1/8<br>( $\bar{1}$   1/4,1/4,1/4)' | (6) d' (1/4,1/4,0) x,y,1/8<br>(m <sub>z</sub>   1/4,1/4,1/4)' | (7) d' (1/4,0,1/4) x,1/8,z<br>(m <sub>y</sub>   1/4,1/4,1/4)' | (8) d' (0,1/4,1/4) 1/8,y,z<br>(m <sub>x</sub>   1/4,1/4,1/4)' |

For (0,1/2,1/2) + set

- |  |   |   |   |
|--|---|---|---|
| (1) t (0,1/2,1/2)<br>(1   0,1/2,1/2)                     | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>   0,1/2,1/2)       | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>   0,1/2,1/2)       | (4) 2 x,1/4,1/4<br>(2 <sub>x</sub>   0,1/2,1/2)               |
| (5) $\bar{1}$ 1/8,3/8,3/8<br>( $\bar{1}$   1/4,3/4,3/4)' | (6) d' (1/4,3/4,0) x,y,3/8<br>(m <sub>z</sub>   1/4,3/4,3/4)' | (7) d' (1/4,0,1/4) x,3/8,z<br>(m <sub>y</sub>   1/4,3/4,3/4)' | (8) d' (0,3/4,3/4) 1/8,y,z<br>(m <sub>x</sub>   1/4,3/4,3/4)' |

For (1/2,0,1/2) + set

- |  |   |   |   |
|--|---|---|---|
| (1) t (1/2,0,1/2)<br>(1   1/2,0,1/2)                     | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>   1/2,0,1/2)       | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,0,1/2)               | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>   1/2,0,1/2)       |
| (5) $\bar{1}$ 3/8,1/8,3/8<br>( $\bar{1}$   3/4,1/4,3/4)' | (6) d' (3/4,1/4,0) x,y,3/8<br>(m <sub>z</sub>   3/4,1/4,3/4)' | (7) d' (3/4,0,3/4) x,1/8,z<br>(m <sub>y</sub>   3/4,1/4,3/4)' | (8) d' (0,1/4,3/4) 3/8,y,z<br>(m <sub>x</sub>   3/4,1/4,3/4)' |

For (1/2,1/2,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)                     | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)               | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)       | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)       |
| (5) $\bar{1}$ 3/8,3/8,1/8<br>( $\bar{1}$   3/4,3/4,1/4)' | (6) d' (3/4,3/4,0) x,y,1/8<br>(m <sub>z</sub>   3/4,3/4,1/4)' | (7) d' (3/4,0,1/4) x,3/8,z<br>(m <sub>y</sub>   3/4,3/4,1/4)' | (8) d' (0,3/4,1/4) 3/8,y,z<br>(m <sub>x</sub>   3/4,3/4,1/4)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5).

**Positions**

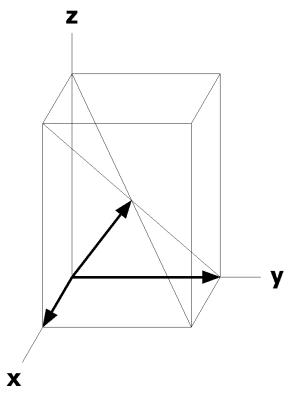
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
32	h 1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
		(5) $\bar{x}+1/4,\bar{y}+1/4,\bar{z}+1/4$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/4,y+1/4,\bar{z}+1/4$ [ $u,v,\bar{w}$ ]	(7) $x+1/4,\bar{y}+1/4,z+1/4$ [ $u,\bar{v},w$ ]	(8) $\bar{x}+1/4,y+1/4,z+1/4$ [ $\bar{u},v,w$ ]
16	g ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/4,1/4, $\bar{z}+1/4$ [0,0, $\bar{w}$ ]	1/4,1/4,z+1/4 [0,0,w]
16	f .2.	0,y,0 [0,v,0]	0, $\bar{y}$ ,0 [0, $\bar{v}$ ,0]	1/4, $\bar{y}+1/4$ ,1/4 [0, $\bar{v}$ ,0]	1/4,y+1/4,1/4 [0,v,0]
16	e 2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0]	$\bar{x}+1/4$ ,1/4,1/4 [ $\bar{u}$ ,0,0]	x+1/4,1/4,1/4 [u,0,0]
16	d $\bar{1}$ '	5/8,5/8,5/8 [0,0,0]	3/8,3/8,5/8 [0,0,0]	3/8,5/8,3/8 [0,0,0]	5/8,3/8,3/8 [0,0,0]
16	c $\bar{1}$ '	1/8,1/8,1/8 [0,0,0]	7/8,7/8,1/8 [0,0,0]	7/8,1/8,7/8 [0,0,0]	1/8,7/8,7/8 [0,0,0]
8	b 222	0,0,1/2 [0,0,0]	1/4,1/4,3/4 [0,0,0]		
8	a 222	0,0,0 [0,0,0]	1/4,1/4,1/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $c2m'm'$   
 $a^* = a/2$   $b^* = b/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2m'm'$   
 $a^* = b/2$   $b^* = c/2$   
 Origin at x,0,0

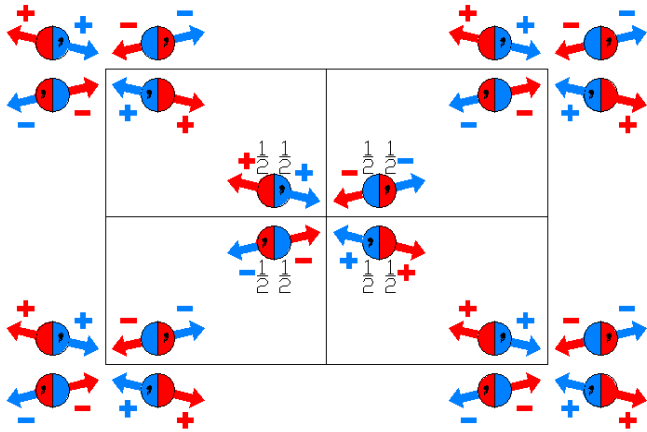
Along [0,1,0]  $c2m'm'$   
 $a^* = c/2$   $b^* = a/2$   
 Origin at 0,y,0



Immm  
71.1.621

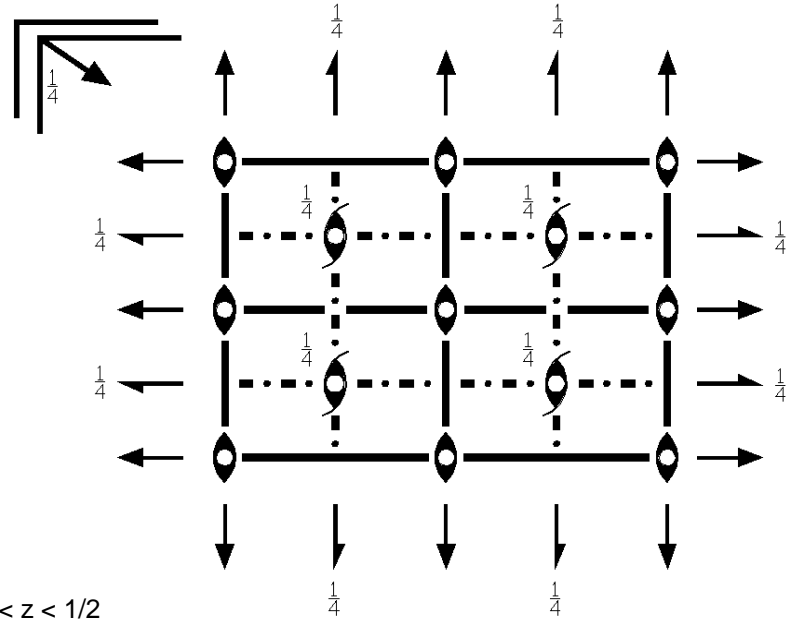
mmm  
I2/m2/m2/m

Orthorhombic



Origin at center (mmm)

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$



### Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (8) m 0,y,z<br>(m <sub>x</sub>  0,0,0) |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                 | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (4) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2) | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (7) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (8) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

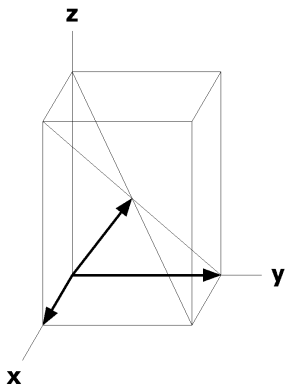
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},\bar{v},\bar{w}$ ]
8 n ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0, $\bar{w}$ ]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
8 m .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]	$\bar{x},0,\bar{z}$ [0,v,0]	x,0, $\bar{z}$ [0, $\bar{v}$ ,0]
8 l m..	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u}$ ,0,0]	0,y, $\bar{z}$ [ $\bar{u}$ ,0,0]	0, $\bar{y},\bar{z}$ [u,0,0]
8 k $\bar{1}$	1/4,1/4,1/4 [u,v,w]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,3/4 [ $\bar{u},v,\bar{w}$ ]	1/4,3/4,3/4 [u, $\bar{v},\bar{w}$ ]
4 j mm2	1/2,0,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
4 i mm2	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 h m2m	0,y,1/2 [0,0,0]	0, $\bar{y}$ ,1/2 [0,0,0]		
4 g m2m	0,y,0 [0,0,0]	0, $\bar{y}$ ,0 [0,0,0]		
4 f 2mm	x,1/2,0 [0,0,0]	$\bar{x}$ ,1/2,0 [0,0,0]		
4 e 2mm	x,0,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0]		
2 d mmm	1/2,0,1/2 [0,0,0]			
2 c mmm	1/2,1/2,0 [0,0,0]			
2 b mmm	0,1/2,1/2 [0,0,0]			
2 a mmm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Immm1'

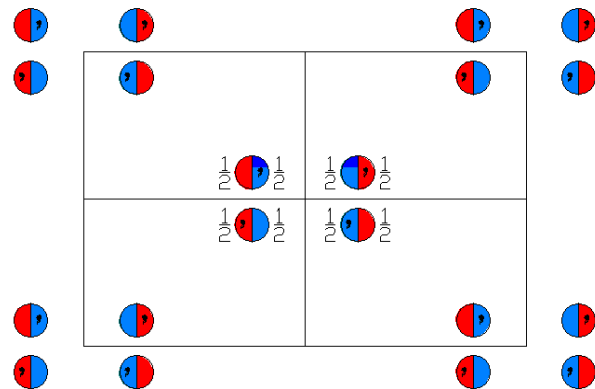
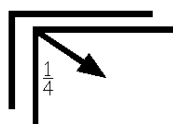
71.2.622

mmm1'

I2/m2/m2/m1'

Orthorhombic

1'



Origin at center (mmm1')

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0) | (3) 2 0,y,0<br>(2 <sub>y</sub>   0,0,0) | (4) 2 x,0,0<br>(2 <sub>x</sub>   0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>   0,0,0) | (7) m x,0,z<br>(m <sub>y</sub>   0,0,0) | (8) m 0,y,z<br>(m <sub>x</sub>   0,0,0) |

For (1/2,1/2,1/2) + set

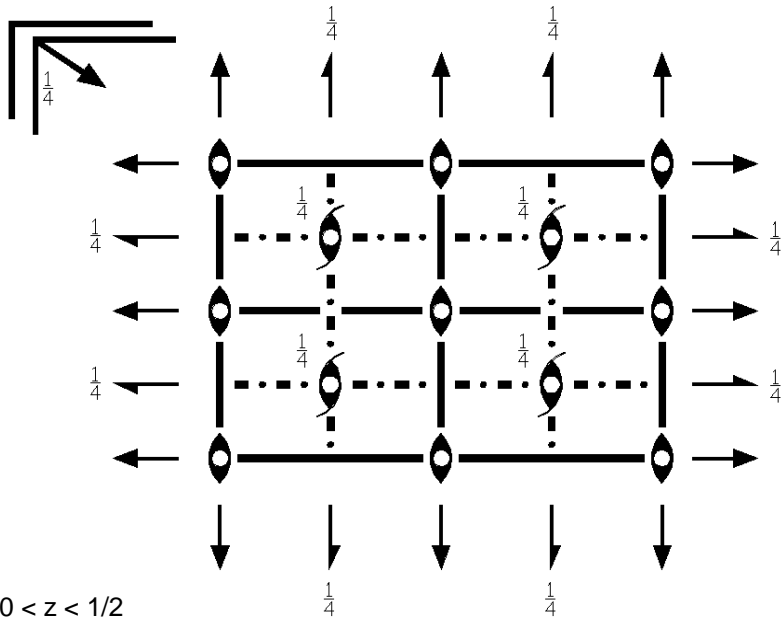
- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)                | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2) | (3) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,1/2,1/2) | (4) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>   1/2,1/2,1/2) |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$   1/2,1/2,1/2) | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>   1/2,1/2,1/2) | (7) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,1/2) | (8) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,1/2) |

For (0,0,0)' + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1'<br>(1   0,0,0)'                         | (2) 2' 0,0,z<br>(2 <sub>z</sub>   0,0,0)' | (3) 2' 0,y,0<br>(2 <sub>y</sub>   0,0,0)' | (4) 2' x,0,0<br>(2 <sub>x</sub>   0,0,0)' |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$   0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>   0,0,0)' | (7) m' x,0,z<br>(m <sub>y</sub>   0,0,0)' | (8) m' 0,y,z<br>(m <sub>x</sub>   0,0,0)' |

For (1/2,1/2,1/2)' + set

- |  |   |   |   |
|--|---|---|---|
| (1) t' (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)'                 | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2)' | (3) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,1/2,1/2)' | (4) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>   1/2,1/2,1/2)' |
| (5) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$   1/2,1/2,1/2)' | (6) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>   1/2,1/2,1/2)' | (7) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,1/2)' | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,1/2)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

**Positions**

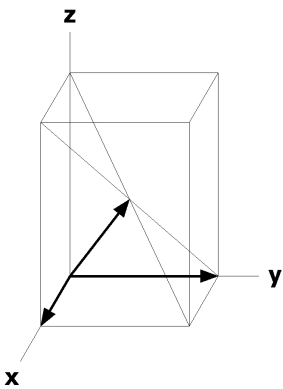
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'		
16 o 11'	(1) x,y,z [0,0,0] (5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0] (6) x,y, $\bar{z}$ [0,0,0]	(3) $\bar{x},y,\bar{z}$ [0,0,0] (7) x, $\bar{y},z$ [0,0,0]	(4) x, $\bar{y},\bar{z}$ [0,0,0] (8) $\bar{x},y,z$ [0,0,0]
8 n ..m1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{x},y,0$ [0,0,0]	x, $\bar{y},0$ [0,0,0]
8 m .m.1'	x,0,z [0,0,0]	$\bar{x},0,z$ [0,0,0]	$\bar{x},0,\bar{z}$ [0,0,0]	x,0, $\bar{z}$ [0,0,0]
8 l m..1'	0,y,z [0,0,0]	0, $\bar{y},z$ [0,0,0]	0,y, $\bar{z}$ [0,0,0]	0, $\bar{y},\bar{z}$ [0,0,0]
8 k $\bar{1}1'$ 1/4,1/4,1/4 [0,0,0]		3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]
4 j mm21'	1/2,0,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
4 i mm21'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 h m2m1'	0,y,1/2 [0,0,0]	0, $\bar{y},1/2$ [0,0,0]		
4 g m2m1'	0,y,0 [0,0,0]	0, $\bar{y},0$ [0,0,0]		
4 f 2mm1'	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]		
4 e 2mm1'	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
2 d mmm1'	1/2,0,1/2 [0,0,0]			
2 c mmm1'	1/2,1/2,0 [0,0,0]			
2 b mmm1'	0,1/2,1/2 [0,0,0]			
2 a mmm1'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



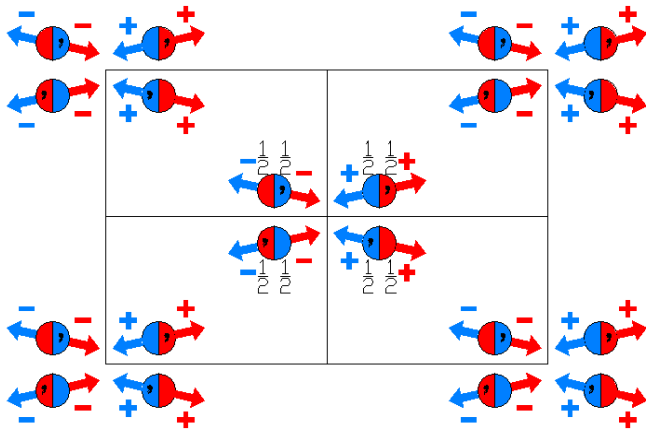
Im'mm

71.3.623

m'mm

I2/m'2'/m2'/m

Orthorhombic



Origin at center (m'mm)

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

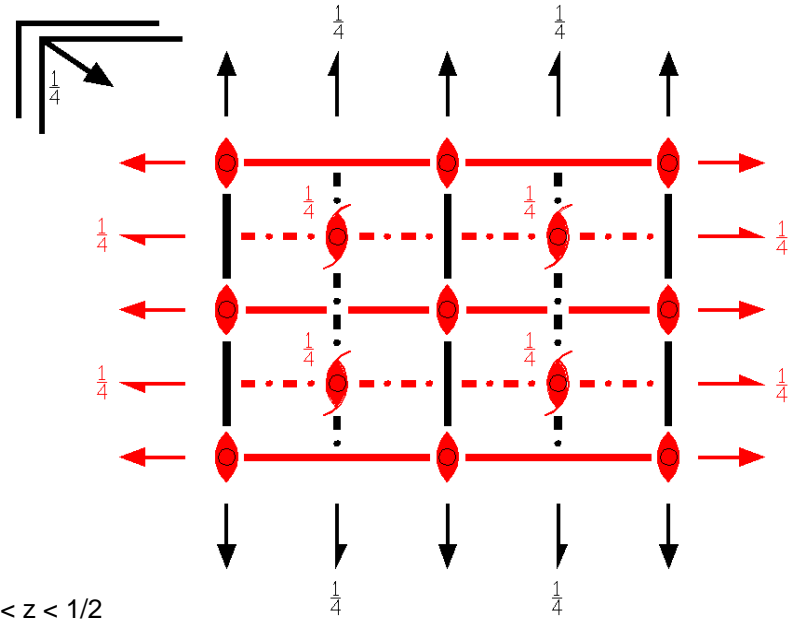
**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0)   | (7) m x,0,z<br>(m <sub>y</sub>  0,0,0)   | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

For (1/2,1/2,1/2) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                    | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (4) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)   |
| (5) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)' | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)   | (7) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)   | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

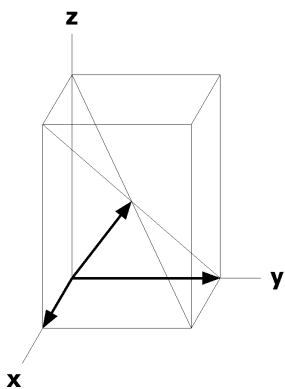
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 n ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]
8 m .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0,v,0]	$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	x,0, $\bar{z}$ [0, $\bar{v},0$ ]
8 l m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0,v, $\bar{w}$ ]	0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 k $\bar{1}'$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]
4 j m'm2'	1/2,0,z [0,v,0]	1/2,0, $\bar{z}$ [0, $\bar{v},0$ ]		
4 i m'm2'	0,0,z [0,v,0]	0,0, $\bar{z}$ [0, $\bar{v},0$ ]		
4 h m'2'm	0,y,1/2 [0,0,w]	0, $\bar{y},1/2$ [0,0, $\bar{w}$ ]		
4 g m'2'm	0,y,0 [0,0,w]	0, $\bar{y},0$ [0,0, $\bar{w}$ ]		
4 f 2mm	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]		
4 e 2mm	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]		
2 d m'mm	1/2,0,1/2 [0,0,0]			
2 c m'mm	1/2,1/2,0 [0,0,0]			
2 b m'mm	0,1/2,1/2 [0,0,0]			
2 a m'mm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c2mm  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

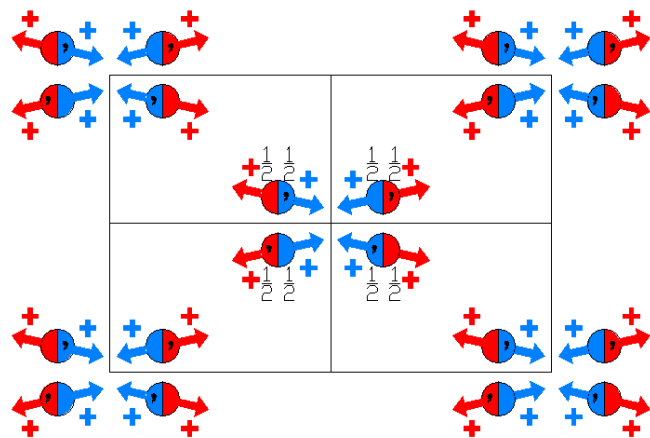
Along [0,1,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



$Im'm'm$   
71.4.624

$m'm'm$   
 $I2'/m'2'/m'2/m$

Orthorhombic



Origin at center ( $m'm'm$ )

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

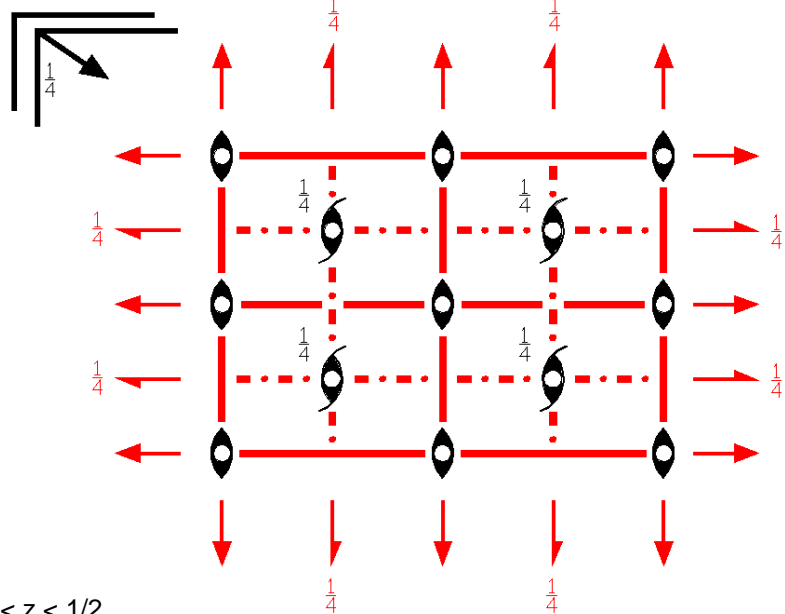
**Symmetry Operations**

For (0,0,0) + set

- |  |                                  |                                    |                                    |
|--|----------------------------------|------------------------------------|------------------------------------|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) 2' $0,y,0$<br>( $2_y$  0,0,0)' | (4) 2' $x,0,0$<br>( $2_x$  0,0,0)' |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0) | (6) m $x,y,0$<br>( $m_z$  0,0,0) | (7) m' $x,0,z$<br>( $m_y$  0,0,0)' | (8) m' $0,y,z$<br>( $m_x$  0,0,0)' |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                   | (2) 2 (0,0,1/2) $1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2) | (3) 2' (0,1/2,0) $1/4,y,1/4$<br>( $2_y$  1/2,1/2,1/2)' | (4) 2' (1/2,0,0) $x,1/4,1/4$<br>( $2_x$  1/2,1/2,1/2)' |
| (5) $\bar{1}$ $1/4,1/4,1/4$<br>( $\bar{1}$  1/2,1/2,1/2) | (6) n (1/2,1/2,0) $x,y,1/4$<br>( $m_z$  1/2,1/2,1/2) | (7) n' (1/2,0,1/2) $x,1/4,z$<br>( $m_y$  1/2,1/2,1/2)' | (8) n' (0,1/2,1/2) $1/4,y,z$<br>( $m_x$  1/2,1/2,1/2)' |





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

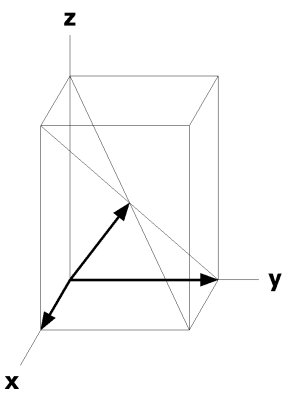
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 n ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0,w]
8 m .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$\bar{x},0,\bar{z}$ [u,0,w]	x,0, $\bar{z}$ [ $\bar{u},0,w$ ]
8 l m..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
8 k $\bar{1}$	1/4,1/4,1/4 [u,v,w]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,3/4 [u, $\bar{v},w$ ]	1/4,3/4,3/4 [ $\bar{u},v,w$ ]
4 j m'm'2	1/2,0,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]		
4 i m'm'2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
4 h m'2'm	0,y,1/2 [0,0,w]	0, $\bar{y},1/2$ [0,0,w]		
4 g m'2'm	0,y,0 [0,0,w]	0, $\bar{y},0$ [0,0,w]		
4 f 2'm'm	x,1/2,0 [0,0,w]	$\bar{x},1/2,0$ [0,0,w]		
4 e 2'm'm	x,0,0 [0,0,w]	$\bar{x},0,0$ [0,0,w]		
2 d m'm'm	1/2,0,1/2 [0,0,w]			
2 c m'm'm	1/2,1/2,0 [0,0,w]			
2 b m'm'm	0,1/2,1/2 [0,0,w]			
2 a m'm'm	0,0,0 [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [0,1,0] c2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



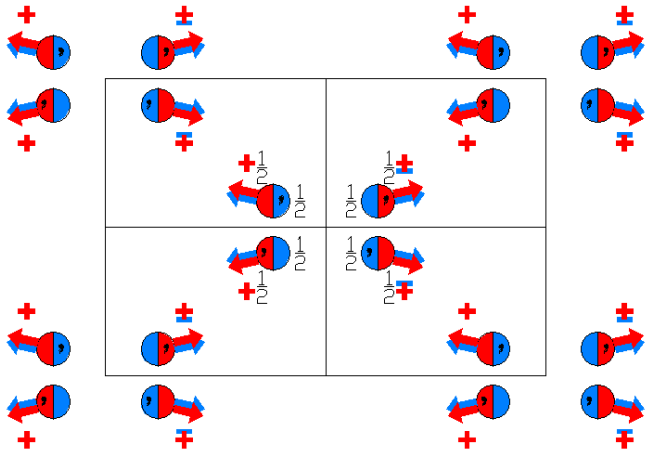
$Im'm'm'$

71.5.625

$m'm'm'$

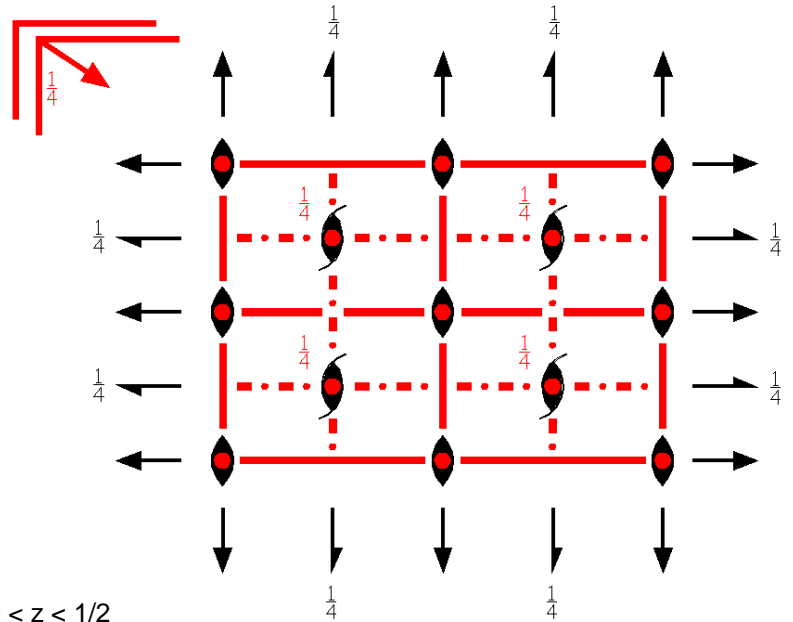
$I2/m'2/m'2/m'$

Orthorhombic



Origin at center ( $m'm'm'$ )

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$



**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                   | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)   | (3) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)   | (4) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)   |
| (5) $\bar{1}'$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)' | (6) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (7) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

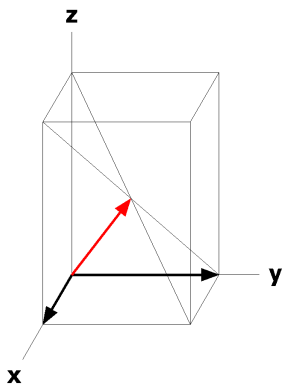
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 o 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 n ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,0$ [ $\bar{u},v,0$ ]	x, $\bar{y},0$ [u, $\bar{v},0$ ]
8 m .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$\bar{x},0,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	x,0, $\bar{z}$ [u,0, $\bar{w}$ ]
8 l m'..	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	0,y, $\bar{z}$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 k $\bar{1}$ '	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]
4 j m'm'2	1/2,0,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 i m'm'2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 h m'2m'	0,y,1/2 [0,v,0]	0, $\bar{y},1/2$ [0, $\bar{v},0$ ]		
4 g m'2m'	0,y,0 [0,v,0]	0, $\bar{y},0$ [0, $\bar{v},0$ ]		
4 f 2m'm'	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]		
4 e 2m'm'	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]		
2 d m'm'm'	1/2,0,1/2 [0,0,0]			
2 c m'm'm'	1/2,1/2,0 [0,0,0]			
2 b m'm'm'	0,1/2,1/2 [0,0,0]			
2 a m'm'm'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



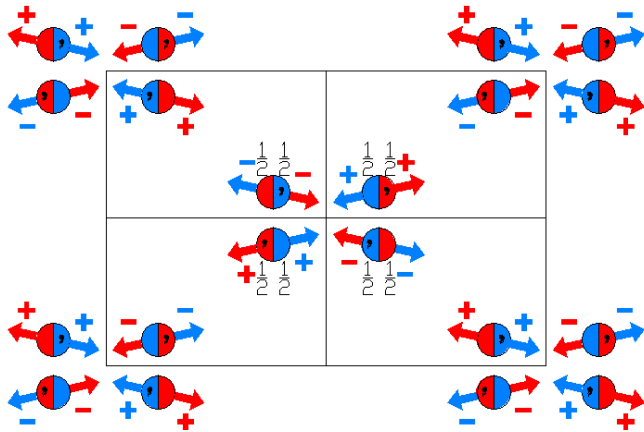
$I_p mmm$

71.6.626

$mmm1'$

$I_p 2/m2/m2/m$

Orthorhombic



Origin at center ( $mmm$ )

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

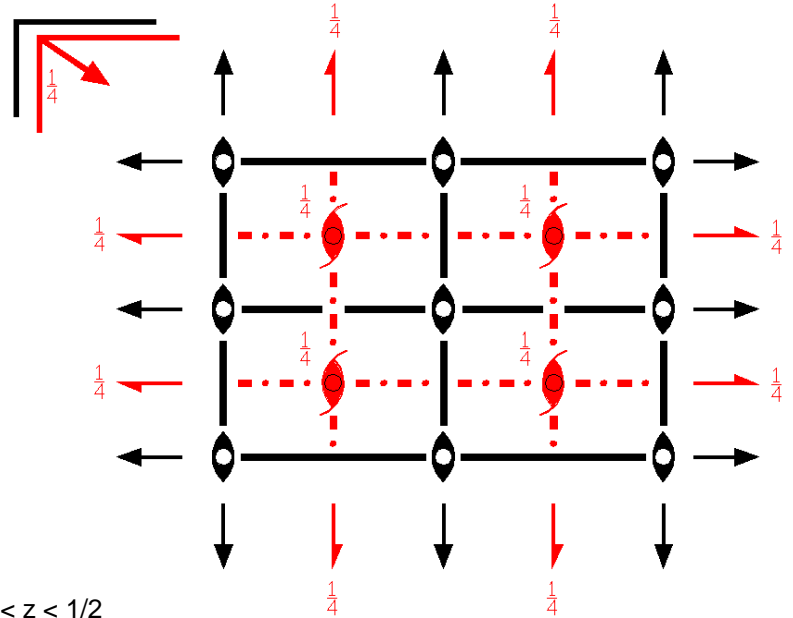
**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |                                   |                                   |                                   |
|---|-----------------------------------|-----------------------------------|-----------------------------------|
| (1) 1<br>(1   0,0,0)                          | (2) 2 $0,0,z$<br>( $2_z$   0,0,0) | (3) 2 $0,y,0$<br>( $2_y$   0,0,0) | (4) 2 $x,0,0$<br>( $2_x$   0,0,0) |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   0,0,0) | (6) m $x,y,0$<br>( $m_z$   0,0,0) | (7) m $x,0,z$<br>( $m_y$   0,0,0) | (8) m $0,y,z$<br>( $m_x$   0,0,0) |

For  $(1/2,1/2,1/2)'$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t'$ $(1/2,1/2,1/2)$<br>(1   $1/2,1/2,1/2$ )'               | (2) $2'$ $(0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1/2$ )' | (3) $2'$ $(0,1/2,0)$ $1/4,y,1/4$<br>( $2_y$   $1/2,1/2,1/2$ )' | (4) $2'$ $(1/2,0,0)$ $x,1/4,1/4$<br>( $2_x$   $1/2,1/2,1/2$ )' |
| (5) $\bar{1}'$ $1/4,1/4,1/4$<br>( $\bar{1}'$   $1/2,1/2,1/2$ )' | (6) $n'$ $(1/2,1/2,0)$ $x,y,1/4$<br>( $m_z$   $1/2,1/2,1/2$ )' | (7) $n'$ $(1/2,0,1/2)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,1/2$ )' | (8) $n'$ $(0,1/2,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,1/2$ )' |



**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(1/2,1/2,1/2)$ ; (2); (3); (5).

**Positions**

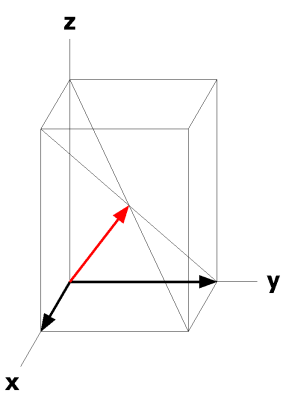
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
16 o 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]
8 n ..m	$x,y,0$ [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,0$ [0,0, $\bar{w}$ ]	$x,\bar{y},0$ [0,0, $\bar{w}$ ]
8 m .m.	$x,0,z$ [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]	$\bar{x},0,\bar{z}$ [0,v,0]	$x,0,\bar{z}$ [0, $\bar{v}$ ,0]
8 l m..	$0,y,z$ [u,0,0]	$0,\bar{y},z$ [ $\bar{u}$ ,0,0]	$0,y,\bar{z}$ [ $\bar{u}$ ,0,0]	$0,\bar{y},\bar{z}$ [u,0,0]
8 k $\bar{1}'$	$1/4,1/4,1/4$ [0,0,0]	$3/4,3/4,1/4$ [0,0,0]	$3/4,1/4,3/4$ [0,0,0]	$1/4,3/4,3/4$ [0,0,0]
4 j mm2	$1/2,0,z$ [0,0,0]	$1/2,0,\bar{z}$ [0,0,0]		
4 i mm2	$0,0,z$ [0,0,0]	$0,0,\bar{z}$ [0,0,0]		
4 h m2m	$0,y,1/2$ [0,0,0]	$0,\bar{y},1/2$ [0,0,0]		
4 g m2m	$0,y,0$ [0,0,0]	$0,\bar{y},0$ [0,0,0]		
4 f 2mm	$x,1/2,0$ [0,0,0]	$\bar{x},1/2,0$ [0,0,0]		
4 e 2mm	$x,0,0$ [0,0,0]	$\bar{x},0,0$ [0,0,0]		
2 d mmm	$1/2,0,1/2$ [0,0,0]			
2 c mmm	$1/2,1/2,0$ [0,0,0]			
2 b mmm	$0,1/2,1/2$ [0,0,0]			
2 a mmm	$0,0,0$ [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $c2mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [0,1,0]  $c2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



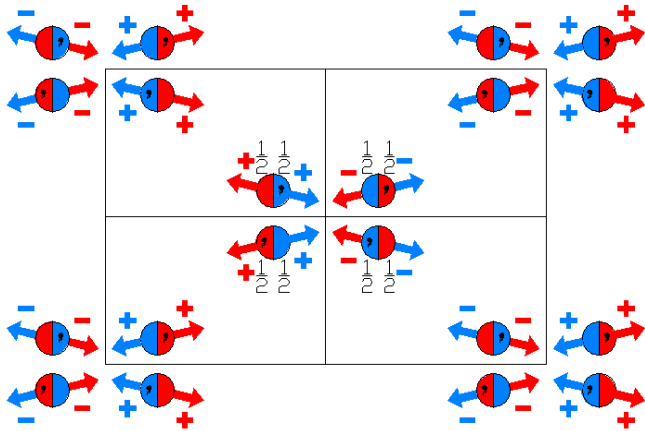
$I_p m' mm$

71.7.627

$mmm1'$

$I_p 2/m'2'/m2'/m$

Orthorhombic



Origin at center ( $m'mm$ )

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

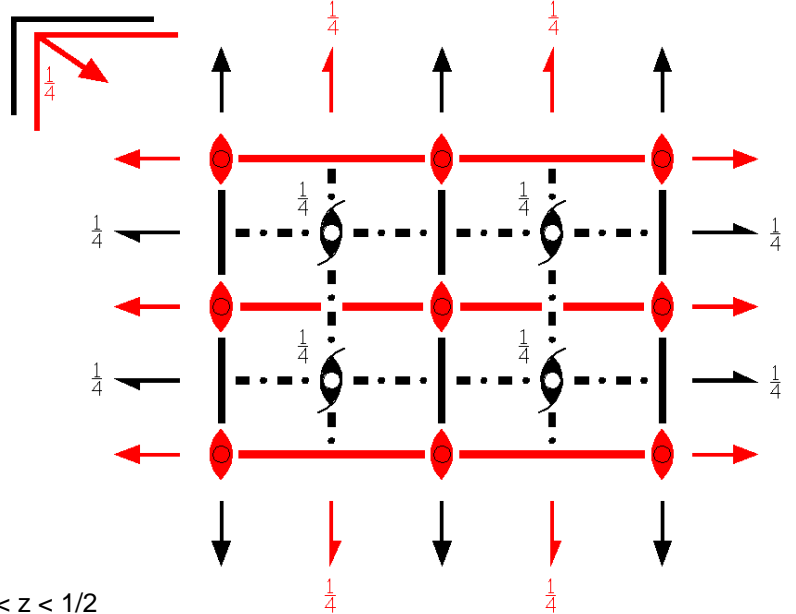
**Symmetry Operations**

For (0,0,0) + set

- |  |                                    |                                    |                                    |
|--|------------------------------------|------------------------------------|------------------------------------|
| (1) 1<br>(1 0,0,0)                           | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $2'$ 0,y,0<br>( $2_y$  0,0,0)' | (4) $2$ x,0,0<br>( $2_x$  0,0,0)   |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m x,y,0<br>( $m_z$  0,0,0)     | (7) m x,0,z<br>( $m_y$  0,0,0)     | (8) $m'$ 0,y,z<br>( $m_x$  0,0,0)' |

For (1/2,1/2,1/2)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'             | (2) $2$ (0,0,1/2) 1/4,1/4,z<br>( $2_z$  1/2,1/2,1/2)   | (3) $2$ (0,1/2,0) 1/4,y,1/4<br>( $2_y$  1/2,1/2,1/2)   | (4) $2'$ (1/2,0,0) x,1/4,1/4<br>( $2_x$  1/2,1/2,1/2)' |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2) | (6) $n'$ (1/2,1/2,0) x,y,1/4<br>( $m_z$  1/2,1/2,1/2)' | (7) $n'$ (1/2,0,1/2) x,1/4,z<br>( $m_y$  1/2,1/2,1/2)' | (8) n (0,1/2,1/2) 1/4,y,z<br>( $m_x$  1/2,1/2,1/2)     |



**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(1/2,1/2,1/2)$ ; (2); (3); (5).

**Positions**

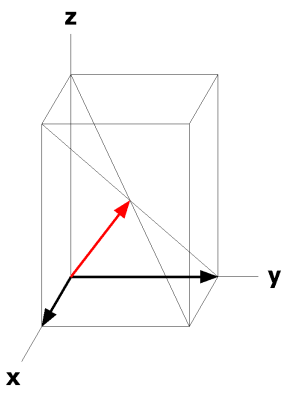
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 o 1	(1) $x,y,z [u,v,w]$ (5) $\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$	(2) $\bar{x},\bar{y},z [u,v,\bar{w}]$ (6) $x,y,\bar{z} [\bar{u},\bar{v},w]$	(3) $\bar{x},y,\bar{z} [u,\bar{v},w]$ (7) $x,\bar{y},z [\bar{u},v,\bar{w}]$	(4) $x,\bar{y},z [u,\bar{v},\bar{w}]$ (8) $\bar{x},y,z [\bar{u},v,w]$
8 n ..m	$x,y,0 [0,0,w]$	$\bar{x},\bar{y},0 [0,0,\bar{w}]$	$\bar{x},y,0 [0,0,w]$	$x,\bar{y},0 [0,0,\bar{w}]$
8 m .m.	$x,0,z [0,v,0]$	$\bar{x},0,z [0,v,0]$	$\bar{x},0,\bar{z} [0,\bar{v},0]$	$x,0,\bar{z} [0,\bar{v},0]$
8 l m'..	$0,y,z [0,v,w]$	$0,\bar{y},z [0,v,\bar{w}]$	$0,y,\bar{z} [0,\bar{v},w]$	$0,\bar{y},z [0,\bar{v},\bar{w}]$
8 k $\bar{1}$	$1/4,1/4,1/4 [u,v,w]$	$3/4,3/4,1/4 [\bar{u},\bar{v},w]$	$3/4,1/4,3/4 [\bar{u},v,\bar{w}]$	$1/4,3/4,3/4 [u,\bar{v},\bar{w}]$
4 j $m'm2'$	$1/2,0,z [0,v,0]$	$1/2,0,\bar{z} [0,\bar{v},0]$		
4 i $m'm2'$	$0,0,z [0,v,0]$	$0,0,\bar{z} [0,\bar{v},0]$		
4 h $m'2'm$	$0,y,1/2 [0,0,w]$	$0,\bar{y},1/2 [0,0,\bar{w}]$		
4 g $m'2'm$	$0,y,0 [0,0,w]$	$0,\bar{y},0 [0,0,\bar{w}]$		
4 f 2mm	$x,1/2,0 [0,0,0]$	$\bar{x},1/2,0 [0,0,0]$		
4 e 2mm	$x,0,0 [0,0,0]$	$\bar{x},0,0 [0,0,0]$		
2 d $m'mm$	$1/2,0,1/2 [0,0,0]$			
2 c $m'mm$	$1/2,1/2,0 [0,0,0]$			
2 b $m'mm$	$0,1/2,1/2 [0,0,0]$			
2 a $m'mm$	$0,0,0 [0,0,0]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $c2mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c_p2mm$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $c2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at  $0,y,0$



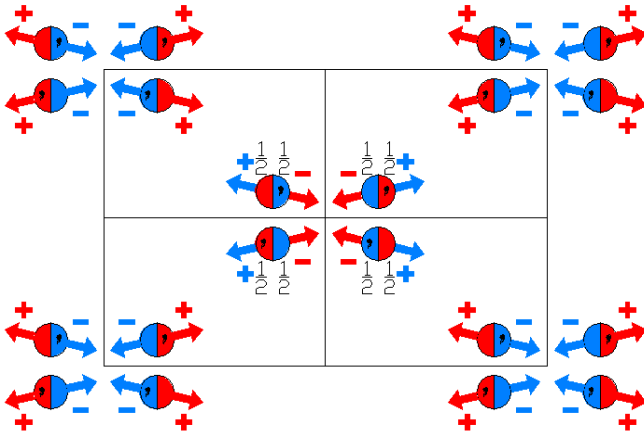
$I_p m' m' m'$

71.8.628

$mmm1'$

$I_p 2'/m'2'/m'2'/m'$

Orthorhombic



Origin at center ( $m' m' m'$ )

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

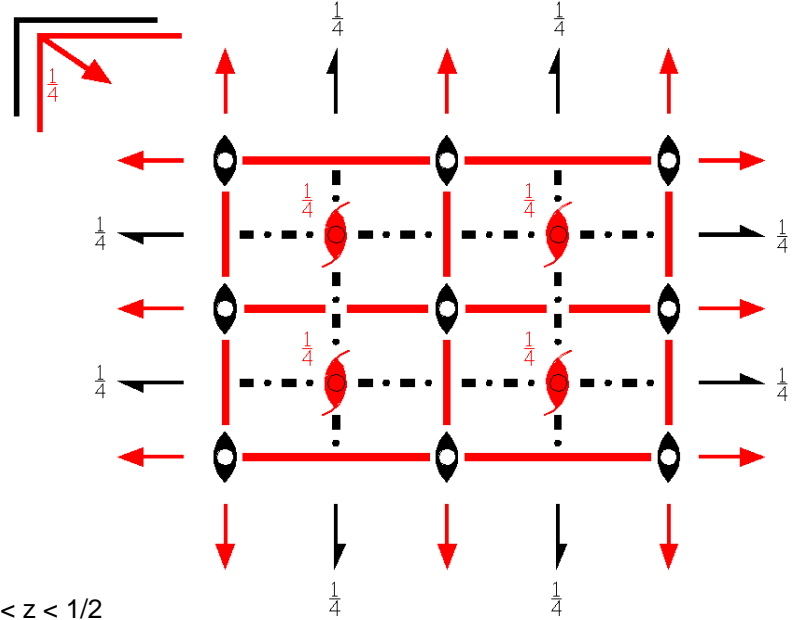
**Symmetry Operations**

For (0,0,0) + set

- |   |                                   |                                     |                                     |
|---|-----------------------------------|-------------------------------------|-------------------------------------|
| (1) 1<br>(1   0,0,0)                          | (2) 2 $0,0,z$<br>( $2_z$   0,0,0) | (3) 2' $0,y,0$<br>( $2_y$   0,0,0)' | (4) 2' $x,0,0$<br>( $2_x$   0,0,0)' |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   0,0,0) | (6) m $x,y,0$<br>( $m_z$   0,0,0) | (7) m' $x,0,z$<br>( $m_y$   0,0,0)' | (8) m' $0,y,z$<br>( $m_x$   0,0,0)' |

For (1/2,1/2,1/2)' + set

- |  |   |   |   |
|--|---|---|---|
| (1) t' (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)'                   | (2) 2' (0,0,1/2) $1/4,1/4,z$<br>( $2_z$   1/2,1/2,1/2)' | (3) 2 (0,1/2,0) $1/4,y,1/4$<br>( $2_y$   1/2,1/2,1/2) | (4) 2 (1/2,0,0) $x,1/4,1/4$<br>( $2_x$   1/2,1/2,1/2) |
| (5) $\bar{1}$ ' $1/4,1/4,1/4$<br>( $\bar{1}$   1/2,1/2,1/2)' | (6) n' (1/2,1/2,0) $x,y,1/4$<br>( $m_z$   1/2,1/2,1/2)' | (7) n (1/2,0,1/2) $x,1/4,z$<br>( $m_y$   1/2,1/2,1/2) | (8) n (0,1/2,1/2) $1/4,y,z$<br>( $m_x$   1/2,1/2,1/2) |





**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(1/2,1/2,1/2)$ ; (2); (3); (5).

### Positions

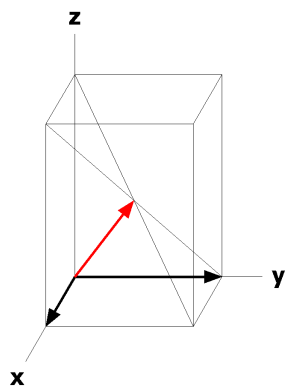
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
16 o 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $\bar{x},y,\bar{z} [u,\bar{v},w]$	(4) $x,\bar{y},\bar{z} [\bar{u},v,w]$
	(5) $\bar{x},\bar{y},\bar{z} [u,v,w]$	(6) $x,y,\bar{z} [\bar{u},\bar{v},w]$	(7) $x,\bar{y},z [u,\bar{v},w]$	(8) $\bar{x},y,z [\bar{u},v,w]$
8 n ..m	$x,y,0 [0,0,w]$	$\bar{x},\bar{y},0 [0,0,w]$	$\bar{x},y,0 [0,0,w]$	$x,\bar{y},0 [0,0,w]$
8 m .m'	$x,0,z [u,0,w]$	$\bar{x},0,z [\bar{u},0,w]$	$\bar{x},0,\bar{z} [u,0,w]$	$x,0,\bar{z} [\bar{u},0,w]$
8 l m..	$0,y,z [0,v,w]$	$0,\bar{y},z [0,\bar{v},w]$	$0,y,\bar{z} [0,\bar{v},w]$	$0,\bar{y},z [0,v,w]$
8 k $\bar{1}'$	$1/4,1/4,1/4 [0,0,0]$	$3/4,3/4,1/4 [0,0,0]$	$3/4,1/4,3/4 [0,0,0]$	$1/4,3/4,3/4 [0,0,0]$
4 j $m'm'2$	$1/2,0,z [0,0,w]$	$1/2,0,\bar{z} [0,0,w]$		
4 i $m'm'2$	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,w]$		
4 h $m'2'm$	$0,y,1/2 [0,0,w]$	$0,\bar{y},1/2 [0,0,w]$		
4 g $m'2'm$	$0,y,0 [0,0,w]$	$0,\bar{y},0 [0,0,w]$		
4 f $2'm'm$	$x,1/2,0 [0,0,w]$	$\bar{x},1/2,0 [0,0,w]$		
4 e $2'm'm$	$x,0,0 [0,0,w]$	$\bar{x},0,0 [0,0,w]$		
2 d $m'm'm$	$1/2,0,1/2 [0,0,w]$			
2 c $m'm'm$	$1/2,1/2,0 [0,0,w]$			
2 b $m'm'm$	$0,1/2,1/2 [0,0,w]$			
2 a $m'm'm$	$0,0,0 [0,0,w]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $c2mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c_p-2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $x,0,0$

Along  $[0,1,0]$   $c_p-2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at  $0,y,0$



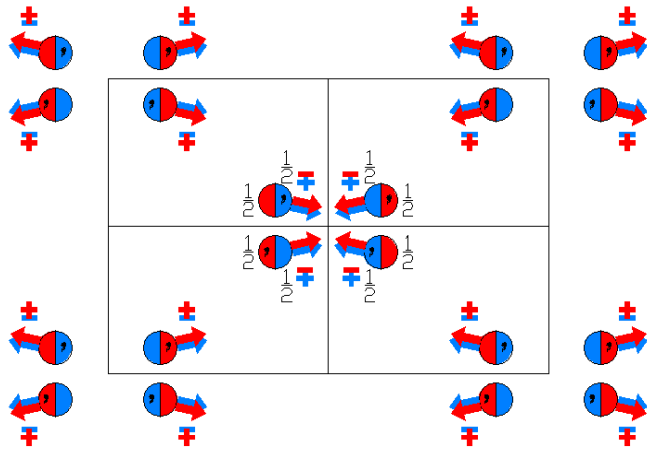
$I_p m' m' m'$

71.9.629

$mmm1'$

$I_p 2/m'2/m'2/m'$

Orthorhombic



Origin at center ( $m'm'm'$ )

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

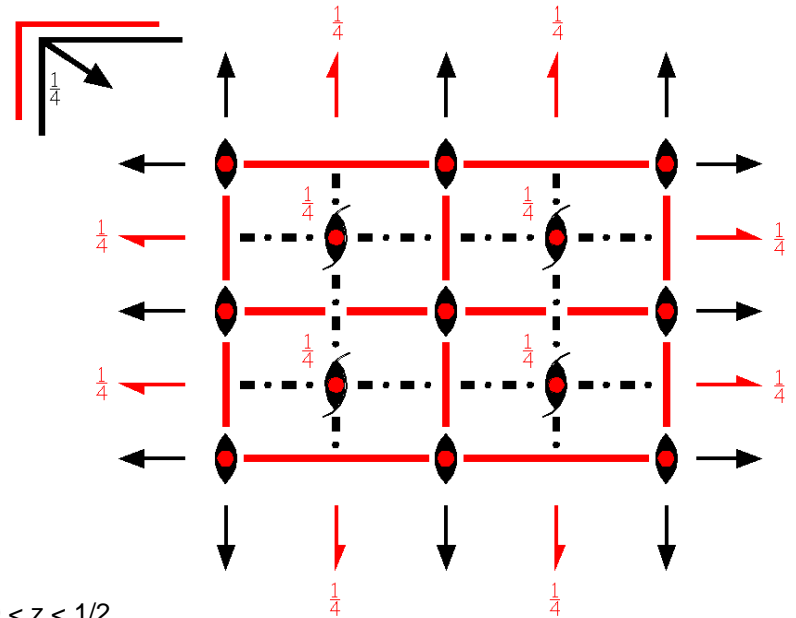
### Symmetry Operations

For (0,0,0) + set

- |  |                                       |                                       |                                       |
|--|---------------------------------------|---------------------------------------|---------------------------------------|
| (1) 1<br>(1   0,0,0)                           | (2) 2 $0,0,z$<br>( $2_z$   0,0,0)     | (3) 2 $0,y,0$<br>( $2_y$   0,0,0)     | (4) 2 $x,0,0$<br>( $2_x$   0,0,0)     |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   0,0,0)' | (6) $m'$ $x,y,0$<br>( $m_z$   0,0,0)' | (7) $m'$ $x,0,z$<br>( $m_y$   0,0,0)' | (8) $m'$ $0,y,z$<br>( $m_x$   0,0,0)' |

For (1/2,1/2,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) $t'$ (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)'              | (2) 2' (0,0,1/2) $1/4,1/4,z$<br>( $2_z$   1/2,1/2,1/2)' | (3) 2' (0,1/2,0) $1/4,y,1/4$<br>( $2_y$   1/2,1/2,1/2)' | (4) 2' (1/2,0,0) $x,1/4,1/4$<br>( $2_x$   1/2,1/2,1/2)' |
| (5) $\bar{1}$ $1/4,1/4,1/4$<br>( $\bar{1}$   1/2,1/2,1/2) | (6) $n$ (1/2,1/2,0) $x,y,1/4$<br>( $m_z$   1/2,1/2,1/2) | (7) $n$ (1/2,0,1/2) $x,1/4,z$<br>( $m_y$   1/2,1/2,1/2) | (8) $n$ (0,1/2,1/2) $1/4,y,z$<br>( $m_x$   1/2,1/2,1/2) |



**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(1/2,1/2,1/2)$ ; (2); (3); (5).

### Positions

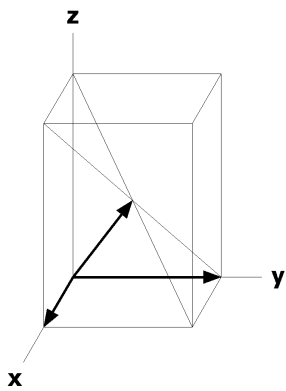
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	$(1/2,1/2,1/2)'$ +		
16 o 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $\bar{x},y,\bar{z} [\bar{u},v,\bar{w}]$	(4) $x,\bar{y},\bar{z} [u,\bar{v},\bar{w}]$
	(5) $\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$	(6) $x,y,\bar{z} [u,v,\bar{w}]$	(7) $x,\bar{y},z [u,\bar{v},w]$	(8) $\bar{x},y,z [\bar{u},v,w]$
8 n $..m'$	$x,y,0 [u,v,0]$	$\bar{x},\bar{y},0 [\bar{u},\bar{v},0]$	$\bar{x},y,0 [\bar{u},v,0]$	$x,\bar{y},0 [u,\bar{v},0]$
8 m $.m'$	$x,0,z [u,0,w]$	$\bar{x},0,z [\bar{u},0,w]$	$\bar{x},0,\bar{z} [\bar{u},0,\bar{w}]$	$x,0,\bar{z} [u,0,\bar{w}]$
8 l $m'..$	$0,y,z [0,v,w]$	$0,\bar{y},z [0,\bar{v},w]$	$0,y,\bar{z} [0,v,\bar{w}]$	$0,\bar{y},z [0,\bar{v},\bar{w}]$
8 k $\bar{1}$	$1/4,1/4,1/4 [u,v,w]$	$3/4,3/4,1/4 [\bar{u},\bar{v},w]$	$3/4,1/4,3/4 [\bar{u},v,\bar{w}]$	$1/4,3/4,3/4 [u,\bar{v},\bar{w}]$
4 j $m'm'2$	$1/2,0,z [0,0,w]$	$1/2,0,\bar{z} [0,0,\bar{w}]$		
4 i $m'm'2$	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,\bar{w}]$		
4 h $m'2m'$	$0,y,1/2 [0,v,0]$	$0,\bar{y},1/2 [0,\bar{v},0]$		
4 g $m'2m'$	$0,y,0 [0,v,0]$	$0,\bar{y},0 [0,\bar{v},0]$		
4 f $2m'm'$	$x,1/2,0 [u,0,0]$	$\bar{x},1/2,0 [\bar{u},0,0]$		
4 e $2m'm'$	$x,0,0 [u,0,0]$	$\bar{x},0,0 [\bar{u},0,0]$		
2 d $m'm'm'$	$1/2,0,1/2 [0,0,0]$			
2 c $m'm'm'$	$1/2,1/2,0 [0,0,0]$			
2 b $m'm'm'$	$0,1/2,1/2 [0,0,0]$			
2 a $m'm'm'$	$0,0,0 [0,0,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

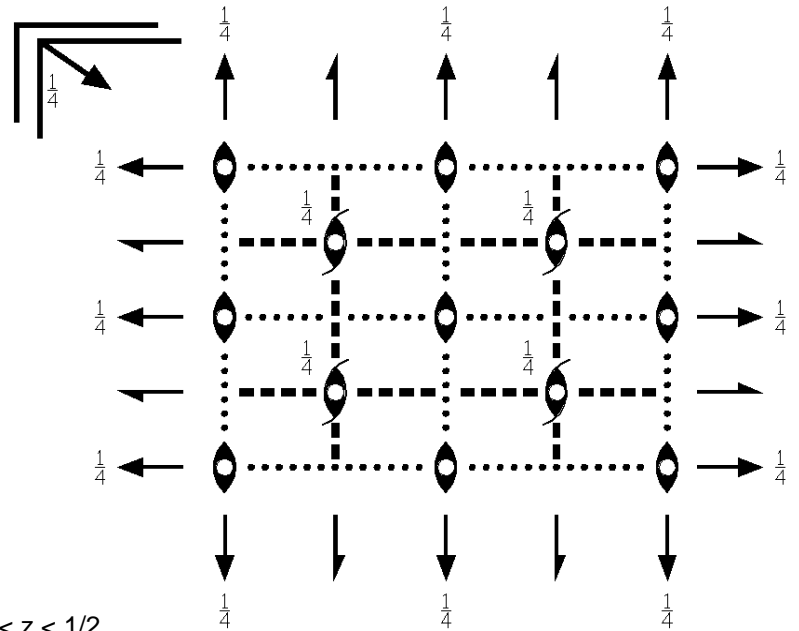
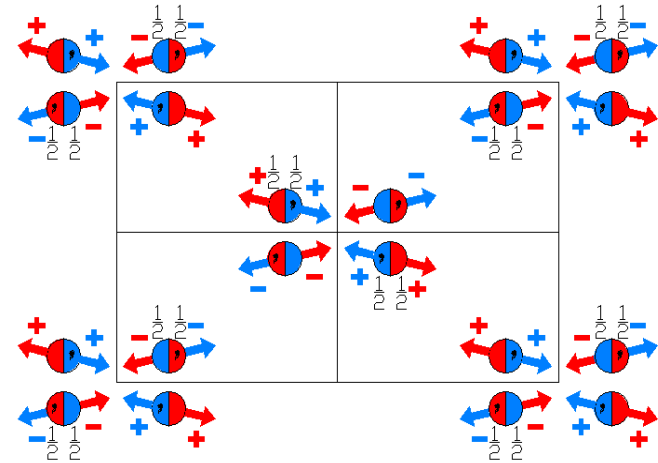
Along  $[0,1,0]$   $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at  $0,y,0$



Ibam  
72.1.630

mmm  
I2/b2/a2/m

Orthorhombic



Origin at center (2/m) at cc2/m

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0) | (3) 2 0,y,1/4<br>(2 <sub>y</sub>   0,0,1/2)         | (4) 2 x,0,1/4<br>(2 <sub>x</sub>   0,0,1/2)         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>   0,0,0) | (7) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>   0,0,1/2) | (8) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>   0,0,1/2) |

For (1/2,1/2,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)                | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2) | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$   1/2,1/2,1/2) | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>   1/2,1/2,1/2) | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

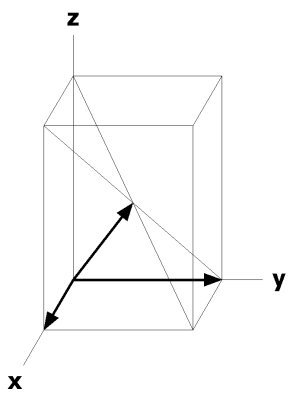
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 k 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},\bar{y},z+1/2$ [u, $\bar{v},\bar{w}$ ]
8 j ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
8 i ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
8 h ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]
8 g .2.	0,y,1/4 [0,v,0]	0, $\bar{y},1/4$ [0, $\bar{v},0$ ]	0,y,3/4 [0, $\bar{v},0$ ]	0, $\bar{y},3/4$ [0,v,0]
8 f 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [ $\bar{u},0,0$ ]	$\bar{x},0,3/4$ [u,0,0]
8 e $\bar{1}$	1/4,1/4,1/4 [u,v,w]	1/4,3/4,1/4 [u, $\bar{v},\bar{w}$ ]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,1/4 [ $\bar{u},v,\bar{w}$ ]
4 d ..2/m	1/2,0,0 [0,0,w]	1/2,0,1/2 [0,0, $\bar{w}$ ]		
4 c ..2/m	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		
4 b 222	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]		
4 a 222	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a}2'mm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



lbam1'

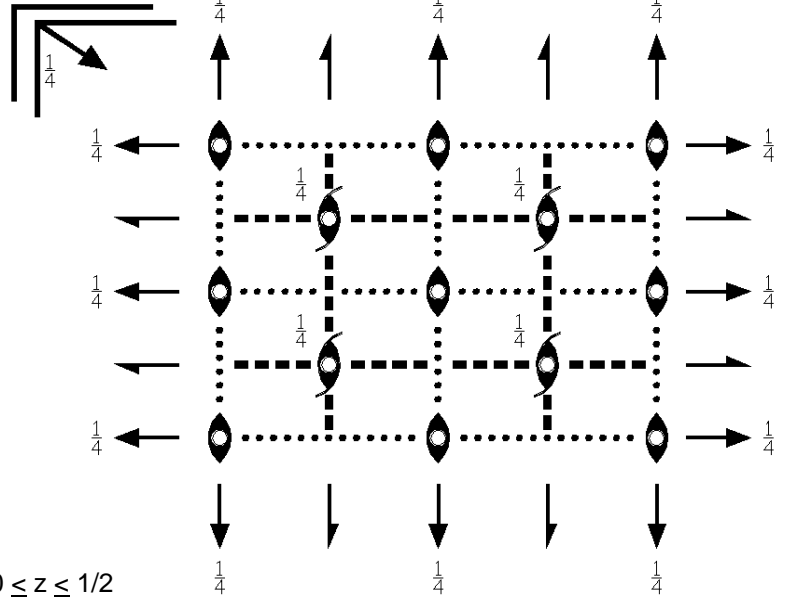
72.2.631

mmm1'

l2/b2/a2/m1'

Orthorhombic

1'



Origin at center ( $2/m1'$ ) at  $cc2/m1'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)         | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (8) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                 | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2) | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |

For (0,0,0)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1'<br>(1 0,0,0)'                          | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'         | (4) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'         |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (8) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |

For (1/2,1/2,1/2)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'                  | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)' | (6) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

### Positions

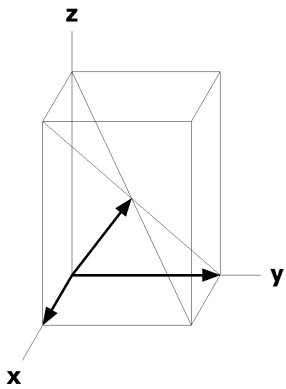
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'		
16 k 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{x},y,\bar{z}+1/2$ [0,0,0]	(4) $x,\bar{y},\bar{z}+1/2$ [0,0,0]
	(5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(6) x,y, $\bar{z}$ [0,0,0]	(7) x, $\bar{y},z+1/2$ [0,0,0]	(8) $\bar{x},y,z+1/2$ [0,0,0]
8 j ..m1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{x},y,1/2$ [0,0,0]	x, $\bar{y},1/2$ [0,0,0]
8 i ..21'	0,1/2,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	0,1/2, $\bar{z}+1/2$ [0,0,0]	0,1/2,z+1/2 [0,0,0]
8 h ..21'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0,z+1/2 [0,0,0]
8 g .2.1'	0,y,1/4 [0,0,0]	0, $\bar{y},1/4$ [0,0,0]	0,y,3/4 [0,0,0]	0, $\bar{y},3/4$ [0,0,0]
8 f 2..1'	x,0,1/4 [0,0,0]	$\bar{x},0,1/4$ [0,0,0]	x,0,3/4 [0,0,0]	$\bar{x},0,3/4$ [0,0,0]
8 e $\bar{1}1'$	1/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
4 d ..2/m1'	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 c ..2/m1'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
4 b 2221'	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]		
4 a 2221'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

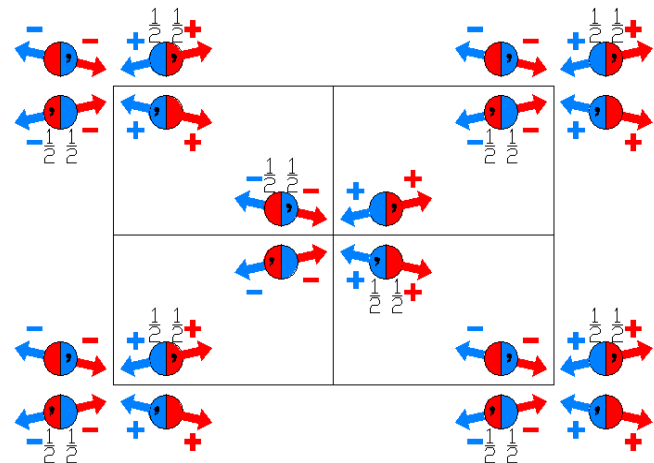
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Ib'am  
72.3.632

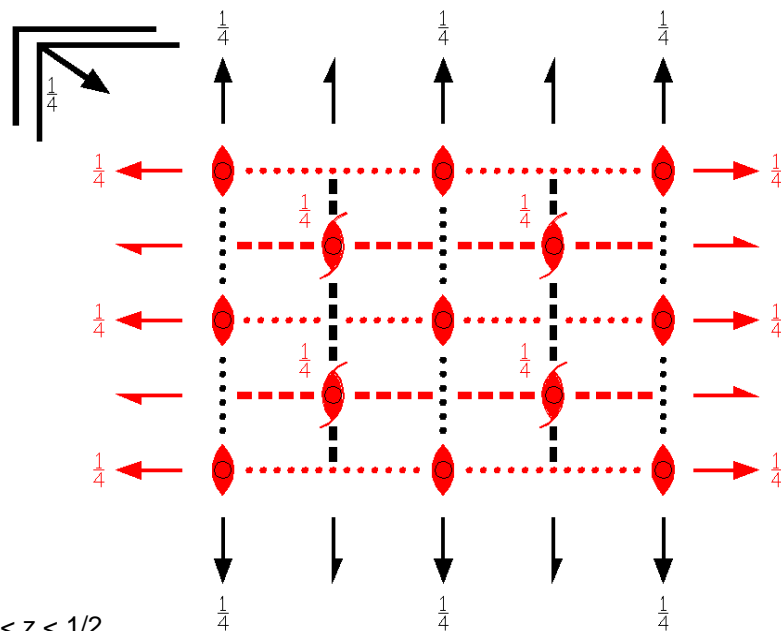
m'mm  
I2/b'2'/a2'/m

Orthorhombic



Origin at center ( $2'/m$ ) at  $c'c2'/m$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$



### Symmetry Operations

For (0,0,0) + set

- |  |                                    |  |  |
|--|------------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $2'$ 0,y,1/4<br>( $2_y$  0,0,1/2)'     | (4) 2 x,0,1/4<br>( $2_x$  0,0,1/2)             |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m x,y,0<br>( $m_z$  0,0,0)     | (7) c (0,0,1/2) x,0,z<br>( $m_y$  0,0,1/2) | (8) $c'$ (0,0,1/2) 0,y,z<br>( $m_x$  0,0,1/2)' |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                   | (2) $2'$ (0,0,1/2) 1/4,1/4,z<br>( $2_z$  1/2,1/2,1/2)' | (3) $2'$ (0,1/2,0) 1/4,y,0<br>( $2_y$  1/2,1/2,0)' | (4) 2 (1/2,0,0) x,1/4,0<br>( $2_x$  1/2,1/2,0)     |
| (5) $\bar{1}'$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)' | (6) n (1/2,1/2,0) x,y,1/4<br>( $m_z$  1/2,1/2,1/2)     | (7) a (1/2,0,0) x,1/4,z<br>( $m_y$  1/2,1/2,0)     | (8) $b'$ (0,1/2,0) 1/4,y,z<br>( $m_x$  1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

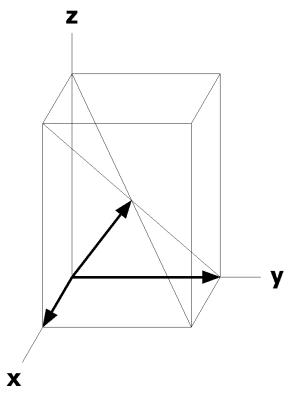
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 k 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
8 j ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
8 i ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	0,1/2, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	0,1/2,z+1/2 [ $\bar{u},v,0$ ]
8 h ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	0,0, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	0,0,z+1/2 [ $\bar{u},v,0$ ]
8 g .2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [u,0, $\bar{w}$ ]	0,y,3/4 [ $\bar{u},0,w$ ]	0, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]
8 f 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [u,0,0]	x,0,3/4 [ $\bar{u},0,0$ ]	$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]
8 e $\bar{1}'$	1/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
4 d ..2'/m	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 c ..2'/m	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
4 b 22'2'	1/2,0,1/4 [u,0,0]	1/2,0,3/4 [ $\bar{u},0,0$ ]		
4 a 22'2'	0,0,1/4 [u,0,0]	0,0,3/4 [ $\bar{u},0,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

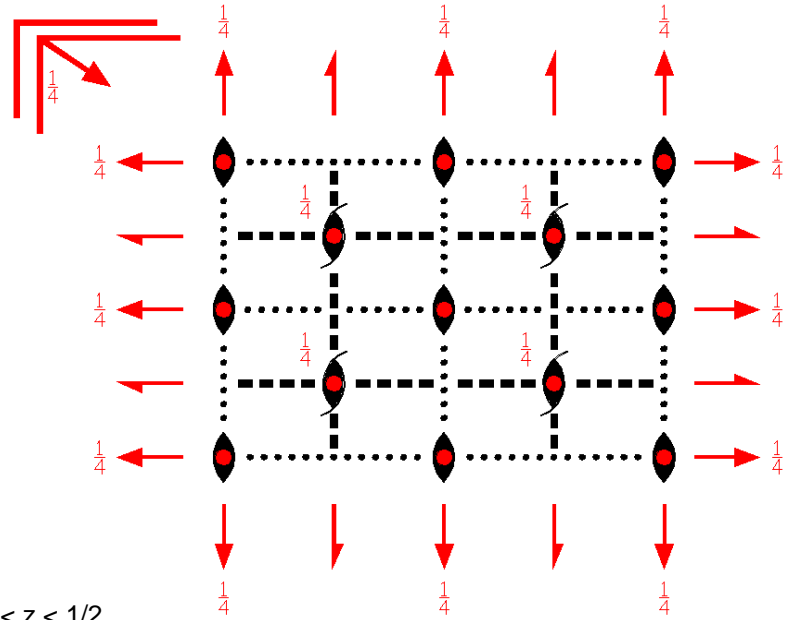
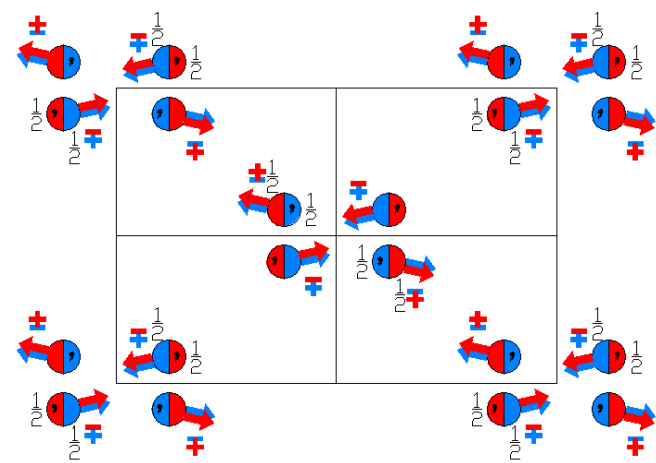
Along [0,1,0] p<sub>2a</sub>·2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Ibam'  
72.4.633

mmm'  
I2'/b2'/a2/m'

Orthorhombic



Origin at center ( $2/m'$ ) at  $cc2/m'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'       | (4) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'       |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (8) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) |

For (1/2,1/2,1/2) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                    | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)   | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)' | (6) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (7) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)   | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

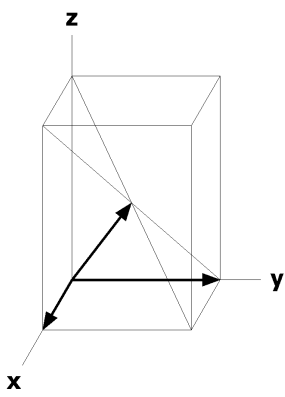
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 k 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z+1/2$ [u, $\bar{v},\bar{w}$ ]
8 j ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [u, $\bar{v},0$ ]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]
8 i ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
8 h ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]
8 g .2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	0,y,3/4 [u,0, $\bar{w}$ ]	0, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]
8 f 2'..	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	x,0,3/4 [0,v, $\bar{w}$ ]	$\bar{x},0,3/4$ [0, $\bar{v},\bar{w}$ ]
8 e $\bar{1}$ '	1/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
4 d ..2/m'	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 c ..2/m'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
4 b 2'2'2	1/2,0,1/4 [0,0,w]	1/2,0,3/4 [0,0, $\bar{w}$ ]		
4 a 2'2'2	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



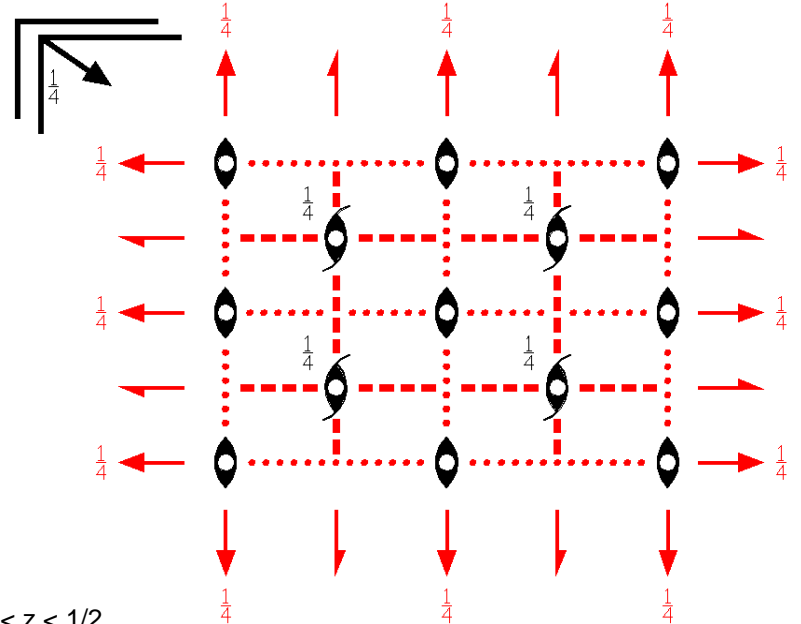
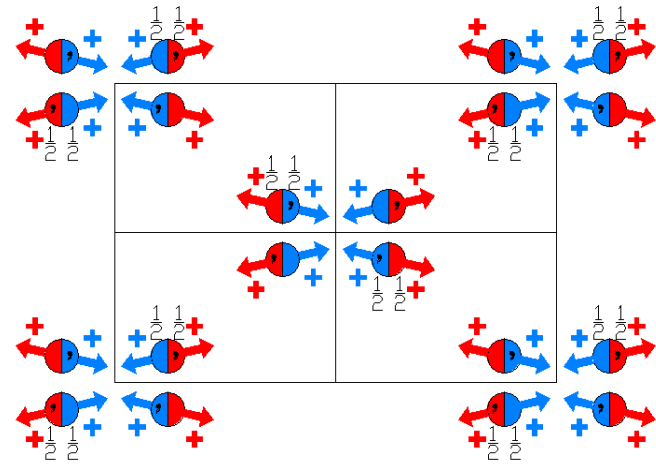
Ib'a'm

72.5.634

m'm'm

I2'/b'2'/a'2'/m

Orthorhombic



Origin at center (2/m) at c'c'2/m

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'         | (4) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (8) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                 | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2) | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

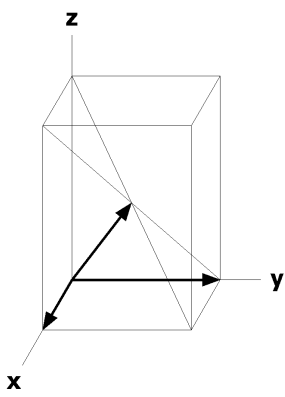
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 k 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
8 j ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0,w]
8 i ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	0,1/2,z+1/2 [0,0,w]
8 h ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0,z+1/2 [0,0,w]
8 g .2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	0,y,3/4 [ $\bar{u},0,w$ ]	0, $\bar{y},3/4$ [u,0,w]
8 f 2'..	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	x,0,3/4 [0, $\bar{v},w$ ]	$\bar{x},0,3/4$ [0,v,w]
8 e $\bar{1}$	1/4,1/4,1/4 [u,v,w]	1/4,3/4,1/4 [ $\bar{u},v,w$ ]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,1/4 [u, $\bar{v},w$ ]
4 d ..2/m	1/2,0,0 [0,0,w]	1/2,0,1/2 [0,0,w]		
4 c ..2/m	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]		
4 b 2'2'2	1/2,0,1/4 [0,0,w]	1/2,0,3/4 [0,0,w]		
4 a 2'2'2	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

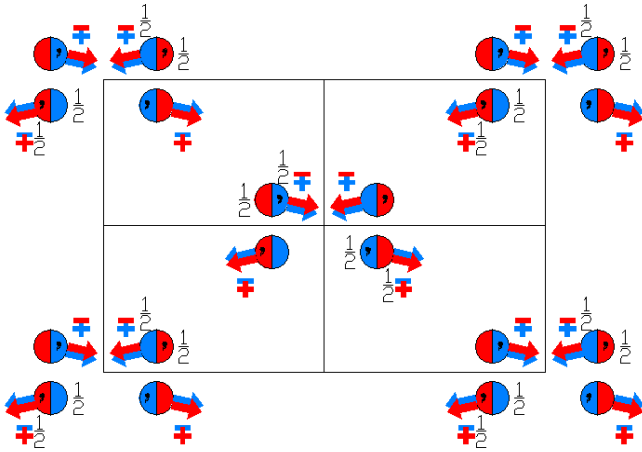
Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



Iba'm'  
72.6.635

mm'm'  
I2/b2'/a'2'/m'

Orthorhombic



Origin at center ( $2'/m'$ ) at  $cc'2'/m'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

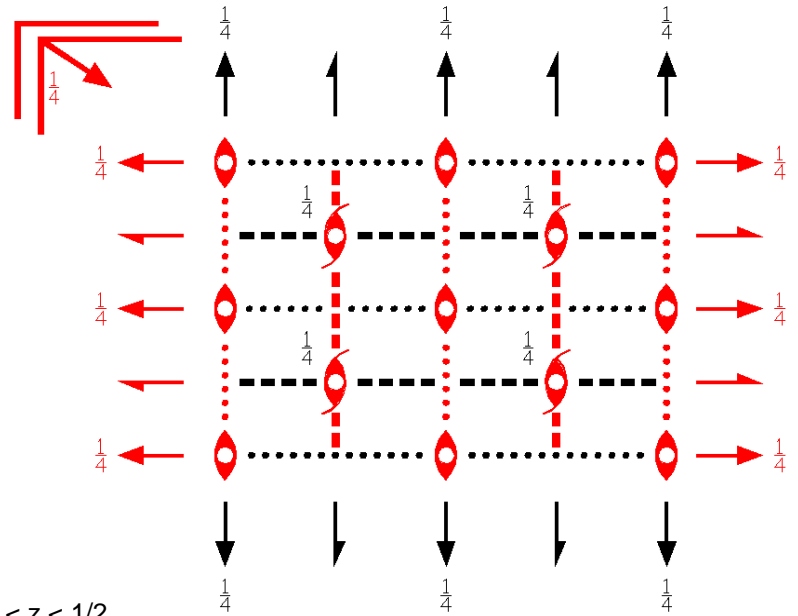
**Symmetry Operations**

For (0,0,0) + set

- |  |                                    |  |  |
|--|------------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $2'$ 0,y,1/4<br>( $2_y$  0,0,1/2)'         | (4) $2$ x,0,1/4<br>( $2_x$  0,0,1/2)         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) $m'$ x,y,0<br>( $m_z$  0,0,0)' | (7) $c'$ (0,0,1/2) x,0,z<br>( $m_y$  0,0,1/2)' | (8) $c$ (0,0,1/2) 0,y,z<br>( $m_x$  0,0,1/2) |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t$ (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)               | (2) $2'$ (0,0,1/2) 1/4,1/4,z<br>( $2_z$  1/2,1/2,1/2)' | (3) $2'$ (0,1/2,0) 1/4,y,0<br>( $2_y$  1/2,1/2,0)' | (4) $2$ (1/2,0,0) x,1/4,0<br>( $2_x$  1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2) | (6) $n'$ (1/2,1/2,0) x,y,1/4<br>( $m_z$  1/2,1/2,1/2)' | (7) $a'$ (1/2,0,0) x,1/4,z<br>( $m_y$  1/2,1/2,0)' | (8) $b$ (0,1/2,0) 1/4,y,z<br>( $m_x$  1/2,1/2,0) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

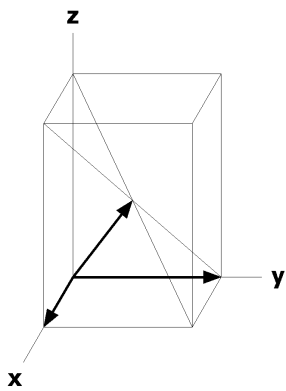
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 k 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v}$ ,w] (7) x, $\bar{y},z+1/2$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z+1/2$ [u, $\bar{v},\bar{w}$ ]
8 j ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [u,v,0]	$\bar{x},y,1/2$ [u, $\bar{v}$ ,0]	x, $\bar{y},1/2$ [u, $\bar{v}$ ,0]
8 i ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}$ [u,v,0]	0,1/2, $\bar{z}+1/2$ [u, $\bar{v}$ ,0]	0,1/2,z+1/2 [u, $\bar{v}$ ,0]
8 h ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [u,v,0]	0,0, $\bar{z}+1/2$ [u, $\bar{v}$ ,0]	0,0,z+1/2 [u, $\bar{v}$ ,0]
8 g .2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [u,0, $\bar{w}$ ]	0,y,3/4 [u,0, $\bar{w}$ ]	0, $\bar{y},3/4$ [u,0,w]
8 f 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [u,0,0]	x,0,3/4 [u,0,0]	$\bar{x},0,3/4$ [u,0,0]
8 e $\bar{1}$	1/4,1/4,1/4 [u,v,w]	1/4,3/4,1/4 [u, $\bar{v},\bar{w}$ ]	3/4,3/4,1/4 [u,v, $\bar{w}$ ]	3/4,1/4,1/4 [u, $\bar{v},w$ ]
4 d ..2'/m'	1/2,0,0 [u,v,0]	1/2,0,1/2 [u, $\bar{v}$ ,0]		
4 c ..2'/m'	0,0,0 [u,v,0]	0,0,1/2 [u, $\bar{v}$ ,0]		
4 b 22'2'	1/2,0,1/4 [u,0,0]	1/2,0,3/4 [u,0,0]		
4 a 22'2'	0,0,1/4 [u,0,0]	0,0,3/4 [u,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}$ -2mm  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,1/4

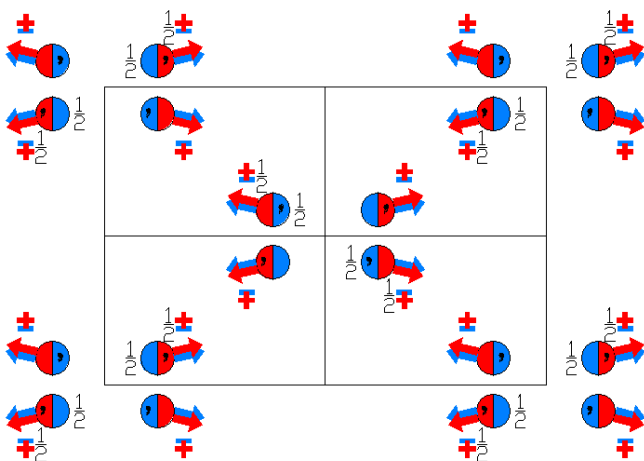
Along [0,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



$Ib'a'm'$   
72.7.636

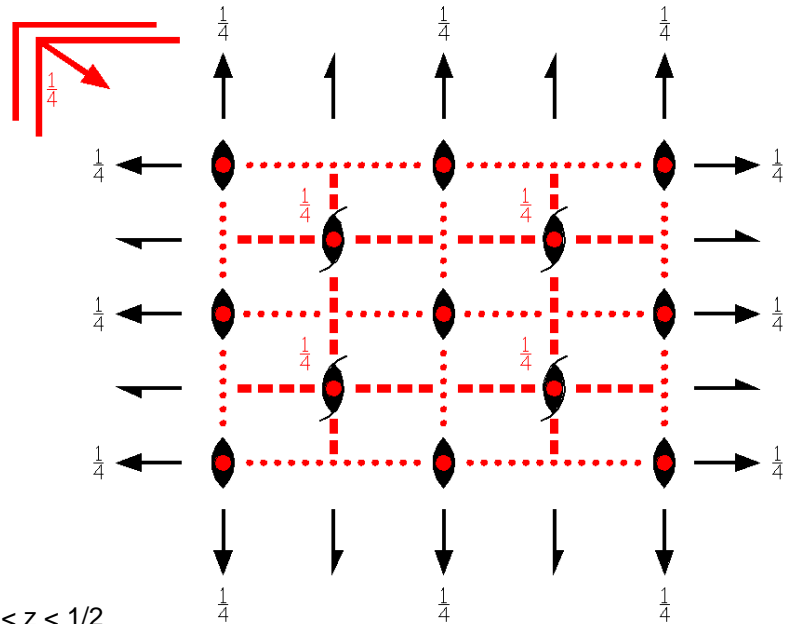
$m'm'm'$   
 $I2/b'2/a'2/m'$

Orthorhombic



Origin at center ( $2/m'$ ) at  $c'c'2/m'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$



**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)     | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)     |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) $m'$ x,y,0<br>( $m_z$  0,0,0)'     | (7) $c'$ (0,0,1/2) x,0,z<br>( $m_y$  0,0,1/2)' | (8) $c'$ (0,0,1/2) 0,y,z<br>( $m_x$  0,0,1/2)' |

For (1/2,1/2,1/2) + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t$ (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                  | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)' | (6) $n'$ (1/2,1/2,0) x,y,1/4<br>( $m_z$  1/2,1/2,1/2)'     | (7) $a'$ (1/2,0,0) x,1/4,z<br>( $m_y$  1/2,1/2,0)'     | (8) $b'$ (0,1/2,0) 1/4,y,z<br>( $m_x$  1/2,1/2,0)'     |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

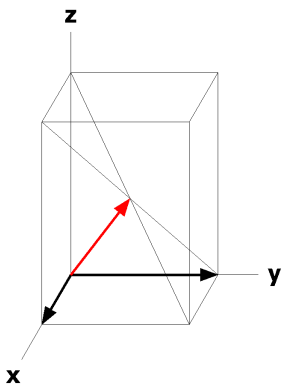
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 k 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ] (7) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
8 j ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	x, $\bar{y},1/2$ [u, $\bar{v},0$ ]
8 i ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0,w]
8 h ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]
8 g .2.	0,y,1/4 [0,v,0]	0, $\bar{y},1/4$ [0, $\bar{v},0$ ]	0,y,3/4 [0,v,0]	0, $\bar{y},3/4$ [0, $\bar{v},0$ ]
8 f 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [u,0,0]	$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]
8 e $\bar{1}$ '	1/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
4 d ..2/m'	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 c ..2/m'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
4 b 222	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]		
4 a 222	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



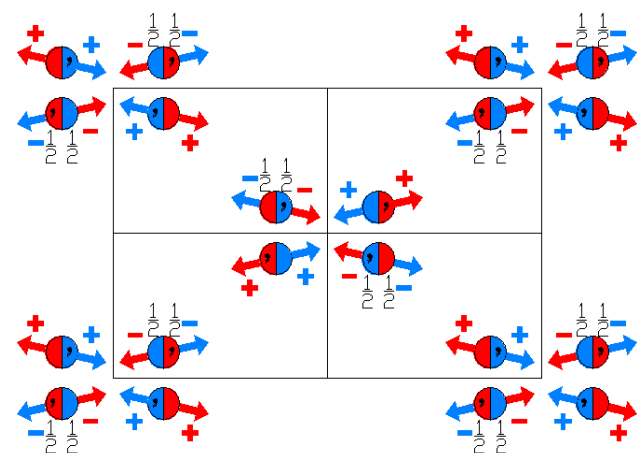
$I_{pbam}$

72.8.637

$mmm1'$

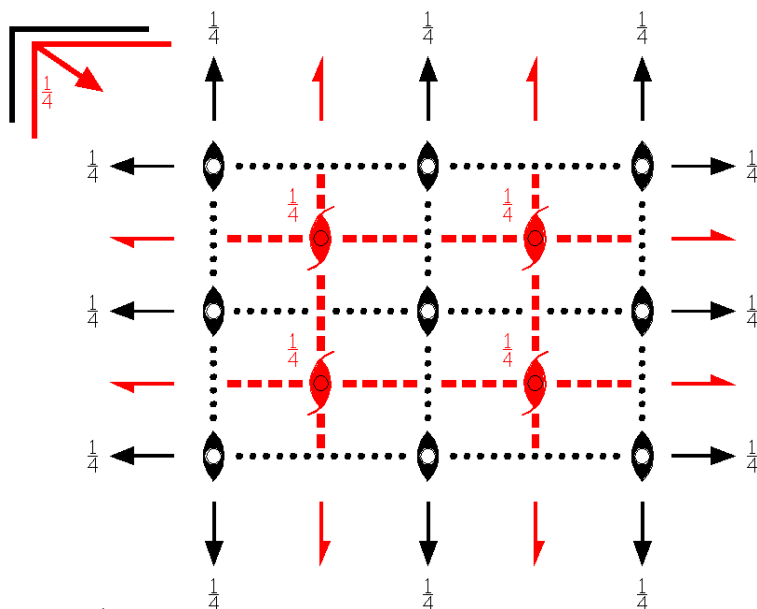
$I_{p2/b2/a2/m}$

Orthorhombic



Origin at center ( $2/m$ ) at  $cc2/m$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$



### Symmetry Operations

For  $(0,0,0)$  + set

- |   |                                   |   |   |
|---|-----------------------------------|---|---|
| (1) 1<br>(1   0,0,0)                          | (2) 2 $0,0,z$<br>( $2_z$   0,0,0) | (3) 2 $0,y,1/4$<br>( $2_y$   0,0,1/2)           | (4) 2 $x,0,1/4$<br>( $2_x$   0,0,1/2)           |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   0,0,0) | (6) m $x,y,0$<br>( $m_z$   0,0,0) | (7) c $(0,0,1/2)$ $x,0,z$<br>( $m_y$   0,0,1/2) | (8) c $(0,0,1/2)$ $0,y,z$<br>( $m_x$   0,0,1/2) |

For  $(1/2,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,1/2)$<br>(1   $1/2,1/2,1/2$ )'              | (2) $2'$ $(0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1/2$ )' | (3) $2'$ $(0,1/2,0)$ $1/4,y,0$<br>( $2_y$   $1/2,1/2,0$ )' | (4) $2'$ $(1/2,0,0)$ $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )' |
| (5) $\bar{1}'$ $1/4,1/4,1/4$<br>( $\bar{1}$   $1/2,1/2,1/2$ )' | (6) $n'$ $(1/2,1/2,0)$ $x,y,1/4$<br>( $m_z$   $1/2,1/2,1/2$ )' | (7) $a'$ $(1/2,0,0)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,0$ )' | (8) $b'$ $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

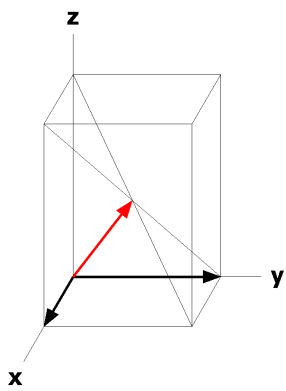
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
16 k 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(4) $x,\bar{y},\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(6) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $x,\bar{y},z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(8) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]
8 j ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	$x,\bar{y},1/2$ [0,0, $\bar{w}$ ]
8 i ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
8 h ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]
8 g .2.	0,y,1/4 [0,v,0]	0, $\bar{y},1/4$ [0, $\bar{v},0$ ]	0,y,3/4 [0, $\bar{v},0$ ]	0, $\bar{y},3/4$ [0,v,0]
8 f 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [ $\bar{u},0,0$ ]	$\bar{x},0,3/4$ [u,0,0]
8 e $\bar{1}'$	1/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
4 d ..2/m	1/2,0,0 [0,0,w]	1/2,0,1/2 [0,0, $\bar{w}$ ]		
4 c ..2/m	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		
4 b 222	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]		
4 a 222	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a}2'mm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



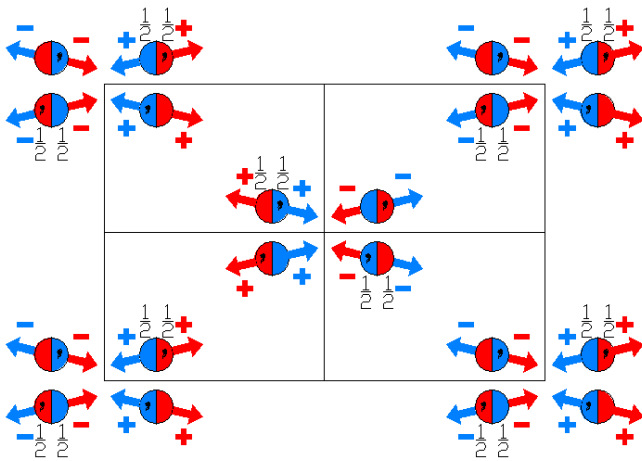
$I_p b' am$

72.9.638

$mmm1'$

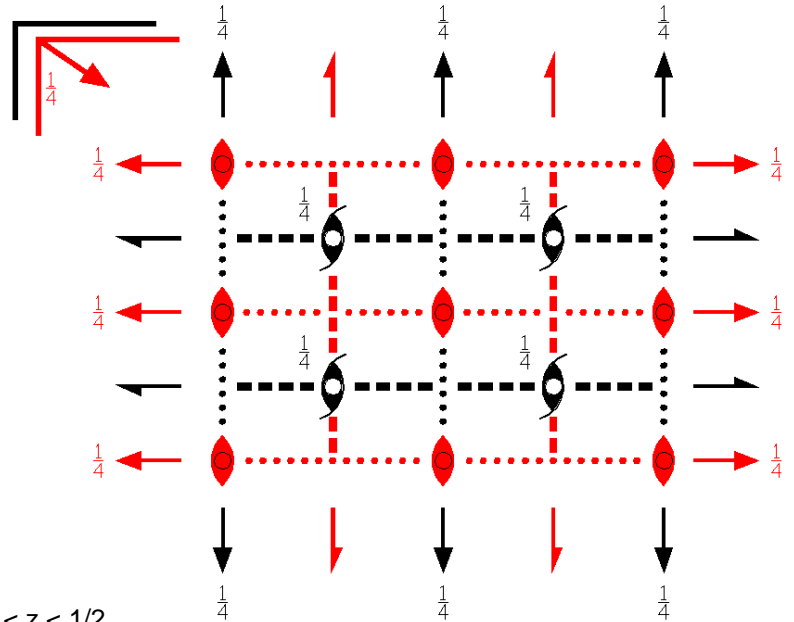
$I_p 2/b'2'/a2'/m$

Orthorhombic



Origin at center ( $2'/m$ ) at  $c'c2'/m$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$



**Symmetry Operations**

For (0,0,0) + set

- |  |                                    |  |  |
|--|------------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $2'$ 0,y,1/4<br>( $2_y$  0,0,1/2)'     | (4) $2$ x,0,1/4<br>( $2_x$  0,0,1/2)           |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m x,y,0<br>( $m_z$  0,0,0)     | (7) c (0,0,1/2) x,0,z<br>( $m_y$  0,0,1/2) | (8) $c'$ (0,0,1/2) 0,y,z<br>( $m_x$  0,0,1/2)' |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'             | (2) $2$ (0,0,1/2) 1/4,1/4,z<br>( $2_z$  1/2,1/2,1/2)   | (3) $2$ (0,1/2,0) 1/4,y,0<br>( $2_y$  1/2,1/2,0)   | (4) $2'$ (1/2,0,0) x,1/4,0<br>( $2_x$  1/2,1/2,0)' |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2) | (6) $n'$ (1/2,1/2,0) x,y,1/4<br>( $m_z$  1/2,1/2,1/2)' | (7) $a'$ (1/2,0,0) x,1/4,z<br>( $m_y$  1/2,1/2,0)' | (8) b (0,1/2,0) 1/4,y,z<br>( $m_x$  1/2,1/2,0)     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

### Positions

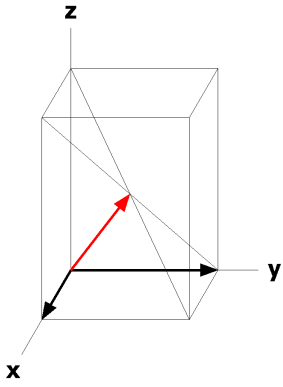
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
16 k 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ] (8) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
8 j ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]
8 i ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	0,1/2, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	0,1/2,z+1/2 [ $\bar{u},v,0$ ]
8 h ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	0,0, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	0,0,z+1/2 [ $\bar{u},v,0$ ]
8 g .2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [u,0, $\bar{w}$ ]	0,y,3/4 [ $\bar{u},0,w$ ]	0, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]
8 f 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [u,0,0]	x,0,3/4 [ $\bar{u},0,0$ ]	$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]
8 e $\bar{1}$	1/4,1/4,1/4 [u,v,w]	1/4,3/4,1/4 [u, $\bar{v},\bar{w}$ ]	3/4,3/4,1/4 [u,v, $\bar{w}$ ]	3/4,1/4,1/4 [u, $\bar{v},w$ ]
4 d ..2'/m	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 c ..2'/m	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
4 b 22'2'	1/2,0,1/4 [u,0,0]	1/2,0,3/4 [ $\bar{u},0,0$ ]		
4 a 22'2'	0,0,1/4 [u,0,0]	0,0,3/4 [ $\bar{u},0,0$ ]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>·2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

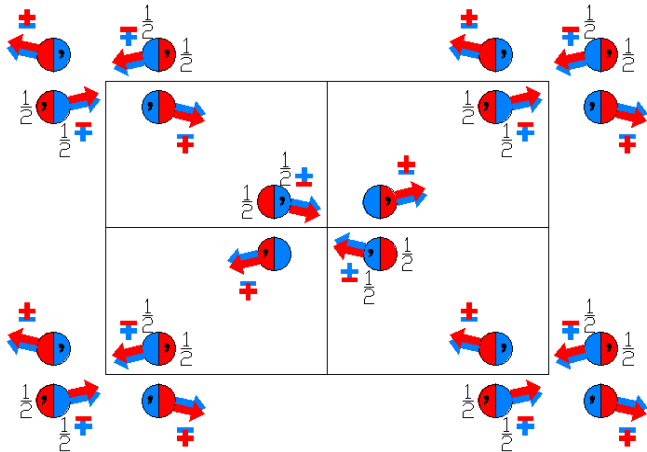
Along [0,1,0] p<sub>2a</sub>·2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



$I_{pbam}'$   
72.10.639

$mmm1'$   
 $I_{p2}'/b2'/a2/m'$

Orthorhombic



Origin at center ( $2/m'$ ) at  $cc2/m'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

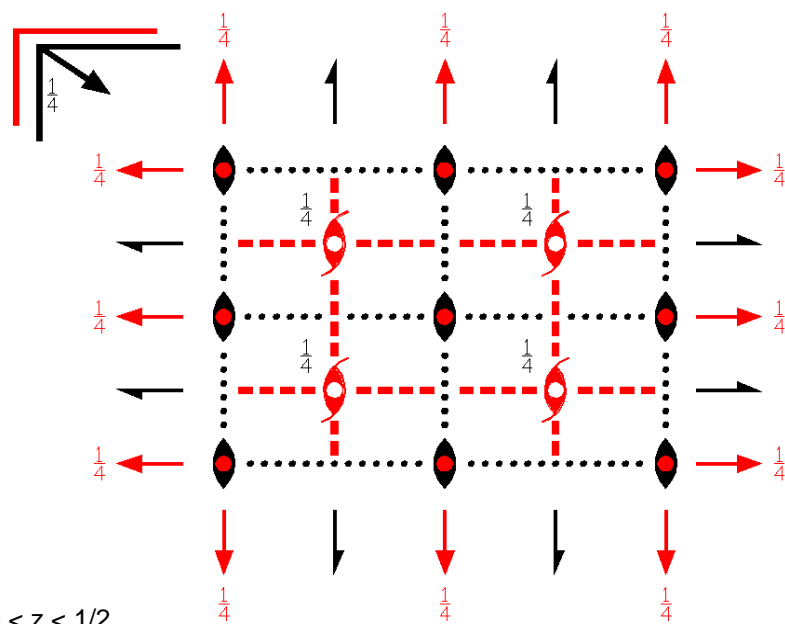
**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1   0,0,0)                           | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0)   | (3) 2' 0,y,1/4<br>(2 <sub>y</sub>   0,0,1/2)'       | (4) 2' x,0,1/4<br>(2 <sub>x</sub>   0,0,1/2)'       |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$   0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>   0,0,0)' | (7) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>   0,0,1/2) | (8) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>   0,0,1/2) |

For (1/2,1/2,1/2)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) t' (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)'              | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2)' | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)   |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$   1/2,1/2,1/2) | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>   1/2,1/2,1/2)   | (7) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

### Positions

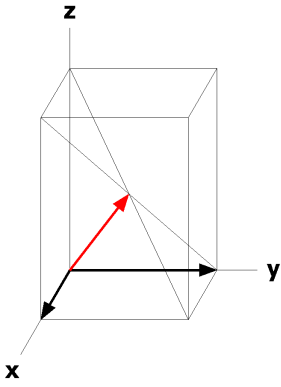
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
16 k 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z+1/2$ [u, $\bar{v},\bar{w}$ ]
8 j ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [u, $\bar{v},0$ ]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]
8 i ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
8 h ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]
8 g .2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	0,y,3/4 [u,0, $\bar{w}$ ]	0, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]
8 f 2'..	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	x,0,3/4 [0,v, $\bar{w}$ ]	$\bar{x},0,3/4$ [0, $\bar{v},\bar{w}$ ]
8 e $\bar{1}$	1/4,1/4,1/4 [u,v,w]	1/4,3/4,1/4 [ $\bar{u},v,w$ ]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,1/4 [u, $\bar{v},w$ ]
4 d ..2/m'	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 c ..2/m'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
4 b 2'2'2	1/2,0,1/4 [0,0,w]	1/2,0,3/4 [0,0, $\bar{w}$ ]		
4 a 2'2'2	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1]  $c_p$ -2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}$ -2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

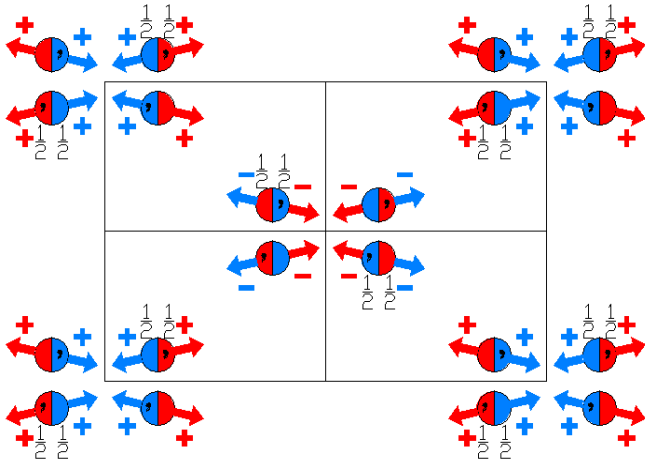
Along [0,1,0]  $p_{2a}$ -2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



$I_p b'a'm$   
72.11.640

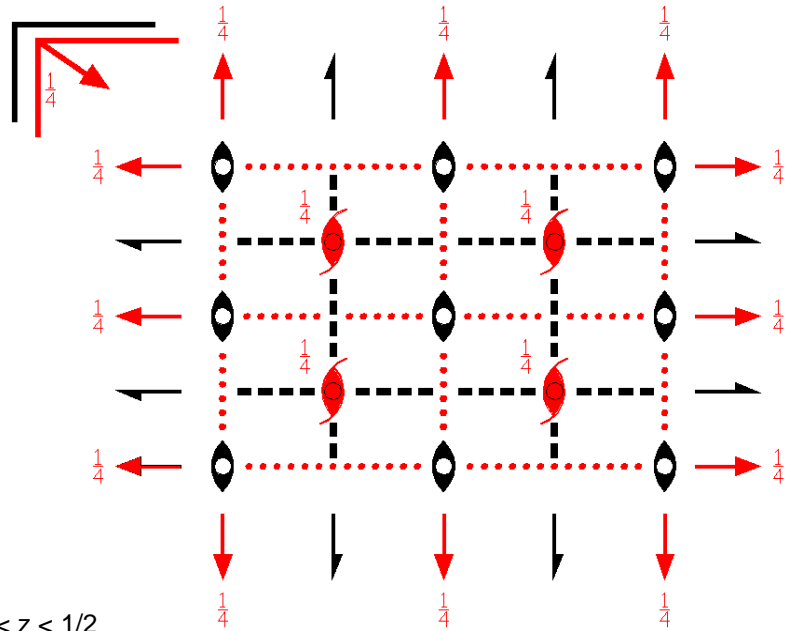
$mmm1'$   
 $I_p 2'/b'2'/a'2'/m$

Orthorhombic



Origin at center ( $2/m$ ) at  $c'c'2/m$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$



**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |                                  |  |  |
|--|----------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) 2' $0,y,1/4$<br>( $2_y$  0,0,1/2)'           | (4) 2' $x,0,1/4$<br>( $2_x$  0,0,1/2)'           |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0) | (6) m $x,y,0$<br>( $m_z$  0,0,0) | (7) c' $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2)' | (8) c' $(0,0,1/2)$ $0,y,z$<br>( $m_x$  0,0,1/2)' |

For  $(1/2,1/2,1/2)$ ' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' $(1/2,1/2,1/2)$<br>(1 1/2,1/2,1/2)'                  | (2) 2' $(0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2)' | (3) 2 $(0,1/2,0)$ $1/4,y,0$<br>( $2_y$  1/2,1/2,0) | (4) 2 $(1/2,0,0)$ $x,1/4,0$<br>( $2_x$  1/2,1/2,0) |
| (5) $\bar{1}$ ' $1/4,1/4,1/4$<br>( $\bar{1}$  1/2,1/2,1/2)' | (6) n' $(1/2,1/2,0)$ $x,y,1/4$<br>( $m_z$  1/2,1/2,1/2)' | (7) a $(1/2,0,0)$ $x,1/4,z$<br>( $m_y$  1/2,1/2,0) | (8) b $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$  1/2,1/2,0) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

### Positions

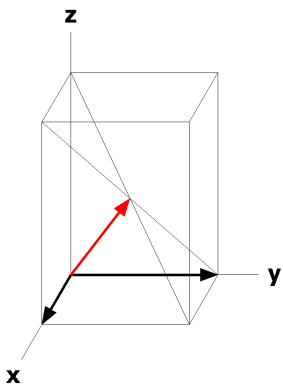
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
16 k 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
8 j ..m	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0,w]
8 i ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	0,1/2,z+1/2 [0,0,w]
8 h ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0,z+1/2 [0,0,w]
8 g .2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	0,y,3/4 [ $\bar{u},0,w$ ]	0, $\bar{y},3/4$ [u,0,w]
8 f 2'..	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	x,0,3/4 [0, $\bar{v},w$ ]	$\bar{x},0,3/4$ [0,v,w]
8 e $\bar{1}'$	1/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
4 d ..2/m	1/2,0,0 [0,0,w]	1/2,0,1/2 [0,0,w]		
4 c ..2/m	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]		
4 b 2'2'2	1/2,0,1/4 [0,0,w]	1/2,0,3/4 [0,0,w]		
4 a 2'2'2	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,1/4

Along [0,1,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,1/4



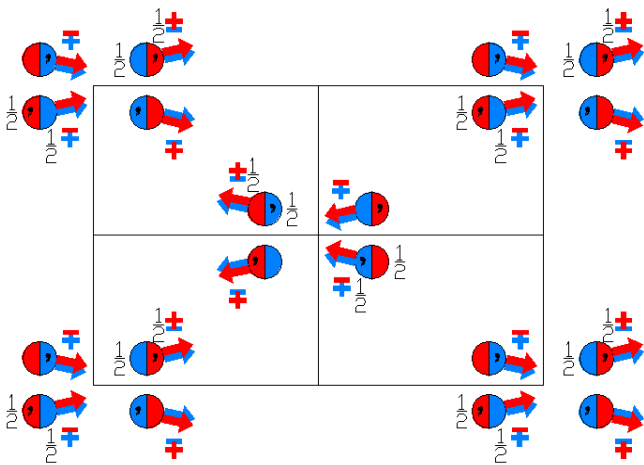
$I_p b' a m'$

72.12.641

$m m m 1'$

$I_p 2' b' 2' a 2' m'$

Orthorhombic



Origin at center ( $2'/m'$ ) at  $c'c'2'/m'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |                                     |   |   |
|---|-------------------------------------|---|---|
| (1) 1<br>(1   0,0,0)                        | (2) $2'$ 0,0,z<br>( $2_z$   0,0,0)' | (3) $2$ 0,y,1/4<br>( $2_y$   0,0,1/2)         | (4) $2'$ x,0,1/4<br>( $2_x$   0,0,1/2)'         |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0) | (6) $m'$ x,y,0<br>( $m_z$   0,0,0)' | (7) $c$ (0,0,1/2) x,0,z<br>( $m_y$   0,0,1/2) | (8) $c'$ (0,0,1/2) 0,y,z<br>( $m_x$   0,0,1/2)' |

For (1/2,1/2,1/2) + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t'$ (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)'               | (2) $2$ (0,0,1/2) 1/4,1/4,z<br>( $2_z$   1/2,1/2,1/2) | (3) $2'$ (0,1/2,0) 1/4,y,0<br>( $2_y$   1/2,1/2,0)' | (4) $2$ (1/2,0,0) x,1/4,0<br>( $2_x$   1/2,1/2,0) |
| (5) $\bar{1}'$ 1/4,1/4,1/4<br>( $\bar{1}'$   1/2,1/2,1/2)' | (6) $n$ (1/2,1/2,0) x,y,1/4<br>( $m_z$   1/2,1/2,1/2) | (7) $a'$ (1/2,0,0) x,1/4,z<br>( $m_y$   1/2,1/2,0)' | (8) $b$ (0,1/2,0) 1/4,y,z<br>( $m_x$   1/2,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

### Positions

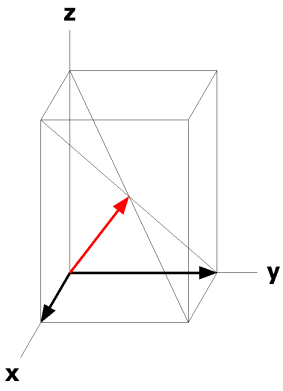
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
16 k 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
8 j ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [u,v,0]	$\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]
8 i ..2'	0,1/2,z [u,v,0]	0,1/2, $\bar{z}$ [u,v,0]	0,1/2, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	0,1/2,z+1/2 [ $\bar{u},v,0$ ]
8 h ..2'	0,0,z [u,v,0]	0,0, $\bar{z}$ [u,v,0]	0,0, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]	0,0,z+1/2 [ $\bar{u},v,0$ ]
8 g .2.	0,y,1/4 [0,v,0]	0, $\bar{y},1/4$ [0,v,0]	0,y,3/4 [0,v,0]	0, $\bar{y},3/4$ [0,v,0]
8 f 2'..	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0,v, $\bar{w}$ ]	x,0,3/4 [0,v, $\bar{w}$ ]	$\bar{x},0,3/4$ [0,v,w]
8 e $\bar{1}'$	1/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
4 d ..2'/m'	1/2,0,0 [u,v,0]	1/2,0,1/2 [ $\bar{u},v,0$ ]		
4 c ..2'/m'	0,0,0 [u,v,0]	0,0,1/2 [ $\bar{u},v,0$ ]		
4 b 2'22'	1/2,0,1/4 [0,v,0]	1/2,0,3/4 [0,v,0]		
4 a 2'22'	0,0,1/4 [0,v,0]	0,0,3/4 [0,v,0]		

### Symmetry of Special Projections

Along [0,0,1]  $c_p-2'mm'$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}-2'mm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

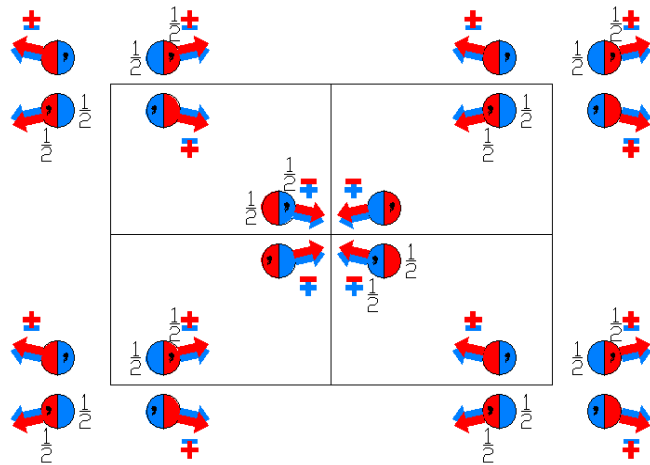
Along [0,1,0]  $p_{2a}-2mm$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



$I_p b' a' m'$   
72.13.642

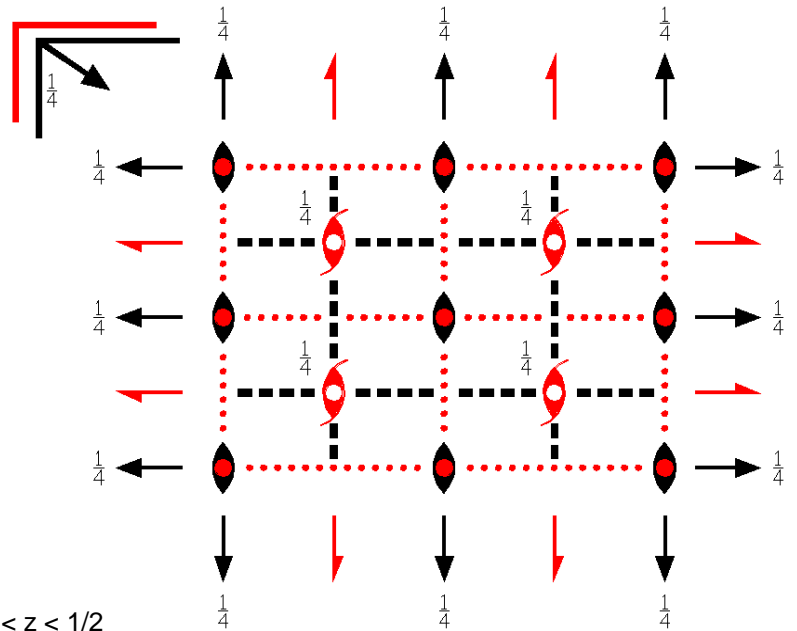
$mmm1'$   
 $I_p 2/b' 2/a' 2/m'$

Orthorhombic



Origin at center ( $2/m'$ ) at  $c'c'2/m'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$



### Symmetry Operations

For (0,0,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1   0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0) | (3) 2 0,y,1/4<br>(2 <sub>y</sub>   0,0,1/2)     | (4) 2 x,0,1/4<br>(2 <sub>x</sub>   0,0,1/2)     |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0)' | (6) $m'$ x,y,0<br>( $m_z$   0,0,0)'     | (7) $c'$ (0,0,1/2) x,0,z<br>( $m_y$   0,0,1/2)' | (8) $c'$ (0,0,1/2) 0,y,z<br>( $m_x$   0,0,1/2)' |

For (1/2,1/2,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) $t'$ (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)'            | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2)' | (3) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)' |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$   1/2,1/2,1/2) | (6) $n$ (1/2,1/2,0) x,y,1/4<br>( $m_z$   1/2,1/2,1/2)         | (7) $a$ (1/2,0,0) x,1/4,z<br>( $m_y$   1/2,1/2,0)         | (8) $b$ (0,1/2,0) 1/4,y,z<br>( $m_x$   1/2,1/2,0)         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

### Positions

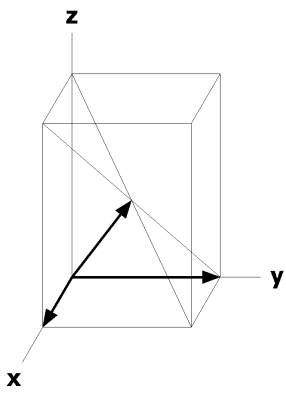
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
16 k 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ] (7) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]
8 j ..m'	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	x, $\bar{y},1/2$ [u, $\bar{v},0$ ]
8 i ..2	0,1/2,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0,w]
8 h ..2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]
8 g .2.	0,y,1/4 [0,v,0]	0, $\bar{y},1/4$ [0, $\bar{v},0$ ]	0,y,3/4 [0,v,0]	0, $\bar{y},3/4$ [0, $\bar{v},0$ ]
8 f 2..	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [u,0,0]	$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]
8 e $\bar{1}$	1/4,1/4,1/4 [u,v,w]	1/4,3/4,1/4 [u, $\bar{v},\bar{w}$ ]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,1/4 [ $\bar{u},v,\bar{w}$ ]
4 d ..2/m'	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 c ..2/m'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
4 b 222	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]		
4 a 222	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>.2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

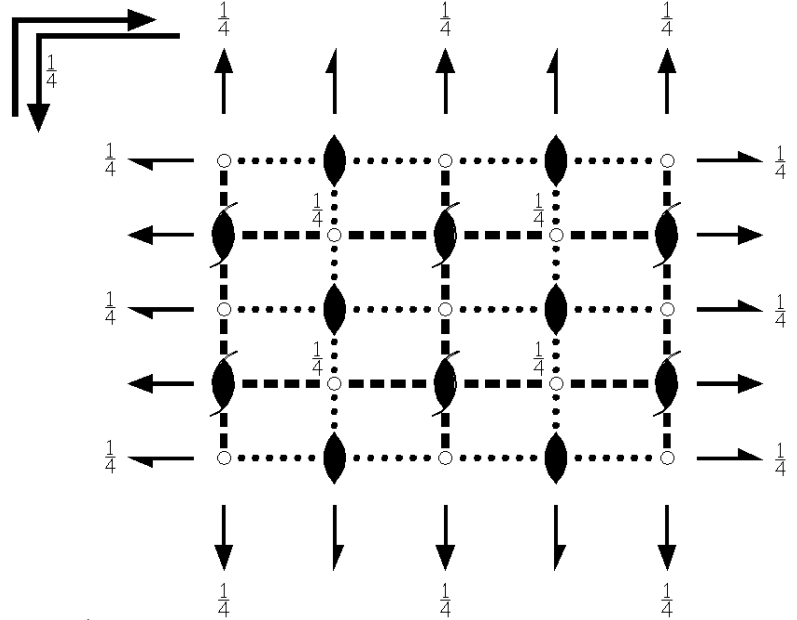
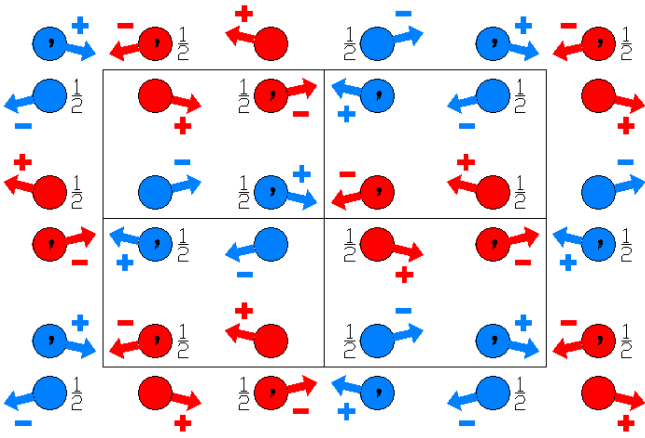
Along [0,1,0] p<sub>2a</sub>.2m'm'  
 $\mathbf{a}^* = -\mathbf{a}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at 0,y,0



lbca  
73.1.643

mmm  
 $I2_1/b2_1/c2_1/a$

Orthorhombic



Origin at  $\bar{1}$  at cab

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) $1/4,0,z$<br>( $2_z$   $1/2,0,1/2$ ) | (3) 2 (0,1/2,0) $0,y,1/4$<br>( $2_y$   $0,1/2,1/2$ ) | (4) 2 (1/2,0,0) $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ ) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a (1/2,0,0) $x,y,1/4$<br>( $m_z$   $1/2,0,1/2$ ) | (7) c (0,0,1/2) $x,1/4,z$<br>( $m_y$   $0,1/2,1/2$ ) | (8) b (0,1/2,0) $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ ) |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                 | (2) 2 $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )         | (3) 2 $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )         | (4) 2 $x,0,1/4$<br>( $2_x$   $0,0,1/2$ )         |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2) | (6) b (0,1/2,0) $x,y,0$<br>( $m_z$   $0,1/2,0$ ) | (7) a (1/2,0,0) $x,0,z$<br>( $m_y$   $1/2,0,0$ ) | (8) c (0,0,1/2) $0,y,z$<br>( $m_x$   $0,0,1/2$ ) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

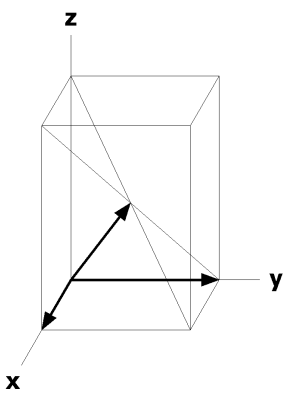
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 f 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ] (7) $x,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ] (8) $\bar{x}+1/2,y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]
8 e ..2	0,1/4,z [0,0,w]	0,3/4, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,3/4, $\bar{z}$ [0,0,w]	0,1/4,z+1/2 [0,0, $\bar{w}$ ]
8 d .2.	1/4,y,0 [0,v,0]	1/4, $\bar{y},1/2$ [0, $\bar{v},0$ ]	3/4, $\bar{y},0$ [0,v,0]	3/4,y,1/2 [0, $\bar{v},0$ ]
8 c 2..	x,0,1/4 [u,0,0]	$\bar{x}+1/2,0,3/4$ [ $\bar{u},0,0$ ]	$\bar{x},0,3/4$ [u,0,0]	$x+1/2,0,1/4$ [ $\bar{u},0,0$ ]
8 b $\bar{1}$	1/4,1/4,1/4 [u,v,w]	1/4,3/4,3/4 [ $\bar{u},\bar{v},w$ ]	3/4,3/4,1/4 [ $\bar{u},v,\bar{w}$ ]	3/4,1/4,3/4 [ $u,\bar{v},\bar{w}$ ]
8 a $\bar{1}$	0,0,0 [u,v,w]	1/2,0,1/2 [ $\bar{u},\bar{v},w$ ]	0,1/2,1/2 [ $\bar{u},v,\bar{w}$ ]	1/2,1/2,0 [ $u,\bar{v},\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1]  $p_c$ -2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,1/4,z

Along [1,0,0]  $p_{2a}$ -2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,0

Along [0,1,0]  $p_{2a}$ -2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0

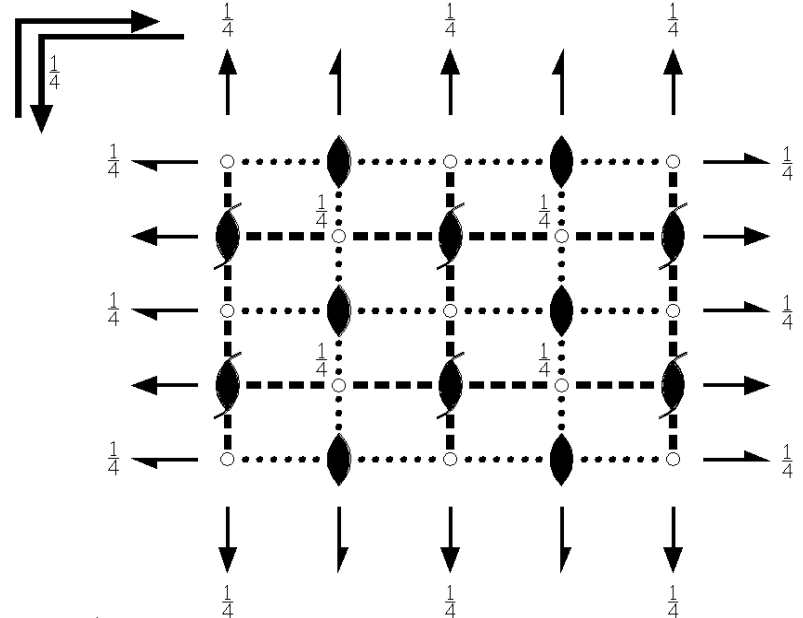
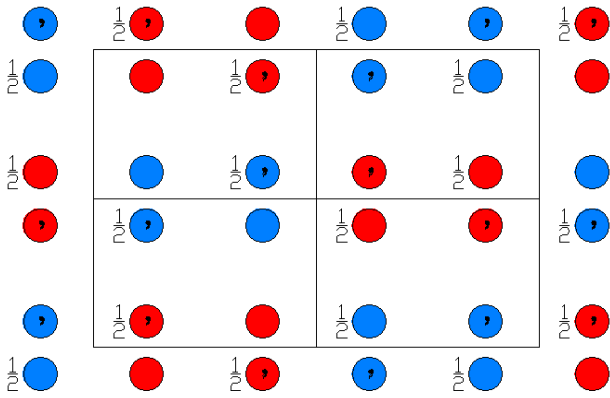


lbca1'  
73.2.644

mmm1'  
I2<sub>1</sub>/b2<sub>1</sub>/c2<sub>1</sub>/a1'

Orthorhombic

1'



Origin at  $\bar{1}1'$  at cab

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2) | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2) | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2) | (8) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                 | (2) 2 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,0)         | (3) 2 1/4,y,0<br>(2 <sub>y</sub>  1/2,0,0)         | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)         |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2) | (6) b (0,1/2,0) x,y,0<br>(m <sub>z</sub>  0,1/2,0) | (7) a (1/2,0,0) x,0,z<br>(m <sub>y</sub>  1/2,0,0) | (8) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) |

For (0,0,0)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1'<br>(1 0,0,0)'                          | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

For (1/2,1/2,1/2)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'                  | (2) 2' 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,0)'         | (3) 2' 1/4,y,0<br>(2 <sub>y</sub>  1/2,0,0)'         | (4) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'         |
| (5) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)' | (6) b' (0,1/2,0) x,y,0<br>(m <sub>z</sub>  0,1/2,0)' | (7) a' (1/2,0,0) x,0,z<br>(m <sub>y</sub>  1/2,0,0)' | (8) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

**Positions**

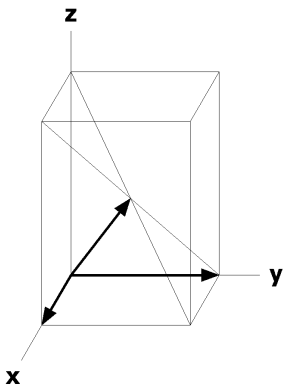
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) + (0,0,0)' +		(1/2,1/2,1/2) + (1/2,1/2,1/2)' +	
16	f 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [0,0,0]	(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [0,0,0]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [0,0,0]
		(5) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]	(6) $x+1/2, y, \bar{z}+1/2$ [0,0,0]	(7) $x, \bar{y}+1/2, z+1/2$ [0,0,0]	(8) $\bar{x}+1/2, y+1/2, z$ [0,0,0]
8	e ..21'	0,1/4,z [0,0,0]	0,3/4, $\bar{z}+1/2$ [0,0,0]	0,3/4, $\bar{z}$ [0,0,0]	0,1/4,z+1/2 [0,0,0]
8	d .2.1'	1/4,y,0 [0,0,0]	1/4, $\bar{y}, 1/2$ [0,0,0]	3/4, $\bar{y}, 0$ [0,0,0]	3/4,y,1/2 [0,0,0]
8	c 2..1'	x,0,1/4 [0,0,0]	$\bar{x}+1/2, 0, 3/4$ [0,0,0]	$\bar{x}, 0, 3/4$ [0,0,0]	x+1/2,0,1/4 [0,0,0]
8	b $\bar{1}1'$	1/4,1/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]
8	a $\bar{1}1'$	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

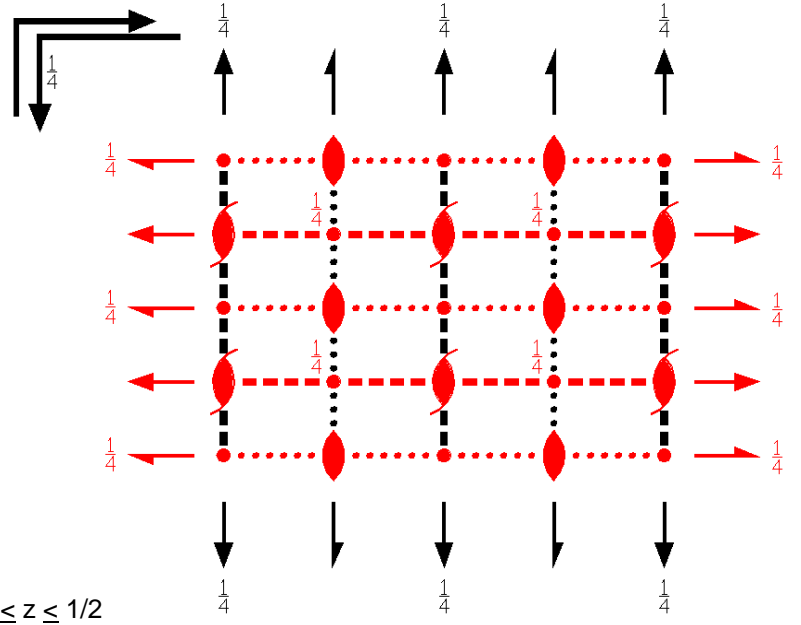
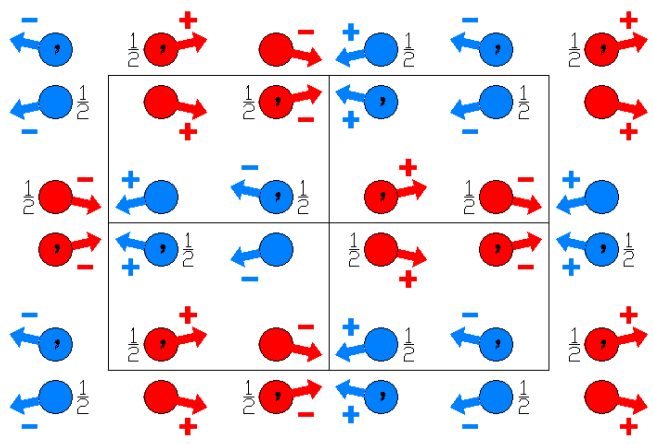
Along [0,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



lb'ca  
73.3.645

m'mm  
I2<sub>1</sub>/b'2<sub>1</sub>'/c2<sub>1</sub>'/a

Orthorhombic



Origin at  $\bar{1}$ ' at c'ab

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)   | (7) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)   | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

For (1/2,1/2,1/2) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                    | (2) 2' 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,0)'       | (3) 2' 1/4,y,0<br>(2 <sub>y</sub>  1/2,0,0)'       | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)           |
| (5) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)' | (6) b (0,1/2,0) x,y,0<br>(m <sub>z</sub>  0,1/2,0) | (7) a (1/2,0,0) x,0,z<br>(m <sub>y</sub>  1/2,0,0) | (8) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

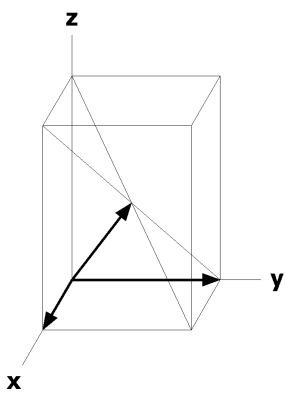
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 f 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [u,v, $\bar{w}$ ] (6) x+1/2,y, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x+1/2, $\bar{y}+1/2,\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]
8 e ..2'	0,1/4,z [u,v,0]	0,3/4, $\bar{z}+1/2$ [u, $\bar{v},0$ ]	0,3/4, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	0,1/4,z+1/2 [ $\bar{u},v,0$ ]
8 d .2'	1/4,y,0 [u,0,w]	1/4, $\bar{y},1/2$ [u,0, $\bar{w}$ ]	3/4, $\bar{y},0$ [ $\bar{u},0,\bar{w}$ ]	3/4,y,1/2 [ $\bar{u},0,w$ ]
8 c 2..	x,0,1/4 [u,0,0]	$\bar{x}+1/2,0,3/4$ [u,0,0]	$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x+1/2,0,1/4 [ $\bar{u},0,0$ ]
8 b $\bar{1}'$	1/4,1/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]
8 a $\bar{1}'$	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2a}2mm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $p2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [0,1,0]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



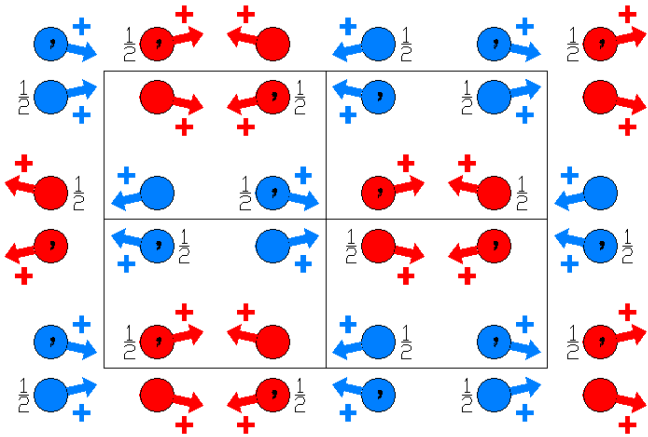
lb'c'a

73.4.646

m'm'm

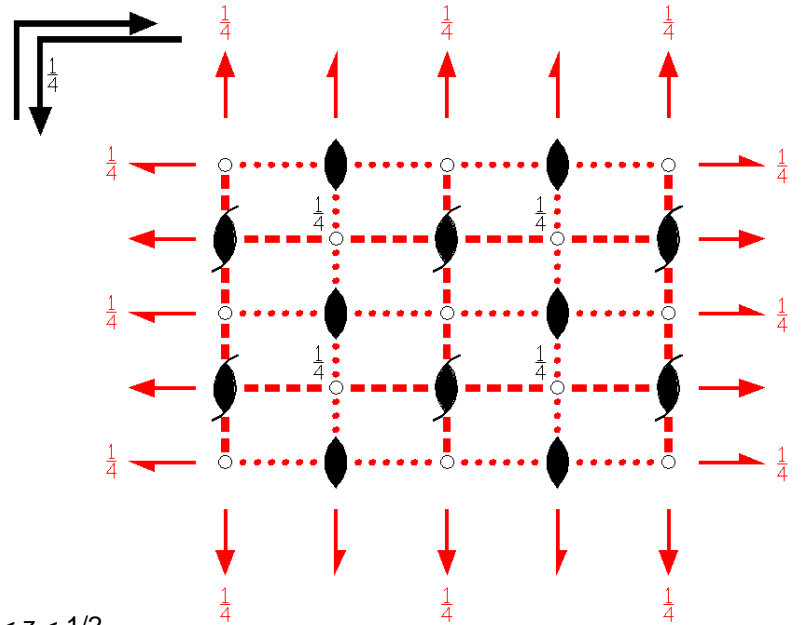
$I2_1'/b'2_1'/c'2_1/a$

Orthorhombic



Origin at  $\bar{1}$  at c'a'b

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$



**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2) | (3) 2' (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)' | (4) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2) | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                 | (2) 2 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,0)         | (3) 2' 1/4,y,0<br>(2 <sub>y</sub>  1/2,0,0)'         | (4) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'         |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2) | (6) b (0,1/2,0) x,y,0<br>(m <sub>z</sub>  0,1/2,0) | (7) a' (1/2,0,0) x,0,z<br>(m <sub>y</sub>  1/2,0,0)' | (8) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

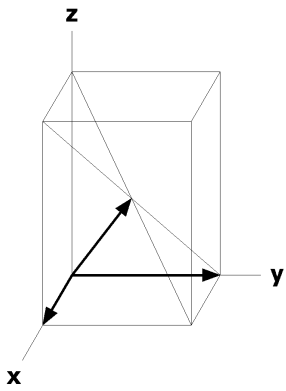
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 f 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ] (6) $x+1/2,y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [ $u,\bar{v},w$ ] (7) $x,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]
8 e ..2	0,1/4,z [0,0,w]	0,3/4, $\bar{z}+1/2$ [0,0,w]	0,3/4, $\bar{z}$ [0,0,w]	0,1/4,z+1/2 [0,0,w]
8 d .2'	1/4,y,0 [u,0,w]	1/4, $\bar{y},1/2$ [ $\bar{u},0,w$ ]	3/4, $\bar{y},0$ [u,0,w]	3/4,y,1/2 [ $\bar{u},0,w$ ]
8 c 2'..	x,0,1/4 [0,v,w]	$\bar{x}+1/2,0,3/4$ [0, $\bar{v},w$ ]	$\bar{x},0,3/4$ [0,v,w]	$x+1/2,0,1/4$ [0, $\bar{v},w$ ]
8 b $\bar{1}$	1/4,1/4,1/4 [u,v,w]	1/4,3/4,3/4 [ $\bar{u},\bar{v},w$ ]	3/4,3/4,1/4 [u, $\bar{v},w$ ]	3/4,1/4,3/4 [ $\bar{u},v,w$ ]
8 a $\bar{1}$	0,0,0 [u,v,w]	1/2,0,1/2 [ $\bar{u},\bar{v},w$ ]	0,1/2,1/2 [u, $\bar{v},w$ ]	1/2,1/2,0 [ $\bar{u},v,w$ ]

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,0,z

Along [1,0,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

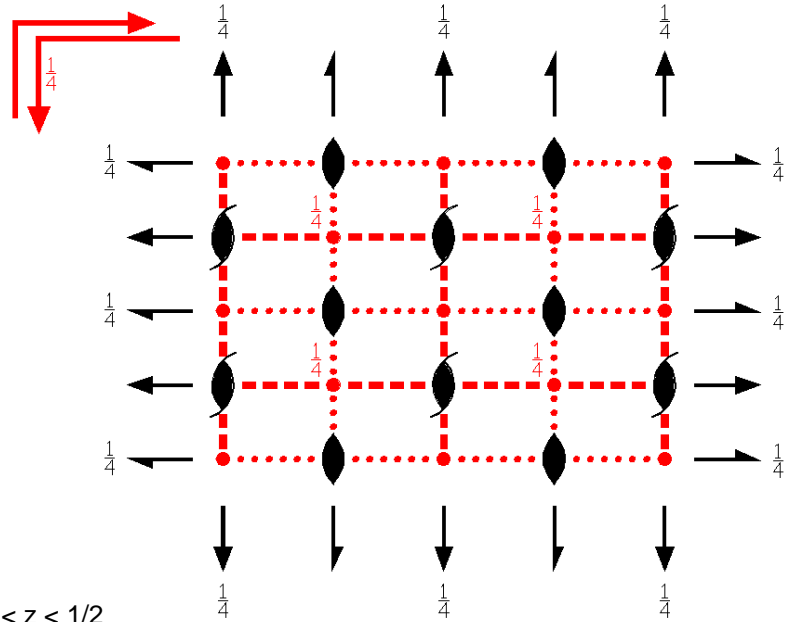
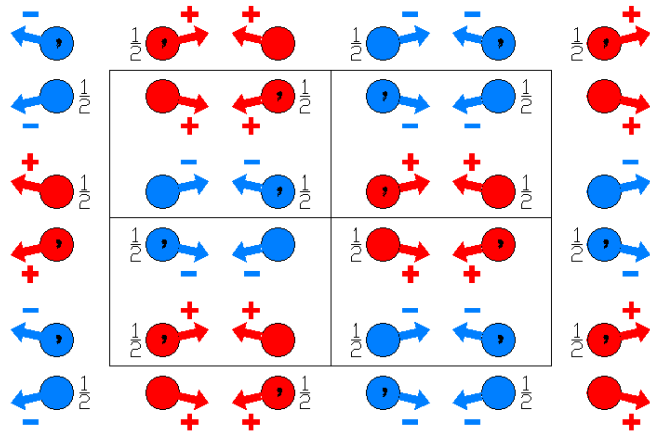
Along [0,1,0]  $p2'mm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



lb'c'a'  
73.5.647

m'm'm'  
I2<sub>1</sub>/b'2<sub>1</sub>/c'2<sub>1</sub>/a'

Orthorhombic



Origin at  $\bar{1}$ ' at cab

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)' | (7) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)' | (8) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' |

For (1/2,1/2,1/2) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                    | (2) 2 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,0)           | (3) 2 1/4,y,0<br>(2 <sub>y</sub>  1/2,0,0)           | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)           |
| (5) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)' | (6) b' (0,1/2,0) x,y,0<br>(m <sub>z</sub>  0,1/2,0)' | (7) a' (1/2,0,0) x,0,z<br>(m <sub>y</sub>  1/2,0,0)' | (8) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

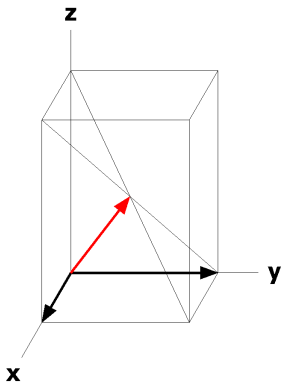
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +		(1/2,1/2,1/2) +	
16	f 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]
		(5) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(6) $x+1/2, y, \bar{z}+1/2$ [ $u, v, \bar{w}$ ]	(7) $x, \bar{y}+1/2, z+1/2$ [ $u, \bar{v}, w$ ]	(8) $\bar{x}+1/2, y+1/2, z$ [ $\bar{u}, v, w$ ]
8	e ..2	0,1/4,z [0,0,w]	0,3/4, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/4,z+1/2 [0,0,w]
8	d .2.	1/4,y,0 [0,v,0]	1/4, $\bar{y}, 1/2$ [0, $\bar{v}, 0$ ]	3/4, $\bar{y}, 0$ [0, $\bar{v}, 0$ ]	3/4,y,1/2 [0,v,0]
8	c 2..	x,0,1/4 [u,0,0]	$\bar{x}+1/2, 0, 3/4$ [ $\bar{u}, 0, 0$ ]	$\bar{x}, 0, 3/4$ [ $\bar{u}, 0, 0$ ]	x+1/2,0,1/4 [u,0,0]
8	b $\bar{1}'$	1/4,1/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]
8	a $\bar{1}'$	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

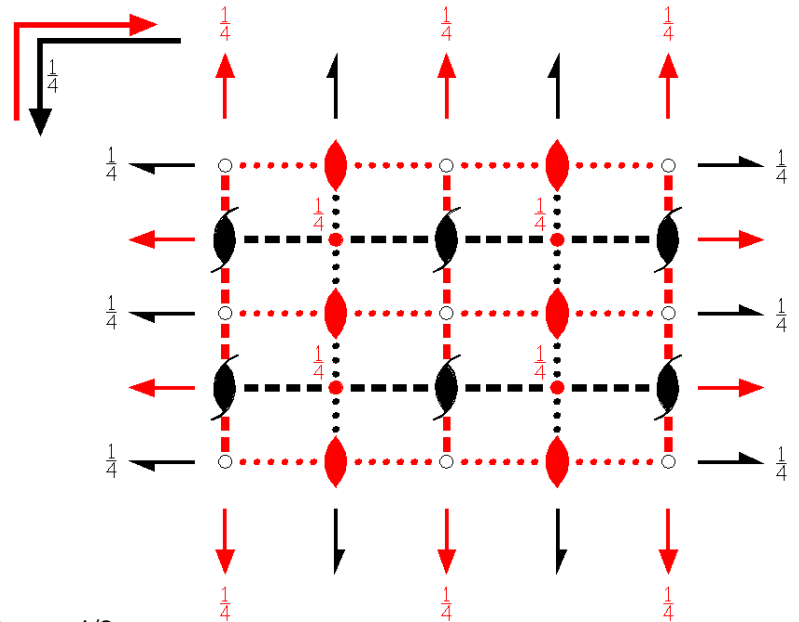
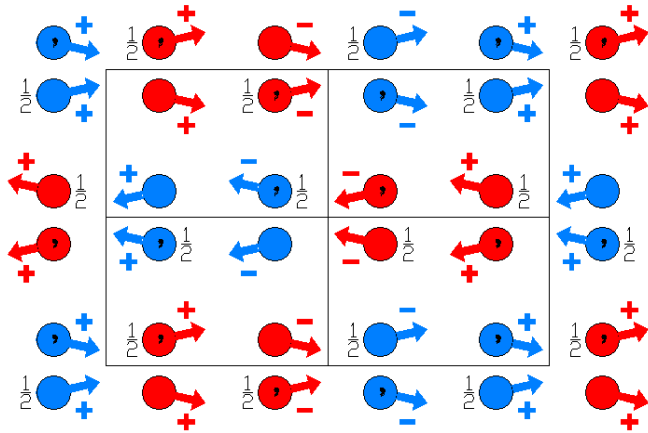
Along [0,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



$I_p bca$   
73.6.648

$mmm1'$   
 $I_p 2_1/b2_1/c2_1/a$

Orthorhombic



Origin at  $\bar{1}$  at  $c'a'b'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                               | (2) 2 $(0,0,1/2)$ $1/4,0,z$<br>( $2_z$   $1/2,0,1/2$ ) | (3) 2 $(0,1/2,0)$ $0,y,1/4$<br>( $2_y$   $0,1/2,1/2$ ) | (4) 2 $(1/2,0,0)$ $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ ) |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ ) | (6) a $(1/2,0,0)$ $x,y,1/4$<br>( $m_z$   $1/2,0,1/2$ ) | (7) c $(0,0,1/2)$ $x,1/4,z$<br>( $m_y$   $0,1/2,1/2$ ) | (8) b $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ ) |

For  $(1/2,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,1/2)$<br>(1  $1/2,1/2,1/2$ )'               | (2) $2'$ $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )'           | (3) $2'$ $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )'           | (4) $2'$ $x,0,1/4$<br>( $2_x$   $0,0,1/2$ )'           |
| (5) $\bar{1}'$ $1/4,1/4,1/4$<br>( $\bar{1}$   $1/2,1/2,1/2$ )' | (6) $b'$ $(0,1/2,0)$ $x,y,0$<br>( $m_z$   $0,1/2,0$ )' | (7) $a'$ $(1/2,0,0)$ $x,0,z$<br>( $m_y$   $1/2,0,0$ )' | (8) $c'$ $(0,0,1/2)$ $0,y,z$<br>( $m_x$   $0,0,1/2$ )' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

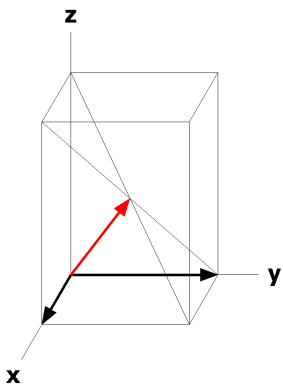
		Coordinates			
		(0,0,0) + (1/2,1/2,1/2)' +			
Multiplicity,	Wyckoff letter,				
Site Symmetry.					
16 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]	(5) $\bar{x}, \bar{y}, \bar{z}$ [ $u, v, w$ ]
	(5) $\bar{x}, \bar{y}, \bar{z}$ [ $u, v, w$ ]	(6) $x+1/2, y, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(7) $x, \bar{y}+1/2, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(8) $\bar{x}+1/2, y+1/2, z$ [ $u, \bar{v}, \bar{w}$ ]	
8 e .2'	0,1/4,z [u,v,0]	0,3/4, $\bar{z}+1/2$ [ $\bar{u}, v, 0$ ]	0,3/4, $\bar{z}$ [u,v,0]	0,1/4,z+1/2 [ $\bar{u}, v, 0$ ]	
8 d .2'	1/4,y,0 [u,0,w]	1/4, $\bar{y}, 1/2$ [ $\bar{u}, 0, w$ ]	3/4, $\bar{y}, 0$ [u,0,w]	3/4,y,1/2 [ $\bar{u}, 0, w$ ]	
8 c 2'..	x,0,1/4 [0,v,w]	$\bar{x}+1/2, 0, 3/4$ [0, $\bar{v}, w$ ]	$\bar{x}, 0, 3/4$ [0,v,w]	x+1/2,0,1/4 [0, $\bar{v}, w$ ]	
8 b $\bar{1}'$	1/4,1/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	
8 a $\bar{1}$	0,0,0 [u,v,w]	1/2,0,1/2 [ $\bar{u}, \bar{v}, w$ ]	0,1/2,1/2 [ $\bar{u}, v, \bar{w}$ ]	1/2,1/2,0 [ $u, \bar{v}, \bar{w}$ ]	

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2a}$ -2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,0,z

Along [1,0,0]  $p_{2a}$ -2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,0

Along [0,1,0]  $p_{2a}$ -2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,1/4



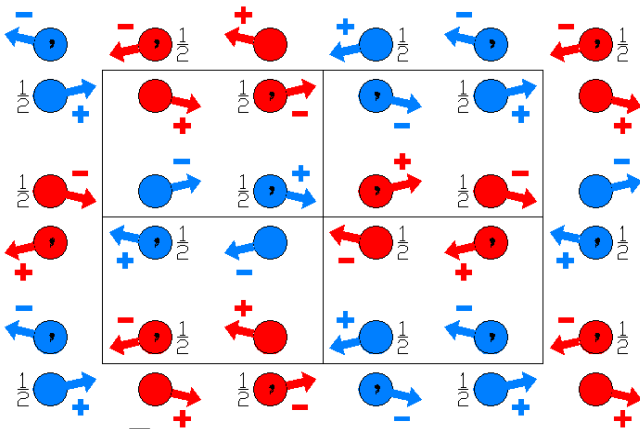
$I_p b'ca$

73.7.649

$mmm1'$

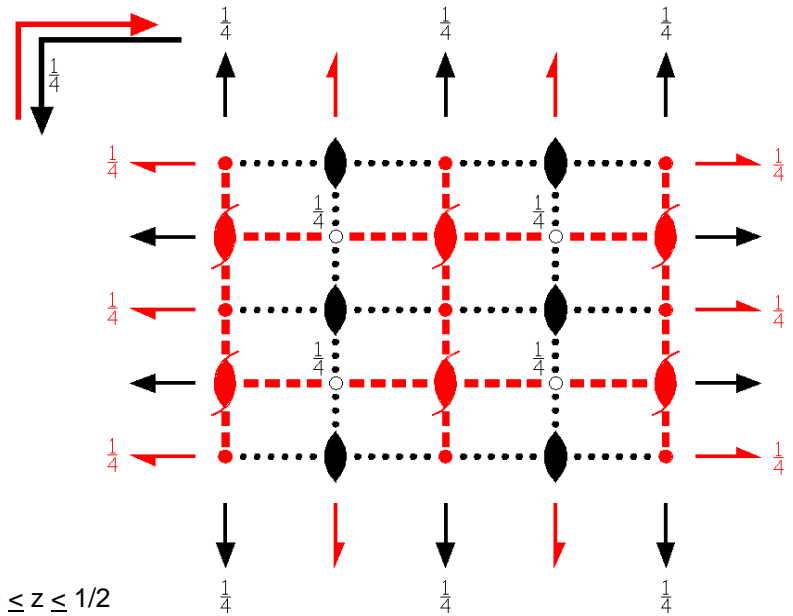
$I_p 2_1/b'2_1'/c2_1'/a$

Orthorhombic



Origin at  $\bar{1}'$  at  $ca'b'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$



### Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) $2' (0,0,1/2)$ $1/4,0,z$<br>( $2_z$   $1/2,0,1/2$ )' | (3) $2' (0,1/2,0)$ $0,y,1/4$<br>( $2_y$   $0,1/2,1/2$ )' | (4) $2 (1/2,0,0)$ $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )   |
| (5) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) a ( $1/2,0,0$ ) $x,y,1/4$<br>( $m_z$   $1/2,0,1/2$ ) | (7) c ( $0,0,1/2$ ) $x,1/4,z$<br>( $m_y$   $0,1/2,1/2$ ) | (8) $b' (0,1/2,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' |

For (1/2,1/2,1/2)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t' (1/2,1/2,1/2)$<br>(1  $1/2,1/2,1/2$ )'               | (2) $2$ $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )           | (3) $2$ $1/4,y,0$<br>( $2_y$   $1/2,0,0$ )           | (4) $2'$ $x,0,1/4$<br>( $2_x$   $0,0,1/2$ )'         |
| (5) $\bar{1}$ $1/4,1/4,1/4$<br>( $\bar{1}$   $1/2,1/2,1/2$ ) | (6) $b' (0,1/2,0)$ $x,y,0$<br>( $m_z$   $0,1/2,0$ )' | (7) $a' (1/2,0,0)$ $x,0,z$<br>( $m_y$   $1/2,0,0$ )' | (8) c ( $0,0,1/2$ ) $0,y,z$<br>( $m_x$   $0,0,1/2$ ) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

### Positions

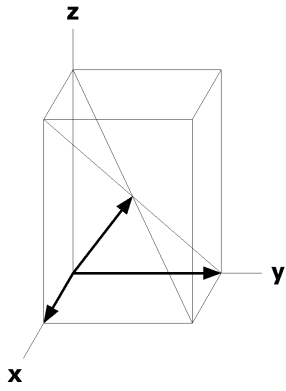
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
16 f 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [u,v, $\bar{w}$ ] (6) x+1/2,y, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [u, $\bar{v},w$ ] (7) x, $\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(4) x+1/2, $\bar{y}+1/2,\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]
8 e ..2	0,1/4,z [0,0,w]	0,3/4, $\bar{z}+1/2$ [0,0,w]	0,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/4,z+1/2 [0,0, $\bar{w}$ ]
8 d .2.	1/4,y,0 [0,v,0]	1/4, $\bar{y},1/2$ [0,v,0]	3/4, $\bar{y},0$ [0, $\bar{v},0$ ]	3/4,y,1/2 [0, $\bar{v},0$ ]
8 c 2'..	x,0,1/4 [0,v,w]	$\bar{x}+1/2,0,3/4$ [0,v, $\bar{w}$ ]	$\bar{x},0,3/4$ [0, $\bar{v},\bar{w}$ ]	x+1/2,0,1/4 [0, $\bar{v},w$ ]
8 b $\bar{1}$	1/4,1/4,1/4 [u,v,w]	1/4,3/4,3/4 [u,v, $\bar{w}$ ]	3/4,3/4,1/4 [u, $\bar{v},w$ ]	3/4,1/4,3/4 [u, $\bar{v},\bar{w}$ ]
8 a $\bar{1}'$	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p_{2a}2mm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

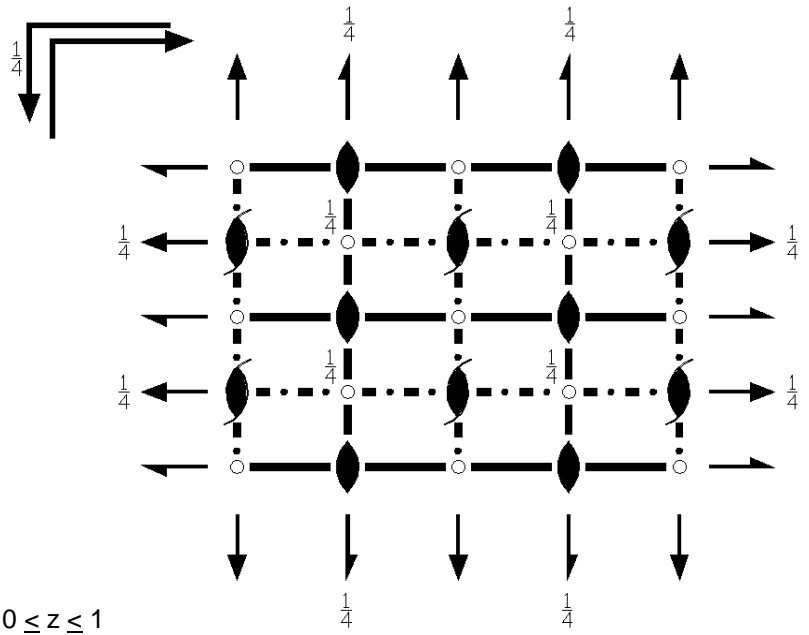
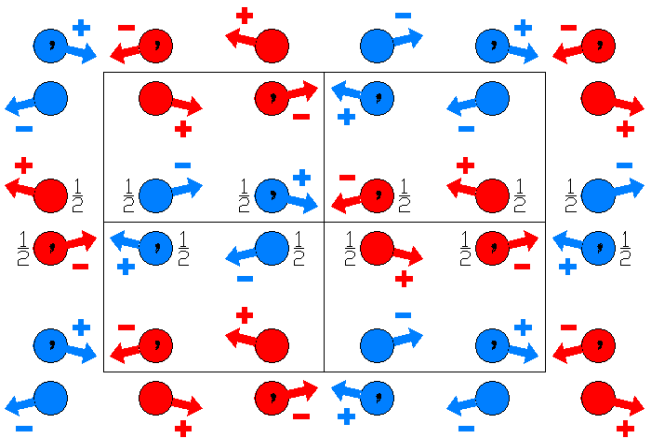
Along [0,1,0]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,y,0



**Imma**  
74.1.650

**mmm**  
 $I2_1/m2_1/m2_1/a$

**Orthorhombic**



**Origin at center (2/m) at  $2/m2_1/nb$**

**Asymmetric unit**  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1   0,0,0)                                 | (2) 2 $0, 1/4, z$<br>( $2_z$   $0, 1/2, 0$ )           | (3) 2 (0, 1/2, 0) $0, y, 0$<br>( $2_y$   $0, 1/2, 0$ ) | (4) 2 $x, 0, 0$<br>( $2_x$   $0, 0, 0$ ) |
| (5) $\bar{1}$ $0, 0, 0$<br>( $\bar{1}$   $0, 0, 0$ ) | (6) b (0, 1/2, 0) $x, y, 0$<br>( $m_z$   $0, 1/2, 0$ ) | (7) m $x, 1/4, z$<br>( $m_y$   $0, 1/2, 0$ )           | (8) m $0, y, z$<br>( $m_x$   $0, 0, 0$ ) |

For (1/2, 1/2, 1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2, 1/2, 1/2)<br>(1   1/2, 1/2, 1/2)                  | (2) 2 (0, 0, 1/2) $1/4, 0, z$<br>( $2_z$   1/2, 0, 1/2) | (3) 2 $1/4, y, 1/4$<br>( $2_y$   1/2, 0, 1/2)           | (4) 2 (1/2, 0, 0) $x, 1/4, 1/4$<br>( $2_x$   1/2, 1/2, 1/2) |
| (5) $\bar{1}$ $1/4, 1/4, 1/4$<br>( $\bar{1}$   1/2, 1/2, 1/2) | (6) a (1/2, 0, 0) $x, y, 1/4$<br>( $m_z$   1/2, 0, 1/2) | (7) n (1/2, 0, 1/2) $x, 0, z$<br>( $m_y$   1/2, 0, 1/2) | (8) n (0, 1/2, 1/2) $1/4, y, z$<br>( $m_x$   1/2, 1/2, 1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

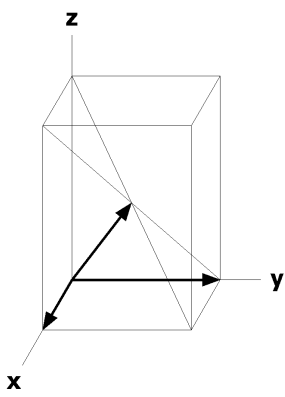
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 j 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y}+1/2,z$ [ $\bar{u},\bar{v},w$ ] (6) x,y+1/2, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 i .m.	x,1/4,z [0,v,0]	$\bar{x},1/4,z$ [0, $\bar{v},0$ ]	$\bar{x},3/4,\bar{z}$ [0,v,0]	x,3/4, $\bar{z}$ [0, $\bar{v},0$ ]
8 h m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z$ [ $\bar{u},0,0$ ]	0,y+1/2, $\bar{z}$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]
8 g .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y}+1/2,1/4$ [0, $\bar{v},0$ ]	3/4, $\bar{y},3/4$ [0,v,0]	1/4,y+1/2,3/4 [0, $\bar{v},0$ ]
8 f 2..	x,0,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	$\bar{x},0,0$ [u,0,0]	x,1/2,0 [ $\bar{u},0,0$ ]
4 e mm2	0,1/4,z [0,0,0]	0,3/4, $\bar{z}$ [0,0,0]		
4 d .2/m.	1/4,1/4,3/4 [0,v,0]	3/4,1/4,3/4 [0, $\bar{v},0$ ]		
4 c .2/m.	1/4,1/4,1/4 [0,v,0]	3/4,1/4,1/4 [0, $\bar{v},0$ ]		
4 b 2/m..	0,0,1/2 [u,0,0]	0,1/2,1/2 [ $\bar{u},0,0$ ]		
4 a 2/m..	0,0,0 [u,0,0]	0,1/2,0 [ $\bar{u},0,0$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2a}2mm$   
 $a^* = a/2$   $b^* = b/2$   
 Origin at 0,1/4,z

Along [1,0,0]  $c2mm1'$   
 $a^* = b$   $b^* = c$   
 Origin at x,1/4,1/4

Along [0,1,0]  $c2mm1'$   
 $a^* = c$   $b^* = a$   
 Origin at 0,y,0



Imma1'

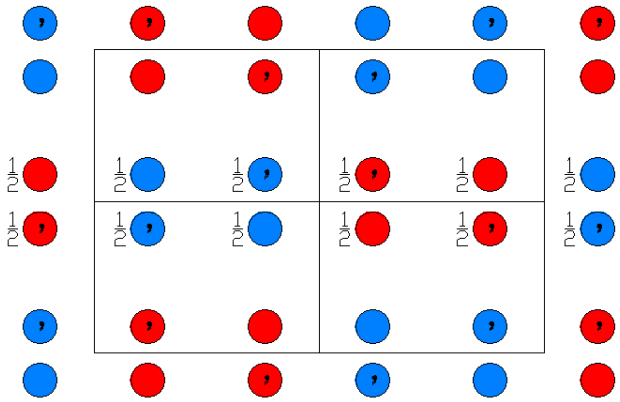
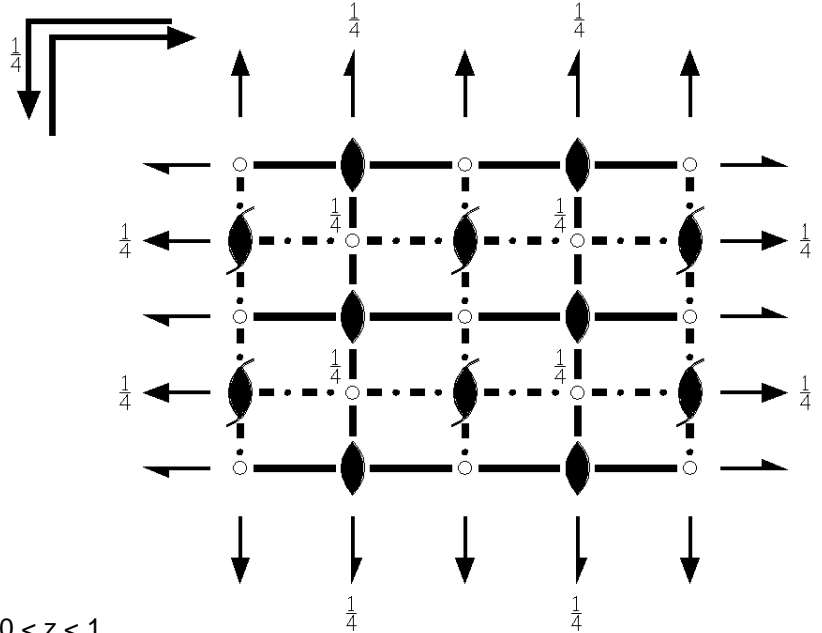
74.2.651

mmm1'

$I2_1/m2_1/m2_1/a1'$

Orthorhombic

1'



Origin at center ( $2/m1'$ ) at  $2/m2_1/nb1'$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |                                      |
|--|--|--|--------------------------------------|
| (1) 1<br>(1 0,0,0)                               | (2) 2 $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )         | (3) 2 (0,1/2,0) $0,y,0$<br>( $2_y$   $0,1/2,0$ ) | (4) 2 $x,0,0$<br>( $2_x$   $0,0,0$ ) |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   $0,0,0$ ) | (6) b (0,1/2,0) $x,y,0$<br>( $m_z$   $0,1/2,0$ ) | (7) m $x,1/4,z$<br>( $m_y$   $0,1/2,0$ )         | (8) m $0,y,z$<br>( $m_x$   $0,0,0$ ) |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                       | (2) 2 (0,0,1/2) $1/4,0,z$<br>( $2_z$   $1/2,0,1/2$ ) | (3) 2 $1/4,y,1/4$<br>( $2_y$   $1/2,0,1/2$ )         | (4) 2 (1/2,0,0) $x,1/4,1/4$<br>( $2_x$   $1/2,1/2,1/2$ ) |
| (5) $\bar{1}$ $1/4,1/4,1/4$<br>( $\bar{1}$   $1/2,1/2,1/2$ ) | (6) a (1/2,0,0) $x,y,1/4$<br>( $m_z$   $1/2,0,1/2$ ) | (7) n (1/2,0,1/2) $x,0,z$<br>( $m_y$   $1/2,0,1/2$ ) | (8) n (0,1/2,1/2) $1/4,y,z$<br>( $m_x$   $1/2,1/2,1/2$ ) |

For (0,0,0)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1'<br>(1 0,0,0)'                                | (2) 2' $0,1/4,z$<br>( $2_z$   $0,1/2,0$ )'         | (3) 2' (0,1/2,0) $0,y,0$<br>( $2_y$   $0,1/2,0$ )' | (4) 2' $x,0,0$<br>( $2_x$   $0,0,0$ )' |
| (5) $\bar{1}$ ' $0,0,0$<br>( $\bar{1}$   $0,0,0$ )' | (6) b' (0,1/2,0) $x,y,0$<br>( $m_z$   $0,1/2,0$ )' | (7) m' $x,1/4,z$<br>( $m_y$   $0,1/2,0$ )'         | (8) m' $0,y,z$<br>( $m_x$   $0,0,0$ )' |

For (1/2,1/2,1/2)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'                        | (2) 2' (0,0,1/2) $1/4,0,z$<br>( $2_z$   $1/2,0,1/2$ )' | (3) 2' $1/4,y,1/4$<br>( $2_y$   $1/2,0,1/2$ )'         | (4) 2' (1/2,0,0) $x,1/4,1/4$<br>( $2_x$   $1/2,1/2,1/2$ )' |
| (5) $\bar{1}$ ' $1/4,1/4,1/4$<br>( $\bar{1}$   $1/2,1/2,1/2$ )' | (6) a' (1/2,0,0) $x,y,1/4$<br>( $m_z$   $1/2,0,1/2$ )' | (7) n' (1/2,0,1/2) $x,0,z$<br>( $m_y$   $1/2,0,1/2$ )' | (8) n' (0,1/2,1/2) $1/4,y,z$<br>( $m_x$   $1/2,1/2,1/2$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

### Positions

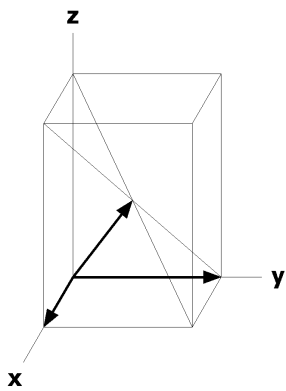
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'		
16 j 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y} + 1/2, z$ [0,0,0]	(3) $\bar{x}, y + 1/2, \bar{z}$ [0,0,0]	(4) x, $\bar{y}, \bar{z}$ [0,0,0]
	(5) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]	(6) x, y + 1/2, $\bar{z}$ [0,0,0]	(7) x, $\bar{y} + 1/2, z$ [0,0,0]	(8) $\bar{x}, y, z$ [0,0,0]
8 i .m.1'	x, 1/4, z [0,0,0]	$\bar{x}, 1/4, z$ [0,0,0]	$\bar{x}, 3/4, \bar{z}$ [0,0,0]	x, 3/4, $\bar{z}$ [0,0,0]
8 h m..1'	0, y, z [0,0,0]	0, $\bar{y} + 1/2, z$ [0,0,0]	0, y + 1/2, $\bar{z}$ [0,0,0]	0, $\bar{y}, \bar{z}$ [0,0,0]
8 g .2.1'	1/4, y, 1/4 [0,0,0]	3/4, $\bar{y} + 1/2, 1/4$ [0,0,0]	3/4, $\bar{y}, 3/4$ [0,0,0]	1/4, y + 1/2, 3/4 [0,0,0]
8 f 2..1'	x, 0, 0 [0,0,0]	$\bar{x}, 1/2, 0$ [0,0,0]	$\bar{x}, 0, 0$ [0,0,0]	x, 1/2, 0 [0,0,0]
4 e mm21'	0, 1/4, z [0,0,0]	0, 3/4, $\bar{z}$ [0,0,0]		
4 d .2/m.1'	1/4, 1/4, 3/4 [0,0,0]	3/4, 1/4, 3/4 [0,0,0]		
4 c .2/m.1'	1/4, 1/4, 1/4 [0,0,0]	3/4, 1/4, 1/4 [0,0,0]		
4 b 2/m..1'	0, 0, 1/2 [0,0,0]	0, 1/2, 1/2 [0,0,0]		
4 a 2/m..1'	0, 0, 0 [0,0,0]	0, 1/2, 0 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x, 1/4, 1/4

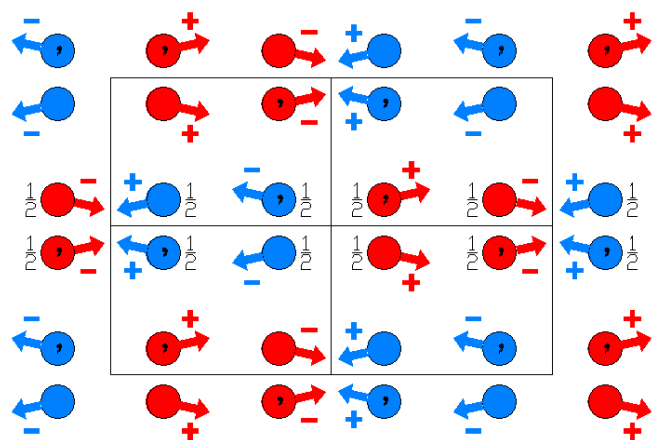
Along [0,1,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



Im'ma  
74.3.652

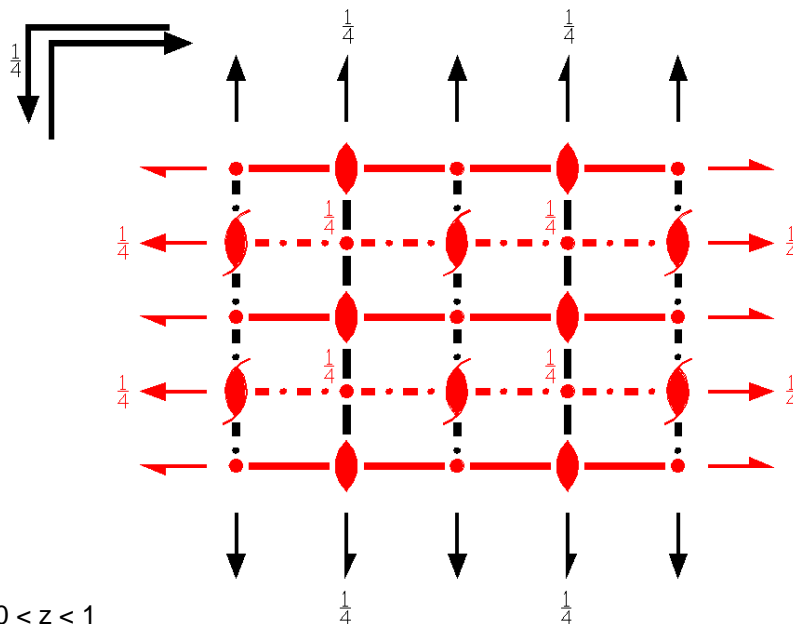
m'mm  
I2<sub>1</sub>/m'2<sub>1</sub>'/m2<sub>1</sub>'/a

Orthorhombic



Origin at center (2/m') at 2/m'2<sub>1</sub>'/nb

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$



**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2' 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,0)'       | (3) 2' (0,1/2,0) 0,y,0<br>(2 <sub>y</sub>  0,1/2,0)' | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) b (0,1/2,0) x,y,0<br>(m <sub>z</sub>  0,1/2,0) | (7) m x,1/4,z<br>(m <sub>y</sub>  0,1/2,0)           | (8) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' |

For (1/2,1/2,1/2) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                    | (2) 2' (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)' | (3) 2' 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)'       | (4) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)   |
| (5) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)' | (6) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)   | (7) n (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2) | (8) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

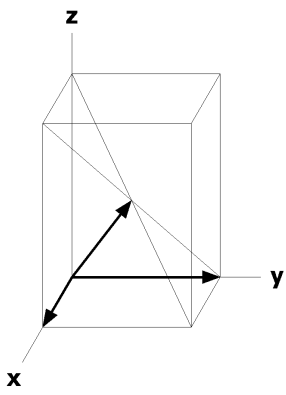
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 j 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y}+1/2,z$ [u,v, $\bar{w}$ ] (6) x,y+1/2, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 i .m.	x,1/4,z [0,v,0]	$\bar{x},1/4,z$ [0,v,0]	$\bar{x},3/4,\bar{z}$ [0, $\bar{v},0$ ]	x,3/4, $\bar{z}$ [0, $\bar{v},0$ ]
8 h m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z$ [0,v, $\bar{w}$ ]	0,y+1/2, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 g .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,1/4$ [u,0, $\bar{w}$ ]	3/4, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,3/4 [ $\bar{u},0,w$ ]
8 f 2..	x,0,0 [u,0,0]	$\bar{x},1/2,0$ [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	x,1/2,0 [ $\bar{u},0,0$ ]
4 e m'm2'	0,1/4,z [0,v,0]	0,3/4, $\bar{z}$ [0, $\bar{v},0$ ]		
4 d .2'/m.	1/4,1/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]		
4 c .2'/m.	1/4,1/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]		
4 b 2/m'..	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 a 2/m'..	0,0,0 [0,0,0]	0,1/2,0 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = -\mathbf{b}^*/2$   $\mathbf{b}^* = \mathbf{a}^*/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2mm$   
 $\mathbf{a}^* = \mathbf{b}^*$   $\mathbf{b}^* = \mathbf{c}^*$   
 Origin at x,1/4,1/4

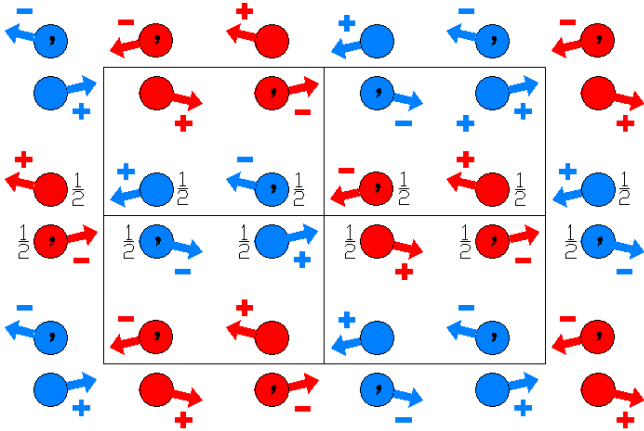
Along [0,1,0]  $c2mm1'$   
 $\mathbf{a}^* = \mathbf{c}^*$   $\mathbf{b}^* = \mathbf{a}^*$   
 Origin at 0,y,0



$Imma'$   
74.4.653

$mmm'$   
 $I2_1'/m2_1'/m2_1'/a'$

Orthorhombic



Origin at center ( $2'/m$ ) at  $2'/m2_1'/nb'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

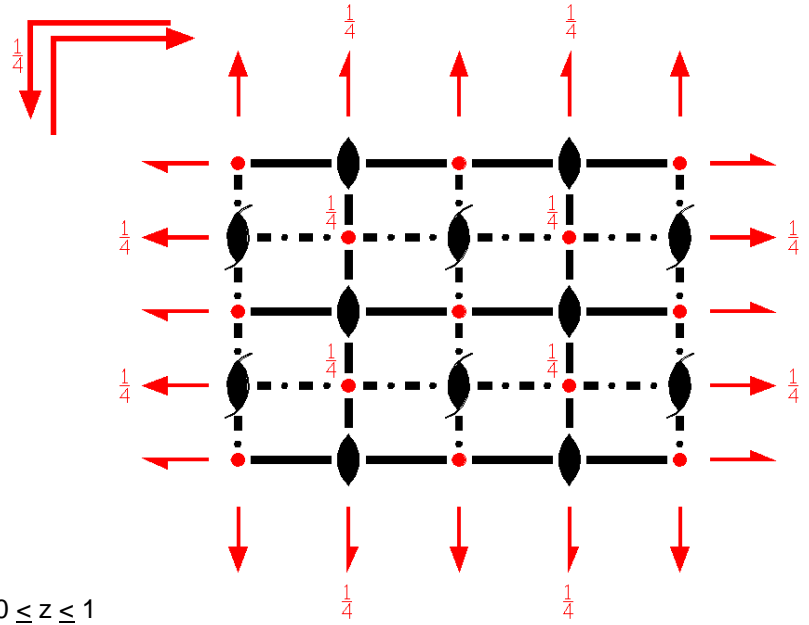
**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |                                    |
|---|--|--|------------------------------------|
| (1) 1<br>(1 0,0,0)                              | (2) 2 $0,1/4,z$<br>( $2_z$  0,1/2,0)             | (3) 2' (0,1/2,0) $0,y,0$<br>( $2_y$  0,1/2,0)' | (4) 2' $x,0,0$<br>( $2_x$  0,0,0)' |
| (5) $\bar{1}$ ' $0,0,0$<br>( $\bar{1}$  0,0,0)' | (6) $b'$ (0,1/2,0) $x,y,0$<br>( $m_z$  0,1/2,0)' | (7) $m$ $x,1/4,z$<br>( $m_y$  0,1/2,0)         | (8) $m$ $0,y,z$<br>( $m_x$  0,0,0) |

For (1/2,1/2,1/2) + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t$ (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                    | (2) 2 (0,0,1/2) $1/4,0,z$<br>( $2_z$  1/2,0,1/2)     | (3) 2' $1/4,y,1/4$<br>( $2_y$  1/2,0,1/2)'         | (4) 2' (1/2,0,0) $x,1/4,1/4$<br>( $2_x$  1/2,1/2,1/2)' |
| (5) $\bar{1}$ ' $1/4,1/4,1/4$<br>( $\bar{1}$  1/2,1/2,1/2)' | (6) $a'$ (1/2,0,0) $x,y,1/4$<br>( $m_z$  1/2,0,1/2)' | (7) $n$ (1/2,0,1/2) $x,0,z$<br>( $m_y$  1/2,0,1/2) | (8) $n$ (0,1/2,1/2) $1/4,y,z$<br>( $m_x$  1/2,1/2,1/2) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

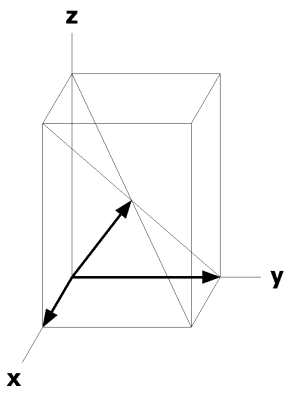
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(1/2,1/2,1/2) +	
16 j 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y}+1/2,z$ [ $\bar{u},\bar{v},w$ ] (6) x,y+1/2, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 i .m.	x,1/4,z [0,v,0]	$\bar{x},1/4,z$ [0, $\bar{v},0$ ]	$\bar{x},3/4,\bar{z}$ [0, $\bar{v},0$ ]	x,3/4, $\bar{z}$ [0,v,0]
8 h m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z$ [ $\bar{u},0,0$ ]	0,y+1/2, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]
8 g .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,1/4$ [ $\bar{u},0,w$ ]	3/4, $\bar{y},3/4$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,3/4 [u,0, $\bar{w}$ ]
8 f 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,0$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0, $\bar{v},\bar{w}$ ]	x,1/2,0 [0,v, $\bar{w}$ ]
4 e mm2	0,1/4,z [0,0,0]	0,3/4, $\bar{z}$ [0,0,0]		
4 d .2'/m.	1/4,1/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]		
4 c .2'/m.	1/4,1/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]		
4 b 2'/m..	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 a 2'/m..	0,0,0 [0,0,0]	0,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [0,1,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



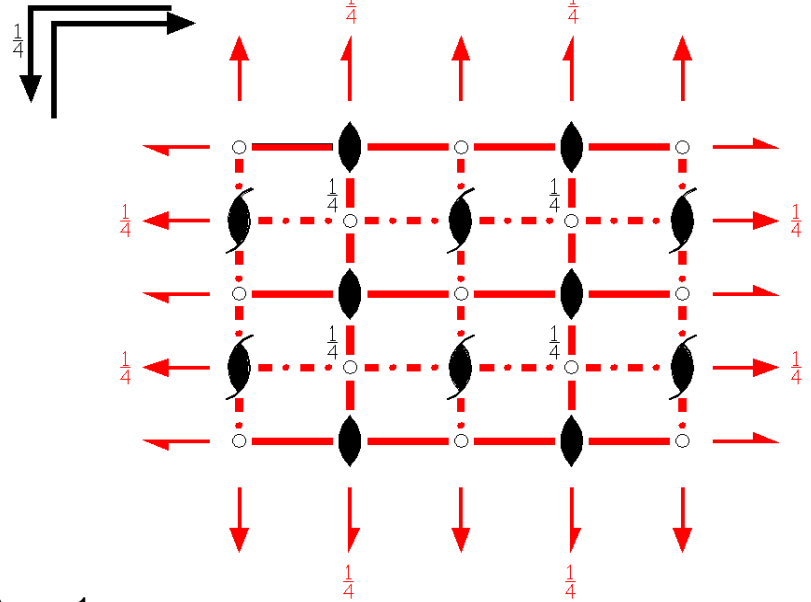
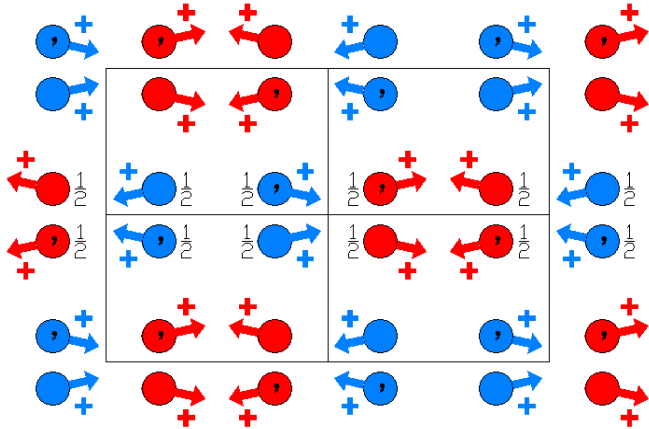
$Im'm'a$

74.5.654

$m'm'm$

$I2_1'/m'2_1'/m'2_1'/a$

Orthorhombic



Origin at center ( $2'/m'$ ) at  $2'/m'2_1'/n'b$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |                                     |
|---|---|---|-------------------------------------|
| (1) 1<br>(1   0,0,0)                          | (2) 2 $0,1/4,z$<br>( $2_z$   0,1/2,0)           | (3) $2' (0,1/2,0)$ $0,y,0$<br>( $2_y$   0,1/2,0)' | (4) $2' x,0,0$<br>( $2_x$   0,0,0)' |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$   0,0,0) | (6) b $(0,1/2,0)$ $x,y,0$<br>( $m_z$   0,1/2,0) | (7) $m' x,1/4,z$<br>( $m_y$   0,1/2,0)'           | (8) $m' 0,y,z$<br>( $m_x$   0,0,0)' |

For (1/2,1/2,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t $(1/2,1/2,1/2)$<br>(1   1/2,1/2,1/2)                | (2) 2 $(0,0,1/2)$ $1/4,0,z$<br>( $2_z$   1/2,0,1/2) | (3) $2' 1/4,y,1/4$<br>( $2_y$   1/2,0,1/2)'           | (4) $2' (1/2,0,0)$ $x,1/4,1/4$<br>( $2_x$   1/2,1/2,1/2)' |
| (5) $\bar{1}$ $1/4,1/4,1/4$<br>( $\bar{1}$   1/2,1/2,1/2) | (6) a $(1/2,0,0)$ $x,y,1/4$<br>( $m_z$   1/2,0,1/2) | (7) $n' (1/2,0,1/2)$ $x,0,z$<br>( $m_y$   1/2,0,1/2)' | (8) $n' (0,1/2,1/2)$ $1/4,y,z$<br>( $m_x$   1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

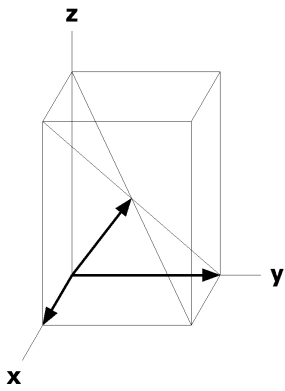
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 j 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y}+1/2,z$ [ $\bar{u},\bar{v},w$ ] (6) x,y+1/2, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y+1/2,\bar{z}$ [u, $\bar{v},w$ ] (7) x, $\bar{y}+1/2,z$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 i .m'	x,1/4,z [u,0,w]	$\bar{x},1/4,z$ [ $\bar{u},0,w$ ]	$\bar{x},3/4,\bar{z}$ [u,0,w]	x,3/4, $\bar{z}$ [ $\bar{u},0,w$ ]
8 h m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z$ [0, $\bar{v},w$ ]	0,y+1/2, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
8 g .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,1/4$ [ $\bar{u},0,w$ ]	3/4, $\bar{y},3/4$ [u,0,w]	1/4,y+1/2,3/4 [ $\bar{u},0,w$ ]
8 f 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,0$ [0, $\bar{v},w$ ]	$\bar{x},0,0$ [0,v,w]	x,1/2,0 [0, $\bar{v},w$ ]
4 e m'm'2	0,1/4,z [0,0,w]	0,3/4, $\bar{z}$ [0,0,w]		
4 d .2'/m'	1/4,1/4,3/4 [u,0,w]	3/4,1/4,3/4 [ $\bar{u},0,w$ ]		
4 c .2'/m'	1/4,1/4,1/4 [u,0,w]	3/4,1/4,1/4 [ $\bar{u},0,w$ ]		
4 b 2'/m'..	0,0,1/2 [0,v,w]	0,1/2,1/2 [0, $\bar{v},w$ ]		
4 a 2'/m'..	0,0,0 [0,v,w]	0,1/2,0 [0, $\bar{v},w$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_{2a}2m'm'$   
 $a^* = a/2$   $b^* = b/2$   
 Origin at 0,1/4,z

Along [1,0,0]  $c2'mm'$   
 $a^* = -c$   $b^* = b$   
 Origin at x,1/4,1/4

Along [0,1,0]  $c2'mm'$   
 $a^* = c$   $b^* = a$   
 Origin at 0,y,0



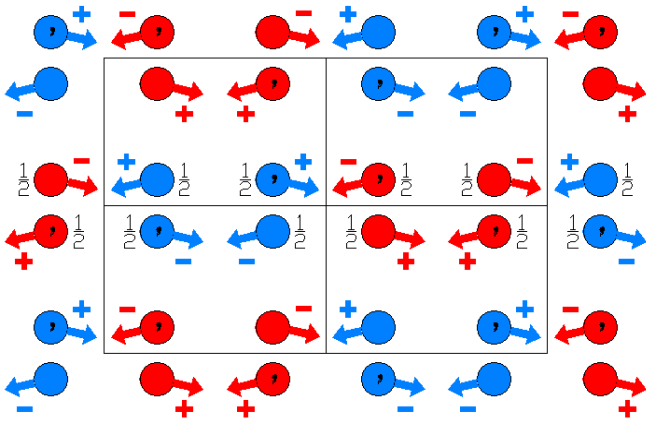
Imm'a'

74.6.655

mm'm'

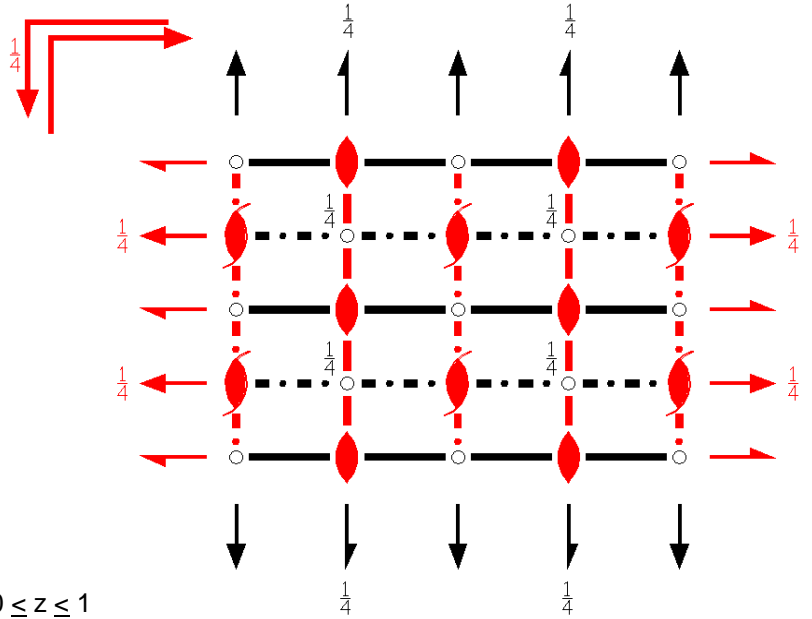
$I2_1/m2_1/m'2_1/a'$

Orthorhombic



Origin at center ( $2/m$ ) at  $2/m2_1/n'b'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$



**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                   | (2) $2'$ $0, 1/4, z$<br>( $2_z$   $0, 1/2, 0$ )'             | (3) $2'$ $(0, 1/2, 0)$ $0, y, 0$<br>( $2_y$   $0, 1/2, 0$ )' | (4) $2$ $x, 0, 0$<br>( $2_x$   $0, 0, 0$ ) |
| (5) $\bar{1}$ $0, 0, 0$<br>( $\bar{1}$   $0, 0, 0$ ) | (6) $b'$ $(0, 1/2, 0)$ $x, y, 0$<br>( $m_z$   $0, 1/2, 0$ )' | (7) $m'$ $x, 1/4, z$<br>( $m_y$   $0, 1/2, 0$ )'             | (8) $m$ $0, y, z$<br>( $m_x$   $0, 0, 0$ ) |

For (1/2, 1/2, 1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t$ $(1/2, 1/2, 1/2)$<br>(1  $1/2, 1/2, 1/2$ )               | (2) $2'$ $(0, 0, 1/2)$ $1/4, 0, z$<br>( $2_z$   $1/2, 0, 1/2$ )' | (3) $2'$ $1/4, y, 1/4$<br>( $2_y$   $1/2, 0, 1/2$ )'             | (4) $2$ $(1/2, 0, 0)$ $x, 1/4, 1/4$<br>( $2_x$   $1/2, 1/2, 1/2$ ) |
| (5) $\bar{1}$ $1/4, 1/4, 1/4$<br>( $\bar{1}$   $1/2, 1/2, 1/2$ ) | (6) $a'$ $(1/2, 0, 0)$ $x, y, 1/4$<br>( $m_z$   $1/2, 0, 1/2$ )' | (7) $n'$ $(1/2, 0, 1/2)$ $x, 0, z$<br>( $m_y$   $1/2, 0, 1/2$ )' | (8) $n$ $(0, 1/2, 1/2)$ $1/4, y, z$<br>( $m_x$   $1/2, 1/2, 1/2$ ) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

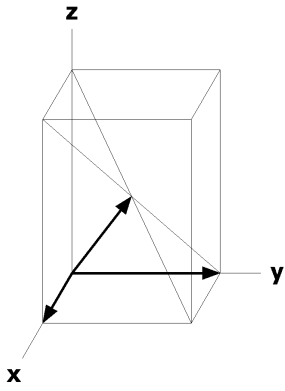
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 j 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y}+1/2,z$ [u,v, $\bar{w}$ ] (6) x,y+1/2, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}$ [u, $\bar{v}$ ,w] (7) x, $\bar{y}+1/2,z$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 i .m'	x,1/4,z [u,0,w]	$\bar{x},1/4,z$ [u,0, $\bar{w}$ ]	$\bar{x},3/4,\bar{z}$ [u,0,w]	x,3/4, $\bar{z}$ [u,0, $\bar{w}$ ]
8 h m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z$ [u,0,0]	0,y+1/2, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [u,0,0]
8 g .2'	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,1/4$ [u,v, $\bar{w}$ ]	3/4, $\bar{y},3/4$ [u,0,w]	1/4,y+1/2,3/4 [u,v, $\bar{w}$ ]
8 f 2..	x,0,0 [u,0,0]	$\bar{x},1/2,0$ [u,0,0]	$\bar{x},0,0$ [u,0,0]	x,1/2,0 [u,0,0]
4 e mm'2'	0,1/4,z [u,0,0]	0,3/4, $\bar{z}$ [u,0,0]		
4 d .2'/m'	1/4,1/4,3/4 [u,0,w]	3/4,1/4,3/4 [u,0, $\bar{w}$ ]		
4 c .2'/m'	1/4,1/4,1/4 [u,0,w]	3/4,1/4,1/4 [u,0, $\bar{w}$ ]		
4 b 2/m..	0,0,1/2 [u,0,0]	0,1/2,1/2 [u,0,0]		
4 a 2/m..	0,0,0 [u,0,0]	0,1/2,0 [u,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [0,1,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



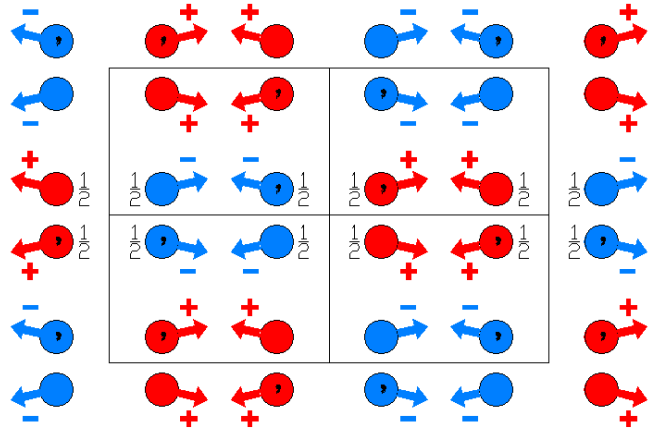
$Im'm'a'$

74.7.656

$m'm'm'$

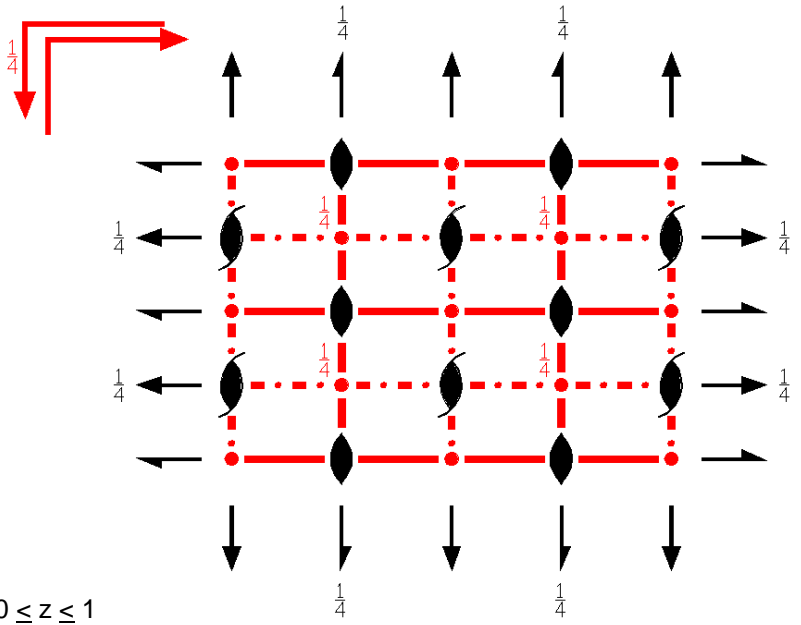
$I2_1/m'2_1/m'2_1/a'$

Orthorhombic



Origin at center ( $2/m'$ ) at  $2/m'2_1/n'b'$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$



**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 $0, 1/4, z$<br>( $2_z$   $0, 1/2, 0$ )             | (3) 2 (0,1/2,0) $0, y, 0$<br>( $2_y$   $0, 1/2, 0$ ) | (4) 2 $x, 0, 0$<br>( $2_x$   $0, 0, 0$ )     |
| (5) $\bar{1}'$ $0, 0, 0$<br>( $\bar{1}$   $0, 0, 0$ )' | (6) $b'$ (0,1/2,0) $x, y, 0$<br>( $m_z$   $0, 1/2, 0$ )' | (7) $m'$ $x, 1/4, z$<br>( $m_y$   $0, 1/2, 0$ )'     | (8) $m'$ $0, y, z$<br>( $m_x$   $0, 0, 0$ )' |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t$ (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                           | (2) 2 (0,0,1/2) $1/4, 0, z$<br>( $2_z$   $1/2, 0, 1/2$ )     | (3) 2 $1/4, y, 1/4$<br>( $2_y$   $1/2, 0, 1/2$ )             | (4) 2 (1/2,0,0) $x, 1/4, 1/4$<br>( $2_x$   $1/2, 1/2, 1/2$ )     |
| (5) $\bar{1}'$ $1/4, 1/4, 1/4$<br>( $\bar{1}$   $1/2, 1/2, 1/2$ )' | (6) $a'$ (1/2,0,0) $x, y, 1/4$<br>( $m_z$   $1/2, 0, 1/2$ )' | (7) $n'$ (1/2,0,1/2) $x, 0, z$<br>( $m_y$   $1/2, 0, 1/2$ )' | (8) $n'$ (0,1/2,1/2) $1/4, y, z$<br>( $m_x$   $1/2, 1/2, 1/2$ )' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

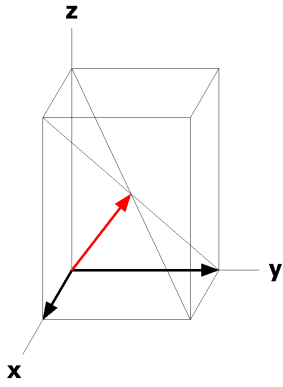
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 j 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y}+1/2,z$ [ $\bar{u},\bar{v},w$ ] (6) x,y+1/2, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ] (7) x, $\bar{y}+1/2,z$ [u, $\bar{v},w$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [u, $\bar{v},w$ ]
8 i .m'	x,1/4,z [u,0,w]	$\bar{x},1/4,z$ [ $\bar{u},0,w$ ]	$\bar{x},3/4,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	x,3/4, $\bar{z}$ [u,0, $\bar{w}$ ]
8 h m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z$ [0, $\bar{v},w$ ]	0,y+1/2, $\bar{z}$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]
8 g .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y}+1/2,1/4$ [0, $\bar{v},0$ ]	3/4, $\bar{y},3/4$ [0, $\bar{v},0$ ]	1/4,y+1/2,3/4 [0,v,0]
8 f 2..	x,0,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	x,1/2,0 [u,0,0]
4 e m'm'2	0,1/4,z [0,0,w]	0,3/4, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 d .2/m'	1/4,1/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]		
4 c .2/m'	1/4,1/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]		
4 b 2/m'..	0,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
4 a 2/m'..	0,0,0 [0,0,0]	0,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [0,1,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



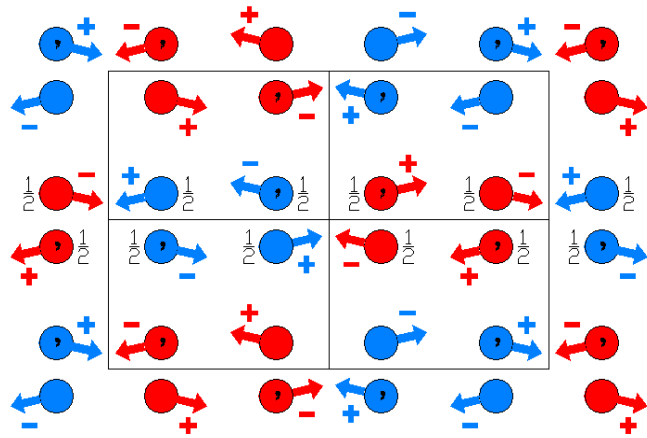
$I_p m m a$

74.8.657

$m m m 1'$

$I_p 2_1/m 2_1/m 2_1/a$

Orthorhombic



Origin at center ( $2/m$ ) at  $2/m 2_1/n'$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

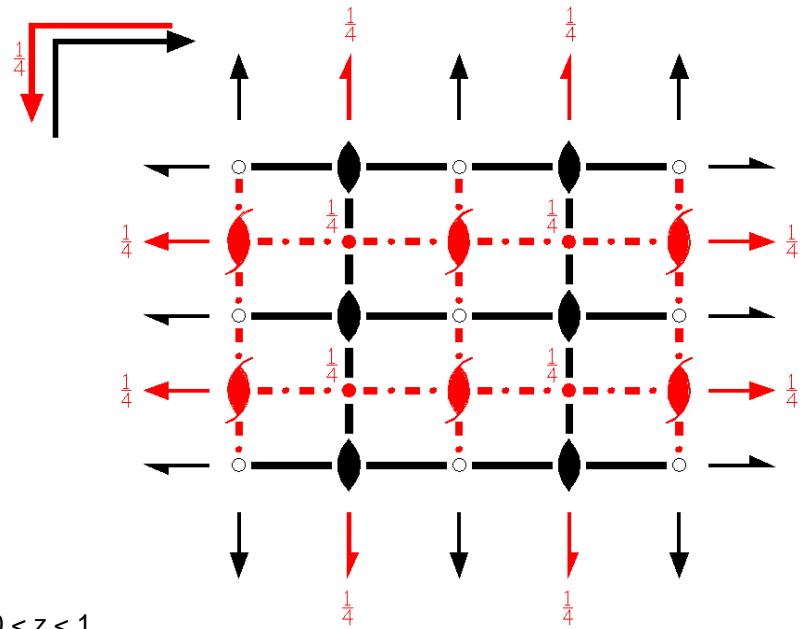
**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                              | (2) 2 $0, 1/4, z$<br>( $2_z$   0, 1/2, 0)               | (3) 2 $(0, 1/2, 0)$ $0, y, 0$<br>( $2_y$   0, 1/2, 0) | (4) 2 $x, 0, 0$<br>( $2_x$   0, 0, 0)   |
| (5) $\bar{1}$ $0, 0, 0$<br>( $\bar{1}$   0, 0, 0) | (6) $b$ $(0, 1/2, 0)$ $x, y, 0$<br>( $m_z$   0, 1/2, 0) | (7) $m$ $x, 1/4, z$<br>( $m_y$   0, 1/2, 0)           | (8) $m$ $0, y, z$<br>( $m_x$   0, 0, 0) |

For  $(1/2, 1/2, 1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2, 1/2, 1/2)$<br>(1   $1/2, 1/2, 1/2$ )'              | (2) $2'$ $(0, 0, 1/2)$ $1/4, 0, z$<br>( $2_z$   $1/2, 0, 1/2$ )' | (3) $2'$ $1/4, y, 1/4$<br>( $2_y$   $1/2, 0, 1/2$ )'             | (4) $2'$ $(1/2, 0, 0)$ $x, 1/4, 1/4$<br>( $2_x$   $1/2, 1/2, 1/2$ )' |
| (5) $\bar{1}'$ $1/4, 1/4, 1/4$<br>( $\bar{1}$   $1/2, 1/2, 1/2$ )' | (6) $a'$ $(1/2, 0, 0)$ $x, y, 1/4$<br>( $m_z$   $1/2, 0, 1/2$ )' | (7) $n'$ $(1/2, 0, 1/2)$ $x, 0, z$<br>( $m_y$   $1/2, 0, 1/2$ )' | (8) $n'$ $(0, 1/2, 1/2)$ $1/4, y, z$<br>( $m_x$   $1/2, 1/2, 1/2$ )' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

### Positions

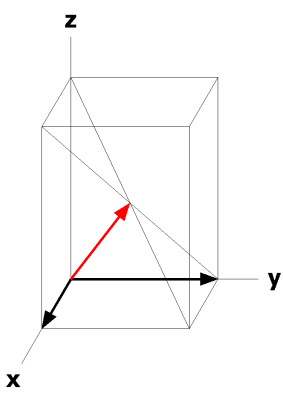
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
16 j 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y}+1/2,z [\bar{u},\bar{v},w]$	(3) $\bar{x},y+1/2,\bar{z} [\bar{u},v,\bar{w}]$	(4) $x,\bar{y},\bar{z} [u,\bar{v},\bar{w}]$
	(5) $\bar{x},\bar{y},\bar{z} [u,v,w]$	(6) $x,y+1/2,\bar{z} [\bar{u},\bar{v},w]$	(7) $x,\bar{y}+1/2,z [\bar{u},v,\bar{w}]$	(8) $\bar{x},y,z [u,\bar{v},\bar{w}]$
8 i .m.	x,1/4,z [0,v,0]	$\bar{x},1/4,z [0,\bar{v},0]$	$\bar{x},3/4,\bar{z} [0,v,0]$	$x,3/4,\bar{z} [0,\bar{v},0]$
8 h m..	0,y,z [u,0,0]	$0,\bar{y}+1/2,z [\bar{u},0,0]$	$0,y+1/2,\bar{z} [\bar{u},0,0]$	$0,\bar{y},\bar{z} [u,0,0]$
8 g .2'	1/4,y,1/4 [u,0,w]	$3/4,\bar{y}+1/2,1/4 [\bar{u},0,w]$	$3/4,\bar{y},3/4 [\bar{u},0,\bar{w}]$	$1/4,y+1/2,3/4 [u,0,\bar{w}]$
8 f 2..	x,0,0 [u,0,0]	$\bar{x},1/2,0 [\bar{u},0,0]$	$\bar{x},0,0 [u,0,0]$	$x,1/2,0 [\bar{u},0,0]$
4 e mm2	0,1/4,z [0,0,0]	$0,3/4,\bar{z} [0,0,0]$		
4 d .2'/m.	1/4,1/4,3/4 [0,0,0]	$3/4,1/4,3/4 [0,0,0]$		
4 c .2'/m.	1/4,1/4,1/4 [0,0,0]	$3/4,1/4,1/4 [0,0,0]$		
4 b 2/m..	0,0,1/2 [u,0,0]	$0,1/2,1/2 [\bar{u},0,0]$		
4 a 2/m..	0,0,0 [u,0,0]	$0,1/2,0 [\bar{u},0,0]$		

### Symmetry of Special Projections

Along [0,0,1]  $p_{2a}$ -2mm  
 $\mathbf{a}^* = -\mathbf{b}/2$   $\mathbf{b}^* = \mathbf{a}/2$   
 Origin at 0,1/4,z

Along [1,0,0]  $c2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [0,1,0]  $c2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,y,0



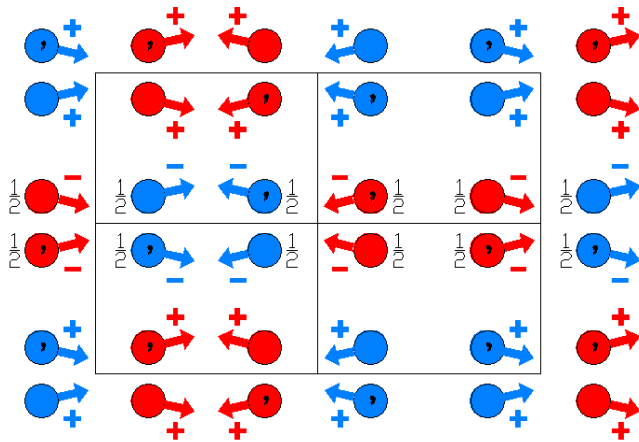
$I_p m' m' a$

74.9.658

$mmm1'$

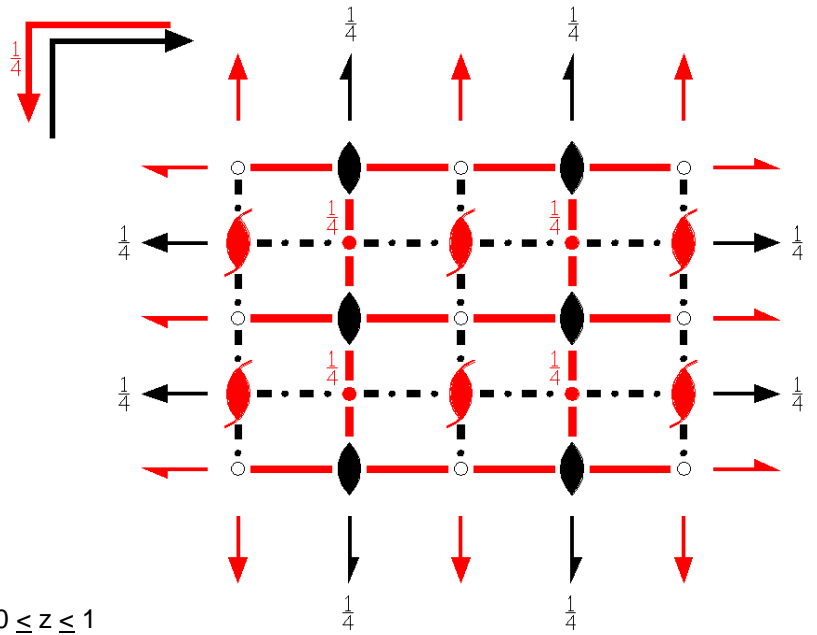
$I_{p2_1'} m' 2_1' m' 2_1' / a$

Orthorhombic



Origin at center ( $2'/m'$ ) at  $2'/m'2_1'/n'b$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$



**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1   0,0,0)                              | (2) 2 $0, 1/4, z$<br>( $2_z$   0, 1/2, 0)           | (3) $2'$ (0, 1/2, 0) $0, y, 0$<br>( $2_y$   0, 1/2, 0)' | (4) $2'$ $x, 0, 0$<br>( $2_x$   0, 0, 0)' |
| (5) $\bar{1}$ $0, 0, 0$<br>( $\bar{1}$   0, 0, 0) | (6) b (0, 1/2, 0) $x, y, 0$<br>( $m_z$   0, 1/2, 0) | (7) $m'$ $x, 1/4, z$<br>( $m_y$   0, 1/2, 0)'           | (8) $m'$ $0, y, z$<br>( $m_x$   0, 0, 0)' |

For (1/2, 1/2, 1/2)' + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t'$ (1/2, 1/2, 1/2)<br>(1   1/2, 1/2, 1/2)'                 | (2) $2'$ (0, 0, 1/2) $1/4, 0, z$<br>( $2_z$   1/2, 0, 1/2)' | (3) 2 $1/4, y, 1/4$<br>( $2_y$   1/2, 0, 1/2)           | (4) 2 (1/2, 0, 0) $x, 1/4, 1/4$<br>( $2_x$   1/2, 1/2, 1/2) |
| (5) $\bar{1}'$ $1/4, 1/4, 1/4$<br>( $\bar{1}'$   1/2, 1/2, 1/2)' | (6) $a'$ (1/2, 0, 0) $x, y, 1/4$<br>( $m_z$   1/2, 0, 1/2)' | (7) n (1/2, 0, 1/2) $x, 0, z$<br>( $m_y$   1/2, 0, 1/2) | (8) n (0, 1/2, 1/2) $1/4, y, z$<br>( $m_x$   1/2, 1/2, 1/2) |

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(1/2,1/2,1/2)$ ; (2); (3); (5).

**Positions**

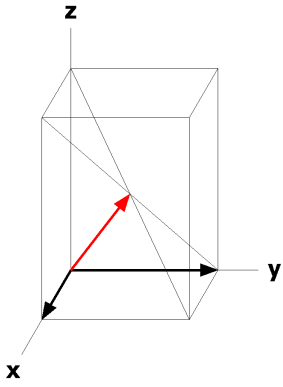
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +		$(1/2,1/2,1/2)' +$	
16 j 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y}+1/2,z [\bar{u},\bar{v},w]$	(3) $\bar{x},y+1/2,\bar{z} [u,\bar{v},w]$	(4) $x,\bar{y},\bar{z} [\bar{u},v,w]$
	(5) $\bar{x},\bar{y},\bar{z} [u,v,w]$	(6) $x,y+1/2,\bar{z} [\bar{u},\bar{v},w]$	(7) $x,\bar{y}+1/2,z [u,\bar{v},w]$	(8) $\bar{x},y,z [\bar{u},v,w]$
8 i $.m'$	$x,1/4,z [u,0,w]$	$\bar{x},1/4,z [\bar{u},0,w]$	$\bar{x},3/4,\bar{z} [u,0,w]$	$x,3/4,\bar{z} [\bar{u},0,w]$
8 h $m'..$	$0,y,z [0,v,w]$	$0,\bar{y}+1/2,z [0,\bar{v},w]$	$0,y+1/2,\bar{z} [0,\bar{v},w]$	$0,\bar{y},\bar{z} [0,v,w]$
8 g $.2.$	$1/4,y,1/4 [0,v,0]$	$3/4,\bar{y}+1/2,1/4 [0,\bar{v},0]$	$3/4,\bar{y},3/4 [0,v,0]$	$1/4,y+1/2,3/4 [0,\bar{v},0]$
8 f $2'..$	$x,0,0 [0,v,w]$	$\bar{x},1/2,0 [0,\bar{v},w]$	$\bar{x},0,0 [0,v,w]$	$x,1/2,0 [0,\bar{v},w]$
4 e $m'm'2$	$0,1/4,z [0,0,w]$	$0,3/4,\bar{z} [0,0,w]$		
4 d $.2/m'$	$1/4,1/4,3/4 [0,0,0]$	$3/4,1/4,3/4 [0,0,0]$		
4 c $.2/m'$	$1/4,1/4,1/4 [0,0,0]$	$3/4,1/4,1/4 [0,0,0]$		
4 b $2'/m'..$	$0,0,1/2 [0,v,w]$	$0,1/2,1/2 [0,\bar{v},w]$		
4 a $2'/m'..$	$0,0,0 [0,v,w]$	$0,1/2,0 [0,\bar{v},w]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_{2a}2m'm'$   
 $a^* = -b/2$   $b^* = a/2$   
 Origin at  $0,1/4,z$

Along  $[1,0,0]$   $c_p2'mm'$   
 $a^* = -c$   $b^* = b$   
 Origin at  $x,1/4,1/4$

Along  $[0,1,0]$   $c_p2'mm'$   
 $a^* = c$   $b^* = a$   
 Origin at  $0,y,0$



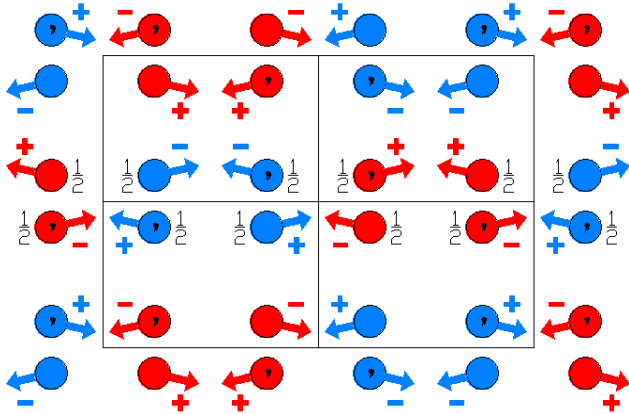
$I_pmm'a'$

74.10.659

$mmm1'$

$I_p2_1/m'2_1'/a'$

Orthorhombic



Origin at center ( $2/m$ ) at  $2/m2_1'/n'b'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

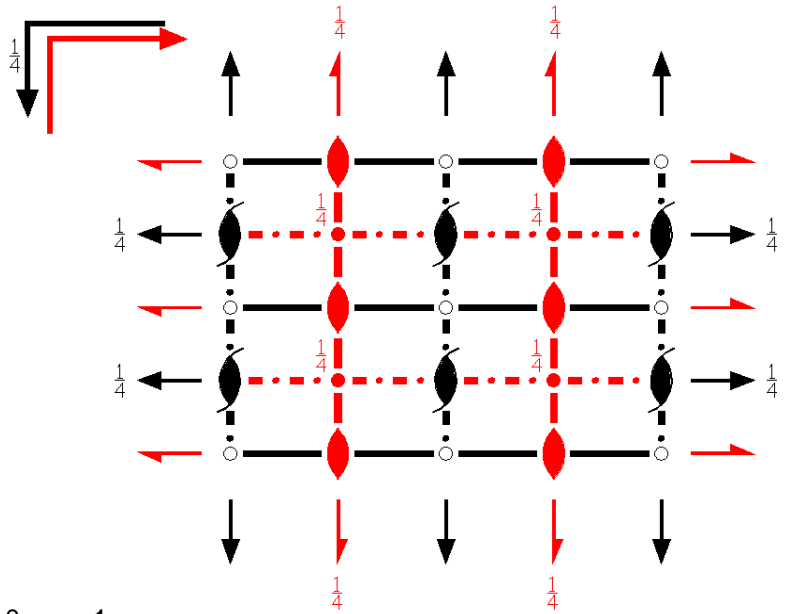
**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                   | (2) $2'$ $0, 1/4, z$<br>( $2_z$   $0, 1/2, 0$ )'             | (3) $2'$ $(0, 1/2, 0)$ $0, y, 0$<br>( $2_y$   $0, 1/2, 0$ )' | (4) $2$ $x, 0, 0$<br>( $2_x$   $0, 0, 0$ ) |
| (5) $\bar{1}$ $0, 0, 0$<br>( $\bar{1}$   $0, 0, 0$ ) | (6) $b'$ $(0, 1/2, 0)$ $x, y, 0$<br>( $m_z$   $0, 1/2, 0$ )' | (7) $m'$ $x, 1/4, z$<br>( $m_y$   $0, 1/2, 0$ )'             | (8) $m$ $0, y, z$<br>( $m_x$   $0, 0, 0$ ) |

For (1/2, 1/2, 1/2)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t'$ $(1/2, 1/2, 1/2)$<br>(1  $1/2, 1/2, 1/2$ )'                | (2) $2$ $(0, 0, 1/2)$ $1/4, 0, z$<br>( $2_z$   $1/2, 0, 1/2$ ) | (3) $2$ $1/4, y, 1/4$<br>( $2_y$   $1/2, 0, 1/2$ )             | (4) $2'$ $(1/2, 0, 0)$ $x, 1/4, 1/4$<br>( $2_x$   $1/2, 1/2, 1/2$ )' |
| (5) $\bar{1}'$ $1/4, 1/4, 1/4$<br>( $\bar{1}'$   $1/2, 1/2, 1/2$ )' | (6) $a$ $(1/2, 0, 0)$ $x, y, 1/4$<br>( $m_z$   $1/2, 0, 1/2$ ) | (7) $n$ $(1/2, 0, 1/2)$ $x, 0, z$<br>( $m_y$   $1/2, 0, 1/2$ ) | (8) $n'$ $(0, 1/2, 1/2)$ $1/4, y, z$<br>( $m_x$   $1/2, 1/2, 1/2$ )' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

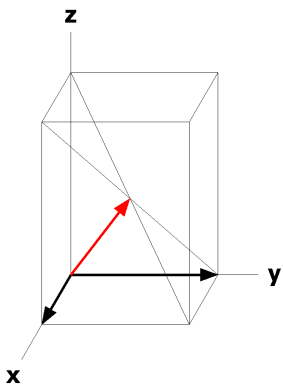
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
16 j 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y}+1/2,z$ [u,v, $\bar{w}$ ] (6) x,y+1/2, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}$ [u, $\bar{v}$ ,w] (7) x, $\bar{y}+1/2,z$ [u, $\bar{v}$ ,w]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (8) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]
8 i .m'	x,1/4,z [u,0,w]	$\bar{x},1/4,z$ [u,0, $\bar{w}$ ]	$\bar{x},3/4,\bar{z}$ [u,0,w]	x,3/4, $\bar{z}$ [u,0, $\bar{w}$ ]
8 h m..	0,y,z [u,0,0]	0, $\bar{y}+1/2,z$ [u,0,0]	0,y+1/2, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [u,0,0]
8 g .2.	1/4,y,1/4 [0,v,0]	3/4, $\bar{y}+1/2,1/4$ [0,v,0]	3/4, $\bar{y},3/4$ [0, $\bar{v}$ ,0]	1/4,y+1/2,3/4 [0, $\bar{v}$ ,0]
8 f 2..	x,0,0 [u,0,0]	$\bar{x},1/2,0$ [u,0,0]	$\bar{x},0,0$ [u,0,0]	x,1/2,0 [u,0,0]
4 e mm'2'	0,1/4,z [u,0,0]	0,3/4, $\bar{z}$ [u,0,0]		
4 d .2/m'	1/4,1/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]		
4 c .2/m'	1/4,1/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]		
4 b 2/m..	0,0,1/2 [u,0,0]	0,1/2,1/2 [u,0,0]		
4 a 2/m..	0,0,0 [u,0,0]	0,1/2,0 [u,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

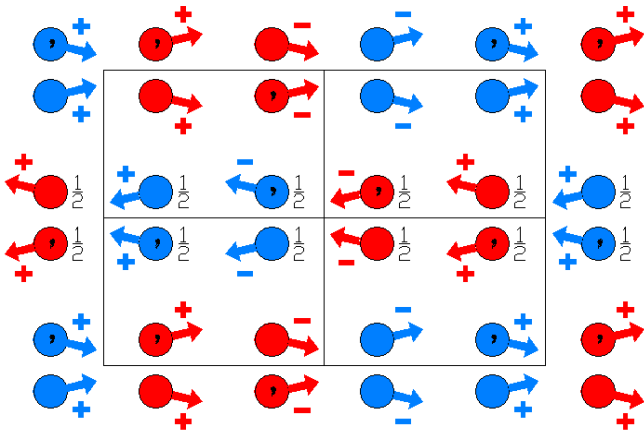
Along [0,1,0] c<sub>p</sub>-2'mm'  
 $\mathbf{a}^* = -\mathbf{a}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at 0,y,0



$I_p m' ma'$   
74.11.660

$mmm1'$   
 $I_p 2_1' / m' 2_1' / m' 2_1' / a'$

Orthorhombic



Origin at center ( $2'/m'$ ) at  $2'/m'2_1'/n'b'$

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1$

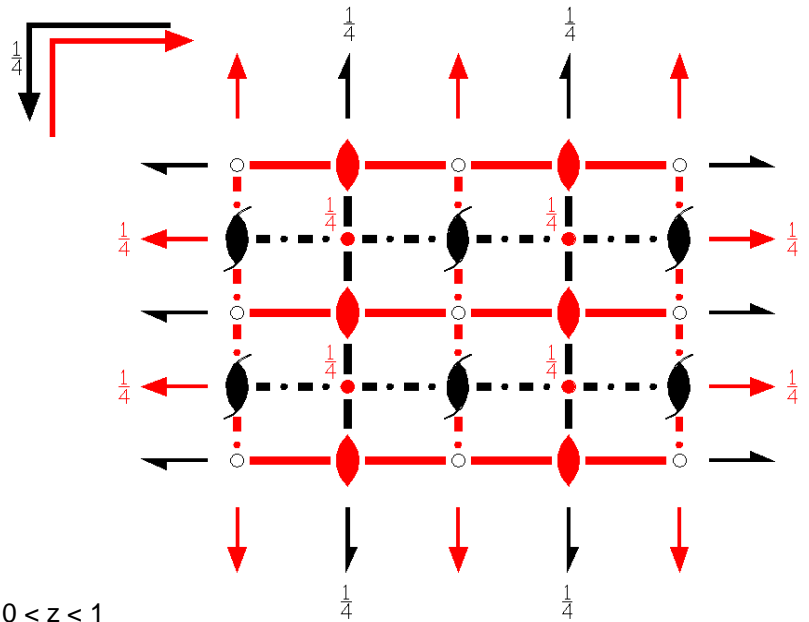
**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1   0,0,0)                                 | (2) $2'$ $0, 1/4, z$<br>( $2_z$   $0, 1/2, 0$ )'         | (3) $2$ (0,1/2,0) $0, y, 0$<br>( $2_y$   $0, 1/2, 0$ ) | (4) $2'$ $x, 0, 0$<br>( $2_x$   $0, 0, 0$ )' |
| (5) $\bar{1}$ $0, 0, 0$<br>( $\bar{1}$   $0, 0, 0$ ) | (6) $b'$ (0,1/2,0) $x, y, 0$<br>( $m_z$   $0, 1/2, 0$ )' | (7) $m$ $x, 1/4, z$<br>( $m_y$   $0, 1/2, 0$ )         | (8) $m'$ $0, y, z$<br>( $m_x$   $0, 0, 0$ )' |

For (1/2,1/2,1/2)' + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t'$ (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)'                   | (2) $2$ (0,0,1/2) $1/4, 0, z$<br>( $2_z$   1/2,0,1/2) | (3) $2'$ $1/4, y, 1/4$<br>( $2_y$   1/2,0,1/2)'         | (4) $2$ (1/2,0,0) $x, 1/4, 1/4$<br>( $2_x$   1/2,1/2,1/2) |
| (5) $\bar{1}'$ $1/4, 1/4, 1/4$<br>( $\bar{1}'$   1/2,1/2,1/2)' | (6) $a$ (1/2,0,0) $x, y, 1/4$<br>( $m_z$   1/2,0,1/2) | (7) $n'$ (1/2,0,1/2) $x, 0, z$<br>( $m_y$   1/2,0,1/2)' | (8) $n$ (0,1/2,1/2) $1/4, y, z$<br>( $m_x$   1/2,1/2,1/2) |





**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

### Positions

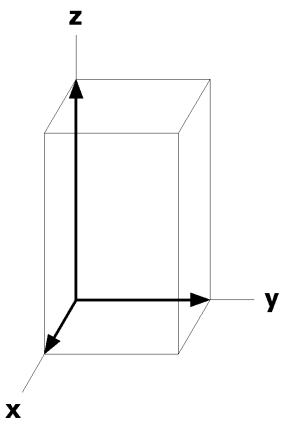
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
16 j 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y}+1/2,z$ [u,v, $\bar{w}$ ]	(3) $\bar{x},y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) x,y+1/2, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) x, $\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(8) $\bar{x},y,z$ [ $\bar{u},v,w$ ]
8 i .m.	x,1/4,z [0,v,0]	$\bar{x},1/4,z$ [0,v,0]	$\bar{x},3/4,\bar{z}$ [0,v,0]	x,3/4, $\bar{z}$ [0,v,0]
8 h m'..	0,y,z [0,v,w]	0, $\bar{y}+1/2,z$ [0,v, $\bar{w}$ ]	0,y+1/2, $\bar{z}$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0,v,w]
8 g .2'.	1/4,y,1/4 [u,0,w]	3/4, $\bar{y}+1/2,1/4$ [u,0, $\bar{w}$ ]	3/4, $\bar{y},3/4$ [u,0,w]	1/4,y+1/2,3/4 [u,0, $\bar{w}$ ]
8 f 2'..	x,0,0 [0,v,w]	$\bar{x},1/2,0$ [0,v, $\bar{w}$ ]	$\bar{x},0,0$ [0,v,w]	x,1/2,0 [0,v, $\bar{w}$ ]
4 e m'm2'	0,1/4,z [0,v,0]	0,3/4, $\bar{z}$ [0,v,0]		
4 d .2'/m.	1/4,1/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]		
4 c .2'/m.	1/4,1/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]		
4 b 2'/m'..	0,0,1/2 [0,v,w]	0,1/2,1/2 [0,v, $\bar{w}$ ]		
4 a 2'/m'..	0,0,0 [0,v,w]	0,1/2,0 [0,v, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p2'mm'  
 $\mathbf{a}^* = -\mathbf{b}^*/2$   $\mathbf{b}^* = \mathbf{a}^*/2$   
 Origin at 0,0,z

Along [1,0,0] c<sub>p</sub>-2mm  
 $\mathbf{a}^* = \mathbf{b}^*$   $\mathbf{b}^* = \mathbf{c}^*$   
 Origin at x,1/4,1/4

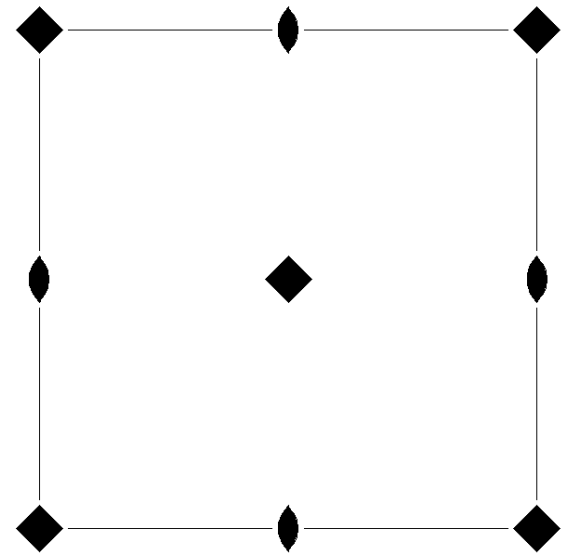
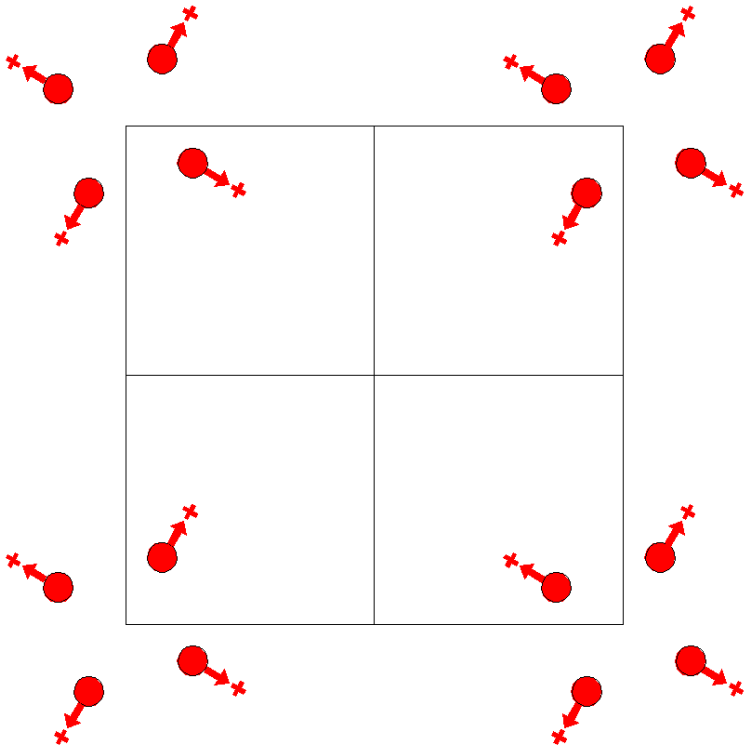
Along [0,1,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{c}^*$   $\mathbf{b}^* = \mathbf{a}^*$   
 Origin at 0,y,0



P4  
75.1.661

4  
P4

Tetragonal



Origin on 4

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 4<sup>+</sup> 0,0,z  
(4<sub>z</sub><sup>+</sup>|0,0,0)

(4) 4<sup>-</sup> 0,0,z  
(4<sub>z</sub><sup>-</sup>|0,0,0)

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3).

### Positions

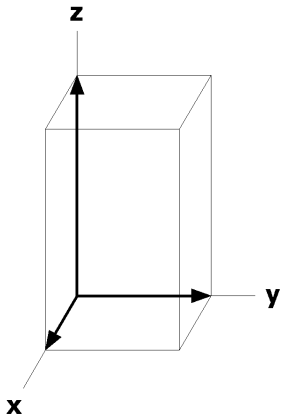
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
4	d	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]
2	c	2..	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,w$ ]		
1	b	4..	$1/2,1/2,z$ [ $0,0,w$ ]			
1	a	4..	$0,0,z$ [ $0,0,w$ ]			

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$

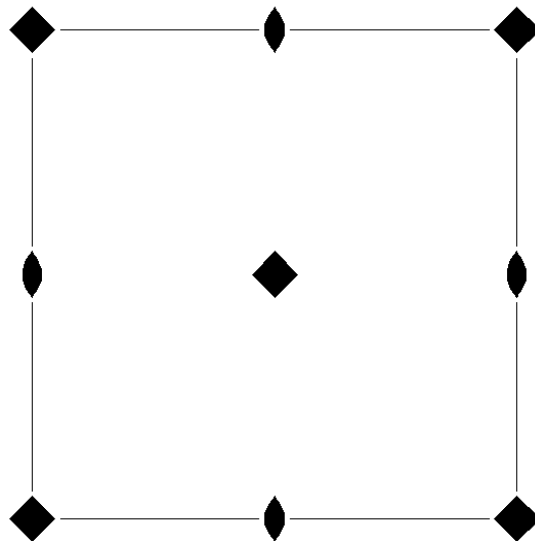
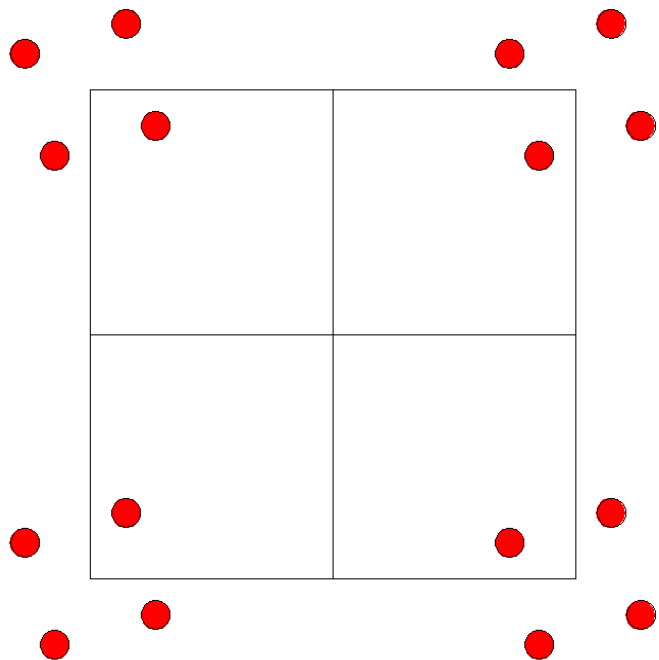


P41'  
75.2.662

41'  
P41'

Tetragonal

1'



Origin on 41'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For 1 + set

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 4<sup>+</sup> 0,0,z  
(4<sub>z</sub><sup>+</sup>|0,0,0)

(4) 4<sup>-</sup> 0,0,z  
(4<sub>z</sub><sup>-</sup>|0,0,0)

For 1' + set

(1) 1'  
(1|0,0,0)'

(2) 2' 0,0,z  
(2<sub>z</sub>'|0,0,0)'

(3) 4<sup>+</sup> 0,0,z  
(4<sub>z</sub><sup>+</sup>|0,0,0)'

(4) 4<sup>-</sup> 0,0,z  
(4<sub>z</sub><sup>-</sup>'|0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

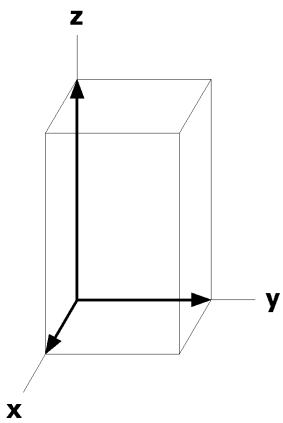
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
4 d 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z$ [0,0,0]	(4) $y,\bar{x},z$ [0,0,0]
2 c 2..1'	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]		
1 b 4..1'	1/2,1/2,z [0,0,0]			
1 a 4..1'	0,0,z [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

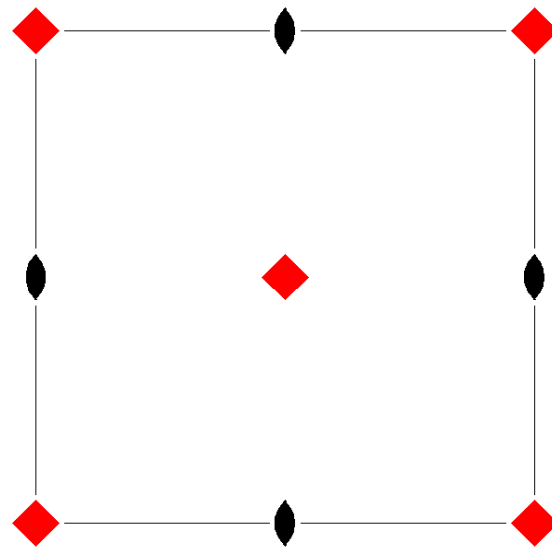
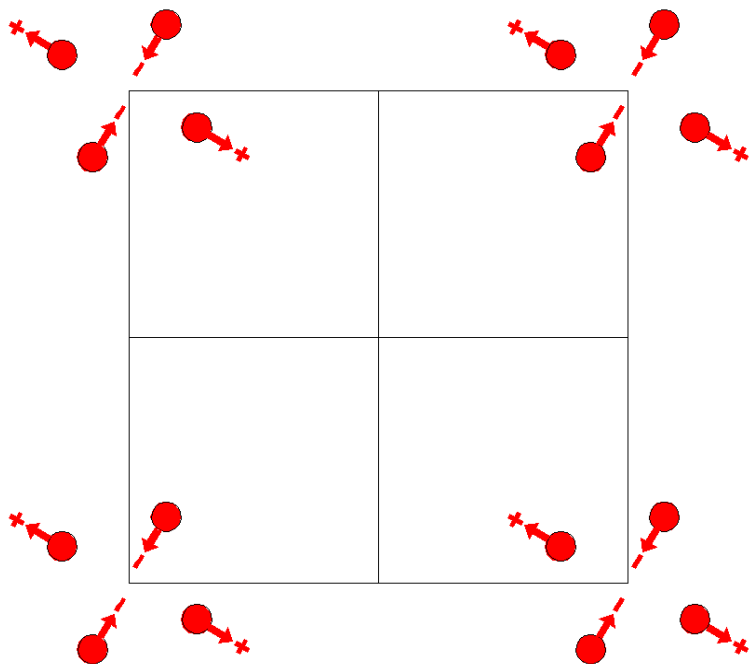
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4'  
75.3.663

4'  
P4'

Tetragonal



Origin on 4'

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 4<sup>+</sup> 0,0,z  
(4<sub>z</sub><sup>+</sup>|0,0,0)'

(4) 4<sup>-</sup> 0,0,z  
(4<sub>z</sub><sup>-</sup>|0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

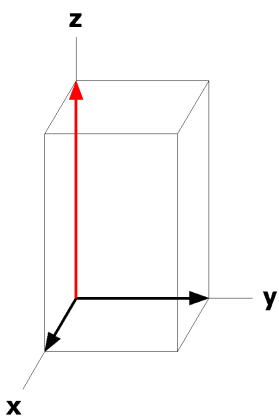
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
4	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
2	c	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]		
1	b	4'..	1/2,1/2,z [0,0,0]			
1	a	4'..	0,0,z [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $p4'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

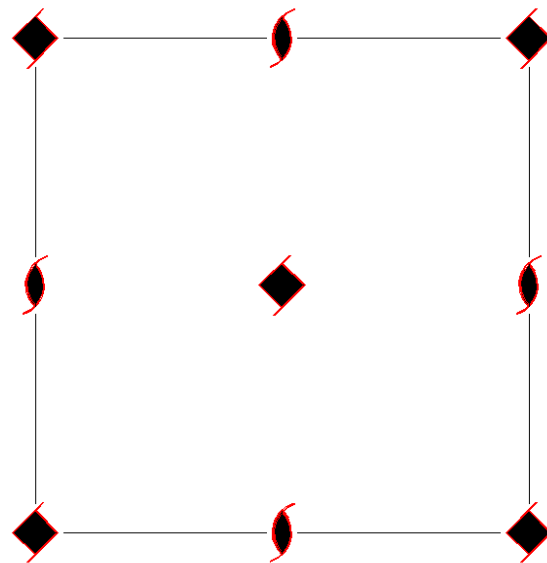
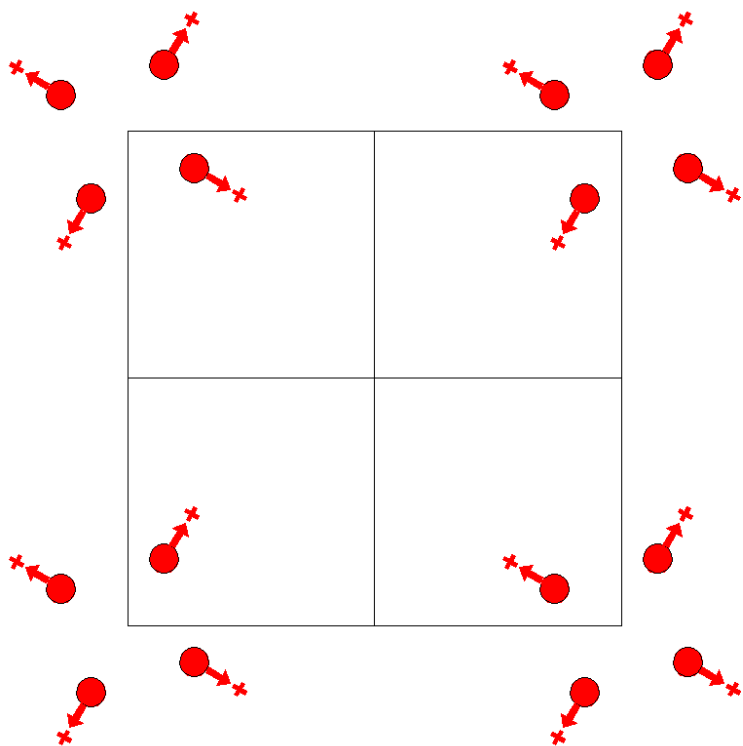
Along [1,1,0]  $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_{2c}4$   
75.4.664

$41'$   
 $P_{2c}4$

Tetragonal



Origin on 4

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0)$  + set

(1) 1  
 $(1|0,0,0)$

(2)  $2_{0,0,z}$   
 $(2_z|0,0,0)$

(3)  $4^+_{0,0,z}$   
 $(4_z^+|0,0,0)$

(4)  $4^-_{0,0,z}$   
 $(4_z^-|0,0,0)$

For  $(0,0,1)$ ' + set

(1)  $t'(0,0,1)$   
 $(1|0,0,1)'$

(2)  $2'_{(0,0,1)}$   $0,0,z$   
 $(2_z'|0,0,1)'$

(3)  $4^{+'}_{(0,0,1)}$   $0,0,z$   
 $(4_z^{+'}|0,0,1)'$

(4)  $4^{-'}_{(0,0,1)}$   $0,0,z$   
 $(4_z^{-'}|0,0,1)'$



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

### Positions

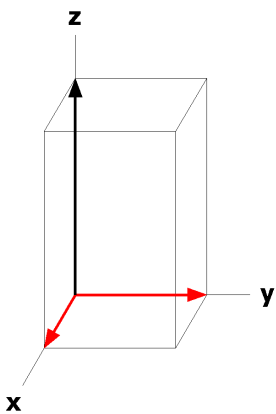
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(0,0,1)' +		
8	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z$ [ $\bar{v}, u, w$ ]	(4) $y, \bar{x}, z$ [ $v, \bar{u}, w$ ]
4	c	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]		
2	b	4..	1/2,1/2,z [0,0,w]			
2	a	4..	0,0,z [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>\*1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

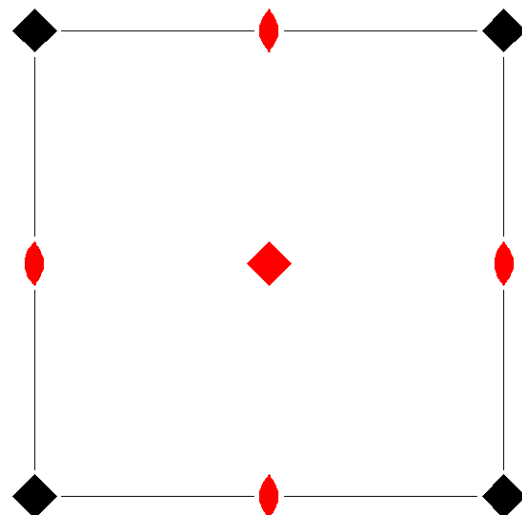
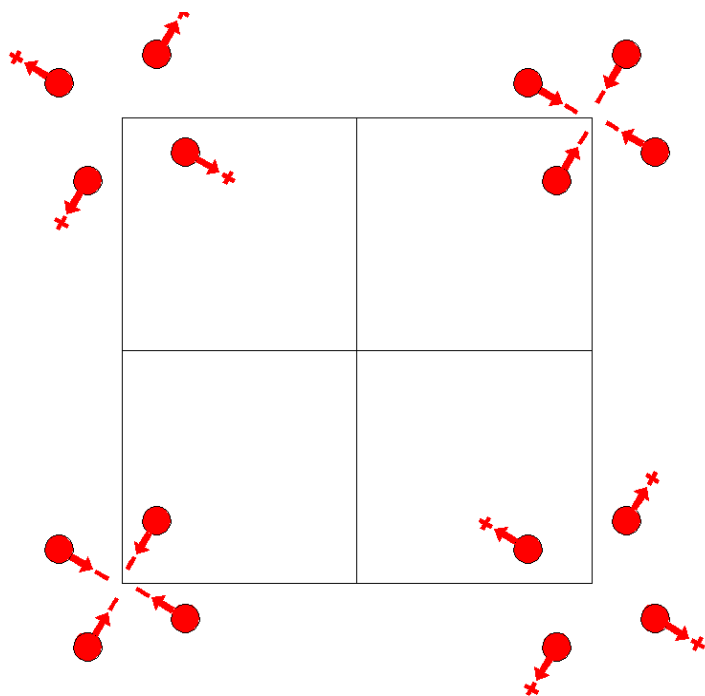
Along [1,1,0] p<sub>2b</sub>\*1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_4$   
75.5.665

$4_2'$   
 $P_4$

Tetragonal



Origin on 4

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $4^+$   $0,0,z$   
( $4_z$ |0,0,0)

(4)  $4^-$   $0,0,z$   
( $4_z^{-1}$ |0,0,0)

For  $(1,0,0)'$  + set

(1)  $t'$   $(1,0,0)$   
(1|1,0,0)'

(2)  $2'$   $1/2,0,z$   
( $2_z$ |1,0,0)'

(3)  $4^{+ '}$   $1/2,1/2,z$   
( $4_z$ |1,0,0)'

(4)  $4^{- '}$   $1/2,1/2,z$   
( $4_z^{-1}$ |1,0,0)'

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3).

**Positions**

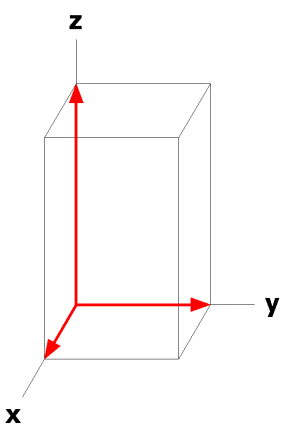
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(1,0,0)' +		
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z$ [ $\bar{v}, u, w$ ]	(4) $y, \bar{x}, z$ [ $v, \bar{u}, w$ ]
4	c 2'..	0,1/2,z [u,v,0]	1/2,0,z [ $v, \bar{u}, 0$ ]		
2	b 4'..	1/2,1/2,z [0,0,0]			
2	a 4..	0,0,z [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub>·4  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

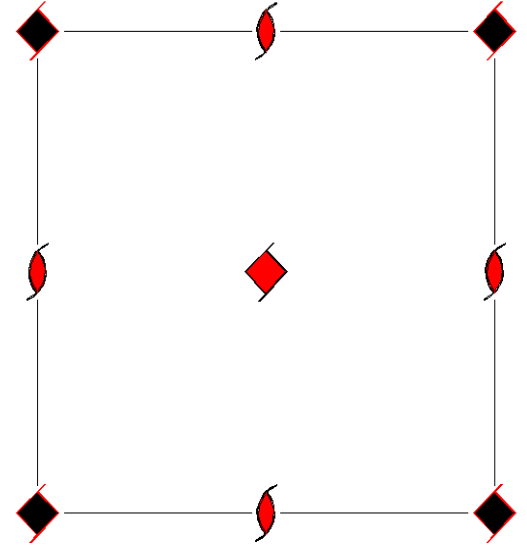
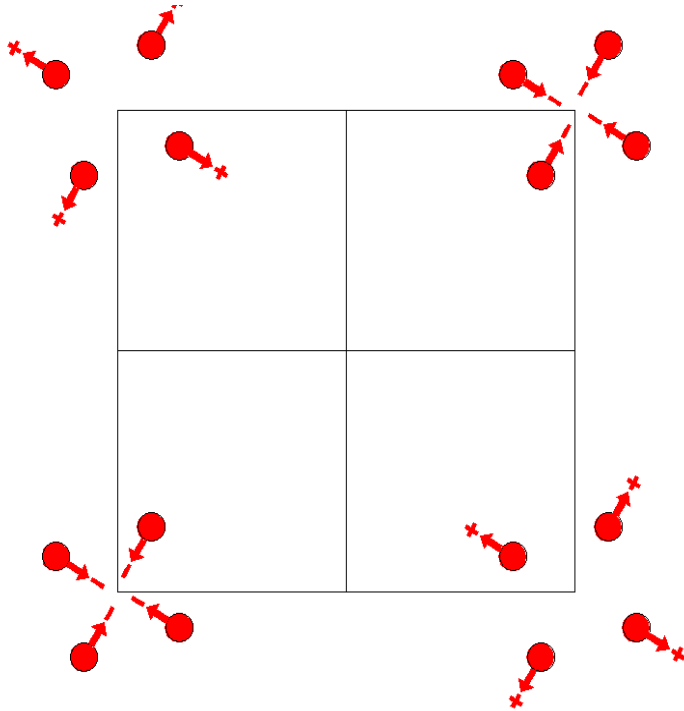
Along [1,1,0] p<sub>2a</sub>·1m1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x-1/4,x+1/4,0



$P_14$   
75.6.666

$41'$   
 $P_14$

Tetragonal



Origin on 4

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0)$  + set

- |                    |                                  |                                      |   |
|--------------------|----------------------------------|--------------------------------------|---|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $4^+$ $0,0,z$<br>( $4_z$  0,0,0) | (4) $4^-$ $0,0,z$<br>( $4_z^{-1}$  0,0,0) |
|--------------------|----------------------------------|--------------------------------------|---|

For  $(1,0,0)'$  + set

- |                                  |  |   |  |
|----------------------------------|--|---|--|
| (1) $t'$ $(1,0,0)$<br>(1 1,0,0)' | (2) $2'$ $1/2,0,z$<br>( $2_z$  1,0,0)' | (3) $4^{+ '}$ $1/2,1/2,z$<br>( $4_z$  1,0,0)' | (4) $4^{- '}$ $1/2,1/2,z$<br>( $4_z^{-1}$  1,0,0)' |
|----------------------------------|--|---|--|

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3).

**Positions**

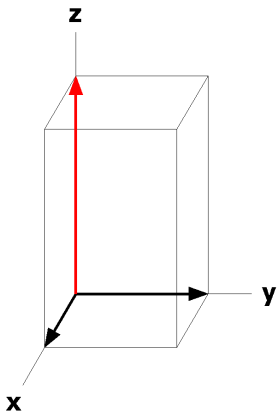
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(1,0,0)' +		
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z$ [ $\bar{v}, u, w$ ]	(4) $y, \bar{x}, z$ [ $v, \bar{u}, w$ ]
4	c 2'..	0,1/2,z [u,v,0]	1/2,0,z [ $v, \bar{u}, 0$ ]		
2	b 4'..	1/2,1/2,z [0,0,0]			
2	a 4..	0,0,z [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

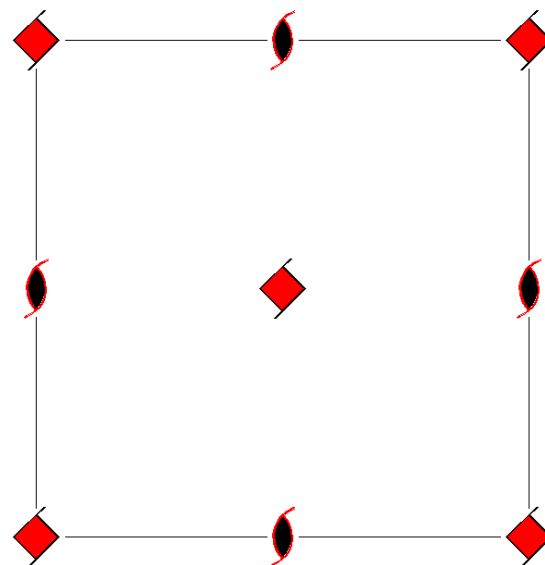
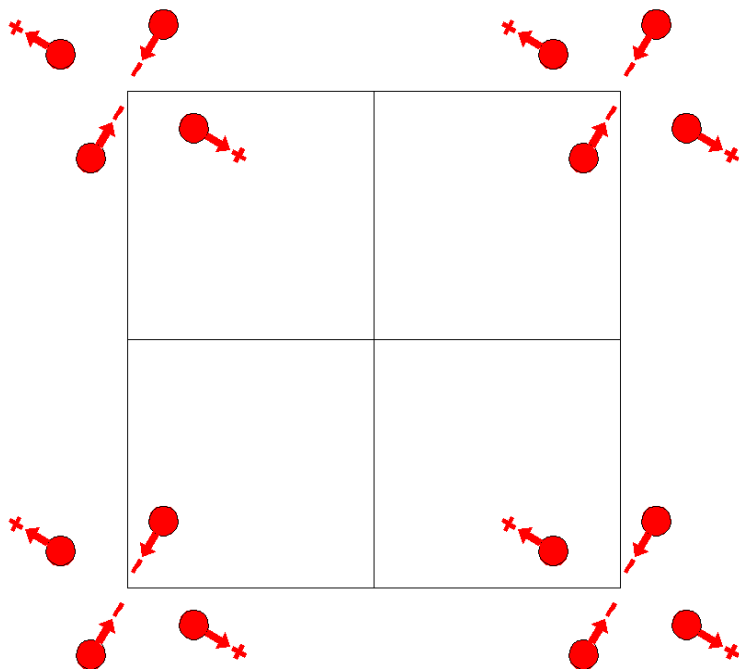
Along [1,1,0] p<sub>c</sub>-1m1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x-1/4,x+1/4,0



$P_{2c} 4'$   
75.7.667

$41'$   
 $P_{2c} 4'$

Tetragonal



Origin on 4

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $4^+ 0,0,z$   
( $4_z^+$ |0,0,0)'

(4)  $4^- 0,0,z$   
( $4_z^-$ |0,0,0)'

For  $(0,0,1)$ ' + set

(1)  $t' (0,0,1)$   
(1|0,0,1)'

(2)  $2' (0,0,1) 0,0,z$   
( $2_z'$ |0,0,1)'

(3)  $4^+ (0,0,1) 0,0,z$   
( $4_z^+$ |0,0,1)

(4)  $4^- (0,0,1) 0,0,z$   
( $4_z^-$ |0,0,1)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

### Positions

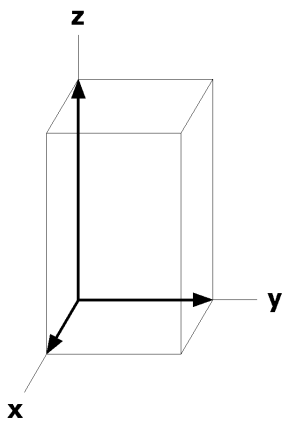
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z$ [ $v, \bar{u}, \bar{w}$ ]	(4) $y, \bar{x}, z$ [ $\bar{v}, u, \bar{w}$ ]
4 c 2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]		
2 b 4..	1/2,1/2,z [0,0,w]			
2 a 4..	0,0,z [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>\*1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

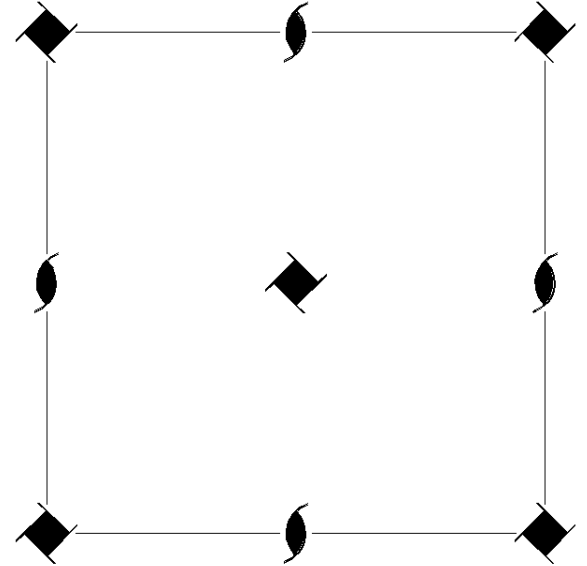
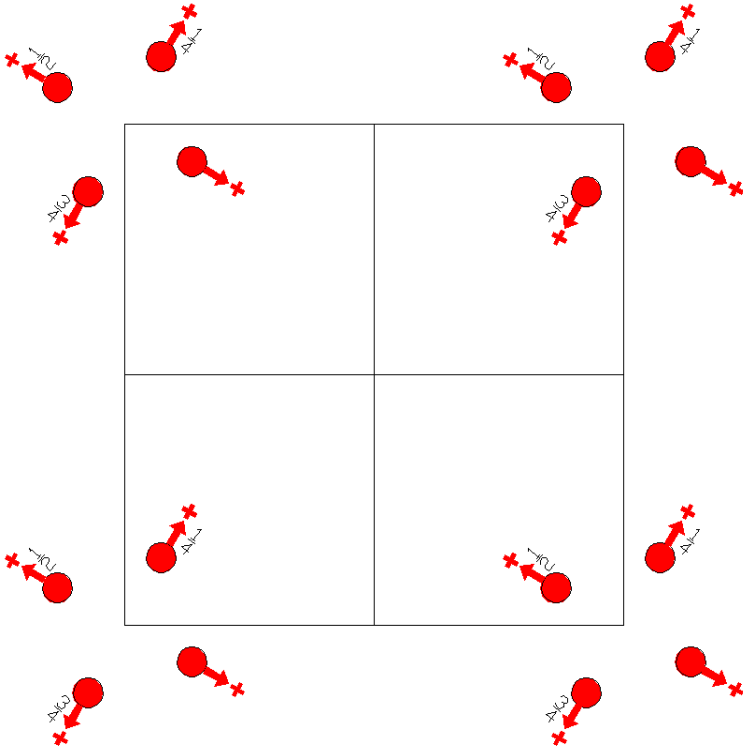
Along [1,1,0] p<sub>2b</sub>\*1m1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P4_1$   
76.1.668

4  
 $P4_1$

Tetragonal



Origin on  $4_1$

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)

(3) 4<sup>+</sup> (0,0,1/4) 0,0,z  
(4<sub>z</sub>|0,0,1/4)

(4) 4<sup>-</sup> (0,0,3/4) 0,0,z  
(4<sub>z</sub><sup>-1</sup>|0,0,3/4)



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

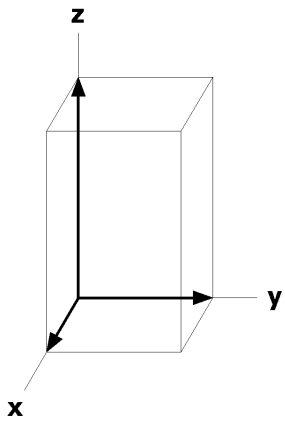
4 a 1 (1) x,y,z [u,v,w] (2)  $\bar{x}, \bar{y}, z+1/2$  [ $\bar{u}, \bar{v}, w$ ] (3)  $\bar{y}, x, z+1/4$  [ $\bar{v}, u, w$ ] (4)  $y, \bar{x}, z+3/4$  [ $v, \bar{u}, w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p1g'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,0,0

Along [1,1,0] p1g'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,x,0

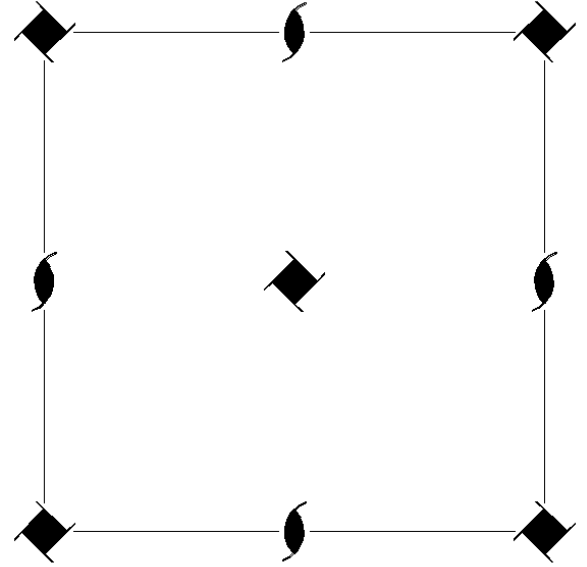
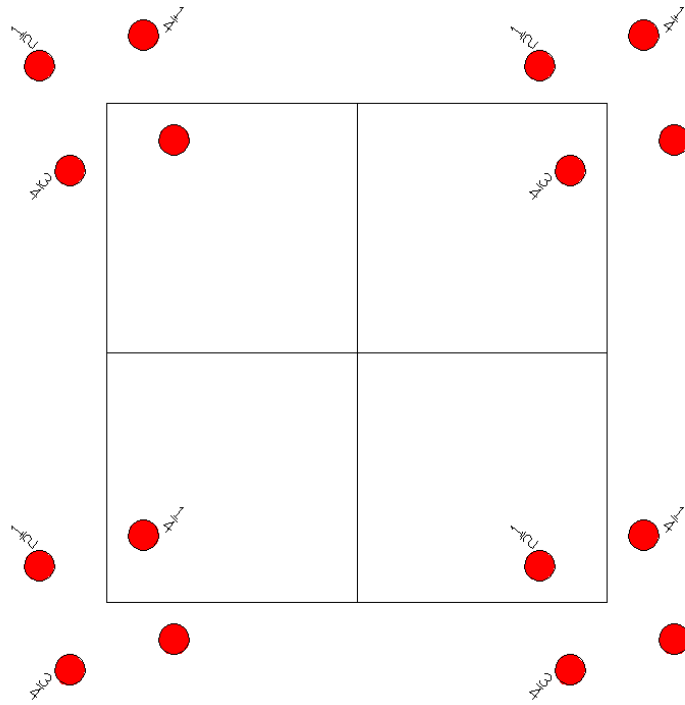


$P4_11'$   
76.2.669

$41'$   
 $P4_11'$

Tetragonal

$1'$



Origin on  $4_11'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For  $1 +$  set

- |                        |  |  |   |
|------------------------|--|--|---|
| (1) $1$<br>$(1 0,0,0)$ | (2) $2 (0,0,1/2) \ 0,0,z$<br>$(2_z 0,0,1/2)$ | (3) $4^+ (0,0,1/4) \ 0,0,z$<br>$(4_z 0,0,1/4)$ | (4) $4^- (0,0,3/4) \ 0,0,z$<br>$(4_z^{-1} 0,0,3/4)$ |
|------------------------|--|--|---|

For  $1' +$  set

- |                          |  |  |   |
|--------------------------|--|--|---|
| (1) $1'$<br>$(1 0,0,0)'$ | (2) $2' (0,0,1/2) \ 0,0,z$<br>$(2_z 0,0,1/2)'$ | (3) $4^{+'} (0,0,1/4) \ 0,0,z$<br>$(4_z 0,0,1/4)'$ | (4) $4^{-'} (0,0,3/4) \ 0,0,z$<br>$(4_z^{-1} 0,0,3/4)'$ |
|--------------------------|--|--|---|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

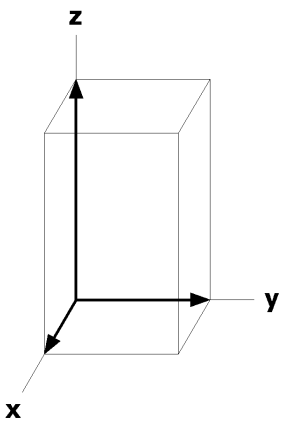
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
4 a 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z+1/2$ [0,0,0]	(3) $\bar{y},x,z+1/4$ [0,0,0]	(4) $y,\bar{x},z+3/4$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

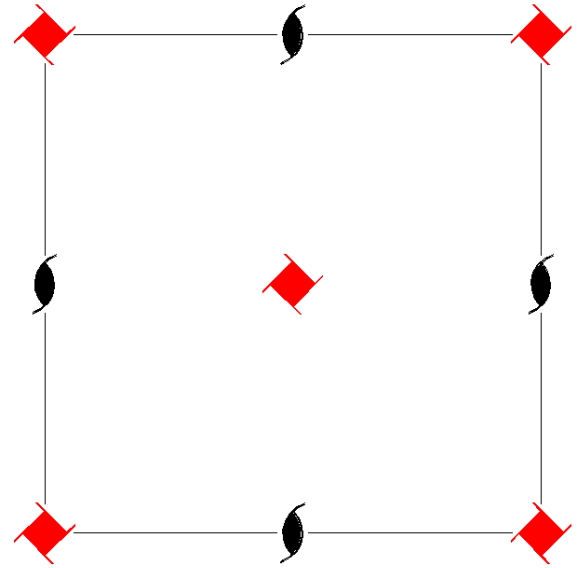
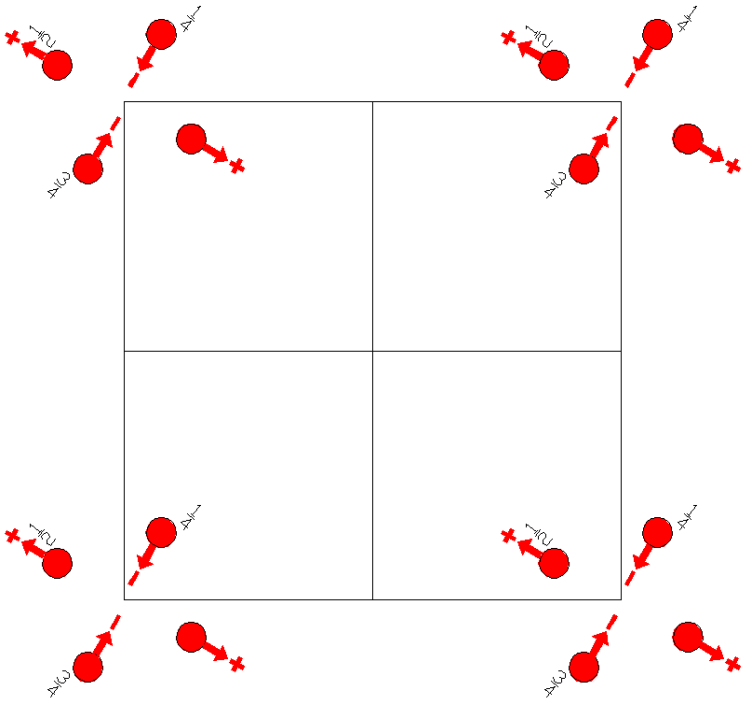
Along [1,1,0] p1g11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P4_1'$   
76.3.670

$4'$   
 $P4_1'$

Tetragonal



Origin on  $4_1'$

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z  
(2<sub>z</sub>|0,0,1/2)

(3) 4<sup>+</sup> (0,0,1/4) 0,0,z  
(4<sub>z</sub><sup>+</sup>|0,0,1/4)'

(4) 4<sup>-</sup> (0,0,3/4) 0,0,z  
(4<sub>z</sub><sup>-</sup>|0,0,3/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

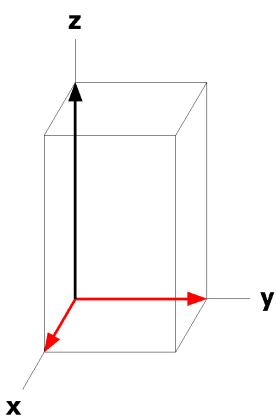
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
4	a 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/4$ [ $v,\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+3/4$ [ $\bar{v},u,\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

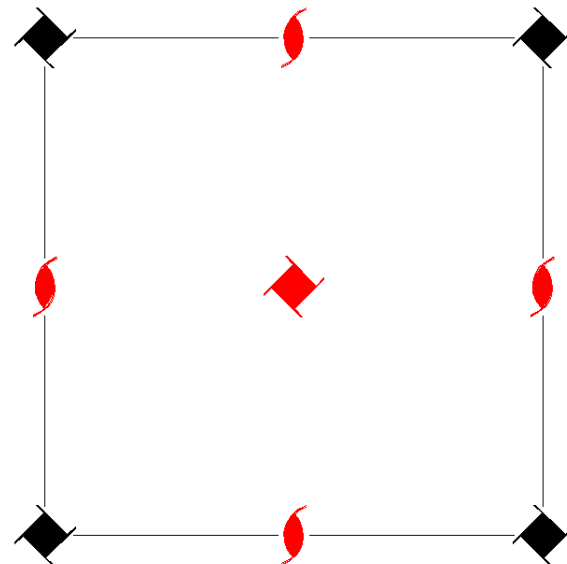
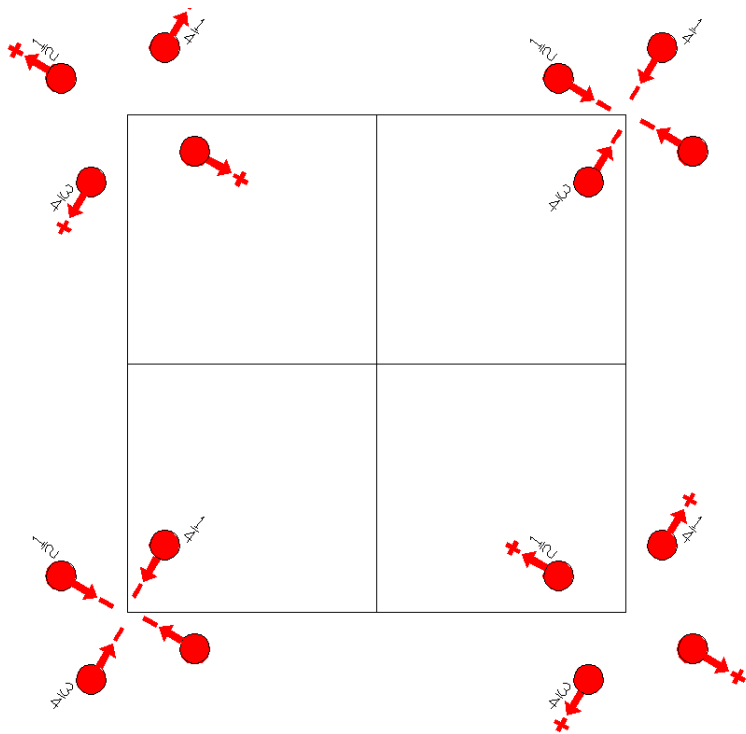
Along [1,1,0] p1g'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_P 4_1$   
76.4.671

$41'$   
 $P_P 4_1$

Tetragonal



Origin on  $4_1$

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0)$  + set

- |                    |  |   |   |
|--------------------|--|---|---|
| (1) 1<br>(1 0,0,0) | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 4 <sup>+</sup> (0,0,1/4) 0,0,z<br>(4 <sub>z</sub>  0,0,1/4) | (4) 4 <sup>-</sup> (0,0,3/4) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,3/4) |
|--------------------|--|---|---|

For  $(1,0,0)'$  + set

- |                              |  |  |  |
|------------------------------|--|--|--|
| (1) t' (1,0,0)<br>(1 1,0,0)' | (2) 2' (0,0,1/2) 1/2,0,z<br>(2 <sub>z</sub>  1,0,1/2)' | (3) 4 <sup>+</sup> ' (0,0,1/4) 1/2,1/2,z<br>(4 <sub>z</sub>  1,0,1/4)' | (4) 4 <sup>-</sup> ' (0,0,3/4) 1/2,1/2,z<br>(4 <sub>z</sub> <sup>-1</sup>  1,0,3/4)' |
|------------------------------|--|--|--|

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3).

**Positions**

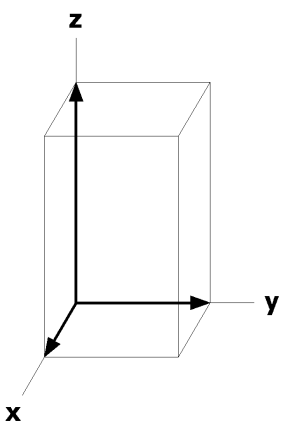
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1,0,0)' +		
8	a 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z+1/4$ [ $\bar{v}, u, w$ ]	(4) $y, \bar{x}, z+3/4$ [ $v, \bar{u}, w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub>\*4  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

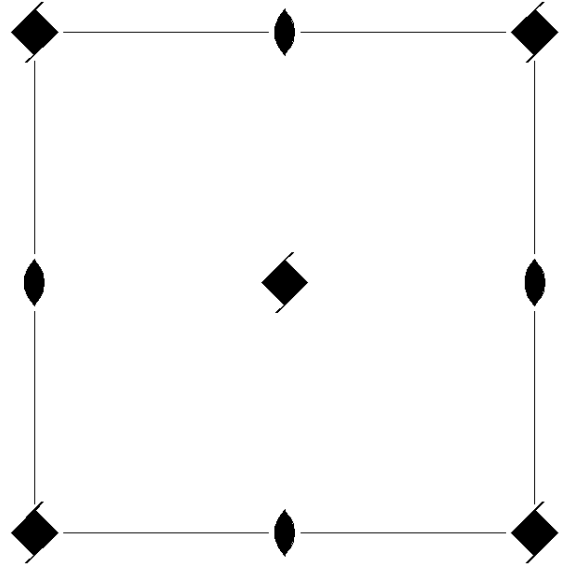
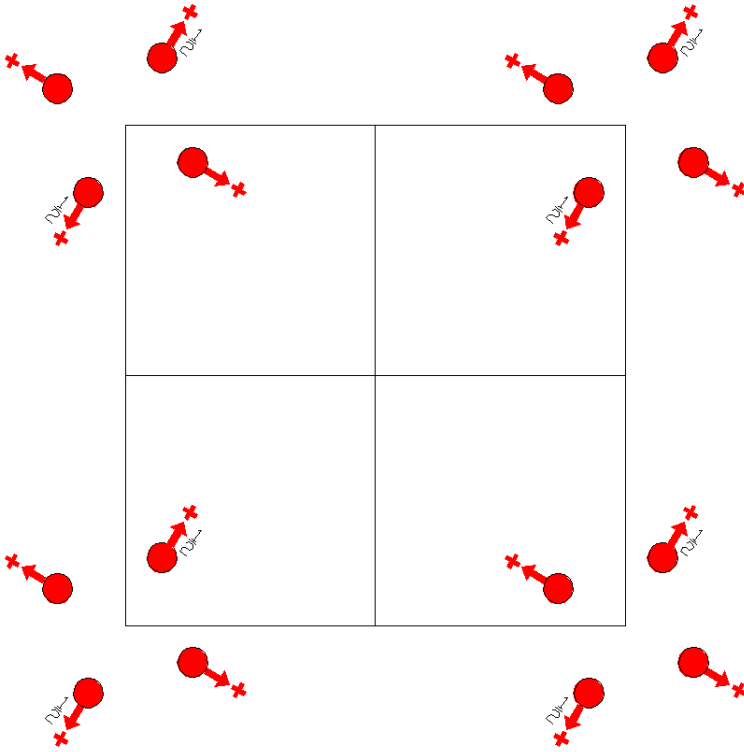
Along [1,1,0] p<sub>2a</sub>\*1g1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x-1/4,x+1/4,0



$P4_2$   
77.1.672

4  
 $P4_2$

Tetragonal



Origin on 2 on  $4_2$

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $4^+$   $(0,0,1/2)$   $0,0,z$   
( $4_z$ |0,0,1/2)

(4)  $4^-$   $(0,0,1/2)$   $0,0,z$   
( $4_z^{-1}$ |0,0,1/2)



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

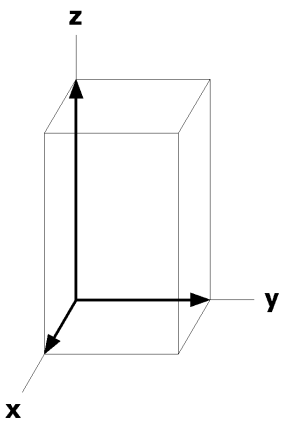
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
4	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]
2	c	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0,w]		
2	b	2..	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]		
2	a	2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p4  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0

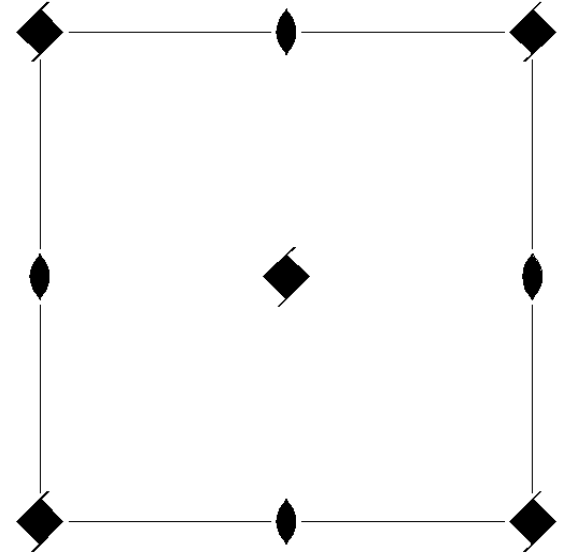
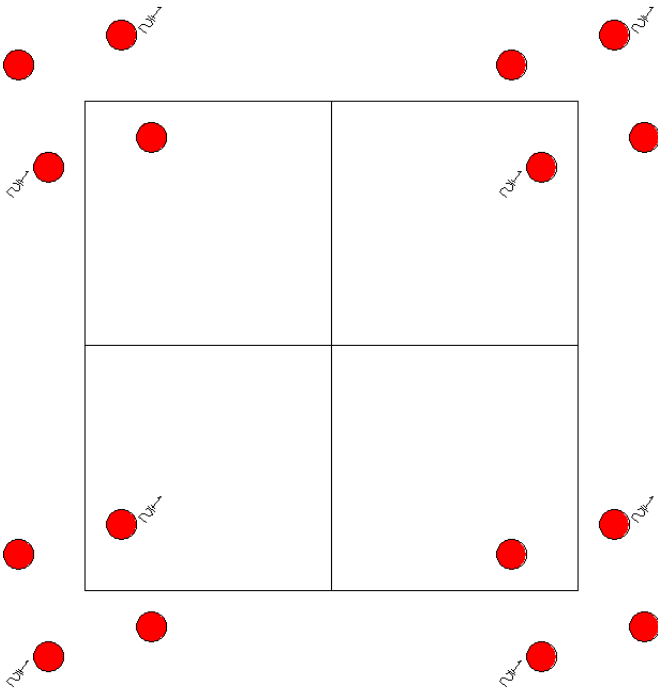


$P4_21'$   
77.2.673

$41'$   
 $P4_21'$

Tetragonal

$1'$



Origin on  $21'$  on  $4_21'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For  $1 + \text{set}$

- |                        |                                  |  |   |
|------------------------|----------------------------------|--|---|
| (1) $1$<br>$(1 0,0,0)$ | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$ | (3) $4^+$ $(0,0,1/2)$ $0,0,z$<br>$(4_z 0,0,1/2)$ | (4) $4^-$ $(0,0,1/2)$ $0,0,z$<br>$(4_z^{-1} 0,0,1/2)$ |
|------------------------|----------------------------------|--|---|

For  $1' + \text{set}$

- |                          |                                    |   |  |
|--------------------------|------------------------------------|---|--|
| (1) $1'$<br>$(1 0,0,0)'$ | (2) $2'$ $0,0,z$<br>$(2_z 0,0,0)'$ | (3) $4^{+ '}$ $(0,0,1/2)$ $0,0,z$<br>$(4_z 0,0,1/2)'$ | (4) $4^{- '}$ $(0,0,1/2)$ $0,0,z$<br>$(4_z^{-1} 0,0,1/2)'$ |
|--------------------------|------------------------------------|---|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

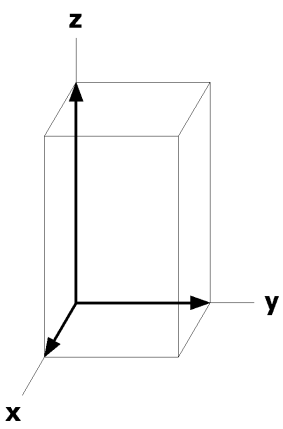
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
4 d 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z+1/2$ [0,0,0]	(4) $y,\bar{x},z+1/2$ [0,0,0]
2 c 2..1'	0,1/2,z [0,0,0]	1/2,0,z+1/2 [0,0,0]		
2 b 2..1'	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]		
2 a 2..1'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

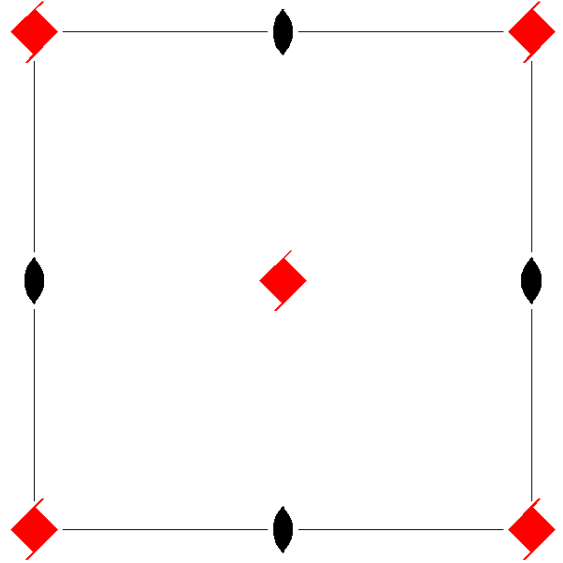
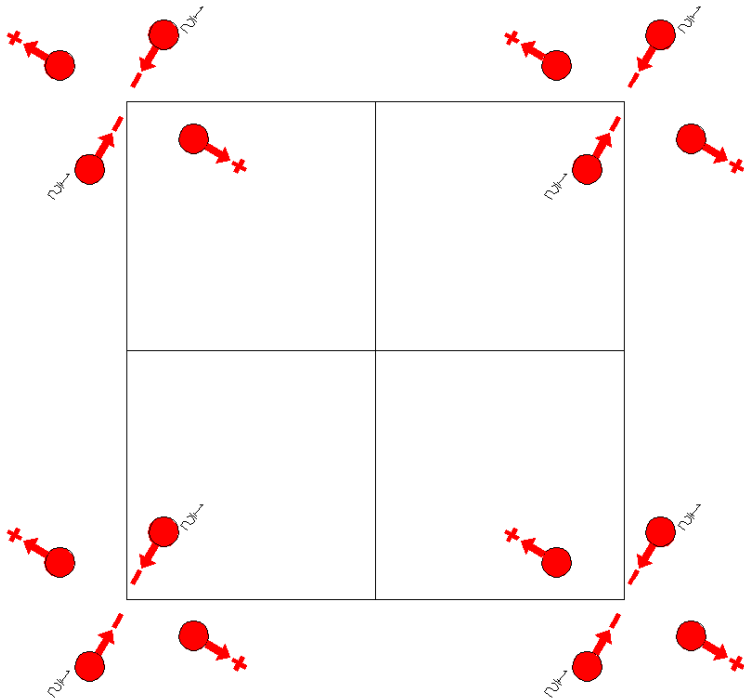
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P4_2'$   
77.3.674

$4'$   
 $P4_2'$

Tetragonal



Origin on 2 on  $4_2'$

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $4^+$   $(0,0,1/2)$   $0,0,z$   
( $4_z$ | $0,0,1/2$ )'

(4)  $4^-$   $(0,0,1/2)$   $0,0,z$   
( $4_z^{-1}$ | $0,0,1/2$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

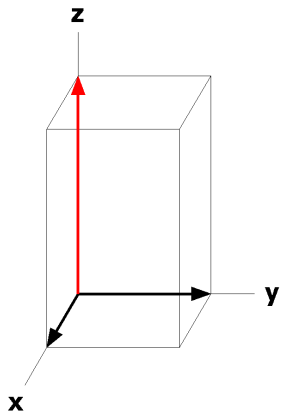
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
4	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ]
2	c	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]		
2	b	2..	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]		
2	a	2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p4  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

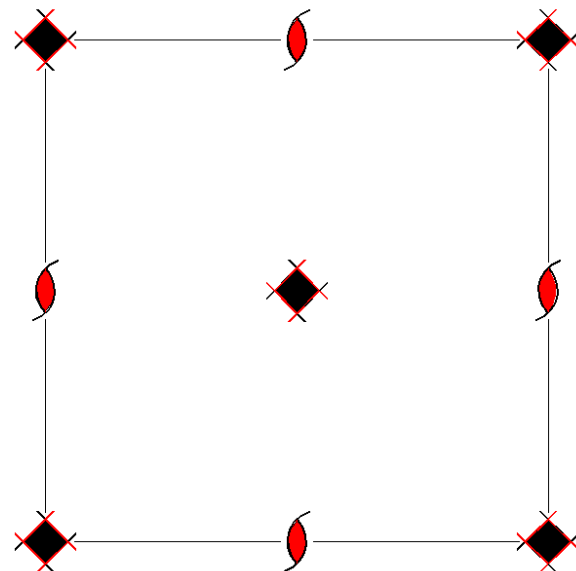
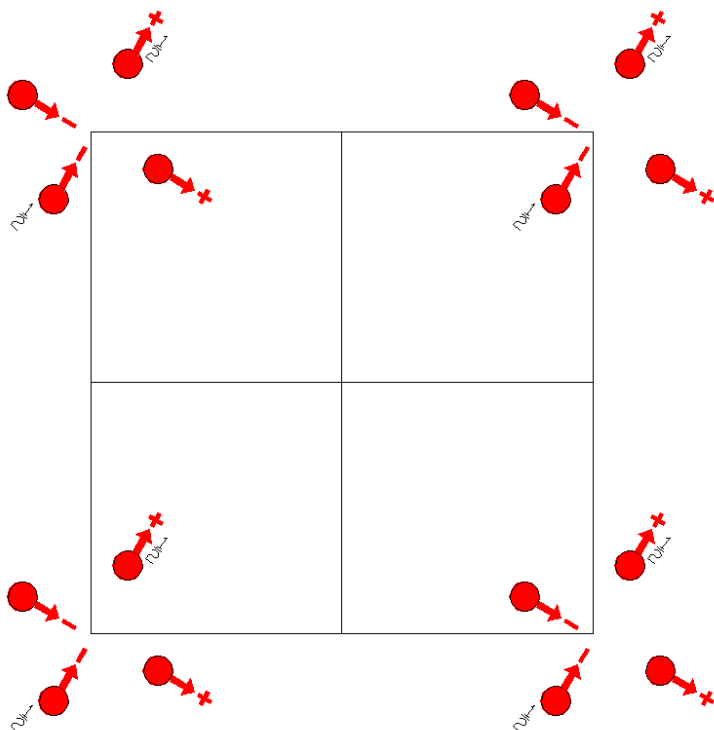
Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_{2c} 4_2$   
77.4.675

$41'$   
 $P_{2c} 4_2$

Tetragonal



Origin on  $2'$  on  $4_2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0) +$

- |                    |                                      |  |  |
|--------------------|--------------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) $2'$ $0,0,z$<br>( $2_z$  0,0,0)' | (3) $4^+$ $(0,0,1/2) 0,0,z$<br>( $4_z$  0,0,1/2) | (4) $4^-$ $(0,0,1/2) 0,0,z$<br>( $4_z^{-1}$  0,0,1/2)' |
|--------------------|--------------------------------------|--|--|

For  $(0,0,1)' +$

- |                                 |  |  |   |
|---------------------------------|--|--|---|
| (1) $t'$ $(0,0,1)$<br>(1 0,0,1) | (2) 2 $(0,0,1) 0,0,z$<br>( $2_z$  0,0,1) | (3) $4^+'$ $(0,0,3/2) 0,0,z$<br>( $4_z$  0,0,3/2)' | (4) $4^-'$ $(0,0,3/2) 0,0,z$<br>( $4_z^{-1}$  0,0,3/2)' |
|---------------------------------|--|--|---|

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3).

**Positions**

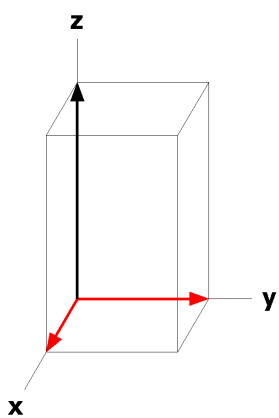
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +		(0,0,1)' +	
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ]
4	c 2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]		
4	b 2..	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]		
4	a 2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p4  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

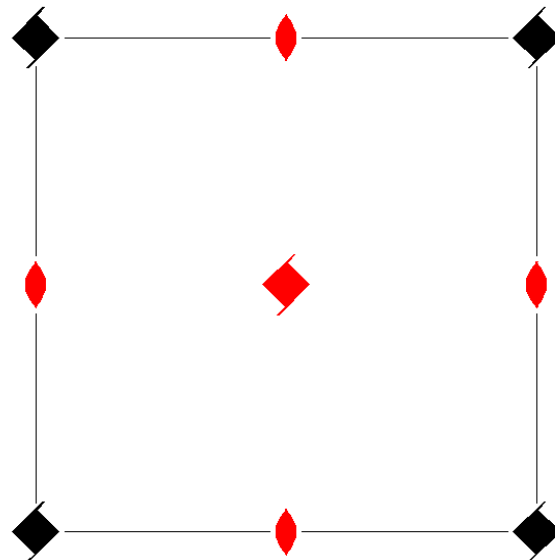
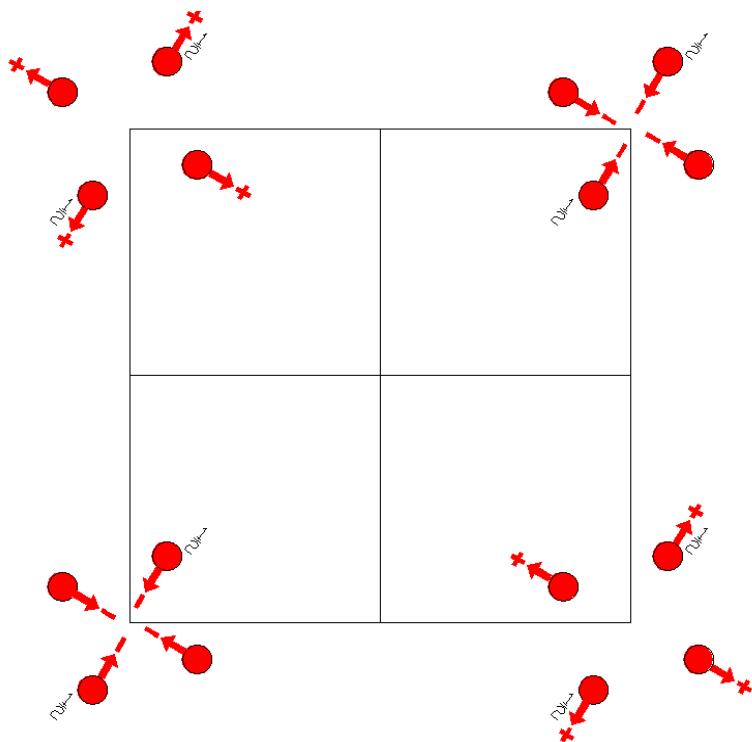
Along [1,1,0] p1m1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_P 4_2$   
77.5.676

$41'$   
 $P_P 4_2$

Tetragonal



Origin on 2 on  $4_2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0)$  + set

- |                    |                                  |  |   |
|--------------------|----------------------------------|--|---|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $4^+$ $(0,0,1/2)$ $0,0,z$<br>( $4_z$  0,0,1/2) | (4) $4^-$ $(0,0,1/2)$ $0,0,z$<br>( $4_z^{-1}$  0,0,1/2) |
|--------------------|----------------------------------|--|---|

For  $(1,0,0)'$  + set

- |                                  |  |   |  |
|----------------------------------|--|---|--|
| (1) $t'$ $(1,0,0)$<br>(1 1,0,0)' | (2) $2'$ $1/2,0,z$<br>( $2_z$  1,0,0)' | (3) $4^{+ '}$ $(0,0,1/2)$ $1/2,1/2,z$<br>( $4_z$  1,0,1/2)' | (4) $4^{- '}$ $(0,0,1/2)$ $1/2,1/2,z$<br>( $4_z^{-1}$  1,0,1/2)' |
|----------------------------------|--|---|--|



**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3).

**Positions**

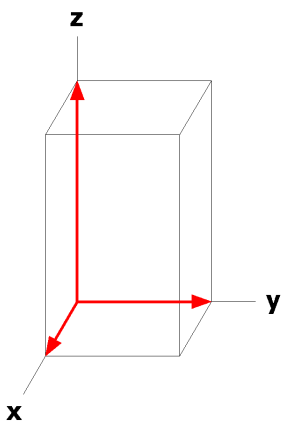
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
8 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]
4 c 2'..	0,1/2,z [u,v,0]	1/2,0,z+1/2 [v, $\bar{u}$ ,0]		
4 b 2..	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]		
4 a 2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub>·4  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

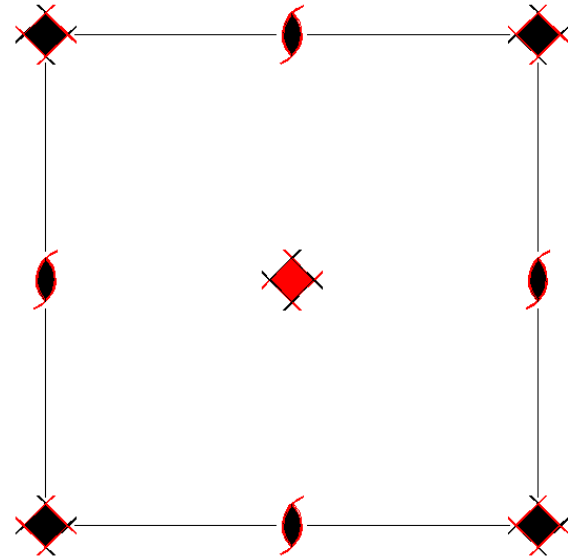
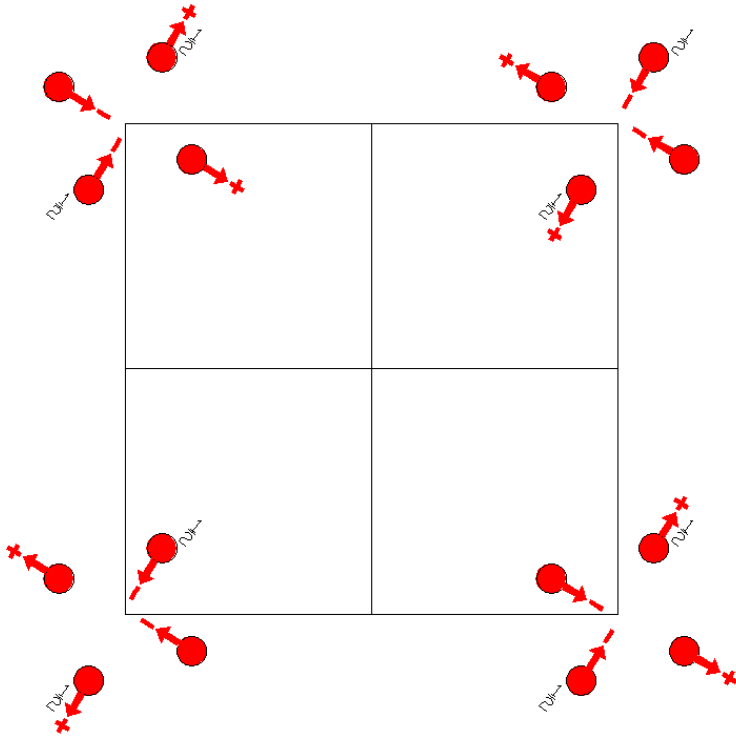
Along [1,1,0] p<sub>2a</sub>·1m1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x-1/4,x+1/4,0



$P_14_2$   
77.6.677

$41'$   
 $P_14_2$

Tetragonal



Origin on  $2'$  on  $4_2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0)$  + set

- |                    |                                    |  |  |
|--------------------|------------------------------------|--|--|
| (1) 1<br>(1 0,0,0) | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $4^+$ (0,0,1/2) 0,0,z<br>( $4_z$  0,0,1/2) | (4) $4^-$ (0,0,1/2) 0,0,z<br>( $4_z^{-1}$  0,0,1/2)' |
|--------------------|------------------------------------|--|--|

For  $(1,0,0)$ ' + set

- |                                |                                    |   |   |
|--------------------------------|------------------------------------|---|---|
| (1) $t'$ (1,0,0)<br>(1 1,0,0)' | (2) $2$ 1/2,0,z<br>( $2_z$  1,0,0) | (3) $4^+$ (0,0,1/2) 1/2,1/2,z<br>( $4_z$  1,0,1/2)' | (4) $4^-$ (0,0,1/2) 1/2,1/2,z<br>( $4_z^{-1}$  1,0,1/2) |
|--------------------------------|------------------------------------|---|---|

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3).

**Positions**

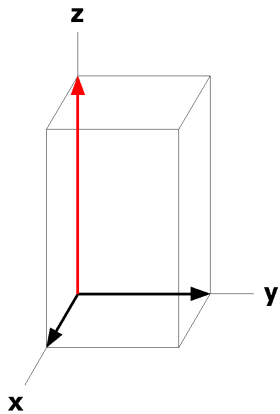
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +		(1,0,0)' +	
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ]
4	c 2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]		
4	b 2'..	1/2,1/2,z [u,v,0]	1/2,1/2,z+1/2 [ $v,\bar{u},0$ ]		
4	a 2'..	0,0,z [u,v,0]	0,0,z+1/2 [ $v,\bar{u},0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

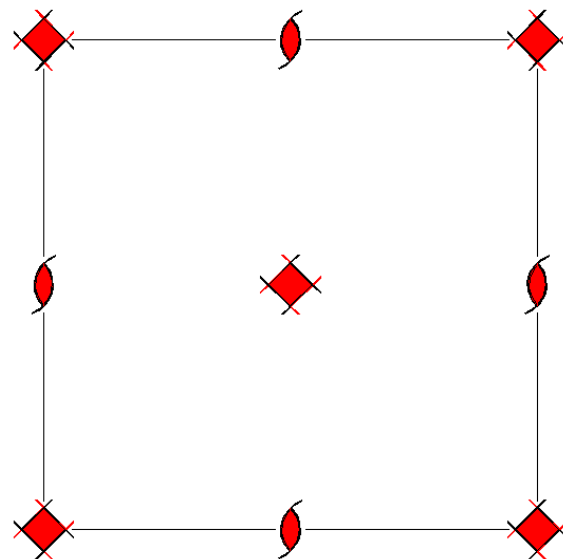
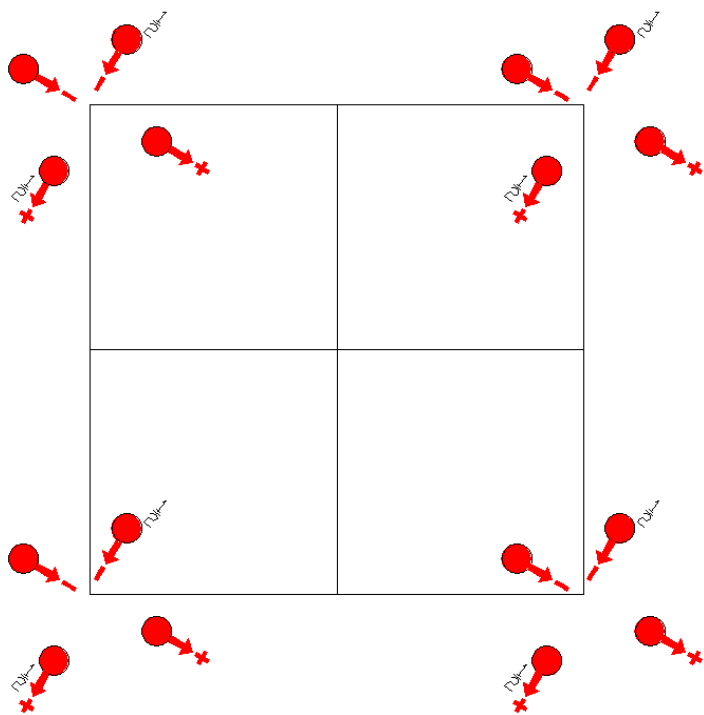
Along [1,1,0] p<sub>c</sub>-1m1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_{2c} 4_2'$   
77.7.678

$41'$   
 $P_{2c} 4_2'$

Tetragonal



Origin on  $2'$  on  $4_2'$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0) +$

- |                        |                                    |   |   |
|------------------------|------------------------------------|---|---|
| (1) $1$<br>$(1 0,0,0)$ | (2) $2'$ $0,0,z$<br>$(2_z 0,0,0)'$ | (3) $4^+ ' (0,0,1/2) \quad 0,0,z$<br>$(4_z 0,0,1/2)'$ | (4) $4^- (0,0,1/2) \quad 0,0,z$<br>$(4_z^{-1} 0,0,1/2)$ |
|------------------------|------------------------------------|---|---|

For  $(0,0,1)' +$

- |                                  |  |  |  |
|----------------------------------|--|--|--|
| (1) $t' (0,0,1)$<br>$(1 0,0,1)'$ | (2) $2 (0,0,1) \quad 0,0,z$<br>$(2_z 0,0,1)$ | (3) $4^+ (0,0,3/2) \quad 0,0,z$<br>$(4_z 0,0,3/2)$ | (4) $4^- ' (0,0,3/2) \quad 0,0,z$<br>$(4_z^{-1} 0,0,3/2)'$ |
|----------------------------------|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3).

**Positions**

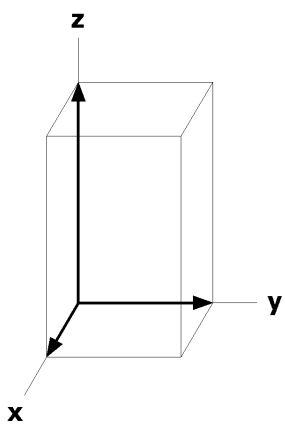
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(0,0,1)' +		
8	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{y},x,z+1/2$ [v, $\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [v, $\bar{u},w$ ]
4	c 2'..	0,1/2,z [u,v,0]	1/2,0,z+1/2 [v, $\bar{u}$ ,0]		
4	b 2'..	1/2,1/2,z [u,v,0]	1/2,1/2,z+1/2 [v, $\bar{u}$ ,0]		
4	a 2'..	0,0,z [u,v,0]	0,0,z+1/2 [v, $\bar{u}$ ,0]		

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>\*1m1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

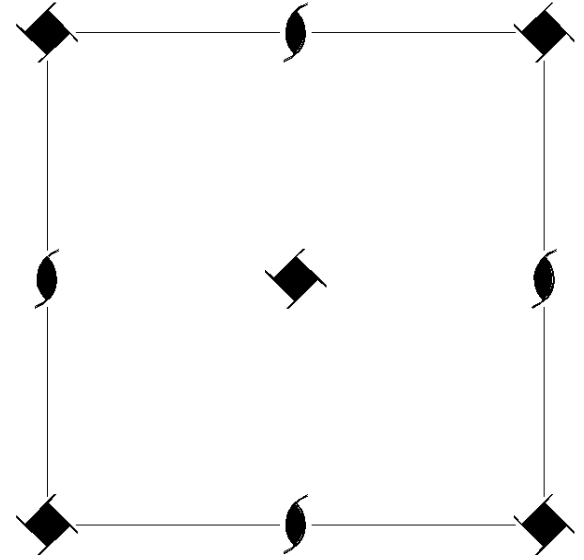
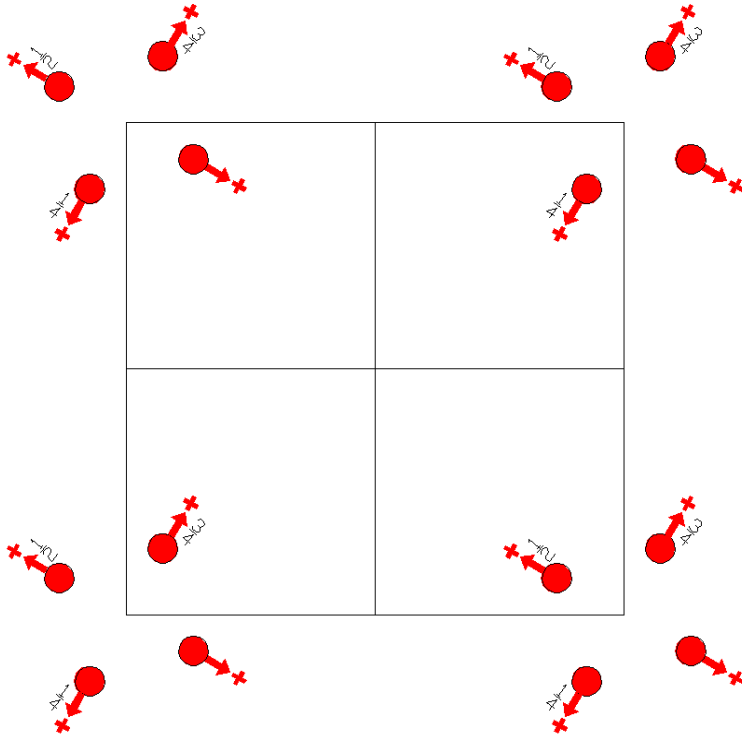
Along [1,1,0] p<sub>2b</sub>\*1m1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P4_3$   
78.1.679

4  
 $P4_3$

Tetragonal



Origin on  $4_3$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

- |                    |  |   |   |
|--------------------|--|---|---|
| (1) 1<br>(1 0,0,0) | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 4 <sup>+</sup> (0,0,3/4) 0,0,z<br>(4 <sub>z</sub>  0,0,3/4) | (4) 4 <sup>-</sup> (0,0,1/4) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/4) |
|--------------------|--|---|---|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

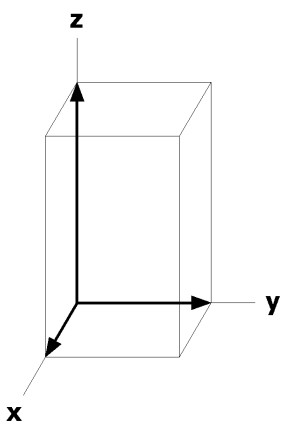
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
4	a 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+3/4$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/4$ [ $v,\bar{u},w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1g'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0

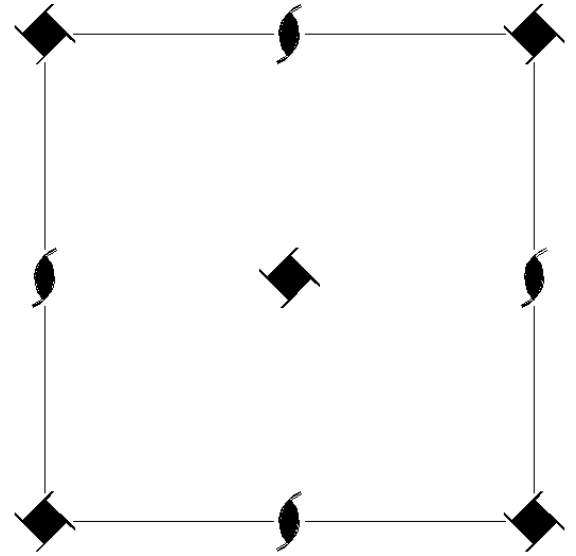
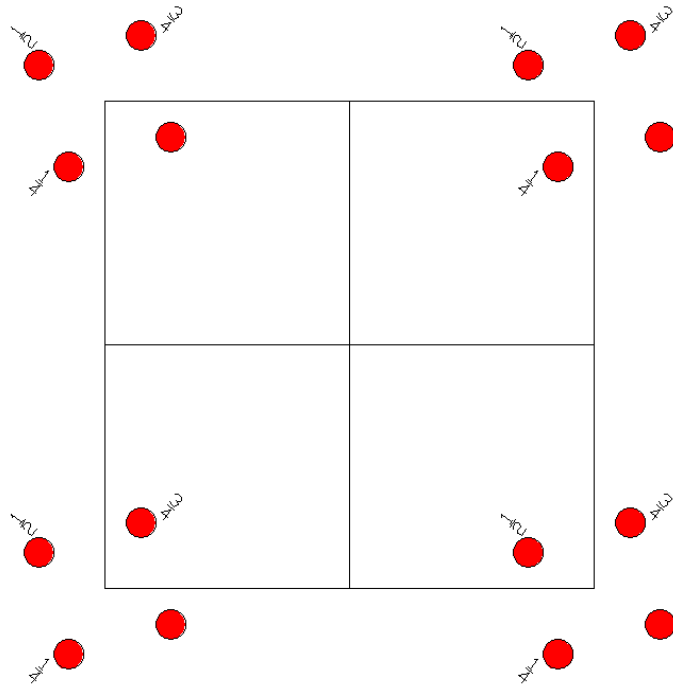


$P4_31'$   
78.2.680

$41'$   
 $P4_31'$

Tetragonal

$1'$



Origin on  $4_31'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For  $1 +$  set

- |                          |  |  |   |
|--------------------------|--|--|---|
| (1) $1$<br>( $1 0,0,0$ ) | (2) $2$ ( $0,0,1/2$ ) $0,0,z$<br>( $2_z 0,0,1/2$ ) | (3) $4^+$ ( $0,0,3/4$ ) $0,0,z$<br>( $4_z 0,0,3/4$ ) | (4) $4^-$ ( $0,0,1/4$ ) $0,0,z$<br>( $4_z^{-1} 0,0,1/4$ ) |
|--------------------------|--|--|---|

For  $1' +$  set

- |                            |  |   |  |
|----------------------------|--|---|--|
| (1) $1'$<br>( $1 0,0,0$ )' | (2) $2'$ ( $0,0,1/2$ ) $0,0,z$<br>( $2_z 0,0,1/2$ )' | (3) $4^{+ '}$ ( $0,0,3/4$ ) $0,0,z$<br>( $4_z 0,0,3/4$ )' | (4) $4^{- '}$ ( $0,0,1/4$ ) $0,0,z$<br>( $4_z^{-1} 0,0,1/4$ )' |
|----------------------------|--|---|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

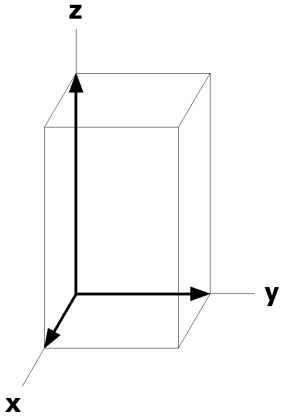
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
4 a 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y}, z+1/2$ [0,0,0]	(3) $\bar{y}, x, z+3/4$ [0,0,0]	(4) $y, \bar{x}, z+1/4$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

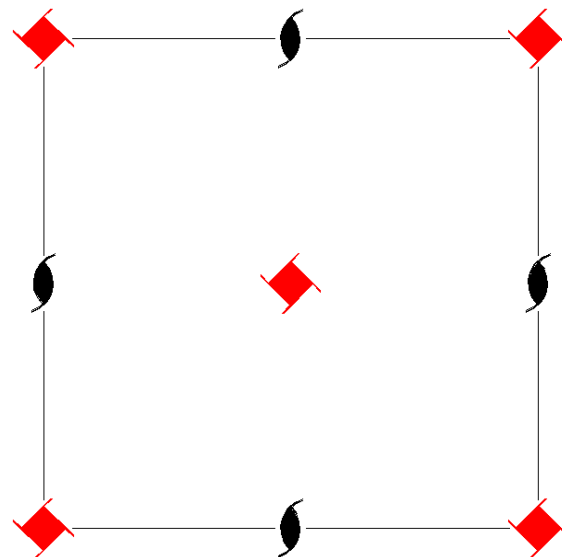
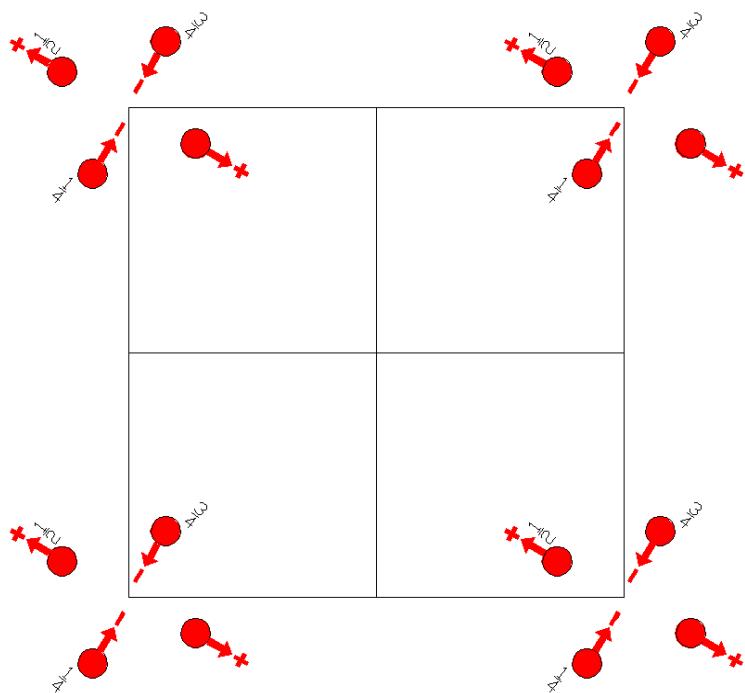
Along [1,1,0] p1g11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P4_3'$   
78.3.681

$4'$   
 $P4_3'$

Tetragonal



Origin on  $4_3'$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

(1)  $1$   
 $(1|0,0,0)$

(2)  $2 (0,0,1/2) \quad 0,0,z$   
 $(2_z|0,0,1/2)$

(3)  $4^+ (0,0,3/4) \quad 0,0,z$   
 $(4_z^+|0,0,3/4)'$

(4)  $4^- (0,0,1/4) \quad 0,0,z$   
 $(4_z^-|0,0,1/4)'$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

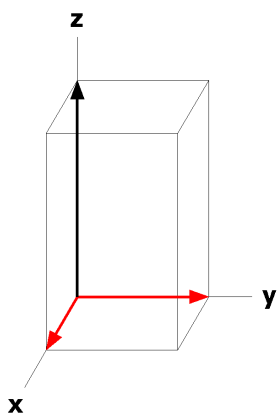
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
4	a 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+3/4$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/4$ [ $\bar{v},u,\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

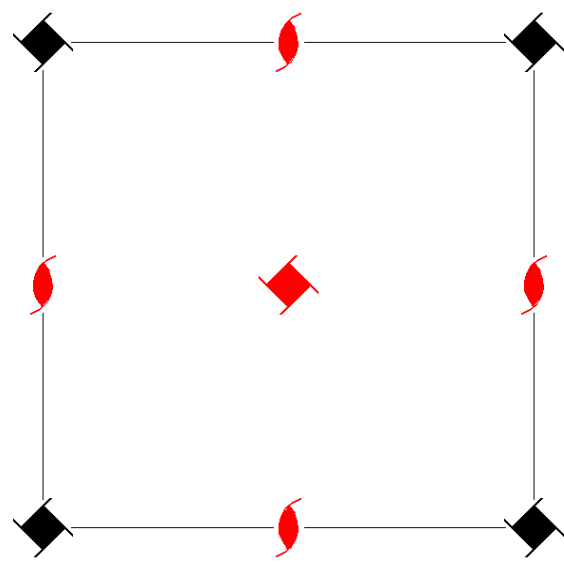
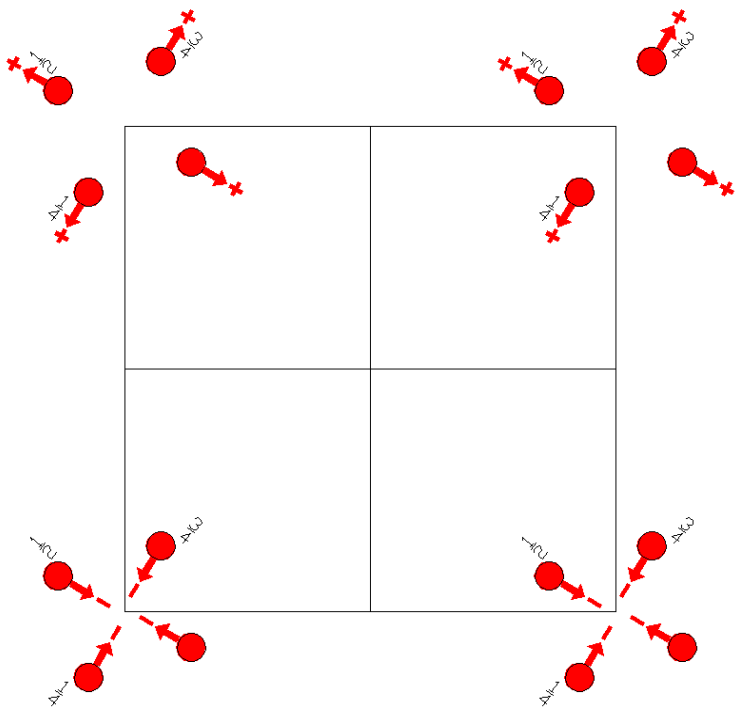
Along [1,1,0] p1g'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_P 4_3$   
78.4.682

$41'$   
 $P_P 4_3$

Tetragonal



Origin on  $4_3$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                    |  |   |   |
|--------------------|--|---|---|
| (1) 1<br>(1 0,0,0) | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 4 <sup>+</sup> (0,0,3/4) 0,0,z<br>(4 <sub>z</sub>  0,0,3/4) | (4) 4 <sup>-</sup> (0,0,1/4) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/4) |
|--------------------|--|---|---|

For  $(1,0,0)'$  + set

- |                              |  |  |  |
|------------------------------|--|--|--|
| (1) t' (1,0,0)<br>(1 1,0,0)' | (2) 2' (0,0,1/2) 1/2,0,z<br>(2 <sub>z</sub>  1,0,1/2)' | (3) 4 <sup>+</sup> ' (0,0,3/4) 1/2,1/2,z<br>(4 <sub>z</sub>  1,0,3/4)' | (4) 4 <sup>-</sup> ' (0,0,1/4) 1/2,1/2,z<br>(4 <sub>z</sub> <sup>-1</sup>  1,0,1/4)' |
|------------------------------|--|--|--|

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3).

**Positions**

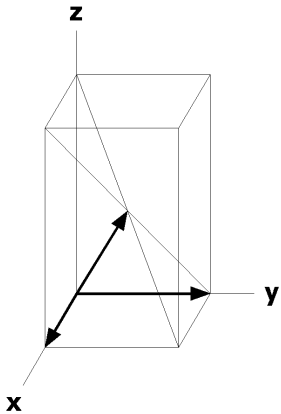
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) + (1,0,0)' +			
8	a 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z+3/4$ [ $\bar{v}, u, w$ ]	(4) $y, \bar{x}, z+1/4$ [ $v, \bar{u}, w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

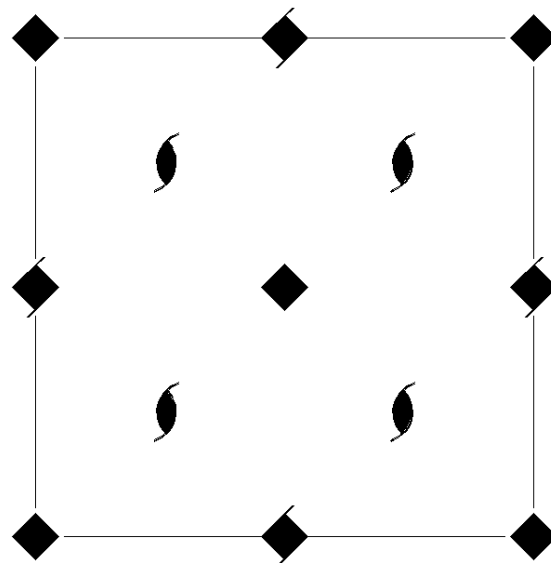
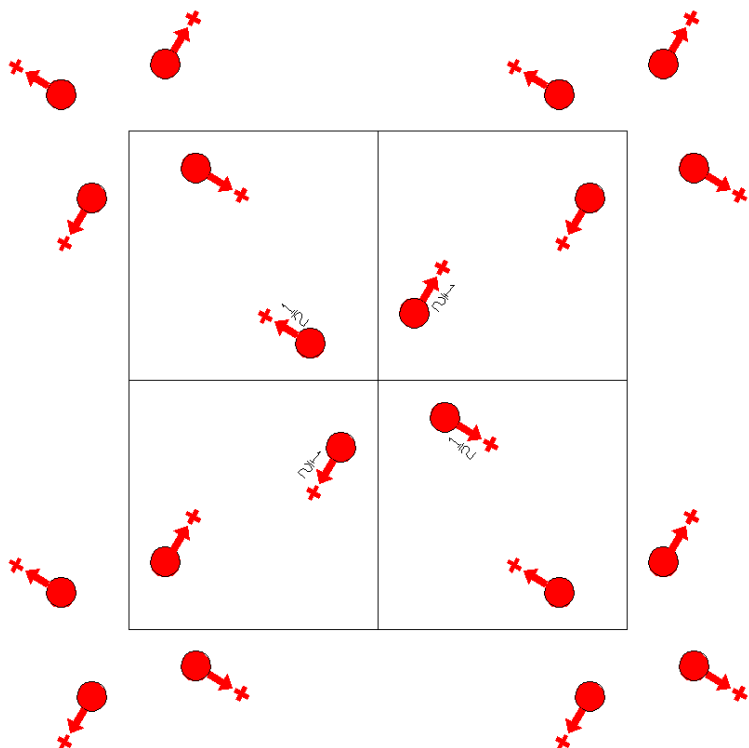
Along [1,1,0] p1g'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



I4  
79.1.683

4  
I4

Tetragonal



Origin on 4

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 4<sup>+</sup> 0,0,z  
(4<sub>z</sub><sup>+</sup>|0,0,0)

(4) 4<sup>-</sup> 0,0,z  
(4<sub>z</sub><sup>-</sup>|0,0,0)

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)  
(1|1/2,1/2,1/2)

(2) 2 (0,0,1/2) 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,1/2)

(3) 4<sup>+</sup> (0,0,1/2) 0,1/2,z  
(4<sub>z</sub><sup>+</sup>|1/2,1/2,1/2)

(4) 4<sup>-</sup> (0,0,1/2) 1/2,0,z  
(4<sub>z</sub><sup>-</sup>|1/2,1/2,1/2)

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,1/2)$ ; (2); (3).

### Positions

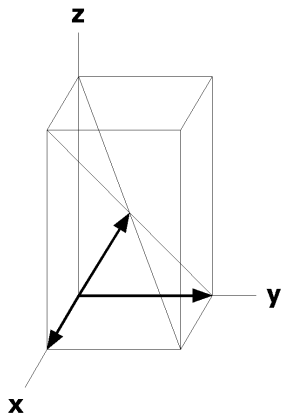
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1/2,1/2,1/2) +		
8	c	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]
4	b	2..	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,w$ ]		
2	a	4..	$0,0,z$ [ $0,0,w$ ]			

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$

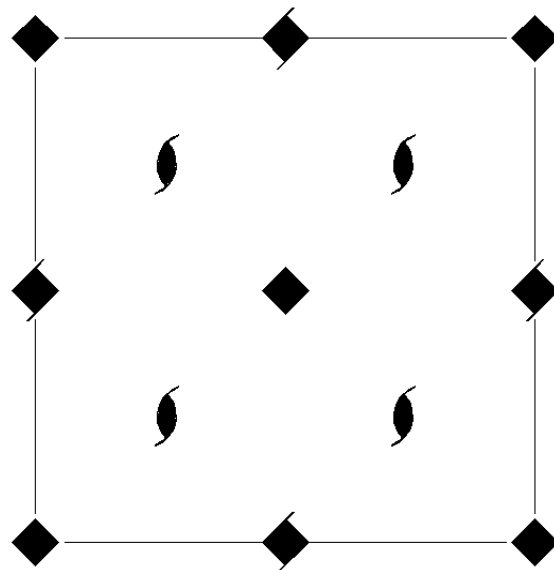
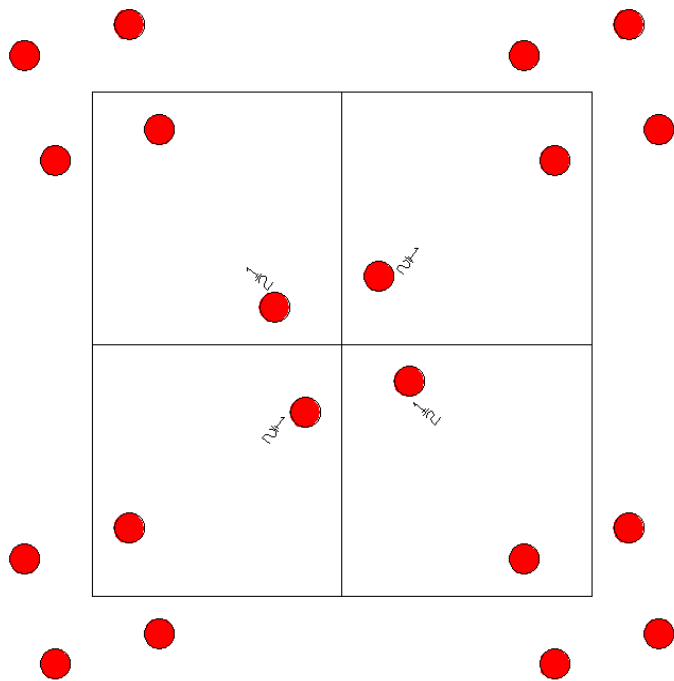


I41'  
79.2.684

41'  
I41'

Tetragonal

1'



Origin on 41'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

- |                    |  |   |   |
|--------------------|--|---|---|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
|--------------------|--|---|---|

For (1/2,1/2,1/2) + set

- |  |  |   |   |
|--|--|---|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2) | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
|--|--|---|---|

For (0,0,0)' + set

- |                      |  |  |  |
|----------------------|--|--|--|
| (1) 1'<br>(1 0,0,0)' | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 4 <sup>+</sup> ' 0,0,z<br>(4 <sub>z</sub>  0,0,0)' | (4) 4 <sup>-</sup> ' 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
|----------------------|--|--|--|

For (1/2,1/2,1/2)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)' | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
|--|--|--|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); 1'.

**Positions**

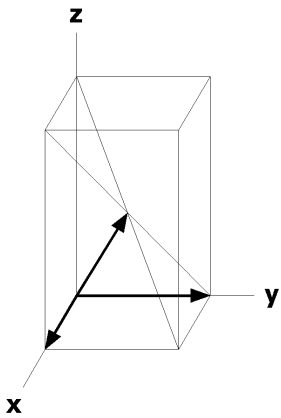
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'		
8	c 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z$ [0,0,0]	(4) $y,\bar{x},z$ [0,0,0]
4	b 2..1'	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]		
2	a 4..1'	0,0,z [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

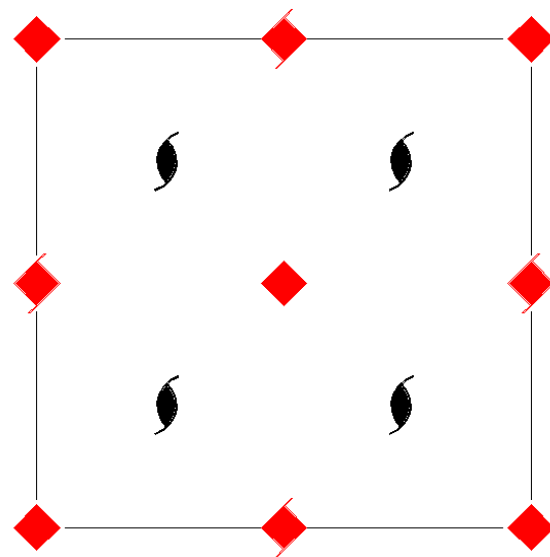
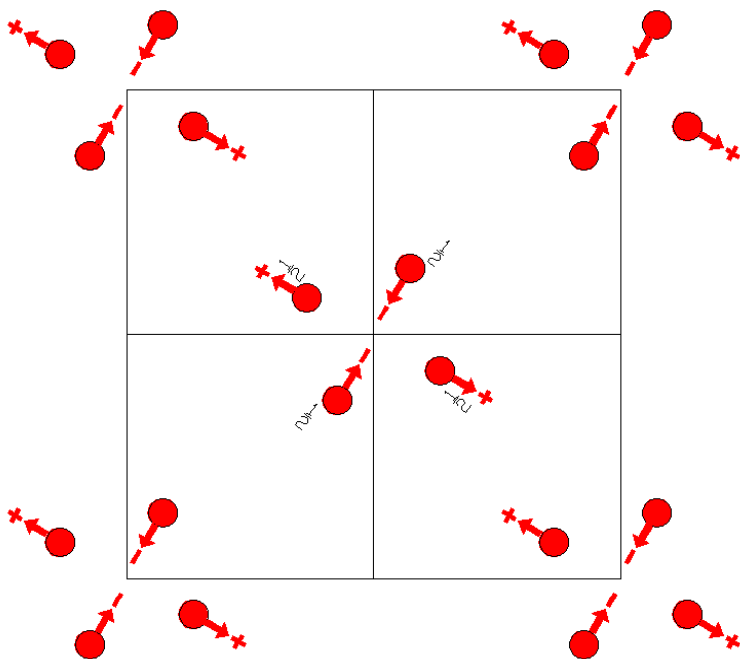
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



I4'  
79.3.685

4'  
I4'

Tetragonal



Origin on 4'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 4<sup>+</sup> 0,0,z  
(4<sub>z</sub>|0,0,0)'

(4) 4<sup>-</sup> 0,0,z  
(4<sub>z</sub><sup>-1</sup>|0,0,0)'

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)  
(1|1/2,1/2,1/2)

(2) 2 (0,0,1/2) 1/4,1/4,z  
(2<sub>z</sub>|1/2,1/2,1/2)

(3) 4<sup>+</sup> (0,0,1/2) 0,1/2,z  
(4<sub>z</sub>|1/2,1/2,1/2)'

(4) 4<sup>-</sup> (0,0,1/2) 1/2,0,z  
(4<sub>z</sub><sup>-1</sup>|1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

### Positions

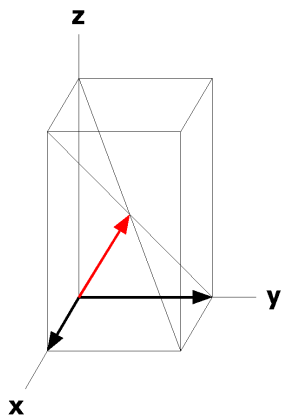
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1/2,1/2,1/2) +		
8	c	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $v,\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
4	b	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]		
2	a	4'..	0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1]  $p4'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

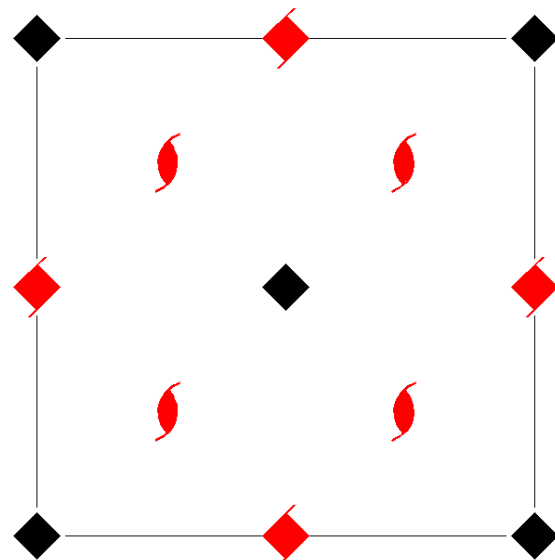
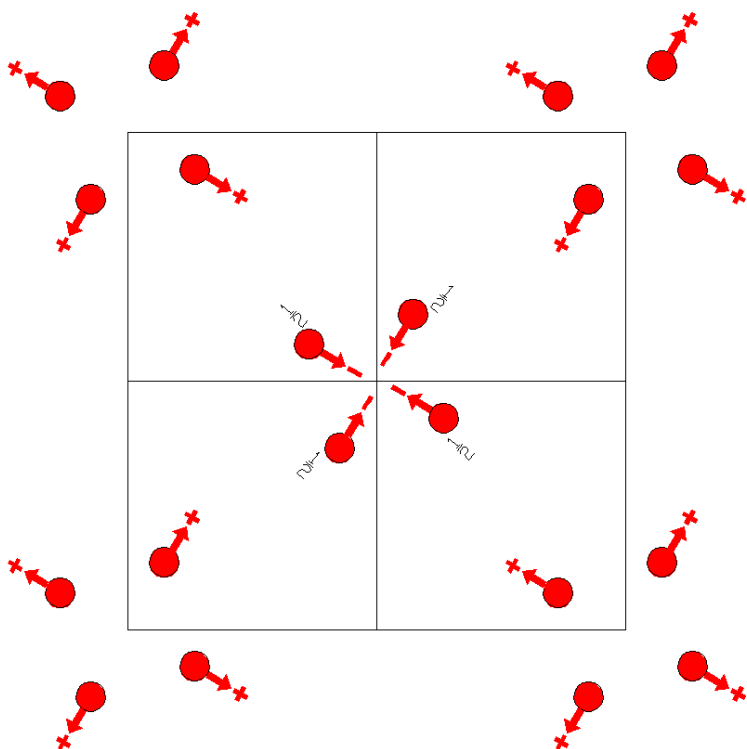
Along [1,1,0]  $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I_p 4$   
79.4.686

$41'$   
 $I_p 4$

Tetragonal



Origin on 4

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $4^+$   $0,0,z$   
( $4_z$ |0,0,0)

(4)  $4^-$   $0,0,z$   
( $4_z^{-1}$ |0,0,0)

For (1/2,1/2,1/2)' + set

(1)  $t'$  (1/2,1/2,1/2)  
(1|1/2,1/2,1/2)'

(2)  $2'$  (0,0,1/2) 1/4,1/4,z  
( $2_z$ |1/2,1/2,1/2)'

(3)  $4^{+ '}$  (0,0,1/2) 0,1/2,z  
( $4_z$ |1/2,1/2,1/2)'

(4)  $4^{- '}$  (0,0,1/2) 1/2,0,z  
( $4_z^{-1}$ |1/2,1/2,1/2)'

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(1/2,1/2,1/2)$ ; (2); (3).

### Positions

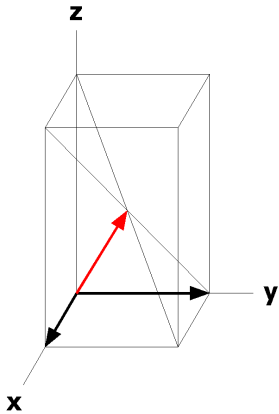
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1/2,1/2,1/2)' +		
8	c	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]
4	b	2..	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,w$ ]		
2	a	4..	$0,0,z$ [ $0,0,w$ ]			

### Symmetry of Special Projections

Along  $[0,0,1]$   $p_p \cdot 4$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c_p \cdot 1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

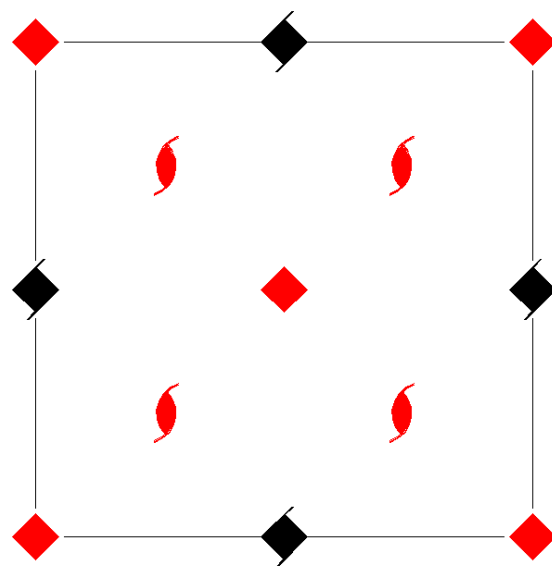
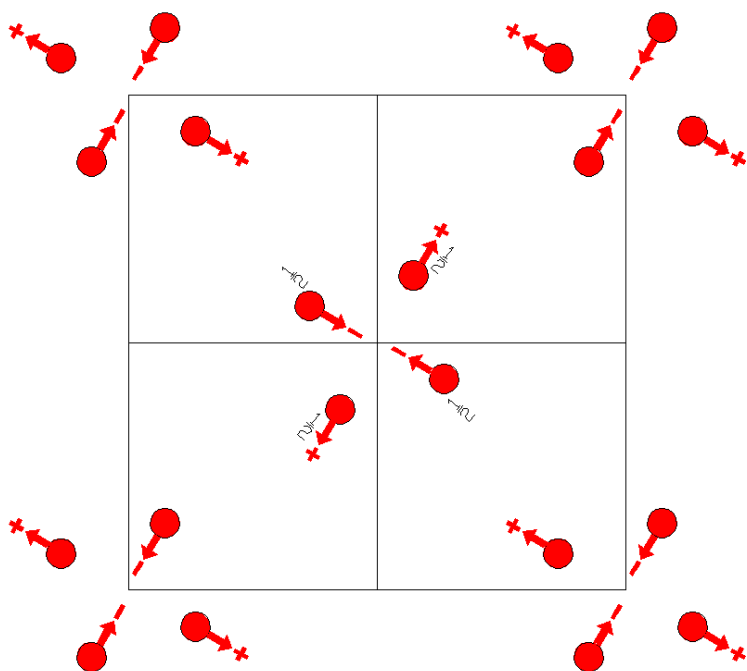
Along  $[1,1,0]$   $p_{2b} \cdot 1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



$I_P 4'$   
79.5.687

$41'$   
 $I_P 4'$

Tetragonal



Origin on  $4'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0)$  + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $4^+ 0,0,z$   
( $4_z$ |0,0,0)'

(4)  $4^- 0,0,z$   
( $4_z^{-1}$ |0,0,0)'

For  $(1/2,1/2,1/2)$ ' + set

(1)  $t' (1/2,1/2,1/2)$   
(1| $1/2,1/2,1/2$ )'

(2)  $2' (0,0,1/2) 1/4,1/4,z$   
( $2_z$ | $1/2,1/2,1/2$ )'

(3)  $4^+ (0,0,1/2) 0,1/2,z$   
( $4_z$ | $1/2,1/2,1/2$ )'

(4)  $4^- (0,0,1/2) 1/2,0,z$   
( $4_z^{-1}$ | $1/2,1/2,1/2$ )'

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(1/2,1/2,1/2)$ ; (2); (3).

### Positions

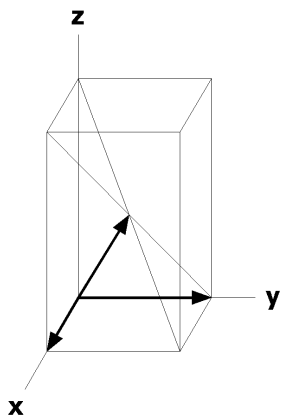
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1/2,1/2,1/2)' +		
8	c	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $v,\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
4	b	2..	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,\bar{w}$ ]		
2	a	4'..	$0,0,z$ [ $0,0,0$ ]			

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $1/2,0,z$

Along  $[1,0,0]$   $c1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

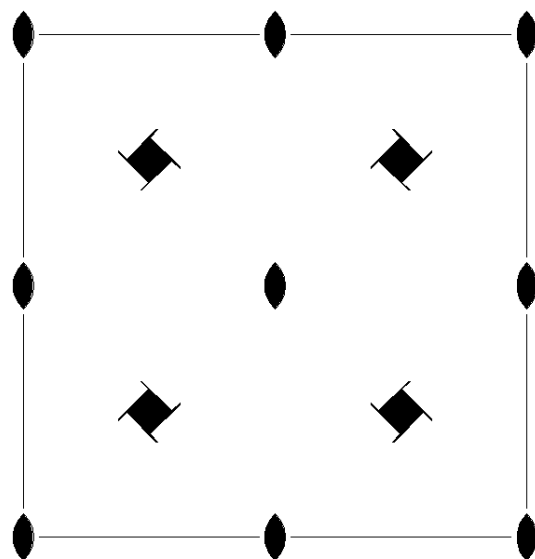
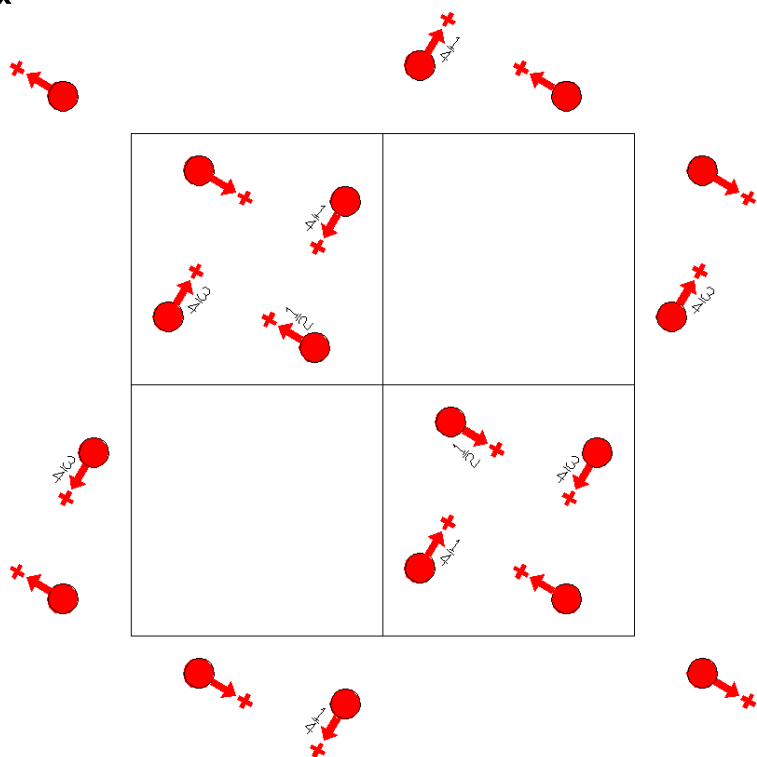
Along  $[1,1,0]$   $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



$I4_1$   
80.1.688

4  
 $I4_1$

Tetragonal



Origin on 2

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |                    |  |  |   |
|--------------------|--|--|---|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> (0,0,1/4) -1/4,1/4,z<br>(4 <sub>z</sub>  0,1/2,1/4) | (4) 4 <sup>-</sup> (0,0,1/4) 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4) |
|--------------------|--|--|---|

For (1/2,1/2,1/2) + set

- |  |  |   |  |
|--|--|---|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2) | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,3/4) 1/4,1/4,z<br>(4 <sub>z</sub>  1/2,0,3/4) | (4) 4 <sup>-</sup> (0,0,3/4) 1/4,-1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,0,3/4) |
|--|--|---|--|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

**Positions**

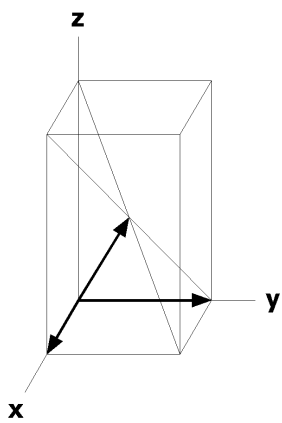
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,1/2) +		
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $v,\bar{u},w$ ]
4	a 2..	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p4  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] c1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

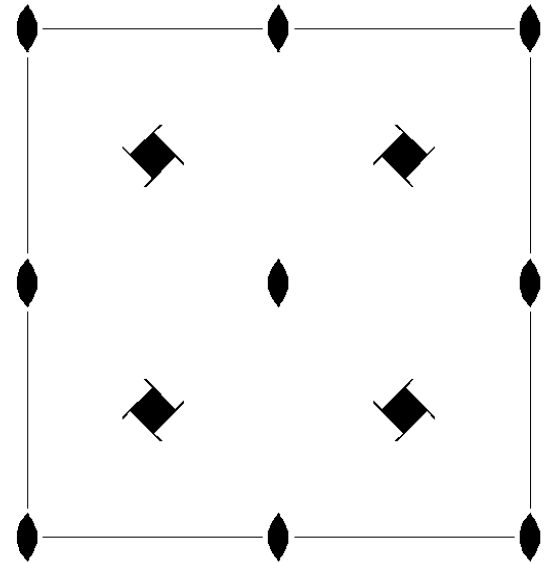
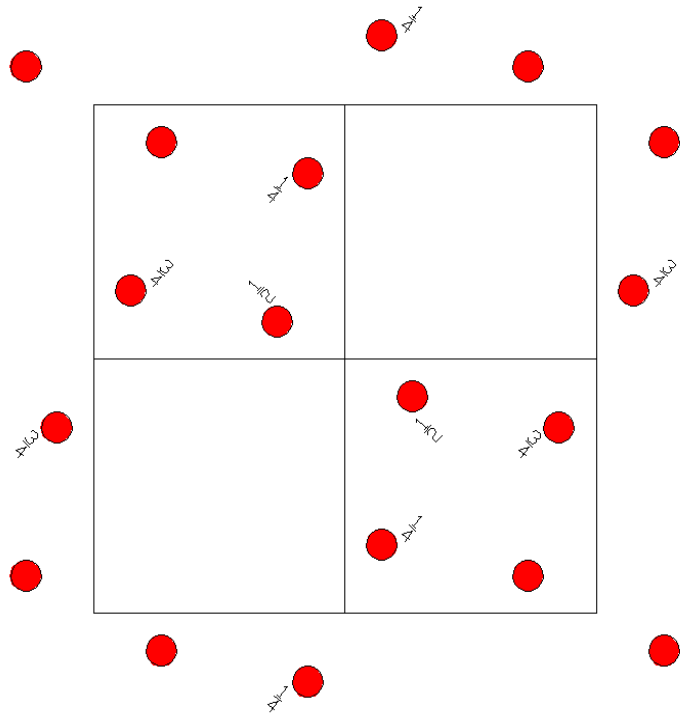


$I4_11'$   
80.2.689

$41'$   
 $I4_11'$

Tetragonal

**1'**



Origin on  $21'$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For  $(0,0,0) + \text{set}$

- |                        |                                      |   |   |
|------------------------|--------------------------------------|---|---|
| (1) $1$<br>$(1 0,0,0)$ | (2) $2 \quad 0,0,z$<br>$(2_z 0,0,0)$ | (3) $4^+ (0,0,1/4) \quad -1/4,1/4,z$<br>$(4_z 0,1/2,1/4)$ | (4) $4^- (0,0,1/4) \quad 1/4,1/4,z$<br>$(4_z^{-1} 0,1/2,1/4)$ |
|------------------------|--------------------------------------|---|---|

For  $(1/2,1/2,1/2) + \text{set}$

- |  |  |  |  |
|--|--|--|--|
| (1) $t (1/2,1/2,1/2)$<br>$(1 1/2,1/2,1/2)$ | (2) $2 (0,0,1/2) \quad 1/4,1/4,z$<br>$(2_z 1/2,1/2,1/2)$ | (3) $4^+ (0,0,3/4) \quad 1/4,1/4,z$<br>$(4_z 1/2,0,3/4)$ | (4) $4^- (0,0,3/4) \quad 1/4,-1/4,z$<br>$(4_z^{-1} 1/2,0,3/4)$ |
|--|--|--|--|

For  $(0,0,0)' + \text{set}$

- |                          |  |   |   |
|--------------------------|--|---|---|
| (1) $1'$<br>$(1 0,0,0)'$ | (2) $2' \quad 0,0,z$<br>$(2_z 0,0,0)'$ | (3) $4^{+'} (0,0,1/4) \quad -1/4,1/4,z$<br>$(4_z 0,1/2,1/4)'$ | (4) $4^{-'} (0,0,1/4) \quad 1/4,1/4,z$<br>$(4_z^{-1} 0,1/2,1/4)'$ |
|--------------------------|--|---|---|

For  $(1/2,1/2,1/2)' + \text{set}$

- |  |  |  |  |
|--|--|--|--|
| (1) $t' (1/2,1/2,1/2)$<br>$(1 1/2,1/2,1/2)'$ | (2) $2' (0,0,1/2) \quad 1/4,1/4,z$<br>$(2_z 1/2,1/2,1/2)'$ | (3) $4^{+'} (0,0,3/4) \quad 1/4,1/4,z$<br>$(4_z 1/2,0,3/4)'$ | (4) $4^{-'} (0,0,3/4) \quad 1/4,-1/4,z$<br>$(4_z^{-1} 1/2,0,3/4)'$ |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); 1'.

**Positions**

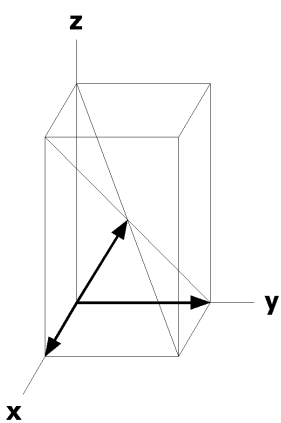
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'		
8	b 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y}, z$ [0,0,0]	(3) $\bar{y}, x+1/2, z+1/4$ [0,0,0]	(4) $y, \bar{x}+1/2, z+1/4$ [0,0,0]
4	a 2..1'	0,0,z [0,0,0]	0,1/2,z+1/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4, 1/4, z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

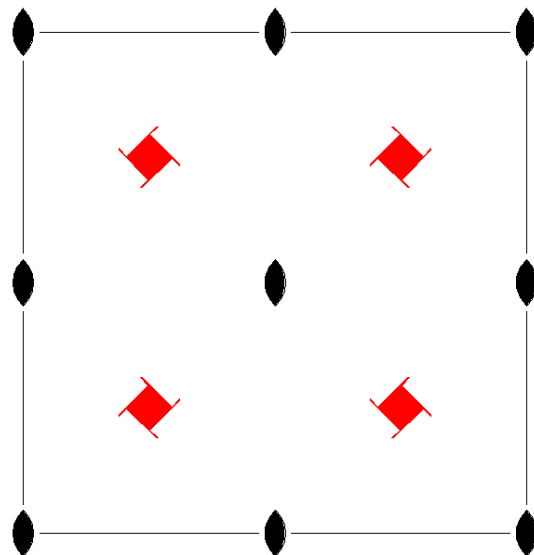
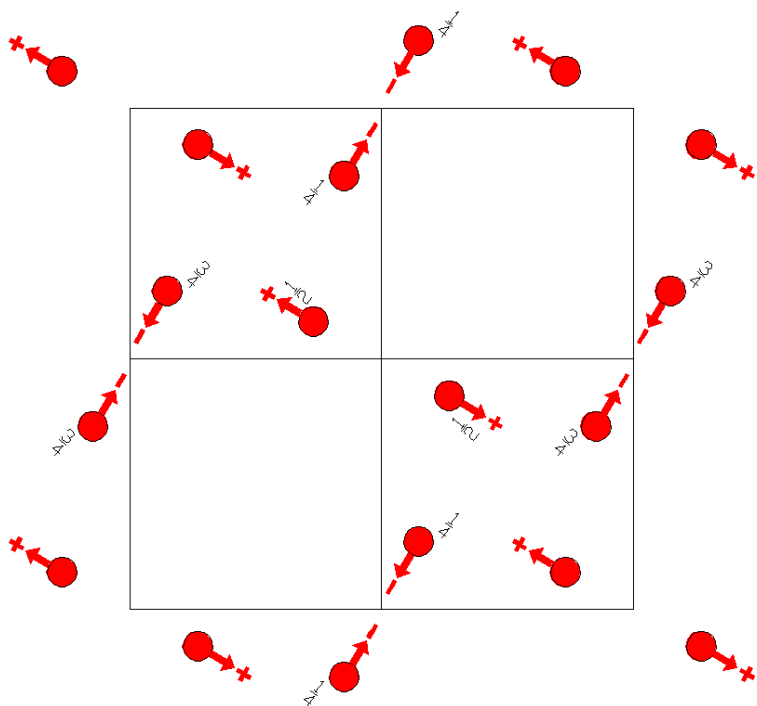
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I4_1'$   
80.3.690

$4'$   
 $I4_1'$

Tetragonal



Origin on 2

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |                    |  |   |  |
|--------------------|--|---|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> (0,0,1/4) -1/4,1/4,z<br>(4 <sub>z</sub>  0,1/2,1/4)' | (4) 4 <sup>-</sup> (0,0,1/4) 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4)' |
|--------------------|--|---|--|

For (1/2,1/2,1/2) + set

- |  |  |  |   |
|--|--|--|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2) | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,3/4) 1/4,1/4,z<br>(4 <sub>z</sub>  1/2,0,3/4)' | (4) 4 <sup>-</sup> (0,0,3/4) 1/4,-1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,0,3/4)' |
|--|--|--|---|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

**Positions**

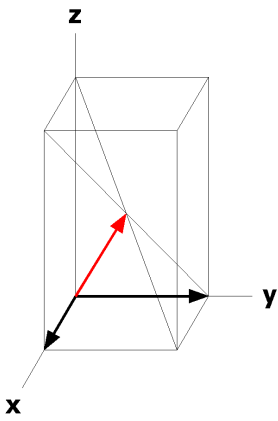
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,1/2) +		
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $\bar{v},u,\bar{w}$ ]
4	a 2..	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p4'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] c1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

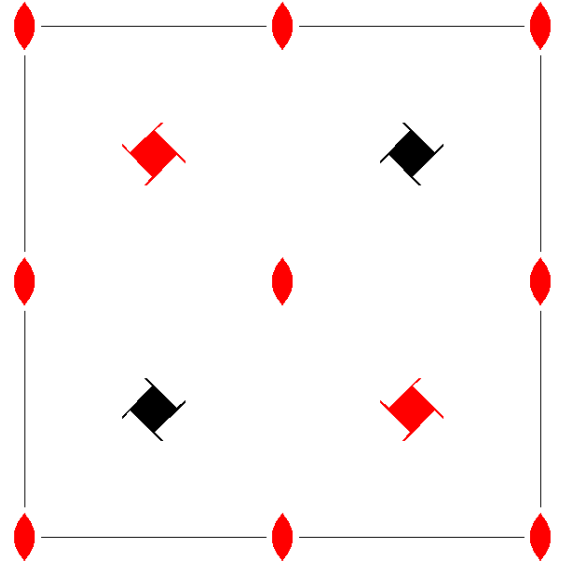
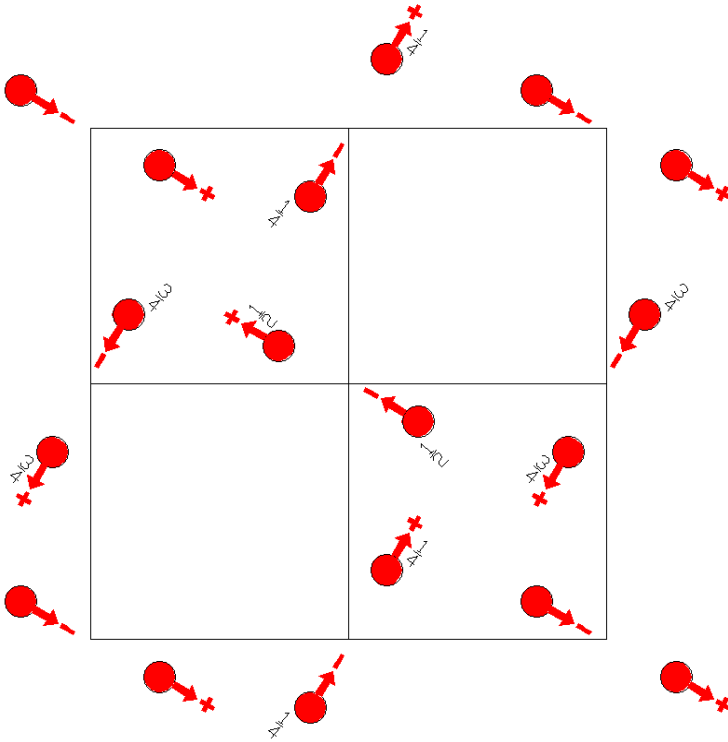
Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I_P 4_1$   
80.4.691

$41'$   
 $I_P 4_1$

Tetragonal



Origin on  $2'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

Symmetry Operations

For  $(0,0,0)$  + set

- |                    |                                      |   |  |
|--------------------|--------------------------------------|---|--|
| (1) 1<br>(1 0,0,0) | (2) $2'$ $0,0,z$<br>( $2_z$  0,0,0)' | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>( $4_z$  0,1/2,1/4) | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>( $4_z^{-1}$  0,1/2,1/4)' |
|--------------------|--------------------------------------|---|--|

For  $(1/2,1/2,1/2)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1/2,1/2,1/2)$<br>(1 1/2,1/2,1/2)' | (2) $2$ $(0,0,1/2) 1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2) | (3) $4^+'$ $(0,0,3/4) 1/4,1/4,z$<br>( $4_z$  1/2,0,3/4)' | (4) $4^-$ $(0,0,3/4) 1/4,-1/4,z$<br>( $4_z^{-1}$  1/2,0,3/4) |
|--|--|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

### Positions

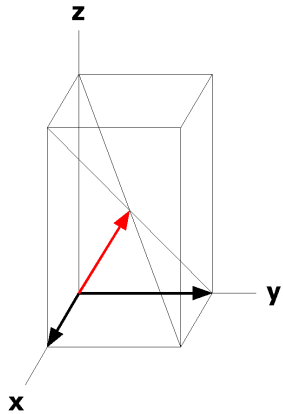
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +	(1/2,1/2,1/2)' +		
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x+1/2, z+1/4$ [ $\bar{v}, u, w$ ]	(4) $y, \bar{x}+1/2, z+1/4$ [ $v, \bar{u}, w$ ]
4	a 2'..	0,0,z [u,v,0]	0,1/2,z+1/4 [ $\bar{v}, u, 0$ ]		

### Symmetry of Special Projections

Along [0,0,1]  $p_p^* 4$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at -1/4, 1/4, z

Along [1,0,0]  $c_p^* 1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

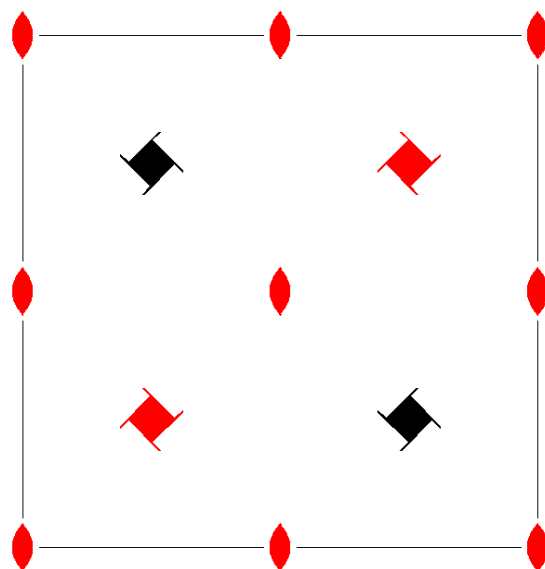
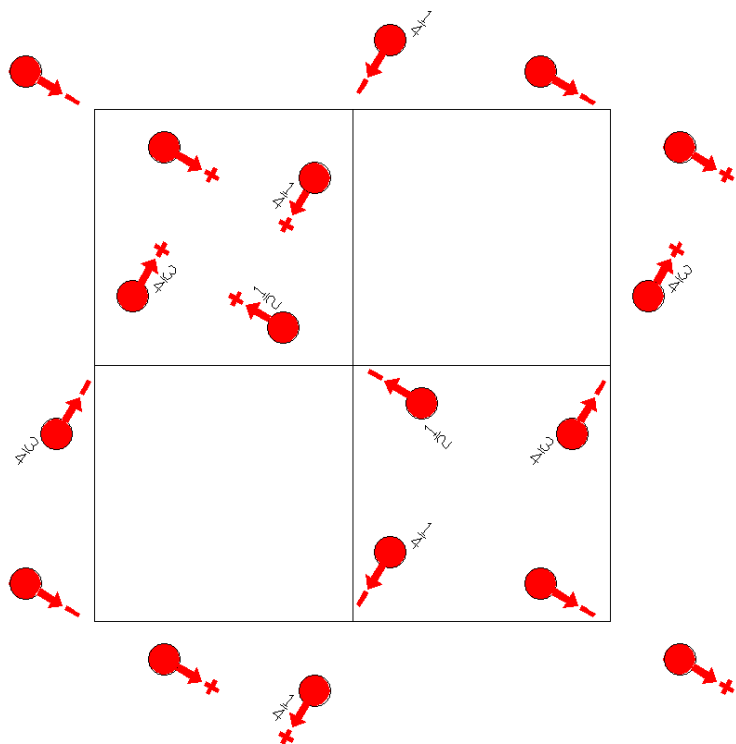
Along [1,1,0]  $p_{2b}^* 1m1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I_P 4_1'$   
80.5.692

$41'$   
 $I_P 4_1'$

Tetragonal



Origin on  $2'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

Symmetry Operations

For  $(0,0,0)$  + set

- |                    |                                      |  |   |
|--------------------|--------------------------------------|--|---|
| (1) 1<br>(1 0,0,0) | (2) $2'$ $0,0,z$<br>( $2_z$  0,0,0)' | (3) $4^+$ $(0,0,1/4)$ $-1/4,1/4,z$<br>( $4_z$  0,1/2,1/4)' | (4) $4^-$ $(0,0,1/4)$ $1/4,1/4,z$<br>( $4_z^{-1}$  0,1/2,1/4) |
|--------------------|--------------------------------------|--|---|

For  $(1/2,1/2,1/2)'$  + set

- |  |  |  |   |
|--|--|--|---|
| (1) $t'$ $(1/2,1/2,1/2)$<br>(1 1/2,1/2,1/2)' | (2) $2$ $(0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2) | (3) $4^+$ $(0,0,3/4)$ $1/4,1/4,z$<br>( $4_z$  1/2,0,3/4) | (4) $4^-$ $(0,0,3/4)$ $1/4,-1/4,z$<br>( $4_z^{-1}$  1/2,0,3/4)' |
|--|--|--|---|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

**Positions**

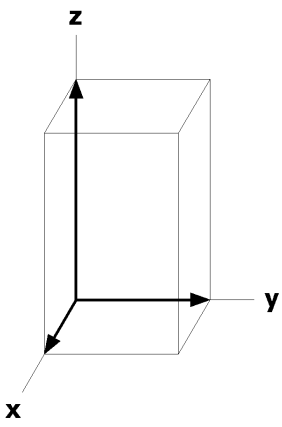
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +		(1/2,1/2,1/2)' +	
8	b 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{y},x+1/2,z+1/4$ [v, $\bar{u},\bar{w}$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [v, $\bar{u},w$ ]
4	a 2'..	0,0,z [u,v,0]	0,1/2,z+1/4 [v, $\bar{u},0$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_{p^*} 4$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at -1/4,1/4,z

Along [1,0,0]  $c_{p^*} 1m1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

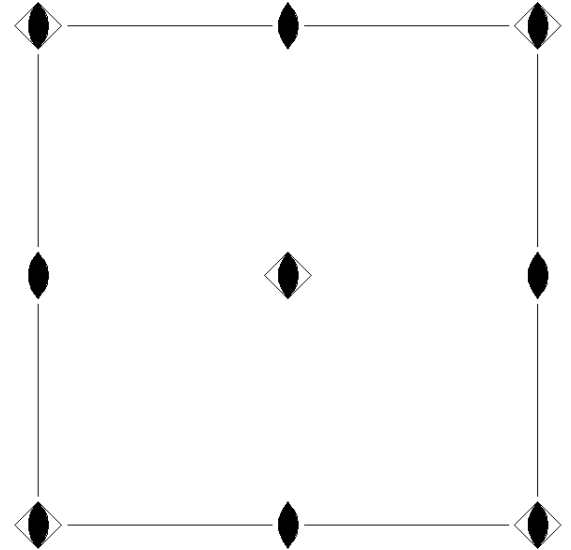
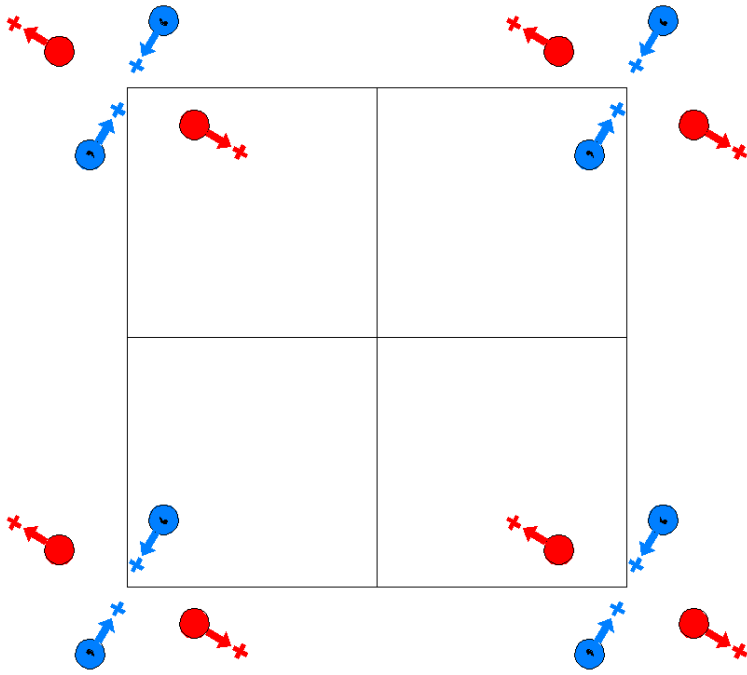
Along [1,1,0]  $p_{2b^*} 1m1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P\bar{4}$   
81.1.693

$\bar{4}$   
 $P\bar{4}$

Tetragonal



Origin on  $\bar{4}$

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3)  $\bar{4}^+$  0,0,z; 0,0,0  
( $\bar{4}_z$ |0,0,0)

(4)  $\bar{4}^-$  0,0,z; 0,0,0  
( $\bar{4}_z^{-1}$ |0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

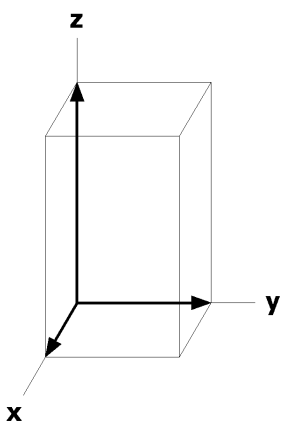
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
4	h	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
2	g	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]		
2	f	2..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
2	e	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
1	d	$\bar{4}$ ..	1/2,1/2,1/2 [0,0,w]			
1	c	$\bar{4}$ ..	1/2,1/2,0 [0,0,w]			
1	b	$\bar{4}$ ..	0,0,1/2 [0,0,w]			
1	a	$\bar{4}$ ..	0,0,0 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1]  $p4'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0

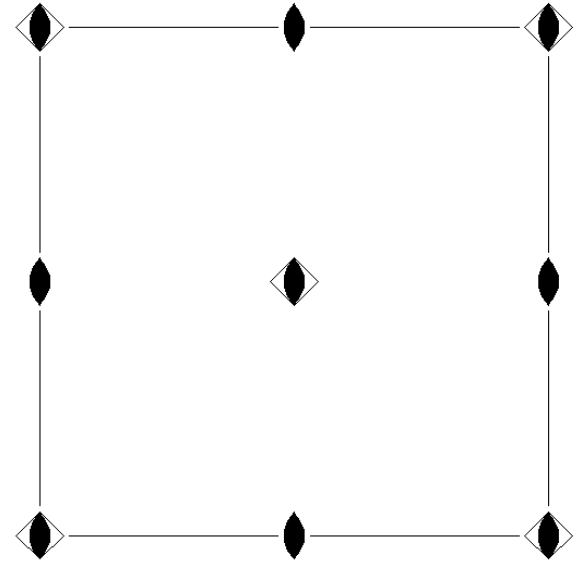
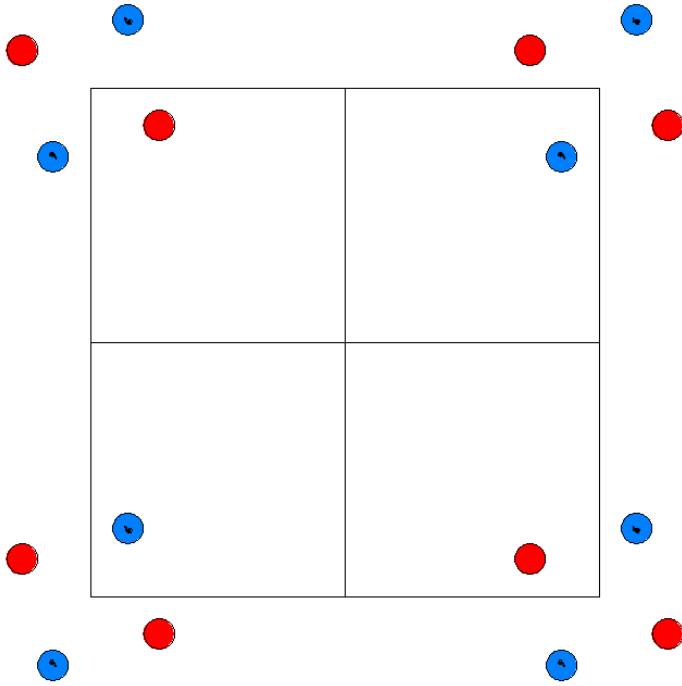


$P\bar{4}1'$   
81.2.694

$\bar{4}1'$   
 $P\bar{4}1'$

Tetragonal

$1'$



Origin on  $\bar{4}1'$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

- |                            |  |  |   |  |
|----------------------------|--|--|---|--|
|                            |  | For $1 +$ set  |   |  |
| (1) $1$<br>( $1 0,0,0$ )   | (2) $2 \quad 0,0,z$<br>( $2_z 0,0,0$ )   | (3) $\bar{4}^+ \quad 0,0,z; \quad 0,0,0$<br>( $\bar{4}_z 0,0,0$ )  | (4) $\bar{4}^- \quad 0,0,z; \quad 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ )  |  |
|                            |  | For $1' +$ set   |   |  |
| (1) $1'$<br>( $1 0,0,0$ )' | (2) $2' \quad 0,0,z$<br>( $2_z 0,0,0$ )' | (3) $\bar{4}^+ \quad 0,0,z; \quad 0,0,0$<br>( $\bar{4}_z 0,0,0$ )' | (4) $\bar{4}^- \quad 0,0,z; \quad 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ )' |  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

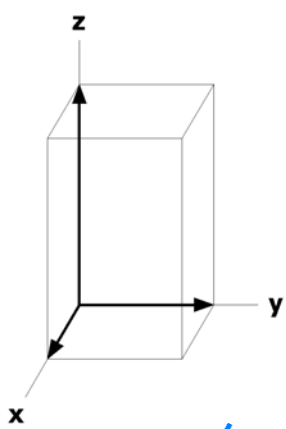
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +	1 +	1' +	1' +
4 h 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $y,\bar{x},\bar{z}$ [0,0,0]	(4) $\bar{y},x,\bar{z}$ [0,0,0]
2 g 2..1'	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
2 f 2..1'	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
2 e 2..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
1 d $\bar{4}..1'$	1/2,1/2,1/2 [0,0,0]			
1 c $\bar{4}..1'$	1/2,1/2,0 [0,0,0]			
1 b $\bar{4}..1'$	0,0,1/2 [0,0,0]			
1 a $\bar{4}..1'$	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $p41'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

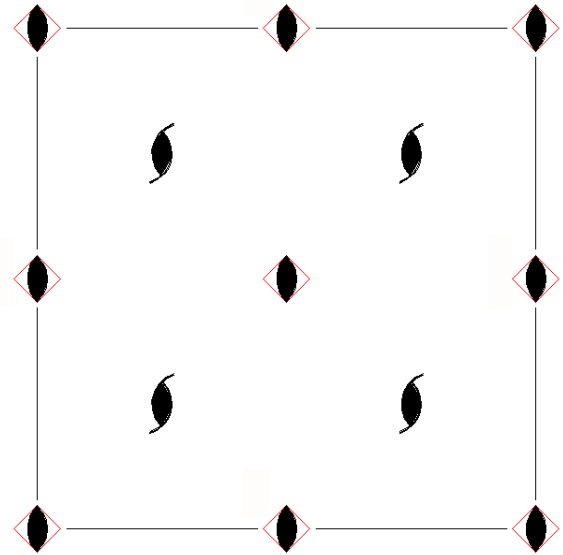
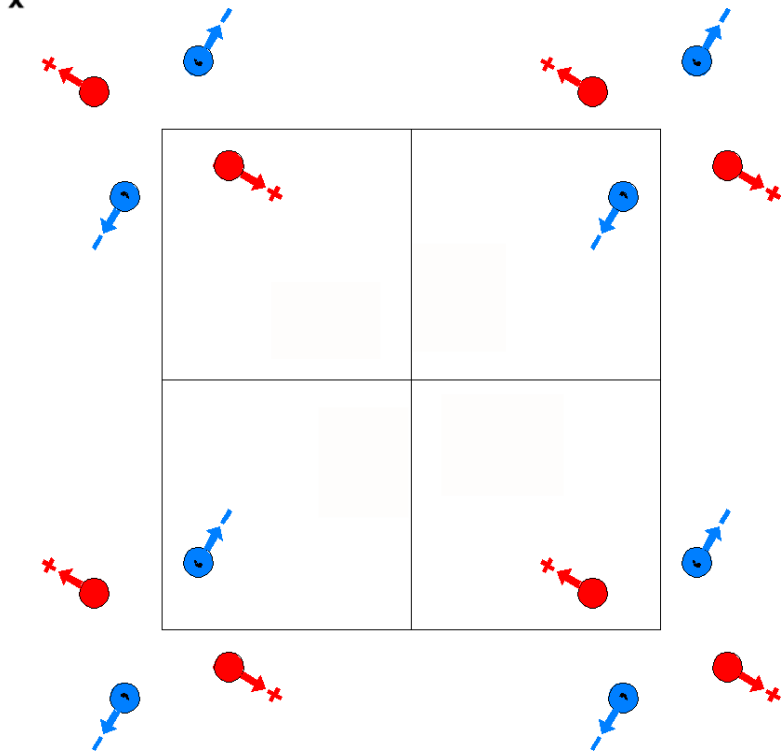
Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P&'  
81.3.695

&'  
P&'

Tetragonal



Origin on &'

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1\*0,0,0)

(2) 2 0,0,z  
(2z\*0,0,0)

(3) &' 0,0,z; 0,0,0  
(&'z\*0,0,0)'

(4) &' 0,0,z; 0,0,0  
(&'z^-1\*0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

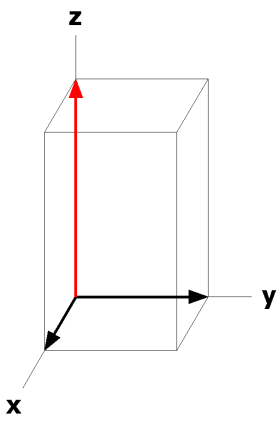
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
4	h 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
2	g 2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	f 2..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	e 2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
1	d $\bar{4}'$ ..	1/2,1/2,1/2 [0,0,0]			
1	c $\bar{4}'$ ..	1/2,1/2,0 [0,0,0]			
1	b $\bar{4}'$ ..	0,0,1/2 [0,0,0]			
1	a $\bar{4}'$ ..	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

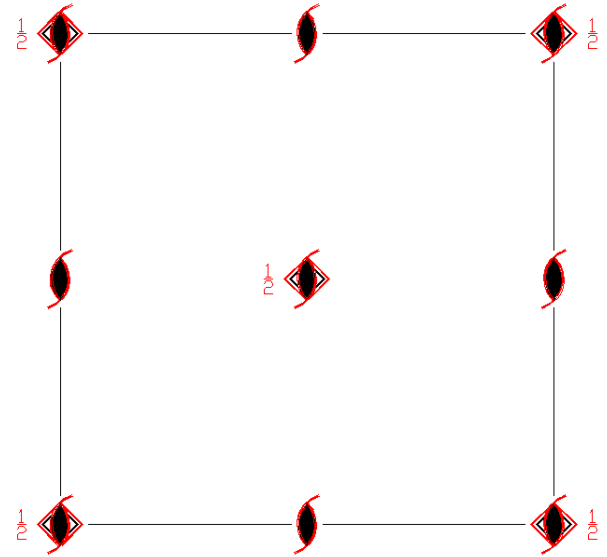
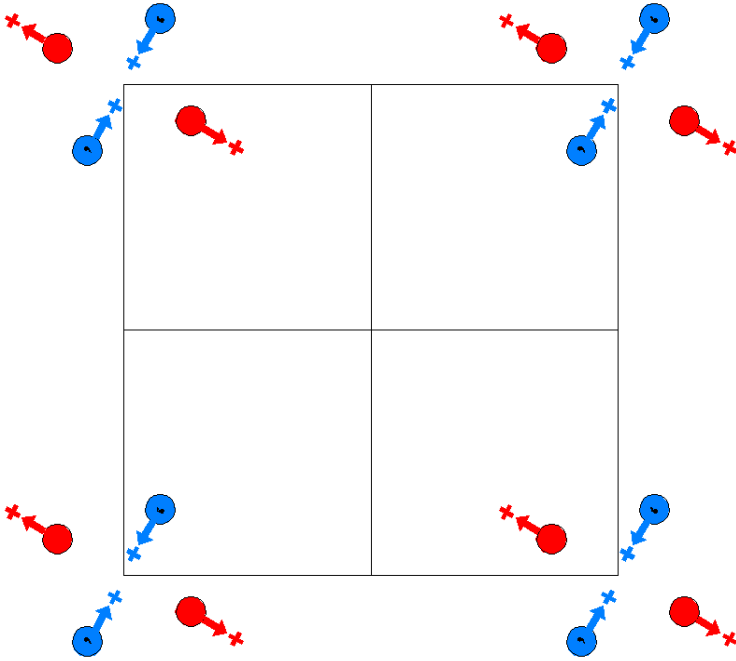
Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_{2c} \bar{4}$   
81.4.696

$\bar{4}1'$   
 $P_{2c} \bar{4}$

Tetragonal



Origin on  $\bar{4}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For  $(0,0,0) + \text{set}$

- |                    |                                  |   |  |
|--------------------|----------------------------------|---|--|
| (1) 1<br>(1 0,0,0) | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1}$  0,0,0) |
|--------------------|----------------------------------|---|--|

For  $(0,0,1)' + \text{set}$

- |                                  |  |  |   |
|----------------------------------|--|--|---|
| (1) $t'$ $(0,0,1)$<br>(1 0,0,1)' | (2) $2'$ $(0,0,1)$ $0,0,z$<br>( $2_z$  0,0,1)' | (3) $\bar{4}^+$ $0,0,z; 0,0,1/2$<br>( $\bar{4}_z$  0,0,1)' | (4) $\bar{4}^-$ $0,0,z; 0,0,1/2$<br>( $\bar{4}_z^{-1}$  0,0,1)' |
|----------------------------------|--|--|---|



**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3).

**Positions**

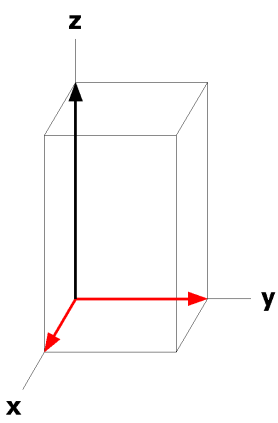
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
8 h 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
4 g 2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]		
4 f 2..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
4 e 2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
2 d $\bar{4}'$ ..	1/2,1/2,1/2 [0,0,0]			
2 c $\bar{4}$ ..	1/2,1/2,0 [0,0,w]			
2 b $\bar{4}'$ ..	0,0,1/2 [0,0,0]			
2 a $\bar{4}$ ..	0,0,0 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>·1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

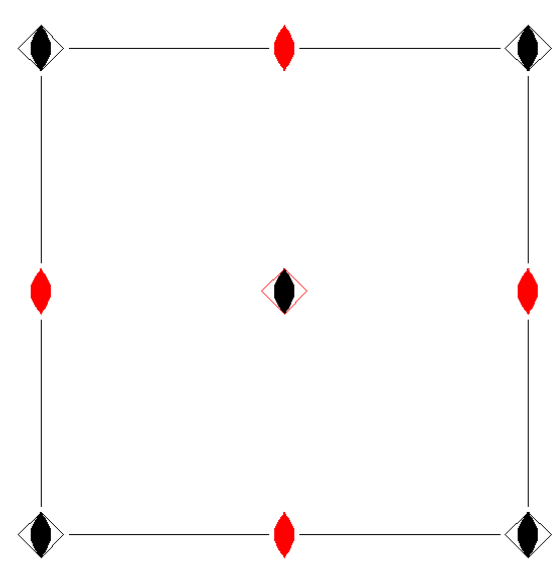
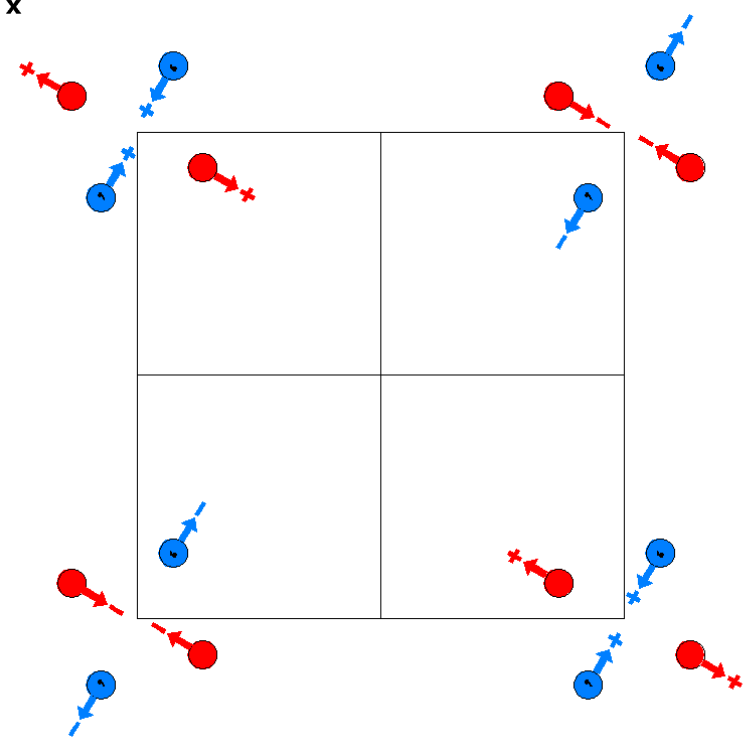
Along [1,1,0] p<sub>2b</sub>·1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_P \bar{4}$   
81.5.697

$\bar{4}1'$   
 $P_P \bar{4}$

Tetragonal



Origin on  $\bar{4}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

- (1) 1  
(1|0,0,0)
- (2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)
- (3)  $\bar{4}^+$  0,0,z; 0,0,0  
( $\bar{4}_z^+$ |0,0,0)
- (4)  $\bar{4}^-$  0,0,z; 0,0,0  
( $\bar{4}_z^{-1}$ |0,0,0)

For (1,0,0)' + set

- (1) t' (1,0,0)  
(1|1,0,0)'
- (2) 2' 1/2,0,z  
(2<sub>z</sub>|1,0,0)'
- (3)  $\bar{4}^+$  ' 1/2,1/2,z; 1/2,1/2,0  
( $\bar{4}_z^+$ |1,0,0)'
- (4)  $\bar{4}^-$  ' 1/2,1/2,z; 1/2,1/2,0  
( $\bar{4}_z^{-1}$ |1,0,0)'

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3).

**Positions**

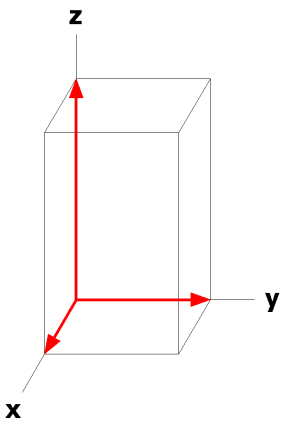
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
8 h 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
4 g 2'..	0,1/2,z [u,v,0]	1/2,0, $\bar{z}$ [ $v,\bar{u},0$ ]		
4 f 2..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
4 e 2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
2 d $\bar{4}'$ ..	1/2,1/2,1/2 [0,0,0]			
2 c $\bar{4}'$ ..	1/2,1/2,0 [0,0,0]			
2 b $\bar{4}'$ ..	0,0,1/2 [0,0,w]			
2 a $\bar{4}'$ ..	0,0,0 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1]  $p_4$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/2,1/2,z

Along [1,0,0]  $p1m1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

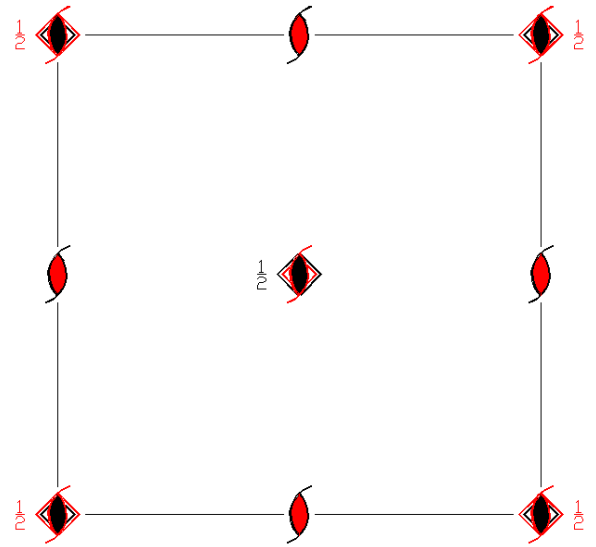
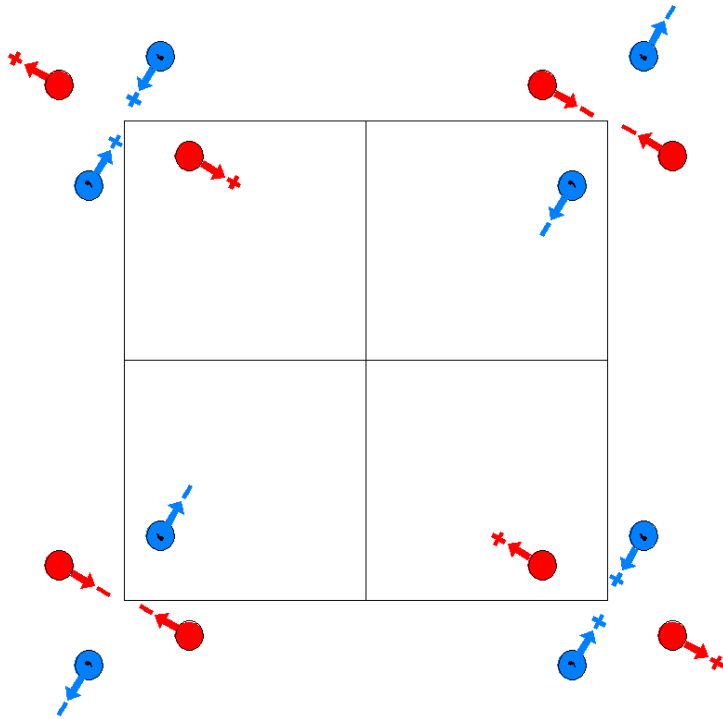
Along [1,1,0]  $p_{2a}1m1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x-1/4, x+1/4, 0$



$P_1\bar{4}$   
81.6.698

$\bar{4}1'$   
 $P_1\bar{4}$

Tetragonal



Origin on  $\bar{4}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

(0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $\bar{4}^+$   $0,0,z; 0,0,0$   
( $\bar{4}_z$ |0,0,0)

(4)  $\bar{4}^-$   $0,0,z; 0,0,0$   
( $\bar{4}_z^{-1}$ |0,0,0)

For (1,0,0)' + set

(1)  $t'$  (1,0,0)  
(1|1,0,0)'

(2)  $2'$   $1/2,0,z$   
( $2_z$ |1,0,0)'

(3)  $\bar{4}^+$   $1/2,1/2,z; 1/2,1/2,0$   
( $\bar{4}_z$ |1,0,0)'

(4)  $\bar{4}^-$   $1/2,1/2,z; 1/2,1/2,0$   
( $\bar{4}_z^{-1}$ |1,0,0)'

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3).

**Positions**

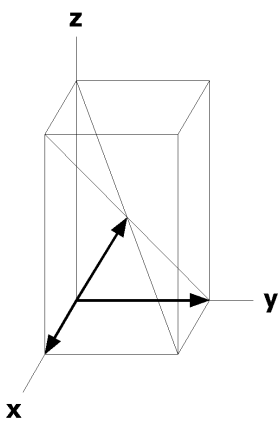
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
8 h 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
4 g 2'..	0,1/2,z [u,v,0]	1/2,0, $\bar{z}$ [ $v,\bar{u},0$ ]		
4 f 2..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
4 e 2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
2 d $\bar{4}$ ..	1/2,1/2,1/2 [0,0,w]			
2 c $\bar{4}$ '..	1/2,1/2,0 [0,0,0]			
2 b $\bar{4}$ '..	0,0,1/2 [0,0,0]			
2 a $\bar{4}$ ..	0,0,0 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

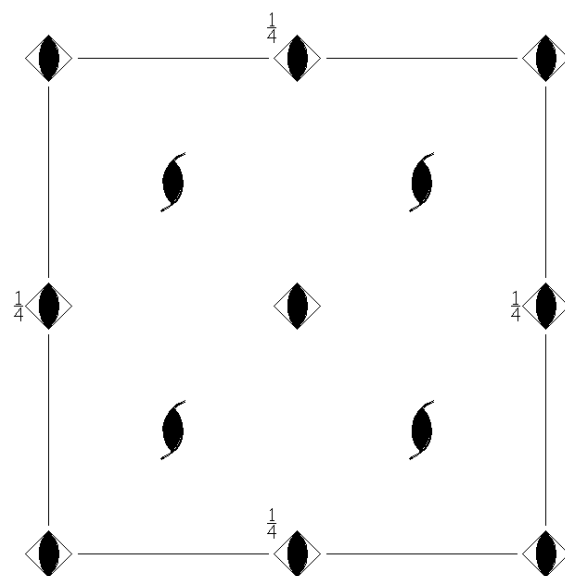
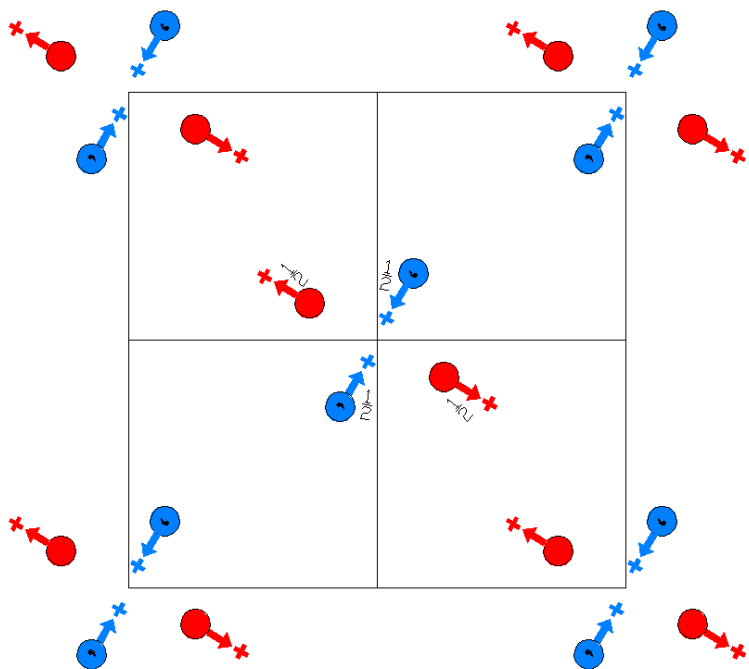
Along [1,1,0]  $p_c\bar{1}m1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x-1/4, x+1/4, 0$



$\bar{4}$   
82.1.699

$\bar{4}$   
 $\bar{4}$

Tetragonal



Origin on  $\bar{4}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

- |                    |  |   |  |
|--------------------|--|---|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0) |
|--------------------|--|---|--|

For (1/2,1/2,1/2) + set

- |  |  |   |  |
|--|--|---|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2) | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2) | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2) |
|--|--|---|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

**Positions**

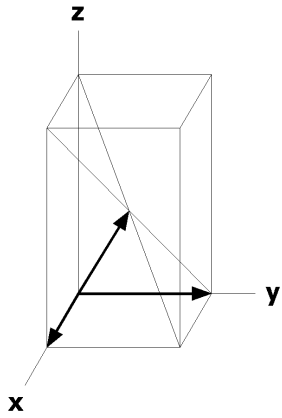
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +		(1/2,1/2,1/2) +	
8	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
4	f	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]		
4	e	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
2	d	$\bar{4}$ ..	0,1/2,3/4 [0,0,w]			
2	c	$\bar{4}$ ..	0,1/2,1/4 [0,0,w]			
2	b	$\bar{4}$ ..	0,0,1/2 [0,0,w]			
2	a	$\bar{4}$ ..	0,0,0 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1]  $p4'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

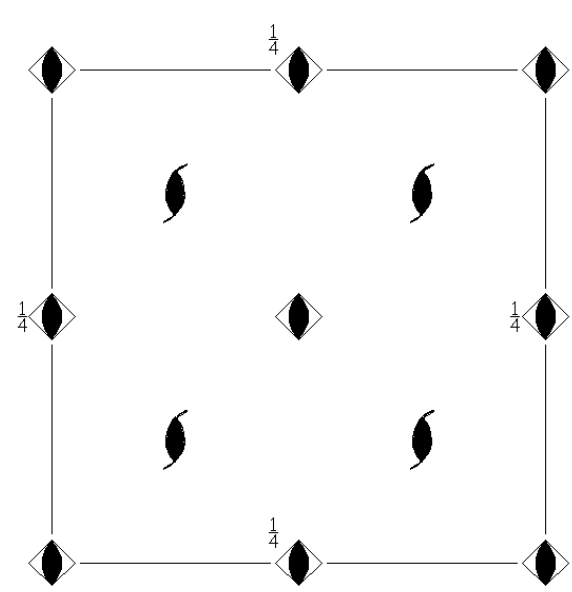
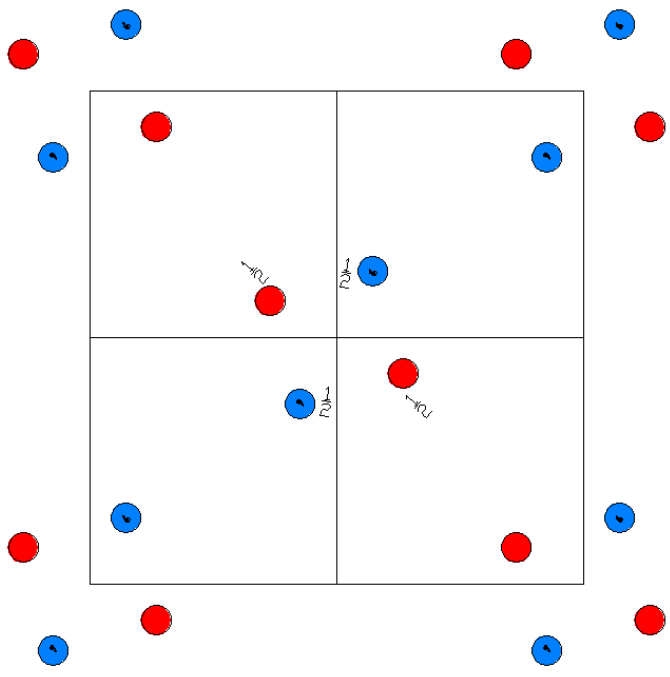


$\bar{4}1'$   
82.2.700

$\bar{4}1'$   
 $\bar{4}1'$

Tetragonal

1'



Origin on  $\bar{4}1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

- |                    |  |   |  |
|--------------------|--|---|--|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0) |
|--------------------|--|---|--|

For (1/2,1/2,1/2) + set

- |  |  |   |  |
|--|--|---|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2) | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2) | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2) |
|--|--|---|--|

For (0,0,0)' + set

- |                      |  |  |   |
|----------------------|--|--|---|
| (1) 1'<br>(1 0,0,0)' | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)' |
|----------------------|--|--|---|

For (1/2,1/2,1/2)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)' | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2)' | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2)' |
|--|--|--|---|



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3);1'.

**Positions**

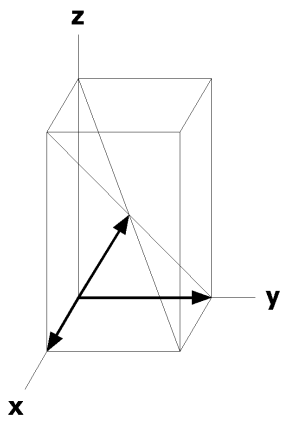
				Coordinates					
Multiplicity, Wyckoff letter, Site Symmetry.				(0,0,0) + (0,0,0)' +	(1/2,1/2,1/2) + (1/2,1/2,1/2)' +				
8	g 11'	(1) x,y,z	[0,0,0]	(2) $\bar{x},\bar{y},z$	[0,0,0]	(3) $y,\bar{x},\bar{z}$	[0,0,0]	(4) $\bar{y},x,\bar{z}$	[0,0,0]
4	f 2..1'	0,1/2,z	[0,0,0]	1/2,0, $\bar{z}$	[0,0,0]				
4	e 2..1'	0,0,z	[0,0,0]	0,0, $\bar{z}$	[0,0,0]				
2	d $\bar{4}..1'$	0,1/2,3/4	[0,0,0]						
2	c $\bar{4}..1'$	0,1/2,1/4	[0,0,0]						
2	b $\bar{4}..1'$	0,0,1/2	[0,0,0]						
2	a $\bar{4}..1'$	0,0,0	[0,0,0]						

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

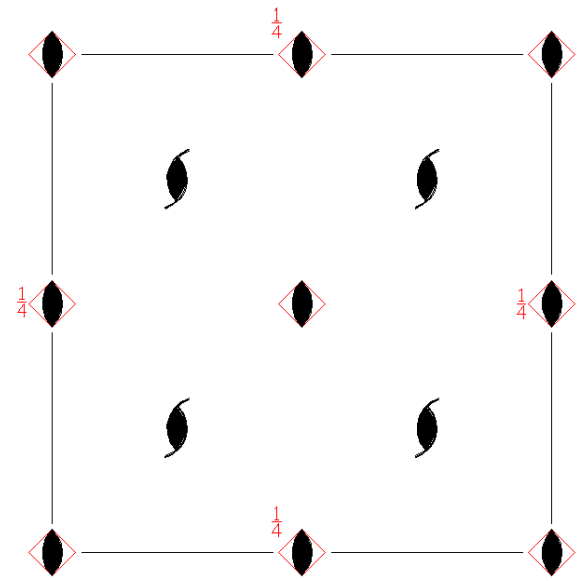
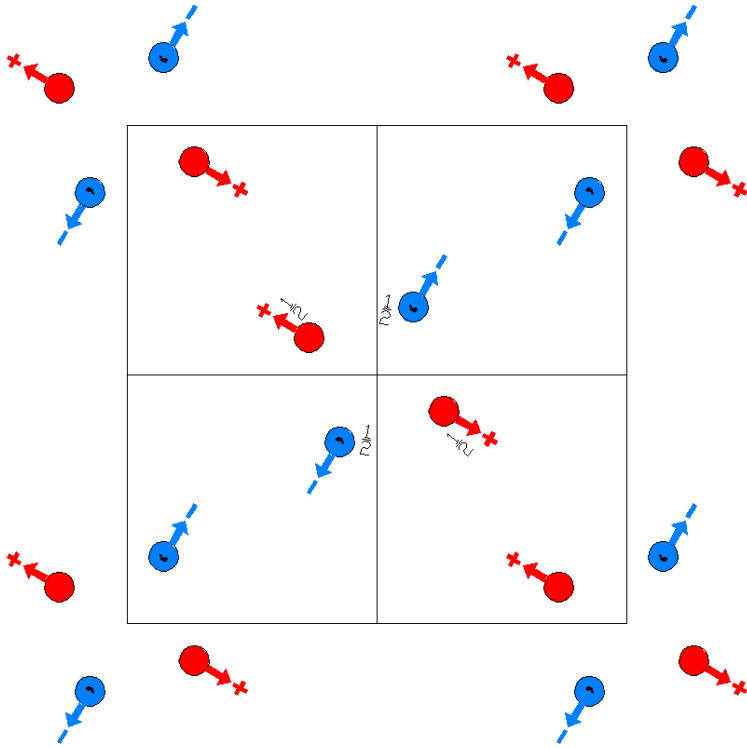
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$\bar{4}'$   
82.3.701

$\bar{4}'$   
 $\bar{4}'$

Tetragonal



Origin on  $\bar{4}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

- |                    |  |  |   |
|--------------------|--|--|---|
| (1) 1<br>(1 0,0,0) | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)' |
|--------------------|--|--|---|

For (1/2,1/2,1/2) + set

- |  |  |  |   |
|--|--|--|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2) | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2)' | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2)' |
|--|--|--|---|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

**Positions**

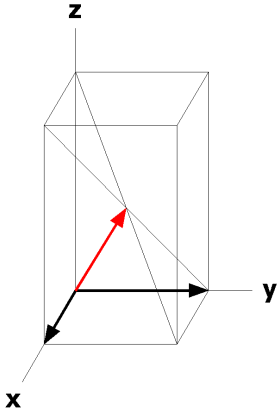
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +		(1/2,1/2,1/2) +	
8	g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
4	f 2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4	e 2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	d $\bar{4}'$ ..	0,1/2,3/4 [0,0,0]			
2	c $\bar{4}'$ ..	0,1/2,1/4 [0,0,0]			
2	b $\bar{4}'$ ..	0,0,1/2 [0,0,0]			
2	a $\bar{4}'$ ..	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

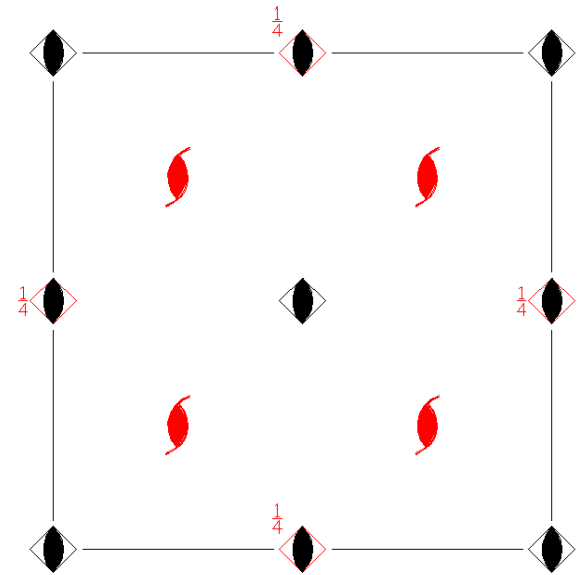
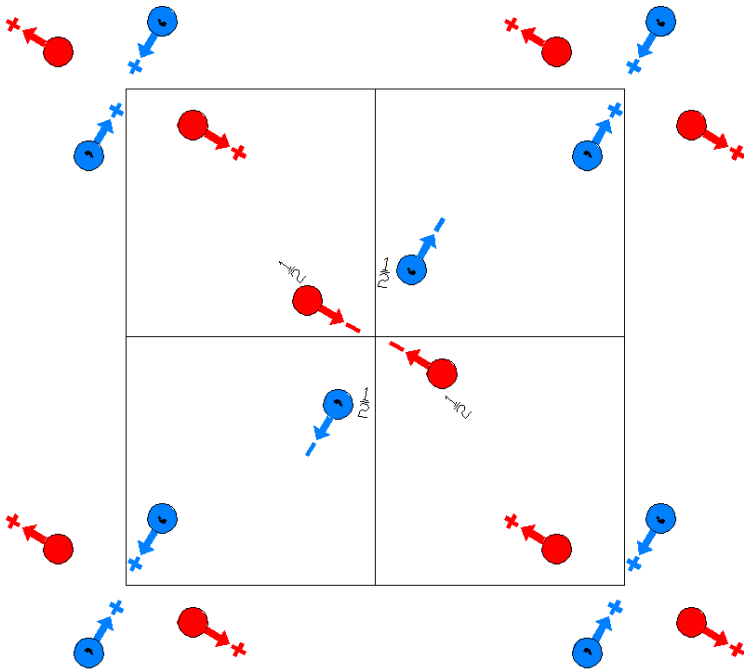
Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I_p \bar{4}$   
82.4.702

$\bar{4}1'$   
 $I_p \bar{4}$

Tetragonal



Origin on  $\bar{4}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $\bar{4}^+$   $0,0,z; 0,0,0$   
( $\bar{4}_z$ |0,0,0)

(4)  $\bar{4}^-$   $0,0,z; 0,0,0$   
( $\bar{4}_z^{-1}$ |0,0,0)

For (1/2,1/2,1/2)' + set

(1)  $t'$  (1/2,1/2,1/2)  
(1|1/2,1/2,1/2)'

(2)  $2'$  (0,0,1/2)  $1/4,1/4,z$   
( $2_z$ |1/2,1/2,1/2)'

(3)  $\bar{4}^+$  '  $1/2,0,z; 1/2,0,1/4$   
( $\bar{4}_z$ |1/2,1/2,1/2)'

(4)  $\bar{4}^-$  '  $0,1/2,z; 0,1/2,1/4$   
( $\bar{4}_z^{-1}$ |1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

**Positions**

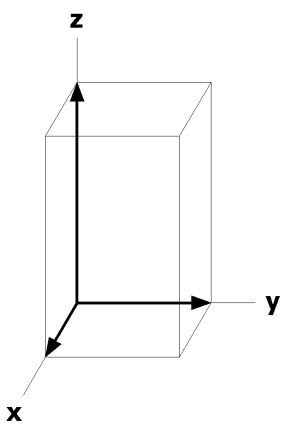
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
8 g 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $y, \bar{x}, \bar{z}$ [ $\bar{v}, u, w$ ]	(4) $\bar{y}, x, \bar{z}$ [ $v, \bar{u}, w$ ]
4 f 2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]		
4 e 2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
2 d $\bar{4}'$ ..	0,1/2,3/4 [0,0,0]			
2 c $\bar{4}'$ ..	0,1/2,1/4 [0,0,0]			
2 b $\bar{4}'$ ..	0,0,1/2 [0,0,0]			
2 a $\bar{4}'$ ..	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $p_{p^*} 4$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/2,0,z

Along [1,0,0]  $c_{p^*} 1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

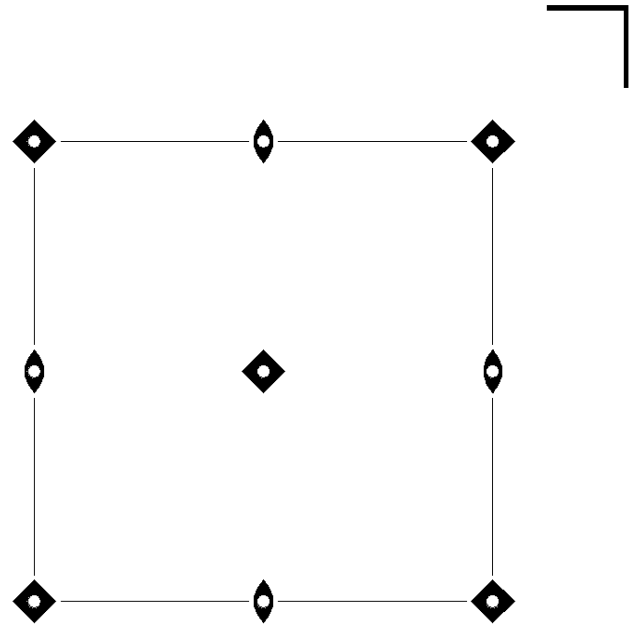
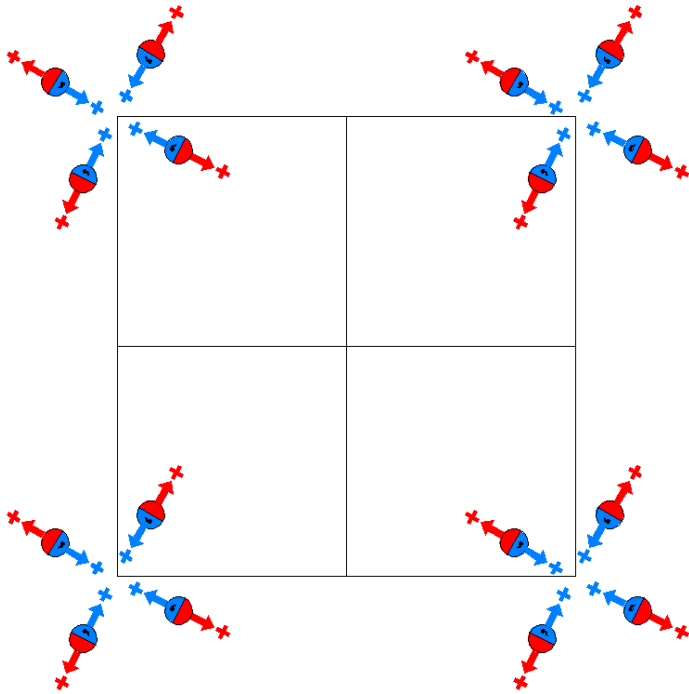
Along [1,1,0]  $p_{2b^*} 1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



P4/m  
83.1.703

4/m  
P4/m

Tetragonal



Origin at center ( 4/m )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 4<sup>+</sup> 0,0,z  
(4<sub>z</sub><sup>+</sup>|0,0,0)

(4) 4<sup>-</sup> 0,0,z  
(4<sub>z</sub><sup>-</sup>|0,0,0)

(5)  $\bar{1}$  0,0,0  
( $\bar{1}$ |0,0,0)

(6) m x,y,0  
(m<sub>z</sub>|0,0,0)

(7)  $\bar{4}^+$  0,0,z; 0,0,0  
( $\bar{4}_z^+$ |0,0,0)

(8)  $\bar{4}^-$  0,0,z; 0,0,0  
( $\bar{4}_z^-$ |0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

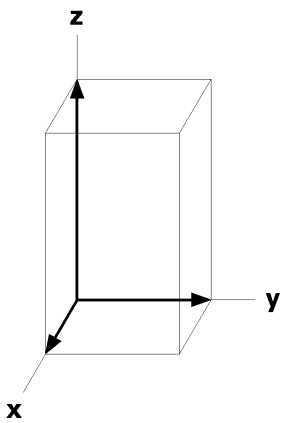
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	l	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]
			(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(8) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
4	k	m..	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0,w]	$\bar{y},x,1/2$ [0,0,w]	y, $\bar{x},1/2$ [0,0,w]
4	j	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0,w]	y, $\bar{x},0$ [0,0,w]
4	l	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]
2	h	4..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
2	g	4..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
2	f	2/m..	0,1/2,1/2 [0,0,w]	1/2,0,1/2 [0,0,w]		
2	e	2/m..	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]		
1	d	4/m..	1/2,1/2,1/2 [0,0,w]			
1	c	4/m..	1/2,1/2,0 [0,0,w]			
1	b	4/m..	0,0,1/2 [0,0,w]			
1	a	4/m..	0,0,0 [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



P4/m1'

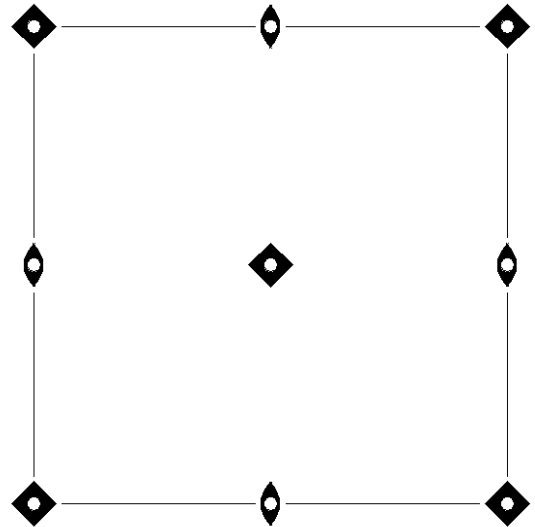
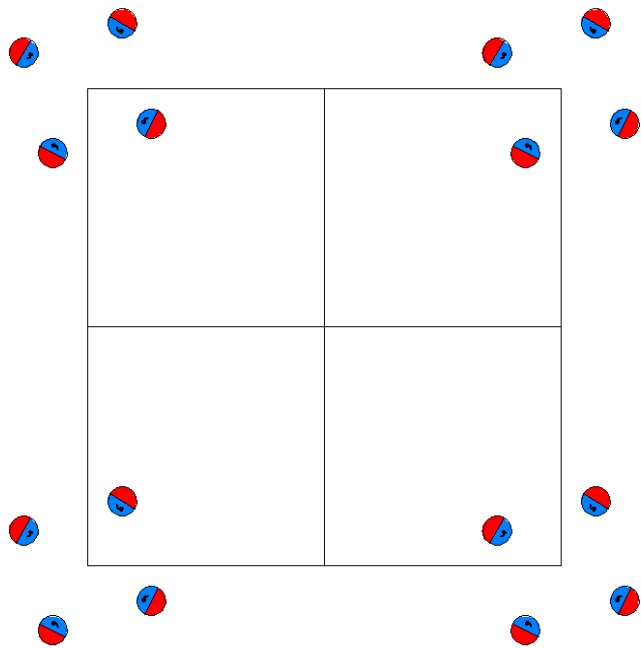
83.2.704

4/m1'

P4/m1'

Tetragonal

1'



Origin at center ( 4/m1' )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For 1 + set

(1) 1  
(1|0,0,0)

(2) 2<sub>z</sub> 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 4<sup>+</sup> 0,0,z  
(4<sub>z</sub><sup>+</sup>|0,0,0)

(4) 4<sup>-</sup> 0,0,z  
(4<sub>z</sub><sup>-</sup>|0,0,0)

(5)  $\bar{1}$  0,0,0  
( $\bar{1}$ |0,0,0)

(6) m<sub>x,y</sub> x,y,0  
(m<sub>z</sub>|0,0,0)

(7)  $\bar{4}^+$  0,0,z; 0,0,0  
( $\bar{4}_z^+$ |0,0,0)

(8)  $\bar{4}^-$  0,0,z; 0,0,0  
( $\bar{4}_z^-$ |0,0,0)

For 1' + set

(1) 1'  
(1|0,0,0)'

(2) 2'<sub>z</sub> 0,0,z  
(2'<sub>z</sub>|0,0,0)'

(3) 4<sup>+</sup>' 0,0,z  
(4<sub>z</sub><sup>+</sup>'|0,0,0)'

(4) 4<sup>-</sup>' 0,0,z  
(4<sub>z</sub><sup>-</sup>'|0,0,0)'

(5)  $\bar{1}$ ' 0,0,0  
( $\bar{1}$ '|0,0,0)'

(6) m'<sub>x,y</sub> x,y,0  
(m'<sub>z</sub>'|0,0,0)'

(7)  $\bar{4}^+$ ' 0,0,z; 0,0,0  
( $\bar{4}_z^+$ '|0,0,0)'

(8)  $\bar{4}^-$ ' 0,0,z; 0,0,0  
( $\bar{4}_z^-$ '|0,0,0)'



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

### Positions

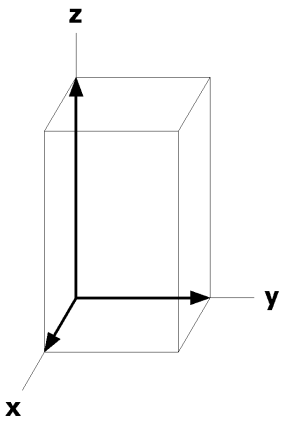
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1+	1+	1'+	1'+
8 l 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z$ [0,0,0]	(4) $y,\bar{x},z$ [0,0,0]
	(5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(6) x,y, $\bar{z}$ [0,0,0]	(7) y, $\bar{x},\bar{z}$ [0,0,0]	(8) $\bar{y},x,\bar{z}$ [0,0,0]
4 k m..1'	x,y,1/2 [0,0,0]	$\bar{x},\bar{y},1/2$ [0,0,0]	$\bar{y},x,1/2$ [0,0,0]	y, $\bar{x},1/2$ [0,0,0]
4 j m..1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{y},x,0$ [0,0,0]	y, $\bar{x},0$ [0,0,0]
4 l 2..1'	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]
2 h 4..1'	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
2 g 4..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2 f 2/m..1'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
2 e 2/m..1'	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
1 d 4/m..1'	1/2,1/2,1/2 [0,0,0]			
1 c 4/m..1'	1/2,1/2,0 [0,0,0]			
1 b 4/m..1'	0,0,1/2 [0,0,0]			
1 a 4/m..1'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

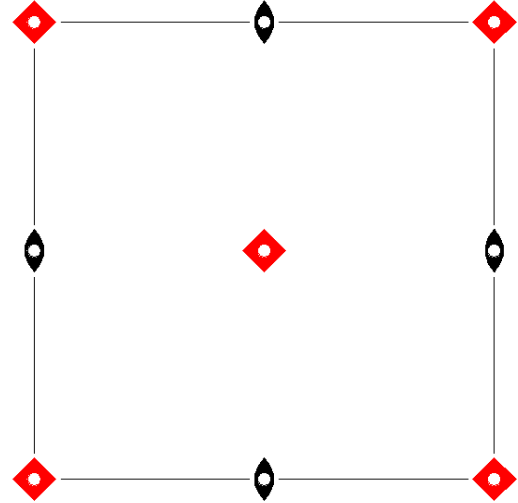
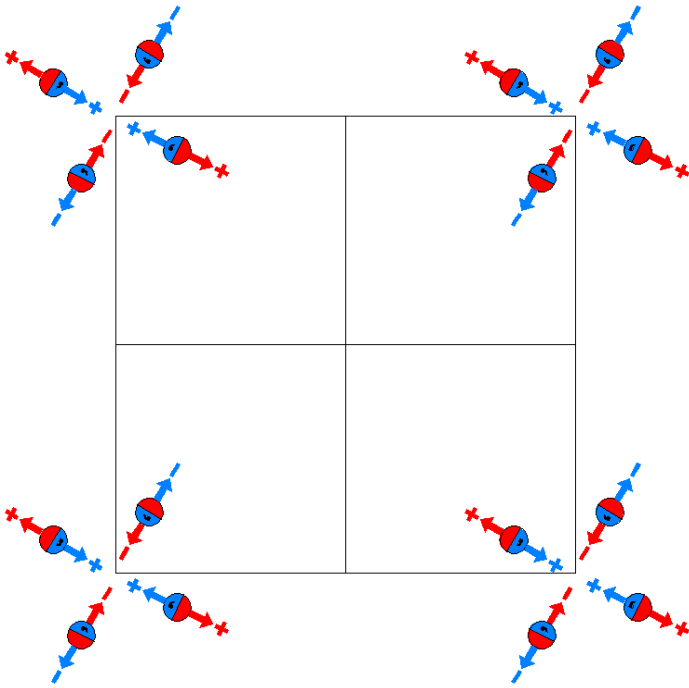
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4'/m  
83.3.705

4'/m  
P4'/m

Tetragonal



Origin at center ( 4'/m )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'          | (8) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

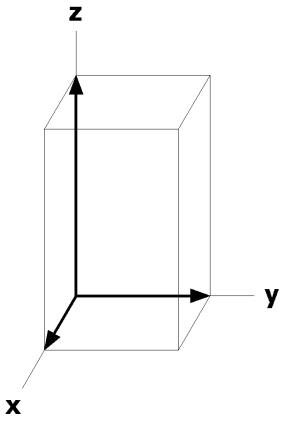
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	l	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $v,\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
			(5) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(6) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(8) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
4	k	m..	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0,w]	$\bar{y},x,1/2$ [0,0, $\bar{w}$ ]	$y,\bar{x},1/2$ [0,0, $\bar{w}$ ]
4	j	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0, $\bar{w}$ ]	$y,\bar{x},0$ [0,0, $\bar{w}$ ]
4	l	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
2	h	4'..	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
2	g	4'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	f	2/m..	0,1/2,1/2 [0,0,w]	1/2,0,1/2 [0,0, $\bar{w}$ ]		
2	e	2/m..	0,1/2,0 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]		
1	d	4'/m..	1/2,1/2,1/2 [0,0,0]			
1	c	4'/m..	1/2,1/2,0 [0,0,0]			
1	b	4'/m..	0,0,1/2 [0,0,0]			
1	a	4'/m..	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

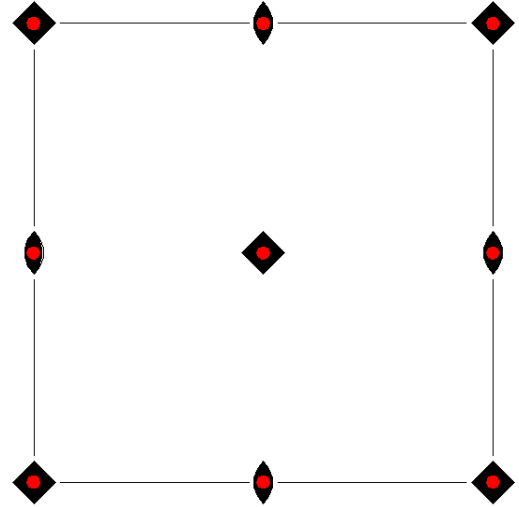
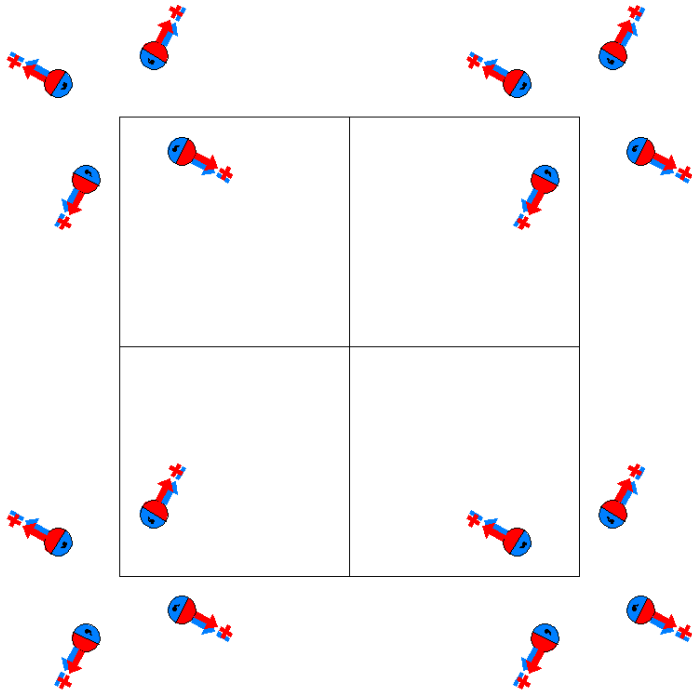
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



P4/m'  
83.4.706

4/m'  
P4/m'

Tetragonal



Origin at center ( 4/m' )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

- |  |   |  |   |
|--|---|--|---|
| (1) 1<br>(1 0,0,0)                             | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)  | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)                             |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$ ' 0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub> ' 0,0,0)' | (7) $\bar{4}$ <sup>+</sup> ' 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>+</sup> ' 0,0,0)' | (8) $\bar{4}$ <sup>-</sup> ' 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>-1</sup> ' 0,0,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

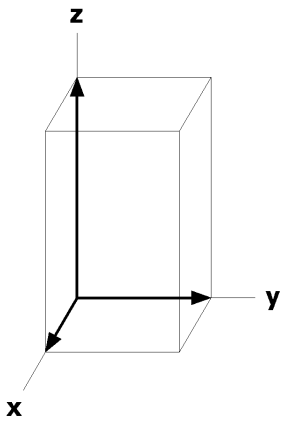
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	l	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]
			(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) y, $\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(8) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
4	k	m'..	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},u,0$ ]	y, $\bar{x},1/2$ [ $v,\bar{u},0$ ]
4	j	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},u,0$ ]	y, $\bar{x},0$ [ $v,\bar{u},0$ ]
4	l	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
2	h	4..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	g	4..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	f	2/m'..	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	e	2/m'..	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
1	d	4/m'..	1/2,1/2,1/2 [0,0,0]			
1	c	4/m'..	1/2,1/2,0 [0,0,0]			
1	b	4/m'..	0,0,1/2 [0,0,0]			
1	a	4/m'..	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

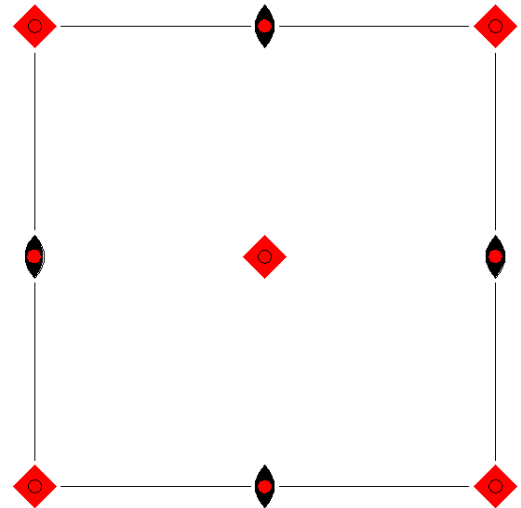
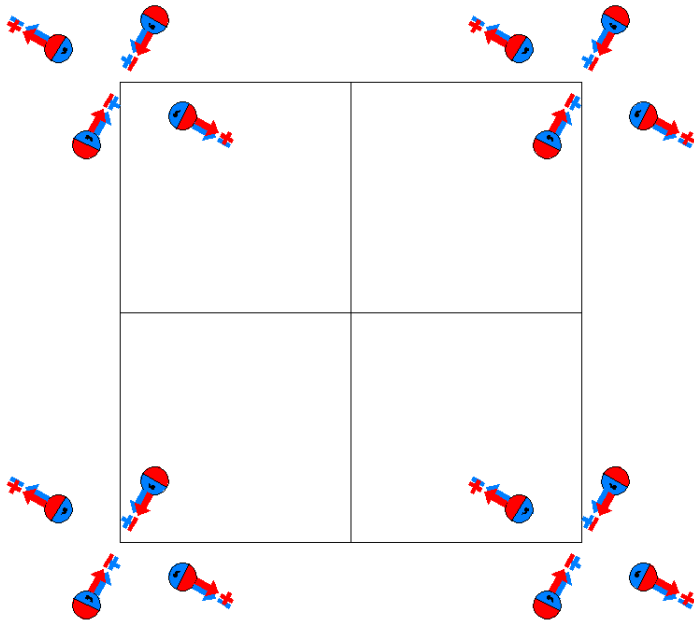
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P4'/m'$   
83.5.707

$4'/m'$   
 $P4'/m'$

Tetragonal



Origin at center ( $4'/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

(1)  $1$   
 $(1|0,0,0)$

(2)  $2 \quad 0,0,z$   
 $(2_z|0,0,0)$

(3)  $4^+ \quad 0,0,z$   
 $(4_z^+|0,0,0)'$

(4)  $4^- \quad 0,0,z$   
 $(4_z^-|0,0,0)'$

(5)  $\bar{1} \quad 0,0,0$   
 $(\bar{1}|0,0,0)'$

(6)  $m' \quad x,y,0$   
 $(m_z|0,0,0)'$

(7)  $\bar{4}^+ \quad 0,0,z; 0,0,0$   
 $(\bar{4}_z^+|0,0,0)$

(8)  $\bar{4}^- \quad 0,0,z; 0,0,0$   
 $(\bar{4}_z^-|0,0,0)$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

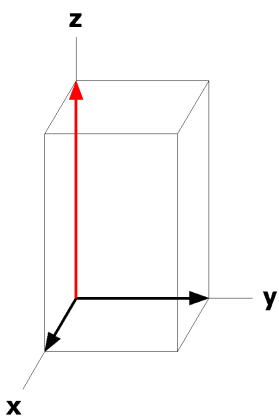
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	l	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
			(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(8) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]
4	k	m'..	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},\bar{u},0$ ]	y, $\bar{x},1/2$ [ $\bar{v},u,0$ ]
4	j	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},\bar{u},0$ ]	y, $\bar{x},0$ [ $\bar{v},u,0$ ]
4	l	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]
2	h	4'..	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
2	g	4'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	f	2/m'..	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	e	2/m'..	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
1	d	4'/m'..	1/2,1/2,1/2 [0,0,0]			
1	c	4'/m'..	1/2,1/2,0 [0,0,0]			
1	b	4'/m'..	0,0,1/2 [0,0,0]			
1	a	4'/m'..	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



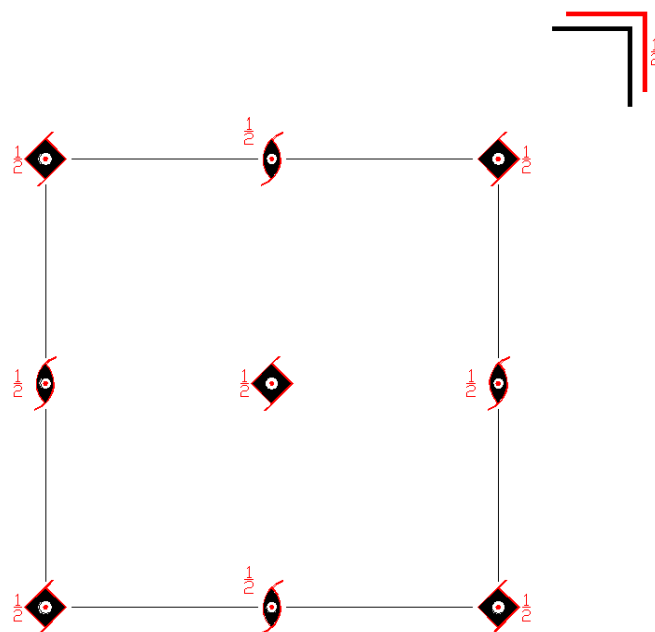
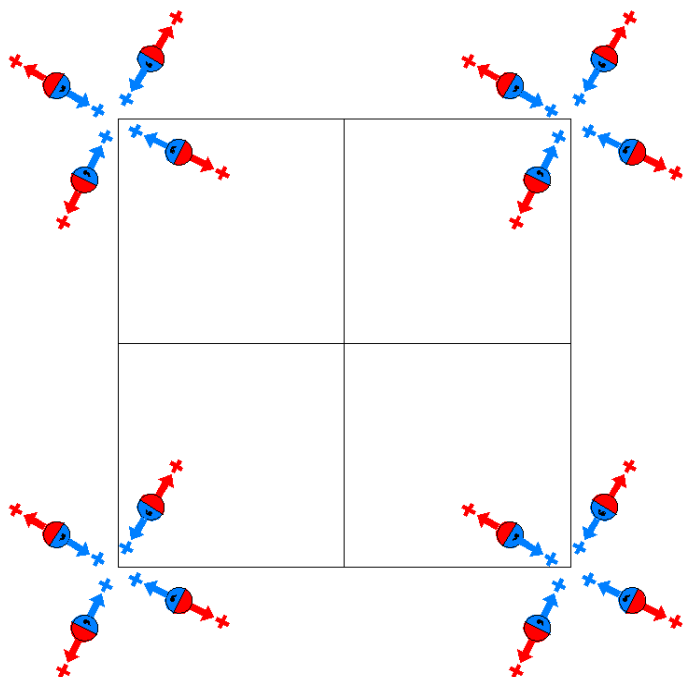
$P_{2c} 4/m$

83.6.708

$4/m\bar{1}'$

$P_{2c} 4/m$

Tetragonal



Origin at center ( $4/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)     | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0) | (8) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)           |

For (0,0,1)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (0,0,1)<br>(1 0,0,1)'                   | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)' | (3) 4 <sup>+</sup> ' (0,0,1) 0,0,z<br>(4 <sub>z</sub>  0,0,1)' | (4) 4 <sup>-</sup> ' (0,0,1) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1)' |
| (5) $\bar{1}'$ 0,0,1/2<br>( $\bar{1}$  0,0,1)' | (6) m' x,y,1/2<br>(m <sub>z</sub>  0,0,1)'       | (7) $\bar{4}^+$ ' 0,0,z; 0,0,1/2<br>( $\bar{4}_z^+$  0,0,1)'   | (8) $\bar{4}^-$ ' 0,0,z; 0,0,1/2<br>( $\bar{4}_z^-$  0,0,1)'                 |



**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

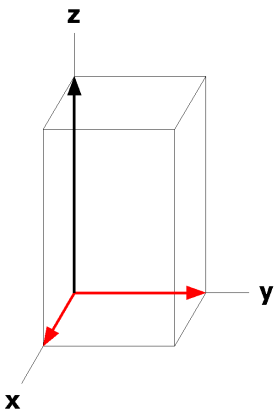
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
16 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(8) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
8 k m'..	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},u,0$ ]	y, $\bar{x},1/2$ [ $v,\bar{u},0$ ]
8 j m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0,w]	y, $\bar{x},0$ [0,0,w]
8 l 2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]
4 h 4..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
4 g 4..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
4 f 2/m'..	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 e 2/m..	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]		
2 d 4/m'..	1/2,1/2,1/2 [0,0,0]			
2 c 4/m..	1/2,1/2,0 [0,0,w]			
2 b 4/m'..	0,0,1/2 [0,0,0]			
2 a 4/m..	0,0,0 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,1/2

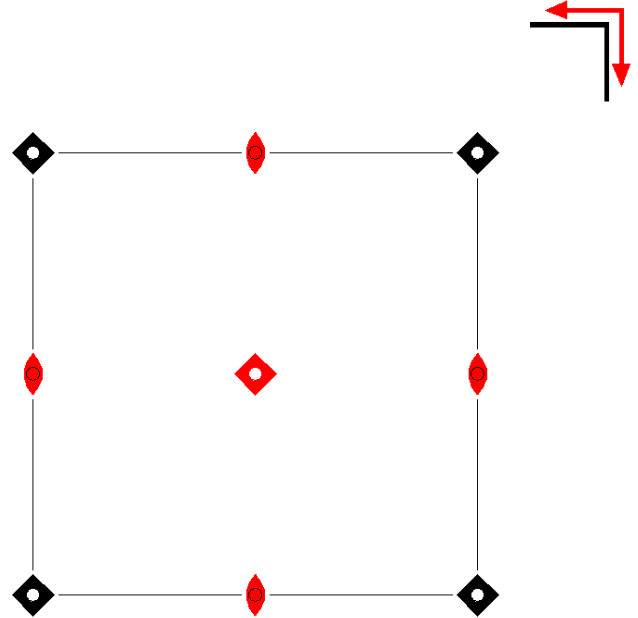
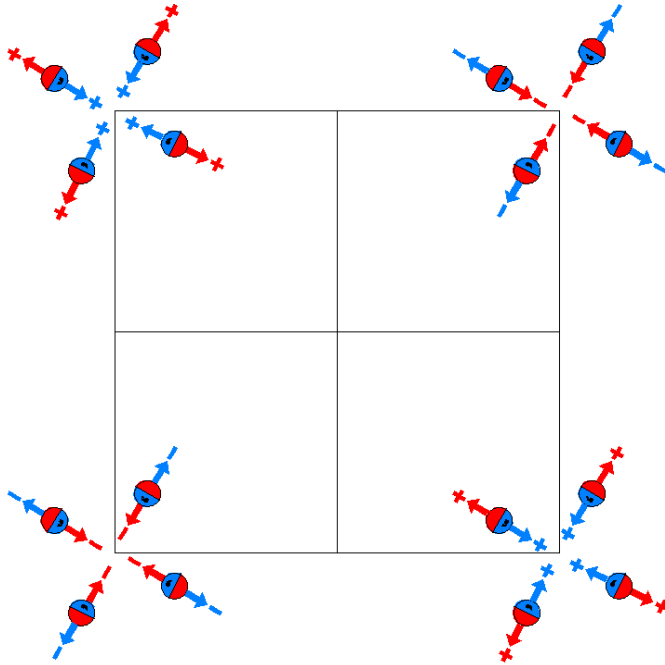
Along [1,1,0] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/2



$P_4/m$   
83.7.709

$4/m\bar{1}'$   
 $P_4/m$

Tetragonal



Origin at center ( $4/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For  $(0,0,0)$  + set

- |  |                                  |   |   |
|--|----------------------------------|---|---|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $4^+$ $0,0,z$<br>( $4_z^+$  0,0,0)                    | (4) $4^-$ $0,0,z$<br>( $4_z^-$  0,0,0)                    |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0) | (6) m $x,y,0$<br>( $m_z$  0,0,0) | (7) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^+$  0,0,0) | (8) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^-$  0,0,0) |

For  $(1,0,0)'$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ $(1,0,0)$<br>(1 1,0,0)'                 | (2) $2'$ $1/2,0,z$<br>( $2_z$  1,0,0)'       | (3) $4^{+'}$ $1/2,1/2,z$<br>( $4_z^{+'}$  1,0,0)'                          | (4) $4^{-'}$ $1/2,-1/2,z$<br>( $4_z^{-'}$  1,0,0)'                       |
| (5) $\bar{1}'$ $1/2,0,0$<br>( $\bar{1}$  1,0,0)' | (6) $a'$ $(1,0,0) x,y,0$<br>( $m_z$  1,0,0)' | (7) $\bar{4}^{+'}$ $1/2,-1/2,z; 1/2,-1/2,0$<br>( $\bar{4}_z^{+'}$  1,0,0)' | (8) $\bar{4}^{-'}$ $1/2,1/2,z; 1/2,1/2,0$<br>( $\bar{4}_z^{-'}$  1,0,0)' |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

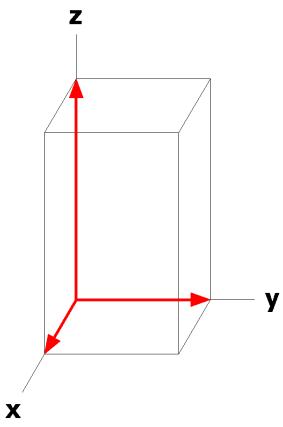
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(6) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(8) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
8 k m..	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0,w]	$\bar{y},x,1/2$ [0,0,w]	$y,\bar{x},1/2$ [0,0,w]
8 j m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0,w]	$y,\bar{x},0$ [0,0,w]
8 l 2'..	0,1/2,z [u,v,0]	1/2,0,z [ $v,\bar{u},0$ ]	0,1/2, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/2,0, $\bar{z}$ [ $\bar{v},u,0$ ]
4 h 4'..	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
4 g 4..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
4 f 2'/m..	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 e 2'/m..	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
2 d 4'/m..	1/2,1/2,1/2 [0,0,0]			
2 c 4'/m..	1/2,1/2,0 [0,0,0]			
2 b 4/m..	0,0,1/2 [0,0,w]			
2 a 4/m..	0,0,0 [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

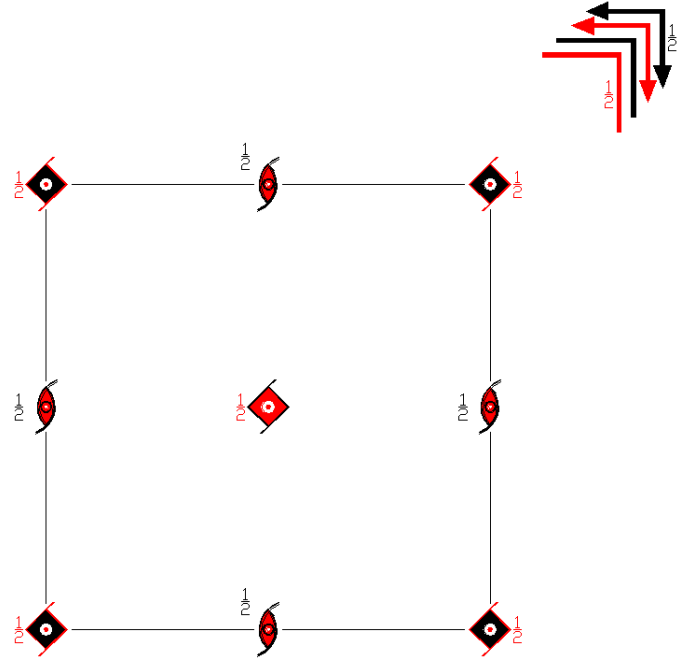
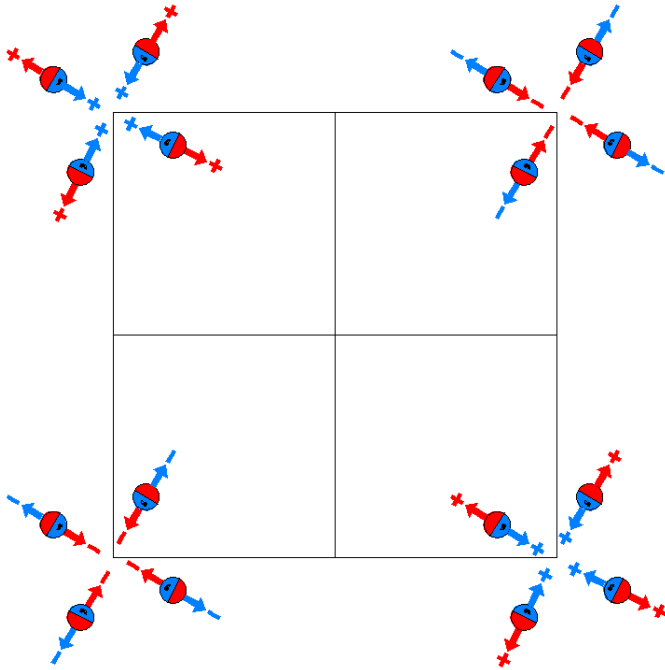
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x-1/4,x+1/4,0



$P_14/m$   
83.8.710

$4/m\bar{1}'$   
 $P_14/m$

Tetragonal



Origin at center ( $4/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |  |  |
|--|---|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)     | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m <sub>x,y</sub> x,y,0<br>(m <sub>x,y</sub>  0,0,0) | (7) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)          | (8) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)          |

For (1,0,0)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) t' (1,0,0)<br>(1 1,0,0)'                     | (2) 2' <sub>z</sub> 1/2,0,z<br>(2' <sub>z</sub>  1,0,0)'           | (3) 4 <sup>+</sup> ' 1/2,1/2,z<br>(4 <sub>z</sub> <sup>+</sup> ' 1,0,0)' | (4) 4 <sup>-</sup> ' 1/2,-1/2,z<br>(4 <sub>z</sub> <sup>-</sup> ' 1,0,0)' |
| (5) $\bar{1}$ ' 1/2,0,0<br>( $\bar{1}$ ' 1,0,0)' | (6) a' <sub>x,y</sub> (1,0,0) x,y,0<br>(m <sub>x,y</sub> ' 1,0,0)' | (7) $\bar{4}^+$ ' 1/2,-1/2,z; 1/2,-1/2,0<br>( $\bar{4}_z^+$ ' 1,0,0)'    | (8) $\bar{4}^-$ ' 1/2,1/2,z; 1/2,1/2,0<br>( $\bar{4}_z^-$ ' 1,0,0)'       |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

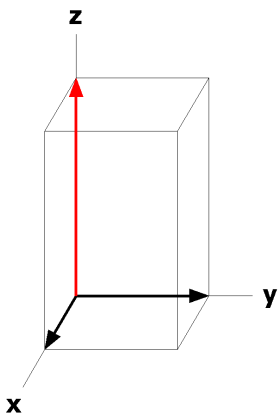
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(8) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
8 k m'..	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},u,0$ ]	$y,\bar{x},1/2$ [ $v,\bar{u},0$ ]
8 j m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0,w]	$y,\bar{x},0$ [0,0,w]
8 l 2'..	0,1/2,z [u,v,0]	1/2,0,z [ $\bar{v},\bar{u},0$ ]	0,1/2, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/2,0, $\bar{z}$ [ $\bar{v},u,0$ ]
4 h 4'..	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
4 g 4..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
4 f 2'/m'..	0,1/2,1/2 [u,v,0]	1/2,0,1/2 [ $\bar{v},\bar{u},0$ ]		
4 e 2'/m..	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
2 d 4'/m'..	1/2,1/2,1/2 [0,0,0]			
2 c 4'/m..	1/2,1/2,0 [0,0,0]			
2 b 4'/m'..	0,0,1/2 [0,0,0]			
2 a 4/m..	0,0,0 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x-1/4,x+1/4,0



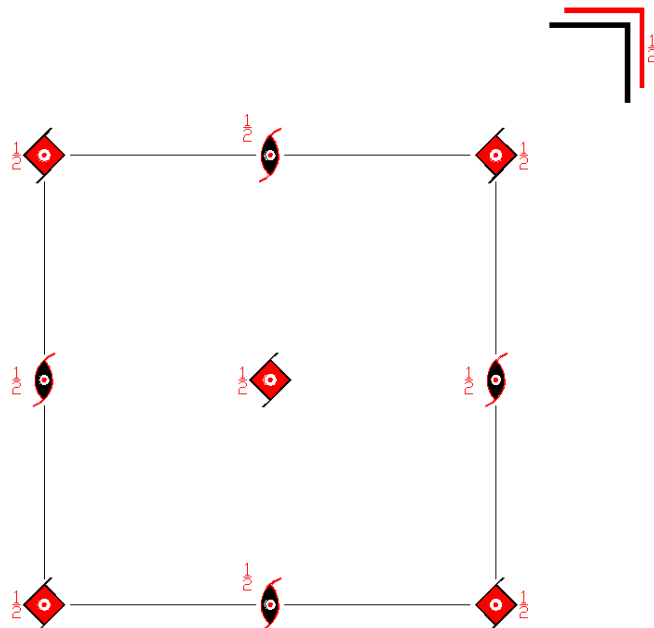
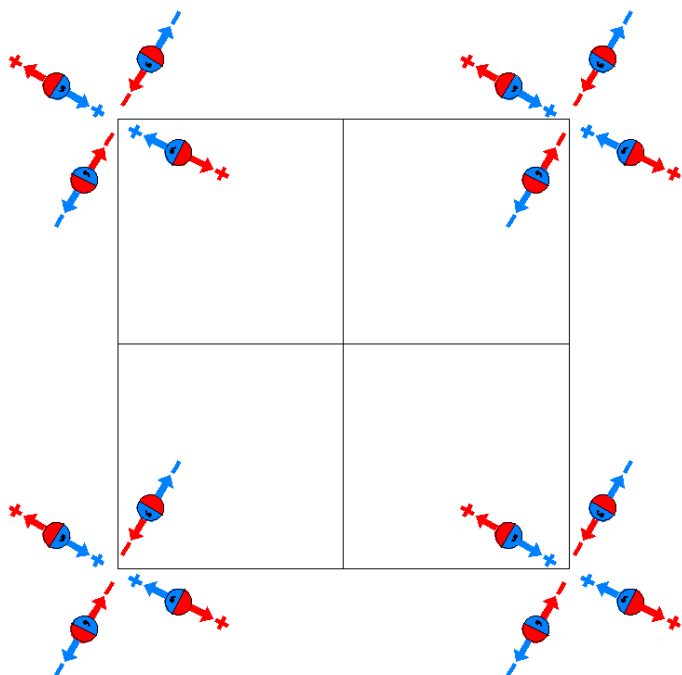
$P_{2c} 4'/m$

83.9.711

$4/m1'$

$P_{2c} 4'/m$

Tetragonal



Origin at center ( $4'/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'   | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)' | (8) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)'        |

For (0,0,1/2) + set

- |   |  |   |   |
|---|--|---|---|
| (1) t' (0,0,1)<br>(1 0,0,1)'                    | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)' | (3) 4 <sup>+</sup> (0,0,1) 0,0,z<br>(4 <sub>z</sub>  0,0,1) | (4) 4 <sup>-</sup> (0,0,1) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1) |
| (5) $\bar{1}$ ' 0,0,1/2<br>( $\bar{1}$  0,0,1)' | (6) m' x,y,1/2<br>(m <sub>z</sub>  0,0,1)'       | (7) $\bar{4}^+$ 0,0,z; 0,0,1/2<br>( $\bar{4}_z$  0,0,1)     | (8) $\bar{4}^-$ 0,0,z; 0,0,1/2<br>( $\bar{4}_z^{-1}$  0,0,1)              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

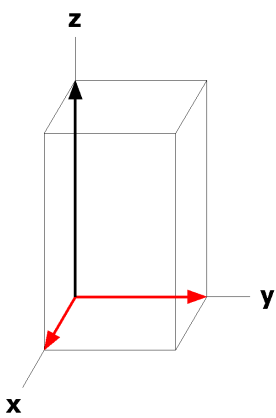
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
16 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) y, $\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
8 k m'..	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},\bar{u},0$ ]	y, $\bar{x},1/2$ [ $\bar{v},u,0$ ]
8 j m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0, $\bar{w}$ ]	y, $\bar{x},0$ [0,0, $\bar{w}$ ]
8 l 2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4 h 4'..	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
4 g 4'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 f 2/m'..	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 e 2/m..	0,1/2,0 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]		
2 d 4'/m'..	1/2,1/2,1/2 [0,0,0]			
2 c 4'/m..	1/2,1/2,0 [0,0,0]			
2 b 4'/m'..	0,0,1/2 [0,0,0]			
2 a 4'/m..	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>-2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

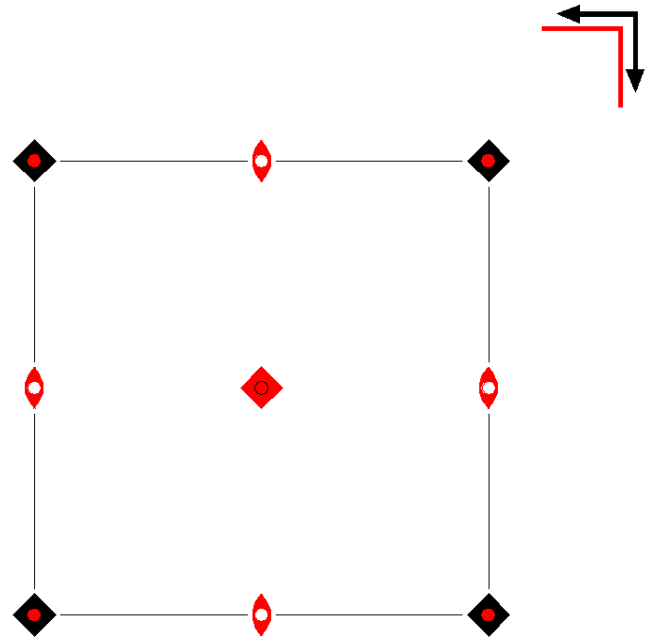
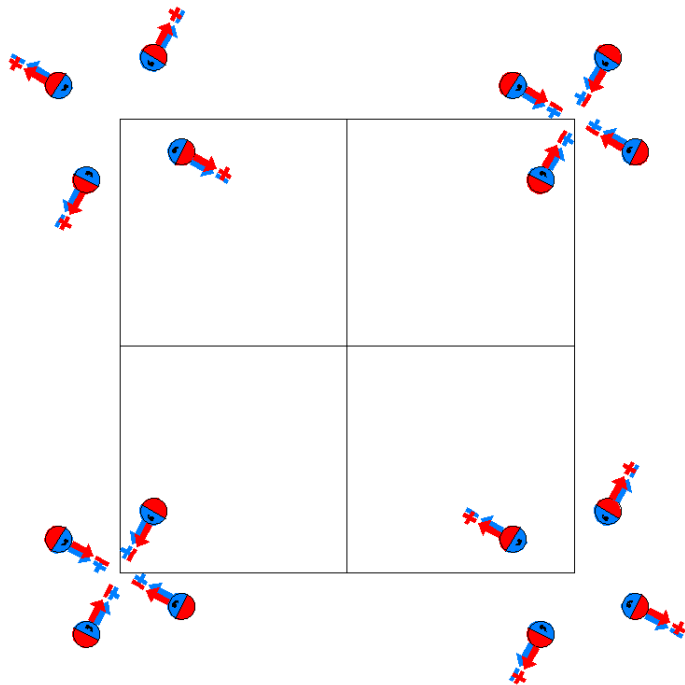
Along [1,1,0] p<sub>2a</sub>-2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$P_4/m'$   
83.10.712

$4/m1'$   
 $P_4/m'$

Tetragonal



Origin at center ( $4/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |   |                                    |  |  |
|---|------------------------------------|--|--|
| (1) $1$<br>$(1 0,0,0)$                      | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$   | (3) $4^+$ $0,0,z$<br>$(4_z^+ 0,0,0)$                     | (4) $4^-$ $0,0,z$<br>$(4_z^- 0,0,0)$                     |
| (5) $\bar{1}$ $0,0,0$<br>$(\bar{1} 0,0,0)'$ | (6) $m'$ $x,y,0$<br>$(m_z 0,0,0)'$ | (7) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^+ 0,0,0)'$ | (8) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^- 0,0,0)'$ |

For (1,0,0)' + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t'$ (1,0,0)<br>$(1 1,0,0)'$             | (2) $2'$ $1/2,0,z$<br>$(2_z' 1,0,0)'$    | (3) $4^{+'}$ $1/2,1/2,z$<br>$(4_z^{+'} 1,0,0)'$                   | (4) $4^{-'}$ $1/2,-1/2,z$<br>$(4_z^{-'} 1,0,0)'$                |
| (5) $\bar{1}$ $1/2,0,0$<br>$(\bar{1} 1,0,0)$ | (6) $a$ (1,0,0) $x,y,0$<br>$(m_z 1,0,0)$ | (7) $\bar{4}^+$ $1/2,-1/2,z; 1/2,-1/2,0$<br>$(\bar{4}_z^+ 1,0,0)$ | (8) $\bar{4}^-$ $1/2,1/2,z; 1/2,1/2,0$<br>$(\bar{4}_z^- 1,0,0)$ |



**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

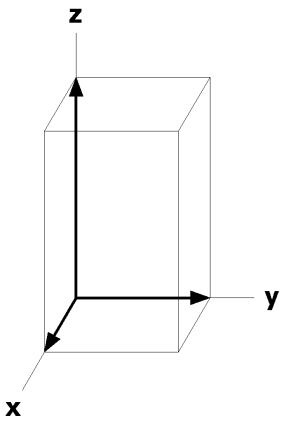
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 l 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ] (7) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ] (8) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
8 k m..	x,y,1/2 [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0,w]	$\bar{y},x,1/2$ [0,0,w]	y, $\bar{x},1/2$ [0,0,w]
8 j m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},u,0$ ]	y, $\bar{x},0$ [v, $\bar{u},0$ ]
8 l 2'..	0,1/2,z [u,v,0]	1/2,0,z [v, $\bar{u},0$ ]	0,1/2, $\bar{z}$ [u,v,0]	1/2,0, $\bar{z}$ [v, $\bar{u},0$ ]
4 h 4'..	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
4 g 4..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 f 2'/m..	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
4 e 2'/m'..	0,1/2,0 [u,v,0]	1/2,0,0 [v, $\bar{u},0$ ]		
2 d 4'/m..	1/2,1/2,1/2 [0,0,0]			
2 c 4'/m'..	1/2,1/2,0 [0,0,0]			
2 b 4/m..	0,0,1/2 [0,0,w]			
2 a 4/m'..	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub>·4  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

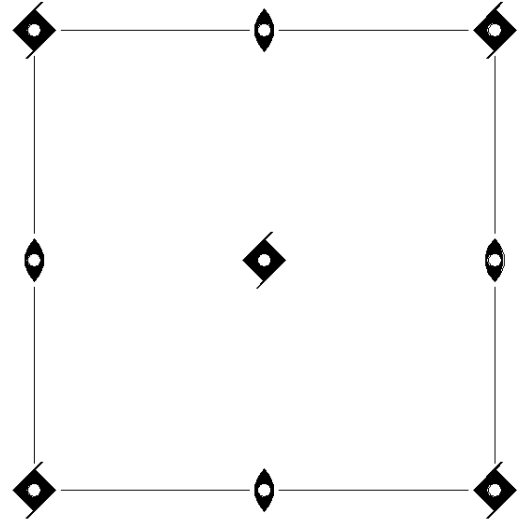
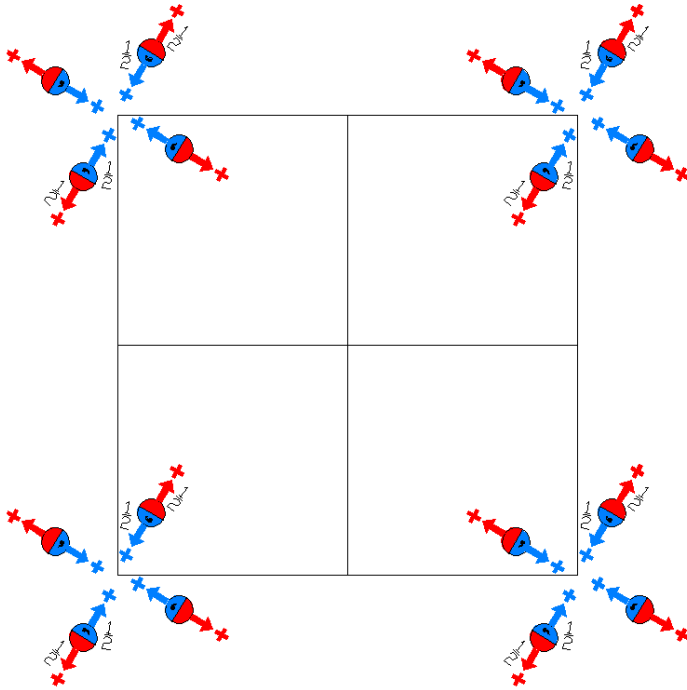
Along [1,1,0] p<sub>2a</sub>·2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P4_2/m$   
84.1.713

$4/m$   
 $P4_2/m$

Tetragonal



Origin at center ( $2/m$ ) on  $4_2$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

- |  |                                    |  |   |
|--|------------------------------------|--|---|
| (1) $1$<br>( $1 0,0,0$ )                     | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ ) | (3) $4^+$ ( $0,0,1/2$ ) $0,0,z$<br>( $4_z 0,0,1/2$ )           | (4) $4^-$ ( $0,0,1/2$ ) $0,0,z$<br>( $4_z^{-1} 0,0,1/2$ )           |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1} 0,0,0$ ) | (6) $m$ $x,y,0$<br>( $m_z 0,0,0$ ) | (7) $\bar{4}^+$ $0,0,z$ ; $0,0,1/4$<br>( $\bar{4}_z 0,0,1/2$ ) | (8) $\bar{4}^-$ $0,0,z$ ; $0,0,1/4$<br>( $\bar{4}_z^{-1} 0,0,1/2$ ) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

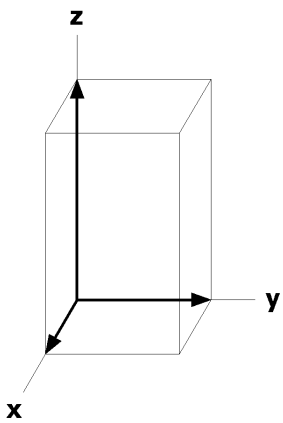
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]
			(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},u,w$ ]	(8) $\bar{y},x,\bar{z}+1/2$ [ $v,\bar{u},w$ ]
4	j	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,1/2$ [0,0,w]	$y,\bar{x},1/2$ [0,0,w]
4	i	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]
4	h	2..	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]
4	g	2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]
2	f	$\bar{4}$ ..	1/2,1/2,1/4 [0,0,w]	1/2,1/2,3/4 [0,0,w]		
2	e	$\bar{4}$ ..	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		
2	d	2/m..	0,1/2,1/2 [0,0,w]	1/2,0,0 [0,0,w]		
2	c	2/m..	0,1/2,0 [0,0,w]	1/2,0,1/2 [0,0,w]		
2	b	2/m..	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]		
2	a	2/m..	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$P4_2/m1'$

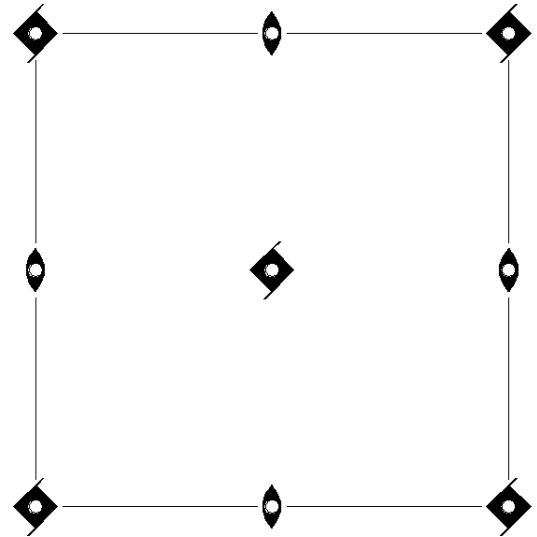
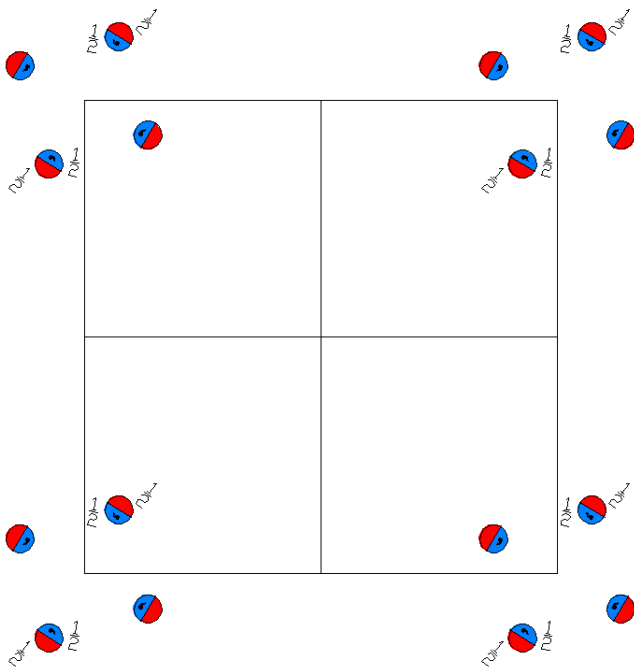
84.2.714

$4/m1'$

$P4_2/m1'$

Tetragonal

$1'$



Origin at center ( $2/m1'$ ) on  $4_21'$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

### Symmetry Operations

For  $1 + \text{set}$

- |  |  |   |  |
|--|--|---|--|
| (1) $1$<br>( $1 0,0,0$ )                         | (2) $2 \quad 0,0,z$<br>( $2_z 0,0,0$ ) | (3) $4^+ (0,0,1/2) \quad 0,0,z$<br>( $4_z 0,0,1/2$ )                  | (4) $4^- (0,0,1/2) \quad 0,0,z$<br>( $4_z^{-1} 0,0,1/2$ )                  |
| (5) $\bar{1} \quad 0,0,0$<br>( $\bar{1} 0,0,0$ ) | (6) $m \quad x,y,0$<br>( $m_z 0,0,0$ ) | (7) $\bar{4}^+ \quad 0,0,z; \quad 0,0,1/4$<br>( $\bar{4}_z 0,0,1/2$ ) | (8) $\bar{4}^- \quad 0,0,z; \quad 0,0,1/4$<br>( $\bar{4}_z^{-1} 0,0,1/2$ ) |

For  $1' + \text{set}$

- |  |  |   |  |
|--|--|---|--|
| (1) $1'$<br>( $1 0,0,0$ )'                         | (2) $2' \quad 0,0,z$<br>( $2_z 0,0,0$ )' | (3) $4^{+'} (0,0,1/2) \quad 0,0,z$<br>( $4_z 0,0,1/2$ )'                  | (4) $4^{-'} (0,0,1/2) \quad 0,0,z$<br>( $4_z^{-1} 0,0,1/2$ )'                  |
| (5) $\bar{1}' \quad 0,0,0$<br>( $\bar{1} 0,0,0$ )' | (6) $m' \quad x,y,0$<br>( $m_z 0,0,0$ )' | (7) $\bar{4}^{+'} \quad 0,0,z; \quad 0,0,1/4$<br>( $\bar{4}_z 0,0,1/2$ )' | (8) $\bar{4}^{-'} \quad 0,0,z; \quad 0,0,1/4$<br>( $\bar{4}_z^{-1} 0,0,1/2$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

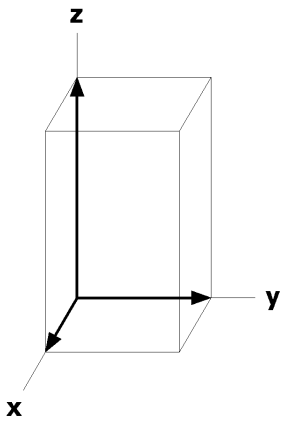
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1+		1'+	
8 k 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z+1/2$ [0,0,0]	(4) $y,\bar{x},z+1/2$ [0,0,0]
	(5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(6) x,y, $\bar{z}$ [0,0,0]	(7) $y,\bar{x},\bar{z}+1/2$ [0,0,0]	(8) $\bar{y},x,\bar{z}+1/2$ [0,0,0]
4 j m..1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{y},x,1/2$ [0,0,0]	$y,\bar{x},1/2$ [0,0,0]
4 i 2..1'	0,1/2,z [0,0,0]	1/2,0,z+1/2 [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]
4 h 2..1'	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]
4 g 2..1'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]
2 f $\bar{4}..1'$	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2 e $\bar{4}..1'$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2 d 2/m..1'	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]		
2 c 2/m..1'	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2 b 2/m..1'	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2 a 2/m..1'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



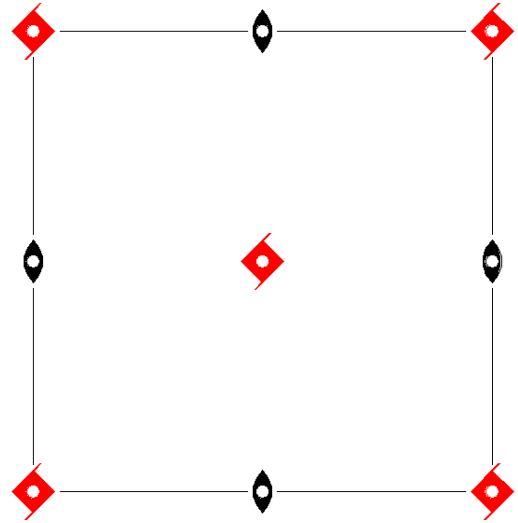
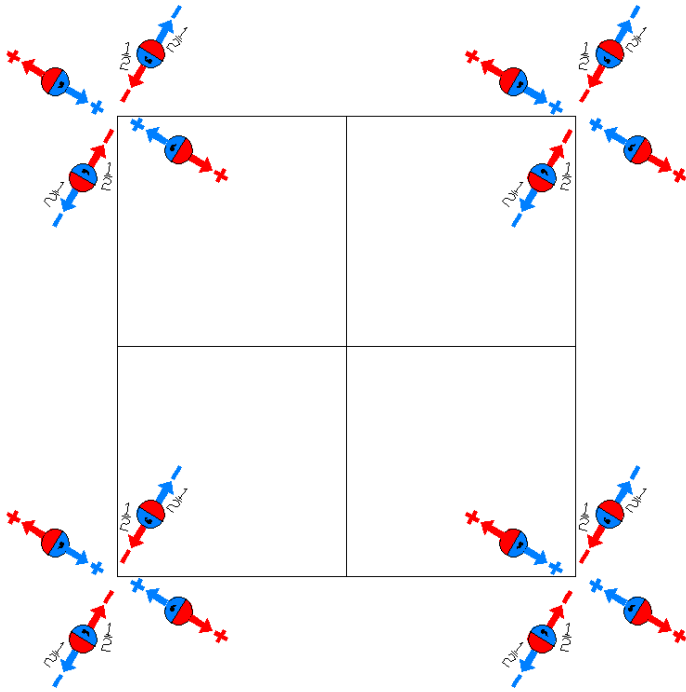
$P4_2'/m$

84.3.715

$4'/m$

$P4_2'/m$

Tetragonal



Origin at center ( $2/m$ ) on  $4_2'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |                                  |  |   |
|--|----------------------------------|--|---|
| (1) $1$<br>$(1 0,0,0)$                     | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$ | (3) $4^+$ $(0,0,1/2) 0,0,z$<br>$(4_z 0,0,1/2)'$            | (4) $4^-$ $(0,0,1/2) 0,0,z$<br>$(4_z^{-1} 0,0,1/2)'$            |
| (5) $\bar{1}$ $0,0,0$<br>$(\bar{1} 0,0,0)$ | (6) $m$ $x,y,0$<br>$(m_z 0,0,0)$ | (7) $\bar{4}^+$ $0,0,z; 0,0,1/4$<br>$(\bar{4}_z 0,0,1/2)'$ | (8) $\bar{4}^-$ $0,0,z; 0,0,1/4$<br>$(\bar{4}_z^{-1} 0,0,1/2)'$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

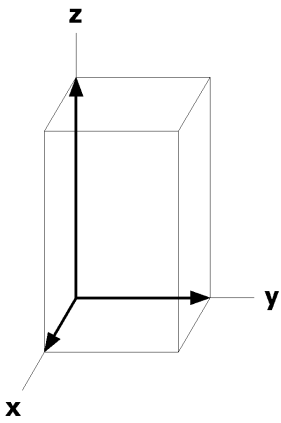
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ]
			(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]
4	j	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,1/2$ [0,0, $\bar{w}$ ]	$y,\bar{x},1/2$ [0,0, $\bar{w}$ ]
4	i	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	h	2..	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	g	2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
2	f	$\bar{4}'..$	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	e	$\bar{4}'..$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	d	2/m..	0,1/2,1/2 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]		
2	c	2/m..	0,1/2,0 [0,0,w]	1/2,0,1/2 [0,0, $\bar{w}$ ]		
2	b	2/m..	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		
2	a	2/m..	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

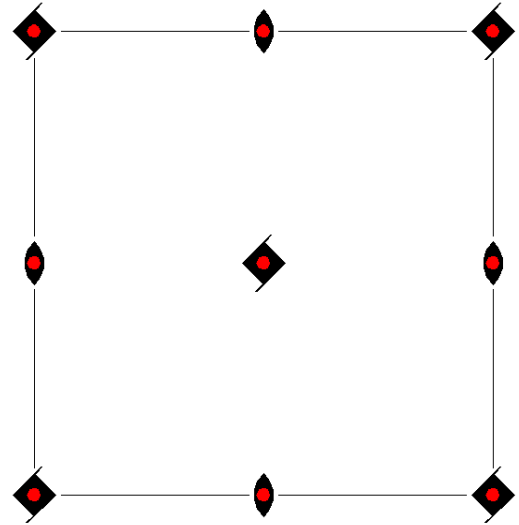
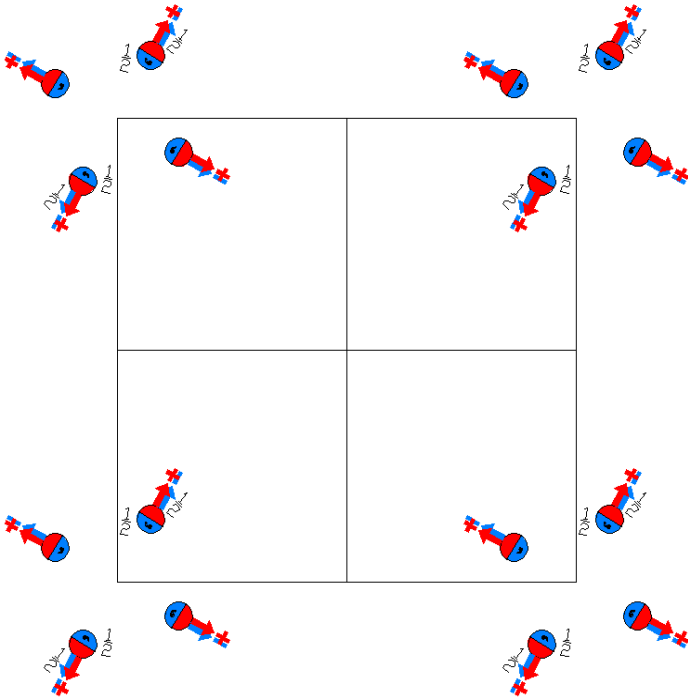
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$P4_2/m'$   
84.4.716

$4/m'$   
 $P4_2/m'$

Tetragonal



Origin at center ( $2/m'$ ) on  $4_2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |                                    |  |   |
|---|------------------------------------|--|---|
| (1) $1$<br>$(1 0,0,0)$                      | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$   | (3) $4^+$ $(0,0,1/2)$ $0,0,z$<br>$(4_z 0,0,1/2)$             | (4) $4^-$ $(0,0,1/2)$ $0,0,z$<br>$(4_z^{-1} 0,0,1/2)$             |
| (5) $\bar{1}$ $0,0,0$<br>$(\bar{1} 0,0,0)'$ | (6) $m'$ $x,y,0$<br>$(m_z 0,0,0)'$ | (7) $\bar{4}^{+}$ $0,0,z; 0,0,1/4$<br>$(\bar{4}_z 0,0,1/2)'$ | (8) $\bar{4}^{-}$ $0,0,z; 0,0,1/4$<br>$(\bar{4}_z^{-1} 0,0,1/2)'$ |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

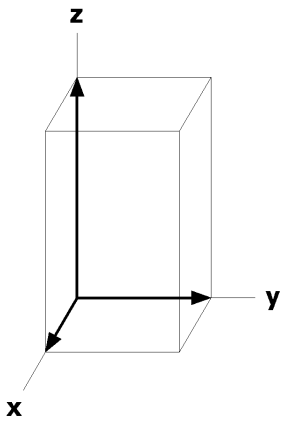
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]
			(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) $y,\bar{x},\bar{z}+1/2$ [ $v,\bar{u},\bar{w}$ ]	(8) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]
4	j	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},u,0$ ]	$y,\bar{x},1/2$ [ $v,\bar{u},0$ ]
4	i	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	h	2..	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	g	2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
2	f	$\bar{4}'..$	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	e	$\bar{4}'..$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	d	2/m'..	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]		
2	c	2/m'..	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	b	2/m'..	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a	2/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



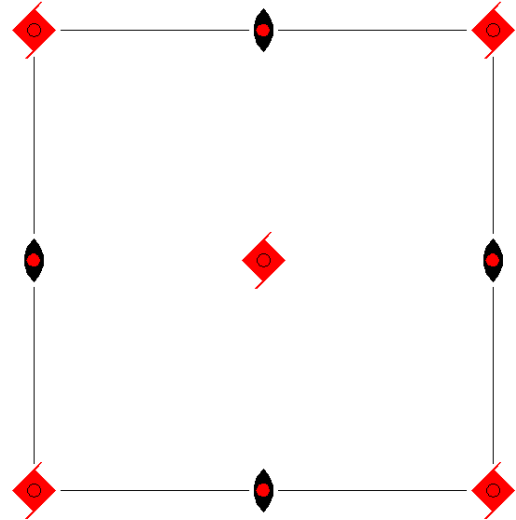
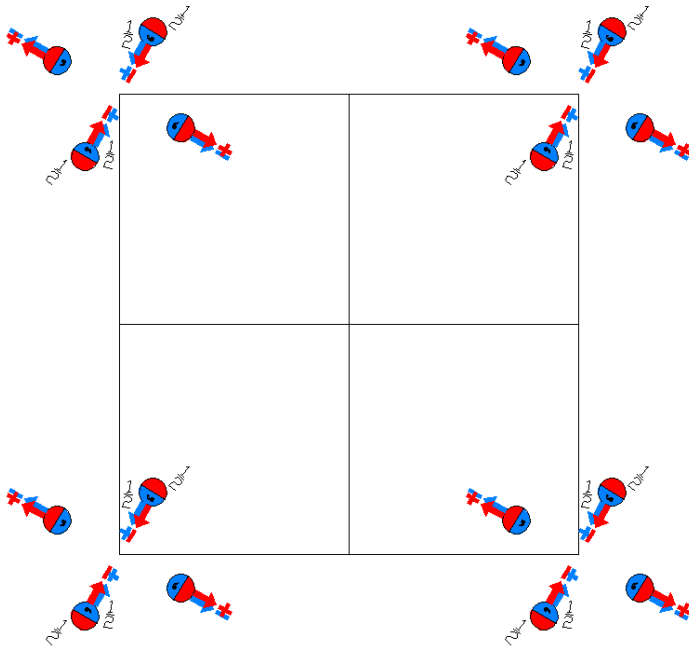
$P4_2'/m'$

84.5.717

$4'/m'$

$P4_2'/m'$

Tetragonal



Origin at center ( $2/m'$ ) on  $4_2'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

- |   |                                    |   |  |
|---|------------------------------------|---|--|
| (1) $1$<br>$(1 0,0,0)$                      | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$   | (3) $4^+$ $(0,0,1/2)$ $0,0,z$<br>$(4_z 0,0,1/2)'$         | (4) $4^-$ $(0,0,1/2)$ $0,0,z$<br>$(4_z^{-1} 0,0,1/2)'$         |
| (5) $\bar{1}$ $0,0,0$<br>$(\bar{1} 0,0,0)'$ | (6) $m'$ $x,y,0$<br>$(m_z 0,0,0)'$ | (7) $\bar{4}^+$ $0,0,z; 0,0,1/4$<br>$(\bar{4}_z 0,0,1/2)$ | (8) $\bar{4}^-$ $0,0,z; 0,0,1/4$<br>$(\bar{4}_z^{-1} 0,0,1/2)$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

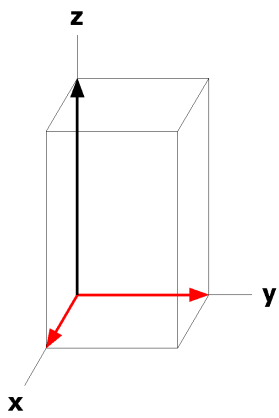
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(7) y, $\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]
4	j	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},\bar{u},0$ ]	y, $\bar{x},1/2$ [ $\bar{v},\bar{u},0$ ]
4	i	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0,w]
4	h	2..	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]
4	g	2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0,w]
2	f	$\bar{4}$ ..	1/2,1/2,1/4 [0,0,w]	1/2,1/2,3/4 [0,0, $\bar{w}$ ]		
2	e	$\bar{4}$ ..	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		
2	d	2/m'..	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]		
2	c	2/m'..	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	b	2/m'..	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a	2/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



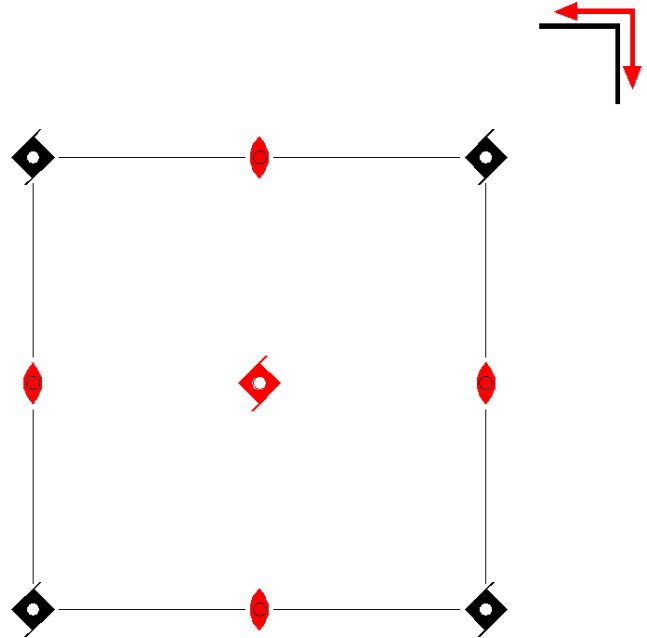
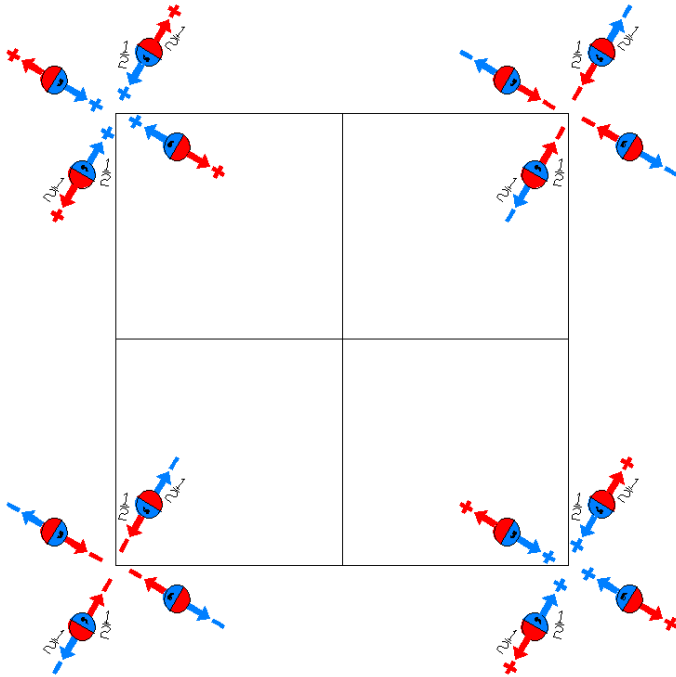
$P_P 4_2/m$

84.6.718

$4/m1'$

$P_P 4_2/m$

Tetragonal



Origin at center ( $2/m$ ) on  $4_2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |                                  |   |  |
|--|----------------------------------|---|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $4^+$ (0,0,1/2) $0,0,z$<br>( $4_z$  0,0,1/2)            | (4) $4^-$ (0,0,1/2) $0,0,z$<br>( $4_z^{-1}$  0,0,1/2)            |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0) | (6) m $x,y,0$<br>( $m_z$  0,0,0) | (7) $\bar{4}^+$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z$  0,0,1/2) | (8) $\bar{4}^-$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z^{-1}$  0,0,1/2) |

For (1,0,0)' + set

- |  |  |   |  |
|--|--|---|--|
| (1) $t'$ (1,0,0)<br>(1 1,0,0)'                   | (2) $2'$ $1/2,0,z$<br>( $2_z$  1,0,0)'       | (3) $4^{+'}$ (0,0,1/2) $1/2,1/2,z$<br>( $4_z$  1,0,1/2)'                  | (4) $4^{-'}$ (0,0,1/2) $1/2,-1/2,z$<br>( $4_z^{-1}$  1,0,1/2)'               |
| (5) $\bar{1}'$ $1/2,0,0$<br>( $\bar{1}$  1,0,0)' | (6) $a'$ (1,0,0) $x,y,0$<br>( $m_z$  1,0,0)' | (7) $\bar{4}^{+'}$ $1/2,-1/2,z; 1/2,-1/2,1/4$<br>( $\bar{4}_z$  1,0,1/2)' | (8) $\bar{4}^{-'}$ $1/2,1/2,z; 1/2,1/2,1/4$<br>( $\bar{4}_z^{-1}$  1,0,1/2)' |

**Generators selected** (1);  $t'(1,0,0)$ ;  $t'(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3); (5).

### Positions

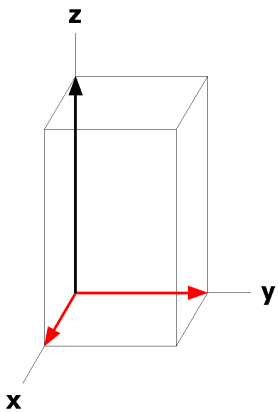
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 k 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(6) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},u,w$ ]	(8) $\bar{y},x,\bar{z}+1/2$ [ $v,\bar{u},w$ ]
8 j m..	$x,y,0$ [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,1/2$ [0,0,w]	$y,\bar{x},1/2$ [0,0,w]
8 i 2'..	$0,1/2,z$ [u,v,0]	$1/2,0,z+1/2$ [ $v,\bar{u},0$ ]	$0,1/2,\bar{z}$ [ $\bar{u},\bar{v},0$ ]	$1/2,0,\bar{z}+1/2$ [ $\bar{v},u,0$ ]
8 h 2..	$1/2,1/2,z$ [0,0,w]	$1/2,1/2,z+1/2$ [0,0,w]	$1/2,1/2,\bar{z}$ [0,0,w]	$1/2,1/2,\bar{z}+1/2$ [0,0,w]
8 g 2..	$0,0,z$ [0,0,w]	$0,0,z+1/2$ [0,0,w]	$0,0,\bar{z}$ [0,0,w]	$0,0,\bar{z}+1/2$ [0,0,w]
4 f $\bar{4}'$ ..	$1/2,1/2,1/4$ [0,0,0]	$1/2,1/2,3/4$ [0,0,0]		
4 e $\bar{4}$ ..	$0,0,1/4$ [0,0,w]	$0,0,3/4$ [0,0,w]		
4 d $2'/m$ ..	$0,1/2,1/2$ [0,0,0]	$1/2,0,0$ [0,0,0]		
4 c $2'/m$ ..	$0,1/2,0$ [0,0,0]	$1/2,0,1/2$ [0,0,0]		
4 b $2'/m$ ..	$1/2,1/2,0$ [0,0,w]	$1/2,1/2,1/2$ [0,0,w]		
4 a $2'/m$ ..	$0,0,0$ [0,0,w]	$0,0,1/2$ [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1]  $p41'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p_{2a}2mm$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x-1/4, x+1/4, 0$



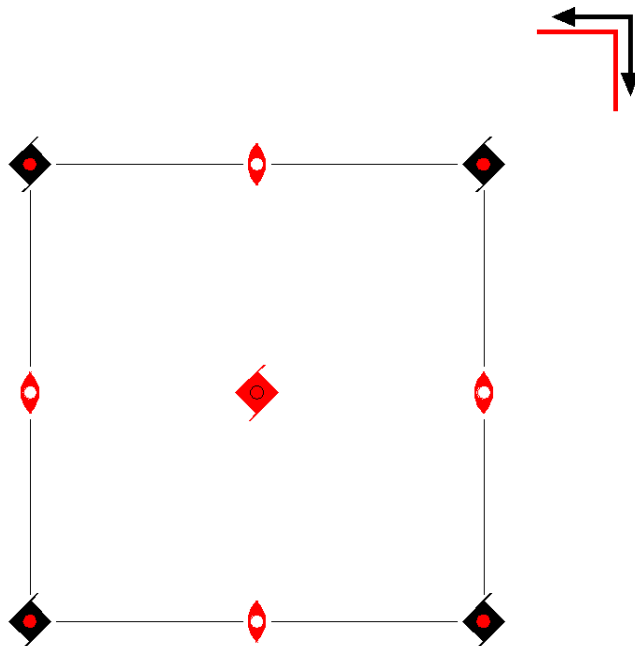
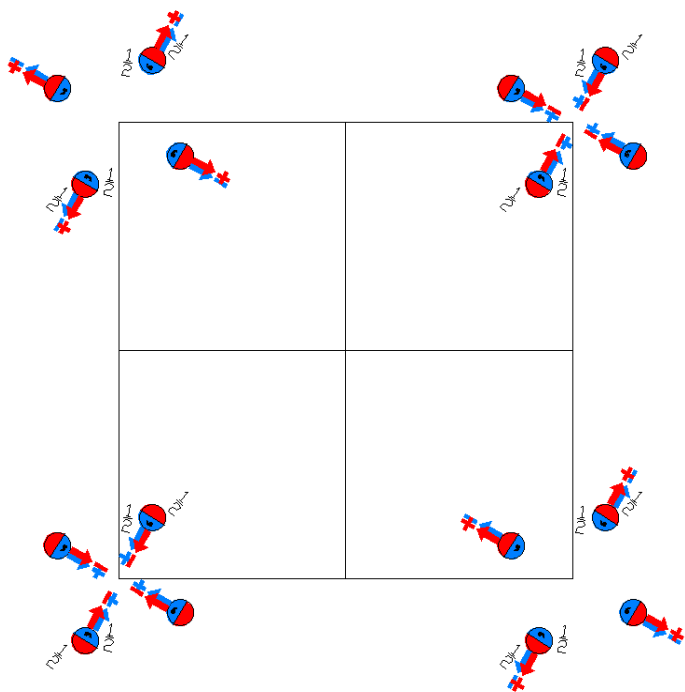
$P_P 4_2/m'$

84.7.719

$4/m1'$

$P_P 4_2/m'$

Tetragonal



Origin at center ( $2/m'$ ) on  $4_2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |                                      |  |   |
|---|--------------------------------------|--|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)     | (3) $4^+$ (0,0,1/2) $0,0,z$<br>( $4_z$  0,0,1/2)       | (4) $4^-$ (0,0,1/2) $0,0,z$<br>( $4_z^{-1}$  0,0,1/2)       |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)' | (6) $m'$ $x,y,0$<br>( $m_z$  0,0,0)' | (7) $\bar{4}^+$ $0,0,z; 0,0,1/4$<br>( $4_z$  0,0,1/2)' | (8) $\bar{4}^-$ $0,0,z; 0,0,1/4$<br>( $4_z^{-1}$  0,0,1/2)' |

For (1,0,0)' + set

- |  |  |   |  |
|--|--|---|--|
| (1) $t'$ (1,0,0)<br>(1 1,0,0)'                 | (2) $2'$ $1/2,0,z$<br>( $2_z$  1,0,0)'     | (3) $4^+$ (0,0,1/2) $1/2,1/2,z$<br>( $4_z$  1,0,1/2)'           | (4) $4^-$ (0,0,1/2) $1/2,-1/2,z$<br>( $4_z^{-1}$  1,0,1/2)'        |
| (5) $\bar{1}$ $1/2,0,0$<br>( $\bar{1}$  1,0,0) | (6) $a$ (1,0,0) $x,y,0$<br>( $m_z$  1,0,0) | (7) $\bar{4}^+$ $1/2,-1/2,z; 1/2,-1/2,1/4$<br>( $4_z$  1,0,1/2) | (8) $\bar{4}^-$ $1/2,1/2,z; 1/2,1/2,1/4$<br>( $4_z^{-1}$  1,0,1/2) |

Continued

84.7.719

$P_P 4_2/m'$

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

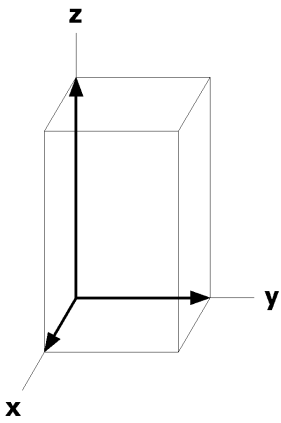
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 k 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ] (7) y, $\bar{x},\bar{z}+1/2$ [v, $\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z+1/2$ [v, $\bar{u},w$ ] (8) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]
8 j m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},u,0$ ]	y, $\bar{x},1/2$ [v, $\bar{u},0$ ]
8 i 2'..	0,1/2,z [u,v,0]	1/2,0,z+1/2 [v, $\bar{u},0$ ]	0,1/2, $\bar{z}$ [u,v,0]	1/2,0, $\bar{z}+1/2$ [v, $\bar{u},0$ ]
8 h 2..	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
8 g 2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4 f $\bar{4}$ '..	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
4 e $\bar{4}$ '..	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		
4 d 2'/m'..	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]		
4 c 2'/m'..	0,1/2,0 [u,v,0]	1/2,0,1/2 [v, $\bar{u},0$ ]		
4 b 2'/m'..	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4 a 2'/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_p \cdot 4$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

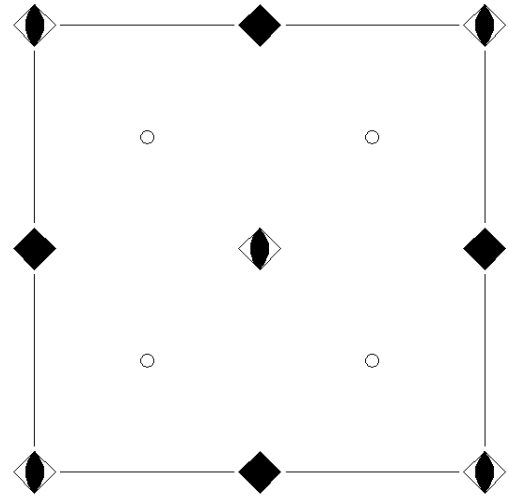
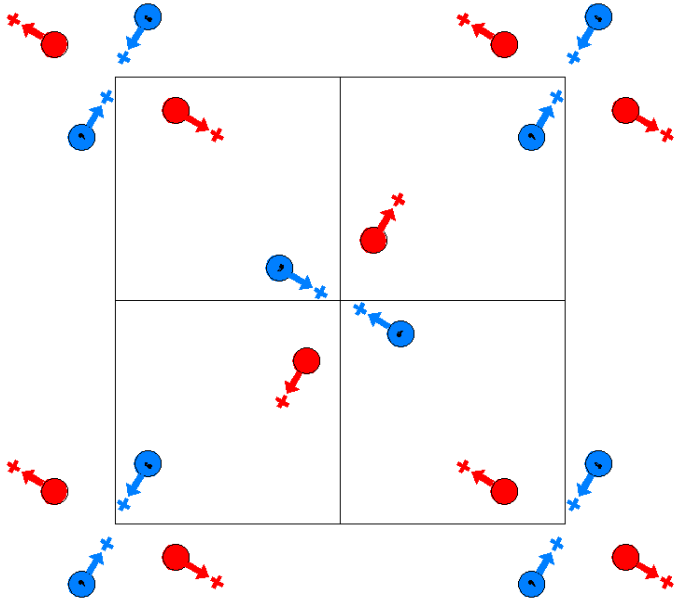
Along [1,1,0]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4/n  
85.1.720

4/m  
P4/n

Tetragonal



Origin at  $\bar{4}$  on  $n$ ,  $-1/4, 1/4, 0$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

(1)  $1$   
 $(1 | 0, 0, 0)$

(2)  $2$   $0, 0, z$   
 $(2_z | 0, 0, 0)$

(3)  $4^+$   $0, 1/2, z$   
 $(4_z | 1/2, 1/2, 0)$

(4)  $4^-$   $1/2, 0, z$   
 $(4_z^{-1} | 1/2, 1/2, 0)$

(5)  $\bar{1}$   $1/4, 1/4, 0$   
 $(\bar{1} | 1/2, 1/2, 0)$

(6)  $n$   $(1/2, 1/2, 0)$   $x, y, 0$   
 $(m_z | 1/2, 1/2, 0)$

(7)  $\bar{4}^+$   $0, 0, z; 0, 0, 0$   
 $(\bar{4}_z | 0, 0, 0)$

(8)  $\bar{4}^-$   $0, 0, z; 0, 0, 0$   
 $(\bar{4}_z^{-1} | 0, 0, 0)$



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

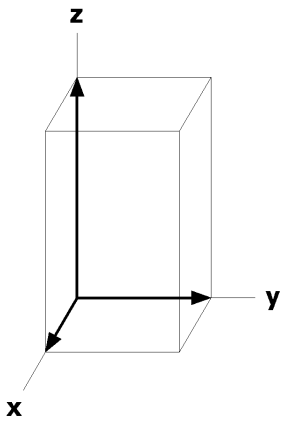
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	g 1	(1) x,y,z [u,v,w]		(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	
		(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},u,w$ ]		(4) $y+1/2,\bar{x}+1/2,z$ [ $v,\bar{u},w$ ]	
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $u,v,w$ ]		(6) $x+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	
		(7) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]		(8) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]	
4	f 2..	0,0,z [0,0,w]	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]
4	e $\bar{1}$	1/4,1/4,1/2 [u,v,w]	3/4,3/4,1/2 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,1/2 [ $\bar{v},u,w$ ]	3/4,1/4,1/2 [ $v,\bar{u},w$ ]
4	d $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,0 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,0 [ $\bar{v},u,w$ ]	3/4,1/4,0 [ $v,\bar{u},w$ ]
2	c 4..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]		
2	b $\bar{4}$ ..	0,0,1/2 [0,0,w]	1/2,1/2,1/2 [0,0,w]		
2	a $\bar{4}$ ..	0,0,0 [0,0,w]	1/2,1/2,0 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p4  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [1,1,0] p2mm  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0

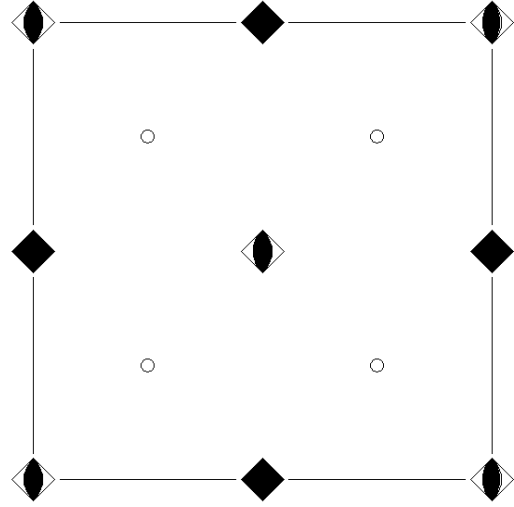
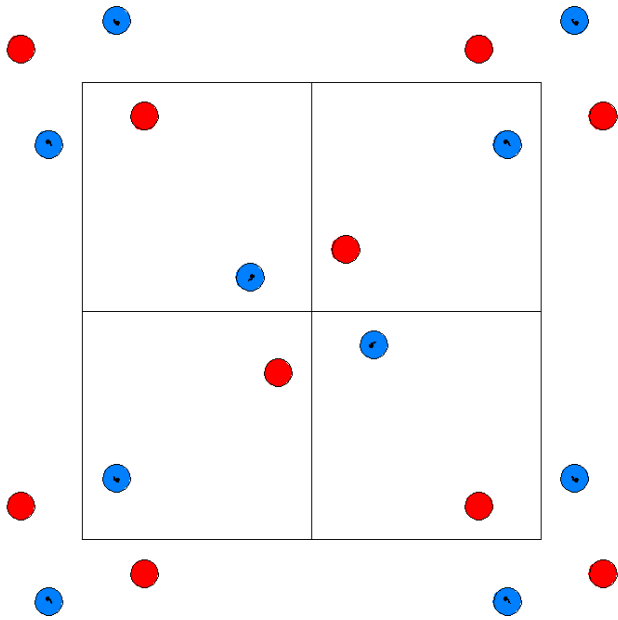


P4/n1'  
85.2.721

4/m1'  
P4/n1'

Tetragonal

1'



Origin at  $\bar{4}1'$  on n,  $-1/4, 1/4, 0$  from  $\bar{1}1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

1 + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0) | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0) |
| (5) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0) | (6) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (7) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)   | (8) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                 |

1' + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1'<br>(1 0,0,0)'                                  | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                 | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0)' | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)' |
| (5) $\bar{1}'$ 1/4,1/4,0<br>( $\bar{1}'$  1/2,1/2,0)' | (6) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (7) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'   | (8) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

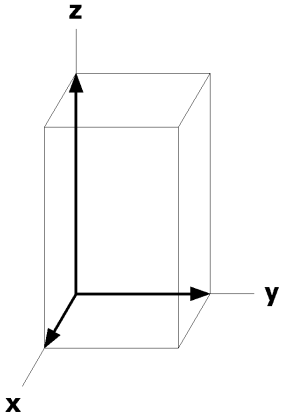
				Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.				1 +	1' +		
8	g 11'	(1) x,y,z [0,0,0]		(2) $\bar{x},\bar{y},z$ [0,0,0]			
		(3) $\bar{y}+1/2,x+1/2,z$ [0,0,0]		(4) $y+1/2,\bar{x}+1/2,z$ [0,0,0]			
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [0,0,0]		(6) $x+1/2,y+1/2,\bar{z}$ [0,0,0]			
		(7) $y,\bar{x},\bar{z}$ [0,0,0]		(8) $\bar{y},x,\bar{z}$ [0,0,0]			
4	f 2..1'	0,0,z [0,0,0]	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		0,0, $\bar{z}$ [0,0,0]	
4	e $\bar{1}1'$	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]		3/4,1/4,1/2 [0,0,0]	
4	d $\bar{1}1'$	1/4,1/4,0 [0,0,0]	3/4,3/4,0 [0,0,0]	1/4,3/4,0 [0,0,0]		3/4,1/4,0 [0,0,0]	
2	c 4..1'	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]				
2	b $\bar{4}..1'$	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]				
2	a $\bar{4}..1'$	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]				

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

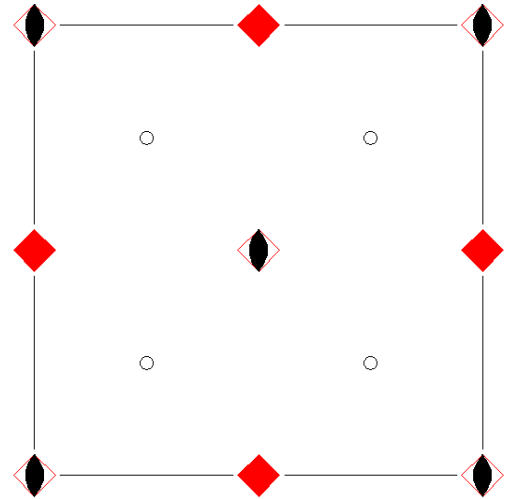
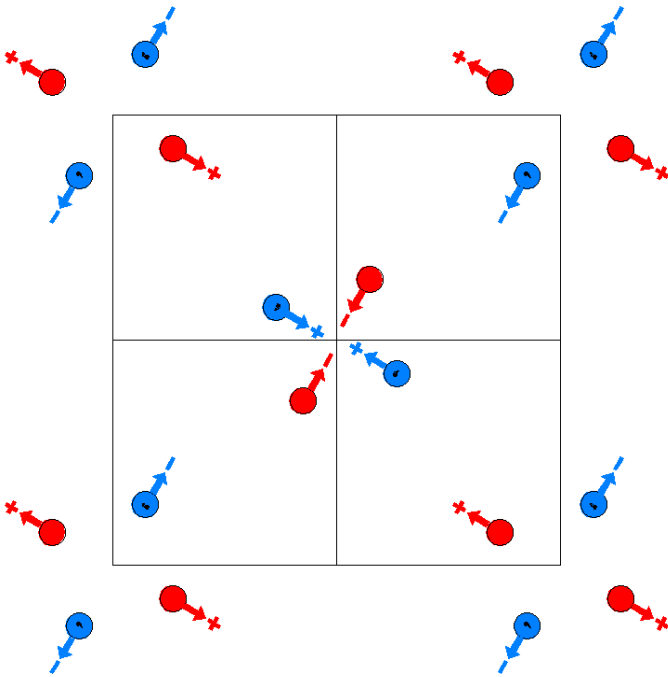
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4'/n  
85.3.722

4'/m  
P4'/n

Tetragonal



Origin at  $\bar{4}'$  on n,  $-1/4, 1/4, 0$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

- |  |  |  |   |
|--|--|--|---|
| (1) $1$<br>$(1   0, 0, 0)$                               | (2) $2$ $0, 0, z$<br>$(2_z   0, 0, 0)$               | (3) $4^+$ $0, 1/2, z$<br>$(4_z   1/2, 1/2, 0)'$                  | (4) $4^-$ $1/2, 0, z$<br>$(4_z^{-1}   1/2, 1/2, 0)'$                |
| (5) $\bar{1}$ $1/4, 1/4, 0$<br>$(\bar{1}   1/2, 1/2, 0)$ | (6) n $(1/2, 1/2, 0)$ x,y,0<br>$(m_z   1/2, 1/2, 0)$ | (7) $\bar{4}^+$ $0, 0, z; 0, 0, 0$<br>$(\bar{4}_z^+   0, 0, 0)'$ | (8) $\bar{4}^-$ $0, 0, z; 0, 0, 0$<br>$(\bar{4}_z^{-1}   0, 0, 0)'$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

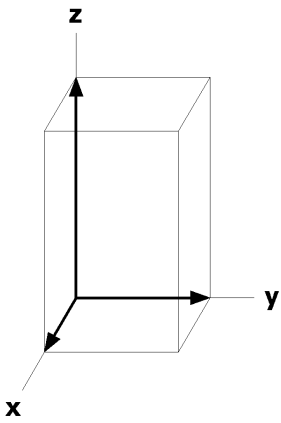
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
		(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z$ [ $\bar{v},u,\bar{w}$ ]		
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [u,v,w]	(6) $x+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]		
		(7) $y,\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
4	f 2..	0,0,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4	e $\bar{1}$	1/4,1/4,1/2 [u,v,w]	3/4,3/4,1/2 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,1/2 [ $\bar{v},\bar{u},\bar{w}$ ]	3/4,1/4,1/2 [ $\bar{v},u,\bar{w}$ ]
4	d $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,0 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,0 [ $\bar{v},\bar{u},\bar{w}$ ]	3/4,1/4,0 [ $\bar{v},u,\bar{w}$ ]
2	c 4'..	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
2	b $\bar{4}'..$	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a $\bar{4}'..$	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

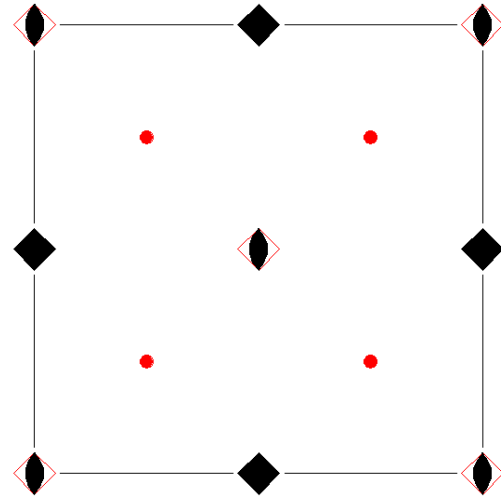
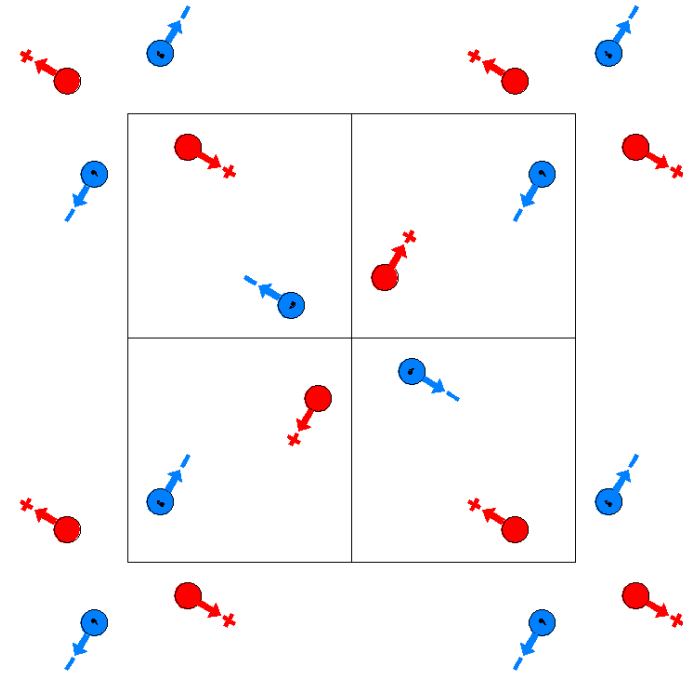
Along [1,1,0] p2mm  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4/n'  
85.4.723

4/m'  
P4/n'

Tetragonal



Origin at  $\bar{4}$  on  $n'$ ,  $-1/4, 1/4, 0$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

- |   |  |  |  |
|---|--|--|--|
| (1) $1$<br>$(1   0,0,0)$                                | (2) $2$ $0,0,z$<br>$(2_z   0,0,0)$                     | (3) $4^+$ $0,1/2,z$<br>$(4_z   1/2,1/2,0)$                 | (4) $4^-$ $1/2,0,z$<br>$(4_z^{-1}   1/2,1/2,0)$            |
| (5) $\bar{1}'$ $1/4,1/4,0$<br>$(\bar{1}'   1/2,1/2,0)'$ | (6) $n'$ $(1/2,1/2,0)$ $x,y,0$<br>$(m_z   1/2,1/2,0)'$ | (7) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^+   0,0,0)'$ | (8) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^-   0,0,0)'$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

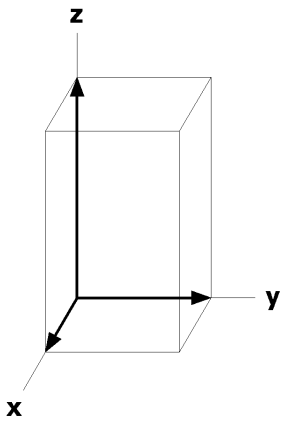
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
		(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z$ [ $v,\bar{u},w$ ]		
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,y+1/2,\bar{z}$ [ $u,v,\bar{w}$ ]		
		(7) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(8) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
4	f 2..	0,0,z [0,0,w]	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4	e $\bar{1}'$	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]
4	d $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,0 [0,0,0]	1/4,3/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]
2	c 4..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	b $\bar{4}'..$	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a $\bar{4}'..$	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_4$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/2,0,z

Along [1,0,0]  $p2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

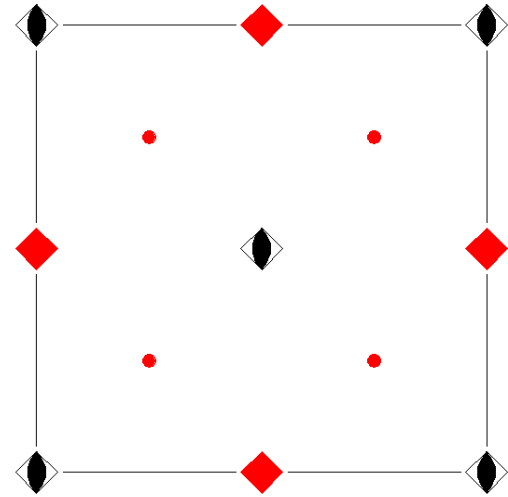
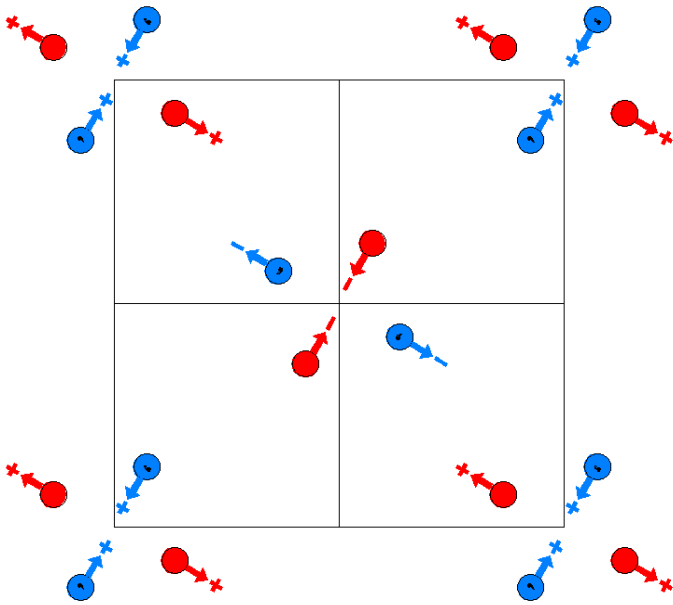
Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4'/n'  
85.5.724

4'/m'  
P4'/n'

Tetragonal



Origin at  $\bar{4}$  on  $n'$ ,  $-1/4, 1/4, 0$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

(1)  $1$   
 $(1 | 0, 0, 0)$

(2)  $2$   $0, 0, z$   
 $(2_z | 0, 0, 0)$

(3)  $4^+$   $0, 1/2, z$   
 $(4_z | 1/2, 1/2, 0)'$

(4)  $4^-$   $1/2, 0, z$   
 $(4_z^{-1} | 1/2, 1/2, 0)'$

(5)  $\bar{1}'$   $1/4, 1/4, 0$   
 $(\bar{1}' | 1/2, 1/2, 0)'$

(6)  $n'$   $(1/2, 1/2, 0)$   $x, y, 0$   
 $(m_z | 1/2, 1/2, 0)'$

(7)  $\bar{4}^+$   $0, 0, z; 0, 0, 0$   
 $(\bar{4}_z^+ | 0, 0, 0)$

(8)  $\bar{4}^-$   $0, 0, z; 0, 0, 0$   
 $(\bar{4}_z^{-1} | 0, 0, 0)$



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

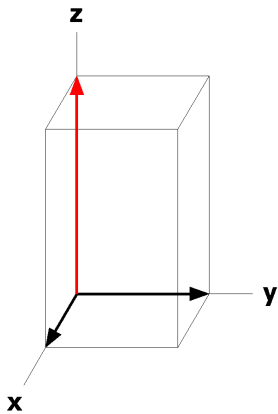
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
		(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z$ [ $\bar{v},u,\bar{w}$ ]		
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,y+1/2,\bar{z}$ [u,v, $\bar{w}$ ]		
		(7) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(8) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]		
4	f 2..	0,0,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]
4	e $\bar{1}'$	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]
4	d $\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,0 [0,0,0]	1/4,3/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]
2	c 4'..	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
2	b $\bar{4}$ ..	0,0,1/2 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		
2	a $\bar{4}$ ..	0,0,0 [0,0,w]	1/2,1/2,0 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_4$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

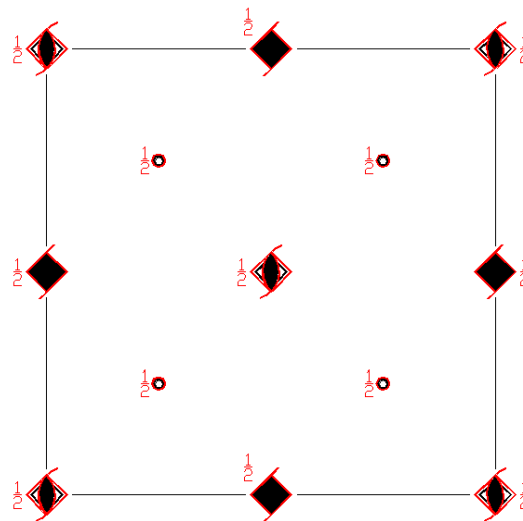
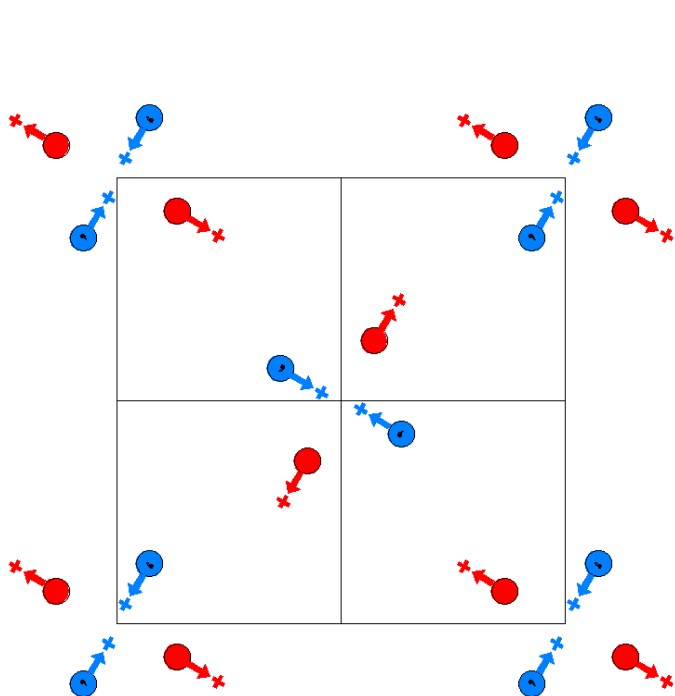
Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_{2c} 4/n$   
85.6.725

$4/m1'$   
 $P_{2c} 4/n$

Tetragonal



Origin at  $\bar{4}$  on  $n$ ,  $-1/4, 1/4, 0$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |   |  |
|--|--|---|--|
| (1) $1$<br>$(1 0,0,0)$                             | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                   | (3) $4^+$ $0,1/2,z$<br>$(4_z 1/2,1/2,0)$              | (4) $4^-$ $1/2,0,z$<br>$(4_z^{-1} 1/2,1/2,0)$              |
| (5) $\bar{1}$ $1/4,1/4,0$<br>$(\bar{1} 1/2,1/2,0)$ | (6) $n$ $(1/2,1/2,0)$ $x,y,0$<br>$(m_z 1/2,1/2,0)$ | (7) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z 0,0,0)$ | (8) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1} 0,0,0)$ |

For  $(0,0,1)'$  + set

- |   |  |   |  |
|---|--|---|--|
| (1) $t'$ $(0,0,1)$<br>$(1 0,0,1)'$                      | (2) $2'$ $(0,0,1)$ $0,0,z$<br>$(2_z 0,0,1)'$           | (3) $4^{+'}$ $(0,0,1)$ $0,1/2,z$<br>$(4_z 1/2,1/2,1)'$      | (4) $4^{-'}$ $(0,0,1)$ $1/2,0,z$<br>$(4_z^{-1} 1/2,1/2,1)'$      |
| (5) $\bar{1}'$ $1/4,1/4,1/2$<br>$(\bar{1}' 1/2,1/2,1)'$ | (6) $n'$ $(1/2,1/2,0)$ $x,y,1/2$<br>$(m_z 1/2,1/2,1)'$ | (7) $\bar{4}^{+'}$ $0,0,z; 0,0,1/2$<br>$(\bar{4}_z 0,0,1)'$ | (8) $\bar{4}^{-'}$ $0,0,z; 0,0,1/2$<br>$(\bar{4}_z^{-1} 0,0,1)'$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

### Positions

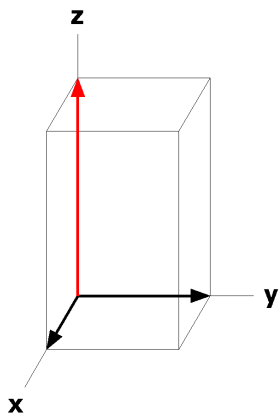
Multiplicity, Wyckoff letter, Site Symmetry.		Coordinates			
		(0,0,0) +		(0,0,1)' +	
16	g 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
		(3) $\bar{y}+1/2, x+1/2, z$ [ $\bar{v}, u, w$ ]	(4) $y+1/2, \bar{x}+1/2, z$ [ $v, \bar{u}, w$ ]		
		(5) $\bar{x}+1/2, \bar{y}+1/2, \bar{z}$ [ $u, v, w$ ]	(6) $x+1/2, y+1/2, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]		
		(7) $y, \bar{x}, \bar{z}$ [ $\bar{v}, u, w$ ]	(8) $\bar{y}, x, z$ [ $v, \bar{u}, w$ ]		
8	f 2..	0,0,z [0,0,w]	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]
8	e $\bar{1}'$	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]
8	d $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,0 [ $\bar{u}, \bar{v}, w$ ]	1/4,3/4,0 [ $\bar{v}, u, w$ ]	3/4,1/4,0 [ $v, \bar{u}, w$ ]
4	c 4..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]		
4	b $\bar{4}'..$	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4	a $\bar{4}..$	0,0,0 [0,0,w]	1/2,1/2,0 [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] p41'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>'-2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/2

Along [1,1,0] p<sub>2a</sub>'-2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/2



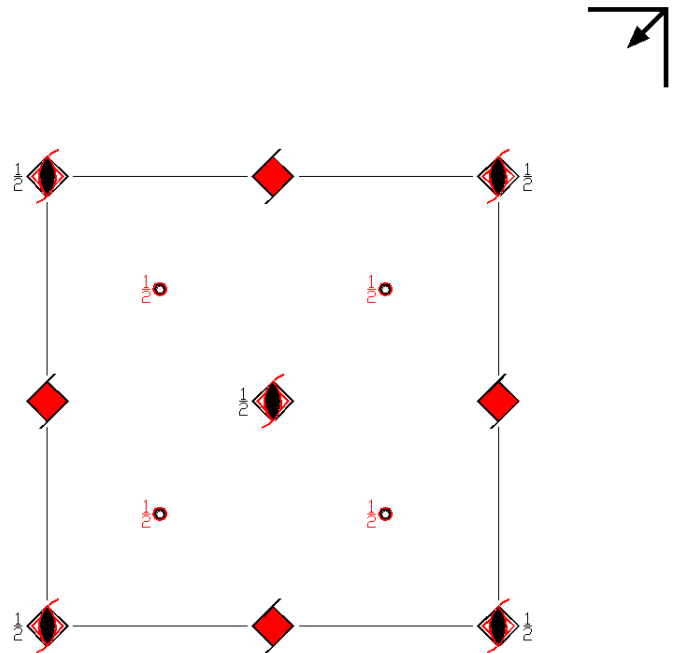
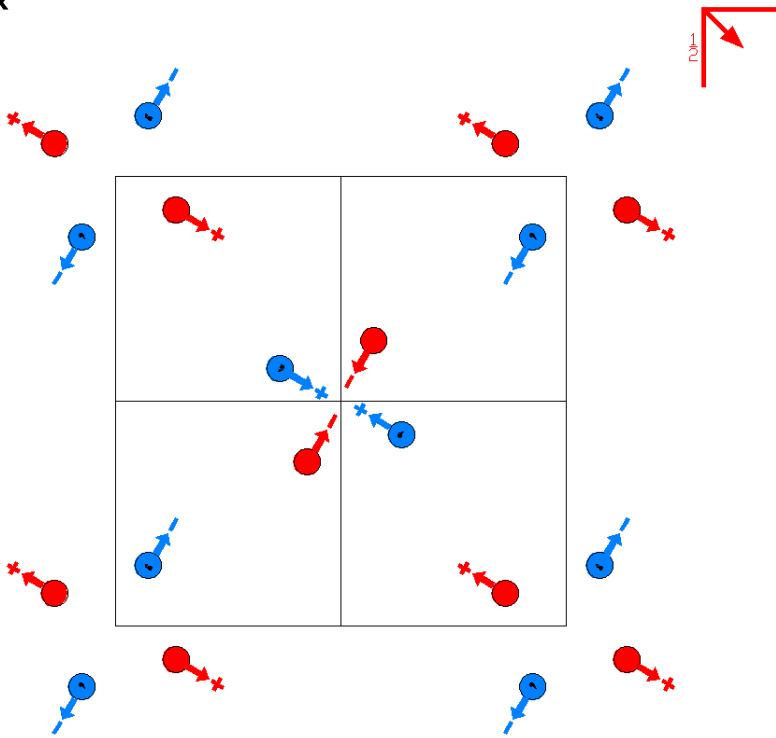
$P_{2c} 4'/n$

85.7.726

$4/m1'$

$P_{2c} 4'/n$

Tetragonal



Origin at  $\bar{4}'$  on  $n$ ,  $-1/4, 1/4, 0$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |  |   |
|--|--|--|---|
| (1) $1$<br>$(1 0,0,0)$                             | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                   | (3) $4^+$ $0,1/2,z$<br>$(4_z 1/2,1/2,0)'$              | (4) $4^-$ $1/2,0,z$<br>$(4_z^{-1} 1/2,1/2,0)'$              |
| (5) $\bar{1}$ $1/4,1/4,0$<br>$(\bar{1} 1/2,1/2,0)$ | (6) $n$ $(1/2,1/2,0)$ $x,y,0$<br>$(m_z 1/2,1/2,0)$ | (7) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z 0,0,0)'$ | (8) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1} 0,0,0)'$ |

For  $(0,0,1)'$  + set

- |   |  |  |   |
|---|--|--|---|
| (1) $t'$ $(0,0,1)$<br>$(1 0,0,1)'$                      | (2) $2'$ $(0,0,1)$ $0,0,z$<br>$(2_z 0,0,1)'$           | (3) $4^+$ $(0,0,1)$ $0,1/2,z$<br>$(4_z 1/2,1/2,1)$       | (4) $4^-$ $(0,0,1)$ $1/2,0,z$<br>$(4_z^{-1} 1/2,1/2,1)$       |
| (5) $\bar{1}'$ $1/4,1/4,1/2$<br>$(\bar{1}' 1/2,1/2,1)'$ | (6) $n'$ $(1/2,1/2,0)$ $x,y,1/2$<br>$(m_z 1/2,1/2,1)'$ | (7) $\bar{4}^+$ $0,0,z; 0,0,1/2$<br>$(\bar{4}_z 0,0,1)'$ | (8) $\bar{4}^-$ $0,0,z; 0,0,1/2$<br>$(\bar{4}_z^{-1} 0,0,1)'$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

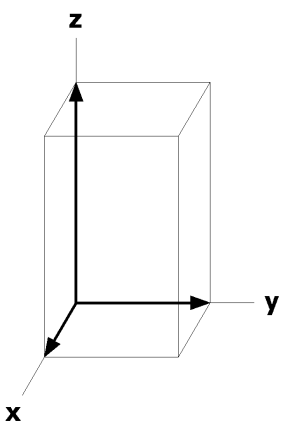
				Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.					
				(0,0,0) +	(0,0,1)' +
16	g 1	(1) x,y,z [u,v,w]		(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	
		(3) $\bar{y}+1/2, x+1/2, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		(4) $y+1/2, \bar{x}+1/2, z$ [ $\bar{v}, u, \bar{w}$ ]	
		(5) $\bar{x}+1/2, \bar{y}+1/2, \bar{z}$ [ $u, v, w$ ]		(6) $x+1/2, y+1/2, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	
		(7) $y, \bar{x}, \bar{z}$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		(8) $\bar{y}, x, \bar{z}$ [ $\bar{v}, u, \bar{w}$ ]	
8	f 2..	0,0,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
8	e $\bar{1}'$	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]
8	d $\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,0 [ $\bar{u}, \bar{v}, w$ ]	1/4,3/4,0 [ $\bar{v}, \bar{u}, \bar{w}$ ]	3/4,1/4,0 [ $\bar{v}, u, \bar{w}$ ]
4	c 4'..	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
4	b $\bar{4}$ ..	0,0,1/2 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		
4	a $\bar{4}'$ ..	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>'-2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/2

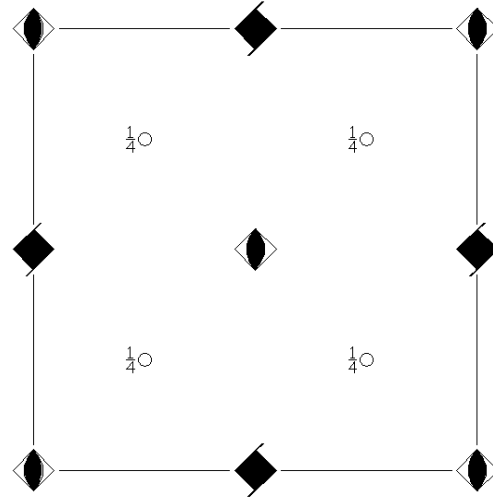
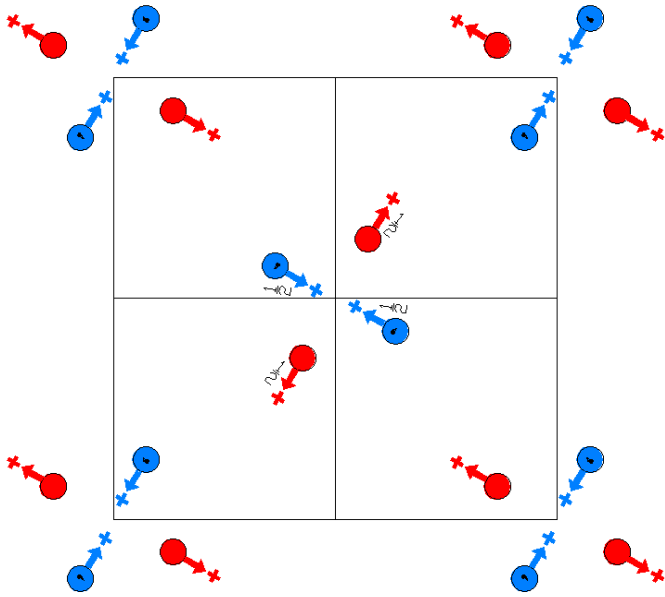
Along [1,1,0] p<sub>2a</sub>'-2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/2



$P4_2/n$   
86.1.727

$4/m$   
 $P4_2/n$

Tetragonal



Origin at  $\bar{4}$  at  $-1/4, -1/4, -1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |  |   |
|--|--|--|---|
| (1) $\bar{1}$<br>(1 0,0,0)                             | (2) $2$ 0,0,z<br>( $2_z$  0,0,0)                     | (3) $4^+$ (0,0,1/2) 0,1/2,z<br>( $4_z$  1/2,1/2,1/2) | (4) $4^-$ (0,0,1/2) 1/2,0,z<br>( $4_z^{-1}$  1/2,1/2,1/2) |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2) | (6) $n$ (1/2,1/2,0) x,y,1/4<br>( $m_z$  1/2,1/2,1/2) | (7) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $4_z$  0,0,0)      | (8) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $4_z^{-1}$  0,0,0)      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

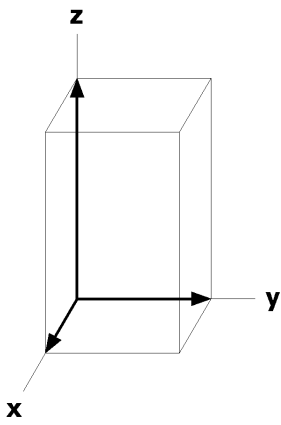
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
		(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]		
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [u,v,w]	(6) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]		
		(7) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(8) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]		
4	f 2..	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]
4	e 2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]
4	d $\bar{1}$	1/4,1/4,3/4 [u,v,w]	3/4,3/4,3/4 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,1/4 [ $\bar{v},u,w$ ]	3/4,1/4,1/4 [ $v,\bar{u},w$ ]
4	c $\bar{1}$	1/4,1/4,1/4 [u,v,w]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,3/4 [ $\bar{v},u,w$ ]	3/4,1/4,3/4 [ $v,\bar{u},w$ ]
2	b $\bar{4}..$	0,0,1/2 [0,0,w]	1/2,1/2,0 [0,0,w]		
2	a $\bar{4}..$	0,0,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p4  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



$P4_2/n1'$

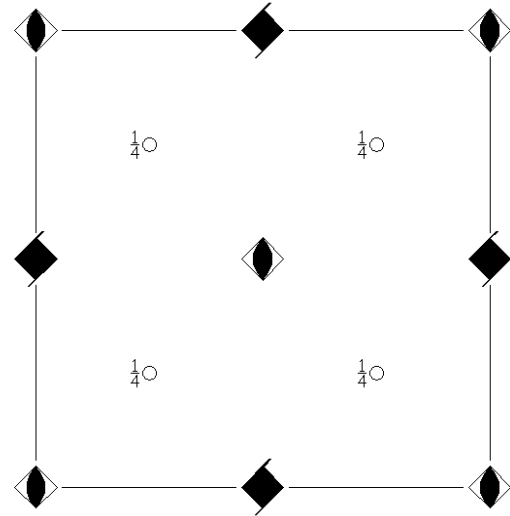
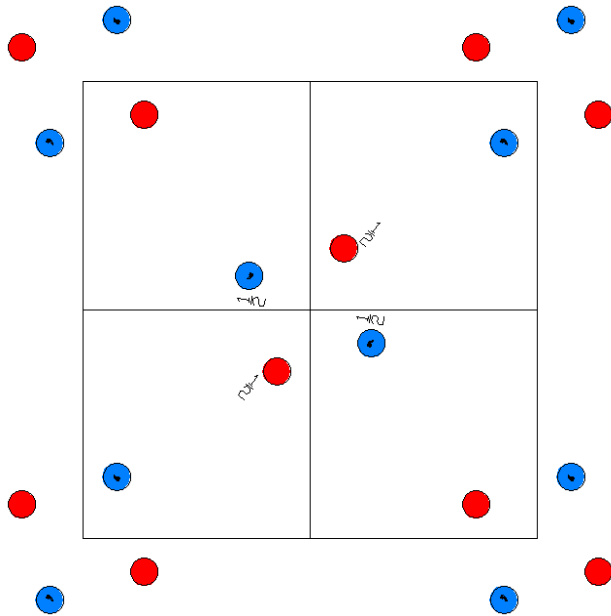
86.2.728

$4/m1'$

$P4_2/n1'$

Tetragonal

$1'$



Origin at  $\bar{4}1'$  at  $-1/4, -1/4, -1/4$  from  $\bar{1}1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

For  $1 +$  set

- |  |  |  |   |
|--|--|--|---|
| (1) $1$<br>( $1   0,0,0$ )                                 | (2) $2$ $0,0,z$<br>( $2_z   0,0,0$ )                     | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>( $4_z   1/2,1/2,1/2$ ) | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1}   1/2,1/2,1/2$ ) |
| (5) $\bar{1}$ $1/4,1/4,1/4$<br>( $\bar{1}   1/2,1/2,1/2$ ) | (6) $n$ $(1/2,1/2,0) x,y,1/4$<br>( $m_z   1/2,1/2,1/2$ ) | (7) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $4_z   0,0,0$ )      | (8) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $4_z^{-1}   0,0,0$ )      |

For  $1' +$  set

- |  |  |  |   |
|--|--|--|---|
| (1) $1'$<br>( $1   0,0,0$ )'                                 | (2) $2'$ $0,0,z$<br>( $2_z   0,0,0$ )'                   | (3) $4^{+'}$ $(0,0,1/2) 0,1/2,z$<br>( $4_z   1/2,1/2,1/2$ )' | (4) $4^{-'}$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1}   1/2,1/2,1/2$ )' |
| (5) $\bar{1}'$ $1/4,1/4,1/2$<br>( $\bar{1}   1/2,1/2,1/2$ )' | (6) $n'$ $(1/2,1/2,0) x,y,0$<br>( $m_z   1/2,1/2,1/2$ )' | (7) $\bar{4}^{+'}$ $0,0,z; 0,0,0$<br>( $4_z   0,0,0$ )'      | (8) $\bar{4}^{-'}$ $0,0,z; 0,0,0$<br>( $4_z^{-1}   0,0,0$ )'      |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

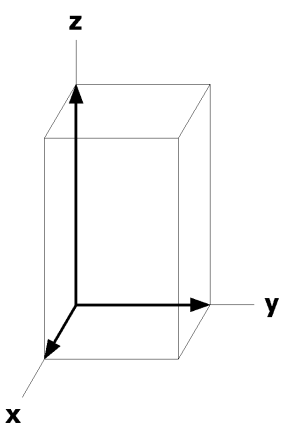
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		1 +	1' +		
8	g 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]		
		(3) $\bar{y}+1/2,x+1/2,z+1/2$ [0,0,0]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [0,0,0]		
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [0,0,0]	(6) $x+1/2,y+1/2,\bar{z}+1/2$ [0,0,0]		
		(7) $y,\bar{x},\bar{z}$ [0,0,0]	(8) $\bar{y},x,\bar{z}$ [0,0,0]		
4	f 2..1'	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	e 2..1'	0,1/2,z [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]
4	d $\bar{1}1'$	1/4,1/4,3/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
4	c $\bar{1}1'$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]
2	b $\bar{4}..1'$	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a $\bar{4}..1'$	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

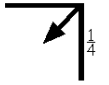
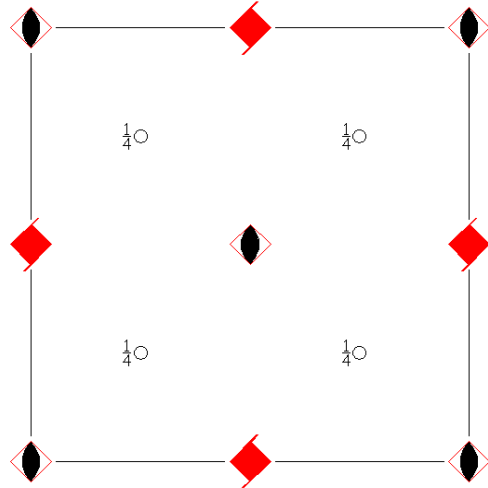
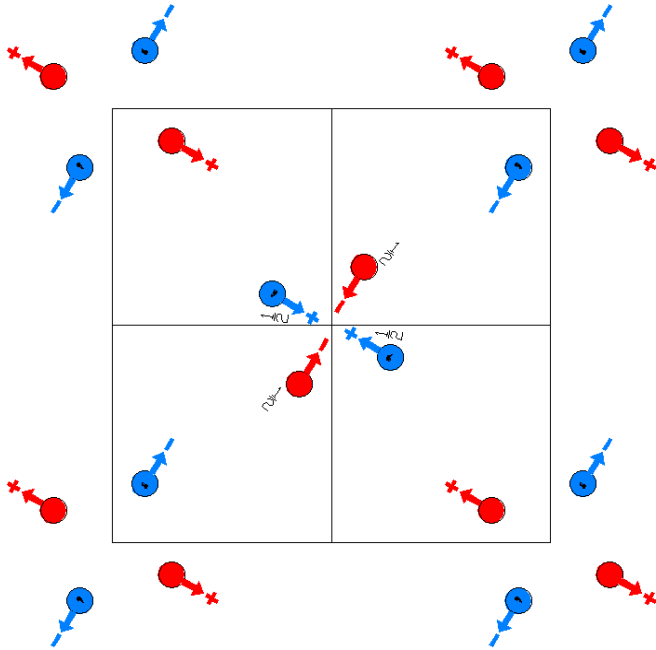
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



$P4_2'/n$   
86.3.729

$4'/m$   
 $P4_2'/n$

Tetragonal



Origin at  $\bar{4}'$  at  $-1/4, -1/4, -1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |  |   |
|--|--|--|---|
| (1) $1$<br>$(1 0,0,0)$                                 | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                     | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>$(4_z 1/2,1/2,1/2)'$  | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>$(4_z^{-1} 1/2,1/2,1/2)'$  |
| (5) $\bar{1}$ $1/4,1/4,1/4$<br>$(\bar{1} 1/2,1/2,1/2)$ | (6) $n$ $(1/2,1/2,0) x,y,1/4$<br>$(m_z 1/2,1/2,1/2)$ | (7) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z 0,0,0)'$ | (8) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1} 0,0,0)'$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

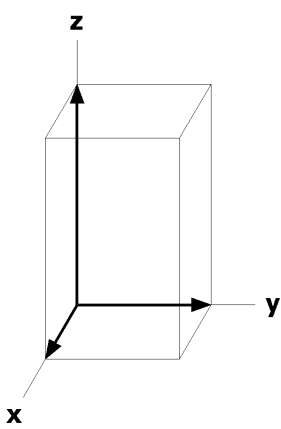
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
		(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]		
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [u,v,w]	(6) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]		
		(7) $y,\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
4	f 2..	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4	e 2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4	d $\bar{1}$	1/4,1/4,3/4 [u,v,w]	3/4,3/4,3/4 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,1/4 [ $\bar{v},\bar{u},\bar{w}$ ]	3/4,1/4,1/4 [ $\bar{v},u,\bar{w}$ ]
4	c $\bar{1}$	1/4,1/4,1/4 [u,v,w]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,3/4 [ $\bar{v},\bar{u},\bar{w}$ ]	3/4,1/4,3/4 [ $\bar{v},u,\bar{w}$ ]
2	b $\bar{4}'$ ..	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a $\bar{4}'$ ..	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

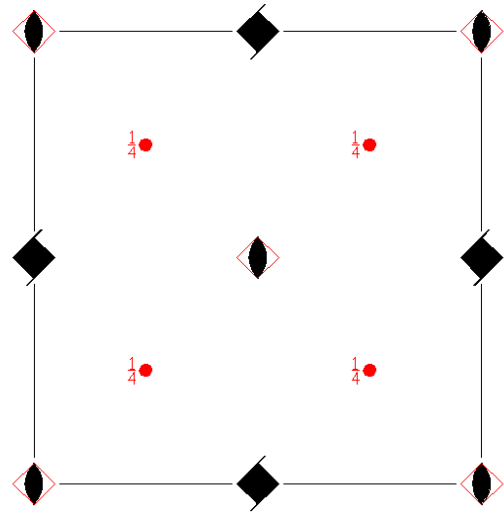
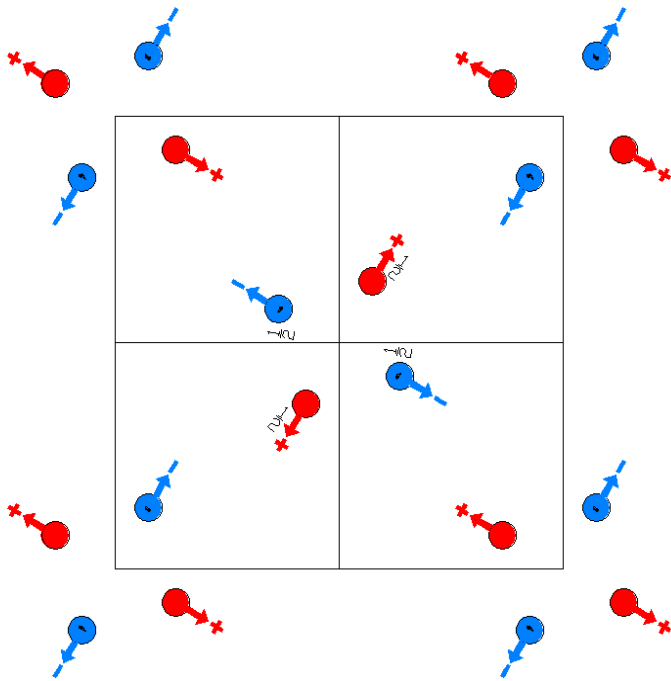
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



$P4_2/n'$   
86.4.730

$4/m'$   
 $P4_2/n'$

Tetragonal



Origin at  $\bar{4}'$  at  $-1/4, -1/4, -1/4$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |  |  |   |
|---|--|--|---|
| (1) $1$<br>$(1 0,0,0)$                                    | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                       | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>$(4_z 1/2,1/2,1/2)$   | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>$(4_z^{-1} 1/2,1/2,1/2)$   |
| (5) $\bar{1}'$ $1/4,1/4,1/4$<br>$(\bar{1}' 1/2,1/2,1/2)'$ | (6) $n'$ $(1/2,1/2,0) x,y,1/4$<br>$(m_z 1/2,1/2,1/2)'$ | (7) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z 0,0,0)'$ | (8) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1} 0,0,0)'$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

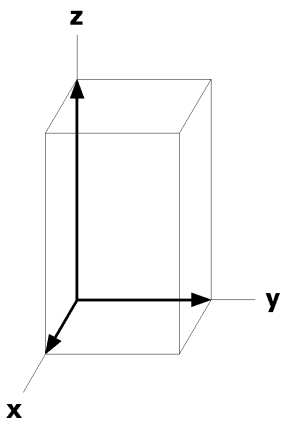
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
		(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]		
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]		
		(7) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(8) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
4	f 2..	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4	e 2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4	d $\bar{1}'$	1/4,1/4,3/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
4	c $\bar{1}'$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]
2	b $\bar{4}'..$	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a $\bar{4}'..$	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_4$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/2,0,z

Along [1,0,0]  $p2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

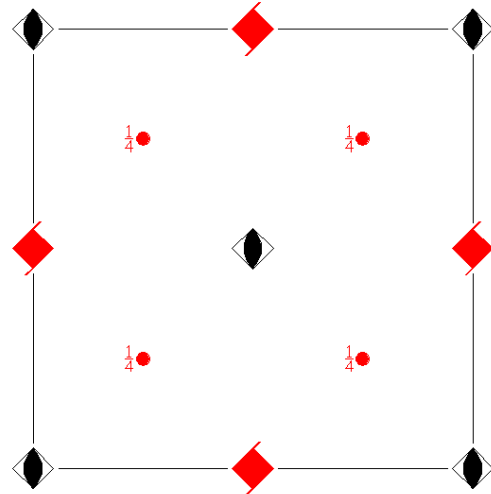
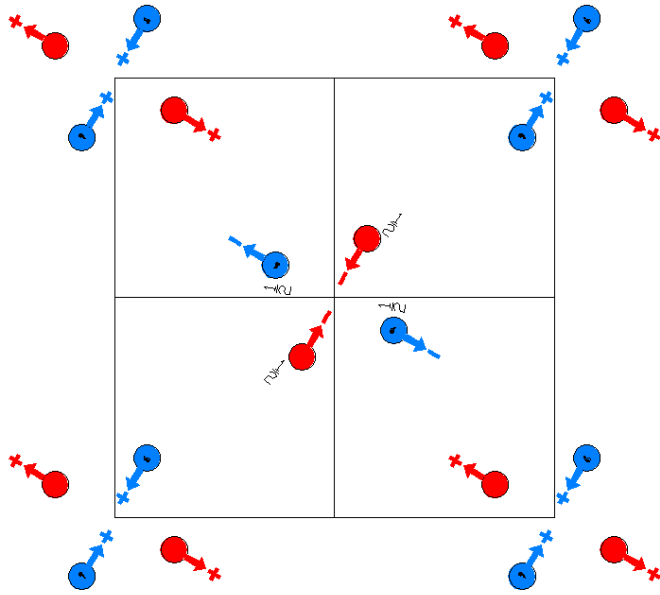
Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



$P4_2'n'$   
86.5.731

$4'/m'$   
 $P4_2'n'$

Tetragonal



Origin at  $\bar{4}$  at  $-1/4, -1/4, -1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |  |   |  |
|---|--|---|--|
| (1) $1$<br>$(1   0,0,0)$                                  | (2) $2$ $0,0,z$<br>$(2_z   0,0,0)$                       | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>$(4_z   1/2,1/2,1/2)'$ | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>$(4_z^{-1}   1/2,1/2,1/2)'$ |
| (5) $\bar{1}$ $1/4,1/4,1/4$<br>$(\bar{1}   1/2,1/2,1/2)'$ | (6) $n'$ $(1/2,1/2,0) x,y,1/4$<br>$(m_z   1/2,1/2,1/2)'$ | (7) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z   0,0,0)$ | (8) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1}   0,0,0)$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

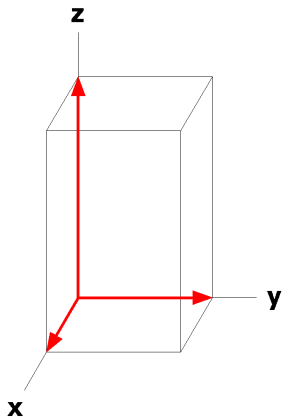
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
		(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]		
		(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]		
		(7) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(8) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]		
4	f 2..	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]
4	e 2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]
4	d $\bar{1}'$	1/4,1/4,3/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
4	c $\bar{1}'$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]
2	b $\bar{4}..$	0,0,1/2 [0,0,w]	1/2,1/2,0 [0,0, $\bar{w}$ ]		
2	a $\bar{4}..$	0,0,0 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_4$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

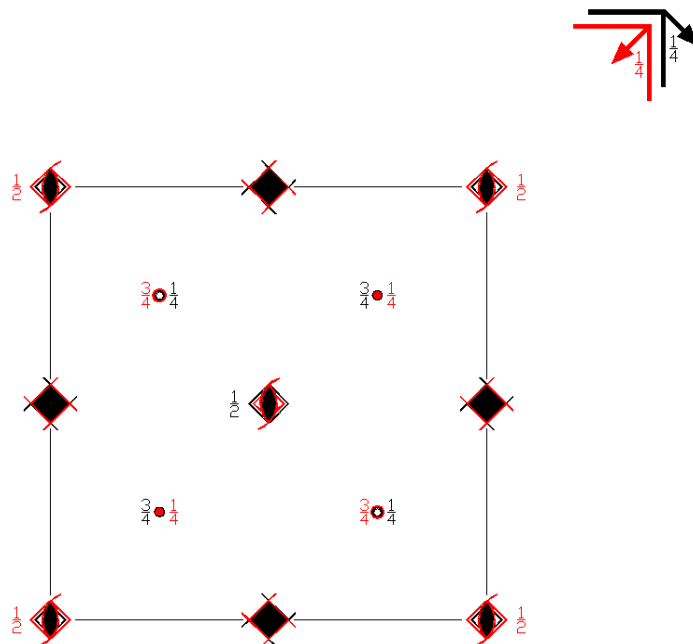
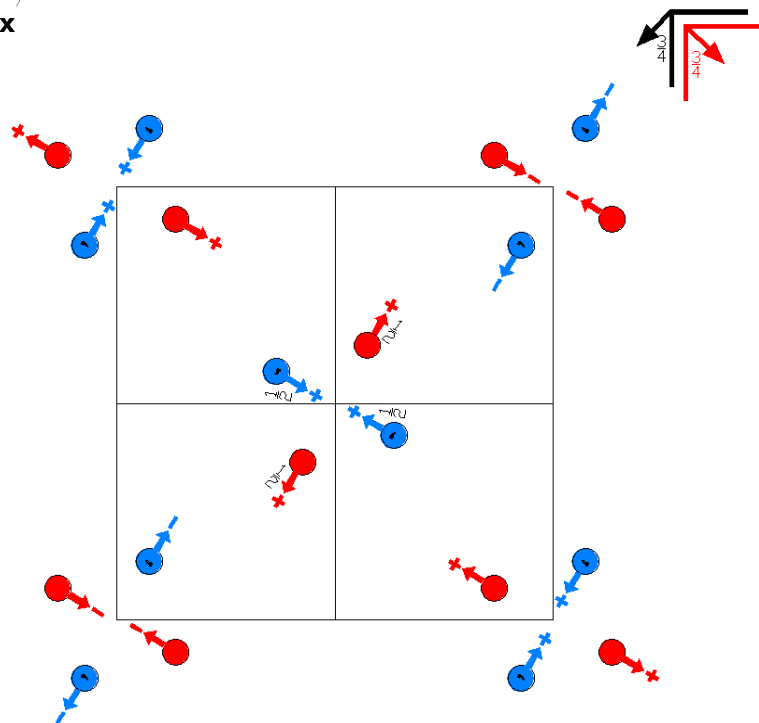
Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



$P_14_2/n$   
86.6.732

$4/m1'$   
 $P_14_2/n$

Tetragonal



Origin at  $\bar{4}$  at  $-1/4, -1/4, -1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |   |  |
|--|--|---|--|
| (1) $1$<br>$(1 0,0,0)$                                 | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                     | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>$(4_z 1/2,1/2,1/2)$  | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>$(4_z^{-1} 1/2,1/2,1/2)$  |
| (5) $\bar{1}$ $1/4,1/4,1/4$<br>$(\bar{1} 1/2,1/2,1/2)$ | (6) $n$ $(1/2,1/2,0) x,y,1/4$<br>$(m_z 1/2,1/2,1/2)$ | (7) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z 0,0,0)$ | (8) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1} 0,0,0)$ |

For  $(1,0,0)'$  + set

- |   |  |  |   |
|---|--|--|---|
| (1) $t'$ $(1,0,0)$<br>$(1 1,0,0)'$                        | (2) $2'$ $1/2,0,z$<br>$(2_z 1,0,0)'$                   | (3) $4^{+ '}$ $(0,0,1/2) 1/2,0,z$<br>$(4_z 3/2,1/2,1/2)'$          | (4) $4^{- '}$ $(0,0,1/2) 0,1/2,z$<br>$(4_z^{-1} 3/2,1/2,1/2)'$          |
| (5) $\bar{1}'$ $3/4,1/4,1/2$<br>$(\bar{1}' 3/2,1/2,1/2)'$ | (6) $n'$ $(3/2,1/2,0) x,y,1/4$<br>$(m_z 3/2,1/2,1/2)'$ | (7) $\bar{4}^{+ '}$ $1/2,1/2,z; 1/2,1/2,0$<br>$(\bar{4}_z 1,0,0)'$ | (8) $\bar{4}^{- '}$ $1/2,1/2,z; 1/2,1/2,0$<br>$(\bar{4}_z^{-1} 1,0,0)'$ |



**Generators selected** (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

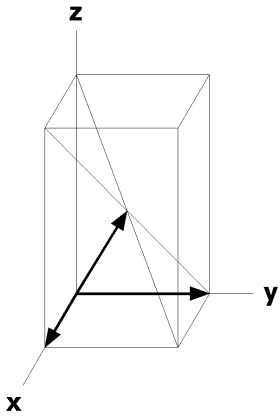
				Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.					
				(0,0,0) +	(1,0,0)' +
16	g 1	(1) x,y,z [u,v,w]		(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	
		(3) $\bar{y}+1/2, x+1/2, z+1/2$ [ $\bar{v}, u, w$ ]		(4) $y+1/2, \bar{x}+1/2, z+1/2$ [ $v, \bar{u}, w$ ]	
		(5) $\bar{x}+1/2, \bar{y}+1/2, \bar{z}+1/2$ [ $u, v, w$ ]		(6) $x+1/2, y+1/2, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]	
		(7) $y, \bar{x}, \bar{z}$ [ $\bar{v}, u, w$ ]		(8) $\bar{y}, x, \bar{z}$ [ $v, \bar{u}, w$ ]	
8	f 2..	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]
8	e 2'..	0,1/2,z [u,v,0]	0,1/2,z+1/2 [ $\bar{v}, u, 0$ ]	1/2,0, $\bar{z}+1/2$ [u,v,0]	1/2,0, $\bar{z}$ [ $\bar{v}, u, 0$ ]
8	d $\bar{1}'$	1/4,1/4,3/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
8	c $\bar{1}$	1/4,1/4,1/4 [u,v,w]	3/4,3/4,1/4 [ $\bar{u}, \bar{v}, w$ ]	1/4,3/4,3/4 [ $\bar{v}, u, w$ ]	3/4,1/4,3/4 [ $v, \bar{u}, w$ ]
4	b $\bar{4}'..$	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
4	a $\bar{4}..$	0,0,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

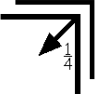
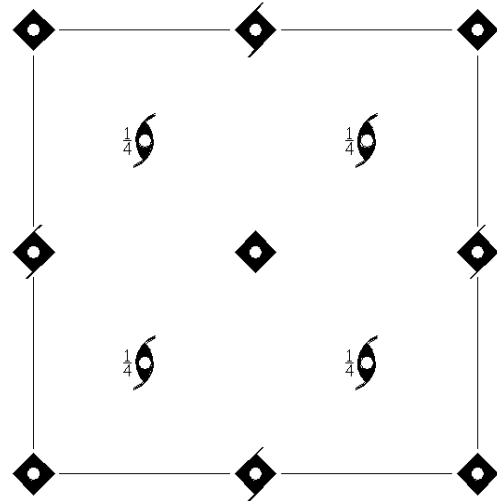
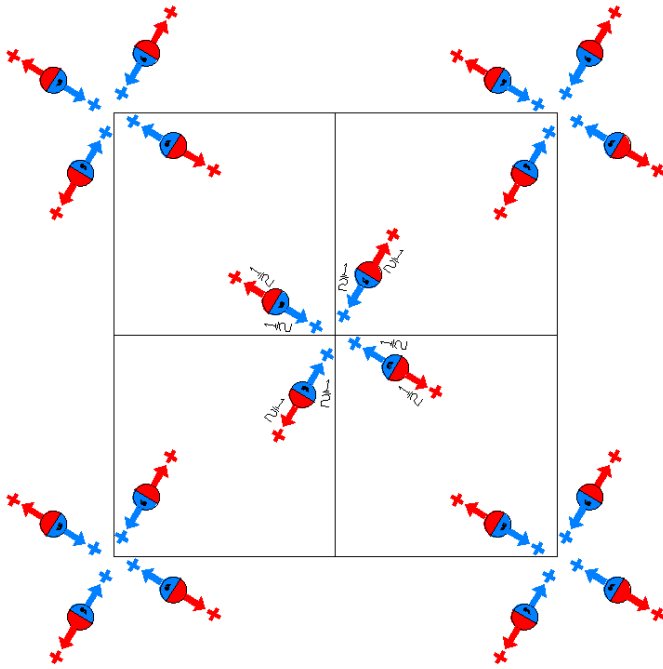
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



I4/m  
87.1.733

4/m  
I4/m

Tetragonal



Origin at center ( 4/m )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1   0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>   0,0,0)     | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>   0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0) | (6) m x,y,0<br>(m <sub>z</sub>   0,0,0) | (7) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$   0,0,0) | (8) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$   0,0,0)           |

For (1/2,1/2,1/2) + set

- |   |   |  |  |
|---|---|--|--|
| (1) t (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)                | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>   1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2) |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$   1/2,1/2,1/2) | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>   1/2,1/2,1/2) | (7) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$   1/2,1/2,1/2)   | (8) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$   1/2,1/2,1/2)                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

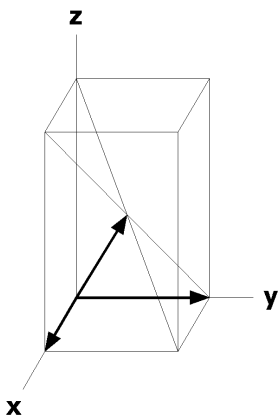
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(8) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
8 h m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0,w]	$y,\bar{x},0$ [0,0,w]
8 g 2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]
8 f $\bar{1}$	1/4,1/4,1/4 [u,v,w]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,1/4 [ $\bar{v},u,w$ ]	1/4,3/4,1/4 [ $v,\bar{u},w$ ]
4 e 4..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
4 d $\bar{4}$ ..	0,1/2,1/4 [0,0,w]	1/2,0,1/4 [0,0,w]		
4 c 2/m..	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]		
2 b 4/m..	0,0,1/2 [0,0,w]			
2 a 4/m..	0,0,0 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] p4  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0

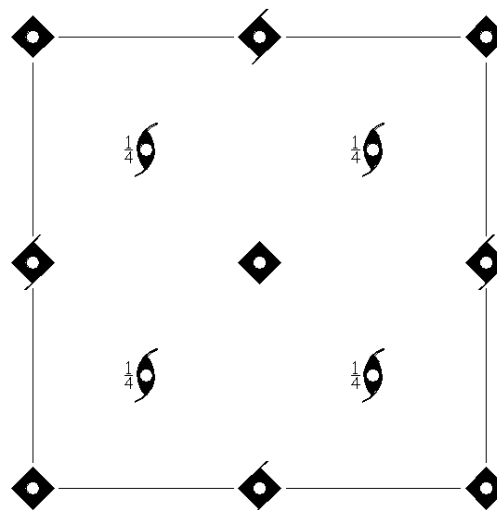
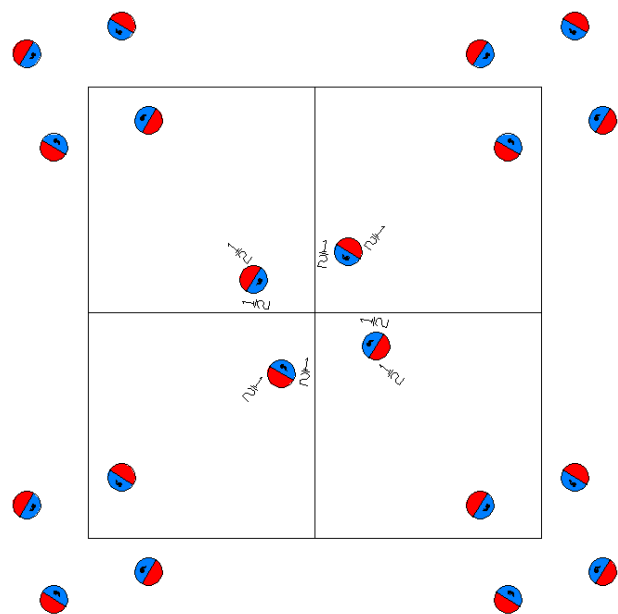
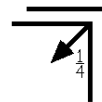


$I4/m1'$   
87.2.734

$4/m1'$   
 $I4/m1'$

Tetragonal

$1'$



Origin at center ( $4/m1'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |  |                                  |   |   |
|--|----------------------------------|---|---|
| (1) $1$<br>$(1 0,0,0)$                     | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$ | (3) $4^+$ $0,0,z$<br>$(4_z^+ 0,0,0)$                    | (4) $4^-$ $0,0,z$<br>$(4_z^- 0,0,0)$                    |
| (5) $\bar{1}$ $0,0,0$<br>$(\bar{1} 0,0,0)$ | (6) $m$ $x,y,0$<br>$(m_z x,y,0)$ | (7) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^+ 0,0,0)$ | (8) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^- 0,0,0)$ |

For (1/2,1/2,1/2) + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t$ $(1/2,1/2,1/2)$<br>$(1 1/2,1/2,1/2)$           | (2) $2$ $(0,0,1/2) 1/4,1/4,z$<br>$(2_z 1/2,1/2,1/2)$ | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>$(4_z^+ 1/2,1/2,1/2)$              | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>$(4_z^- 1/2,1/2,1/2)$              |
| (5) $\bar{1}$ $1/4,1/4,1/4$<br>$(\bar{1} 1/2,1/2,1/2)$ | (6) $n$ $(1/2,1/2,0) x,y,1/4$<br>$(m_z 1/2,1/2,1/2)$ | (7) $\bar{4}^+$ $1/2,0,z; 1/2,0,1/4$<br>$(\bar{4}_z^+ 1/2,1/2,1/2)$ | (8) $\bar{4}^-$ $0,1/2,z; 0,1/2,1/4$<br>$(\bar{4}_z^- 1/2,1/2,1/2)$ |

## For (0,0,0)' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> ' 0,0,z (4 <sub>z</sub>  0,0,0)'	(4) 4 <sup>-</sup> ' 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(5) $\bar{1}$ ' 0,0,0 ( $\bar{1}$  0,0,0)'	(6) m' x,y,0 (m <sub>z</sub>  0,0,0)'	(7) $\bar{4}^+$ ' 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'	(8) $\bar{4}^-$ ' 0,0,z; 0,0,0 ( $\bar{4}_z^{-1}$  0,0,0)'

## For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (1 1/2,1/2,1/2)'	(2) 2' (0,0,1/2 1/4,1/4,z (2 <sub>z</sub>  1/2,1/2,1/2)'	(3) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)'	(4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'
(5) $\bar{1}$ ' 1/4,1/4,1/4 ( $\bar{1}$  1/2,1/2,1/2)'	(6) n' (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>  1/2,1/2,1/2)'	(7) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$  1/2,1/2,1/2)'	(8) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$  1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

**Positions**

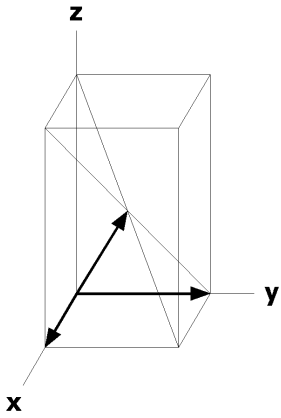
	Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'		
16 i	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z$ [0,0,0]	(4) y, $\bar{x},z$ [0,0,0]
		(5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(6) x,y, $\bar{z}$ [0,0,0]	(7) y, $\bar{x},\bar{z}$ [0,0,0]	(8) $\bar{y},x,\bar{z}$ [0,0,0]
8 h	m..1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{y},x,0$ [0,0,0]	y, $\bar{x},0$ [0,0,0]
8 g	2..1'	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]
8 f	$\bar{1}$ 1'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]
4 e	4..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 d	$\bar{4}$ ..1'	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]		
4 c	2/m..1'	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
2 b	4/m..1'	0,0,1/2 [0,0,0]			
2 a	4/m..1'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



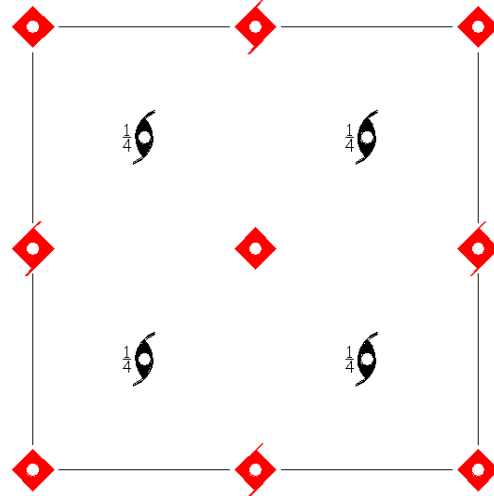
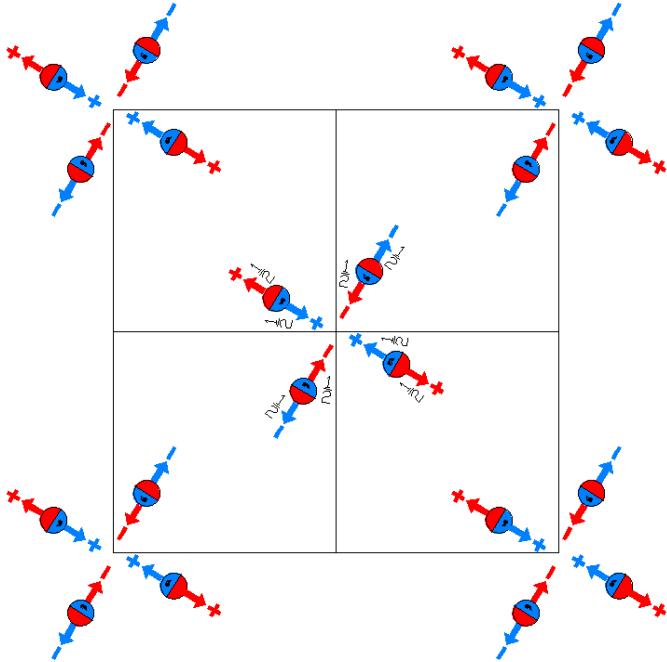
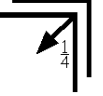
$I4'/m$

87.3.735

$4'/m$

$I4'/m$

Tetragonal



Origin at center ( $4'/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |  |                                  |   |  |
|--|----------------------------------|---|--|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $4^{+1}$ $0,0,z$<br>( $4_z$  0,0,0)'                    | (4) $4^{-1}$ $0,0,z$<br>( $4_z^{-1}$  0,0,0)'                    |
| (5) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0) | (6) m $x,y,0$<br>( $m_z$  0,0,0) | (7) $\bar{4}^{+1}$ $0,0,z; 0,0,0$<br>( $\bar{4}_z$  0,0,0)' | (8) $\bar{4}^{-1}$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1}$  0,0,0)' |

For (1/2,1/2,1/2) + set

- |  |  |   |  |
|--|--|---|--|
| (1) $t$ (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                 | (2) 2 (0,0,1/2) $1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2) | (3) $4^{+1}$ (0,0,1/2) $0,1/2,z$<br>( $4_z$  1/2,1/2,1/2)'              | (4) $4^{-1}$ (0,0,1/2) $1/2,0,z$<br>( $4_z^{-1}$  1/2,1/2,1/2)'              |
| (5) $\bar{1}$ $1/4,1/4,1/4$<br>( $\bar{1}$  1/2,1/2,1/2) | (6) n (1/2,1/2,0) $x,y,1/4$<br>( $m_z$  1/2,1/2,1/2) | (7) $\bar{4}^{+1}$ $1/2,0,z; 1/2,0,1/4$<br>( $\bar{4}_z$  1/2,1/2,1/2)' | (8) $\bar{4}^{-1}$ $0,1/2,z; 0,1/2,1/4$<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

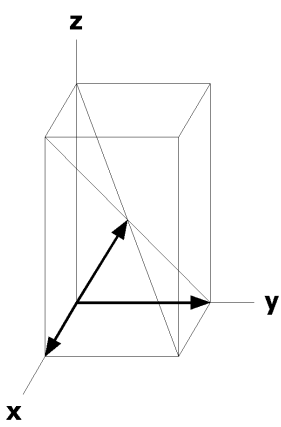
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 i 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [v, $\bar{u},\bar{w}$ ] (7) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ] (8) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
8 h m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0, $\bar{w}$ ]	y, $\bar{x},0$ [0,0, $\bar{w}$ ]
8 g 2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
8 f $\bar{1}$	1/4,1/4,1/4 [u,v,w]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,1/4 [v, $\bar{u},\bar{w}$ ]	1/4,3/4,1/4 [ $\bar{v},u,\bar{w}$ ]
4 e 4'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 d $\bar{4}'..$	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]		
4 c 2/m..	0,1/2,0 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]		
2 b 4'/m..	0,0,1/2 [0,0,0]			
2 a 4'/m..	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p4'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

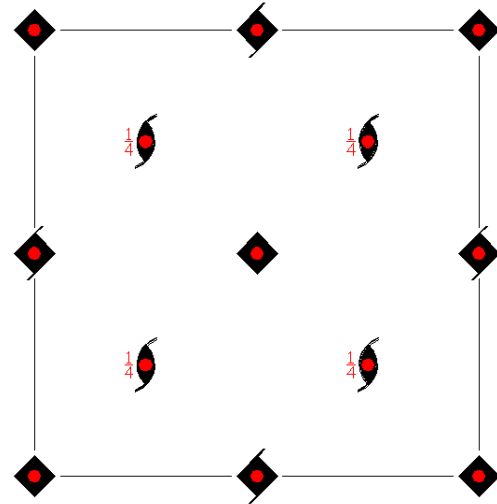
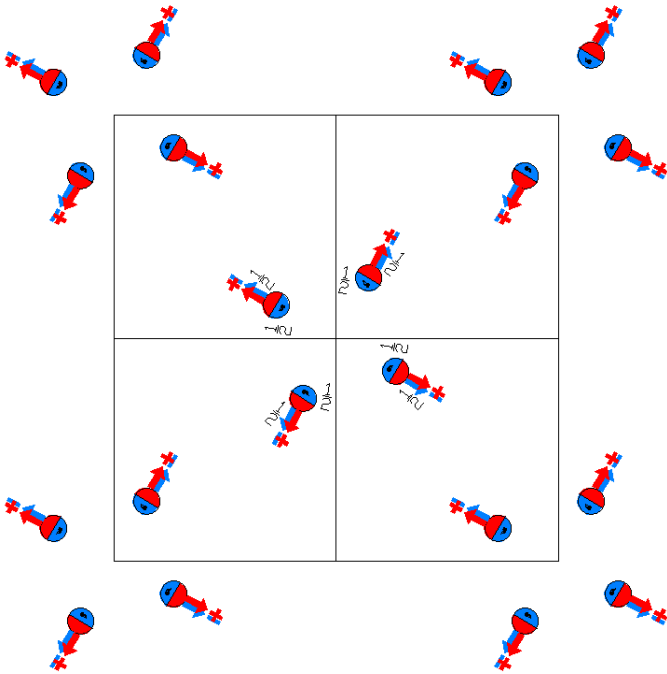
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



14/m'  
87.4.736

4/m'  
14/m'

Tetragonal



Origin at center ( 4/m' )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |  |   |  |  |
|--|---|--|--|
| (1) 1<br>(1   0,0,0)                             | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0)     | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>   0,0,0)                              | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>   0,0,0)                              |
| (5) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$ '   0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub> '   0,0,0)' | (7) $\bar{4}$ <sup>+</sup> ' 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>+</sup> '   0,0,0)' | (8) $\bar{4}$ <sup>-</sup> ' 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>-</sup> '   0,0,0)' |

For (1/2,1/2,1/2) + set

- |  |   |  |  |
|--|---|--|--|
| (1) t (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)                     | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2)     | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub> <sup>+</sup>   1/2,1/2,1/2)                        | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-</sup>   1/2,1/2,1/2)                        |
| (5) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$ '   1/2,1/2,1/2)' | (6) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub> '   1/2,1/2,1/2)' | (7) $\bar{4}$ <sup>+</sup> ' 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}$ <sub>z</sub> <sup>+</sup> '   1/2,1/2,1/2)' | (8) $\bar{4}$ <sup>-</sup> ' 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}$ <sub>z</sub> <sup>-</sup> '   1/2,1/2,1/2)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

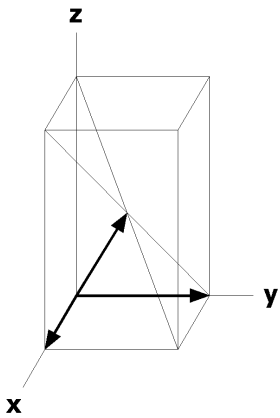
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 i 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ] (7) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ] (8) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
8 h m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},u,0$ ]	y, $\bar{x},0$ [v, $\bar{u},0$ ]
8 g 2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
8 f $\bar{1}'$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]
4 e 4..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 d $\bar{4}'..$	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]		
4 c 2/m'..	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
2 b 4/m'..	0,0,1/2 [0,0,0]			
2 a 4/m'..	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p41'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



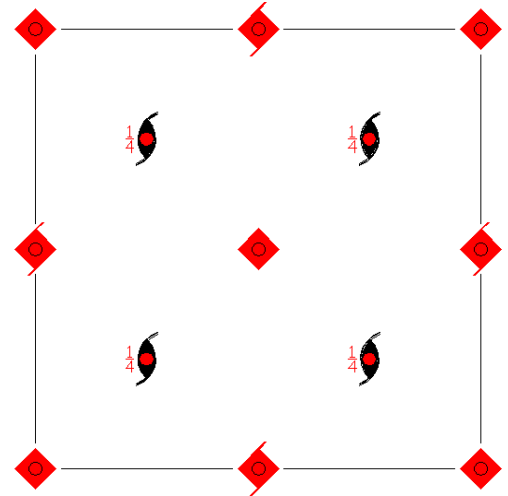
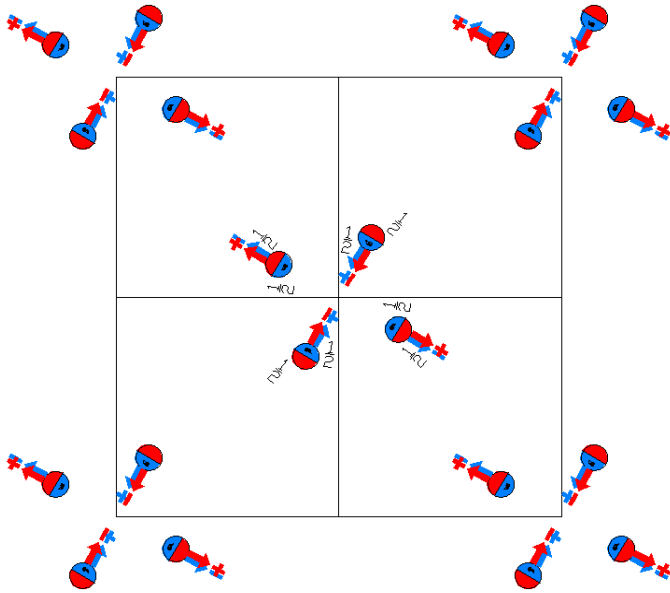
$I4'/m'$

87.5.737

$4'/m'$

$I4'/m'$

Tetragonal



Origin at center ( $4'/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |   |   |
|---|--|---|---|
| (1) 1<br>(1 0,0,0)                          | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'                        | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'                        |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (7) $\bar{4}$ <sup>+</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub>  0,0,0) | (8) $\bar{4}$ <sup>-</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>-1</sup>  0,0,0) |

For (1/2,1/2,1/2) + set

- |   |  |   |   |
|---|--|---|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                  | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)   | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)'                  | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'                  |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)' | (6) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (7) $\bar{4}$ <sup>+</sup> 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}$ <sub>z</sub>  1/2,1/2,1/2) | (8) $\bar{4}$ <sup>-</sup> 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}$ <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

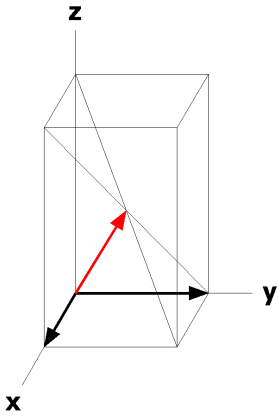
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
16 i 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(3) $\bar{y},x,z$ [v, $\bar{u},\bar{w}$ ] (7) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ] (8) $\bar{y},x,\bar{z}$ [v, $\bar{u},w$ ]
8 h m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [v, $\bar{u},0$ ]	y, $\bar{x},0$ [ $\bar{v},u,0$ ]
8 g 2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]
8 f $\bar{1}'$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]
4 e 4'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 d $\bar{4}$ ..	0,1/2,1/4 [0,0,w]	1/2,0,1/4 [0,0, $\bar{w}$ ]		
4 c 2/m'..	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
2 b 4'/m'..	0,0,1/2 [0,0,0]			
2 a 4'/m'..	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



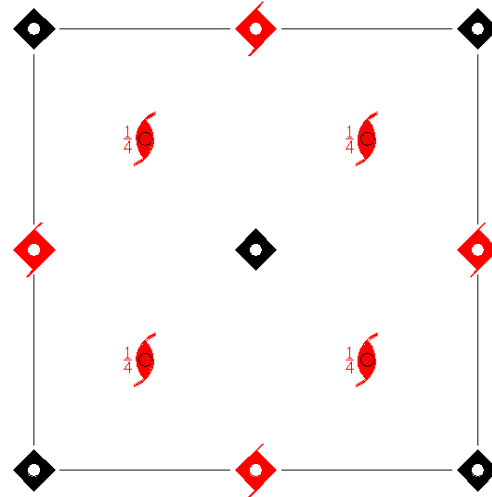
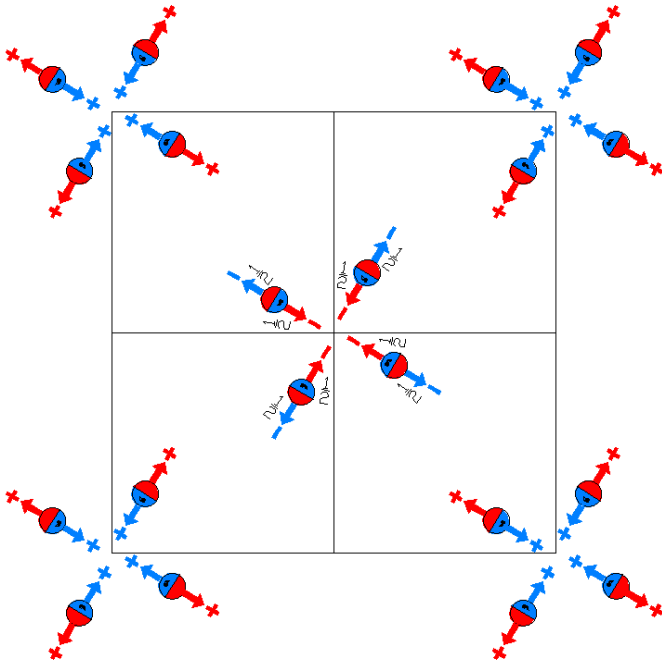
$I_P 4/m$

87.6.738

$4/m\bar{1}'$

$I_P 4/m$

Tetragonal



Origin at center ( $4/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                         | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)     | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (6) m <sub>x,y</sub> x,y,0<br>(m <sub>z</sub>  0,0,0) | (7) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0) | (8) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)           |

For (1/2,1/2,1/2) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'                  | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)' | (6) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (7) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2)'   | (8) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2)'                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

### Positions

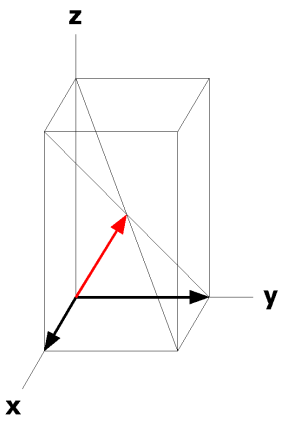
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
16 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(8) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
8 h m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0,w]	$y,\bar{x},0$ [0,0,w]
8 g 2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]
8 f $\bar{1}'$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]
4 e 4..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
4 d $\bar{4}..$	0,1/2,1/4 [0,0,w]	1/2,0,1/4 [0,0,w]		
4 c 2/m..	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]		
2 b 4/m..	0,0,1/2 [0,0,w]			
2 a 4/m..	0,0,0 [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1]  $p_p \cdot 4$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

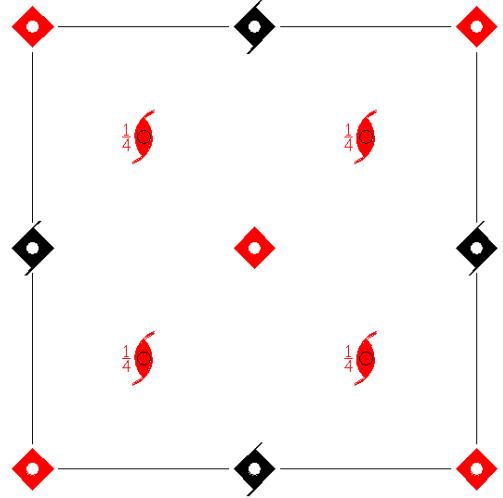
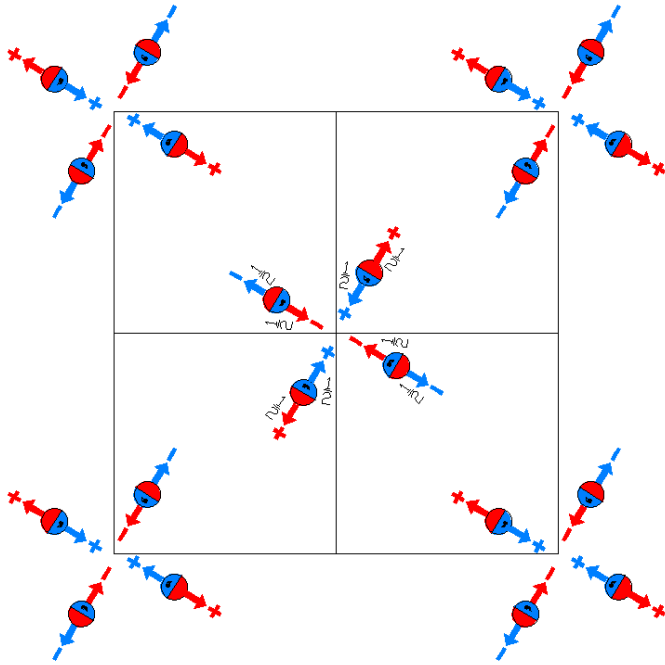
Along [1,1,0]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



$I_P 4'/m$   
87.7.739

$4/m1'$   
 $I_P 4'/m$

Tetragonal



Origin at center ( $4'/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |   |                                   |   |   |
|---|-----------------------------------|---|---|
| (1) 1<br>(1   0,0,0)                        | (2) 2 $0,0,z$<br>( $2_z$   0,0,0) | (3) $4^+ 0,0,z$<br>( $4_z^+$   0,0,0)'                    | (4) $4^- 0,0,z$<br>( $4_z^-$   0,0,0)'                    |
| (5) $\bar{1} 0,0,0$<br>( $\bar{1}$   0,0,0) | (6) m $x,y,0$<br>( $m_z$   0,0,0) | (7) $\bar{4}^+ 0,0,z; 0,0,0$<br>( $\bar{4}_z^+$   0,0,0)' | (8) $\bar{4}^- 0,0,z; 0,0,0$<br>( $\bar{4}_z^-$   0,0,0)' |

For (1/2,1/2,1/2) + set

- |   |   |  |  |
|---|---|--|--|
| (1) $t' (1/2,1/2,1/2)$<br>(1   1/2,1/2,1/2)'              | (2) $2' (0,0,1/2) 1/4,1/4,z$<br>( $2_z$   1/2,1/2,1/2)' | (3) $4^+ (0,0,1/2) 0,1/2,z$<br>( $4_z^+$   1/2,1/2,1/2)              | (4) $4^- (0,0,1/2) 1/2,0,z$<br>( $4_z^-$   1/2,1/2,1/2)              |
| (5) $\bar{1}' 1/4,1/4,1/4$<br>( $\bar{1}$   1/2,1/2,1/2)' | (6) $n' (1/2,1/2,0) x,y,1/4$<br>( $m_z$   1/2,1/2,1/2)' | (7) $\bar{4}^+ 1/2,0,z; 1/2,0,1/4$<br>( $\bar{4}_z^+$   1/2,1/2,1/2) | (8) $\bar{4}^- 0,1/2,z; 0,1/2,1/4$<br>( $\bar{4}_z^-$   1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

### Positions

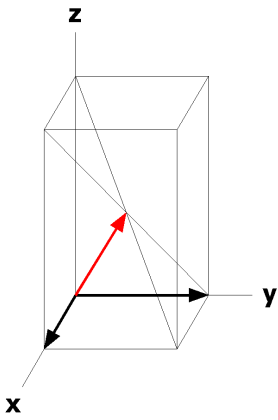
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
16 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $y,\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
8 h m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0, $\bar{w}$ ]	$y,\bar{x},0$ [0,0, $\bar{w}$ ]
8 g 2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
8 f $\bar{1}'$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]
4 e 4'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 d $\bar{4}'..$	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]		
4 c 2/m..	0,1/2,0 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]		
2 b 4'/m..	0,0,1/2 [0,0,0]			
2 a 4'/m..	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1]  $p_p \cdot 4$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/2,0,z

Along [1,0,0]  $c_p \cdot 2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

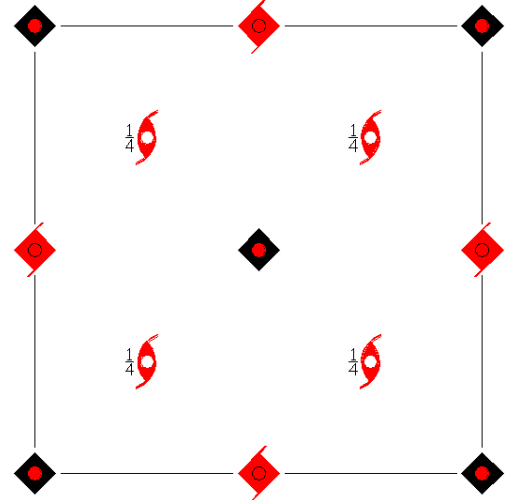
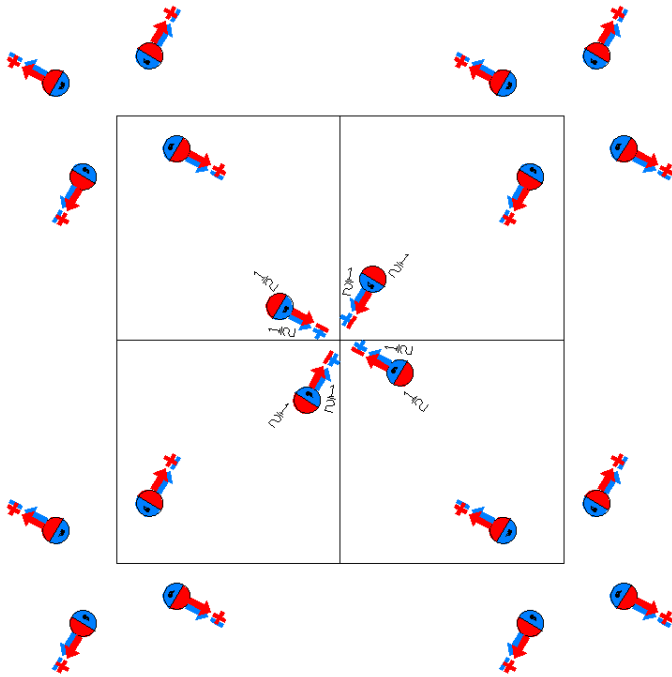
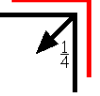
Along [1,1,0]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



$I_p 4/m'$   
87.8.740

$4/m1'$   
 $I_p 4/m'$

Tetragonal



Origin at center ( $4/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                          | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0) |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub> ' 0,0,0)' | (7) $\bar{4}^{+}$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{+}$  0,0,0)'     | (8) $\bar{4}^{-}$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-}$  0,0,0)'     |

For (1/2,1/2,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'                | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub> ' 1/2,1/2,1/2)' | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub> <sup>+</sup>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-</sup>  1/2,1/2,1/2)' |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)' | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)    | (7) $\bar{4}^{+}$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^{+}$  1/2,1/2,1/2)             | (8) $\bar{4}^{-}$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-}$  1/2,1/2,1/2)             |



**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(1/2,1/2,1/2)$ ; (2); (3); (5).

**Positions**

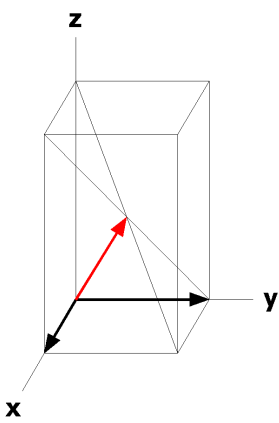
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
16 i 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $\bar{y},x,z [\bar{v},u,w]$	(4) $y,\bar{x},z [v,\bar{u},w]$
	(5) $\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$	(6) $x,y,\bar{z} [u,v,\bar{w}]$	(7) $y,\bar{x},\bar{z} [v,\bar{u},\bar{w}]$	(8) $\bar{y},x,\bar{z} [\bar{v},u,\bar{w}]$
8 h $m'..$	$x,y,0 [u,v,0]$	$\bar{x},\bar{y},0 [\bar{u},\bar{v},0]$	$\bar{y},x,0 [\bar{v},u,0]$	$y,\bar{x},0 [v,\bar{u},0]$
8 g $2..$	$0,1/2,z [0,0,w]$	$1/2,0,z [0,0,w]$	$0,1/2,\bar{z} [0,0,\bar{w}]$	$1/2,0,\bar{z} [0,0,\bar{w}]$
8 f $\bar{1}$	$1/4,1/4,1/4 [u,v,w]$	$3/4,3/4,1/4 [\bar{u},\bar{v},w]$	$3/4,1/4,1/4 [\bar{v},u,w]$	$1/4,3/4,1/4 [v,\bar{u},w]$
4 e $4..$	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,\bar{w}]$		
4 d $\bar{4}'..$	$0,1/2,1/4 [0,0,0]$	$1/2,0,1/4 [0,0,0]$		
4 c $2/m'..$	$0,1/2,0 [0,0,0]$	$1/2,0,0 [0,0,0]$		
2 b $4/m'..$	$0,0,1/2 [0,0,0]$			
2 a $4/m'..$	$0,0,0 [0,0,0]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p41'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c_p 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

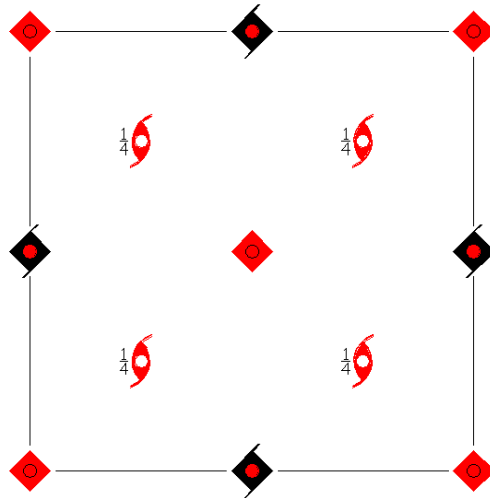
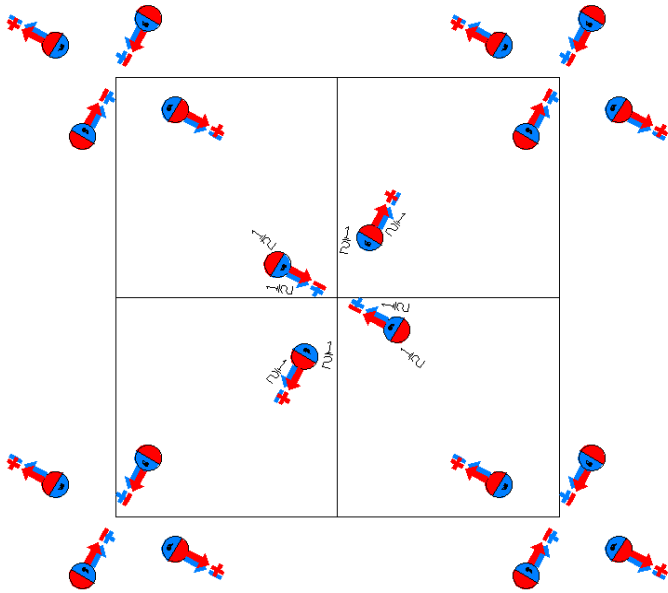
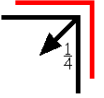
Along  $[1,1,0]$   $p_{2a} 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,0$



$I_P 4'/m'$   
87.9.741

$4/m1'$   
 $I_P 4'/m'$

Tetragonal



Origin at center ( $4'/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                          | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)'                        | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'                        |
| (5) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (6) m' x,y,0<br>(m <sub>z</sub> ' 0,0,0)' | (7) $\bar{4}$ <sup>+</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>+</sup>  0,0,0) | (8) $\bar{4}$ <sup>-</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>-</sup>  0,0,0) |

For (1/2,1/2,1/2) + set

- |  |   |   |   |
|--|---|---|---|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'               | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub> ' 1/2,1/2,1/2)' | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub> <sup>+</sup>  1/2,1/2,1/2)                    | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-</sup>  1/2,1/2,1/2)                    |
| (5) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2) | (6) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)    | (7) $\bar{4}$ <sup>+</sup> 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}$ <sub>z</sub> <sup>+</sup>  1/2,1/2,1/2)' | (8) $\bar{4}$ <sup>-</sup> 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}$ <sub>z</sub> <sup>-</sup>  1/2,1/2,1/2)' |

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(1/2,1/2,1/2)$ ; (2); (3); (5).

### Positions

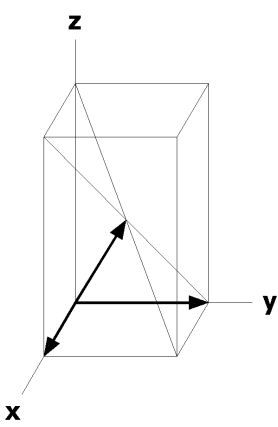
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
16 i 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $v,\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
	(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,y,\bar{z}$ [u,v, $\bar{w}$ ]	(7) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(8) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
8 h $m'..$	$x,y,0$ [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $v,\bar{u},0$ ]	$y,\bar{x},0$ [ $\bar{v},u,0$ ]
8 g $2..$	$0,1/2,z$ [0,0,w]	$1/2,0,z$ [0,0, $\bar{w}$ ]	$0,1/2,\bar{z}$ [0,0, $\bar{w}$ ]	$1/2,0,\bar{z}$ [0,0,w]
8 f $\bar{1}$	$1/4,1/4,1/4$ [u,v,w]	$3/4,3/4,1/4$ [ $\bar{u},\bar{v},w$ ]	$3/4,1/4,1/4$ [ $v,\bar{u},\bar{w}$ ]	$1/4,3/4,1/4$ [ $\bar{v},u,\bar{w}$ ]
4 e $4'..$	$0,0,z$ [0,0,0]	$0,0,\bar{z}$ [0,0,0]		
4 d $\bar{4}..$	$0,1/2,1/4$ [0,0,w]	$1/2,0,1/4$ [0,0, $\bar{w}$ ]		
4 c $2/m'..$	$0,1/2,0$ [0,0,w]	$1/2,0,0$ [0,0,w]		
2 b $4'/m'..$	$0,0,1/2$ [0,0,0]			
2 a $4'/m'..$	$0,0,0$ [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1]  $p41'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



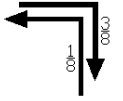
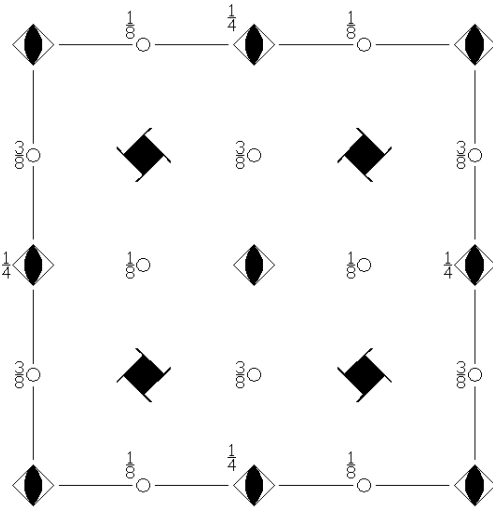
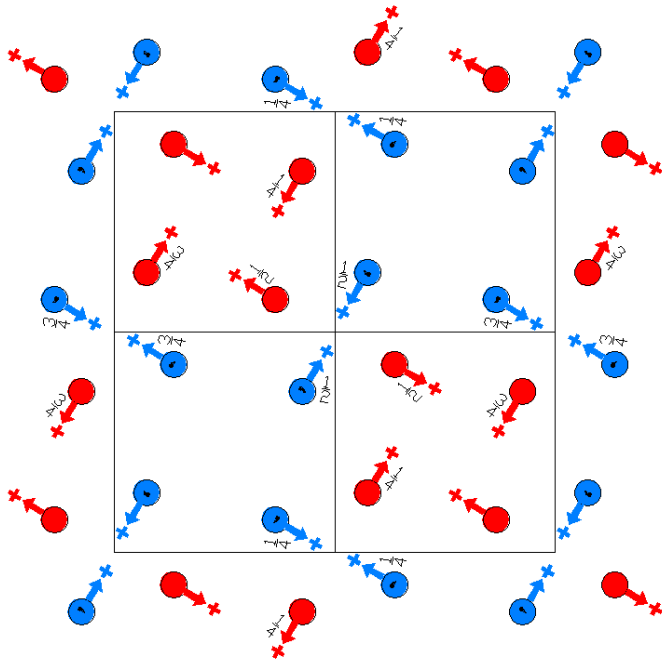
$I4_1/a$

88.1.742

$4/m$

$I4_1/a$

Tetragonal



Origin at  $\bar{4}$  at  $0, -1/4, -1/8$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) $1$<br>$(1 0,0,0)$                             | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                 | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>$(4_z^+ 0,1/2,1/4)$ | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>$(4_z^- 0,1/2,1/4)$  |
| (5) $\bar{1}$ $0,1/4,1/8$<br>$(\bar{1} 0,1/2,1/4)$ | (6) $b$ $(0,1/2,0) x,y,1/8$<br>$(m_z 0,1/2,1/4)$ | (7) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^+ 0,0,0)$ | (8) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^- 0,0,0)$ |

For  $(1/2,1/2,1/2)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t$ $(1/2,1/2,1/2)$<br>$(1 1/2,1/2,1/2)$       | (2) $2$ $(0,0,1/2) 1/4,1/4,z$<br>$(2_z 1/2,1/2,1/2)$ | (3) $4^+$ $(0,0,3/4) 1/4,1/4,z$<br>$(4_z^+ 1/2,0,3/4)$              | (4) $4^-$ $(0,0,3/4) 1/4,-1/4,z$<br>$(4_z^- 1/2,0,3/4)$             |
| (5) $\bar{1}$ $1/4,0,3/8$<br>$(\bar{1} 1/2,0,3/4)$ | (6) $a$ $(1/2,0,0) x,y,3/8$<br>$(m_z 1/2,0,3/4)$     | (7) $\bar{4}^+$ $1/2,0,z; 1/2,0,1/4$<br>$(\bar{4}_z^+ 1/2,1/2,1/2)$ | (8) $\bar{4}^-$ $0,1/2,z; 0,1/2,1/4$<br>$(\bar{4}_z^- 1/2,1/2,1/2)$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

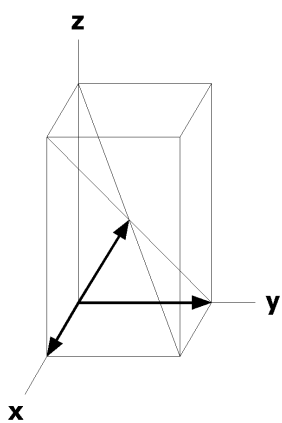
				Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.							
				(0,0,0) +	(1/2,1/2,1/2) +		
16	f 1	(1) x,y,z [u,v,w]		(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]			
		(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},u,w$ ]		(4) $y,\bar{x}+1/2,z+1/4$ [ $v,\bar{u},w$ ]			
		(5) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [u,v,w]		(6) $x,y+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},w$ ]			
		(7) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]		(8) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]			
8	e 2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,1/2,z+1/4 [0,0,w]	0,1/2, $\bar{z}+1/4$ [0,0,w]		
8	d $\bar{1}$	0,1/4,5/8 [u,v,w]	0,3/4,5/8 [ $\bar{u},\bar{v},w$ ]	1/4,0,3/8 [ $\bar{v},u,w$ ]	3/4,0,3/8 [ $v,\bar{u},w$ ]		
8	c $\bar{1}$	0,1/4,1/8 [u,v,w]	0,3/4,1/8 [ $\bar{u},\bar{v},w$ ]	1/4,0,7/8 [ $\bar{v},u,w$ ]	3/4,0,7/8 [ $v,\bar{u},w$ ]		
4	b $\bar{4}..$	0,0,1/2 [0,0,w]	0,1/2,3/4 [0,0,w]				
4	a $\bar{4}..$	0,0,0 [0,0,w]	0,1/2,1/4 [0,0,w]				

**Symmetry of Special Projections**

Along [0,0,1] p4  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,3/8

Along [1,1,0] p2'm'g  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x+1/4,1/8



$I4_1/a1'$

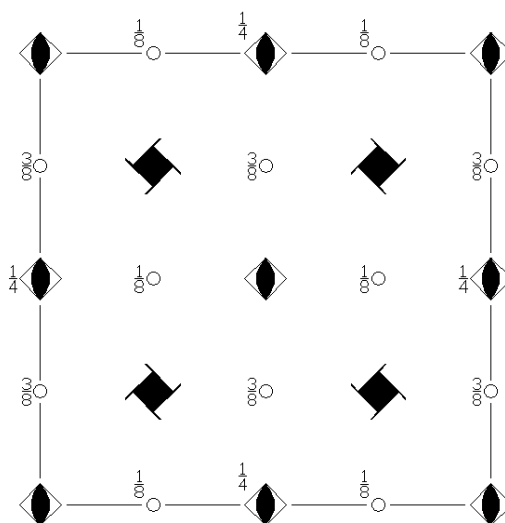
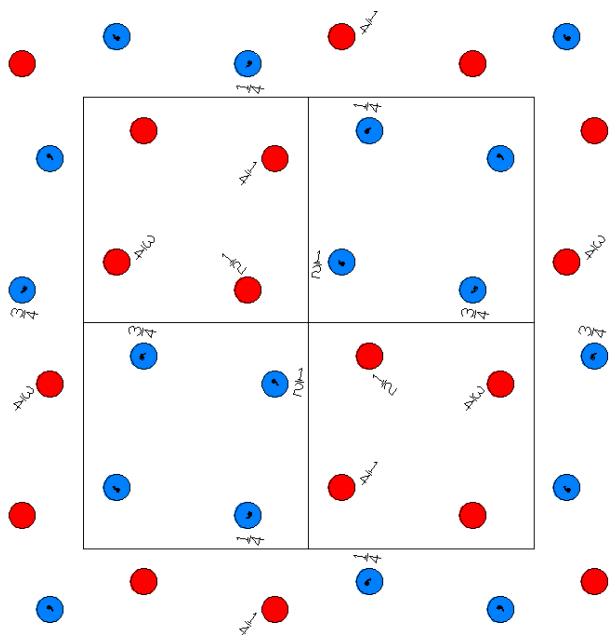
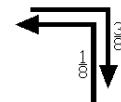
88.2.743

$4/m1'$

$I4_1/a1'$

Tetragonal

1'



Origin at  $\bar{4}1'$  at  $0, -1/4, -1/8$  from  $\bar{1}1'$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) $1$<br>$(1 0,0,0)$                             | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                 | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>$(4_z^+ 0,1/2,1/4)$ | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>$(4_z^- 0,1/2,1/4)$  |
| (5) $\bar{1}$ $0,1/4,1/8$<br>$(\bar{1} 0,1/2,1/4)$ | (6) $b$ $(0,1/2,0) x,y,1/8$<br>$(m_z 0,1/2,1/4)$ | (7) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^+ 0,0,0)$ | (8) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^- 0,0,0)$ |

For  $(1/2,1/2,1/2)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t$ $(1/2,1/2,1/2)$<br>$(1 1/2,1/2,1/2)$       | (2) $2$ $(0,0,1/2) 1/4,1/4,z$<br>$(2_z 1/2,1/2,1/2)$ | (3) $4^+$ $(0,0,3/4) 1/4,1/4,z$<br>$(4_z^+ 1/2,0,3/4)$              | (4) $4^-$ $(0,0,3/4) 1/4,-1/4,z$<br>$(4_z^- 1/2,0,3/4)$             |
| (5) $\bar{1}$ $1/4,0,3/8$<br>$(\bar{1} 1/2,0,3/4)$ | (6) $a$ $(1/2,0,0) x,y,3/8$<br>$(m_z 1/2,0,3/4)$     | (7) $\bar{4}^+$ $1/2,0,z; 1/2,0,1/4$<br>$(\bar{4}_z^+ 1/2,1/2,1/2)$ | (8) $\bar{4}^-$ $0,1/2,z; 0,1/2,1/4$<br>$(\bar{4}_z^- 1/2,1/2,1/2)$ |

## For (0,0,0)' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> ' (0,0,1/4) -1/4,1/4,z (4 <sub>z</sub>  0,1/2,1/4)'	(4) 4 <sup>-</sup> ' (0,0,1/4) 1/4,1/4,z (4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4)'
(5) $\bar{1}$ ' 0,1/4,1/8 ( $\bar{1}$  0,1/2,1/4)'	(6) b' (0,1/2,0) x,y,1/8 (m <sub>z</sub>  0,1/2,1/4)'	(7) $\bar{4}^{+}$ ' 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'	(8) $\bar{4}^{-}$ ' 0,0,z; 0,0,0 ( $\bar{4}_z^{-1}$  0,0,0)'

## For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (1 1/2,1/2,1/2)'	(2) 2' (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>  1/2,1/2,1/2)'	(3) 4 <sup>+</sup> ' (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>  1/2,0,3/4)'	(4) 4 <sup>-</sup> ' (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>  1/2,0,3/4)'
(5) $\bar{1}$ ' 1/4,0,3/8 ( $\bar{1}$  1/2,0,3/4)'	(6) a' (1/2,0,0) x,y,3/8 (m <sub>z</sub>  1/2,0,3/4)'	(7) $\bar{4}^{+}$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$  1/2,1/2,1/2)'	(8) $\bar{4}^{-}$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$  1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

**Positions**

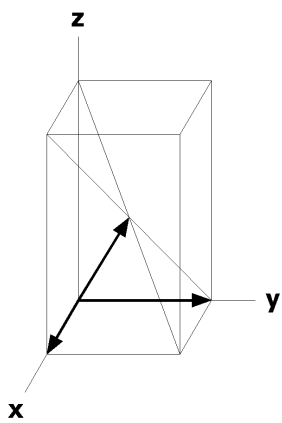
				Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.					
16	f 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'
		(3) $\bar{y},x+1/2,z+1/4$ [0,0,0]	(4) $y,\bar{x}+1/2,z+1/4$ [0,0,0]		
		(5) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [0,0,0]	(6) $x,y+1/2,\bar{z}+1/4$ [0,0,0]		
		(7) $y,\bar{x},\bar{z}$ [0,0,0]	(8) $\bar{y},x,\bar{z}$ [0,0,0]		
8	e 21'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,1/2,z+1/4 [0,0,0]	0,1/2, $\bar{z}+1/4$ [0,0,0]
8	d $\bar{1}1'$	0,1/4,5/8 [0,0,0]	0,3/4,5/8 [0,0,0]	1/4,0,3/8 [0,0,0]	3/4,0,3/8 [0,0,0]
8	c $\bar{1}1'$	0,1/4,1/8 [0,0,0]	0,3/4,1/8 [0,0,0]	1/4,0,7/8 [0,0,0]	3/4,0,7/8 [0,0,0]
4	b $\bar{4}..1'$	0,0,1/2 [0,0,0]	0,1/2,3/4 [0,0,0]		
4	a $\bar{4}..1'$	0,0,0 [0,0,0]	0,1/2,1/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p41'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

Along [1,1,0] p2mg1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x+1/4,1/8



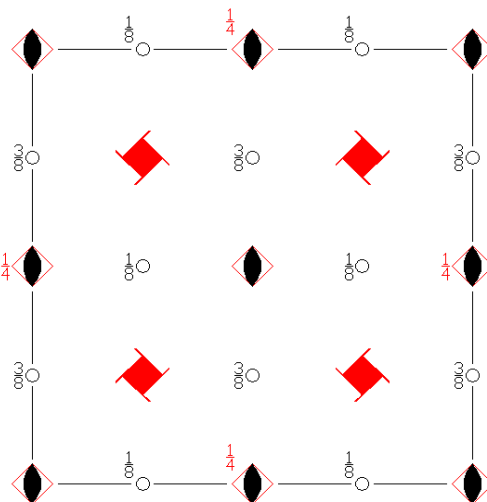
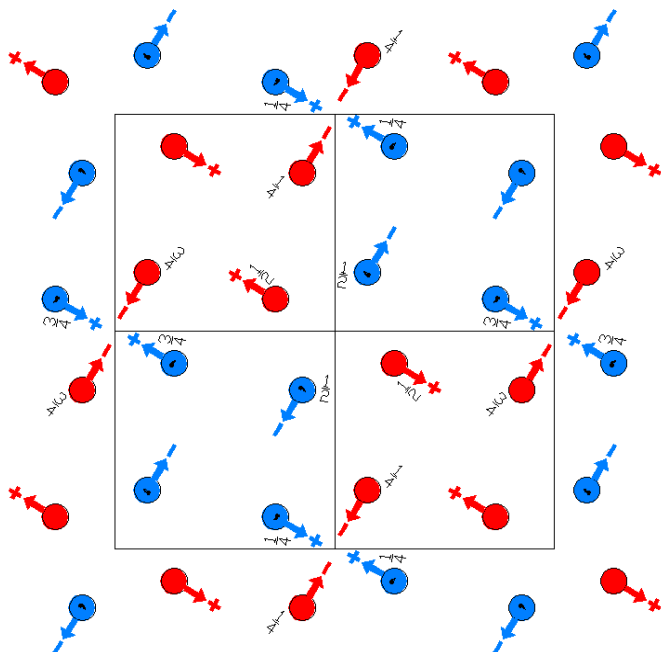
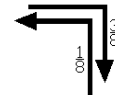
$I4_1'/a$

$4'/m$

Tetragonal

88.3.744

$I4_1'/a$



Origin at  $\bar{4}'$  at  $0, -1/4, -1/8$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |  |   |
|--|--|--|---|
| (1) $1$<br>$(1 0,0,0)$                             | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                 | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>$(4_z 0,1/2,1/4)'$ | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>$(4_z^{-1} 0,1/2,1/4)'$  |
| (5) $\bar{1}$ $0,1/4,1/8$<br>$(\bar{1} 0,1/2,1/4)$ | (6) $b$ $(0,1/2,0) x,y,1/8$<br>$(m_z 0,1/2,1/4)$ | (7) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z 0,0,0)'$ | (8) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1} 0,0,0)'$ |

For  $(1/2,1/2,1/2)$  + set

- |  |  |  |   |
|--|--|--|---|
| (1) $t$ $(1/2,1/2,1/2)$<br>$(1 1/2,1/2,1/2)$       | (2) $2$ $(0,0,1/2) 1/4,1/4,z$<br>$(2_z 1/2,1/2,1/2)$ | (3) $4^+$ $(0,0,3/4) 1/4,1/4,z$<br>$(4_z 1/2,0,3/4)'$              | (4) $4^-$ $(0,0,3/4) 1/4,-1/4,z$<br>$(4_z^{-1} 1/2,0,3/4)'$             |
| (5) $\bar{1}$ $1/4,0,3/8$<br>$(\bar{1} 1/2,0,3/4)$ | (6) $a$ $(1/2,0,0) x,y,3/8$<br>$(m_z 1/2,0,3/4)$     | (7) $\bar{4}^+$ $1/2,0,z; 1/2,0,1/4$<br>$(\bar{4}_z 1/2,1/2,1/2)'$ | (8) $\bar{4}^-$ $0,1/2,z; 0,1/2,1/4$<br>$(\bar{4}_z^{-1} 1/2,1/2,1/2)'$ |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

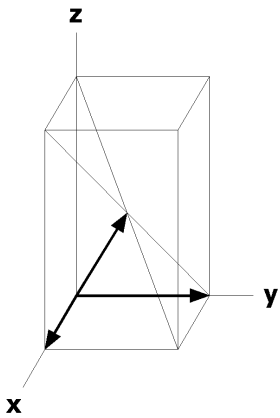
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +		(1/2,1/2,1/2) +
16 f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
	(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $\bar{v},u,\bar{w}$ ]		
	(5) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [u,v,w]	(6) $x,y+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},w$ ]		
	(7) $y,\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},x,z$ [ $\bar{v},u,\bar{w}$ ]		
8 e 2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/4 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/4$ [0,0,w]
8 d $\bar{1}$	0,1/4,5/8 [u,v,w]	0,3/4,5/8 [ $\bar{u},\bar{v},w$ ]	1/4,0,3/8 [ $\bar{v},\bar{u},\bar{w}$ ]	3/4,0,3/8 [ $\bar{v},u,\bar{w}$ ]
8 c $\bar{1}$	0,1/4,1/8 [u,v,w]	0,3/4,1/8 [ $\bar{u},\bar{v},w$ ]	1/4,0,7/8 [ $\bar{v},\bar{u},\bar{w}$ ]	3/4,0,7/8 [ $\bar{v},u,\bar{w}$ ]
4 b $\bar{4}'..$	0,0,1/2 [0,0,0]	0,1/2,3/4 [0,0,0]		
4 a $\bar{4}'..$	0,0,0 [0,0,0]	0,1/2,1/4 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p4'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,3/8

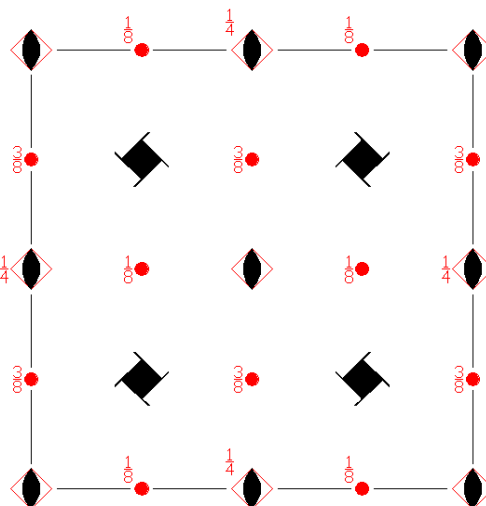
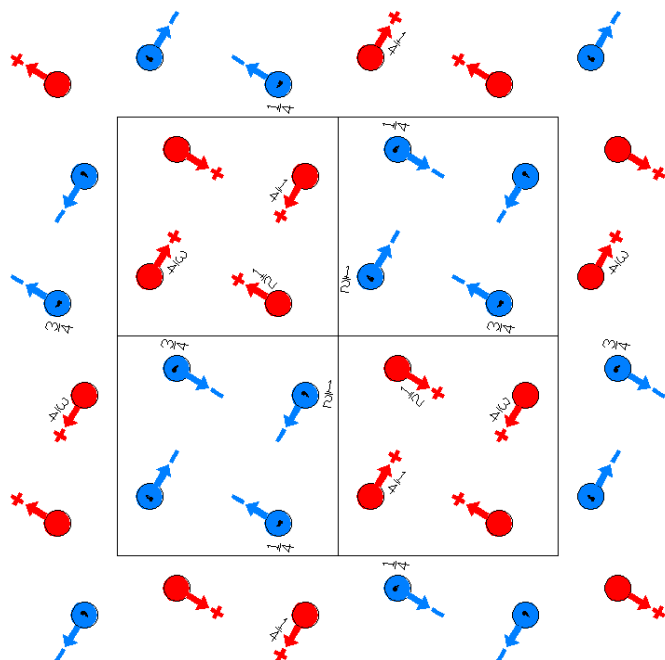
Along [1,1,0] p2'm'g  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x+1/4,1/8



$I4_1/a'$   
88.4.745

$4/m'$   
 $I4_1/a'$

Tetragonal



Origin at  $\bar{4}'$  at  $0, -1/4, -1/8$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

### Symmetry Operations

For  $(0,0,0)$  + set

- |   |  |   |  |
|---|--|---|--|
| (1) $1$<br>$(1 0,0,0)$                                | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                   | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>$(4_z 0,1/2,1/4)$     | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>$(4_z^{-1} 0,1/2,1/4)$    |
| (5) $\bar{1}'$ $0,1/4,1/8$<br>$(\bar{1}' 0,1/2,1/4)'$ | (6) $b'$ $(0,1/2,0) x,y,1/8$<br>$(m_z 0,1/2,1/4)'$ | (7) $\bar{4}^+'$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^+ 0,0,0)'$ | (8) $\bar{4}^-'$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1} 0,0,0)'$ |

For  $(1/2,1/2,1/2)$  + set

- |   |  |   |  |
|---|--|---|--|
| (1) $t$ $(1/2,1/2,1/2)$<br>$(1 1/2,1/2,1/2)$          | (2) $2$ $(0,0,1/2) 1/4,1/4,z$<br>$(2_z 1/2,1/2,1/2)$ | (3) $4^+$ $(0,0,3/4) 1/4,1/4,z$<br>$(4_z 1/2,0,3/4)$                  | (4) $4^-$ $(0,0,3/4) 1/4,-1/4,z$<br>$(4_z^{-1} 1/2,0,3/4)$               |
| (5) $\bar{1}'$ $1/4,0,3/8$<br>$(\bar{1}' 1/2,0,3/4)'$ | (6) $a'$ $(1/2,0,0) x,y,3/8$<br>$(m_z 1/2,0,3/4)'$   | (7) $\bar{4}^+'$ $1/2,0,z; 1/2,0,1/4$<br>$(\bar{4}_z^+ 1/2,1/2,1/2)'$ | (8) $\bar{4}^-'$ $0,1/2,z; 0,1/2,1/4$<br>$(\bar{4}_z^{-1} 1/2,1/2,1/2)'$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

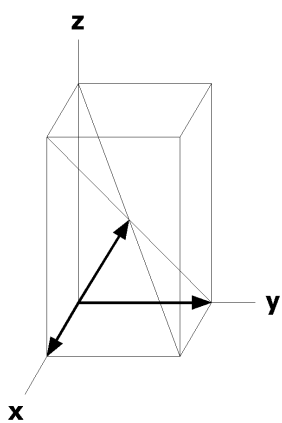
				Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.					
				(0,0,0) +	(1/2,1/2,1/2) +
16	f 1	(1) x,y,z [u,v,w]		(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	
		(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},u,w$ ]		(4) $y,\bar{x}+1/2,z+1/4$ [ $v,\bar{u},w$ ]	
		(5) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},\bar{w}$ ]		(6) $x,y+1/2,\bar{z}+1/4$ [ $u,v,\bar{w}$ ]	
		(7) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]		(8) $\bar{y},x,z$ [ $\bar{v},u,\bar{w}$ ]	
8	e 2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/4 [0,0,w]	0,1/2, $\bar{z}+1/4$ [0,0, $\bar{w}$ ]
8	d $\bar{1}'$	0,1/4,5/8 [0,0,0]	0,3/4,5/8 [0,0,0]	1/4,0,3/8 [0,0,0]	3/4,0,3/8 [0,0,0]
8	c $\bar{1}'$	0,1/4,1/8 [0,0,0]	0,3/4,1/8 [0,0,0]	1/4,0,7/8 [0,0,0]	3/4,0,7/8 [0,0,0]
4	b $\bar{4}'..$	0,0,1/2 [0,0,0]	0,1/2,3/4 [0,0,0]		
4	a $\bar{4}'..$	0,0,0 [0,0,0]	0,1/2,1/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/2,-1/2,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

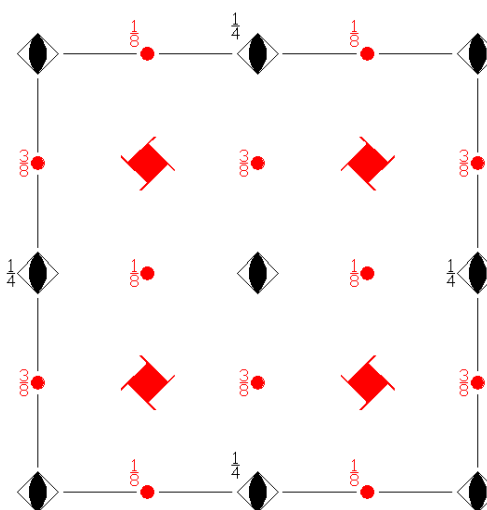
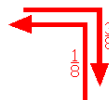
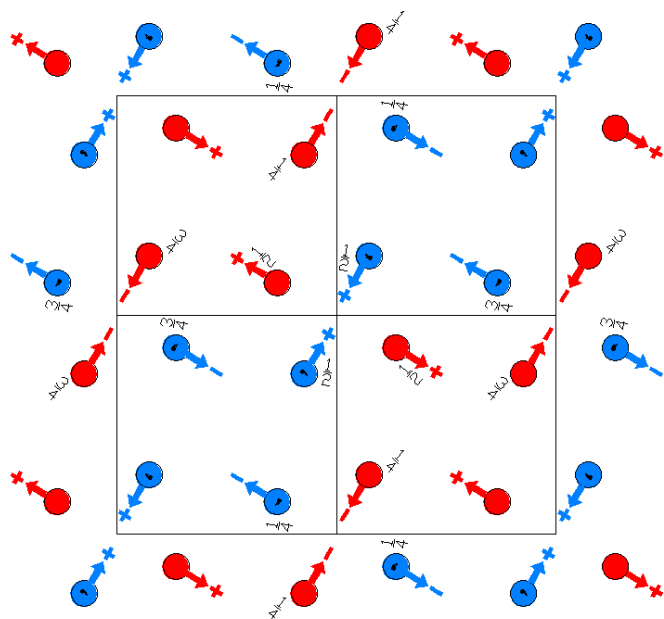
Along [1,1,0] p2m'g'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x+1/4,1/8



$I4_1'/a'$   
88.5.746

$4'/m'$   
 $I4_1'/a'$

Tetragonal



Origin at  $\bar{4}$  at  $0, -1/4, -1/8$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1$

### Symmetry Operations

For  $(0,0,0)$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) $1$<br>$(1 0,0,0)$                                | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                   | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>$(4_z 0,1/2,1/4)'$ | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>$(4_z^{-1} 0,1/2,1/4)'$ |
| (5) $\bar{1}'$ $0,1/4,1/8$<br>$(\bar{1}' 0,1/2,1/4)'$ | (6) $b'$ $(0,1/2,0) x,y,1/8$<br>$(m_z 0,1/2,1/4)'$ | (7) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z 0,0,0)$  | (8) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1} 0,0,0)$ |

For  $(1/2,1/2,1/2)$  + set

- |   |  |   |  |
|---|--|---|--|
| (1) $t$ $(1/2,1/2,1/2)$<br>$(1 1/2,1/2,1/2)$          | (2) $2$ $(0,0,1/2) 1/4,1/4,z$<br>$(2_z 1/2,1/2,1/2)$ | (3) $4^+$ $(0,0,3/4) 1/4,1/4,z$<br>$(4_z 1/2,0,3/4)'$             | (4) $4^-$ $(0,0,3/4) 1/4,-1/4,z$<br>$(4_z^{-1} 1/2,0,3/4)'$            |
| (5) $\bar{1}'$ $1/4,0,3/8$<br>$(\bar{1}' 1/2,0,3/4)'$ | (6) $a'$ $(1/2,0,0) x,y,3/8$<br>$(m_z 1/2,0,3/4)'$   | (7) $\bar{4}^+$ $1/2,0,z; 1/2,0,1/4$<br>$(\bar{4}_z 1/2,1/2,1/2)$ | (8) $\bar{4}^-$ $0,1/2,z; 0,1/2,1/4$<br>$(\bar{4}_z^{-1} 1/2,1/2,1/2)$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

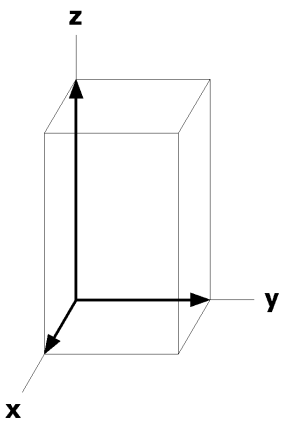
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		(0,0,0) +	(1/2,1/2,1/2) +		
16	f 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
		(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $\bar{v},u,\bar{w}$ ]		
		(5) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,y+1/2,\bar{z}+1/4$ [ $u,v,\bar{w}$ ]		
		(7) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(8) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]		
8	e 2	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,1/2,z+1/4 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/4$ [0,0, $\bar{w}$ ]
8	d $\bar{1}'$	0,1/4,5/8 [0,0,0]	0,3/4,5/8 [0,0,0]	1/4,0,3/8 [0,0,0]	3/4,0,3/8 [0,0,0]
8	c $\bar{1}'$	0,1/4,1/8 [0,0,0]	0,3/4,1/8 [0,0,0]	1/4,0,7/8 [0,0,0]	3/4,0,7/8 [0,0,0]
4	b $\bar{4}..$	0,0,1/2 [0,0,w]	0,1/2,3/4 [0,0, $\bar{w}$ ]		
4	a $\bar{4}..$	0,0,0 [0,0,w]	0,1/2,1/4 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_2$ -4  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2m'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

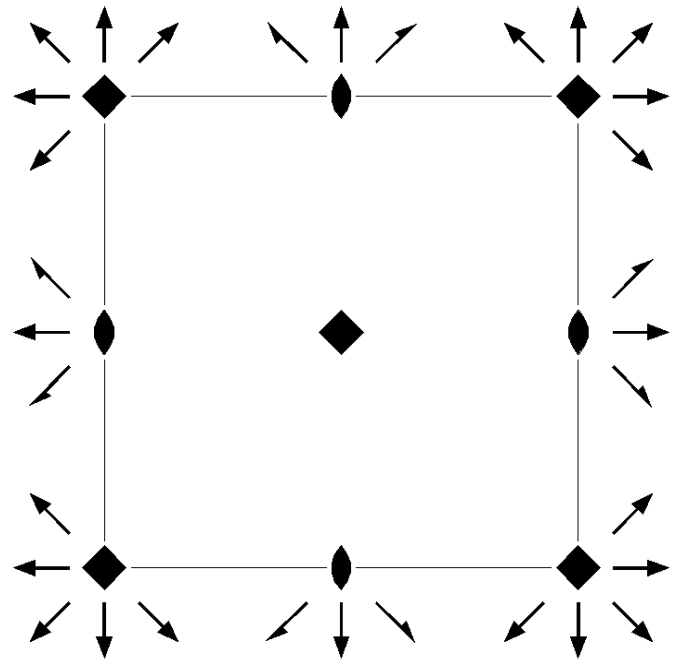
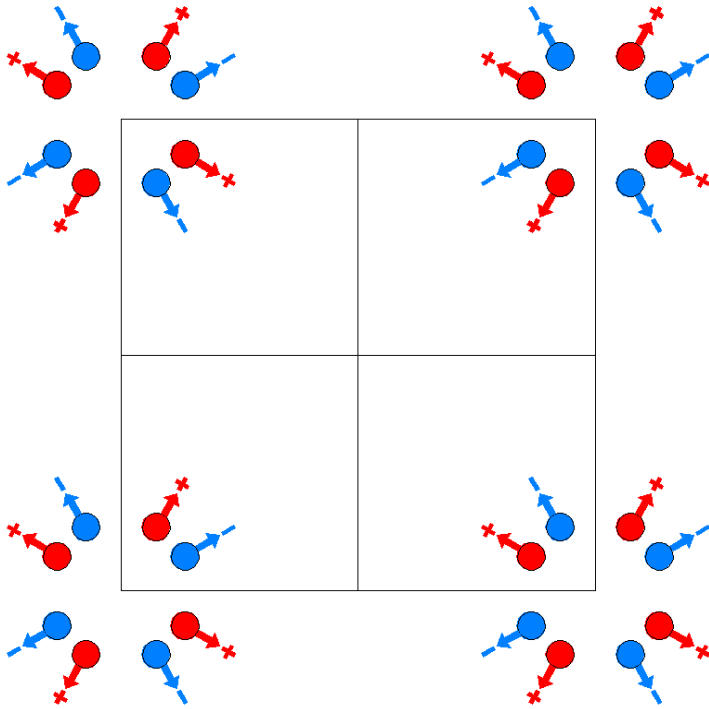
Along [1,1,0]  $p2m'g'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x+1/4,1/8



P422  
89.1.747

422  
P422

Tetragonal



Origin on 422

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

Symmetry Operations

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)    |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)             | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

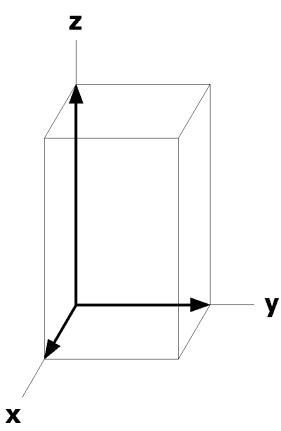
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	p 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]
		(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
4	o .2.	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	1/2,x,0 [0,u,0]	1/2, $\bar{x},0$ [0, $\bar{u},0$ ]
4	n .2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,1/2 [0,u,0]	0, $\bar{x},1/2$ [0, $\bar{u},0$ ]
4	m .2.	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	1/2,x,1/2 [0,u,0]	1/2, $\bar{x},1/2$ [0, $\bar{u},0$ ]
4	l .2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0,u,0]	0, $\bar{x},0$ [0, $\bar{u},0$ ]
4	k ..2	x,x,1/2 [u,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/2$ [ $\bar{u},u,0$ ]	$x,\bar{x},1/2$ [ $u,\bar{u},0$ ]
4	j ..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]	$x,\bar{x},0$ [ $u,\bar{u},0$ ]
4	i 2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
2	h 4..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	g 4..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	f 222.	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	e 222.	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
1	d 422	1/2,1/2,1/2 [0,0,0]			
1	c 422	1/2,1/2,0 [0,0,0]			
1	b 422	0,0,1/2 [0,0,0]			
1	a 422	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0

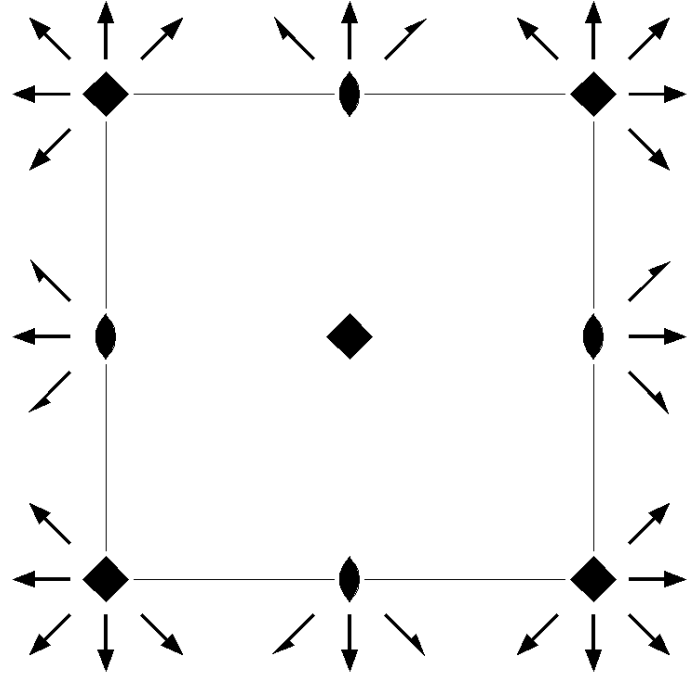
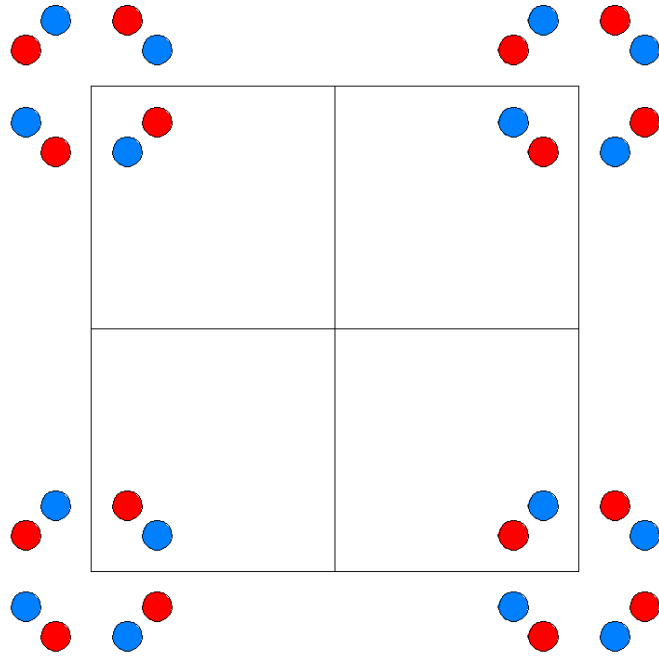


P4221'  
89.2.748

4221'  
P4221'

Tetragonal

1'



Origin on 4221'

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

Symmetry Operations

For 1 + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)    |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)             | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0) |

For 1' + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1'<br>(1 0,0,0)'                     | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'     |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'            | (8) 2' x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

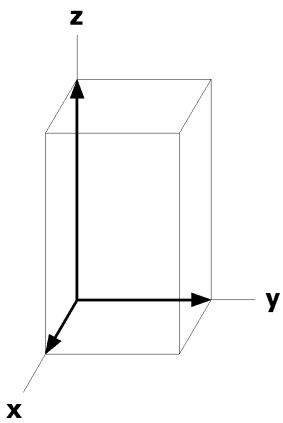
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +		1' +	
8 p 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z$ [0,0,0]	(4) $y,\bar{x},z$ [0,0,0]
	(5) $\bar{x},y,\bar{z}$ [0,0,0]	(6) $x,\bar{y},\bar{z}$ [0,0,0]	(7) $y,x,\bar{z}$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}$ [0,0,0]
4 o .2.1'	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]	1/2,x,0 [0,0,0]	1/2, $\bar{x},0$ [0,0,0]
4 n .2.1'	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]	0,x,1/2 [0,0,0]	0, $\bar{x},1/2$ [0,0,0]
4 m .2.1'	x,1/2,1/2 [0,0,0]	$\bar{x},1/2,1/2$ [0,0,0]	1/2,x,1/2 [0,0,0]	1/2, $\bar{x},1/2$ [0,0,0]
4 l .2.1'	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x},0$ [0,0,0]
4 k ..2 1'	x,x,1/2 [0,0,0]	$\bar{x},\bar{x},1/2$ [0,0,0]	$\bar{x},x,1/2$ [0,0,0]	x, $\bar{x},1/2$ [0,0,0]
4 j ..2 1'	x,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x},x,0$ [0,0,0]	x, $\bar{x},0$ [0,0,0]
4 i 2..1'	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]
2 h 4..1'	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
2 g 4..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2 f 222.1'	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
2 e 222.1'	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
1 d 4221'	1/2,1/2,1/2 [0,0,0]			
1 c 4221'	1/2,1/2,0 [0,0,0]			
1 b 4221'	0,0,1/2 [0,0,0]			
1 a 4221'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

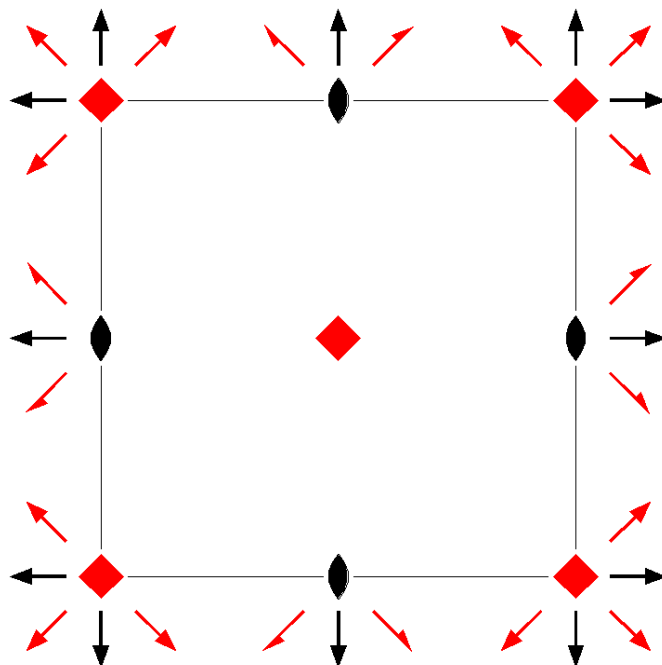
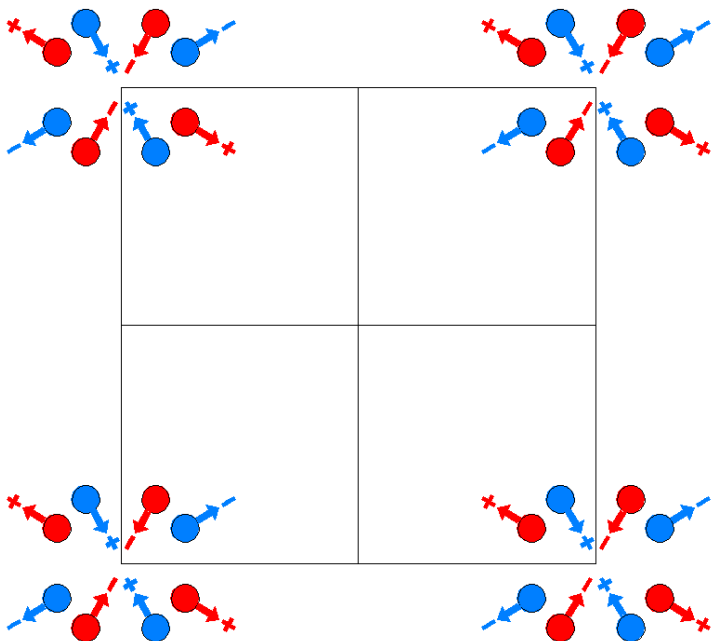
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4'22'  
89.3.749

4'22'  
P4'22'

Tetragonal



Origin on 4'22'

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 4<sup>+</sup> 0,0,z  
(4<sub>z</sub><sup>+</sup>|0,0,0)'

(4) 4<sup>-</sup> 0,0,z  
(4<sub>z</sub><sup>-</sup>|0,0,0)'

(5) 2 0,y,0  
(2<sub>y</sub>|0,0,0)

(6) 2 x,0,0  
(2<sub>x</sub>|0,0,0)

(7) 2' x,x,0  
(2<sub>xy</sub>'|0,0,0)'

(8) 2' x, $\bar{x}$ ,0  
(2 <sub>$\bar{xy}$</sub> '|0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

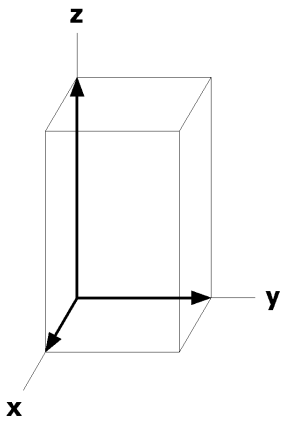
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	p 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
		(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]
4	o .2.	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	1/2,x,0 [0, $\bar{u}$ ,0]	1/2, $\bar{x}$ ,0 [0,u,0]
4	n .2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,1/2 [0, $\bar{u}$ ,0]	0, $\bar{x}$ ,1/2 [0,u,0]
4	m .2.	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	1/2,x,1/2 [0, $\bar{u}$ ,0]	1/2, $\bar{x}$ ,1/2 [0,u,0]
4	l .2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0, $\bar{u}$ ,0]	0, $\bar{x}$ ,0 [0,u,0]
4	k ..2'	x,x,1/2 [u, $\bar{u}$ ,w]	$\bar{x},\bar{x},1/2$ [ $\bar{u},u,w$ ]	$\bar{x},x,1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]	x, $\bar{x},1/2$ [u,u, $\bar{w}$ ]
4	j ..2'	x,x,0 [u, $\bar{u}$ ,w]	$\bar{x},\bar{x},0$ [ $\bar{u},u,w$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},\bar{w}$ ]	x, $\bar{x},0$ [u,u, $\bar{w}$ ]
4	i 2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]
2	h 4'..	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
2	g 4'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	f 222.	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	e 222.	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
1	d 4'22'	1/2,1/2,1/2 [0,0,0]			
1	c 4'22'	1/2,1/2,0 [0,0,0]			
1	b 4'22'	0,0,1/2 [0,0,0]			
1	a 4'22'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

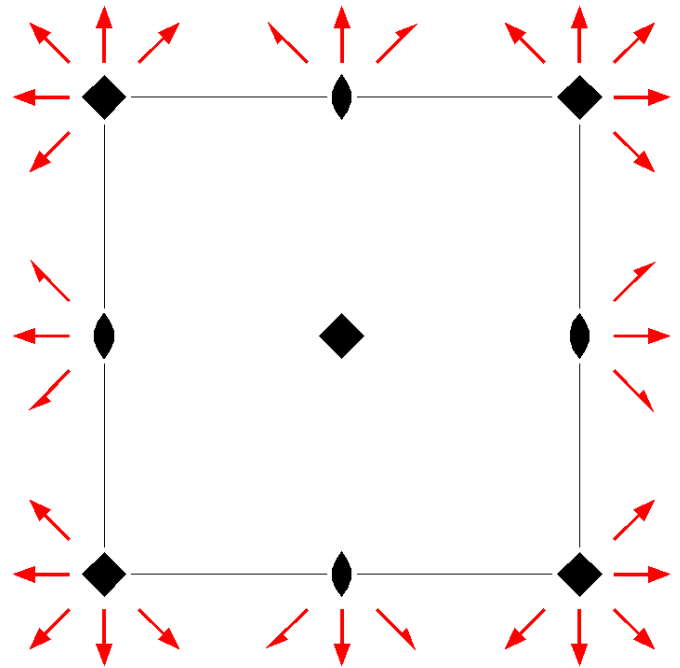
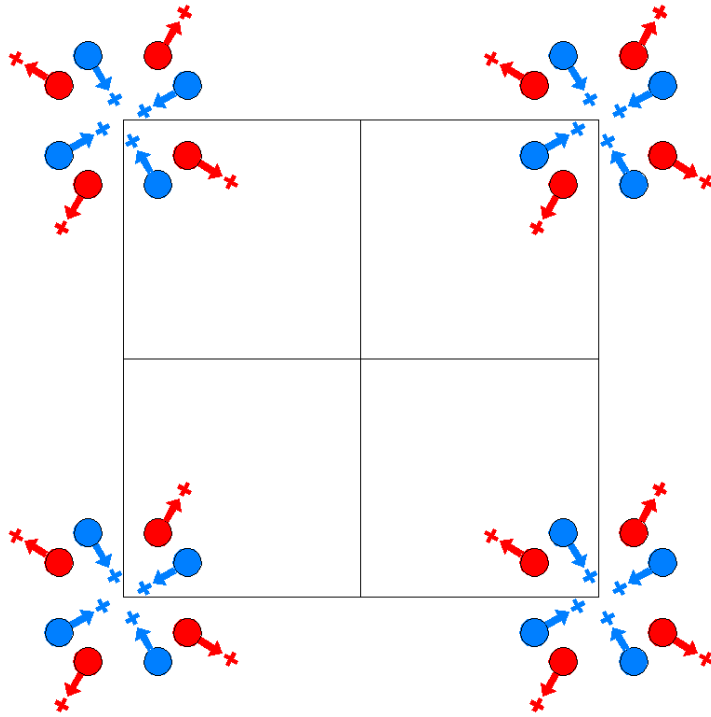
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



P42'2'  
89.4.750

42'2'  
P42'2'

Tetragonal



Origin on 42'2'

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'           | (8) 2' x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)'                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

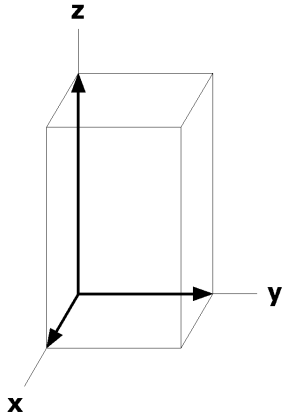
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	p 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]
		(5) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]
4	o .2'	x,1/2,0 [u,0,w]	$\bar{x},1/2,0$ [ $\bar{u},0,w$ ]	1/2,x,0 [0,u,w]	1/2, $\bar{x},0$ [0, $\bar{u},w$ ]
4	n .2'	x,0,1/2 [u,0,w]	$\bar{x},0,1/2$ [ $\bar{u},0,w$ ]	0,x,1/2 [0,u,w]	0, $\bar{x},1/2$ [0, $\bar{u},w$ ]
4	m .2'	x,1/2,1/2 [u,0,w]	$\bar{x},1/2,1/2$ [ $\bar{u},0,w$ ]	1/2,x,1/2 [0,u,w]	1/2, $\bar{x},1/2$ [0, $\bar{u},w$ ]
4	l .2'	x,0,0 [u,0,w]	$\bar{x},0,0$ [ $\bar{u},0,w$ ]	0,x,0 [0,u,w]	0, $\bar{x},0$ [0, $\bar{u},w$ ]
4	k ..2'	x,x,1/2 [u, $\bar{u},w$ ]	$\bar{x},\bar{x},1/2$ [ $\bar{u},u,w$ ]	$\bar{x},x,1/2$ [u,u,w]	x, $\bar{x},1/2$ [ $\bar{u},\bar{u},w$ ]
4	j ..2'	x,x,0 [u, $\bar{u},w$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},u,w$ ]	$\bar{x},x,0$ [u,u,w]	x, $\bar{x},0$ [ $\bar{u},\bar{u},w$ ]
4	i 2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]
2	h 4..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
2	g 4..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
2	f 22'2'	1/2,0,1/2 [0,0,w]	0,1/2,1/2 [0,0,w]		
2	e 22'2'	1/2,0,0 [0,0,w]	0,1/2,0 [0,0,w]		
1	d 42'2'	1/2,1/2,1/2 [0,0,w]			
1	c 42'2'	1/2,1/2,0 [0,0,w]			
1	b 42'2'	0,0,1/2 [0,0,w]			
1	a 42'2'	0,0,0 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



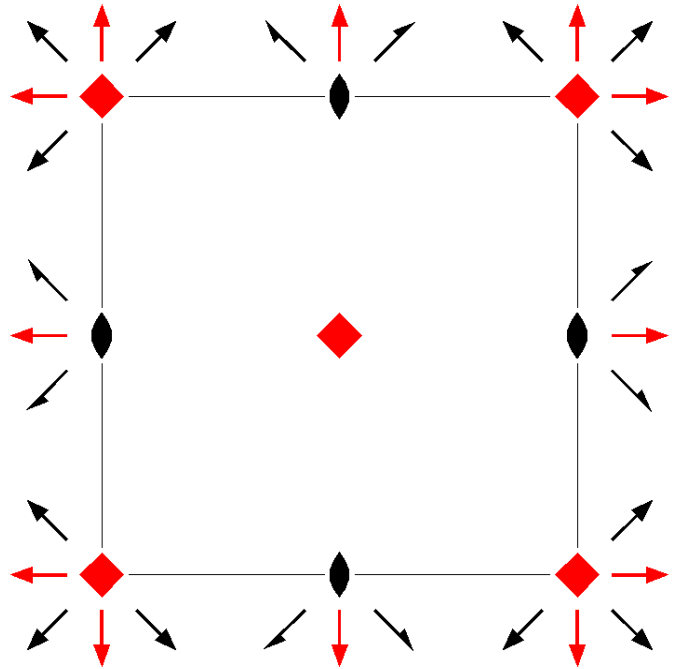
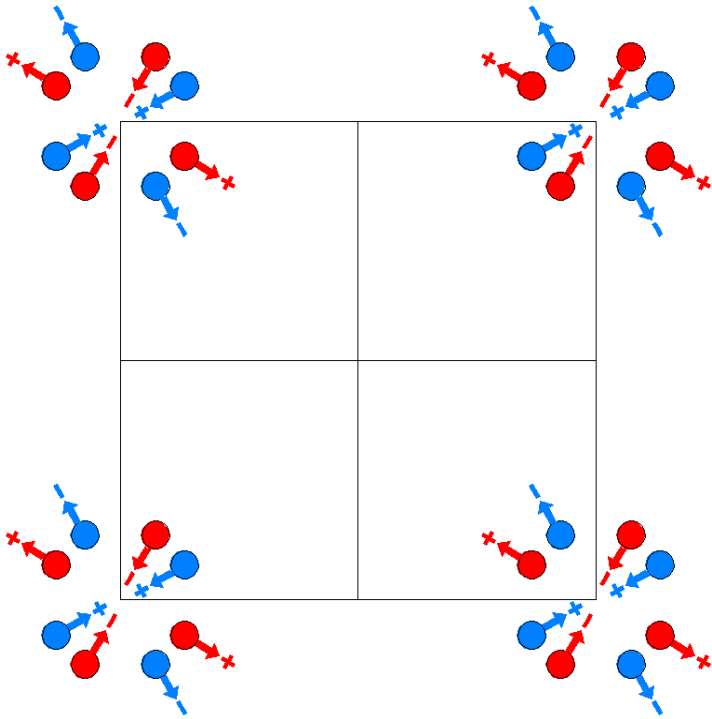
P4'2'2

89.5.751

4'2'2

P4'2'2

Tetragonal



Origin on 4'2'2

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 4<sup>+</sup> 0,0,z  
(4<sub>z</sub>|0,0,0)'

(4) 4<sup>-</sup> 0,0,z  
(4<sub>z</sub><sup>-1</sup>|0,0,0)'

(5) 2' 0,y,0  
(2<sub>y</sub>|0,0,0)'

(6) 2' x,0,0  
(2<sub>x</sub>|0,0,0)'

(7) 2 x,x,0  
(2<sub>xy</sub>|0,0,0)

(8) 2 x,x̄,0  
(2<sub>xy</sub><sup>-</sup>|0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

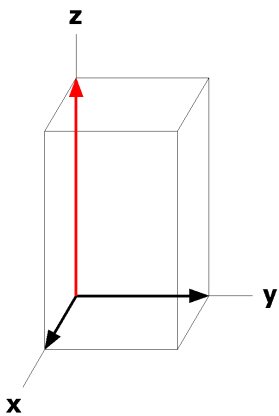
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	p 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $v,\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
		(5) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
4	o .2'	x,1/2,0 [0,v,w]	$\bar{x},1/2,0$ [0, $\bar{v},w$ ]	1/2,x,0 [v,0, $\bar{w}$ ]	1/2, $\bar{x},0$ [ $\bar{v},0,\bar{w}$ ]
4	n .2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	0,x,1/2 [v,0, $\bar{w}$ ]	0, $\bar{x},1/2$ [ $\bar{v},0,\bar{w}$ ]
4	m .2'	x,1/2,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0, $\bar{v},w$ ]	1/2,x,1/2 [v,0, $\bar{w}$ ]	1/2, $\bar{x},1/2$ [ $\bar{v},0,\bar{w}$ ]
4	l .2'	x,0,0 [0,v,w]	$\bar{x},0,0$ [0, $\bar{v},w$ ]	0,x,0 [v,0, $\bar{w}$ ]	0, $\bar{x},0$ [ $\bar{v},0,\bar{w}$ ]
4	k ..2	x,x,1/2 [u,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/2$ [u, $\bar{u},0$ ]	$x,\bar{x},1/2$ [ $\bar{u},u,0$ ]
4	j ..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [u, $\bar{u},0$ ]	$x,\bar{x},0$ [ $\bar{u},u,0$ ]
4	i 2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
2	h 4'..	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
2	g 4'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	f 22'2'.	1/2,0,1/2 [0,0,w]	0,1/2,1/2 [0,0, $\bar{w}$ ]		
2	e 22'2'.	1/2,0,0 [0,0,w]	0,1/2,0 [0,0, $\bar{w}$ ]		
1	d 4'2'2	1/2,1/2,1/2 [0,0,0]			
1	c 4'2'2	1/2,1/2,0 [0,0,0]			
1	b 4'2'2	0,0,1/2 [0,0,0]			
1	a 4'2'2	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4'm'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



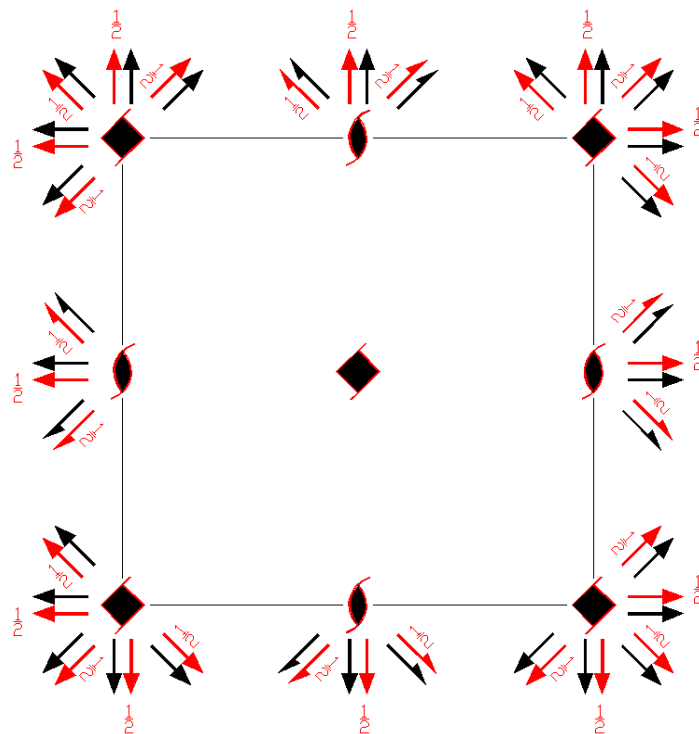
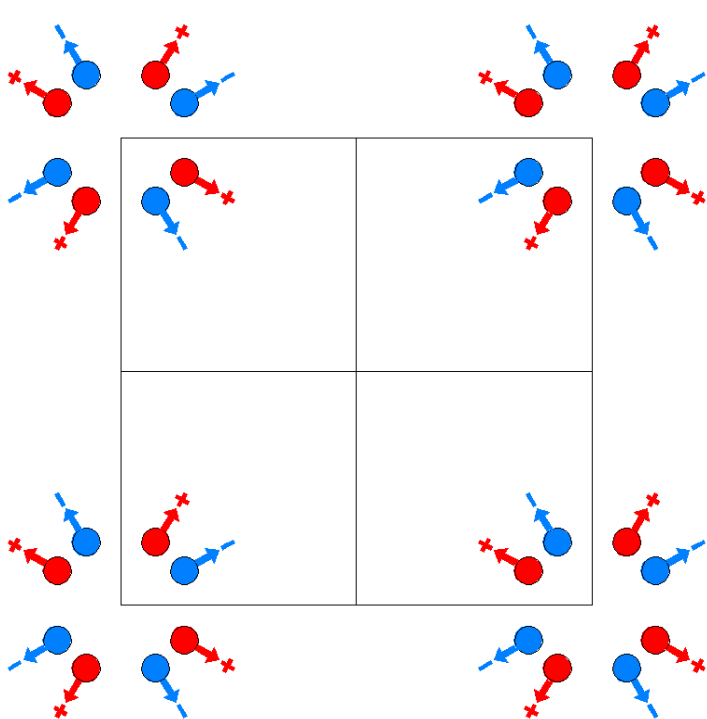
$P_{2c}$  422

89.6.752

4221'

$P_{2c}$  422

Tetragonal



Origin on 422

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)             | (8) 2 x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)                         |

For (0,0,1)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (0,0,1)<br>(1 0,0,1)'               | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)' | (3) 4 <sup>+</sup> ' (0,0,1) 0,0,z<br>(4 <sub>z</sub>  0,0,1)' | (4) 4 <sup>-</sup> ' (0,0,1) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1)' |
| (5) 2' 0,y,1/2<br>(2 <sub>y</sub>  0,0,1)' | (6) 2' x,0,1/2<br>(2 <sub>x</sub>  0,0,1)'       | (7) 2' x,x,1/2<br>(2 <sub>xy</sub>  0,0,1)'                    | (8) 2' x,x̄,1/2<br>(2 <sub>xȳ</sub>  0,0,1)'                                |



**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

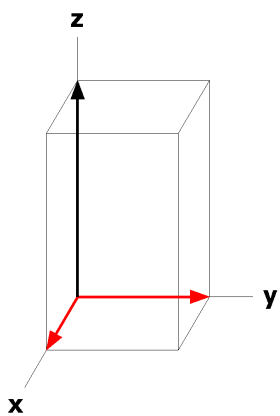
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
16 p 1	(1) x,y,z [u,v,w] (5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ] (7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
8 o .2.	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	1/2,x,0 [0,u,0]	1/2, $\bar{x},0$ [0, $\bar{u},0$ ]
8 n .2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	0,x,1/2 [ $\bar{v},0,w$ ]	0, $\bar{x},1/2$ [v,0,w]
8 m .2'	x,1/2,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0, $\bar{v},w$ ]	1/2,x,1/2 [ $\bar{v},0,w$ ]	1/2, $\bar{x},1/2$ [v,0,w]
8 l .2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0,u,0]	0, $\bar{x},0$ [0, $\bar{u},0$ ]
8 k ..2'	x,x,1/2 [u, $\bar{u},w$ ]	$\bar{x},\bar{x},1/2$ [ $\bar{u},u,w$ ]	$\bar{x},x,1/2$ [u,u,w]	x, $\bar{x},1/2$ [ $\bar{u},\bar{u},w$ ]
8 j ..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]	x, $\bar{x},0$ [u, $\bar{u},0$ ]
8 i 2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4 h 4..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 g 4..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 f 22'2'	1/2,0,1/2 [0,0,w]	0,1/2,1/2 [0,0,w]		
4 e 222.	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
2 d 42'2'	1/2,1/2,1/2 [0,0,w]			
2 c 422	1/2,1/2,0 [0,0,0]			
2 b 42'2'	0,0,1/2 [0,0,w]			
2 a 422	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>·2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

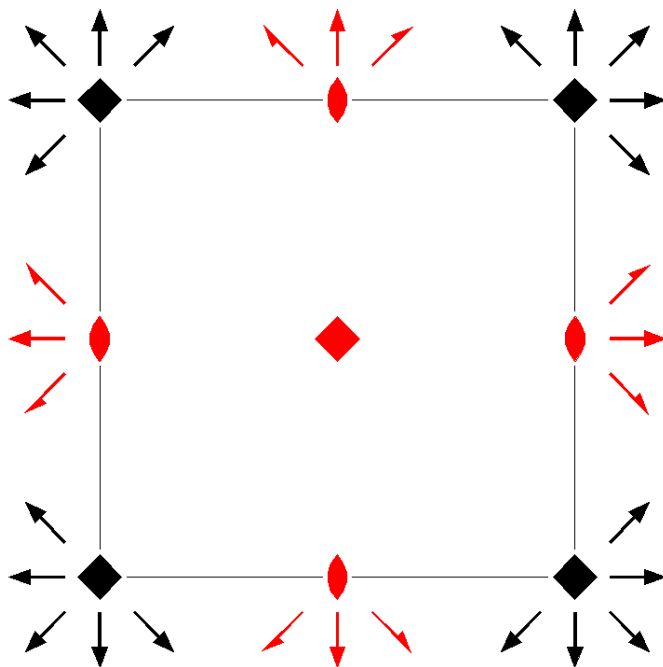
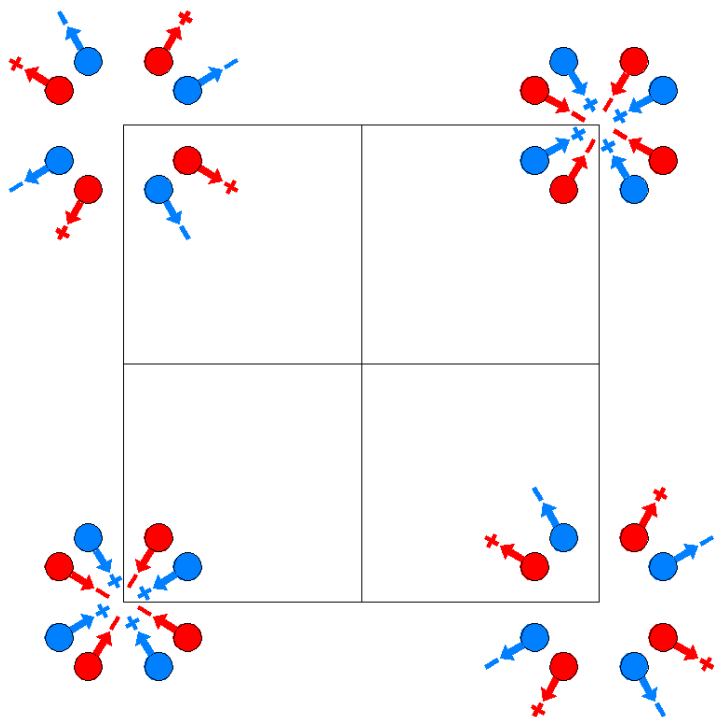
Along [1,1,0] p<sub>2a</sub>·2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



P<sub>p</sub> 422  
89.7.753

4221'  
P<sub>p</sub> 422

Tetragonal



Origin on 422

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)    |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)             | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0) |

For (1,0,0)<sup>'</sup> + set

- |  |  |   |   |
|--|--|---|---|
| (1) t <sup>'</sup> (1,0,0)<br>(1 1,0,0) <sup>'</sup>               | (2) 2 <sup>'</sup> 1/2,0,z<br>(2 <sub>z</sub>  1,0,0) <sup>'</sup>       | (3) 4 <sup>+</sup> 1/2,1/2,z<br>(4 <sub>z</sub>  1,0,0) <sup>'</sup>              | (4) 4 <sup>-</sup> 1/2,-1/2,z<br>(4 <sub>z</sub> <sup>-1</sup>  1,0,0) <sup>'</sup>                             |
| (5) 2 <sup>'</sup> 1/2,y,0<br>(2 <sub>y</sub>  1,0,0) <sup>'</sup> | (6) 2 <sup>'</sup> (1,0,0) x,0,0<br>(2 <sub>x</sub>  1,0,0) <sup>'</sup> | (7) 2 <sup>'</sup> (1/2,1/2,0) x+1/2,x,0<br>(2 <sub>xy</sub>  1,0,0) <sup>'</sup> | (8) 2 <sup>'</sup> (1/2,-1/2,0) x+1/2, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  1,0,0) <sup>'</sup> |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

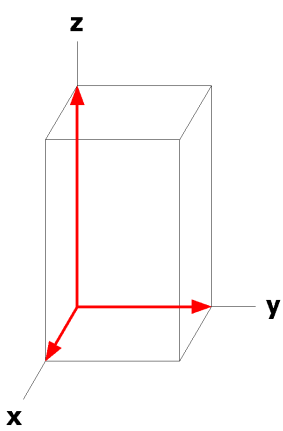
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 p 1	(1) x,y,z [u,v,w] (5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ] (7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
8 o .2'	x,1/2,0 [0,v,w]	$\bar{x},1/2,0$ [0,v, $\bar{w}$ ]	1/2,x,0 [v,0, $\bar{w}$ ]	1/2, $\bar{x},0$ [v,0,w]
8 n .2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,1/2 [0,u,0]	0, $\bar{x},1/2$ [0, $\bar{u},0$ ]
8 m .2'	x,1/2,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0,v, $\bar{w}$ ]	1/2,x,1/2 [v,0, $\bar{w}$ ]	1/2, $\bar{x},1/2$ [v,0,w]
8 l .2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0,u,0]	0, $\bar{x},0$ [0, $\bar{u},0$ ]
8 k ..2	x,x,1/2 [u,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/2$ [ $\bar{u},u,0$ ]	x, $\bar{x},1/2$ [u, $\bar{u},0$ ]
8 j ..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]	x, $\bar{x},0$ [u, $\bar{u},0$ ]
8 i 2'..	0,1/2,z [u,v,0]	1/2,0,z [v, $\bar{u},0$ ]	0,1/2, $\bar{z}$ [ $\bar{u},v,0$ ]	1/2,0, $\bar{z}$ [v,u,0]
4 h 4'..	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
4 g 4..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 f 2'22'	1/2,0,1/2 [u,0,0]	0,1/2,1/2 [0,u,0]		
4 e 2'22'	1/2,0,0 [u,0,0]	0,1/2,0 [0,u,0]		
2 d 4'2'2	1/2,1/2,1/2 [0,0,0]			
2 c 4'2'2	1/2,1/2,0 [0,0,0]			
2 b 422	0,0,1/2 [0,0,0]			
2 a 422	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub> 4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p<sub>2a</sub> 2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



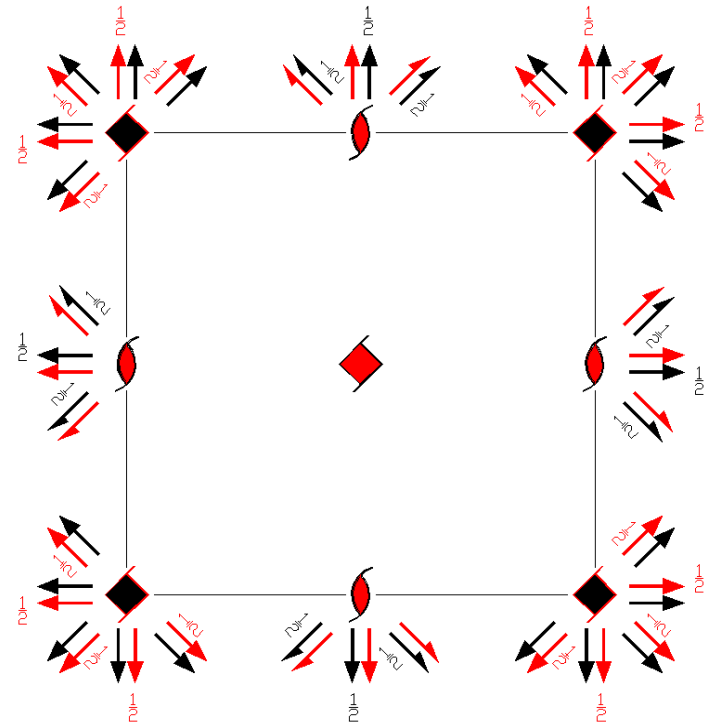
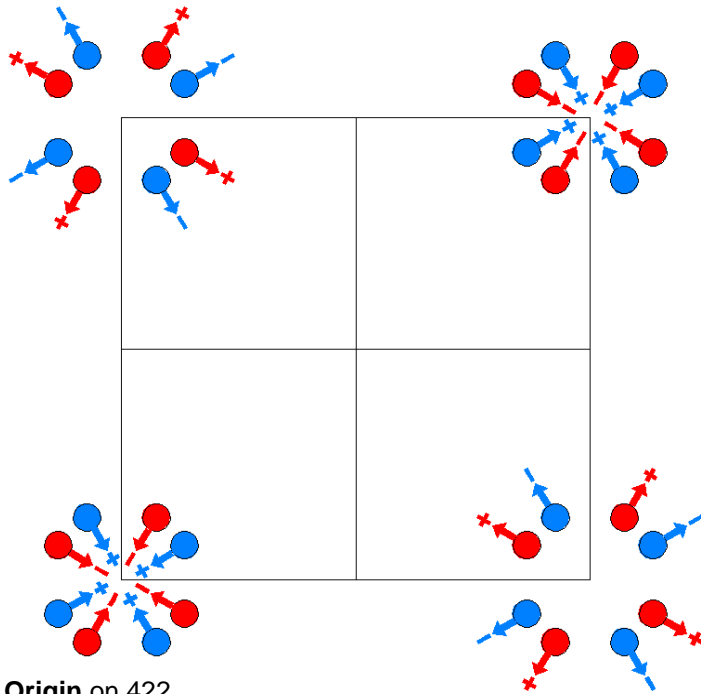
P<sub>1</sub>422

4221'

Tetragonal

89.8.754

P<sub>1</sub>422



Origin on 422

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)             | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub>-xy</sub>  0,0,0)                |

For (1,0,0)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) t' (1,0,0)<br>(1 1,0,0)'               | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'       | (3) 4 <sup>+</sup> ' 1/2,1/2,z<br>(4 <sub>z</sub>  1,0,0)' | (4) 4 <sup>-</sup> ' 1/2,-1/2,z<br>(4 <sub>z</sub> <sup>-1</sup>  1,0,0)' |
| (5) 2' 1/2,y,0<br>(2 <sub>y</sub>  1,0,0)' | (6) 2' (1,0,0) x,0,0<br>(2 <sub>x</sub>  1,0,0)' | (7) 2' (1/2,1/2,0) x+1/2,x,0<br>(2 <sub>xy</sub>  1,0,0)'  | (8) 2' (1/2,-1/2,0) x+1/2, $\bar{x}$ ,0<br>(2 <sub>-xy</sub>  1,0,0)'     |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

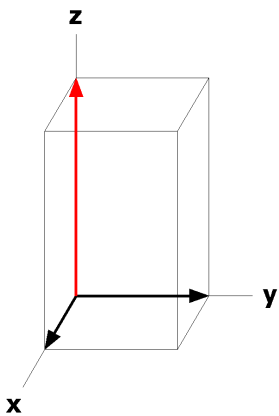
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0) <sup>+</sup>		
16 p 1	(1) x,y,z [u,v,w] (5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ] (7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
8 o .2'	x,1/2,0 [0,v,w]	$\bar{x},1/2,0$ [0,v, $\bar{w}$ ]	1/2,x,0 [v,0, $\bar{w}$ ]	1/2, $\bar{x},0$ [v,0,w]
8 n .2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	0,x,1/2 [ $\bar{v},0,w$ ]	0, $\bar{x},1/2$ [v,0,w]
8 m .2	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	1/2,x,1/2 [0,u,0]	1/2, $\bar{x},1/2$ [0, $\bar{u},0$ ]
8 l .2	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0,u,0]	0, $\bar{x},0$ [0, $\bar{u},0$ ]
8 k ..2'	x,x,1/2 [u, $\bar{u},w$ ]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,1/2$ [u,u,w]	x, $\bar{x},1/2$ [ $\bar{u},\bar{u},w$ ]
8 j ..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]	x, $\bar{x},0$ [u, $\bar{u},0$ ]
8 i 2'..	0,1/2,z [u,v,0]	1/2,0,z [v, $\bar{u},0$ ]	0,1/2, $\bar{z}$ [ $\bar{u},v,0$ ]	1/2,0, $\bar{z}$ [v,u,0]
4 h 4'..	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
4 g 4..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4 f 2'22'	1/2,0,1/2 [u,0,0]	0,1/2,1/2 [0,u,0]		
4 e 2'22'	1/2,0,0 [u,0,0]	0,1/2,0 [0,u,0]		
2 d 4'22'	1/2,1/2,1/2 [0,0,0]			
2 c 4'2'2	1/2,1/2,0 [0,0,0]			
2 b 42'2'	0,0,1/2 [0,0,w]			
2 a 422	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p<sub>c</sub>2mm  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x-1/4,x+1/4,1/2



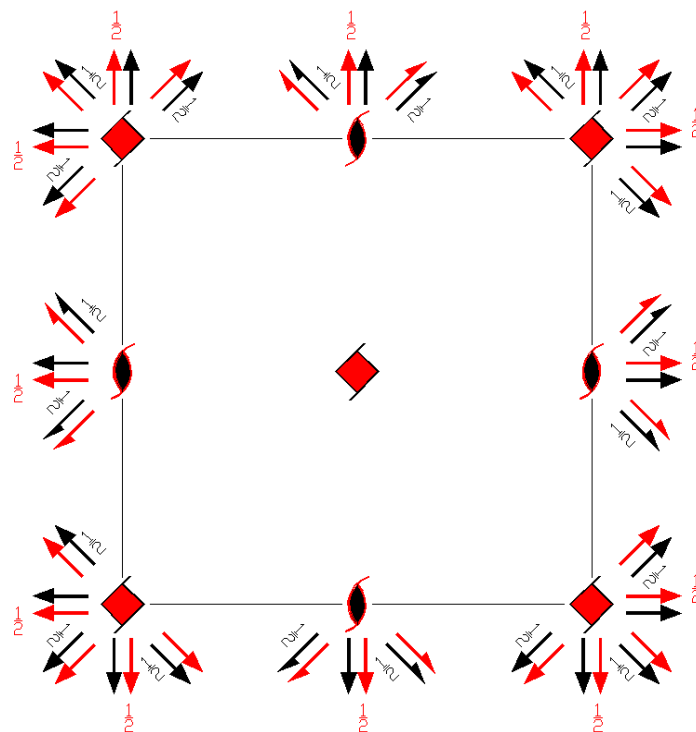
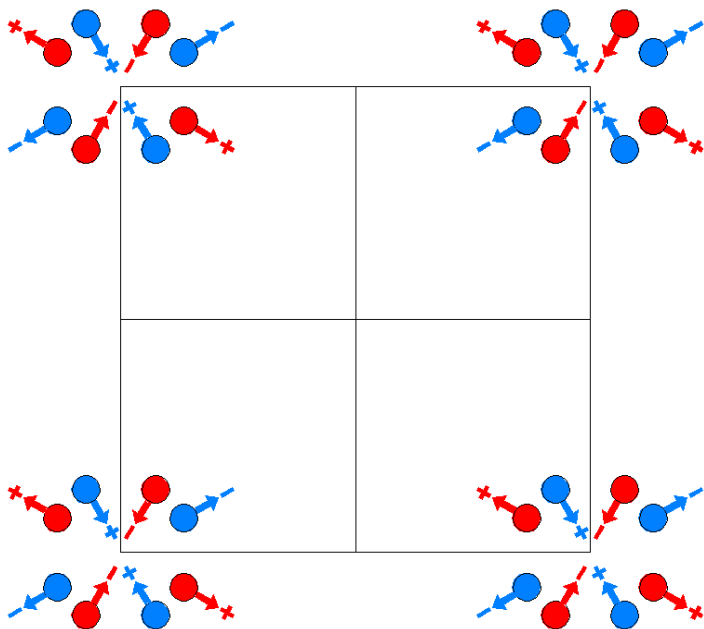
$P_{2c} 4'22'$

89.9.755

4221'

$P_{2c} 4'22'$

Tetragonal



Origin on  $4'22'$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For  $(0,0,0) + \text{set}$

- |                                  |                                  |                                       |   |
|----------------------------------|----------------------------------|---------------------------------------|---|
| (1) 1<br>(1 0,0,0)               | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $4^+ 0,0,z$<br>( $4_z$  0,0,0)'   | (4) $4^- 0,0,z$<br>( $4_z^{-1}$  0,0,0)'          |
| (5) 2 $0,y,0$<br>( $2_y$  0,0,0) | (6) 2 $x,0,0$<br>( $2_x$  0,0,0) | (7) $2' x,x,0$<br>( $2_{xy}$  0,0,0)' | (8) $2' x,\bar{x},0$<br>( $2_{\bar{xy}}$  0,0,0)' |

For  $(0,0,1)' + \text{set}$

- |                                      |  |  |   |
|--------------------------------------|--|--|---|
| (1) $t' (0,0,1)$<br>(1 0,0,1)'       | (2) $2' (0,0,1) \quad 0,0,z$<br>( $2_z$  0,0,1)' | (3) $4^+ (0,0,1) \quad 0,0,z$<br>( $4_z$  0,0,1) | (4) $4^- (0,0,1) \quad 0,0,z$<br>( $4_z^{-1}$  0,0,1) |
| (5) $2' 0,y,1/2$<br>( $2_y$  0,0,1)' | (6) $2' x,0,1/2$<br>( $2_x$  0,0,1)'             | (7) 2 $x,x,1/2$<br>( $2_{xy}$  0,0,1)            | (8) 2 $x,\bar{x},1/2$<br>( $2_{\bar{xy}}$  0,0,1)     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

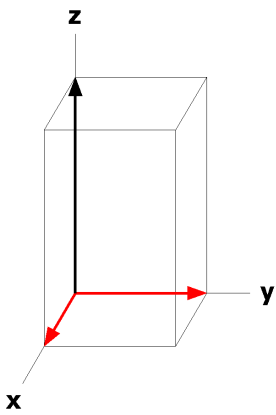
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
16 p 1	(1) x,y,z [u,v,w] (5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ] (7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]
8 o .2.	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	1/2,x,0 [0, $\bar{u},0$ ]	1/2, $\bar{x},0$ [0,u,0]
8 n .2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	0,x,1/2 [v,0, $\bar{w}$ ]	0, $\bar{x},1/2$ [ $\bar{v},0,\bar{w}$ ]
8 m .2'	x,1/2,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0, $\bar{v},w$ ]	1/2,x,1/2 [v,0, $\bar{w}$ ]	1/2, $\bar{x},1/2$ [ $\bar{v},0,\bar{w}$ ]
8 l .2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0, $\bar{u},0$ ]	0, $\bar{x},0$ [0,u,0]
8 k ..2	x,x,1/2 [u,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/2$ [u, $\bar{u},0$ ]	x, $\bar{x},1/2$ [ $\bar{u},u,0$ ]
8 j ..2'	x,x,0 [u, $\bar{u},w$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},u,w$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},\bar{w}$ ]	x, $\bar{x},0$ [u,u, $\bar{w}$ ]
8 i 2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]
4 h 4'..	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
4 g 4'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 f 22'2'	1/2,0,1/2 [0,0,w]	0,1/2,1/2 [0,0, $\bar{w}$ ]		
4 e 222.	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
2 d 4'2'2	1/2,1/2,1/2 [0,0,0]			
2 c 4'22'	1/2,1/2,0 [0,0,0]			
2 b 4'2'2	0,0,1/2 [0,0,0]			
2 a 4'22'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>·2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

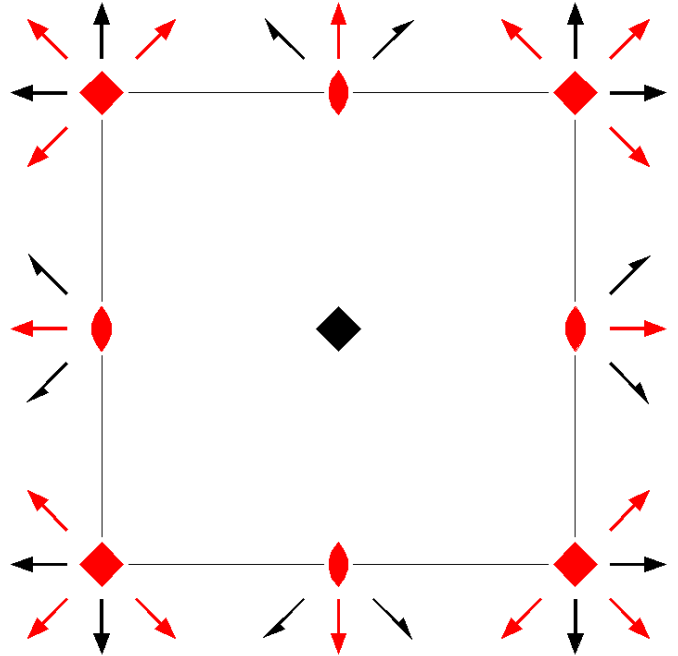
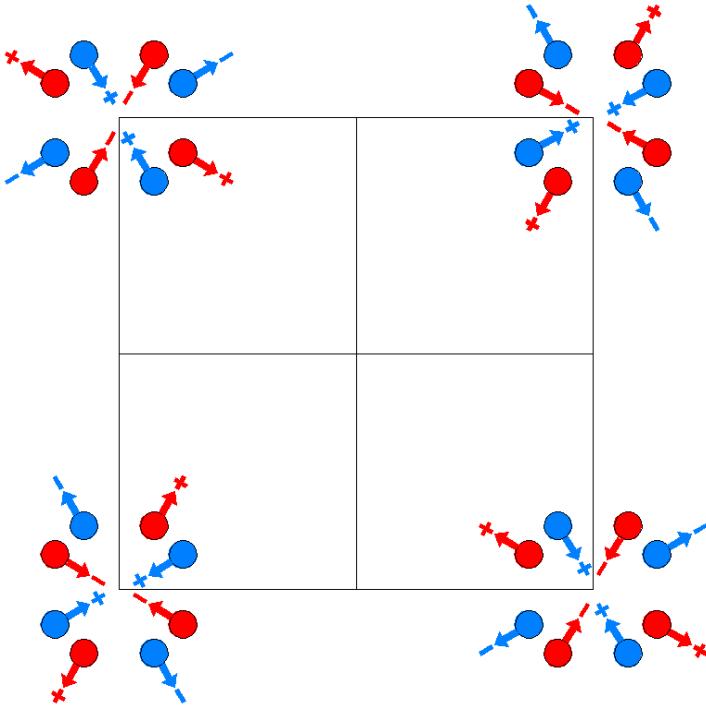
Along [1,1,0] p<sub>2a</sub>·2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/2



$P_p 4'22'$   
89.10.756

$4221'$   
 $P_p 4'22'$

Tetragonal



Origin on  $4'22'$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For  $(0,0,0)$  + set

- |                                |                                |  |   |
|--------------------------------|--------------------------------|--|---|
| (1) 1<br>$(1 0,0,0)$           | (2) 2 $0,0,z$<br>$(2_z 0,0,0)$ | (3) $4^+ 1' 0,0,z$<br>$(4_z^+ 0,0,0)'$ | (4) $4^- 1' 0,0,z$<br>$(4_z^- 0,0,0)'$          |
| (5) 2 $0,y,0$<br>$(2_y 0,0,0)$ | (6) 2 $x,0,0$<br>$(2_x 0,0,0)$ | (7) $2' x,x,0$<br>$(2_{xy} 0,0,0)'$    | (8) $2' x,\bar{x},0$<br>$(2_{\bar{xy}} 0,0,0)'$ |

For  $(1,0,0)'$  + set

- |                                    |  |   |  |
|------------------------------------|--|---|--|
| (1) $t' (1,0,0)$<br>$(1 1,0,0)'$   | (2) $2' 1/2,0,z$<br>$(2_z 1,0,0)'$       | (3) $4^+ 1/2,1/2,z$<br>$(4_z^+ 1,0,0)$            | (4) $4^- 1/2,-1/2,z$<br>$(4_z^- 1,0,0)$                        |
| (5) $2' 1/2,y,0$<br>$(2_y 1,0,0)'$ | (6) $2' (1,0,0) x,0,0$<br>$(2_x 1,0,0)'$ | (7) 2 $(1/2,1/2,0) x+1/2,x,0$<br>$(2_{xy} 1,0,0)$ | (8) 2 $(1/2,-1/2,0) x+1/2,\bar{x},0$<br>$(2_{\bar{xy}} 1,0,0)$ |



**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

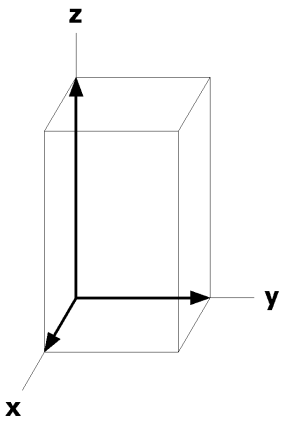
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 p 1	(1) x,y,z [u,v,w] (5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ] (7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]
8 o .2'	x,1/2,0 [0,v,w]	$\bar{x},1/2,0$ [0,v, $\bar{w}$ ]	1/2,x,0 [ $\bar{v},0,w$ ]	1/2, $\bar{x},0$ [ $\bar{v},0,\bar{w}$ ]
8 n .2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,1/2 [0, $\bar{u},0$ ]	0, $\bar{x},1/2$ [0,u,0]
8 m .2'.	x,1/2,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0,v, $\bar{w}$ ]	1/2,x,1/2 [ $\bar{v},0,w$ ]	1/2, $\bar{x},1/2$ [ $\bar{v},0,\bar{w}$ ]
8 l .2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0, $\bar{u},0$ ]	0, $\bar{x},0$ [0,u,0]
8 k ..2'	x,x,1/2 [u, $\bar{u},w$ ]	$\bar{x},\bar{x},1/2$ [ $\bar{u},u,w$ ]	$\bar{x},x,1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]	x, $\bar{x},1/2$ [u,u, $\bar{w}$ ]
8 j ..2'	x,x,0 [u, $\bar{u},w$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},u,w$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},\bar{w}$ ]	x, $\bar{x},0$ [u,u, $\bar{w}$ ]
8 i 2'..	0,1/2,z [u,v,0]	1/2,0,z [ $\bar{v},u,0$ ]	0,1/2, $\bar{z}$ [ $\bar{u},v,0$ ]	1/2,0, $\bar{z}$ [ $\bar{v},\bar{u},0$ ]
4 h 4..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
4 g 4'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4 f 2'22'.	1/2,0,1/2 [u,0,0]	0,1/2,1/2 [0, $\bar{u},0$ ]		
4 e 2'22'.	1/2,0,0 [u,0,0]	0,1/2,0 [0, $\bar{u},0$ ]		
2 d 42'2'	1/2,1/2,1/2 [0,0,w]			
2 c 42'2'	1/2,1/2,0 [0,0,w]			
2 b 4'22'	0,0,1/2 [0,0,0]			
2 a 4'22'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub> 4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/2,1/2,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

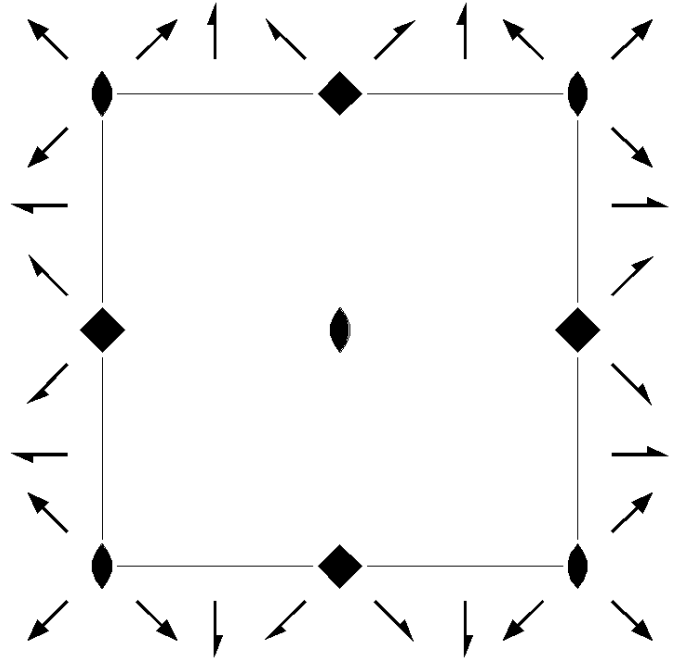
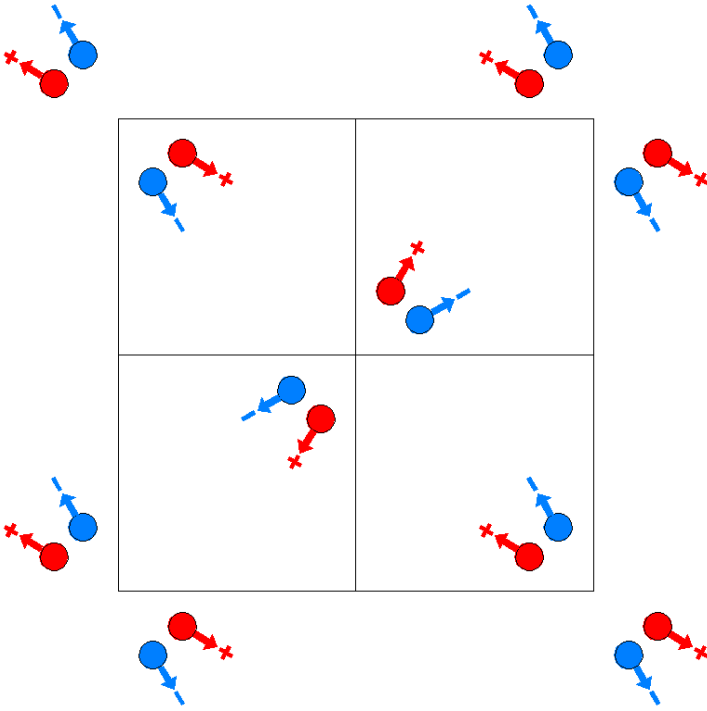
Along [1,1,0] p<sub>2a</sub> 2mm  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x-1/4,x+1/4,0



P42<sub>1</sub>2  
90.1.757

422  
P42<sub>1</sub>2

Tetragonal



Origin at 222 at 212

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

### Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0) | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0) |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                   | (8) 2 x,x̄,0<br>(2 <sub>xy</sub> ̄ 0,0,0)                               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

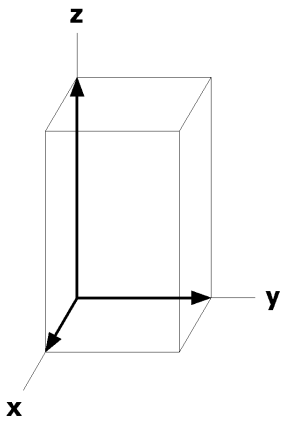
		Coordinates			
		Multiplicity, Wyckoff letter, Site Symmetry.			
8	g 1	(1) x,y,z [u,v,w]		(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	
		(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},u,w$ ]		(4) $y+1/2,\bar{x}+1/2,z$ [ $v,\bar{u},w$ ]	
		(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]		(6) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	
		(7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]		(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	
4	f ..2	x,x,1/2 [u,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $\bar{u},u,0$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $u,\bar{u},0$ ]
4	e ..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,0$ [ $\bar{u},u,0$ ]	$x+1/2,\bar{x}+1/2,0$ [ $u,\bar{u},0$ ]
4	d 2..	0,0,z [0,0,w]	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
2	c 4..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	b 2.22	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a 2.22	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4g'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P42<sub>1</sub>21'

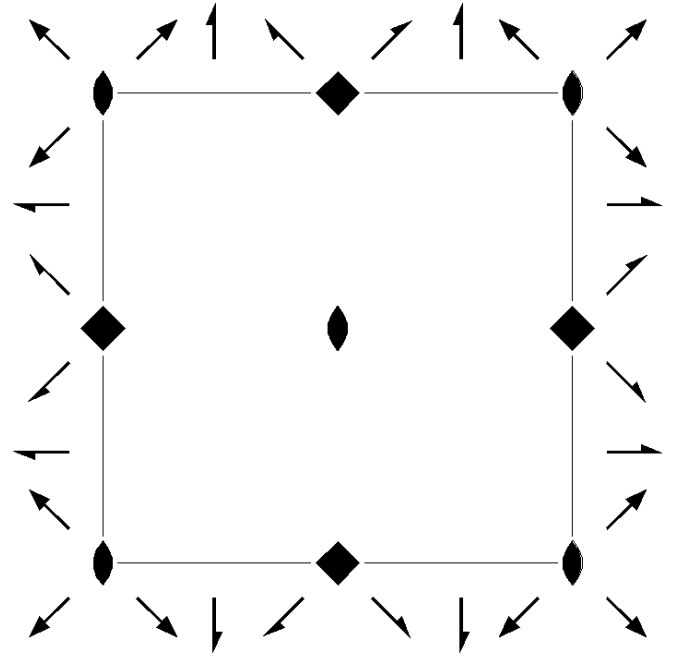
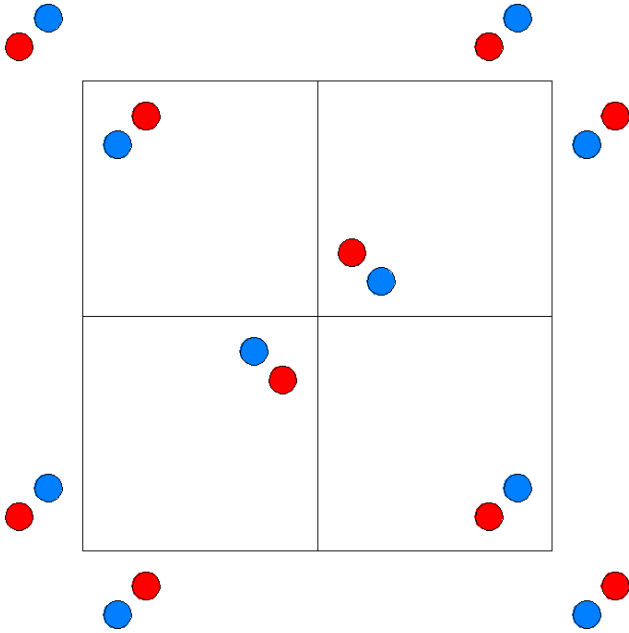
90.2.758

4221'

P42<sub>1</sub>21'

Tetragonal

1'



Origin at 2221' at 2121'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For 1 + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0) | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0) |
| (5) 2 <sub>y</sub> (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (6) 2 <sub>x</sub> (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) | (7) 2 <sub>xy</sub> x,x,0<br>(2 <sub>xy</sub>  0,0,0)     | (8) 2 <sub>xy</sub> x,x̄,0<br>(2 <sub>xy</sub>  0,0,0)                  |

For 1' + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1'<br>(1 0,0,0)'   | (2) 2' <sub>z</sub> 0,0,z<br>(2' <sub>z</sub>  0,0,0)'                 | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0)' | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)' |
| (5) 2' <sub>y</sub> (0,1/2,0) 1/4,y,0<br>(2' <sub>y</sub>  1/2,1/2,0)' | (6) 2' <sub>x</sub> (1/2,0,0) x,1/4,0<br>(2' <sub>x</sub>  1/2,1/2,0)' | (7) 2' <sub>xy</sub> x,x,0<br>(2' <sub>xy</sub>  0,0,0)'   | (8) 2' <sub>xy</sub> x,x̄,0<br>(2' <sub>xy</sub>  0,0,0)'                |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

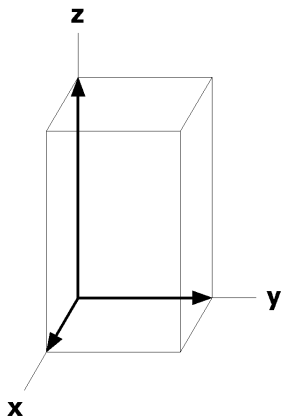
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		1 +		1' +	
8	g 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]		
		(3) $\bar{y}+1/2,x+1/2,z$ [0,0,0]	(4) $y+1/2,\bar{x}+1/2,z$ [0,0,0]		
		(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [0,0,0]	(6) $x+1/2,\bar{y}+1/2,\bar{z}$ [0,0,0]		
		(7) y,x, $\bar{z}$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}$ [0,0,0]		
4	f ..21'	x,x,1/2 [0,0,0]	$\bar{x},\bar{x},1/2$ [0,0,0]	$\bar{x}+1/2,x+1/2,1/2$ [0,0,0]	$x+1/2,\bar{x}+1/2,1/2$ [0,0,0]
4	e ..21'	x,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x}+1/2,x+1/2,0$ [0,0,0]	$x+1/2,\bar{x}+1/2,0$ [0,0,0]
4	d 2..1'	0,0,z [0,0,0]	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]
2	c 4..1'	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
2	b 2.221'	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a 2.221'	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



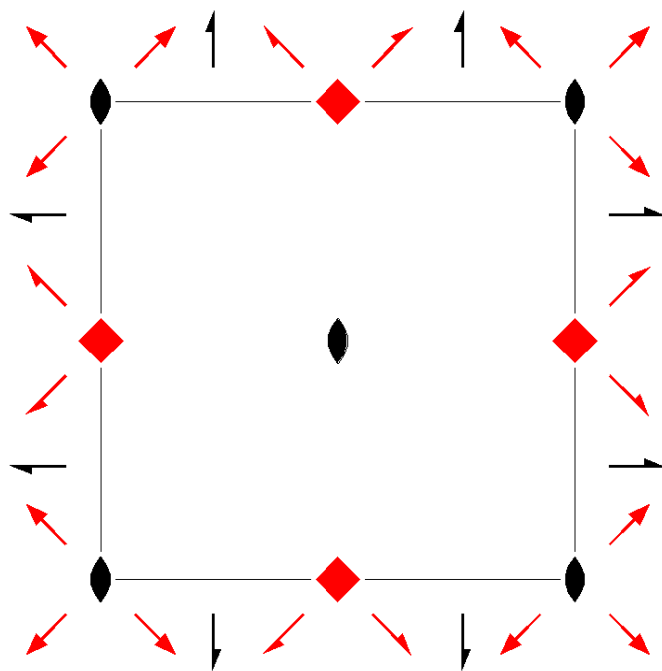
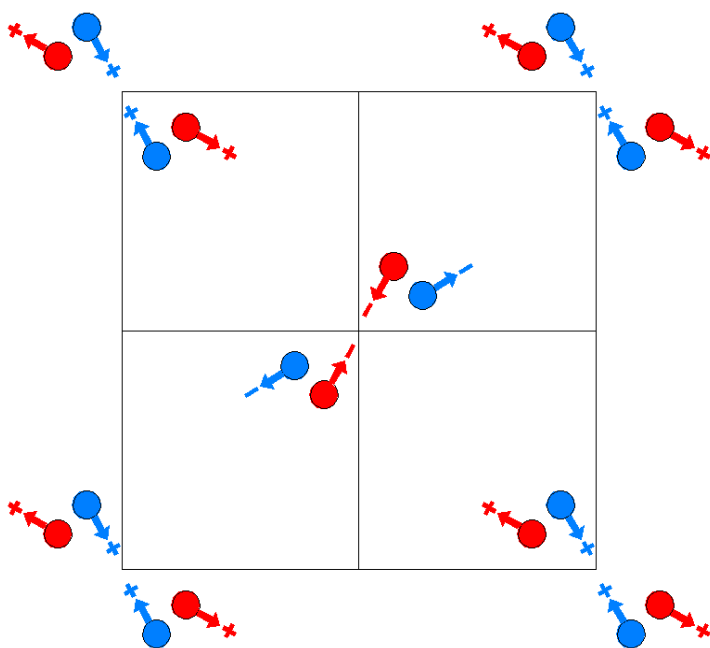
P4'2<sub>1</sub>2'

90.3.759

4'22'

P4'2<sub>1</sub>2'

Tetragonal



Origin at 22'2' at 212'

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 4<sup>+</sup> 0,1/2,z  
(4<sub>z</sub>|1/2,1/2,0)'

(4) 4<sup>-</sup> 1/2,0,z  
(4<sub>z</sub><sup>-1</sup>|1/2,1/2,0)'

(5) 2 (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)

(6) 2 (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)

(7) 2' x,x,0  
(2<sub>xy</sub>|0,0,0)'

(8) 2' x,x̄,0  
(2<sub>xy</sub><sup>-</sup>|0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

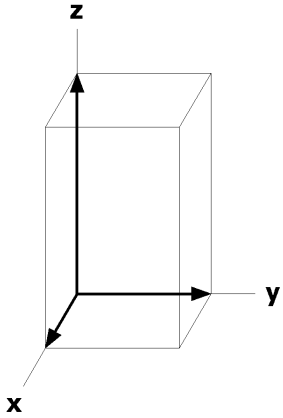
		Coordinates			
		Multiplicity, Wyckoff letter, Site Symmetry.			
8	g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
		(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z$ [ $\bar{v},u,\bar{w}$ ]		
		(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]		
		(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]		
4	f ..2'	x,x,1/2 [u, $\bar{u}$ ,w]	$\bar{x},\bar{x},1/2$ [ $\bar{u},u,w$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]	$x+1/2,\bar{x}+1/2,1/2$ [u,u, $\bar{w}$ ]
4	e ..2'	x,x,0 [u, $\bar{u}$ ,w]	$\bar{x},\bar{x},0$ [ $\bar{u},u,w$ ]	$\bar{x}+1/2,x+1/2,0$ [ $\bar{u},\bar{u},\bar{w}$ ]	$x+1/2,\bar{x}+1/2,0$ [u,u, $\bar{w}$ ]
4	d 2..	0,0,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]
2	c 4'..	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
2	b 2.2'2'	0,0,1/2 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		
2	a 2.2'2'	0,0,0 [0,0,w]	1/2,1/2,0 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p4'g'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



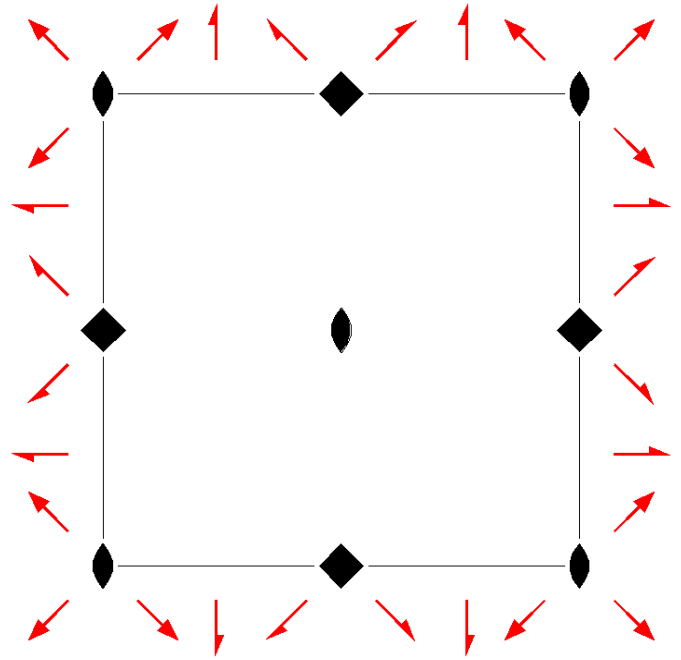
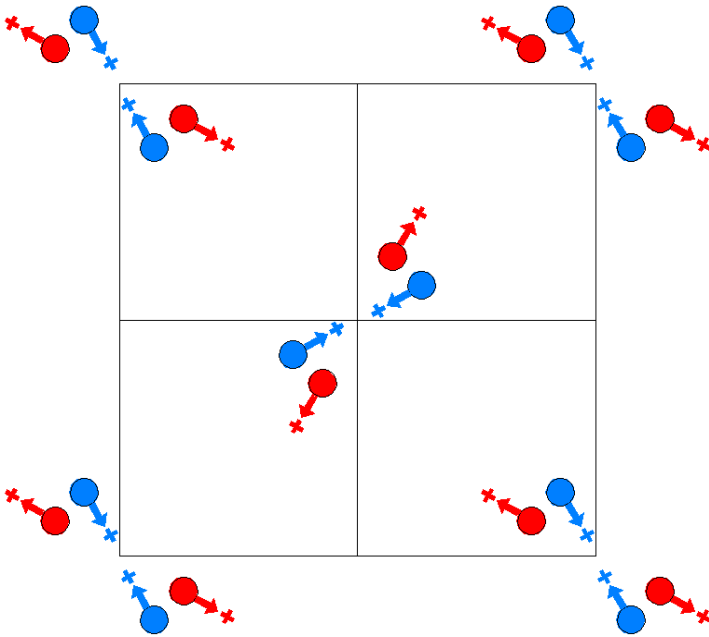
P42<sub>1</sub>'2'

90.4.760

42'2'

P42<sub>1</sub>'2'

Tetragonal



Origin at 22'2' at 212'

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                   | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0) | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0) |
| (5) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (6) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                 | (8) 2' x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)'                             |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

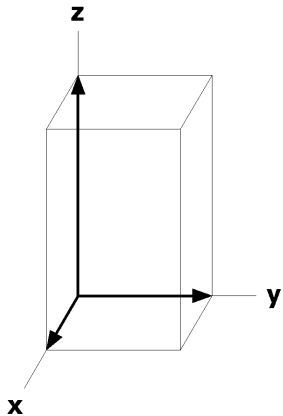
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
		(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z$ [ $v,\bar{u},w$ ]		
		(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]		
		(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]		
4	f ..2'	x,x,1/2 [u, $\bar{u}$ ,w]	$\bar{x},\bar{x},1/2$ [ $\bar{u},u,w$ ]	$\bar{x}+1/2,x+1/2,1/2$ [u,u,w]	$x+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},w$ ]
4	e ..2'	x,x,0 [u, $\bar{u}$ ,w]	$\bar{x},\bar{x},0$ [ $\bar{u},u,w$ ]	$\bar{x}+1/2,x+1/2,0$ [u,u,w]	$x+1/2,\bar{x}+1/2,0$ [ $\bar{u},\bar{u},w$ ]
4	d 2..	0,0,z [0,0,w]	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]
2	c 4..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]		
2	b 2.2'2'	0,0,1/2 [0,0,w]	1/2,1/2,1/2 [0,0,w]		
2	a 2.2'2'	0,0,0 [0,0,w]	1/2,1/2,0 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p4gm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



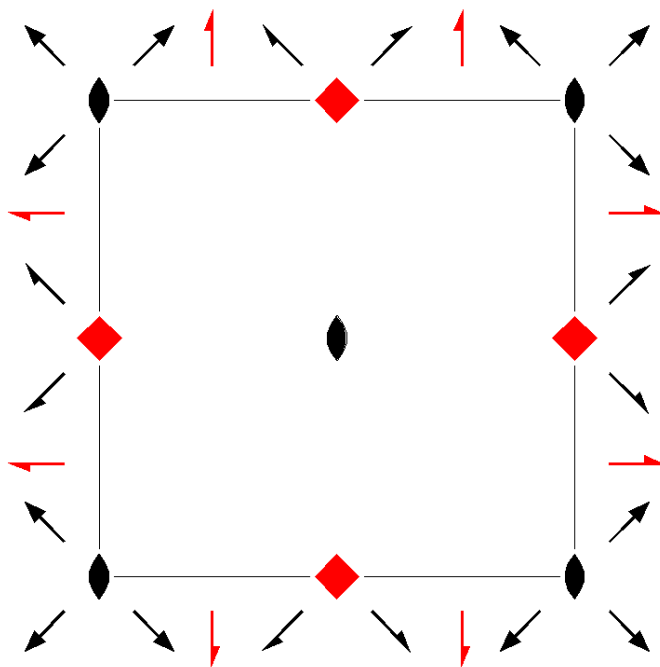
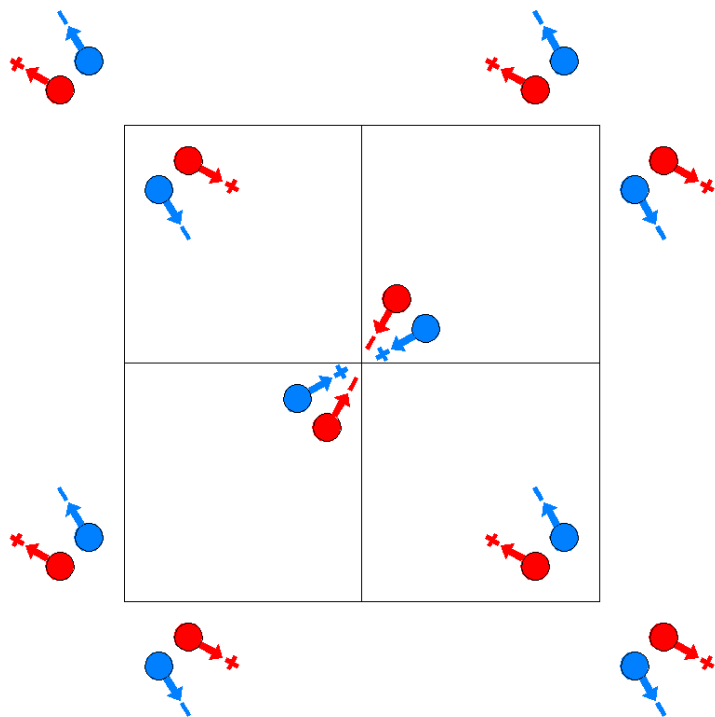
P4'2<sub>1</sub>'2

90.5.761

4'2'2

P4'2<sub>1</sub>'2

Tetragonal



Origin at 222 at 212

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 4<sup>+</sup> 0,1/2,z  
(4<sub>z</sub>|1/2,1/2,0)'

(4) 4<sup>-</sup> 1/2,0,z  
(4<sub>z</sub><sup>-1</sup>|1/2,1/2,0)'

(5) 2' (0,1/2,0) 1/4,y,0  
(2<sub>y</sub>|1/2,1/2,0)'

(6) 2' (1/2,0,0) x,1/4,0  
(2<sub>x</sub>|1/2,1/2,0)'

(7) 2 x,x,0  
(2<sub>xy</sub>|0,0,0)

(8) 2 x,x̄,0  
(2<sub>xy</sub><sup>-</sup>|0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

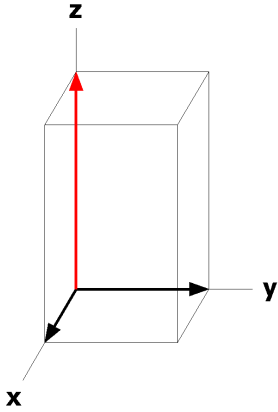
		Coordinates			
		Multiplicity, Wyckoff letter, Site Symmetry.			
8	g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
		(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z$ [ $\bar{v},u,\bar{w}$ ]		
		(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]		
		(7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
4	f ..2	x,x,1/2 [u,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $u,\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},u,0$ ]
4	e ..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,0$ [ $u,\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,0$ [ $\bar{u},u,0$ ]
4	d 2..	0,0,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
2	c 4'..	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
2	b 2.22	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a 2.22	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p4'gm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



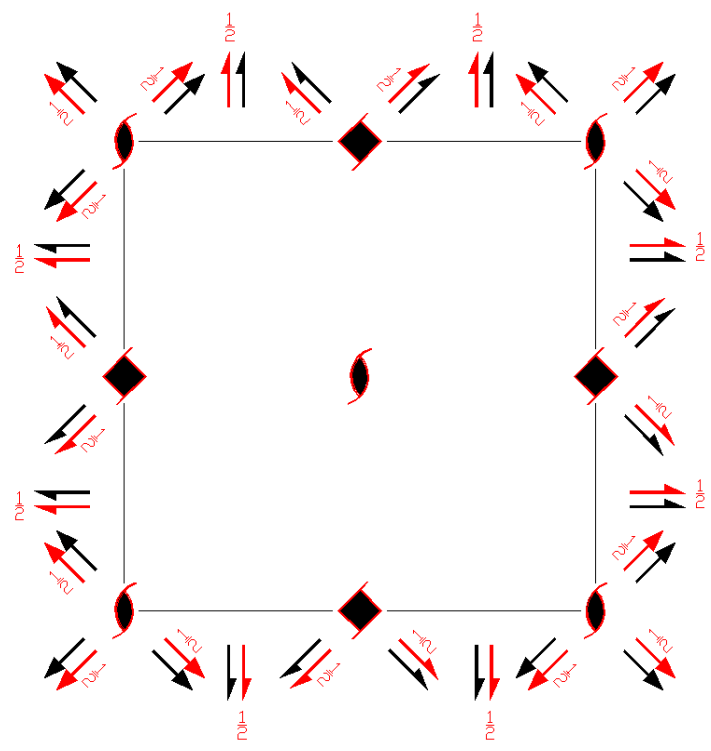
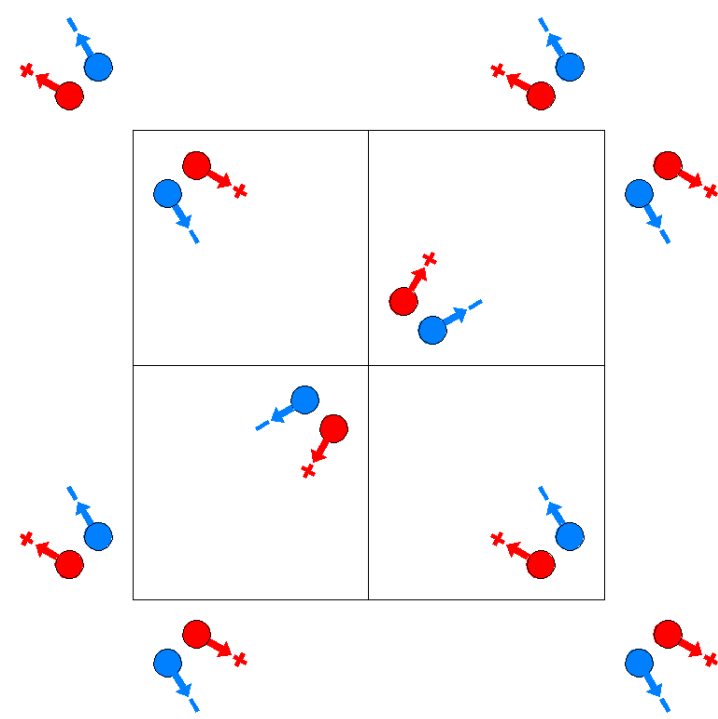
$P_{2c} 42_1 2$

4221'

Tetragonal

90.6.762

$P_{2c} 42_1 2$



Origin at 222 at 212

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0) | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0) |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                   | (8) 2 x,x̄,0<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,0)                  |

For (0,0,1)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (0,0,1)<br>(1 0,0,1)'                               | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)'           | (3) 4 <sup>+</sup> ' (0,0,1) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1)' | (4) 4 <sup>-</sup> ' (0,0,1) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1)' |
| (5) 2' (0,1/2,0) 1/4,y,1/2<br>(2 <sub>y</sub>  1/2,1/2,1)' | (6) 2' (1/2,0,0) x,1/4,1/2<br>(2 <sub>x</sub>  1/2,1/2,1)' | (7) 2' x,x,1/2<br>(2 <sub>xy</sub>  0,0,1)'                          | (8) 2' x,x̄,1/2<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,1)'                         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

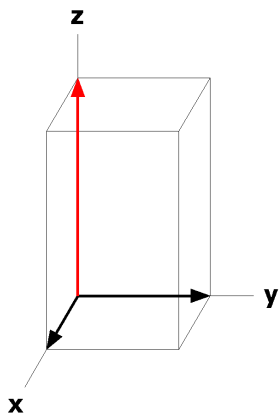
				Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.					
				(0,0,0) +	(0,0,1)' +
16	g 1	(1) x,y,z [u,v,w]		(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	
		(3) $\bar{y}+1/2, x+1/2, z$ [ $\bar{v}, u, w$ ]		(4) $y+1/2, \bar{x}+1/2, z$ [ $v, \bar{u}, w$ ]	
		(5) $\bar{x}+1/2, y+1/2, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]		(6) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]	
		(7) $y, x, \bar{z}$ [ $v, u, \bar{w}$ ]		(8) $\bar{y}, \bar{x}, \bar{z}$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	
8	f ..2'	x,x,1/2 [u, $\bar{u}$ ,w]	$\bar{x}, \bar{x}, 1/2$ [ $\bar{u}, u, w$ ]	$\bar{x}+1/2, x+1/2, 1/2$ [u,u,w]	$x+1/2, \bar{x}+1/2, 1/2$ [ $\bar{u}, \bar{u}, w$ ]
8	e ..2	x,x,0 [u,u,0]	$\bar{x}, \bar{x}, 0$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}+1/2, x+1/2, 0$ [ $\bar{u}, u, 0$ ]	$x+1/2, \bar{x}+1/2, 0$ [u, $\bar{u}$ ,0]
8	d 2..	0,0,z [0,0,w]	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4	c 4..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4	b 2.2'2'	0,0,1/2 [0,0,w]	1/2,1/2,1/2 [0,0,w]		
4	a 2.22	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [1,1,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



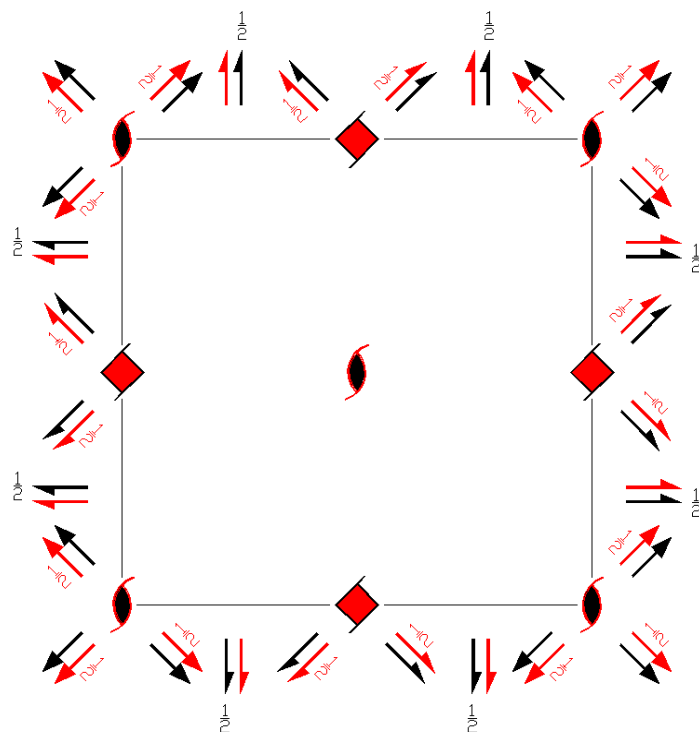
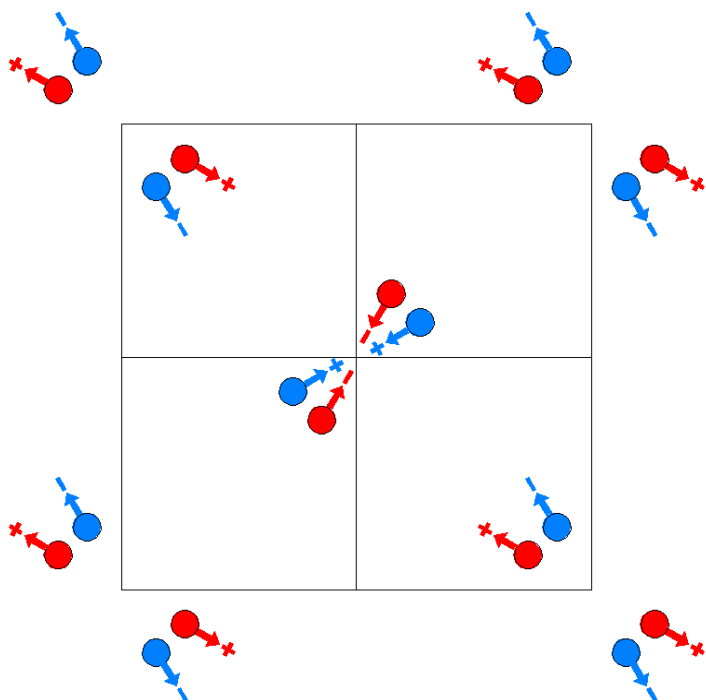
$P_{2c} 4'2_1'2$

4221'

Tetragonal

90.7.763

$P_{2c} 4'2_1'2$



Origin at 222 at 212

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)                    | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0)' | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)' |
| (5) 2 <sub>y</sub> ' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (6) 2 <sub>x</sub> ' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' | (7) 2 <sub>xy</sub> x,x,0<br>(2 <sub>xy</sub>  0,0,0)      | (8) 2 <sub>xy</sub> ' x,x̄,0<br>(2 <sub>xy</sub> ' 0,0,0)                |

For (0,0,1)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) t' (0,0,1)<br>(1 0,0,1)'  | (2) 2 <sub>z</sub> ' (0,0,1) 0,0,z<br>(2 <sub>z</sub> ' 0,0,1)'       | (3) 4 <sup>+</sup> (0,0,1) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1) | (4) 4 <sup>-</sup> (0,0,1) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1) |
| (5) 2 <sub>y</sub> (0,1/2,0) 1/4,y,1/2<br>(2 <sub>y</sub>  1/2,1/2,1) | (6) 2 <sub>x</sub> (1/2,0,0) x,1/4,1/2<br>(2 <sub>x</sub>  1/2,1/2,1) | (7) 2 <sub>xy</sub> ' x,x,1/2<br>(2 <sub>xy</sub> ' 0,0,1)'       | (8) 2 <sub>xy</sub> ' x,x̄,1/2<br>(2 <sub>xy</sub> ' 0,0,1)'                    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

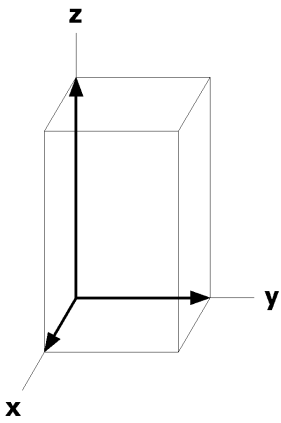
				Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.					
				(0,0,0) +	(0,0,1)' +
16	g 1	(1) x,y,z [u,v,w]		(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	
		(3) $\bar{y}+1/2, x+1/2, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		(4) $y+1/2, \bar{x}+1/2, z$ [ $\bar{v}, u, \bar{w}$ ]	
		(5) $\bar{x}+1/2, y+1/2, \bar{z}$ [ $u, \bar{v}, w$ ]		(6) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $\bar{u}, v, w$ ]	
		(7) $y, x, \bar{z}$ [ $v, u, \bar{w}$ ]		(8) $\bar{y}, \bar{x}, \bar{z}$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	
8	f ..2'	x,x,1/2 [u, $\bar{u}$ ,w]	$\bar{x}, \bar{x}, 1/2$ [ $\bar{u}, u, w$ ]	$\bar{x}+1/2, x+1/2, 1/2$ [ $\bar{u}, \bar{u}, \bar{w}$ ]	$x+1/2, \bar{x}+1/2, 1/2$ [ $u, u, \bar{w}$ ]
8	e ..2	x,x,0 [u,u,0]	$\bar{x}, \bar{x}, 0$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}+1/2, x+1/2, 0$ [ $u, \bar{u}, 0$ ]	$x+1/2, \bar{x}+1/2, 0$ [ $\bar{u}, u, 0$ ]
8	d 2..	0,0,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4	c 4'..	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
4	b 2.2'2'	0,0,1/2 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		
4	a 2.22	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

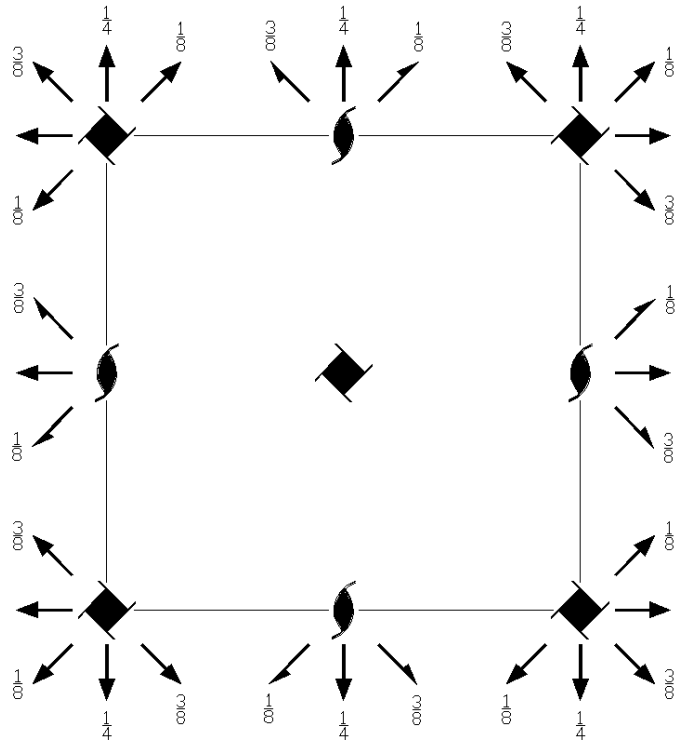
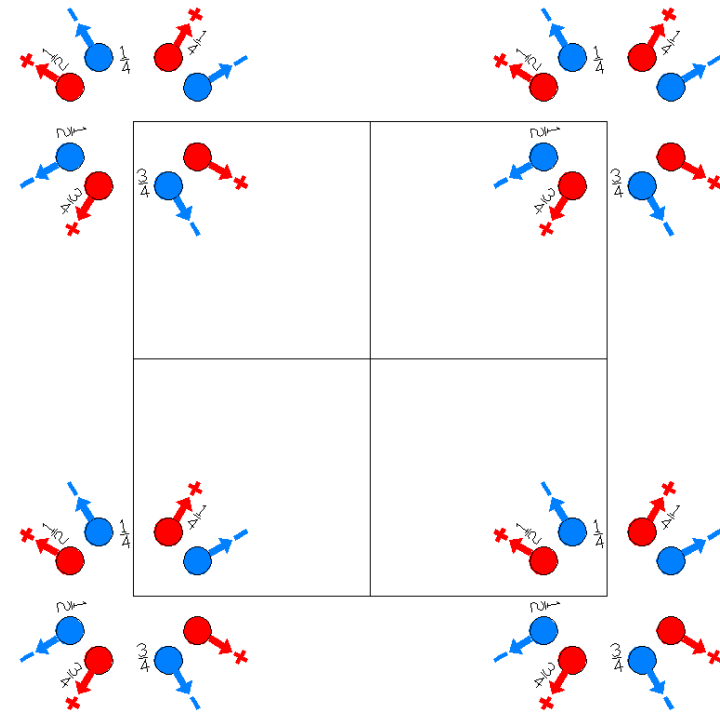
Along [1,1,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



P4<sub>1</sub>22  
91.1.764

422  
P4<sub>1</sub>22

Tetragonal



Origin on 2 [0 1 0] at 4<sub>1</sub> (1,2) 1

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

### Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 4 <sup>+</sup> (0,0,1/4) 0,0,z<br>(4 <sub>z</sub>  0,0,1/4) | (4) 4 <sup>-</sup> (0,0,3/4) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,3/4) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)         | (7) 2 x,x,3/8<br>(2 <sub>xy</sub>  0,0,3/4)                     | (8) 2 x, $\bar{x}$ ,1/8<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,1/4)            |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

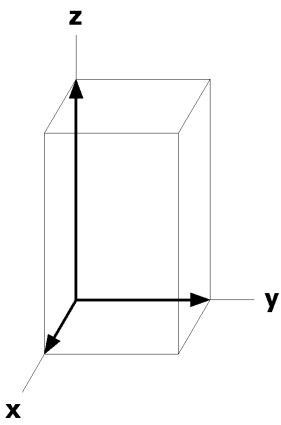
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	d 1	(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z+1/4$ [ $\bar{v}, u, w$ ]	(4) $y, \bar{x}, z+3/4$ [ $v, \bar{u}, w$ ]
		(5) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(6) $x, \bar{y}, \bar{z}+1/2$ [ $u, \bar{v}, \bar{w}$ ]	(7) $y, x, \bar{z}+3/4$ [ $v, u, \bar{w}$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+1/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]
4	c ..2	$x, x, 3/8$ [ $u, u, 0$ ]	$\bar{x}, \bar{x}, 7/8$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}, x, 5/8$ [ $\bar{u}, u, 0$ ]	$x, \bar{x}, 1/8$ [ $u, \bar{u}, 0$ ]
4	b .2.	$1/2, y, 0$ [ $0, v, 0$ ]	$1/2, \bar{y}, 1/2$ [ $0, \bar{v}, 0$ ]	$\bar{y}, 1/2, 1/4$ [ $\bar{v}, 0, 0$ ]	$y, 1/2, 3/4$ [ $v, 0, 0$ ]
4	a .2.	$0, y, 0$ [ $0, v, 0$ ]	$0, \bar{y}, 1/2$ [ $0, \bar{v}, 0$ ]	$\bar{y}, 0, 1/4$ [ $\bar{v}, 0, 0$ ]	$y, 0, 3/4$ [ $v, 0, 0$ ]

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'g'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $x,0,1/4$

Along  $[1,1,0]$   $p2m'g'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,3/8$

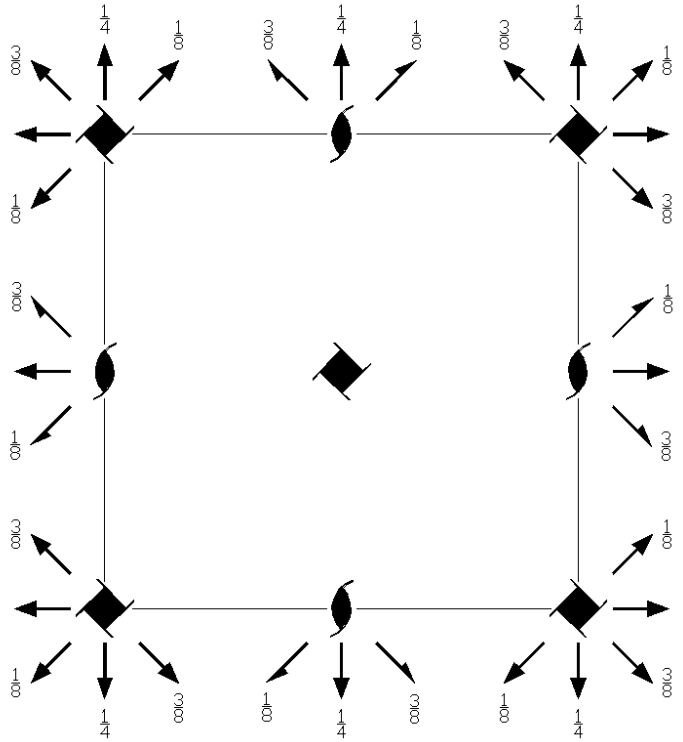
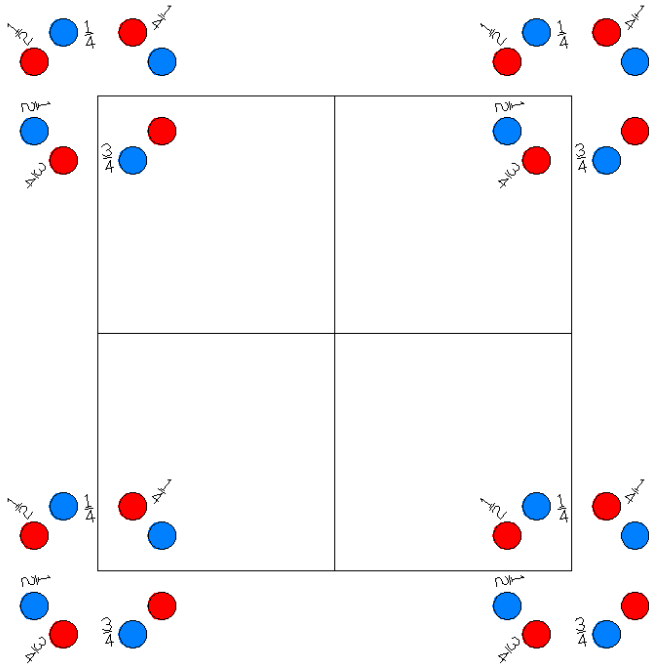


P4<sub>1</sub>221'  
91.2.765

4221'  
P4<sub>1</sub>221'

Tetragonal

1'



Origin on 21' [0 1 0] at 4, (1,2) 11'

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

Symmetry Operations

For 1 + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 4 <sup>+</sup> (0,0,1/4) 0,0,z<br>(4 <sub>z</sub>  0,0,1/4) | (4) 4 <sup>-</sup> (0,0,3/4) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,3/4) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)         | (7) 2 x,x,3/8<br>(2 <sub>xy</sub>  0,0,3/4)                     | (8) 2 x,x̄,1/8<br>(2 <sub>xy</sub>  0,0,1/4)                                  |

For 1' + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1'<br>(1 0,0,0)'                     | (2) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)' | (3) 4 <sup>+</sup> ' (0,0,1/4) 0,0,z<br>(4 <sub>z</sub>  0,0,1/4)' | (4) 4 <sup>-</sup> ' (0,0,3/4) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,3/4)' |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'         | (7) 2' x,x,3/8<br>(2 <sub>xy</sub>  0,0,3/4)'                      | (8) 2' x,x̄,1/8<br>(2 <sub>xy</sub>  0,0,1/4)'                                   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

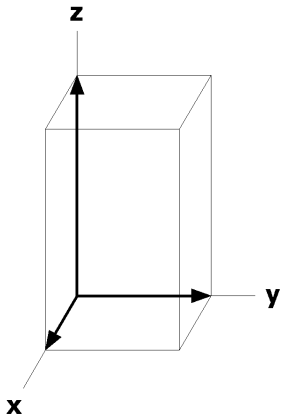
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +		1' +	
8 d 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z+1/2$ [0,0,0]	(3) $\bar{y},x,z+1/4$ [0,0,0]	(4) $y,\bar{x},z+3/4$ [0,0,0]
	(5) $\bar{x},y,\bar{z}$ [0,0,0]	(6) $x,\bar{y},\bar{z}+1/2$ [0,0,0]	(7) $y,x,\bar{z}+3/4$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}+1/4$ [0,0,0]
4 c ..21'	x,x,3/8 [0,0,0]	$\bar{x},\bar{x},7/8$ [0,0,0]	$\bar{x},x,5/8$ [0,0,0]	x, $\bar{x},1/8$ [0,0,0]
4 b .2.1'	1/2,y,0 [0,0,0]	1/2, $\bar{y},1/2$ [0,0,0]	$\bar{y},1/2,1/4$ [0,0,0]	y,1/2,3/4 [0,0,0]
4 a .2.1'	0,y,0 [0,0,0]	0, $\bar{y},1/2$ [0,0,0]	$\bar{y},0,1/4$ [0,0,0]	y,0,3/4 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,1/4

Along [1,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,3/8



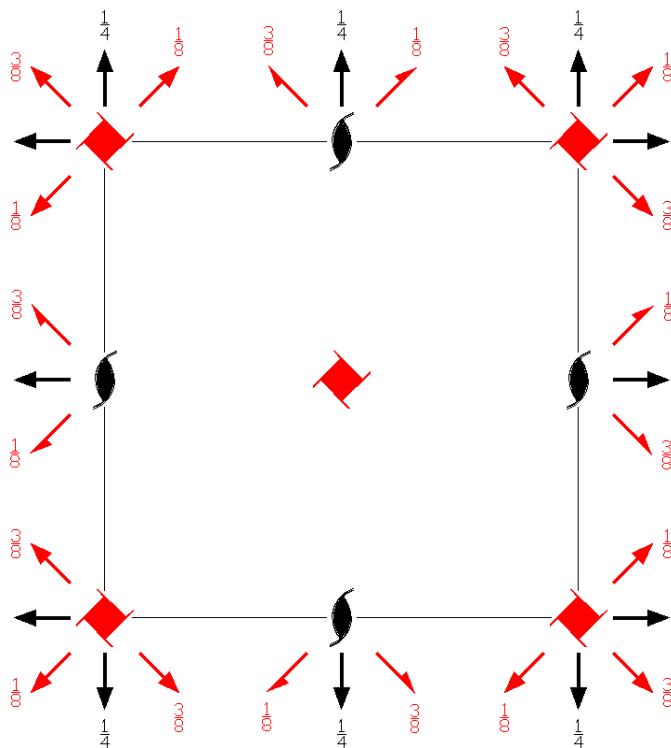
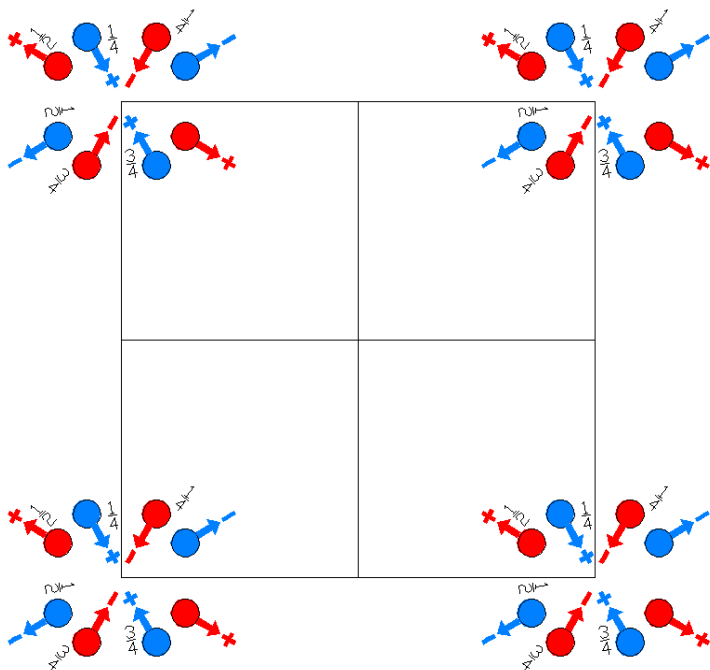
P4<sub>1</sub>'22'

91.3.766

4'22'

P4<sub>1</sub>'22'

Tetragonal



Origin on 2 [0 1 0] at 4<sub>1</sub>' (1,2) 1

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 4 <sup>+</sup> ' (0,0,1/4) 0,0,z<br>(4 <sub>z</sub>  0,0,1/4)' | (4) 4 <sup>-</sup> ' (0,0,3/4) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,3/4)' |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)         | (7) 2' x,x,3/8<br>(2 <sub>xy</sub>  0,0,3/4)'                      | (8) 2' x,x̄,1/8<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,1/4)'                      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

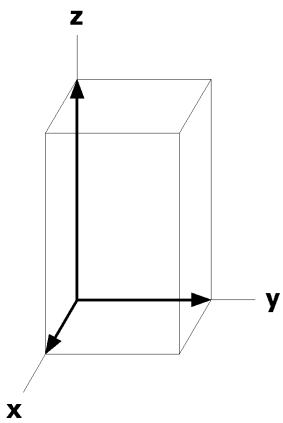
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	d 1	(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z+1/4$ [ $v, \bar{u}, \bar{w}$ ]	(4) $y, \bar{x}, z+3/4$ [ $\bar{v}, u, \bar{w}$ ]
		(5) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(6) $x, \bar{y}, \bar{z}+1/2$ [ $u, \bar{v}, \bar{w}$ ]	(7) $y, x, \bar{z}+3/4$ [ $\bar{v}, \bar{u}, w$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+1/4$ [ $v, u, w$ ]
4	c ..2'	$x, x, 3/8$ [ $u, \bar{u}, w$ ]	$\bar{x}, \bar{x}, 7/8$ [ $\bar{u}, u, w$ ]	$\bar{x}, x, 5/8$ [ $\bar{u}, \bar{u}, \bar{w}$ ]	$x, \bar{x}, 1/8$ [ $u, u, \bar{w}$ ]
4	b .2.	$1/2, y, 0$ [ $0, v, 0$ ]	$1/2, \bar{y}, 1/2$ [ $0, \bar{v}, 0$ ]	$\bar{y}, 1/2, 1/4$ [ $v, 0, 0$ ]	$y, 1/2, 3/4$ [ $\bar{v}, 0, 0$ ]
4	a .2.	$0, y, 0$ [ $0, v, 0$ ]	$0, \bar{y}, 1/2$ [ $0, \bar{v}, 0$ ]	$\bar{y}, 0, 1/4$ [ $v, 0, 0$ ]	$y, 0, 3/4$ [ $\bar{v}, 0, 0$ ]

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4'mm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'g'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $x,0,1/4$

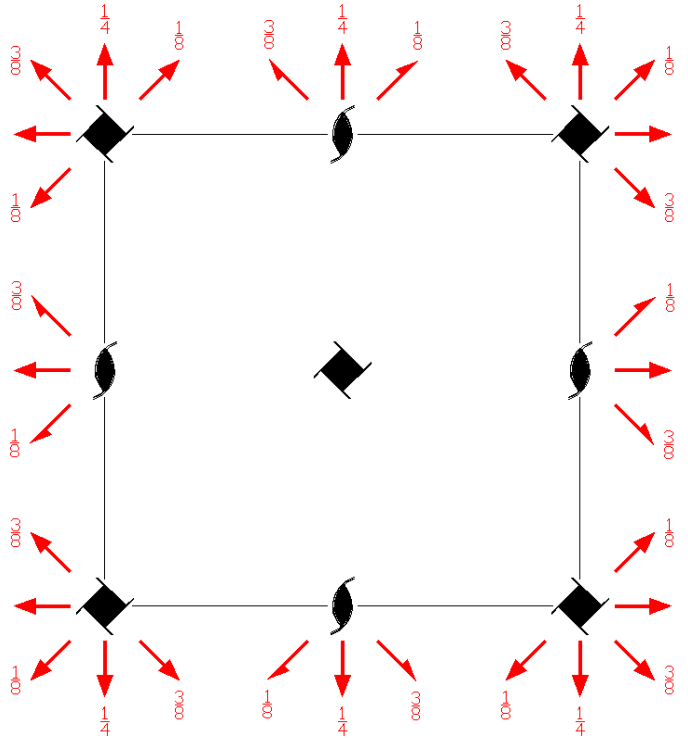
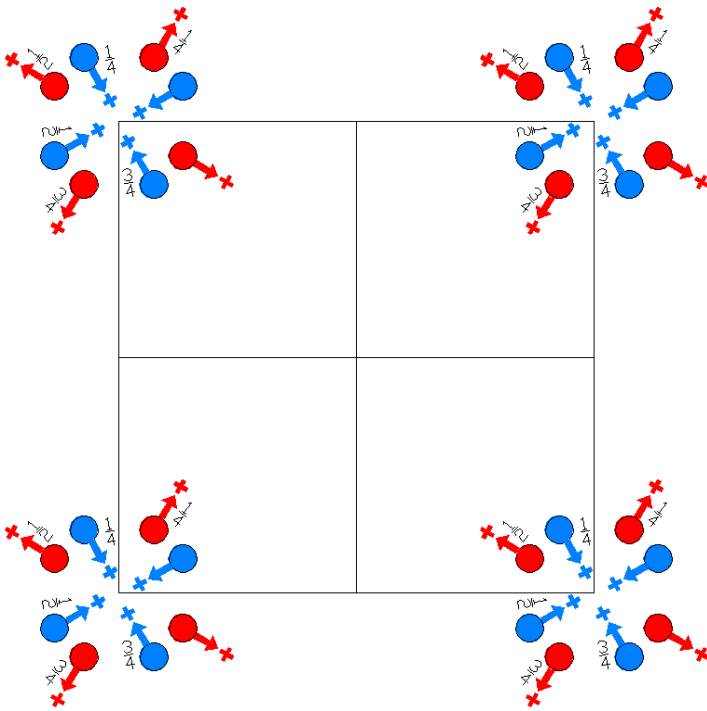
Along  $[1,1,0]$   $p2'mg'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,3/8$



P4<sub>1</sub>2'2'  
91.4.767

42'2'  
P4<sub>1</sub>2'2'

Tetragonal



Origin on 2' [0 1 0] at 4<sub>1</sub> (1,2') 1

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

### Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 4 <sup>+</sup> (0,0,1/4) 0,0,z<br>(4 <sub>z</sub>  0,0,1/4) | (4) 4 <sup>-</sup> (0,0,3/4) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,3/4) |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'       | (7) 2' x,x,3/8<br>(2 <sub>xy</sub>  0,0,3/4)'                   | (8) 2' x,x̄,1/8<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,1/4)'                   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

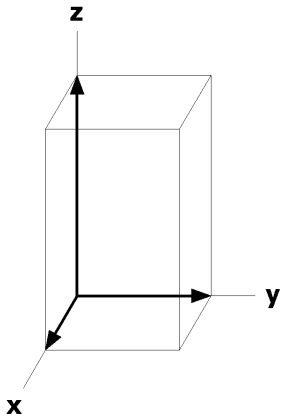
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	d 1	(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z+1/4$ [ $\bar{v}, u, w$ ]	(4) $y, \bar{x}, z+3/4$ [ $v, \bar{u}, w$ ]
		(5) $\bar{x}, y, \bar{z}$ [ $u, \bar{v}, w$ ]	(6) $x, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]	(7) $y, x, \bar{z}+3/4$ [ $\bar{v}, \bar{u}, w$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+1/4$ [ $v, u, w$ ]
4	c ..2'	$x, x, 3/8$ [ $u, \bar{u}, w$ ]	$\bar{x}, \bar{x}, 7/8$ [ $\bar{u}, u, w$ ]	$\bar{x}, x, 5/8$ [ $u, u, w$ ]	$x, \bar{x}, 1/8$ [ $\bar{u}, \bar{u}, w$ ]
4	b .2'	$1/2, y, 0$ [ $u, 0, w$ ]	$1/2, \bar{y}, 1/2$ [ $\bar{u}, 0, w$ ]	$\bar{y}, 1/2, 1/4$ [ $0, u, w$ ]	$y, 1/2, 3/4$ [ $0, \bar{u}, w$ ]
4	a .2'	$0, y, 0$ [ $u, 0, w$ ]	$0, \bar{y}, 1/2$ [ $\bar{u}, 0, w$ ]	$\bar{y}, 0, 1/4$ [ $0, u, w$ ]	$y, 0, 3/4$ [ $0, \bar{u}, w$ ]

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2'mg'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $x,0,1/4$

Along  $[1,1,0]$   $p2'mg'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,3/8$



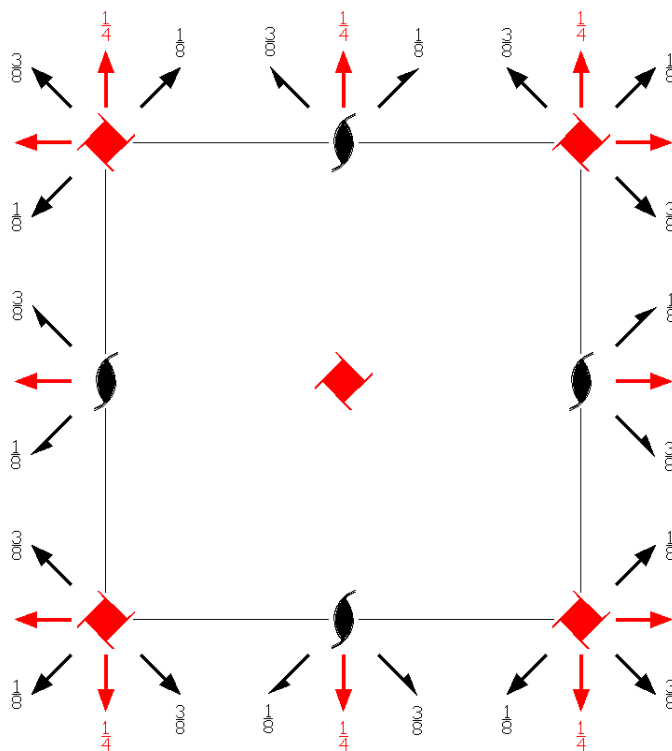
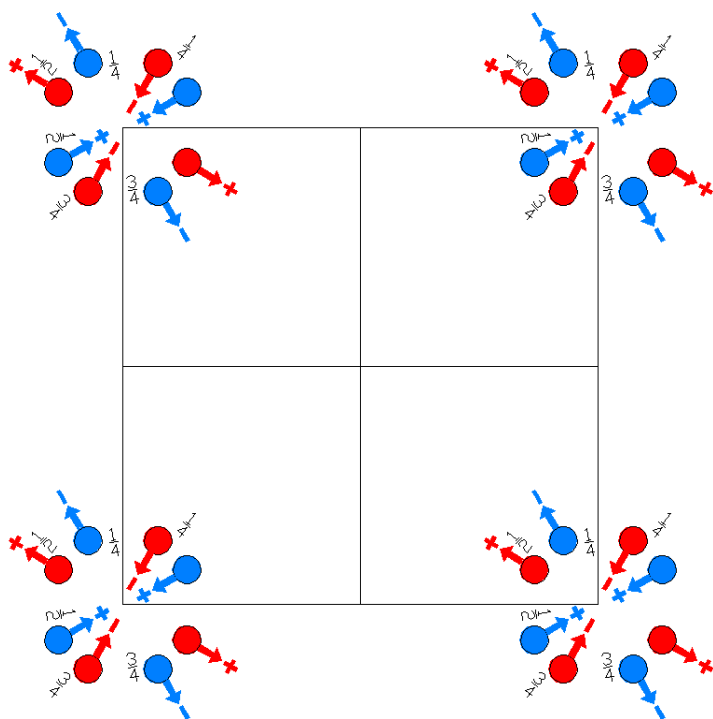
$P4_1'2'2'$

91.5.768

$4'2'2'$

$P4_1'2'2'$

Tetragonal



Origin on  $2'$   $[0\ 1\ 0]$  at  $4_1'$   $(1,2)'\ 1$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/8$

**Symmetry Operations**

- |                                    |  |   |  |
|------------------------------------|--|---|--|
| (1) $1$<br>$(1 0,0,0)$             | (2) $2$ $(0,0,1/2)$ $0,0,z$<br>$(2_z 0,0,1/2)$ | (3) $4^+$ $(0,0,1/4)$ $0,0,z$<br>$(4_z 0,0,1/4)'$ | (4) $4^-$ $(0,0,3/4)$ $0,0,z$<br>$(4_z^{-1} 0,0,3/4)'$ |
| (5) $2'$ $0,y,0$<br>$(2_y 0,0,0)'$ | (6) $2'$ $x,0,1/4$<br>$(2_x 0,0,1/2)'$         | (7) $2$ $x,x,3/8$<br>$(2_{xy} 0,0,3/4)$           | (8) $2$ $x,\bar{x},1/8$<br>$(2_{\bar{xy}} 0,0,1/4)$    |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

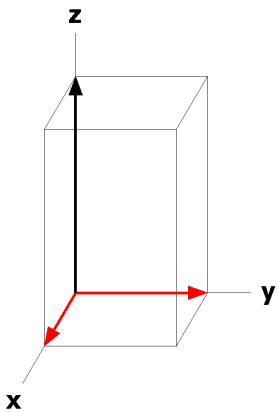
		Coordinates				
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	d	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z+1/4$ [ $v, \bar{u}, \bar{w}$ ]	(4) $y, \bar{x}, z+3/4$ [ $\bar{v}, u, \bar{w}$ ]
			(5) $\bar{x}, y, \bar{z}$ [ $u, \bar{v}, w$ ]	(6) $x, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]	(7) $y, x, \bar{z}+3/4$ [ $v, u, \bar{w}$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+1/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]
4	c	.2	$x, x, 3/8$ [u,u,0]	$\bar{x}, \bar{x}, 7/8$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}, x, 5/8$ [u, $\bar{u}$ ,0]	$x, \bar{x}, 1/8$ [ $\bar{u}, u, 0$ ]
4	b	.2'	$1/2, y, 0$ [u,0,w]	$1/2, \bar{y}, 1/2$ [ $\bar{u}, 0, w$ ]	$\bar{y}, 1/2, 1/4$ [0, $\bar{u}, \bar{w}$ ]	$y, 1/2, 3/4$ [0,u, $\bar{w}$ ]
4	a	.2'	$0, y, 0$ [u,0,w]	$0, \bar{y}, 1/2$ [ $\bar{u}, 0, w$ ]	$\bar{y}, 0, 1/4$ [0, $\bar{u}, \bar{w}$ ]	$y, 0, 3/4$ [0,u, $\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,1/4

Along [1,1,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,3/8



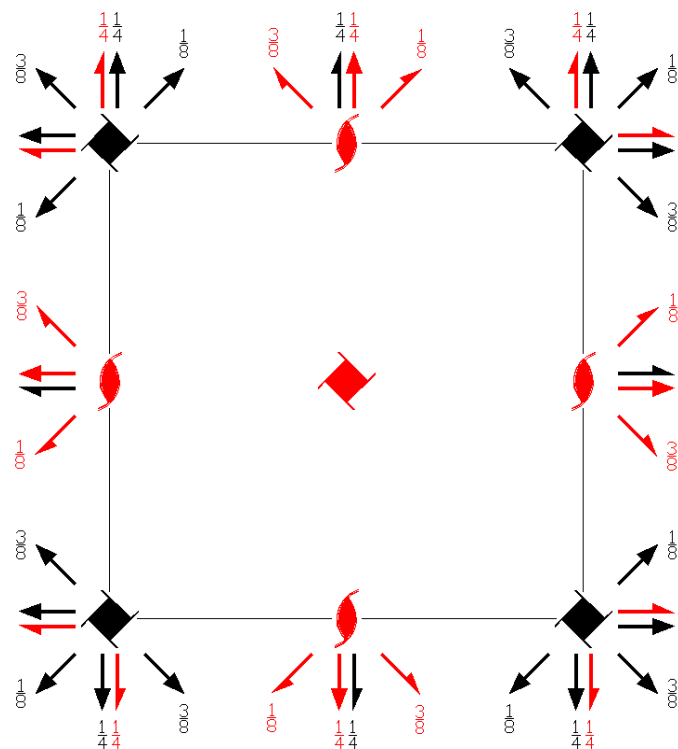
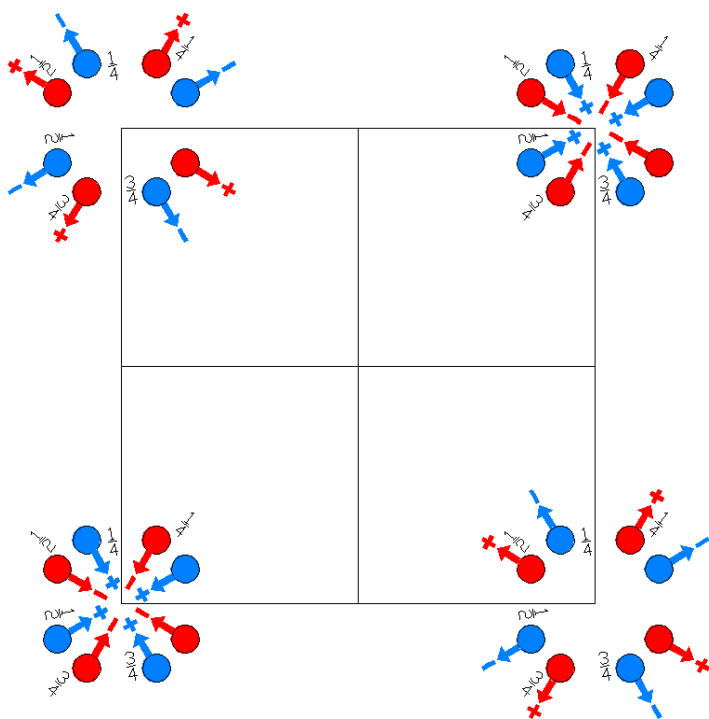
$P_P 4_1 22$

91.6.769

4221'

$P_P 4_1 22$

Tetragonal



Origin on 2 [0 1 0] at  $4_1 (1,2) 1$

Asymmetric unit  $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq 1/8$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 4 <sup>+</sup> (0,0,1/4) 0,0,z<br>(4 <sub>z</sub>  0,0,1/4) | (4) 4 <sup>-</sup> (0,0,3/4) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,3/4) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)         | (7) 2 x,x,3/8<br>(2 <sub>xy</sub>  0,0,3/4)                     | (8) 2 x, $\bar{x}$ ,1/8<br>(2 <sub>-xy</sub>  0,0,1/4)                        |

For (1,0,0)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) t' (1,0,0)<br>(1 1,0,0)'               | (2) 2' (0,0,1/2) 1/2,0,z<br>(2 <sub>z</sub>  1,0,1/2)' | (3) 4 <sup>+</sup> ' (0,0,1/4) 1/2,1/2,z<br>(4 <sub>z</sub>  1,0,1/4)' | (4) 4 <sup>-</sup> ' (0,0,3/4) 1/2,-1/2,z<br>(4 <sub>z</sub> <sup>-1</sup>  1,0,3/4)' |
| (5) 2' 1/2,y,0<br>(2 <sub>y</sub>  1,0,0)' | (6) 2' (1,0,0) x,0,1/4<br>(2 <sub>x</sub>  1,0,1/2)'   | (7) 2' (1/2,1/2,0) x+1/2,x,3/8<br>(2 <sub>xy</sub>  1,0,3/4)'          | (8) 2' (1/2,-1/2,0) x+1/2, $\bar{x}$ ,1/8<br>(2 <sub>-xy</sub>  1,0,1/4)'             |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

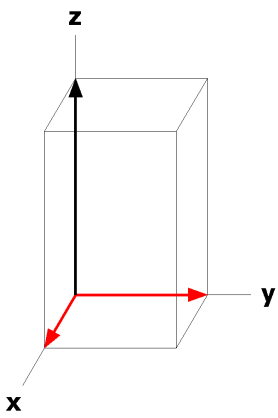
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z+1/4$ [ $\bar{v}, u, w$ ]	(4) $y, \bar{x}, z+3/4$ [ $v, \bar{u}, w$ ]
	(5) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(6) $x, \bar{y}, \bar{z}+1/2$ [ $u, \bar{v}, \bar{w}$ ]	(7) $y, x, \bar{z}+3/4$ [ $v, u, \bar{w}$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+1/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]
8 c ..2	x,x,3/8 [u,u,0]	$\bar{x}, \bar{x}, 7/8$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}, x, 5/8$ [ $\bar{u}, u, 0$ ]	x, $\bar{x}, 1/8$ [ $u, \bar{u}, 0$ ]
8 b .2'	1/2,y,0 [u,0,w]	1/2, $\bar{y}, 1/2$ [ $u, 0, \bar{w}$ ]	$\bar{y}, 1/2, 1/4$ [0,u,w]	y, 1/2, 3/4 [0,u, $\bar{w}$ ]
8 a .2.	0,y,0 [0,v,0]	0, $\bar{y}, 1/2$ [0, $\bar{v}, 0$ ]	$\bar{y}, 0, 1/4$ [ $\bar{v}, 0, 0$ ]	y, 0, 3/4 [v,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub>-4m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,1/4

Along [1,1,0] p<sub>2b</sub>-2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,3/8



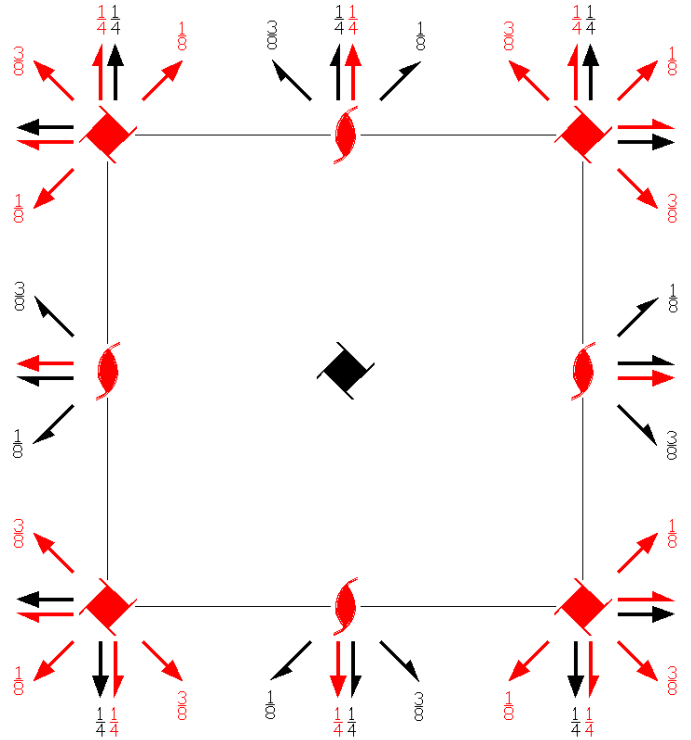
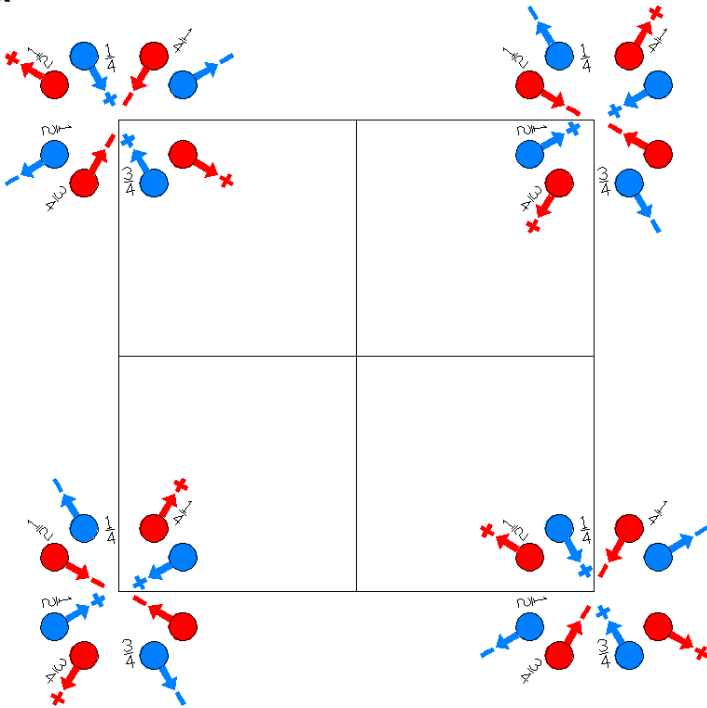
$P_P 4_1'22'$

91.7.770

4221'

$P_P 4_1'22'$

Tetragonal



Origin on  $2 [0\ 1\ 0]$  at  $4_1' (1,2)\ 1$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/8$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 4 <sup>+</sup> (0,0,1/4) 0,0,z<br>(4 <sub>z</sub>  0,0,1/4)' | (4) 4 <sup>-</sup> (0,0,3/4) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,3/4)' |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)         | (7) 2' x,x,3/8<br>(2 <sub>xy</sub>  0,0,3/4)'                    | (8) 2' x,x̄,1/8<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,1/4)'                    |

For  $(1,0,0)$ ' + set

- |  |  |   |  |
|--|--|---|--|
| (1) t' (1,0,0)<br>(1 1,0,0)'               | (2) 2' (0,0,1/2) 1/2,0,z<br>(2 <sub>z</sub>  1,0,1/2)' | (3) 4 <sup>+</sup> (0,0,1/4) 1/2,1/2,z<br>(4 <sub>z</sub>  1,0,1/4) | (4) 4 <sup>-</sup> (0,0,3/4) 1/2,-1/2,z<br>(4 <sub>z</sub> <sup>-1</sup>  1,0,3/4) |
| (5) 2' 1/2,y,0<br>(2 <sub>y</sub>  1,0,0)' | (6) 2' (1,0,0) x,0,1/4<br>(2 <sub>x</sub>  1,0,1/2)'   | (7) 2 (1/2,1/2,0) x+1/2,x,3/8<br>(2 <sub>xy</sub>  1,0,3/4)         | (8) 2 (1/2,-1/2,0) x+1/2,x̄,1/8<br>(2 <sub>xy</sub> <sup>-</sup>  1,0,1/4)         |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

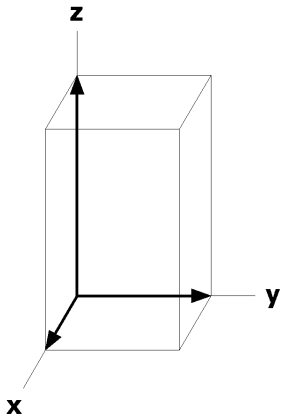
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +		(1,0,0)' +	
16	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z+1/4$ [ $v, \bar{u}, \bar{w}$ ]	(4) $y, \bar{x}, z+3/4$ [ $\bar{v}, u, \bar{w}$ ]
		(5) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(6) $x, \bar{y}, \bar{z}+1/2$ [ $u, \bar{v}, \bar{w}$ ]	(7) $y, x, \bar{z}+3/4$ [ $\bar{v}, \bar{u}, w$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+1/4$ [ $v, u, w$ ]
8	c ..2'	x,x,3/8 [u, $\bar{u}$ ,w]	$\bar{x}, \bar{x}, 7/8$ [ $\bar{u}, u, w$ ]	$\bar{x}, x, 5/8$ [ $\bar{u}, \bar{u}, \bar{w}$ ]	x, $\bar{x}$ ,1/8 [u,u, $\bar{w}$ ]
8	b .2'	1/2,y,0 [u,0,w]	1/2, $\bar{y}$ ,1/2 [u,0, $\bar{w}$ ]	$\bar{y}$ ,1/2,1/4 [0, $\bar{u}, \bar{w}$ ]	y,1/2,3/4 [0, $\bar{u}, w$ ]
8	a .2.	0,y,0 [0,v,0]	0, $\bar{y}$ ,1/2 [0, $\bar{v}$ ,0]	$\bar{y}$ ,0,1/4 [v,0,0]	y,0,3/4 [ $\bar{v}$ ,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,1/4

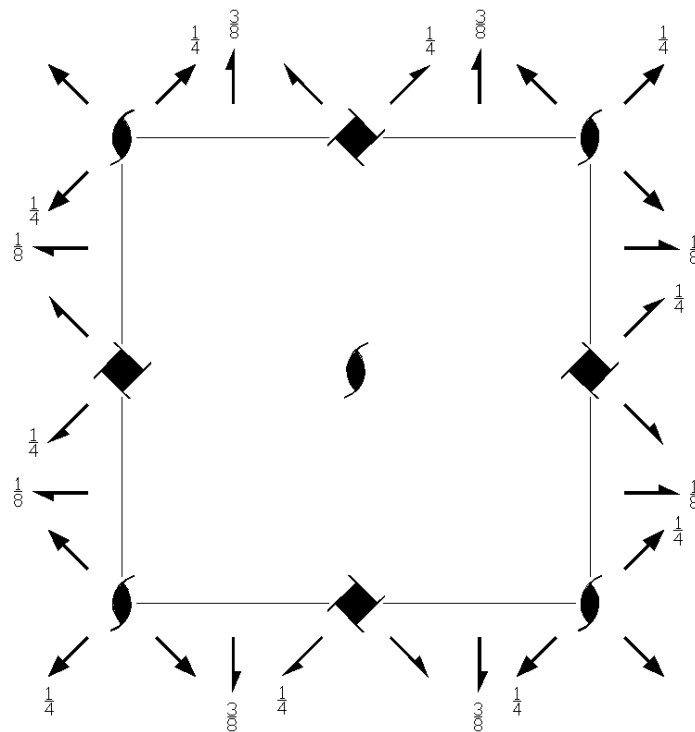
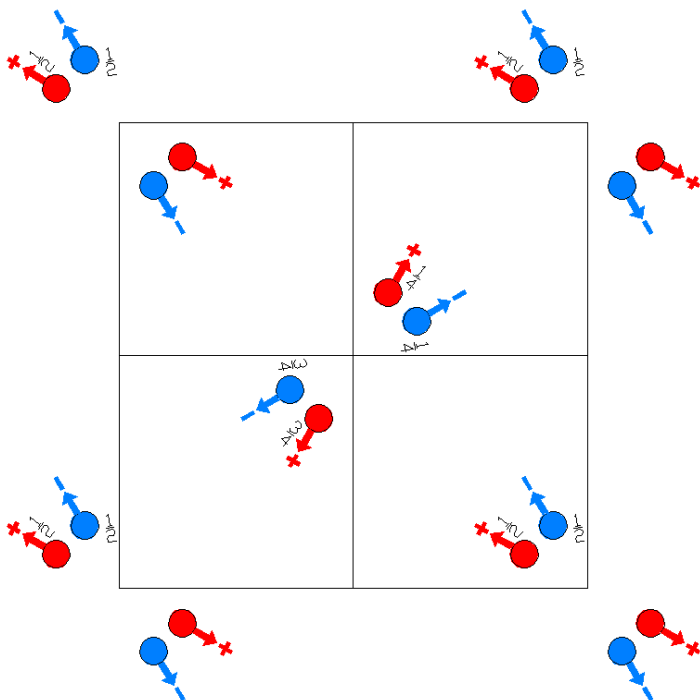
Along [1,1,0] p<sub>2b</sub>'2'mg'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,3/8



P4<sub>1</sub>2<sub>1</sub>2  
92.1.771

422  
P4<sub>1</sub>2<sub>1</sub>2

Tetragonal



Origin on 2 [1 1 0] at 2<sub>1</sub>(1,2)

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

### Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)         | (3) 4 <sup>+</sup> (0,0,1/4) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/4) | (4) 4 <sup>-</sup> (0,0,3/4) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,3/4) |
| (5) 2 (0,1/2,0) 1/4,y,1/8<br>(2 <sub>y</sub>  1/2,1/2,1/4) | (6) 2 (1/2,0,0) x,1/4,3/8<br>(2 <sub>x</sub>  1/2,1/2,3/4) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                               | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,1/2)                  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

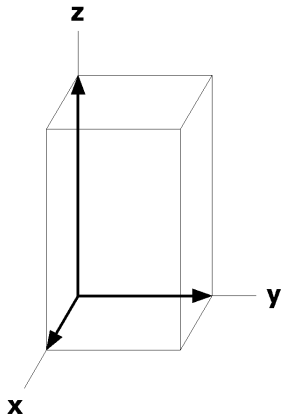
8	b	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}+1/2, x+1/2, z+1/4$ [ $\bar{v}, u, w$ ]	(4) $y+1/2, \bar{x}+1/2, z+3/4$ [v, $\bar{u}, w$ ]		
			(5) $\bar{x}+1/2, y+1/2, \bar{z}+1/4$ [ $\bar{u}, v, \bar{w}$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+3/4$ [u, $\bar{v}, \bar{w}$ ]		
			(7) $y, x, \bar{z}$ [v,u, $\bar{w}$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
4	a	.2	$x, x, 0$ [u,u,0]	$\bar{x}, \bar{x}, 1/2$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}+1/2, x+1/2, 1/4$ [ $\bar{u}, u, 0$ ]	$x+1/2, \bar{x}+1/2, 3/4$ [u, $\bar{u}, 0$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4g'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p2g'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,3/8

Along [1,1,0] p2'mg'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



P4<sub>1</sub>2<sub>1</sub>21'

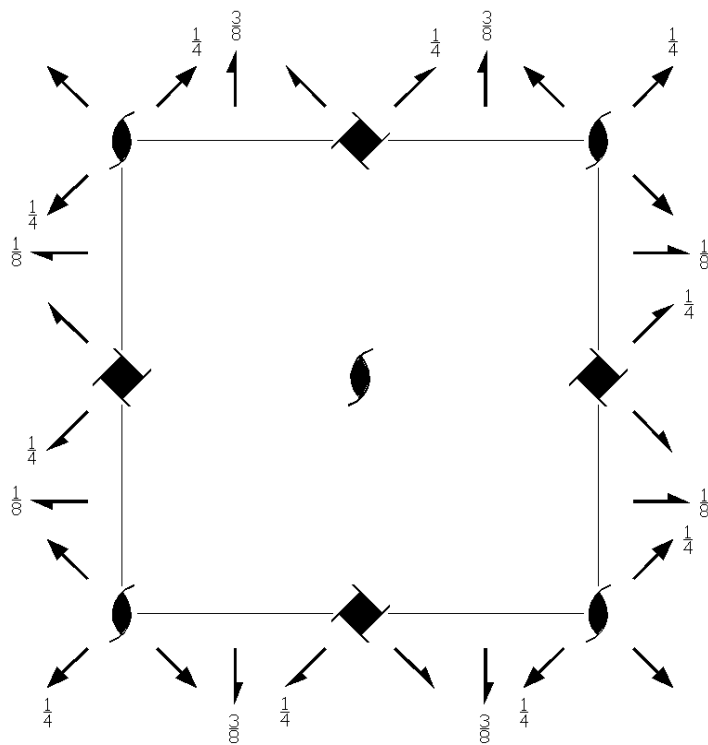
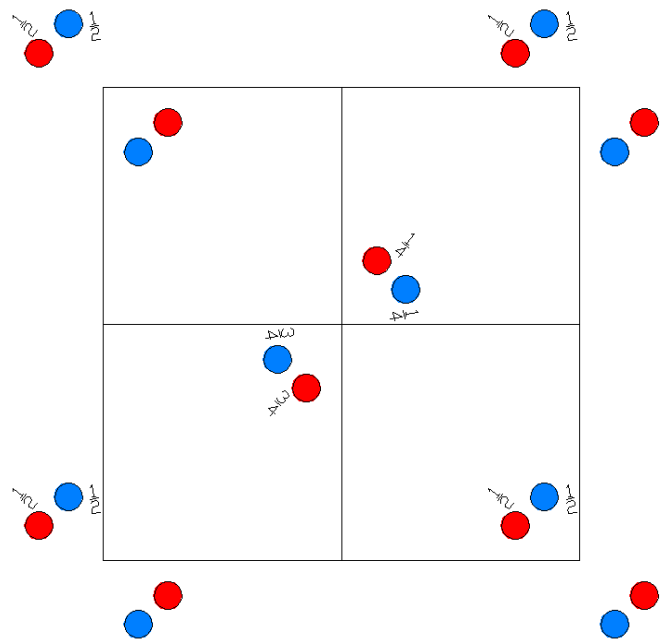
4221'

Tetragonal

92.2.772

P4<sub>1</sub>2<sub>1</sub>21'

1'



Origin on 2 [1 1 0]1' at 2<sub>1</sub>1(1,2)1'

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

### Symmetry Operations

For 1 + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)         | (3) 4 <sup>+</sup> (0,0,1/4) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/4) | (4) 4 <sup>-</sup> (0,0,3/4) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,3/4) |
| (5) 2 (0,1/2,0) 1/4,y,1/8<br>(2 <sub>y</sub>  1/2,1/2,1/4) | (6) 2 (1/2,0,0) x,1/4,3/8<br>(2 <sub>x</sub>  1/2,1/2,3/4) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                               | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                               |

For 1' + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1'<br>(1 0,0,0)'   | (2) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)'         | (3) 4 <sup>+</sup> ' (0,0,1/4) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/4)' | (4) 4 <sup>-</sup> ' (0,0,3/4) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,3/4)' |
| (5) 2' (0,1/2,0) 1/4,y,1/8<br>(2 <sub>y</sub>  1/2,1/2,1/4)' | (6) 2' (1/2,0,0) x,1/4,3/8<br>(2 <sub>x</sub>  1/2,1/2,3/4)' | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                                | (8) 2' x, $\bar{x}$ ,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                                |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

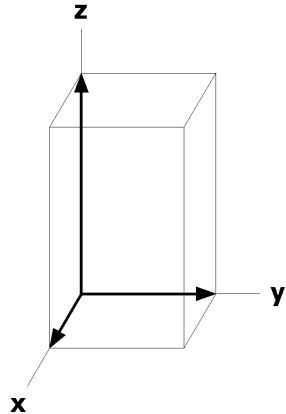
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
		1 +		1' +	
8	b 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z+1/2$ [0,0,0]		
		(3) $\bar{y}+1/2,x+1/2,z+1/4$ [0,0,0]	(4) $y+1/2,\bar{x}+1/2,z+3/4$ [0,0,0]		
		(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/4$ [0,0,0]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+3/4$ [0,0,0]		
		(7) y,x, $\bar{z}$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [0,0,0]		
4	a ..21'	x,x,0 [0,0,0]	$\bar{x},\bar{x},1/2$ [0,0,0]	$\bar{x}+1/2,x+1/2,1/4$ [0,0,0]	$x+1/2,\bar{x}+1/2,3/4$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p2gg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,3/8

Along [1,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



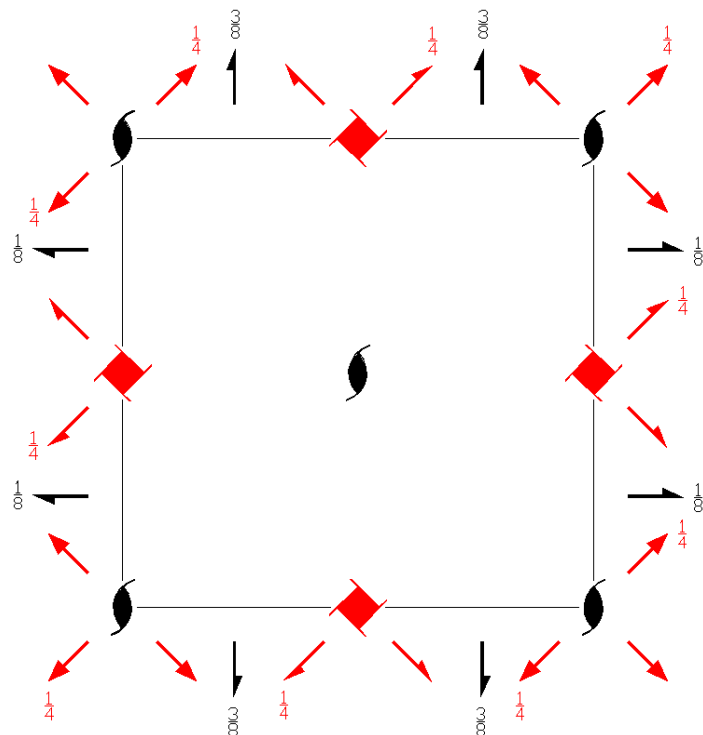
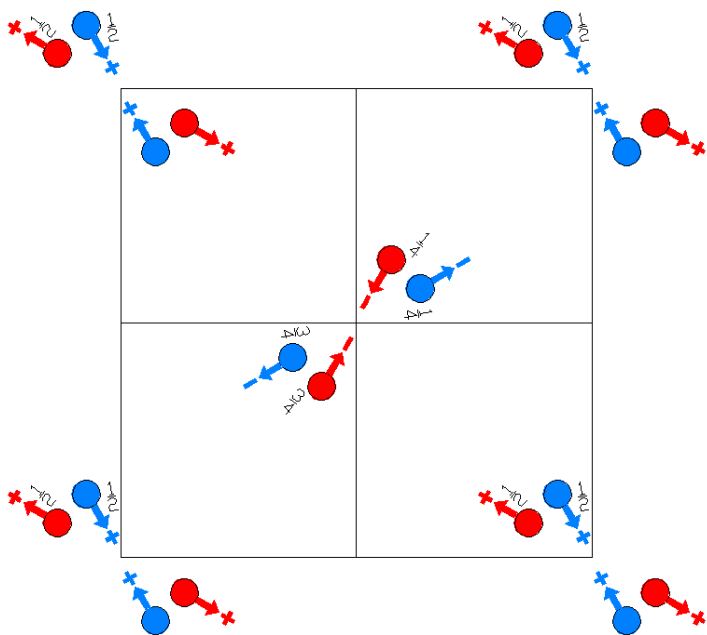
$P4_1'2_1'2'$

92.3.773

$4'22'$

$P4_1'2_1'2'$

Tetragonal



Origin on  $2'$   $[1\ 1\ 0]$  at  $2_1(1,2')$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/8$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)         | (3) 4 <sup>+</sup> (0,0,1/4) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/4)' | (4) 4 <sup>-</sup> (0,0,3/4) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,3/4)' |
| (5) 2 (0,1/2,0) 1/4,y,1/8<br>(2 <sub>y</sub>  1/2,1/2,1/4) | (6) 2 (1/2,0,0) x,1/4,3/8<br>(2 <sub>x</sub>  1/2,1/2,3/4) | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                              | (8) 2' x,x̄,1/4<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,1/2)'                          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

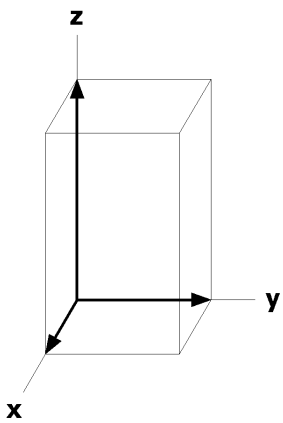
8	b	1	(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}+1/2, x+1/2, z+1/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(4) $y+1/2, \bar{x}+1/2, z+3/4$ [ $\bar{v}, u, \bar{w}$ ]		
			(5) $\bar{x}+1/2, y+1/2, \bar{z}+1/4$ [ $\bar{u}, v, \bar{w}$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+3/4$ [ $u, \bar{v}, \bar{w}$ ]		
			(7) $y, x, \bar{z}$ [ $\bar{v}, \bar{u}, w$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+1/2$ [ $v, u, w$ ]		
4	a	..2'	$x, x, 0$ [ $u, \bar{u}, w$ ]	$\bar{x}, \bar{x}, 1/2$ [ $\bar{u}, u, w$ ]	$\bar{x}+1/2, x+1/2, 1/4$ [ $\bar{u}, \bar{u}, \bar{w}$ ]	$x+1/2, \bar{x}+1/2, 3/4$ [ $u, u, \bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4'gm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p2g'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,3/8

Along [1,1,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



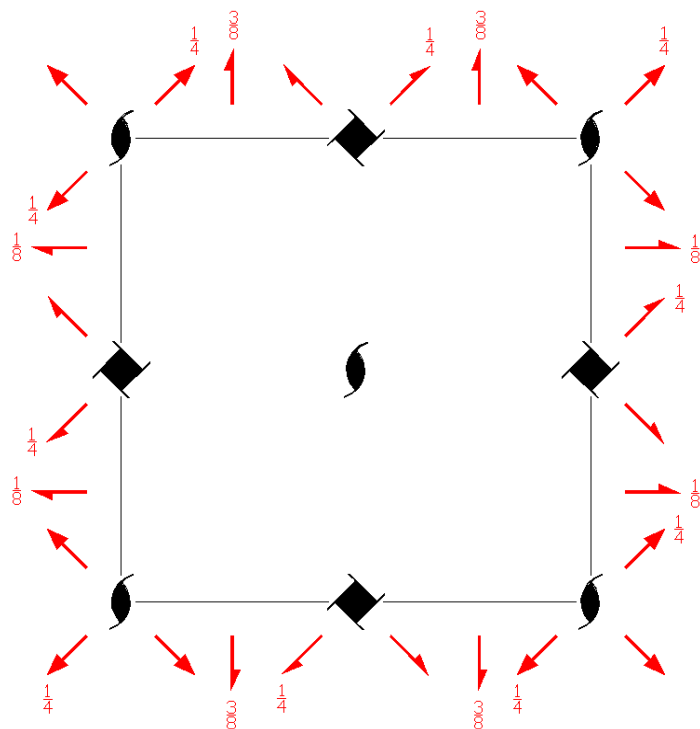
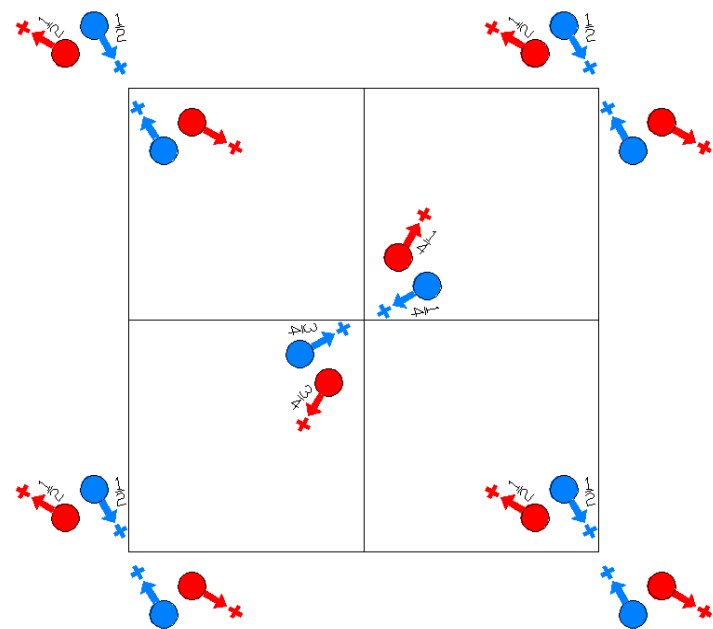
P4<sub>1</sub>2<sub>1</sub>'2'

42'2'

Tetragonal

92.4.774

P4<sub>1</sub>2<sub>1</sub>'2'



Origin on 2' [1 1 0] at 2<sub>1</sub>(1,2')

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

### Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)           | (3) 4 <sup>+</sup> (0,0,1/4) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/4) | (4) 4 <sup>-</sup> (0,0,3/4) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,3/4) |
| (5) 2' (0,1/2,0) 1/4,y,1/8<br>(2 <sub>y</sub>  1/2,1/2,1/4)' | (6) 2' (1/2,0,0) x,1/4,3/8<br>(2 <sub>x</sub>  1/2,1/2,3/4)' | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                             | (8) 2' x,x̄,1/4<br>(2 <sub>xy</sub> ̄ 0,0,1/2)'                                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

8	b	1	(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}+1/2, x+1/2, z+1/4$ [ $\bar{v}, u, w$ ]	(4) $y+1/2, \bar{x}+1/2, z+3/4$ [ $v, \bar{u}, w$ ]		
			(5) $\bar{x}+1/2, y+1/2, \bar{z}+1/4$ [ $u, \bar{v}, w$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+3/4$ [ $\bar{u}, v, w$ ]		
			(7) $y, x, \bar{z}$ [ $\bar{v}, \bar{u}, w$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+1/2$ [ $v, u, w$ ]		
4	a	..2'	$x, x, 0$ [ $u, \bar{u}, w$ ]	$\bar{x}, \bar{x}, 1/2$ [ $\bar{u}, u, w$ ]	$\bar{x}+1/2, x+1/2, 1/4$ [ $u, u, w$ ]	$x+1/2, \bar{x}+1/2, 3/4$ [ $\bar{u}, \bar{u}, w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4gm

$\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$

Origin at 0,1/2,z

Along [1,0,0] p2'gg'

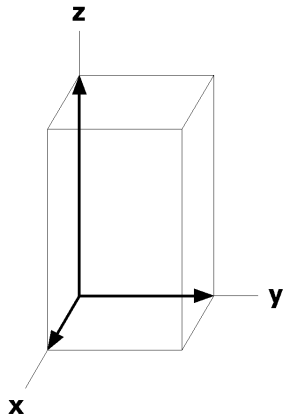
$\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$

Origin at x,1/4,3/8

Along [1,1,0] p2'mg'

$\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$

Origin at x,x,0



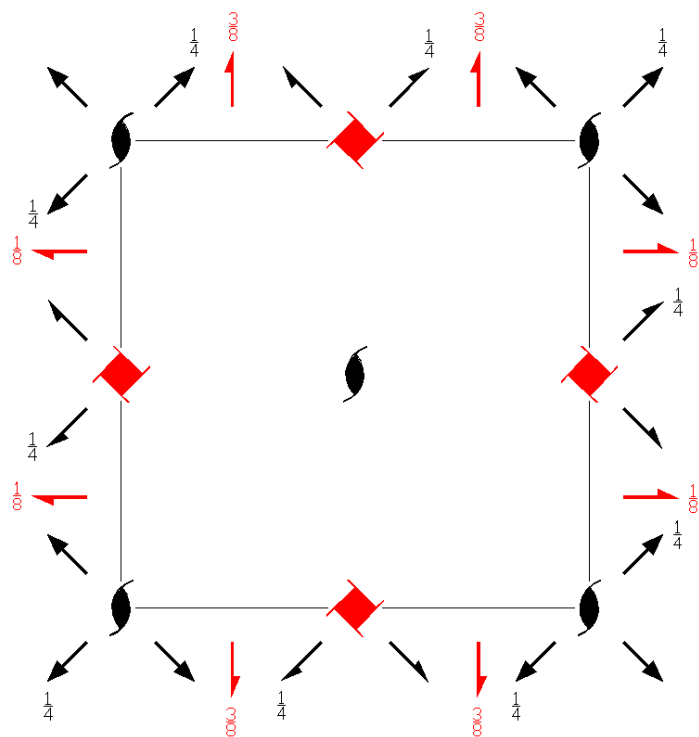
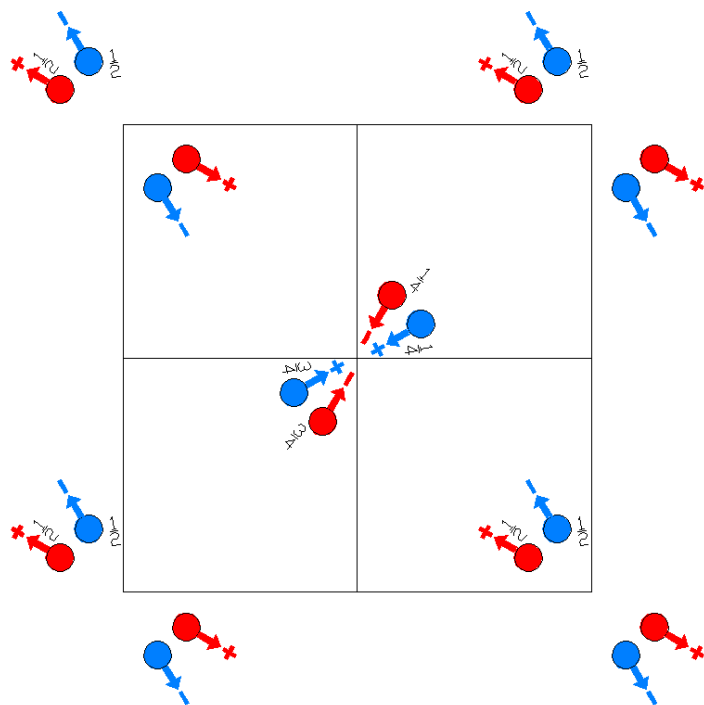
$P4_1'2_1'2$

92.5.775

$4'2'2$

$P4_1'2_1'2$

Tetragonal



Origin on  $2 [1\ 1\ 0]$  at  $2_1(1,2)$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/8$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)           | (3) 4 <sup>+</sup> (0,0,1/4) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/4)' | (4) 4 <sup>-</sup> (0,0,3/4) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,3/4)' |
| (5) 2' (0,1/2,0) 1/4,y,1/8<br>(2 <sub>y</sub>  1/2,1/2,1/4)' | (6) 2' (1/2,0,0) x,1/4,3/8<br>(2 <sub>x</sub>  1/2,1/2,3/4)' | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                | (8) 2 x,x̄,1/4<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,1/2)                            |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

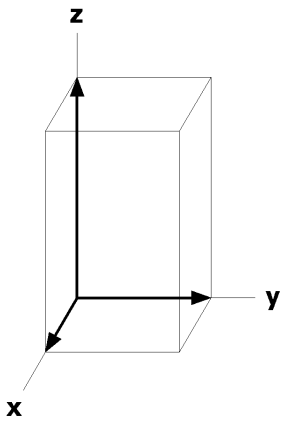
8	b	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}+1/2, x+1/2, z+1/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(4) $y+1/2, \bar{x}+1/2, z+3/4$ [ $\bar{v}, u, \bar{w}$ ]		
			(5) $\bar{x}+1/2, y+1/2, \bar{z}+1/4$ [ $u, \bar{v}, w$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+3/4$ [ $\bar{u}, v, w$ ]		
			(7) $y, x, \bar{z}$ [ $v, u, \bar{w}$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
4	a	..2	$x, x, 0$ [u,u,0]	$\bar{x}, \bar{x}, 1/2$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}+1/2, x+1/2, 1/4$ [ $u, \bar{u}, 0$ ]	$x+1/2, \bar{x}+1/2, 3/4$ [ $\bar{u}, u, 0$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4'g'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,1/2,z

Along [1,0,0] p2g'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,1/4,3/8

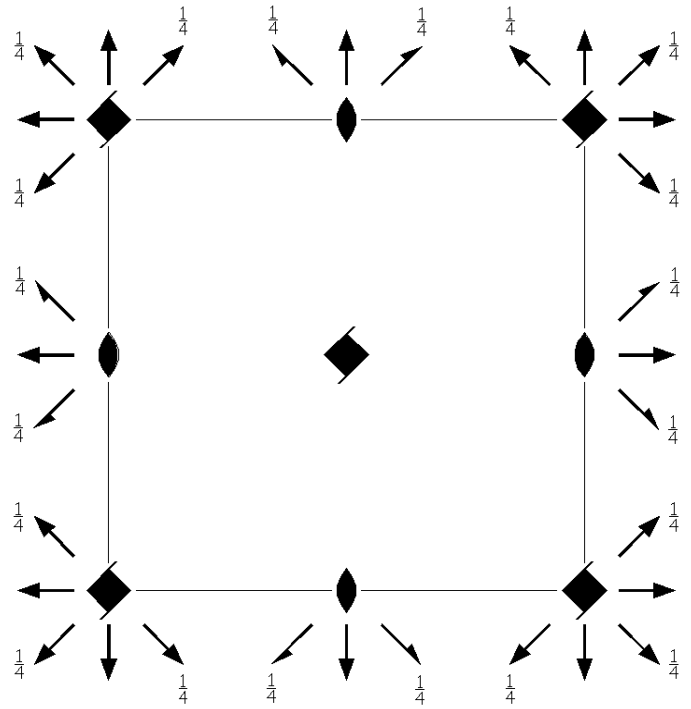
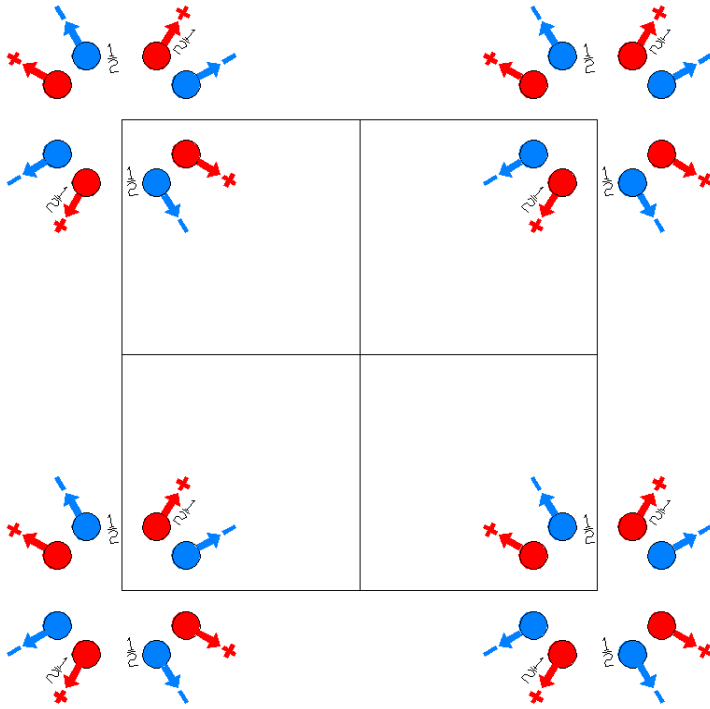
Along [1,1,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at x,x,0



P4<sub>2</sub>22  
93.1.776

422  
P4<sub>2</sub>22

Tetragonal



Origin at 222 at 4<sub>2</sub>21

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                     | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,1/2)            |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

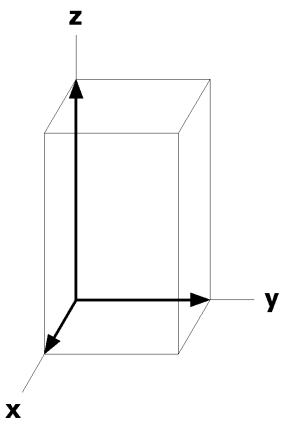
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	p 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]
		(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
4	o ..2	x,x,3/4 [u,u,0]	$\bar{x},\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/4$ [ $\bar{u},u,0$ ]	$x,\bar{x},1/4$ [ $u,\bar{u},0$ ]
4	n ..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]	$x,\bar{x},3/4$ [ $u,\bar{u},0$ ]
4	m .2.	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	1/2,x,1/2 [0,u,0]	1/2, $\bar{x},1/2$ [0, $\bar{u},0$ ]
4	l .2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,0 [0,u,0]	0, $\bar{x},0$ [0, $\bar{u},0$ ]
4	k .2.	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	1/2,x,0 [0,u,0]	1/2, $\bar{x},0$ [0, $\bar{u},0$ ]
4	j .2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,1/2 [0,u,0]	0, $\bar{x},1/2$ [0, $\bar{u},0$ ]
4	i 2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	h 2..	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	g 2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
2	f 2.22	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	e 2.22	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	d 222.	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]		
2	c 222.	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	b 222.	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a 222.	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



P4<sub>2</sub>221'

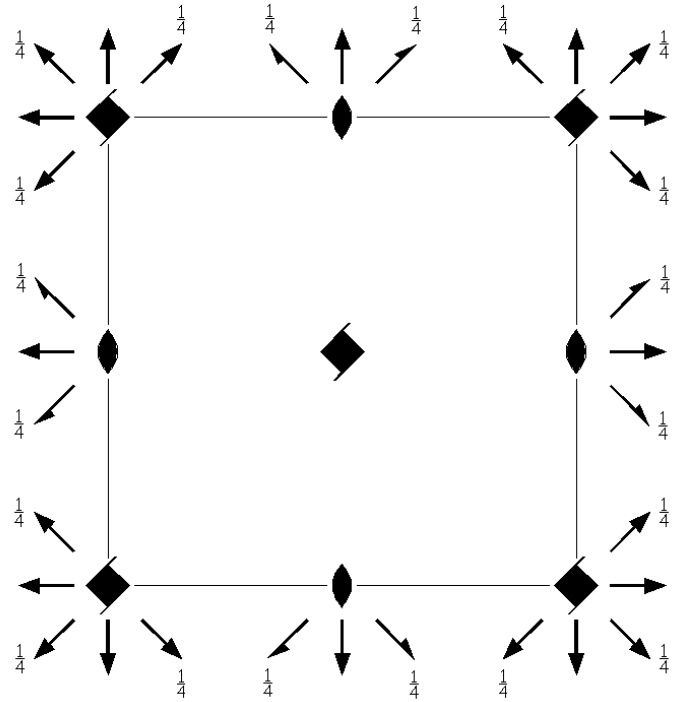
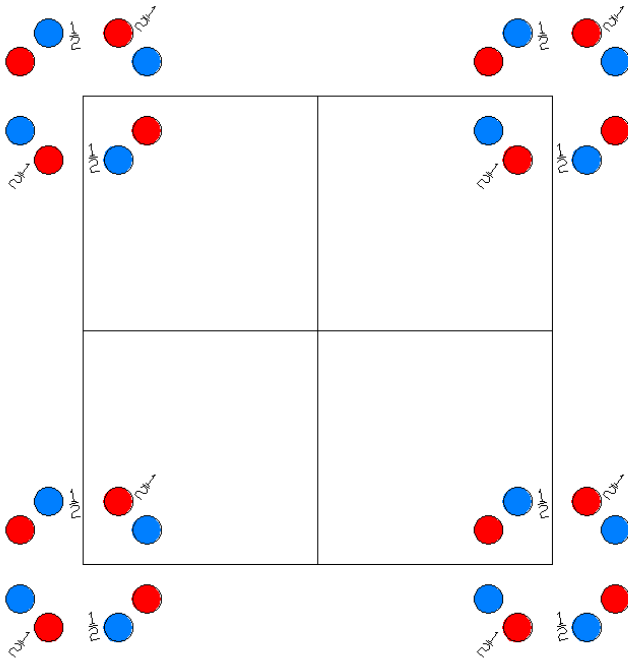
93.2.777

4221'

P4<sub>2</sub>221'

Tetragonal

1'



Origin at 222 at 4<sub>2</sub>21

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

Symmetry Operations

For 1 + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                     | (8) 2 x,x̄,1/4<br>(2 <sub>-xy</sub>  0,0,1/2)                                 |

For 1' + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1'<br>(1 0,0,0)'                     | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 4 <sup>+</sup> ' (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)' | (4) 4 <sup>-</sup> ' (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                      | (8) 2' x,x̄,1/4<br>(2 <sub>-xy</sub>  0,0,1/2)'                                  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

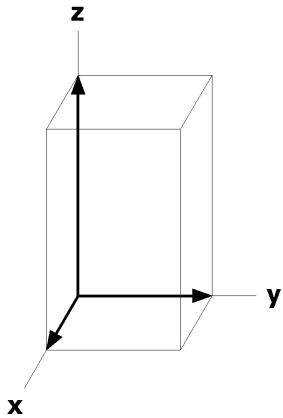
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +		1' +	
8 p 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z+1/2$ [0,0,0]	(4) $y,\bar{x},z+1/2$ [0,0,0]
	(5) $\bar{x},y,\bar{z}$ [0,0,0]	(6) $x,\bar{y},\bar{z}$ [0,0,0]	(7) $y,x,\bar{z}+1/2$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [0,0,0]
4 o ..21'	x,x,3/4 [0,0,0]	$\bar{x},\bar{x},3/4$ [0,0,0]	$\bar{x},x,1/4$ [0,0,0]	$x,\bar{x},1/4$ [0,0,0]
4 n ..21'	x,x,1/4 [0,0,0]	$\bar{x},\bar{x},1/4$ [0,0,0]	$\bar{x},x,3/4$ [0,0,0]	$x,\bar{x},3/4$ [0,0,0]
4 m .2.1'	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]	1/2,x,1/2 [0,0,0]	1/2, $\bar{x},1/2$ [0,0,0]
4 l .2.1'	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x},0$ [0,0,0]
4 k .2.1'	x,1/2,1/2 [0,0,0]	$\bar{x},1/2,1/2$ [0,0,0]	1/2,x,0 [0,0,0]	1/2, $\bar{x},0$ [0,0,0]
4 j .2.1'	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,1/2 [0,0,0]	0, $\bar{x},1/2$ [0,0,0]
4 i 2..1'	0,1/2,z [0,0,0]	1/2,0,z+1/2 [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]
4 h 2..1'	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]
4 g 2..1'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]
2 f 2.221'	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2 e 2.221'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2 d 222.1'	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]		
2 c 222.1'	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2 b 222.1'	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2 a 222.1'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

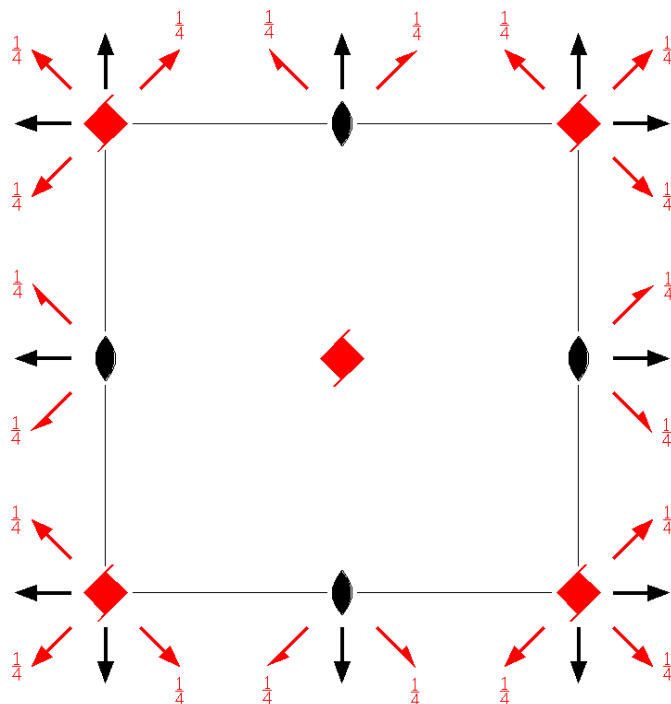
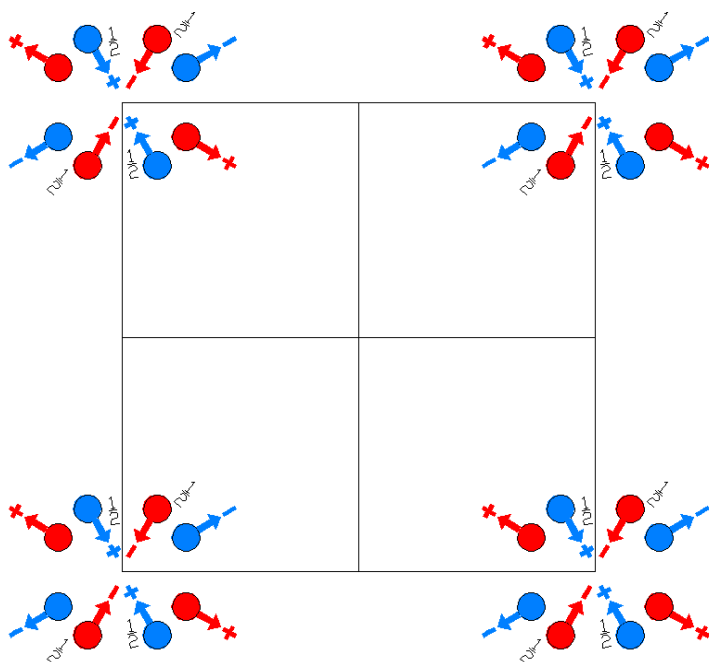
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



$P4_2'22'$   
93.3.778

$4'22'$   
 $P4_2'22'$

Tetragonal



Origin at 222 at  $4_2'21$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                    | (8) 2' x,x̄,1/4<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,1/2)'                    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

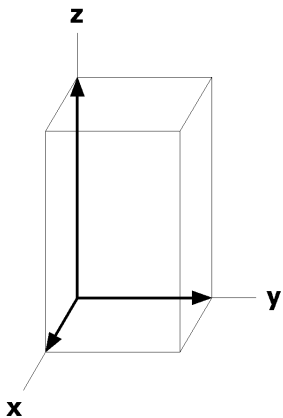
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	p 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ]
		(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $v,u,w$ ]
4	o ..2'	x,x,3/4 [u, $\bar{u}$ ,w]	$\bar{x},\bar{x},3/4$ [ $\bar{u},u,w$ ]	$\bar{x},x,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	x, $\bar{x},1/4$ [u,u, $\bar{w}$ ]
4	n ..2'	x,x,1/4 [u, $\bar{u}$ ,w]	$\bar{x},\bar{x},1/4$ [ $\bar{u},u,w$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	x, $\bar{x},3/4$ [u,u, $\bar{w}$ ]
4	m .2.	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	1/2,x,1/2 [0, $\bar{u}$ ,0]	1/2, $\bar{x},1/2$ [0,u,0]
4	l .2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,0 [0, $\bar{u}$ ,0]	0, $\bar{x},0$ [0,u,0]
4	k .2.	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	1/2,x,0 [0, $\bar{u}$ ,0]	1/2, $\bar{x},0$ [0,u,0]
4	j .2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,1/2 [0, $\bar{u}$ ,0]	0, $\bar{x},1/2$ [0,u,0]
4	i 2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0,w]
4	h 2..	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]
4	g 2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0,w]
2	f 2.2'2'	1/2,1/2,1/4 [0,0,w]	1/2,1/2,3/4 [0,0,w]		
2	e 2.2'2'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		
2	d 222.	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]		
2	c 222.	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	b 222.	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a 222.	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



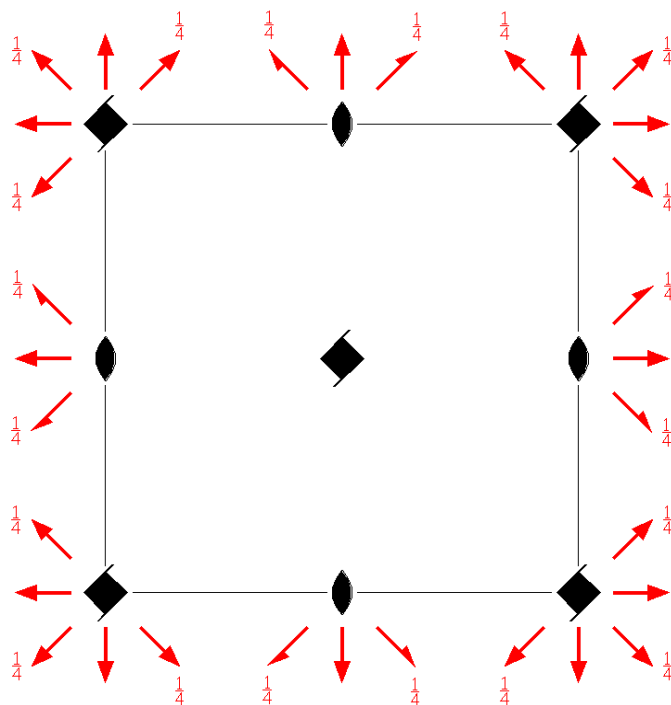
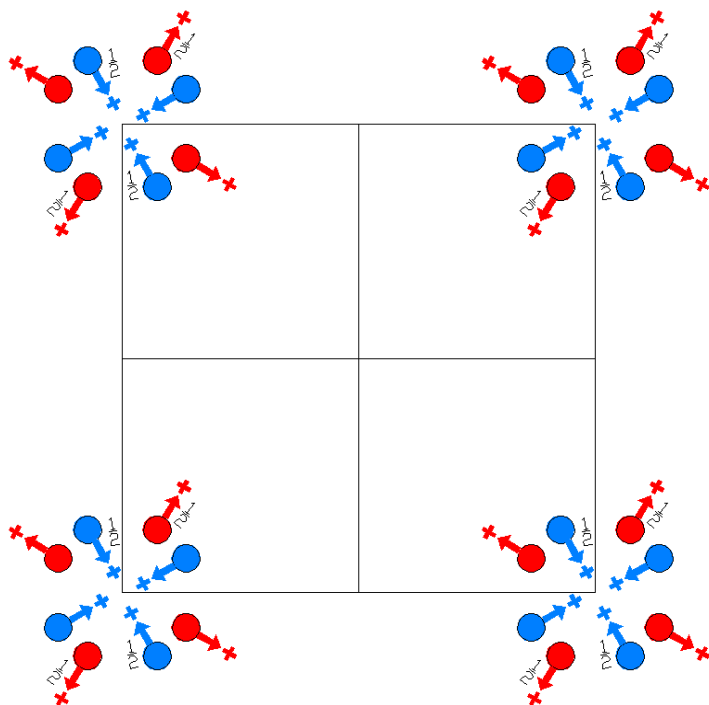
$P4_22'2'$

93.4.779

$42'2'$

$P4_22'2'$

Tetragonal



Origin at  $22'2'$  at  $4_22'1$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

**Symmetry Operations**

- |                                      |                                      |  |   |
|--------------------------------------|--------------------------------------|--|---|
| (1) 1<br>(1 0,0,0)                   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)     | (3) $4^+$ (0,0,1/2) $0,0,z$<br>( $4_z$  0,0,1/2) | (4) $4^-$ (0,0,1/2) $0,0,z$<br>( $4_z^{-1}$  0,0,1/2)   |
| (5) $2'$ $0,y,0$<br>( $2_y$  0,0,0)' | (6) $2'$ $x,0,0$<br>( $2_x$  0,0,0)' | (7) $2'$ $x,x,1/4$<br>( $2_{xy}$  0,0,1/2)'      | (8) $2'$ $x,\bar{x},1/4$<br>( $2_{\bar{xy}}$  0,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

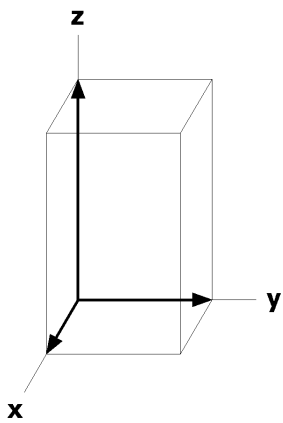
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	p 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]
		(5) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $v,u,w$ ]
4	o ..2'	x,x,3/4 [u, $\bar{u}$ ,w]	$\bar{x},\bar{x},3/4$ [ $\bar{u},u,w$ ]	$\bar{x},x,1/4$ [u,u,w]	x, $\bar{x},1/4$ [ $\bar{u},\bar{u},w$ ]
4	n ..2'	x,x,1/4 [u, $\bar{u}$ ,w]	$\bar{x},\bar{x},1/4$ [ $\bar{u},u,w$ ]	$\bar{x},x,3/4$ [u,u,w]	x, $\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]
4	m .2'	x,1/2,0 [0,v,w]	$\bar{x},1/2,0$ [0, $\bar{v},w$ ]	1/2,x,1/2 [ $\bar{v},0,w$ ]	1/2, $\bar{x},1/2$ [v,0,w]
4	l .2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	0,x,0 [ $\bar{v},0,w$ ]	0, $\bar{x},0$ [v,0,w]
4	k .2'	x,1/2,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0, $\bar{v},w$ ]	1/2,x,0 [ $\bar{v},0,w$ ]	1/2, $\bar{x},0$ [v,0,w]
4	j .2'	x,0,0 [0,v,w]	$\bar{x},0,0$ [0, $\bar{v},w$ ]	0,x,1/2 [ $\bar{v},0,w$ ]	0, $\bar{x},1/2$ [v,0,w]
4	i 2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]
4	h 2..	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]
4	g 2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]
2	f 2.2'2'	1/2,1/2,1/4 [0,0,w]	1/2,1/2,3/4 [0,0,w]		
2	e 2.2'2'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		
2	d 22'2'	0,1/2,1/2 [0,0,w]	1/2,0,0 [0,0,w]		
2	c 22'2'	0,1/2,0 [0,0,w]	1/2,0,1/2 [0,0,w]		
2	b 22'2'	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]		
2	a 22'2'	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

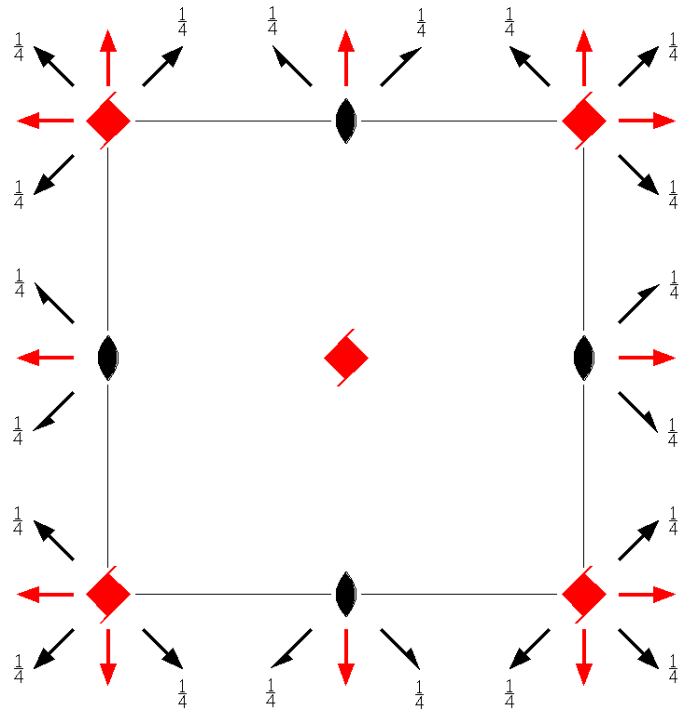
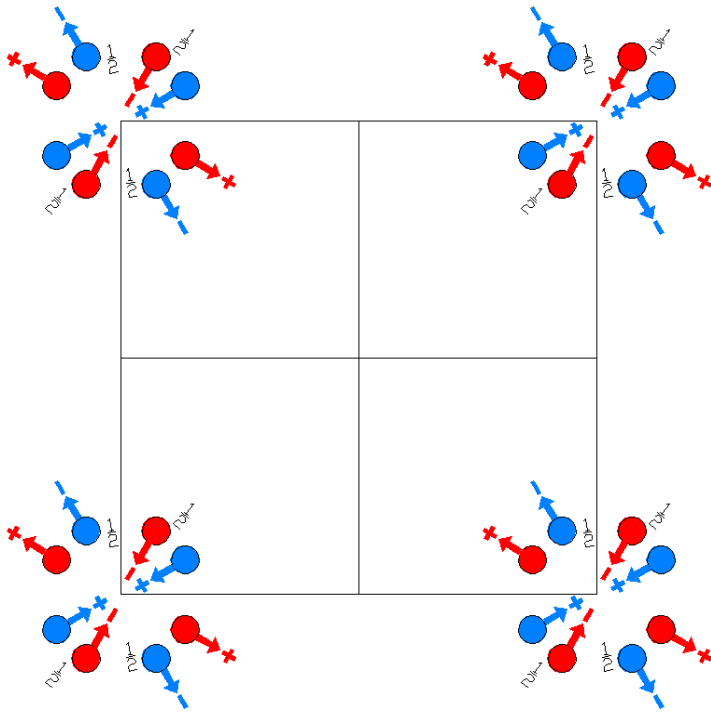
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



$P4_2'2'2'$   
93.5.780

$4'2'2'$   
 $P4_2'2'2'$

Tetragonal



Origin at  $22'2'$  at  $4_2'2'1$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                      | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,1/2)             |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

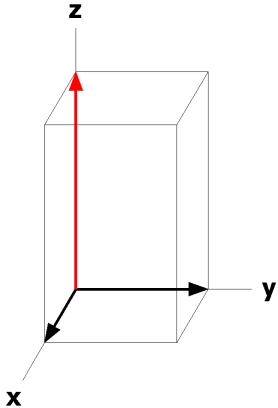
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	p 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $v,\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ]
		(5) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
4	o ..2	x,x,3/4 [u,u,0]	$\bar{x},\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/4$ [ $u,\bar{u},0$ ]	$x,\bar{x},1/4$ [ $\bar{u},u,0$ ]
4	n ..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,3/4$ [ $u,\bar{u},0$ ]	$x,\bar{x},3/4$ [ $\bar{u},u,0$ ]
4	m .2'	x,1/2,0 [0,v,w]	$\bar{x},1/2,0$ [0, $\bar{v},w$ ]	1/2,x,1/2 [v,0, $\bar{w}$ ]	1/2, $\bar{x},1/2$ [ $\bar{v},0,\bar{w}$ ]
4	l .2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	0,x,0 [v,0, $\bar{w}$ ]	0, $\bar{x},0$ [ $\bar{v},0,\bar{w}$ ]
4	k .2'	x,1/2,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0, $\bar{v},w$ ]	1/2,x,0 [v,0, $\bar{w}$ ]	1/2, $\bar{x},0$ [ $\bar{v},0,\bar{w}$ ]
4	j .2'	x,0,0 [0,v,w]	$\bar{x},0,0$ [0, $\bar{v},w$ ]	0,x,1/2 [v,0, $\bar{w}$ ]	0, $\bar{x},1/2$ [ $\bar{v},0,\bar{w}$ ]
4	i 2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	h 2..	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	g 2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
2	f 2.22	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	e 2.22	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	d 22'2'	0,1/2,1/2 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]		
2	c 22'2'	0,1/2,0 [0,0,w]	1/2,0,1/2 [0,0, $\bar{w}$ ]		
2	b 22'2'	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		
2	a 22'2'	0,0,0 [0,0,w]	0,0,1/2 [0,0,0 $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p4'm'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



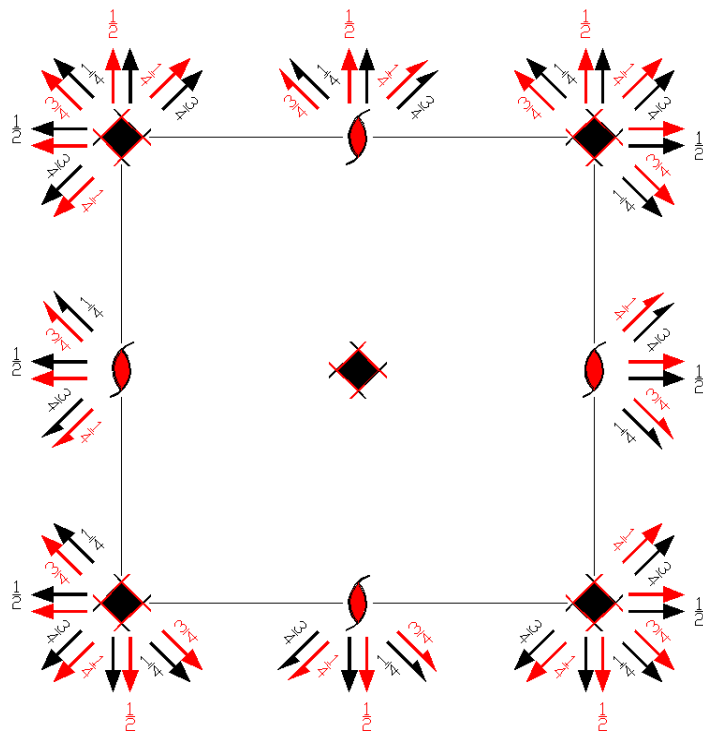
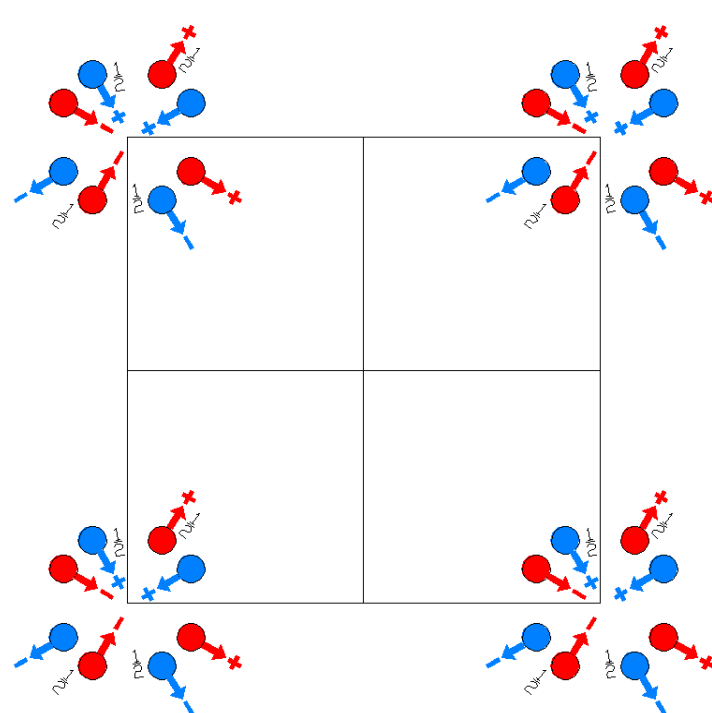
$P_{2c} 4_2 22$

422

Tetragonal

93.6.781

$P_{2c} 4_2 22$



Origin at  $2'22'$  at  $4_2(22')1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                                    |                                    |  |   |
|------------------------------------|------------------------------------|--|---|
| (1) 1<br>(1 0,0,0)                 | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $4^+$ (0,0,1/2) 0,0,z<br>( $4_z$  0,0,1/2) | (4) $4^{-1}$ (0,0,1/2) 0,0,z<br>( $4_z^{-1}$  0,0,1/2)'   |
| (5) $2'$ 0,y,0<br>( $2_y$  0,0,0)' | (6) 2 x,0,0<br>( $2_x$  0,0,0)     | (7) 2 x,x,1/4<br>( $2_{xy}$  0,0,1/2)          | (8) $2'$ x, $\bar{x}$ ,1/4<br>( $2_{\bar{xy}}$  0,0,1/2)' |

For  $(0,0,1)$  + set

- |                                  |  |   |  |
|----------------------------------|--|---|--|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'   | (2) 2 (0,0,1) 0,0,z<br>( $2_z$  0,0,1) | (3) $4^+$ (0,0,3/2) 0,0,z<br>( $4_z$  0,0,3/2)' | (4) $4^{-1}$ (0,0,3/2) 0,0,z<br>( $4_z^{-1}$  0,0,3/2) |
| (5) 2 0,y,1/2<br>( $2_y$  0,0,1) | (6) $2'$ x,0,1/2<br>( $2_x$  0,0,1)'   | (7) $2'$ x,x,3/4<br>( $2_{xy}$  0,0,3/2)'       | (8) 2 x, $\bar{x}$ ,3/4<br>( $2_{\bar{xy}}$  0,0,3/2)  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

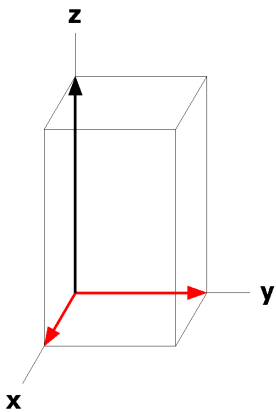
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
16 p 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ]
	(5) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ]	(6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}+1/2$ [v,u, $\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [v,u,w]
8 o ..2'	x,x,3/4 [u, $\bar{u},w$ ]	$\bar{x},\bar{x},3/4$ [u, $\bar{u},\bar{w}$ ]	$\bar{x},x,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	x, $\bar{x},1/4$ [ $\bar{u},\bar{u},w$ ]
8 n ..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]	x, $\bar{x},3/4$ [u, $\bar{u},0$ ]
8 m .2.	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [u,0,0]	1/2,x,1/2 [0,u,0]	1/2, $\bar{x},1/2$ [0,u,0]
8 l .2'.	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0,v, $\bar{w}$ ]	0,x,0 [v,0, $\bar{w}$ ]	0, $\bar{x},0$ [v,0,w]
8 k .2'.	x,1/2,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0,v, $\bar{w}$ ]	1/2,x,0 [v,0, $\bar{w}$ ]	1/2, $\bar{x},0$ [v,0,w]
8 j .2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [u,0,0]	0,x,1/2 [0,u,0]	0, $\bar{x},1/2$ [0,u,0]
8 i 2'..	0,1/2,z [u,v,0]	1/2,0,z+1/2 [ $\bar{v},u,0$ ]	0,1/2, $\bar{z}$ [u, $\bar{v},0$ ]	1/2,0, $\bar{z}+1/2$ [v,u,0]
4 h 2'..	1/2,1/2,z [u,v,0]	1/2,1/2,z+1/2 [ $\bar{v},u,0$ ]	1/2,1/2, $\bar{z}$ [u, $\bar{v},0$ ]	1/2,1/2, $\bar{z}+1/2$ [v,u,0]
4 g 2'..	0,0,z [u,v,0]	0,0,z+1/2 [ $\bar{v},u,0$ ]	0,0, $\bar{z}$ [u, $\bar{v},0$ ]	0,0, $\bar{z}+1/2$ [v,u,0]
4 f 2'.22'	1/2,1/2,1/4 [u,u,0]	1/2,1/2,3/4 [ $\bar{u},u,0$ ]		
4 e 2'.22'	0,0,1/4 [u,u,0]	0,0,3/4 [ $\bar{u},u,0$ ]		
4 d 2'2'2.	0,1/2,1/2 [0,v,0]	1/2,0,0 [v,0,0]		
4 c 2'22'.	0,1/2,0 [u,0,0]	1/2,0,1/2 [0,u,0]		
4 b 2'22'.	1/2,1/2,0 [u,0,0]	1/2,1/2,1/2 [0,u,0]		
4 a 2'22'.	0,0,0 [u,0,0]	0,0,1/2 [0,u,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>·2mm  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0] p<sub>2a</sub>·2mm  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



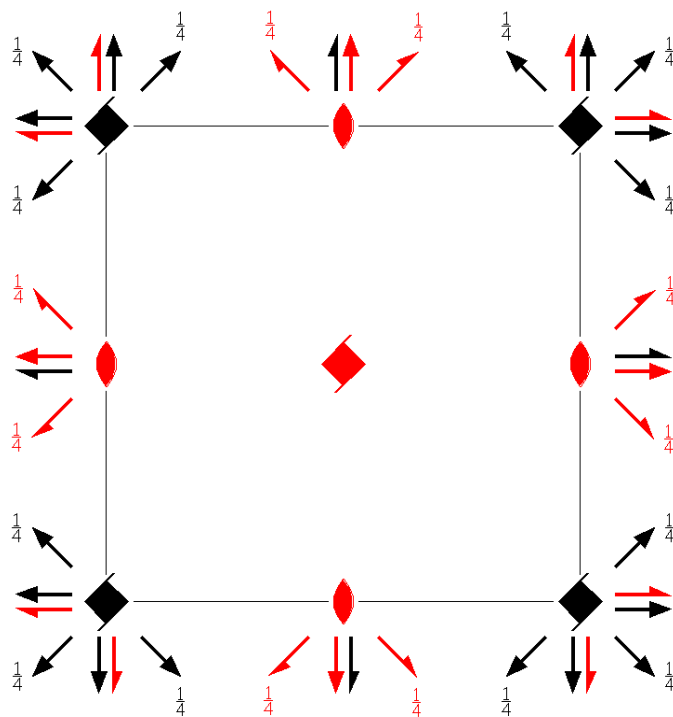
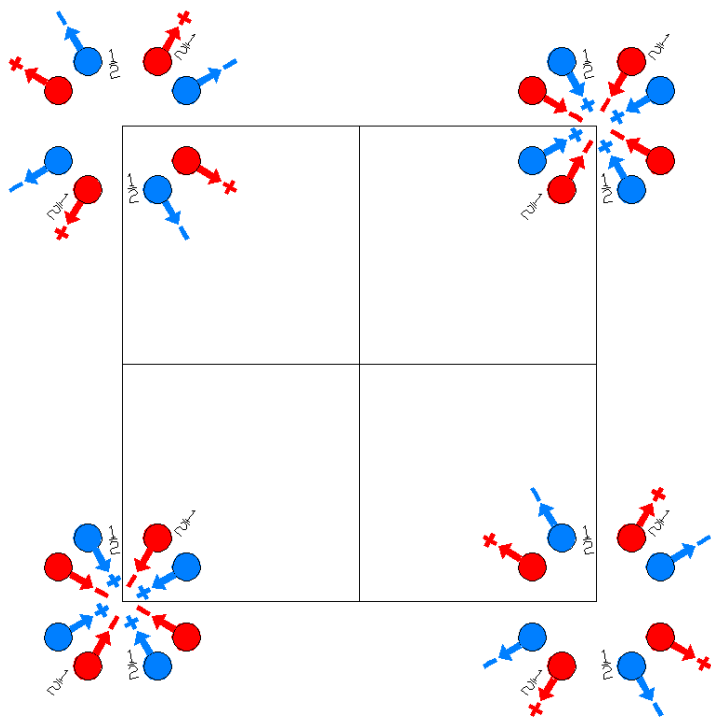
$P_P 4_2 22$

$4221'$

Tetragonal

93.7.782

$P_P 4_2 22$



Origin at 222 at  $4_2 21$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                                  |                                  |  |   |
|----------------------------------|----------------------------------|--|---|
| (1) 1<br>(1 0,0,0)               | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $4^+$ $(0,0,1/2)$ $0,0,z$<br>( $4_z$  0,0,1/2) | (4) $4^-$ $(0,0,1/2)$ $0,0,z$<br>( $4_z^{-1}$  0,0,1/2) |
| (5) 2 $0,y,0$<br>( $2_y$  0,0,0) | (6) 2 $x,0,0$<br>( $2_x$  0,0,0) | (7) 2 $x,x,1/4$<br>( $2_{xy}$  0,0,1/2)            | (8) 2 $x,\bar{x},1/4$<br>( $2_{\bar{xy}}$  0,0,1/2)     |

For  $(1,0,0)'$  + set

- |  |  |   |  |
|--|--|---|--|
| (1) $t'$ $(1,0,0)$<br>(1 1,0,0)'       | (2) $2'$ $1/2,0,z$<br>( $2_z$  1,0,0)'         | (3) $4^+$ $(0,0,1/2)$ $1/2,1/2,z$<br>( $4_z$  1,0,1/2)'       | (4) $4^-$ $(0,0,1/2)$ $1/2,-1/2,z$<br>( $4_z^{-1}$  1,0,1/2)'              |
| (5) $2'$ $1/2,y,0$<br>( $2_y$  1,0,0)' | (6) $2'$ $(1,0,0)$ $x,0,0$<br>( $2_x$  1,0,0)' | (7) $2'$ $(1/2,1/2,0)$ $x+1/2,x,1/4$<br>( $2_{xy}$  1,0,1/2)' | (8) $2'$ $(1/2,-1/2,0)$ $x+1/2,\bar{x},1/4$<br>( $2_{\bar{xy}}$  1,0,1/2)' |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

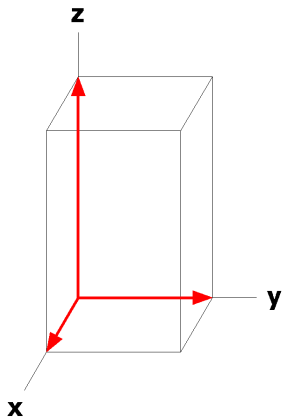
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 p 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ] (7) y,x, $\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]	(4) y, $\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ] (8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8 o ..2	x,x,3/4 [u,u,0]	$\bar{x},\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/4$ [ $\bar{u},u,0$ ]	x, $\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]
8 n ..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]	x, $\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]
8 m .2'	x,1/2,0 [0,v,w]	$\bar{x},1/2,0$ [0,v, $\bar{w}$ ]	1/2,x,1/2 [v,0, $\bar{w}$ ]	1/2, $\bar{x},1/2$ [v,0,w]
8 l .2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,0 [0,u,0]	0, $\bar{x},0$ [0, $\bar{u},0$ ]
8 k .2'	x,1/2,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0,v, $\bar{w}$ ]	1/2,x,0 [v,0, $\bar{w}$ ]	1/2, $\bar{x},0$ [v,0,w]
8 j .2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,1/2 [0,u,0]	0, $\bar{x},1/2$ [0, $\bar{u},0$ ]
8 i 2'..	0,1/2,z [u,v,0]	1/2,0,z+1/2 [v, $\bar{u},0$ ]	0,1/2, $\bar{z}$ [ $\bar{u},v,0$ ]	1/2,0, $\bar{z}+1/2$ [v,u,0]
8 h 2..	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
8 g 2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4 f 2.22	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
4 e 2.22	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
4 d 2'2'.2.	0,1/2,1/2 [0,v,0]	1/2,0,0 [v,0,0]		
4 c 2'2'.2.	0,1/2,0 [0,v,0]	1/2,0,1/2 [v,0,0]		
4 b 22'2'.2.	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		
4 a 222.	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub>-4m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



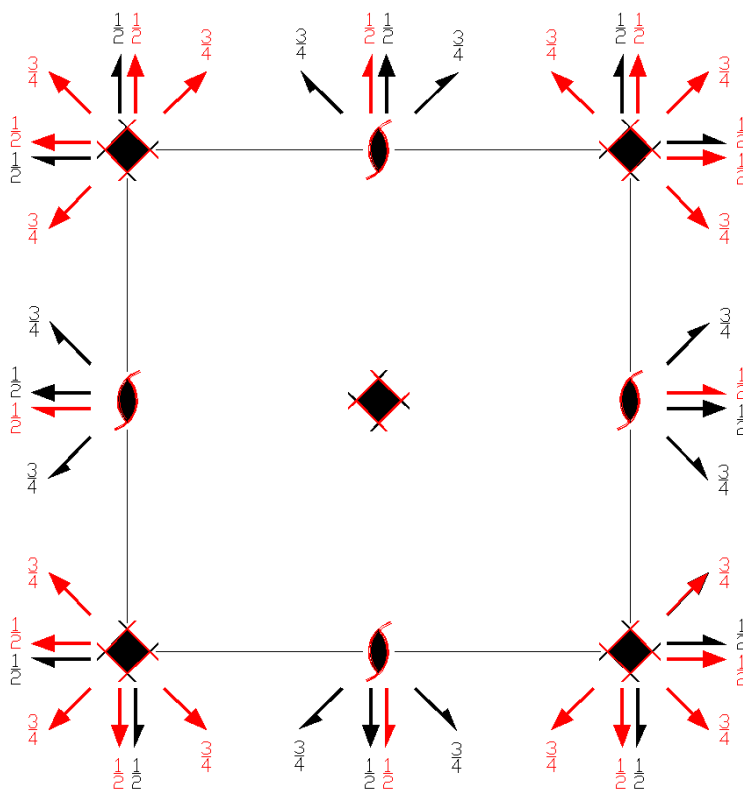
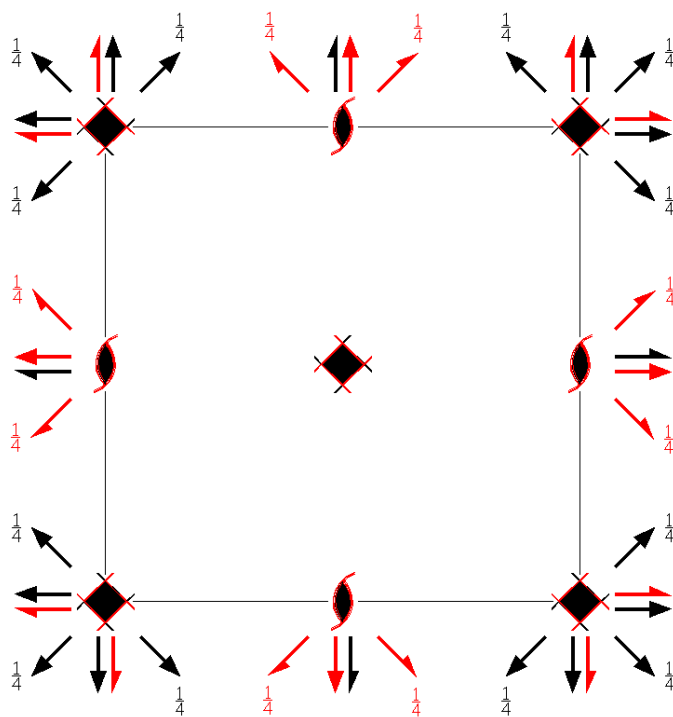
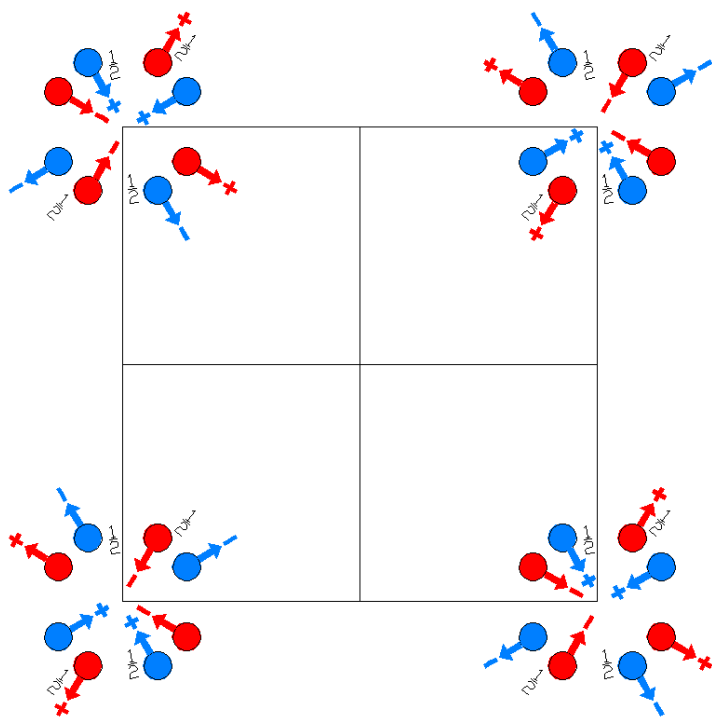
$P_1 4_2 22$

93.8.783

4221'

$P_1 4_2 22$

Tetragonal



Origin at 2'22' at 4<sub>2</sub> (2,2')<sub>1</sub>Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$ 

## Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> (0,0,1/2) 0,0,z (4 <sub>z</sub>  0,0,1/2)	(4) 4 <sup>-</sup> (0,0,1/2) 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)'
(5) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(6) 2 x,0,0 (2 <sub>x</sub>  0,0,0)	(7) 2 x,x,1/4 (2 <sub>xy</sub>  0,0,1/2)	(8) 2' x, $\bar{x}$ ,1/4 (2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)'

For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2 1/2,0,z (2 <sub>z</sub>  1,0,0)	(3) 4 <sup>+</sup> (0,0,1/2) 1/2,1/2,z (4 <sub>z</sub>  1,0,1/2)'	(4) 4 <sup>-</sup> (0,0,1/2) 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,1/2)
(5) 2 1/2,y,0 (2 <sub>y</sub>  1,0,0)	(6) 2' (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)'	(7) 2' (1/2,1/2,0) x+1/2,x,1/4 (2 <sub>xy</sub>  1,0,1/2)'	(8) 2 (1/2,-1/2,0)x+1/2, $\bar{x}$ ,1/4 (2 <sub><math>\bar{xy}</math></sub>  1,0,1/2)

Generators selected (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

		(0,0,0) +		(1,0,0)' +	
16	p 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ]
		(5) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}+1/2$ [v,u, $\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [v,u, $\bar{w}$ ]
8	o ..2'	x,x,3/4 [u, $\bar{u},w$ ]	$\bar{x},\bar{x},3/4$ [u, $\bar{u},\bar{w}$ ]	$\bar{x},x,1/4$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x},1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	n ..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [u,u,0]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]	$x,\bar{x},3/4$ [ $\bar{u},u,0$ ]
8	m .2'	x,1/2,0 [0,v,w]	$\bar{x},1/2,0$ [0, $\bar{v},w$ ]	1/2,x,1/2 [v,0, $\bar{w}$ ]	1/2, $\bar{x},1/2$ [ $\bar{v},0,\bar{w}$ ]
8	l .2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	0,x,0 [v,0, $\bar{w}$ ]	0, $\bar{x},0$ [ $\bar{v},0,\bar{w}$ ]
8	k .2	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [u,0,0]	1/2,x,0 [0,u,0]	1/2, $\bar{x},0$ [0,u,0]
8	j .2	x,0,0 [u,0,0]	$\bar{x},0,0$ [u,0,0]	0,x,1/2 [0,u,0]	0, $\bar{x},1/2$ [0,u,0]
8	i 2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
8	h 2'..	1/2,1/2,z [u,v,0]	1/2,1/2,z+1/2 [v, $\bar{u},0$ ]	1/2,1/2, $\bar{z}$ [u, $\bar{v},0$ ]	1/2,1/2, $\bar{z}+1/2$ [v,u,0]
8	g 2'..	0,0,z [u,v,0]	0,0,z+1/2 [ $\bar{v},u,0$ ]	0,0, $\bar{z}$ [u, $\bar{v},0$ ]	0,0, $\bar{z}+1/2$ [v,u,0]
4	f 2'.22'	1/2,1/2,1/4 [u,u,0]	1/2,1/2,3/4 [u, $\bar{u},0$ ]		
4	e 2'.22'	0,0,1/4 [u,u,0]	0,0,3/4 [ $\bar{u},u,0$ ]		

4	d	222.	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]
4	c	22'2'.	0,1/2,0 [0,0,w]	1/2,0,1/2 [0,0, $\bar{w}$ ]
4	b	2'2'2.	1/2,1/2,0 [0,v,0]	1/2,1/2,1/2 [v,0,0]
4	a	2'22'.	0,0,0 [u,0,0]	0,0,1/2 [0,u,0]

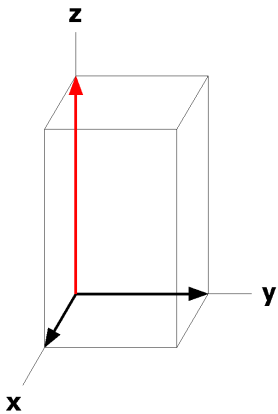
### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4





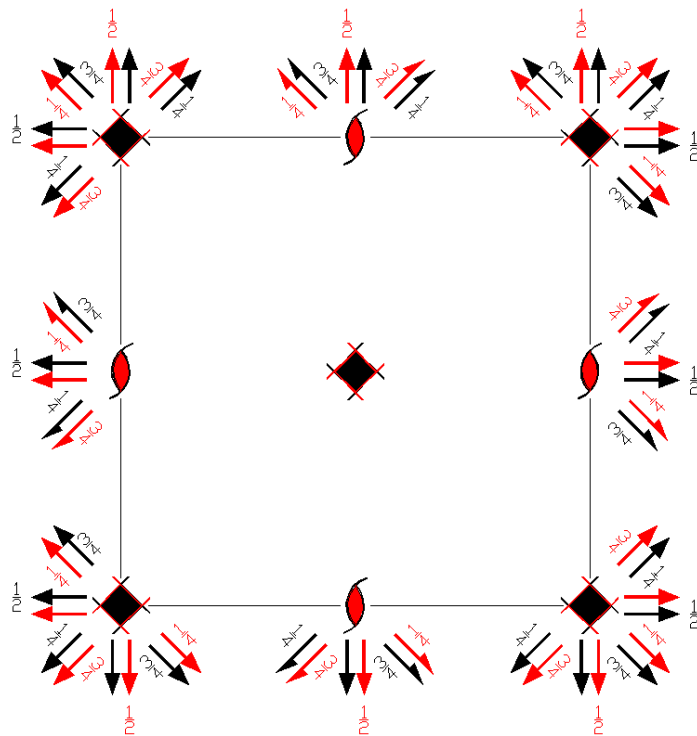
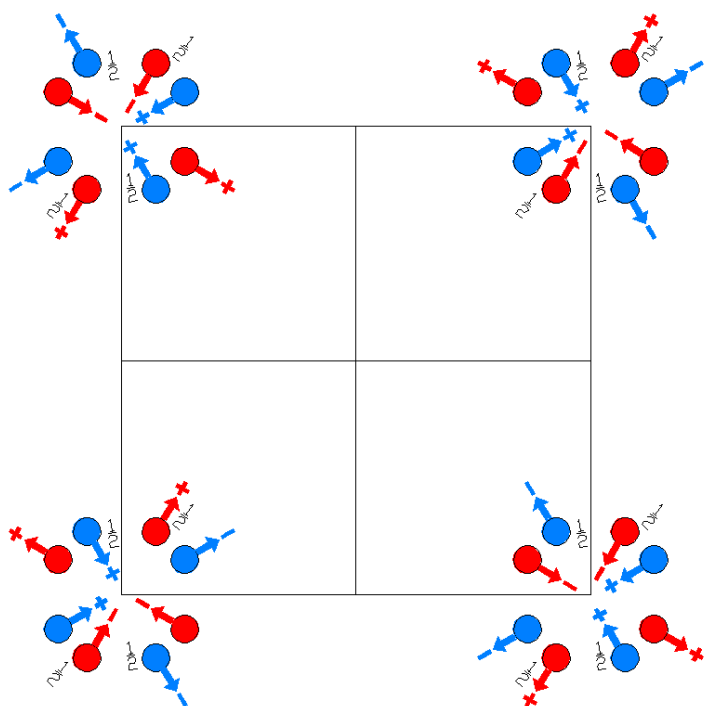
$P_{2c} 4_2'22'$

93.9.784

4221'

$P_{2c} 4_2'22'$

Tetragonal



Origin at  $2'22'$  at  $4_2'21$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

For (0,0,0) + set

- |                                      |                                      |  |   |
|--------------------------------------|--------------------------------------|--|---|
| (1) 1<br>(1 0,0,0)                   | (2) $2'_z$ 0,0,z<br>( $2_z$  0,0,0)' | (3) $4^{+z}$ (0,0,1/2) 0,0,z<br>( $4_z$  0,0,1/2)' | (4) $4^{-z}$ (0,0,1/2) 0,0,z<br>( $4_z^{-1}$  0,0,1/2)              |
| (5) $2'_y$ 0,y,0<br>( $2_y$  0,0,0)' | (6) $2'_x$ x,0,0<br>( $2_x$  0,0,0)  | (7) $2'_{xy}$ x,x,1/4<br>( $2_{xy}$  0,0,1/2)'     | (8) $2'_{\bar{x}y}$ x, $\bar{x}$ ,1/4<br>( $2_{\bar{x}y}$  0,0,1/2) |

For (0,0,1)' + set

- |                                       |   |   |  |
|---------------------------------------|---|---|--|
| (1) $t'_z$ (0,0,1)<br>(1 0,0,1)'      | (2) $2'_z$ (0,0,1) 0,0,z<br>( $2_z$  0,0,1) | (3) $4^{+z}$ (0,0,3/2) 0,0,z<br>( $4_z$  0,0,3/2) | (4) $4^{-z}$ (0,0,3/2) 0,0,z<br>( $4_z^{-1}$  0,0,3/2)'              |
| (5) $2'_y$ 0,y,1/2<br>( $2_y$  0,0,1) | (6) $2'_x$ x,0,1/2<br>( $2_x$  0,0,1)'      | (7) $2'_{xy}$ x,x,3/4<br>( $2_{xy}$  0,0,3/2)     | (8) $2'_{\bar{x}y}$ x, $\bar{x}$ ,3/4<br>( $2_{\bar{x}y}$  0,0,3/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

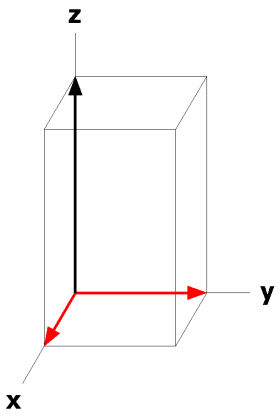
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 p 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
	(5) $\bar{x},y,\bar{z}$ [u, $\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8 o ..2	x,x,3/4 [u,u,0]	$\bar{x},\bar{x},3/4$ [u,u,0]	$\bar{x},x,1/4$ [ $\bar{u},u,0$ ]	$x,\bar{x},1/4$ [ $\bar{u},u,0$ ]
8 n ..2'	x,x,1/4 [u, $\bar{u},w$ ]	$\bar{x},\bar{x},1/4$ [u, $\bar{u},\bar{w}$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	$x,\bar{x},3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
8 m .2.	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [u,0,0]	1/2,x,1/2 [0, $\bar{u},0$ ]	1/2, $\bar{x},1/2$ [0, $\bar{u},0$ ]
8 l .2'.	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0,v, $\bar{w}$ ]	0,x,0 [ $\bar{v},0,w$ ]	0, $\bar{x},0$ [ $\bar{v},0,\bar{w}$ ]
8 k .2'.	x,1/2,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0,v, $\bar{w}$ ]	1/2,x,0 [ $\bar{v},0,w$ ]	1/2, $\bar{x},0$ [ $\bar{v},0,\bar{w}$ ]
8 j .2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [u,0,0]	0,x,1/2 [0, $\bar{u},0$ ]	0, $\bar{x},1/2$ [0, $\bar{u},0$ ]
8 i 2'..	0,1/2,z [u,v,0]	1/2,0,z+1/2 [ $\bar{v},\bar{u},0$ ]	0,1/2, $\bar{z}$ [u, $\bar{v},0$ ]	1/2,0, $\bar{z}+1/2$ [ $\bar{v},\bar{u},0$ ]
8 h 2'..	1/2,1/2,z [u,v,0]	1/2,1/2,z+1/2 [ $\bar{v},\bar{u},0$ ]	1/2,1/2, $\bar{z}$ [u, $\bar{v},0$ ]	1/2,1/2, $\bar{z}+1/2$ [ $\bar{v},\bar{u},0$ ]
8 g 2'..	0,0,z [u,v,0]	0,0,z+1/2 [ $\bar{v},\bar{u},0$ ]	0,0, $\bar{z}$ [u, $\bar{v},0$ ]	0,0, $\bar{z}+1/2$ [ $\bar{v},\bar{u},0$ ]
4 f 2'.2'2	1/2,1/2,1/4 [u, $\bar{u},0$ ]	1/2,1/2,3/4 [ $\bar{u},\bar{u},0$ ]		
4 e 2'.2'2	0,0,1/4 [u, $\bar{u},0$ ]	0,0,3/4 [ $\bar{u},\bar{u},0$ ]		
4 d 2'2'2.	0,1/2,1/2 [0,v,0]	1/2,0,0 [ $\bar{v},0,0$ ]		
4 c 2'22'.	0,1/2,0 [u,0,0]	1/2,0,1/2 [0, $\bar{u},0$ ]		
4 b 2'22'.	1/2,1/2,0 [u,0,0]	1/2,1/2,1/2 [0, $\bar{u},0$ ]		
4 a 2'22'.	0,0,0 [u,0,0]	0,0,1/2 [0, $\bar{u},0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>' 2mm  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0] p<sub>2a</sub>' 2mm  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,3/4



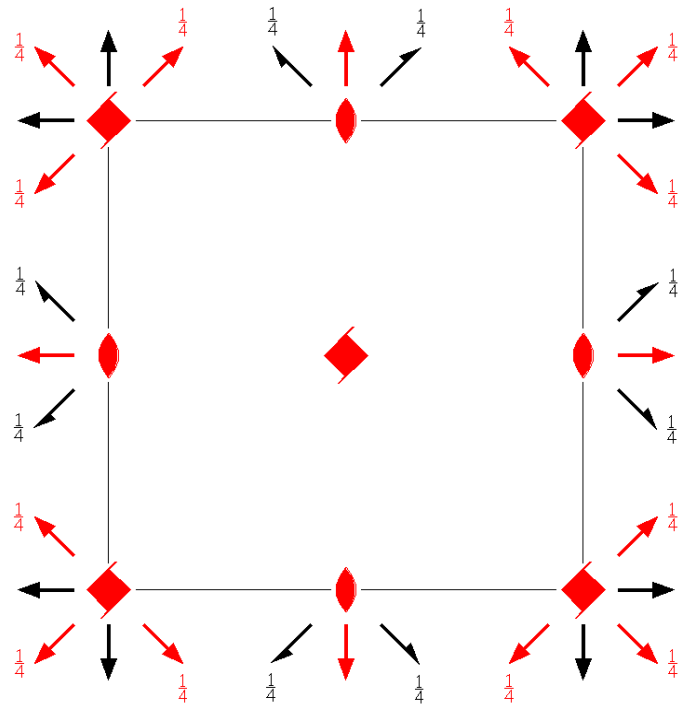
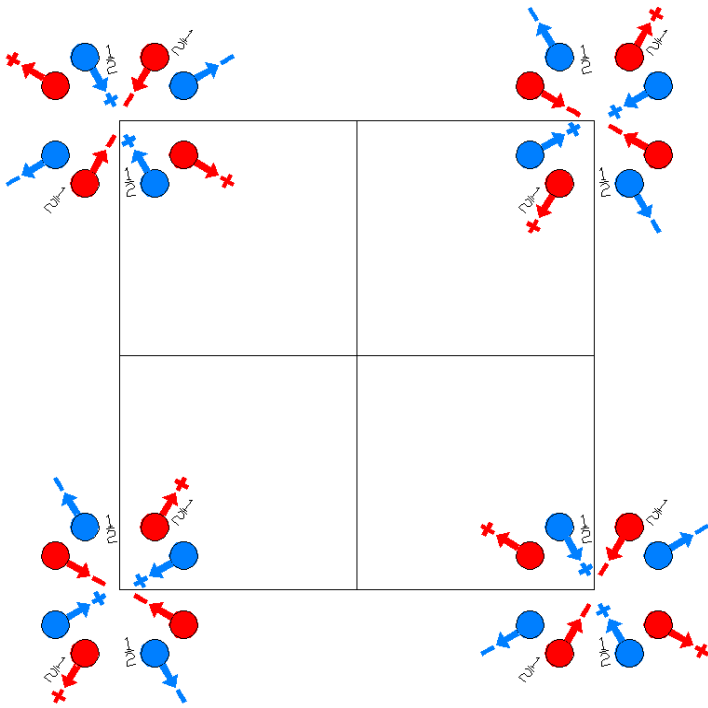
$P_P 4_2'22'$

93.10.785

4221'

$P_P 4_2'22'$

Tetragonal



Origin at 222 at  $4_2'21$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                    | (8) 2' x,x̄,1/4<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,1/2)'                    |

For (1,0,0)' + set

- |  |  |   |  |
|--|--|---|--|
| (1) t' (1,0,0)<br>(1 1,0,0)'               | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'       | (3) 4 <sup>+</sup> (0,0,1/2) 1/2,1/2,z<br>(4 <sub>z</sub>  1,0,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,-1/2,z<br>(4 <sub>z</sub> <sup>-1</sup>  1,0,1/2) |
| (5) 2' 1/2,y,0<br>(2 <sub>y</sub>  1,0,0)' | (6) 2' (1,0,0) x,0,0<br>(2 <sub>x</sub>  1,0,0)' | (7) 2 (1/2,1/2,0) x+1/2,x,1/4<br>(2 <sub>xy</sub>  1,0,1/2)         | (8) 2 (1/2,-1/2,0)x+1/2,x̄,1/4<br>(2 <sub>xy</sub> <sup>-</sup>  1,0,1/2)          |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

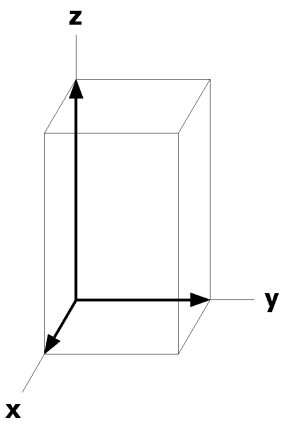
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 p 1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ] (7) y,x, $\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(4) y, $\bar{x},z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ] (8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]
8 o ..2'	x,x,3/4 [u, $\bar{u},w$ ]	$\bar{x},\bar{x},3/4$ [ $\bar{u},u,w$ ]	$\bar{x},x,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	x, $\bar{x},1/4$ [u,u, $\bar{w}$ ]
8 n ..2'	x,x,1/4 [u, $\bar{u},w$ ]	$\bar{x},\bar{x},1/4$ [ $\bar{u},u,w$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	x, $\bar{x},3/4$ [u,u, $\bar{w}$ ]
8 m .2'	x,1/2,0 [0,v,w]	$\bar{x},1/2,0$ [0,v, $\bar{w}$ ]	1/2,x,1/2 [ $\bar{v},0,w$ ]	1/2, $\bar{x},1/2$ [ $\bar{v},0,\bar{w}$ ]
8 l .2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,0 [0, $\bar{u},0$ ]	0, $\bar{x},0$ [0,u,0]
8 k .2'	x,1/2,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0,v, $\bar{w}$ ]	1/2,x,0 [ $\bar{v},0,w$ ]	1/2, $\bar{x},0$ [ $\bar{v},0,\bar{w}$ ]
8 j .2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,1/2 [0, $\bar{u},0$ ]	0, $\bar{x},1/2$ [0,u,0]
8 i 2'..	0,1/2,z [u,v,0]	1/2,0,z+1/2 [ $\bar{v},u,0$ ]	0,1/2, $\bar{z}$ [ $\bar{u},v,0$ ]	1/2,0, $\bar{z}+1/2$ [ $\bar{v},\bar{u},0$ ]
8 h 2..	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]
8 g 2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0,w]
4 f 2.2'2'	1/2,1/2,1/4 [0,0,w]	1/2,1/2,3/4 [0,0,w]		
4 e 2.2'2'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		
4 d 2'2'2.	0,1/2,1/2 [0,v,0]	1/2,0,0 [ $\bar{v},0,0$ ]		
4 c 2'2'2.	0,1/2,0 [0,v,0]	1/2,0,1/2 [ $\bar{v},0,0$ ]		
4 b 22'2'.	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]		
4 a 222.	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub>-4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/2,1/2,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x-1/4,x+1/4,1/4



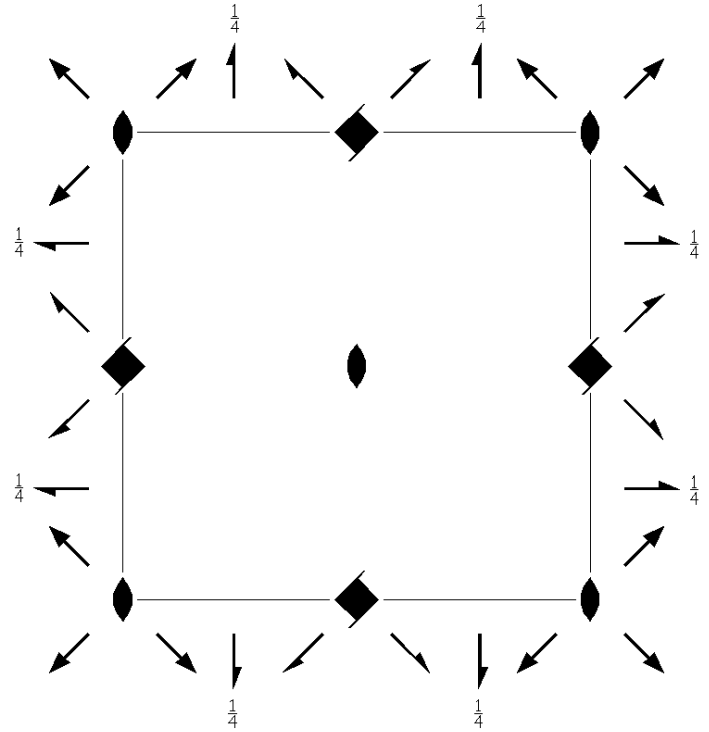
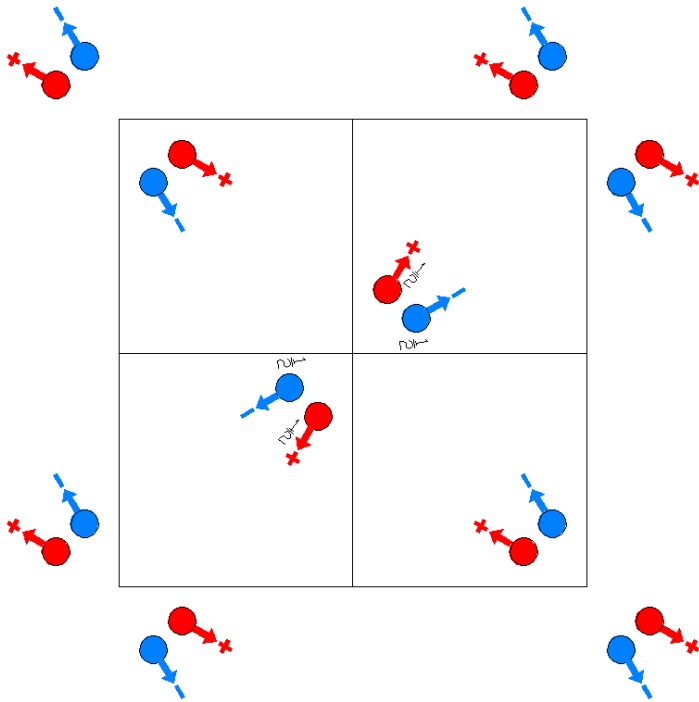
$P4_2 2_1 2$

422

Tetragonal

94.1.786

$P4_2 2_1 2$



Origin on 222 at 212

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                               | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,0)                      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

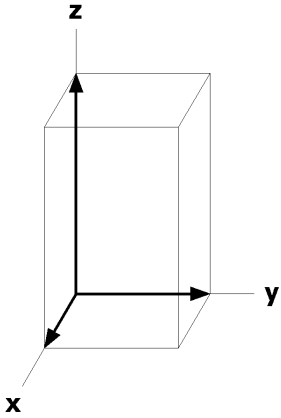
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]
		(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
4	f ..2	x,x,1/2 [u,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,0$ [ $\bar{u},u,0$ ]	$x+1/2,\bar{x}+1/2,0$ [ $u,\bar{u},0$ ]
4	e ..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $\bar{u},u,0$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $u,\bar{u},0$ ]
4	d 2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4	c 2..	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
2	b 2.22	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a 2.22	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4g'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P4_2 2_1 21'$

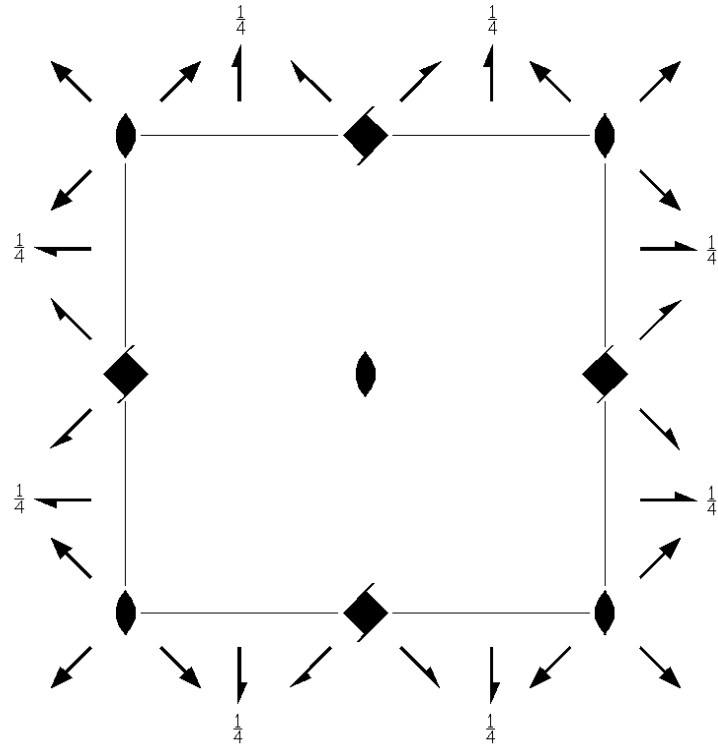
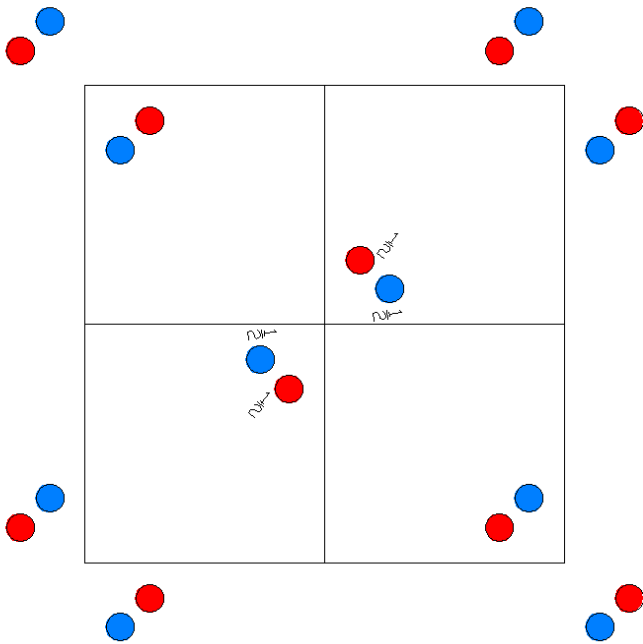
$4221'$

Tetragonal

94.2.787

$P4_2 2_1 21'$

1'



Origin on  $2221'$  at  $2121'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For 1 + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                               | (8) 2 x,x̄,0<br>(2 <sub>xy</sub>  0,0,0)  |

For 1' + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1'<br>(1 0,0,0)'   | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                     | (3) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                                | (8) 2' x,x̄,0<br>(2 <sub>xy</sub>  0,0,0)'   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.		Coordinates							
		1 +		1' +					
8	g 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}, \bar{y}, z$ [0,0,0]	(3) $\bar{y}+1/2, x+1/2, z+1/2$ [0,0,0]	(4) $y+1/2, \bar{x}+1/2, z+1/2$ [0,0,0]	(5) $\bar{x}+1/2, y+1/2, \bar{z}+1/2$ [0,0,0]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+1/2$ [0,0,0]	(7) $y, x, \bar{z}$ [0,0,0]	(8) $\bar{y}, \bar{x}, \bar{z}$ [0,0,0]
4	f ..21'	x,x,1/2 [0,0,0]	$\bar{x}, \bar{x}, 1/2$ [0,0,0]	$\bar{x}+1/2, x+1/2, 0$ [0,0,0]	$x+1/2, \bar{x}+1/2, 0$ [0,0,0]				
4	e ..21'	x,x,0 [0,0,0]	$\bar{x}, \bar{x}, 0$ [0,0,0]	$\bar{x}+1/2, x+1/2, 1/2$ [0,0,0]	$x+1/2, \bar{x}+1/2, 1/2$ [0,0,0]				
4	d 2..1'	0,1/2,z [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]				
4	c 2..1'	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]				
2	b 2.221'	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]						
2	a 2.221'	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]						

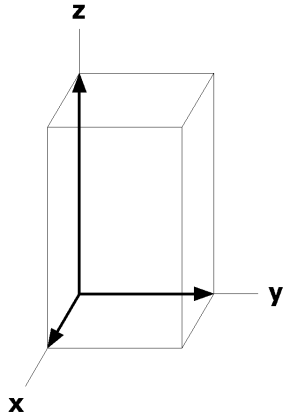
**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0





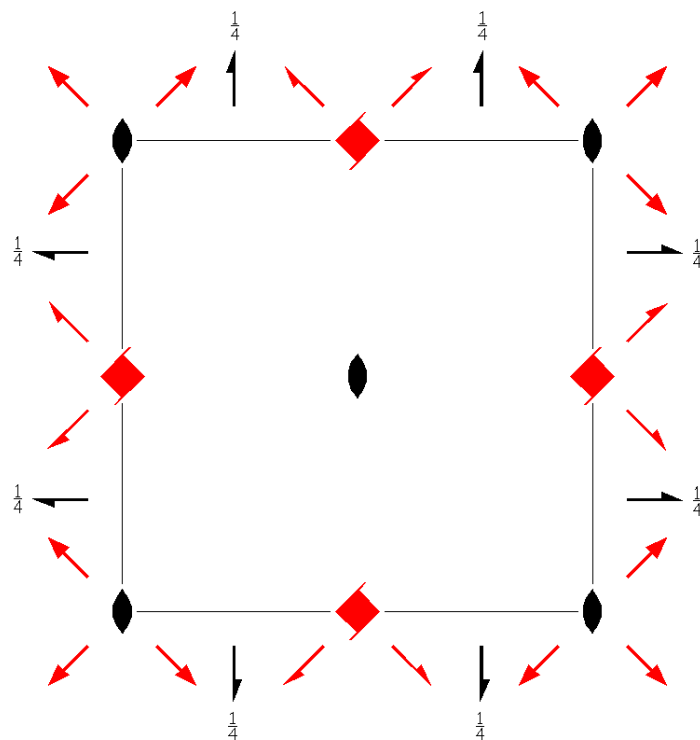
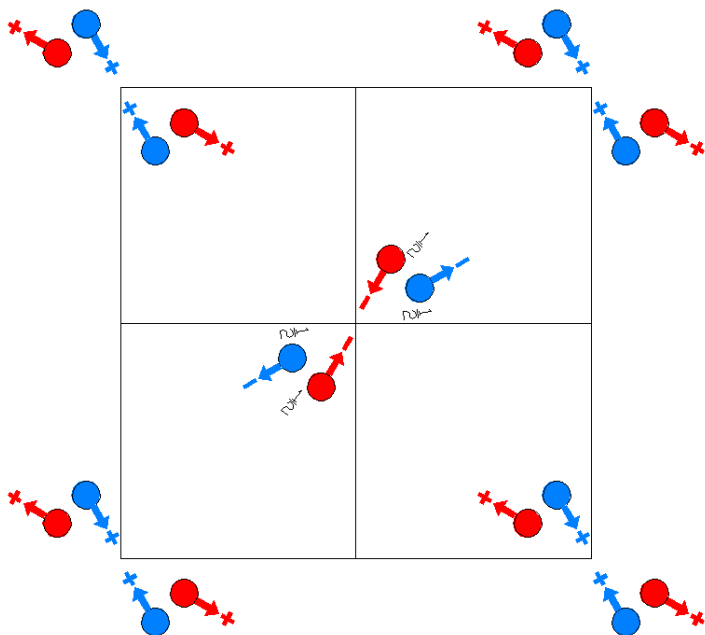
$P4_2'2_1'2'$

94.3.788

$4'22'$

$P4_2'2_1'2'$

Tetragonal



Origin on  $22'2'$  at  $212'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                              | (8) 2' x,x̄,0<br>(2 <sub>-xy</sub>  0,0,0)'  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

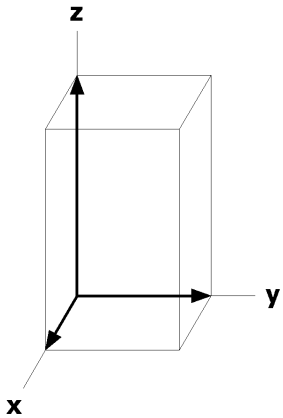
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]
		(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]
4	f ..2'	x,x,1/2 [u, $\bar{u}$ ,w]	$\bar{x},\bar{x},1/2$ [ $\bar{u},u,w$ ]	$\bar{x}+1/2,x+1/2,0$ [ $\bar{u},\bar{u},\bar{w}$ ]	$x+1/2,\bar{x}+1/2,0$ [ $u,u,\bar{w}$ ]
4	e ..2'	x,x,0 [u, $\bar{u}$ ,w]	$\bar{x},\bar{x},0$ [ $\bar{u},u,w$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $u,u,\bar{w}$ ]
4	d 2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]
4	c 2..	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]
2	b 2.2'2'	0,0,1/2 [0,0,w]	1/2,1/2,0 [0,0, $\bar{w}$ ]		
2	a 2.2'2'	0,0,0 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p4g'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



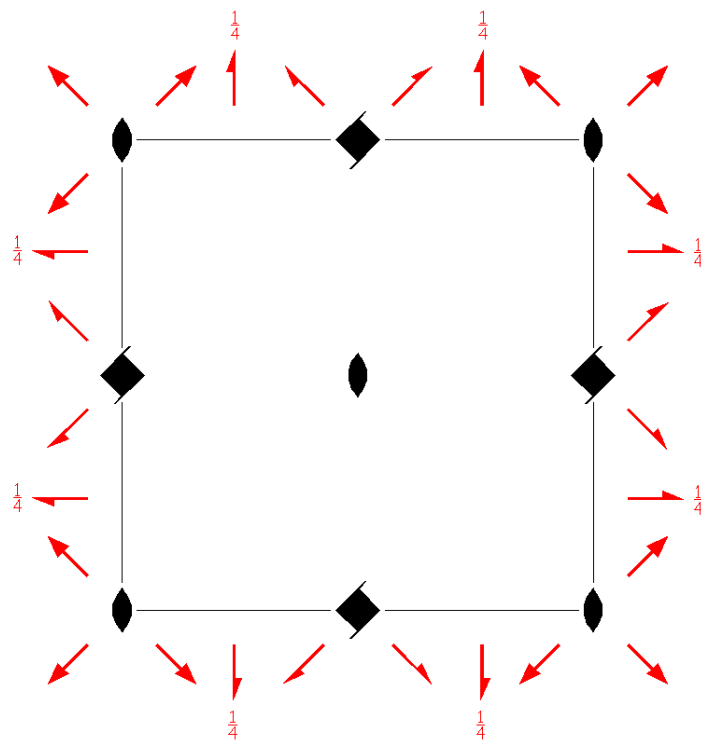
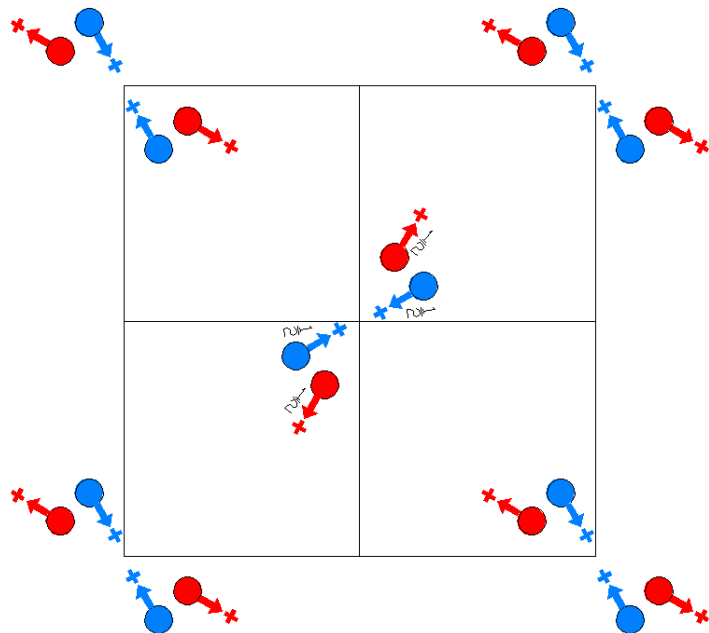
$P4_2 2_1 '2'$

$42'2'$

Tetragonal

94.4.789

$P4_2 2_1 '2'$



Origin on  $22'2'$  at  $212'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 <sub>0,0,z</sub><br>(2 <sub>z</sub>  0,0,0)             | (3) 4 <sup>+</sup> <sub>(0,0,1/2)</sub><br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> <sub>(0,0,1/2)</sub><br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) 2' <sub>(0,1/2,0)</sub><br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (6) 2' <sub>(1/2,0,0)</sub><br>(2 <sub>x</sub>  1/2,1/2,1/2)' | (7) 2' <sub>x,x,0</sub><br>(2 <sub>xy</sub>  0,0,0)'                     | (8) 2' <sub>x,x̄,0</sub><br>(2 <sub>xy</sub> <sup>-</sup>  0,0,0)'                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

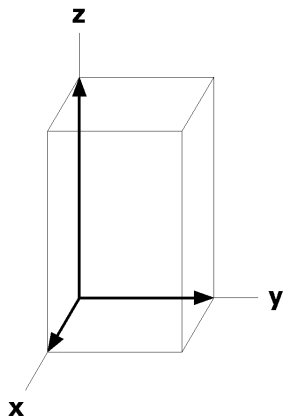
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
8	g 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
		(3) $\bar{y}+1/2, x+1/2, z+1/2$ [ $\bar{v}, u, w$ ]	(4) $y+1/2, \bar{x}+1/2, z+1/2$ [ $v, \bar{u}, w$ ]		
		(5) $\bar{x}+1/2, y+1/2, \bar{z}+1/2$ [ $u, \bar{v}, w$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]		
		(7) y,x, $\bar{z}$ [ $\bar{v}, \bar{u}, w$ ]	(8) $\bar{y}, \bar{x}, \bar{z}$ [ $v, u, w$ ]		
4	f ..2'	x,x,1/2 [u, $\bar{u}$ ,w]	$\bar{x}, \bar{x}, 1/2$ [ $\bar{u}, u, w$ ]	$\bar{x}+1/2, x+1/2, 0$ [u,u,w]	$x+1/2, \bar{x}+1/2, 0$ [ $\bar{u}, \bar{u}, w$ ]
4	e ..2'	x,x,0 [u, $\bar{u}$ ,w]	$\bar{x}, \bar{x}, 0$ [ $\bar{u}, u, w$ ]	$\bar{x}+1/2, x+1/2, 1/2$ [u,u,w]	$x+1/2, \bar{x}+1/2, 1/2$ [ $\bar{u}, \bar{u}, w$ ]
4	d 2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]
4	c 2..	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]
2	b 2.2'2'	0,0,1/2 [0,0,w]	1/2,1/2,0 [0,0,w]		
2	a 2.2'2'	0,0,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p4gm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



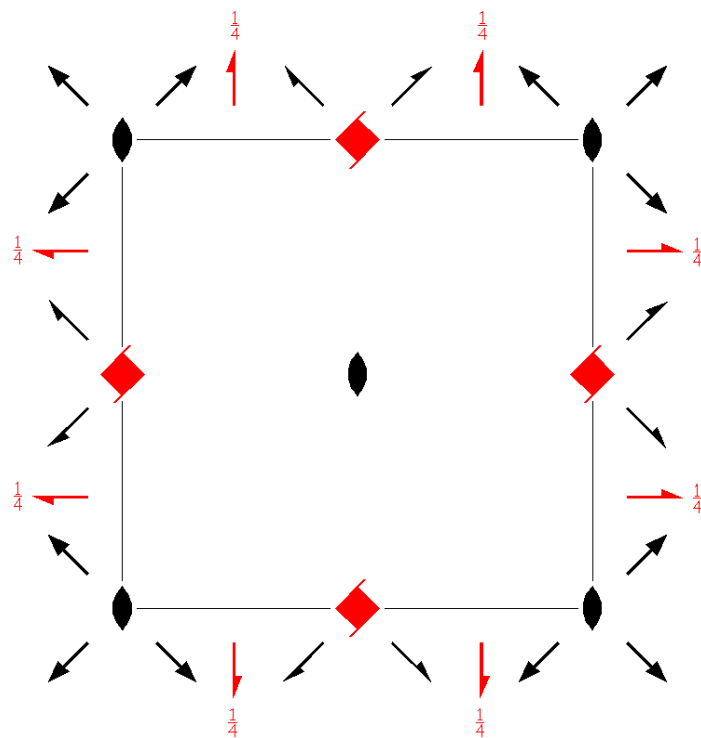
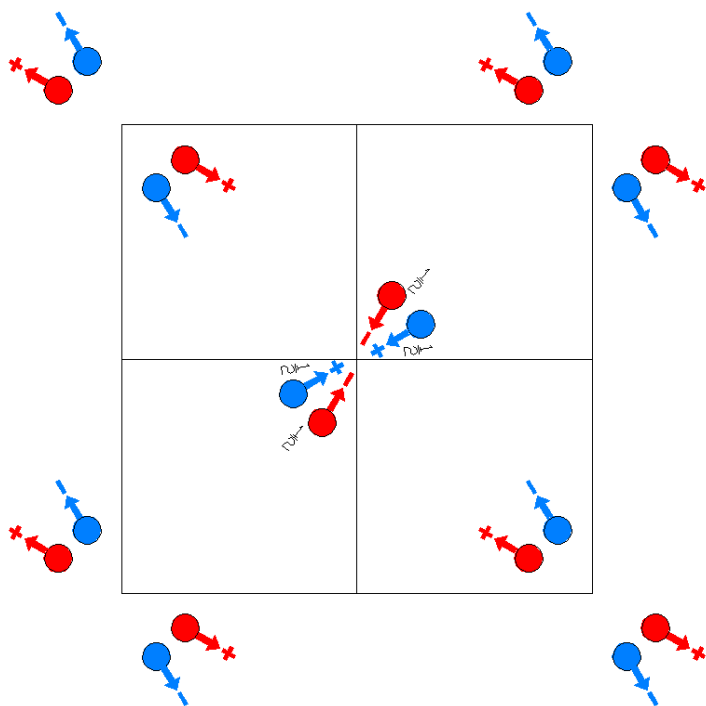
$P4_2'2_1'2$

94.5.790

$4'2'2$

$P4_2'2_1'2$

Tetragonal



Origin on 222 at 212

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                       | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,0)                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

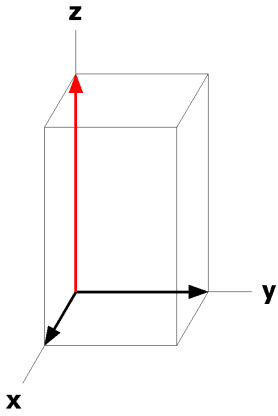
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	g 1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
		(3) $\bar{y}+1/2, x+1/2, z+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(4) $y+1/2, \bar{x}+1/2, z+1/2$ [ $\bar{v}, u, \bar{w}$ ]		
		(5) $\bar{x}+1/2, y+1/2, \bar{z}+1/2$ [u, $\bar{v}$ ,w]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]		
		(7) $y, x, \bar{z}$ [ $\bar{v}, u, \bar{w}$ ]	(8) $\bar{y}, \bar{x}, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
4	f ..2	$x, x, 1/2$ [u,u,0]	$\bar{x}, \bar{x}, 1/2$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}+1/2, x+1/2, 0$ [u, $\bar{u}$ ,0]	$x+1/2, \bar{x}+1/2, 0$ [ $\bar{u}, u, 0$ ]
4	e ..2	$x, x, 0$ [u,u,0]	$\bar{x}, \bar{x}, 0$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}+1/2, x+1/2, 1/2$ [u, $\bar{u}$ ,0]	$x+1/2, \bar{x}+1/2, 1/2$ [ $\bar{u}, u, 0$ ]
4	d 2..	$0, 1/2, z$ [0,0,w]	$0, 1/2, z+1/2$ [0,0, $\bar{w}$ ]	$1/2, 0, \bar{z}+1/2$ [0,0,w]	$1/2, 0, \bar{z}$ [0,0, $\bar{w}$ ]
4	c 2..	$0, 0, z$ [0,0,w]	$1/2, 1/2, z+1/2$ [0,0, $\bar{w}$ ]	$1/2, 1/2, \bar{z}+1/2$ [0,0,w]	$0, 0, \bar{z}$ [0,0, $\bar{w}$ ]
2	b 2.22	$0, 0, 1/2$ [0,0,0]	$1/2, 1/2, 0$ [0,0,0]		
2	a 2.22	$0, 0, 0$ [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4g'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



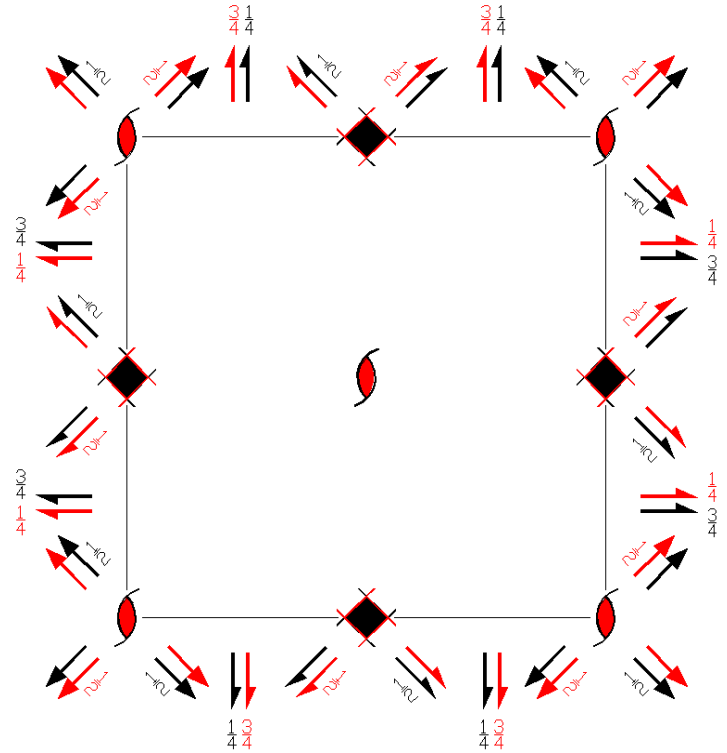
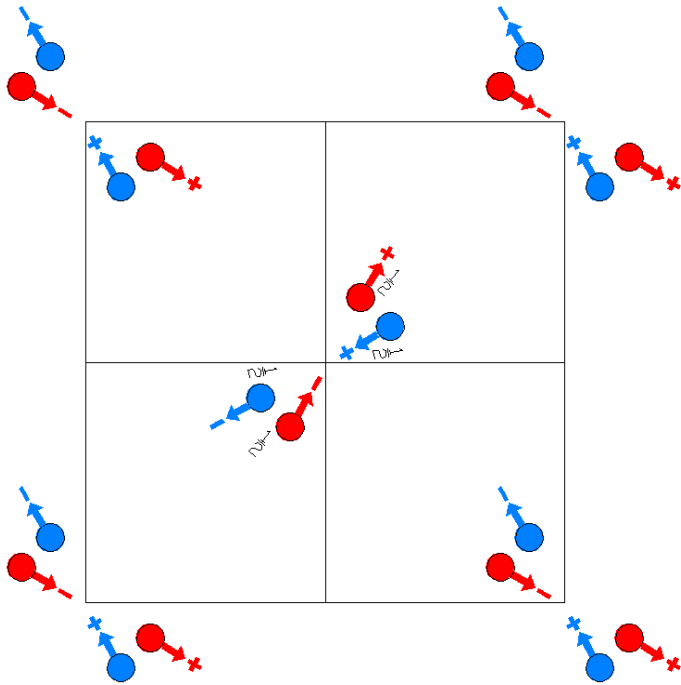
$P_{2c} 4_2 2_1 2$

4221'

Tetragonal

94.6.791

$P_{2c} 4_2 2_1 2$



Origin on 2'22 at 2'12

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                   | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                             | (8) 2 x,x̄,0<br>(2 <sub>xy</sub>  0,0,0)   |

For (0,0,1)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) t' (0,0,1)<br>(1 0,0,1)'                               | (2) 2 (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)               | (3) 4 <sup>+</sup> ' (0,0,3/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,3/2)' | (4) 4 <sup>-</sup> ' (0,0,3/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,3/2) |
| (5) 2 (0,1/2,0) 1/4,y,3/4<br>(2 <sub>y</sub>  1/2,1/2,3/2) | (6) 2' (1/2,0,0) x,1/4,3/4<br>(2 <sub>x</sub>  1/2,1/2,3/2)' | (7) 2 x,x,1/2<br>(2 <sub>xy</sub>  0,0,1)                                | (8) 2' x,x̄,1/2<br>(2 <sub>xy</sub>  0,0,1)'  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.		Coordinates			
			(0,0,0) +	(0,0,1)' +	
16	g 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]		
		(3) $\bar{y}+1/2, x+1/2, z+1/2$ [ $\bar{v}, u, w$ ]	(4) $y+1/2, \bar{x}+1/2, z+1/2$ [ $\bar{v}, u, \bar{w}$ ]		
		(5) $\bar{x}+1/2, y+1/2, \bar{z}+1/2$ [u, $\bar{v}, w$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+1/2$ [u, $\bar{v}, \bar{w}$ ]		
		(7) $y, x, \bar{z}$ [ $\bar{v}, \bar{u}, w$ ]	(8) $\bar{y}, \bar{x}, z$ [ $\bar{v}, u, \bar{w}$ ]		
8	f ..2	x,x,1/2 [u,u,0]	$\bar{x}, \bar{x}, 1/2$ [u,u,0]	$\bar{x}+1/2, x+1/2, 0$ [u, $\bar{u}, 0$ ]	$x+1/2, \bar{x}+1/2, 0$ [u, $\bar{u}, 0$ ]
8	e ..2'	x,x,0 [u, $\bar{u}, w$ ]	$\bar{x}, \bar{x}, 0$ [u, $\bar{u}, \bar{w}$ ]	$\bar{x}+1/2, x+1/2, 1/2$ [ $\bar{u}, u, w$ ]	$x+1/2, \bar{x}+1/2, 1/2$ [ $\bar{u}, u, \bar{w}$ ]
8	d 2'..	0,1/2,z [u,v,0]	0,1/2,z+1/2 [ $\bar{v}, u, 0$ ]	1/2,0, $\bar{z}+1/2$ [u, $\bar{v}, 0$ ]	1/2,0, $\bar{z}$ [ $\bar{v}, \bar{u}, 0$ ]
8	c 2'..	0,0,z [u,v,0]	1/2,1/2,z+1/2 [ $\bar{v}, u, 0$ ]	1/2,1/2, $\bar{z}+1/2$ [u, $\bar{v}, 0$ ]	0,0, $\bar{z}$ [ $\bar{v}, \bar{u}, 0$ ]
4	b 2'.22'	0,0,1/2 [u,u,0]	1/2,1/2,0 [u, $\bar{u}, 0$ ]		
4	a 2'.2'2	0,0,0 [u, $\bar{u}, 0$ ]	1/2,1/2,1/2 [u,u,0]		

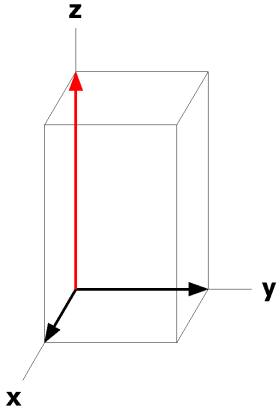
**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p<sub>2b</sub> 2mg  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [1,1,0] p<sub>2a</sub> 2mm  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/2





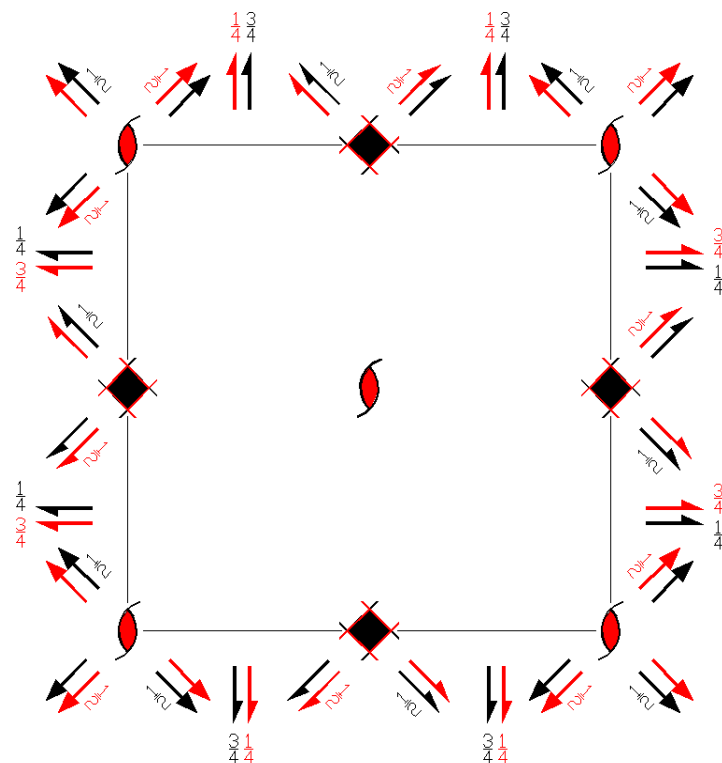
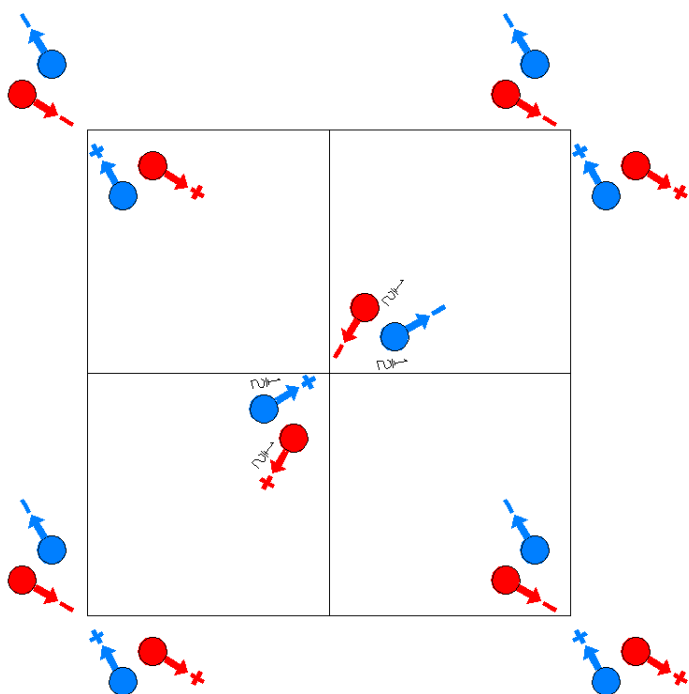
$P_{2c} 4_2' 2_1' 2$

94.7.792

4221'

$P_{2c} 4_2' 2_1' 2$

Tetragonal



Origin on  $2'2'2'$  at  $2(1,2')(2',1)$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

For  $(0,0,0) +$  set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                   | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)'                     | (3) $4^+$ (0,0,1/2) 0,1/2,z<br>( $4_z$  1/2,1/2,1/2)' | (4) $4^-$ (0,0,1/2) 1/2,0,z<br>( $4_z^{-1}$  1/2,1/2,1/2) |
| (5) $2$ (0,1/2,0) 1/4,y,1/4<br>( $2_y$  1/2,1/2,1/2) | (6) $2'$ (1/2,0,0) x,1/4,1/4<br>( $2_x$  1/2,1/2,1/2)' | (7) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)'                 | (8) $2$ $x, \bar{x}, 0$<br>( $2_{\bar{xy}}$  0,0,0)       |

For  $(0,0,1) +$  set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'                         | (2) $2$ (0,0,1) 0,0,z<br>( $2_z$  0,0,1)             | (3) $4^+$ (0,0,3/2) 0,1/2,z<br>( $4_z$  1/2,1/2,3/2) | (4) $4^-$ (0,0,3/2) 1/2,0,z<br>( $4_z^{-1}$  1/2,1/2,3/2)' |
| (5) $2'$ (0,1/2,0) 1/4,y,3/4<br>( $2_y$  1/2,1/2,3/2)' | (6) $2$ (1/2,0,0) x,1/4,3/4<br>( $2_x$  1/2,1/2,3/2) | (7) $2$ x,x,1/2<br>( $2_{xy}$  0,0,1)                | (8) $2'$ $x, \bar{x}, 1/2$<br>( $2_{\bar{xy}}$  0,0,1)'    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

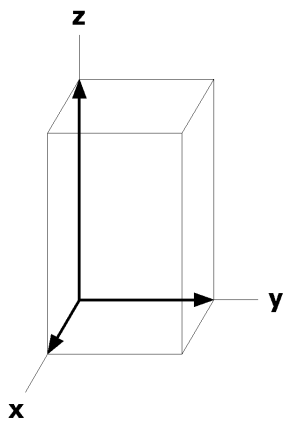
Multiplicity, Wyckoff letter, Site Symmetry.		Coordinates			
		(0,0,0) +		(0,0,1)' +	
16 g 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]			
	(3) $\bar{y}+1/2, x+1/2, z+1/2$ [v, $\bar{u}, \bar{w}$ ]	(4) $y+1/2, \bar{x}+1/2, z+1/2$ [v, $\bar{u}, w$ ]			
	(5) $\bar{x}+1/2, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]			
	(7) $y, x, \bar{z}$ [ $\bar{v}, \bar{u}, w$ ]	(8) $\bar{y}, \bar{x}, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]			
8 f ..2	x,x,1/2 [u,u,0]	$\bar{x}, \bar{x}, 1/2$ [u,u,0]	$\bar{x}+1/2, x+1/2, 0$ [ $\bar{u}, u, 0$ ]	$x+1/2, \bar{x}+1/2, 0$ [ $\bar{u}, u, 0$ ]	
8 e ..2'	x,x,0 [u, $\bar{u}, w$ ]	$\bar{x}, \bar{x}, 0$ [u, $\bar{u}, \bar{w}$ ]	$\bar{x}+1/2, x+1/2, 1/2$ [ $\bar{u}, \bar{u}, \bar{w}$ ]	$x+1/2, \bar{x}+1/2, 1/2$ [ $\bar{u}, \bar{u}, w$ ]	
8 d 2'..	0,1/2,z [u,v,0]	0,1/2,z+1/2 [v, $\bar{u}, 0$ ]	1/2,0, $\bar{z}+1/2$ [ $\bar{u}, v, 0$ ]	1/2,0, $\bar{z}$ [ $\bar{v}, \bar{u}, 0$ ]	
8 c 2'..	0,0,z [u,v,0]	1/2,1/2,z+1/2 [v, $\bar{u}, 0$ ]	1/2,1/2, $\bar{z}+1/2$ [ $\bar{u}, v, 0$ ]	0,0, $\bar{z}$ [ $\bar{v}, \bar{u}, 0$ ]	
4 b 2'.22'	0,0,1/2 [u,u,0]	1/2,1/2,0 [ $\bar{u}, u, 0$ ]			
4 a 2'.22'	0,0,0 [u,u,0]	1/2,1/2,1/2 [u, $\bar{u}, 0$ ]			

**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] p<sub>2b</sub>'-2mg  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,3/4

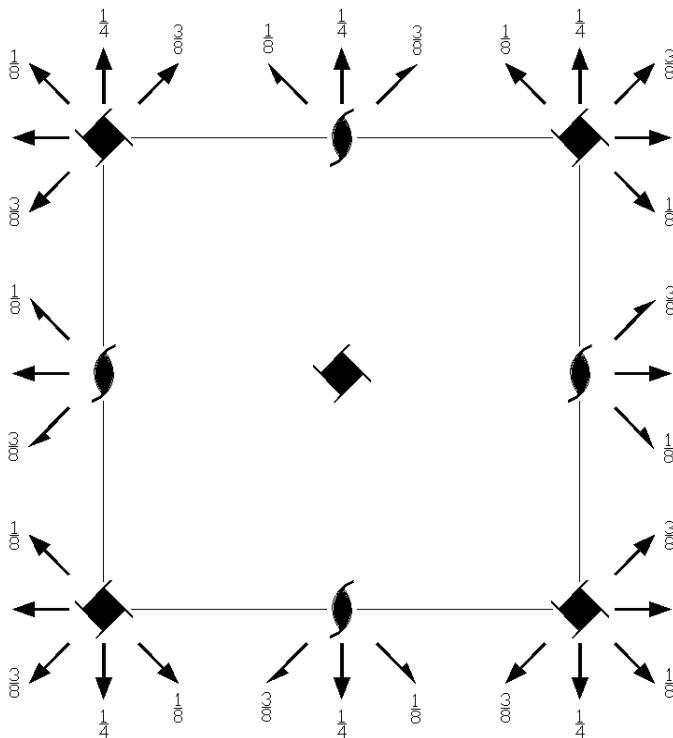
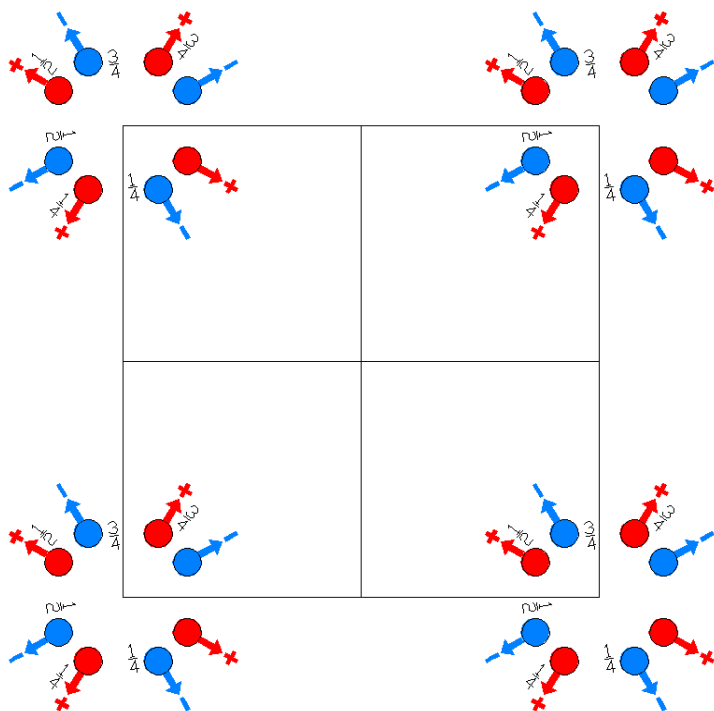
Along [1,1,0] p<sub>2a</sub>'-2mm  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/2



P4<sub>3</sub>22  
95.1.793

422  
P4<sub>3</sub>22

Tetragonal



Origin on 2 [0,1,0] at 4<sub>3</sub> (1,2) 1

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 4 <sup>+</sup> (0,0,3/4) 0,0,z<br>(4 <sub>z</sub>  0,0,3/4) | (4) 4 <sup>-</sup> (0,0,1/4) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/4) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)         | (7) 2 x,x,1/8<br>(2 <sub>xy</sub>  0,0,1/4)                     | (8) 2 x,x̄,3/8<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,3/4)                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

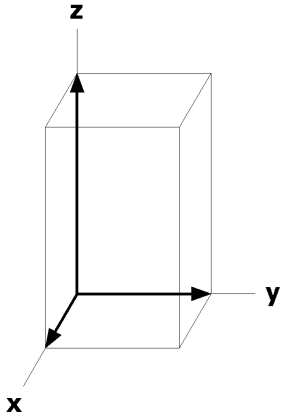
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	d 1	(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z+3/4$ [ $\bar{v}, u, w$ ]	(4) $y, \bar{x}, z+1/4$ [ $v, \bar{u}, w$ ]
		(5) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(6) $x, \bar{y}, \bar{z}+1/2$ [ $u, \bar{v}, \bar{w}$ ]	(7) $y, x, \bar{z}+1/4$ [ $v, u, \bar{w}$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+3/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]
4	c ..2	$x, x, 5/8$ [ $u, u, 0$ ]	$\bar{x}, \bar{x}, 1/8$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}, x, 3/8$ [ $\bar{u}, u, 0$ ]	$x, \bar{x}, 7/8$ [ $u, \bar{u}, 0$ ]
4	b .2.	$1/2, y, 0$ [ $0, v, 0$ ]	$1/2, \bar{y}, 1/2$ [ $0, \bar{v}, 0$ ]	$\bar{y}, 1/2, 3/4$ [ $\bar{v}, 0, 0$ ]	$y, 1/2, 1/4$ [ $v, 0, 0$ ]
4	a .2.	$0, y, 0$ [ $0, v, 0$ ]	$0, \bar{y}, 1/2$ [ $0, \bar{v}, 0$ ]	$\bar{y}, 0, 3/4$ [ $\bar{v}, 0, 0$ ]	$y, 0, 1/4$ [ $v, 0, 0$ ]

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'g'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $x,0,1/4$

Along  $[1,1,0]$   $p2m'g'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,1/8$



P4<sub>3</sub>221'

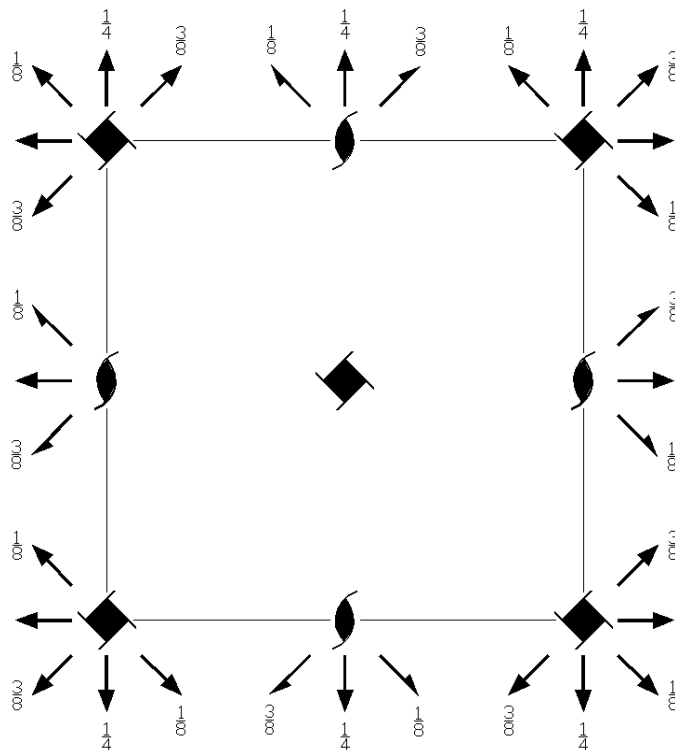
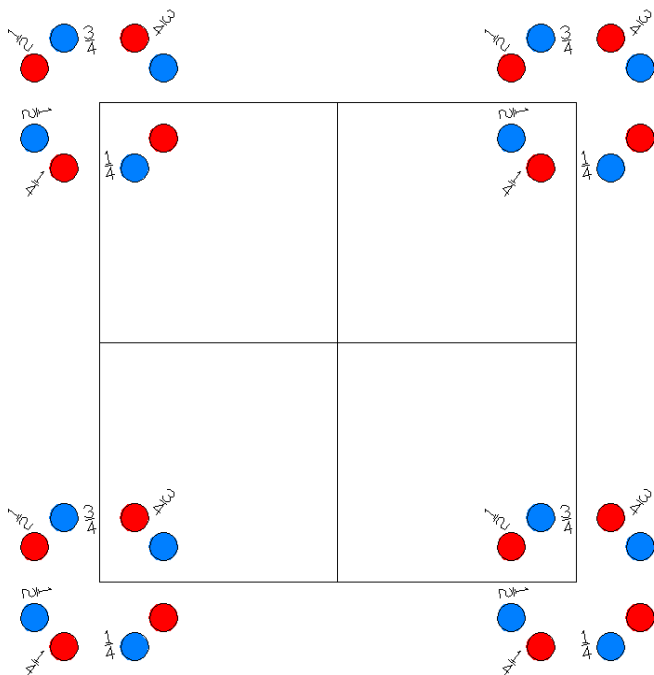
95.2.794

4221'

P4<sub>3</sub>221'

Tetragonal

1'



Origin on 2 [0,1,0]1' at 4<sub>3</sub> (1,2) 11'

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

### Symmetry Operations

For 1 + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 4 <sup>+</sup> (0,0,3/4) 0,0,z<br>(4 <sub>z</sub>  0,0,3/4) | (4) 4 <sup>-</sup> (0,0,1/4) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/4) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)         | (7) 2 x,x,1/8<br>(2 <sub>xy</sub>  0,0,1/4)                     | (8) 2 x,x̄,3/8<br>(2 <sub>xy</sub>  0,0,3/4)                                  |

For 1' + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1'<br>(1 0,0,0)'                     | (2) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)' | (3) 4 <sup>+</sup> ' (0,0,3/4) 0,0,z<br>(4 <sub>z</sub>  0,0,3/4)' | (4) 4 <sup>-</sup> ' (0,0,1/4) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/4)' |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'         | (7) 2' x,x,1/8<br>(2 <sub>xy</sub>  0,0,1/4)'                      | (8) 2' x,x̄,3/8<br>(2 <sub>xy</sub>  0,0,3/4)'                                   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

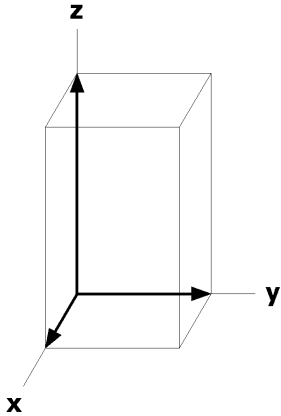
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +		1' +	
8 d 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z+1/2$ [0,0,0]	(3) $\bar{y},x,z+3/4$ [0,0,0]	(4) $y,\bar{x},z+1/4$ [0,0,0]
	(5) $\bar{x},y,\bar{z}$ [0,0,0]	(6) $x,\bar{y},\bar{z}+1/2$ [0,0,0]	(7) $y,x,\bar{z}+1/4$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}+3/4$ [0,0,0]
4 c ..21'	x,x,5/8 [0,0,0]	$\bar{x},\bar{x},1/8$ [0,0,0]	$\bar{x},x,3/8$ [0,0,0]	$x,\bar{x},7/8$ [0,0,0]
4 b .2.1'	1/2,y,0 [0,0,0]	1/2, $\bar{y},1/2$ [0,0,0]	$\bar{y},1/2,3/4$ [0,0,0]	y,1/2,1/4 [0,0,0]
4 a .2.1'	0,y,0 [0,0,0]	0, $\bar{y},1/2$ [0,0,0]	$\bar{y},0,3/4$ [0,0,0]	y,0,1/4 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,1/4

Along [1,1,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/8



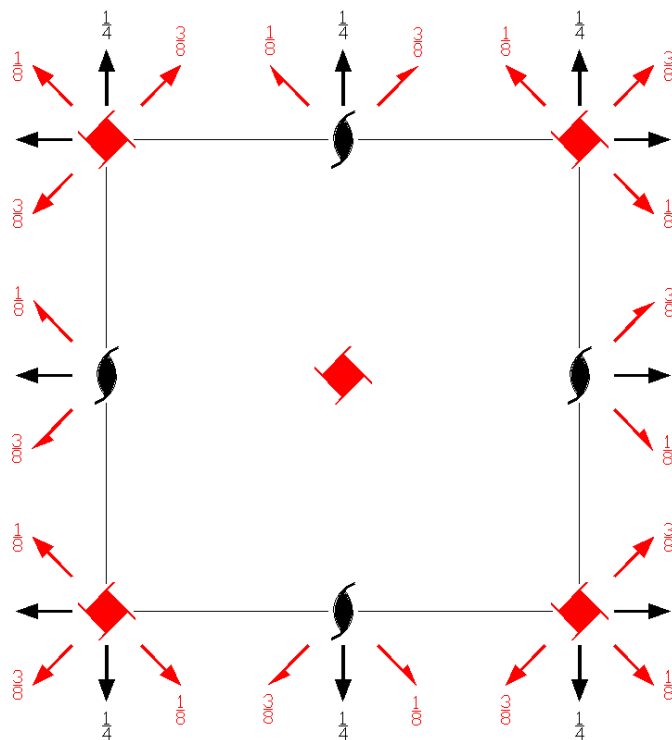
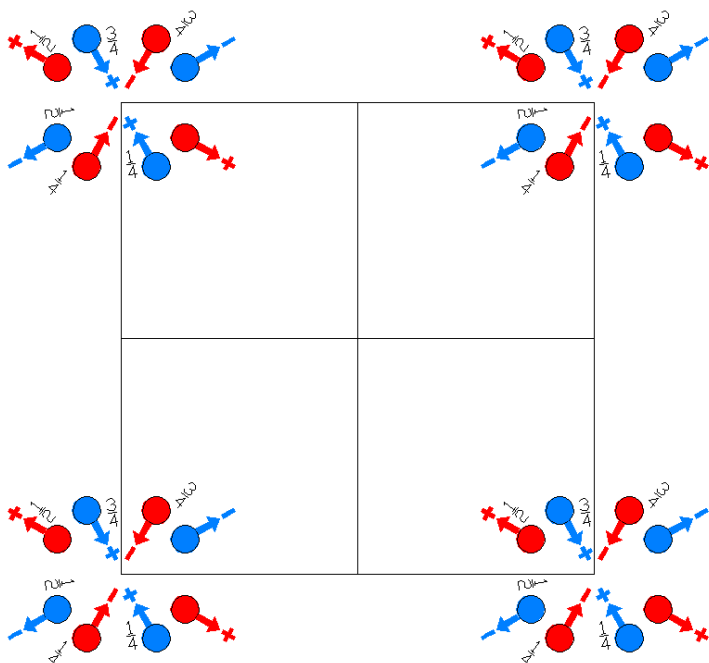
$P4_3'22'$

95.3.795

$4'22'$

$P4_3'22'$

Tetragonal



Origin on 2  $[0,1,0]$  at  $4_3'$   $(1,2) 1$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/8$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 4 <sup>+</sup> (0,0,3/4) 0,0,z<br>(4 <sub>z</sub>  0,0,3/4)' | (4) 4 <sup>-</sup> (0,0,1/4) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/4)' |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)         | (7) 2' x,x,1/8<br>(2 <sub>xy</sub>  0,0,1/4)'                    | (8) 2' x,x,3/8<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,3/4)'                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	d 1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+3/4$ [ $v,\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/4$ [ $\bar{v},u,\bar{w}$ ]
		(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}+1/4$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+3/4$ [ $v,u,w$ ]
4	c ..2'	$x,x,5/8$ [ $u,\bar{u},w$ ]	$\bar{x},\bar{x},1/8$ [ $\bar{u},u,w$ ]	$\bar{x},x,3/8$ [ $\bar{u},\bar{u},\bar{w}$ ]	$x,\bar{x},7/8$ [ $u,u,\bar{w}$ ]
4	b .2.	$1/2,y,0$ [ $0,v,0$ ]	$1/2,\bar{y},1/2$ [ $0,\bar{v},0$ ]	$\bar{y},1/2,3/4$ [ $v,0,0$ ]	$y,1/2,1/4$ [ $\bar{v},0,0$ ]
4	a .2.	$0,y,0$ [ $0,v,0$ ]	$0,\bar{y},1/2$ [ $0,\bar{v},0$ ]	$\bar{y},0,3/4$ [ $v,0,0$ ]	$y,0,1/4$ [ $\bar{v},0,0$ ]

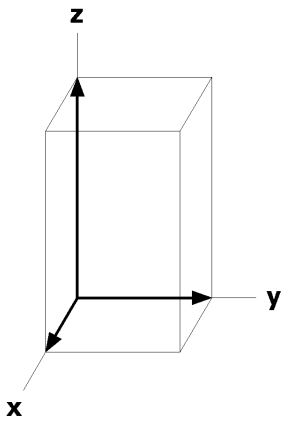
**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4'm'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'g'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $x,0,1/4$

Along  $[1,1,0]$   $p2'mg'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,1/8$

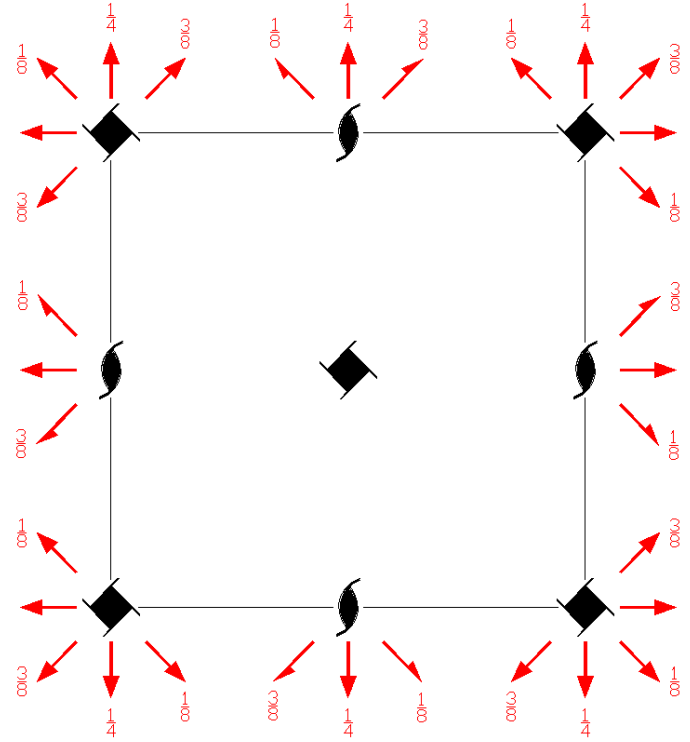
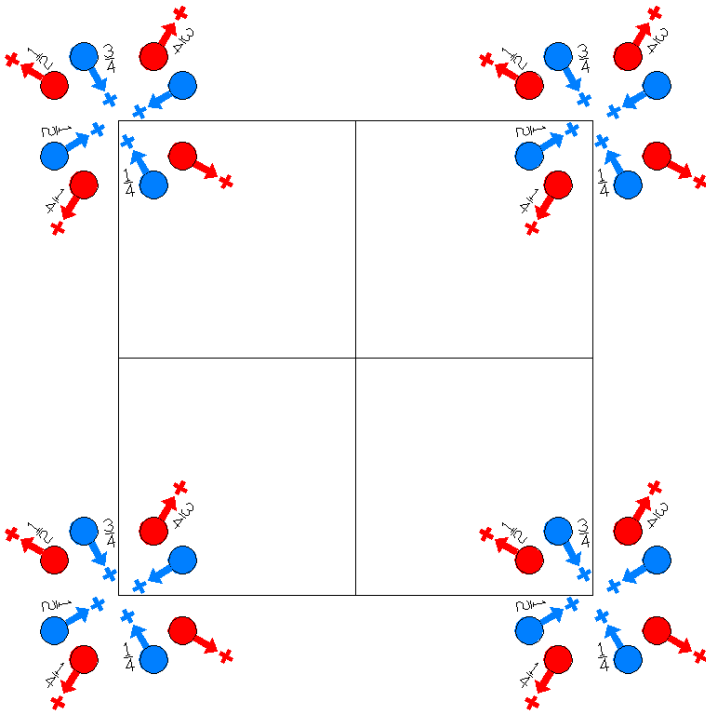




$P4_3 2' 2'$   
95.4.796

$42' 2'$   
 $P4_3 2' 2'$

Tetragonal



Origin on  $2'$   $[0,1,0]$  at  $4_3 (1,2') 1$

Asymmetric unit  $0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 4 <sup>+</sup> (0,0,3/4) 0,0,z<br>(4 <sub>z</sub>  0,0,3/4) | (4) 4 <sup>-</sup> (0,0,1/4) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/4) |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'       | (7) 2' x,x,1/8<br>(2 <sub>xy</sub>  0,0,1/4)'                   | (8) 2' x,x̄,3/8<br>(2 <sub>xy</sub> ̄ 0,0,3/4)'                               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

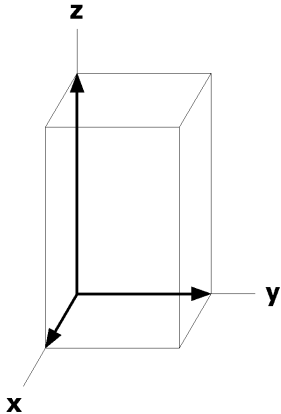
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	d 1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+3/4$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/4$ [ $v,\bar{u},w$ ]
		(5) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}+1/4$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+3/4$ [ $v,u,w$ ]
4	c ..2'	$x,x,5/8$ [ $u,\bar{u},w$ ]	$\bar{x},\bar{x},1/8$ [ $\bar{u},u,w$ ]	$\bar{x},x,3/8$ [ $u,u,w$ ]	$x,\bar{x},7/8$ [ $\bar{u},\bar{u},w$ ]
4	b .2'	$1/2,y,0$ [ $u,0,w$ ]	$1/2,\bar{y},1/2$ [ $\bar{u},0,w$ ]	$\bar{y},1/2,3/4$ [ $0,u,w$ ]	$y,1/2,1/4$ [ $0,\bar{u},w$ ]
4	a .2'	$0,y,0$ [ $u,0,w$ ]	$0,\bar{y},1/2$ [ $\bar{u},0,w$ ]	$\bar{y},0,3/4$ [ $0,u,w$ ]	$y,0,1/4$ [ $0,\bar{u},w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,1/4

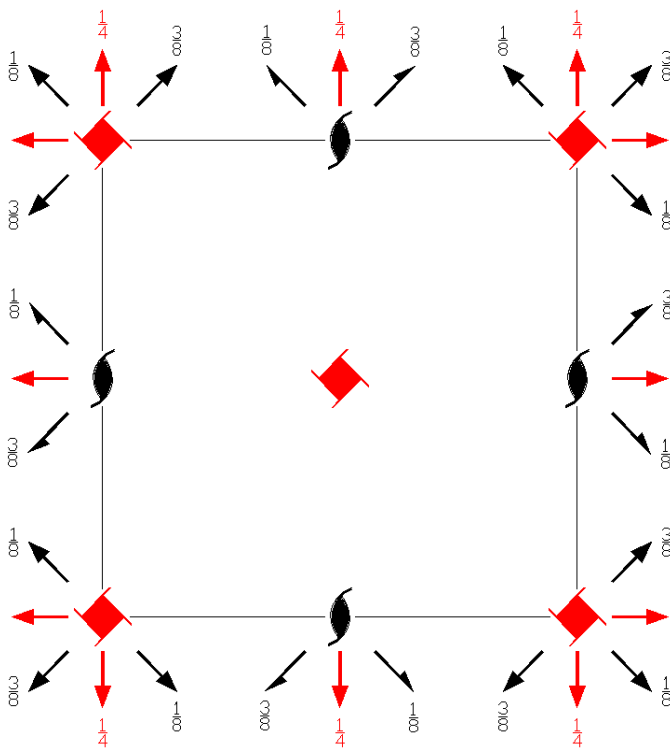
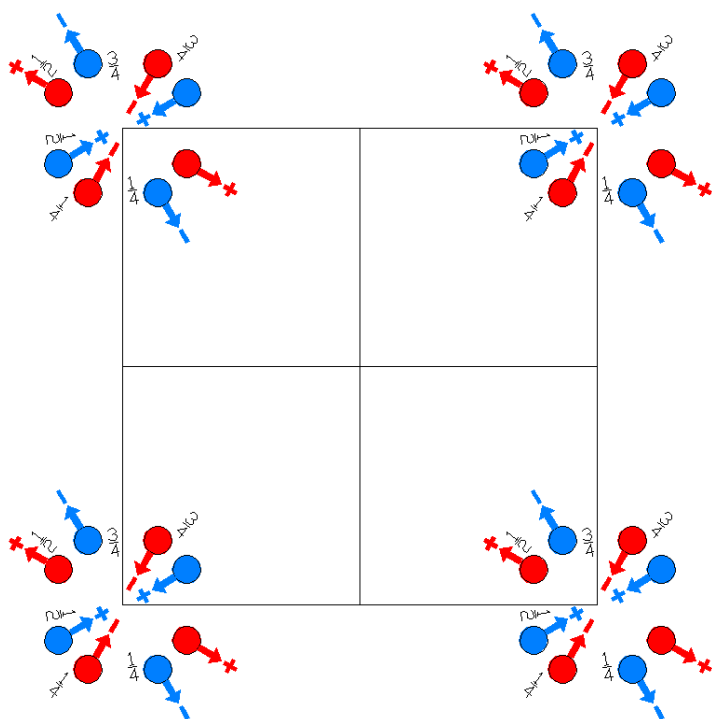
Along [1,1,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/8



$P4_3'2'2$   
95.5.797

$4'2'2$   
 $P4_3'2'2$

Tetragonal



Origin on 2  $[0,1,0]$  at  $4_3 (1,2) 1$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                       | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 4 <sup>+</sup> (0,0,3/4) 0,0,z<br>(4 <sub>z</sub>  0,0,3/4)' | (4) 4 <sup>-</sup> (0,0,1/4) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/4)' |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'       | (7) 2 x,x,1/8<br>(2 <sub>xy</sub>  0,0,1/4)                      | (8) 2 x, $\bar{x}$ ,3/8<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,3/4)             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

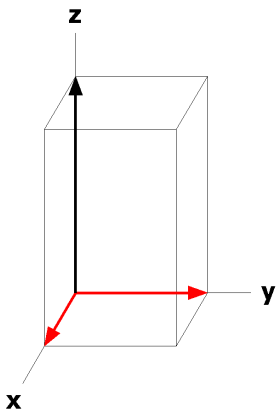
		Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.			
8	d 1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z+3/4$ [ $v, \bar{u}, \bar{w}$ ]	(4) $y, \bar{x}, z+1/4$ [ $\bar{v}, u, \bar{w}$ ]
		(5) $\bar{x}, y, \bar{z}$ [ $u, \bar{v}, w$ ]	(6) $x, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]	(7) $y, x, \bar{z}+1/4$ [ $v, u, \bar{w}$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+3/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]
4	c ..2	$x, x, 5/8$ [u,u,0]	$\bar{x}, \bar{x}, 1/8$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}, x, 3/8$ [u, $\bar{u}$ ,0]	$x, \bar{x}, 7/8$ [ $\bar{u}, u, 0$ ]
4	b .2'	$1/2, y, 0$ [u,0,w]	$1/2, \bar{y}, 1/2$ [ $\bar{u}, 0, w$ ]	$\bar{y}, 1/2, 3/4$ [0, $\bar{u}, \bar{w}$ ]	$y, 1/2, 1/4$ [0,u, $\bar{w}$ ]
4	a .2'	$0, y, 0$ [u,0,w]	$0, \bar{y}, 1/2$ [ $\bar{u}, 0, w$ ]	$\bar{y}, 0, 3/4$ [0, $\bar{u}, \bar{w}$ ]	$y, 0, 1/4$ [0,u, $\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4'm'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,1/4

Along [1,1,0] p2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/8



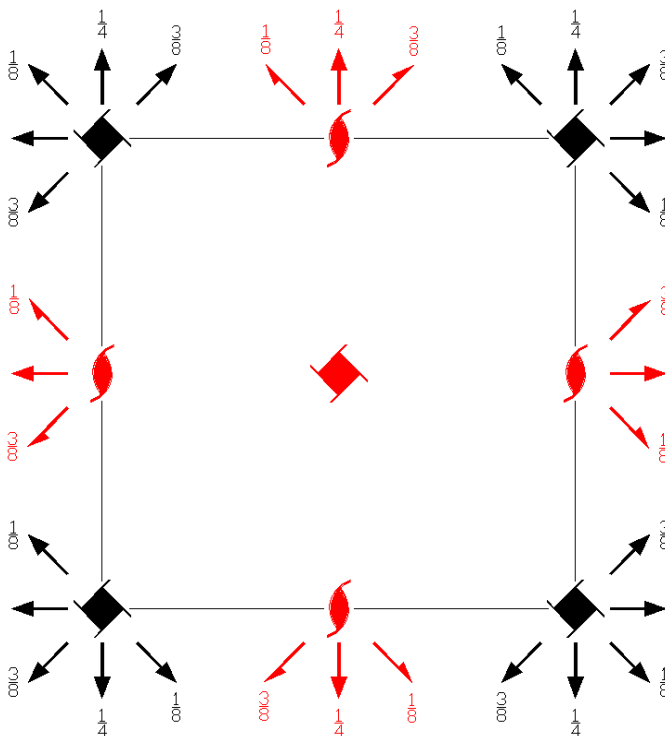
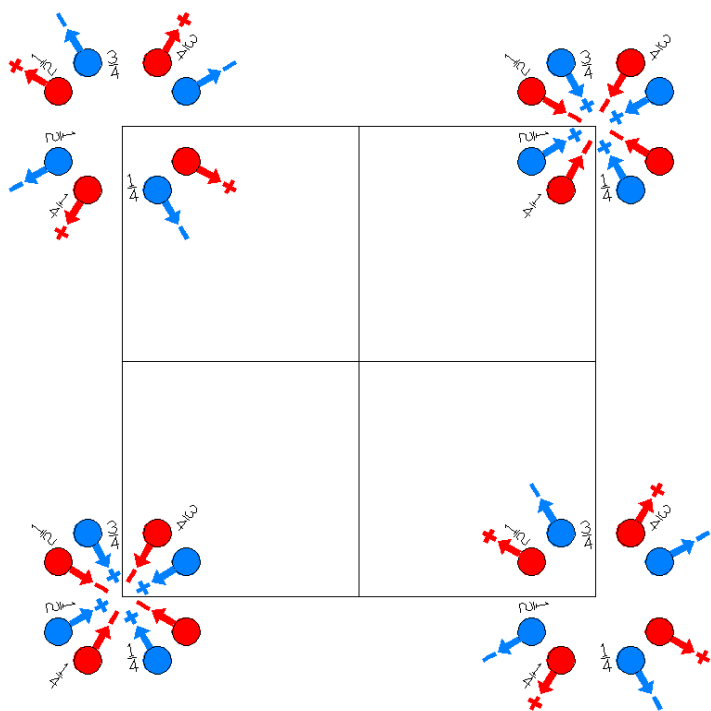
$P_4 4_3 22$

4221'

Tetragonal

95.6.798

$P_4 4_3 22$



Origin on 2  $[0,1,0]$  at  $4_3 (1,2) 1$

Asymmetric unit  $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq 1/8$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                                      |  |  |   |
|--------------------------------------|--|--|---|
| (1) 1<br>(1 0,0,0)                   | (2) 2 $(0,0,1/2)$ $0,0,z$<br>( $2_z$   $0,0,1/2$ ) | (3) $4^+$ $(0,0,3/4)$ $0,0,z$<br>( $4_z$   $0,0,3/4$ ) | (4) $4^-$ $(0,0,1/4)$ $0,0,z$<br>( $4_z^{-1}$   $0,0,1/4$ ) |
| (5) 2 $0,y,0$<br>( $2_y$   $0,0,0$ ) | (6) 2 $x,0,1/4$<br>( $2_x$   $0,0,1/2$ )           | (7) 2 $x,x,1/8$<br>( $2_{xy}$   $0,0,1/4$ )            | (8) 2 $x,\bar{x},3/8$<br>( $2_{\bar{xy}}$   $0,0,3/4$ )     |

For  $(1,0,0)$ ' + set

- |  |  |   |  |
|--|--|---|--|
| (1) $t'$ $(1,0,0)$<br>(1  $1,0,0$ )'       | (2) 2 $(0,0,1/2)$ $1/2,0,z$<br>( $2_z$   $1,0,1/2$ )'  | (3) $4^+$ $(0,0,3/4)$ $1/2,1/2,z$<br>( $4_z$   $1,0,3/4$ )'       | (4) $4^-$ $(0,0,1/4)$ $1/2,-1/2,z$<br>( $4_z^{-1}$   $1,0,1/4$ )'              |
| (5) $2'$ $1/2,y,0$<br>( $2_y$   $1,0,0$ )' | (6) $2'$ $(1,0,0)$ $x,0,1/4$<br>( $2_x$   $1,0,1/2$ )' | (7) $2'$ $(1/2,1/2,0)$ $x+1/2,x,1/8$<br>( $2_{xy}$   $1,0,1/4$ )' | (8) $2'$ $(1/2,-1/2,0)$ $x+1/2,\bar{x},3/8$<br>( $2_{\bar{xy}}$   $1,0,3/4$ )' |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

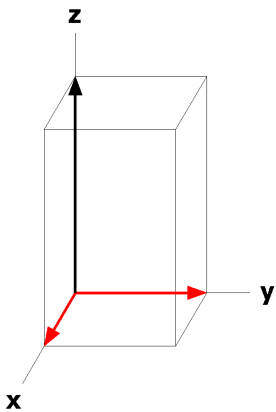
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		(0,0,0) +		(1,0,0)' +	
16	d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z+3/4$ [ $\bar{v}, u, w$ ]	(4) $y, \bar{x}, z+1/4$ [ $v, \bar{u}, w$ ]
		(5) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(6) $x, \bar{y}, \bar{z}+1/2$ [ $u, \bar{v}, \bar{w}$ ]	(7) $y, x, \bar{z}+1/4$ [ $v, u, \bar{w}$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+3/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]
8	c ..2	x,x,5/8 [u,u,0]	$\bar{x}, \bar{x}, 1/8$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}, x, 3/8$ [ $\bar{u}, u, 0$ ]	$x, \bar{x}, 7/8$ [ $u, \bar{u}, 0$ ]
8	b .2'	1/2,y,0 [u,0,w]	1/2, $\bar{y}, 1/2$ [ $u, 0, \bar{w}$ ]	$\bar{y}, 1/2, 3/4$ [0,u,w]	y,1/2,1/4 [0,u, $\bar{w}$ ]
8	a .2.	0,y,0 [0,v,0]	0, $\bar{y}, 1/2$ [0, $\bar{v}, 0$ ]	$\bar{y}, 0, 3/4$ [ $\bar{v}, 0, 0$ ]	y,0,1/4 [v,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p<sub>4</sub>-4m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,1/4

Along [1,1,0] p<sub>2b</sub>-2m'g'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/8



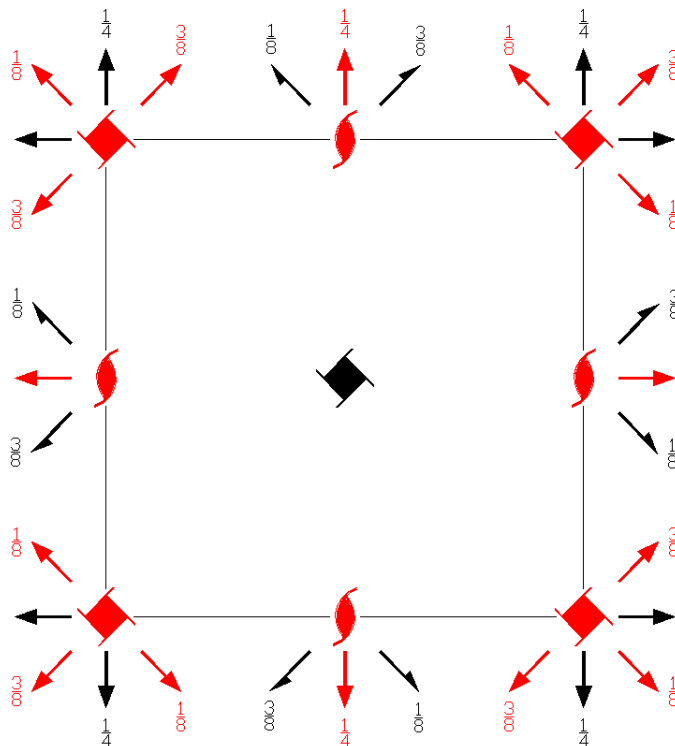
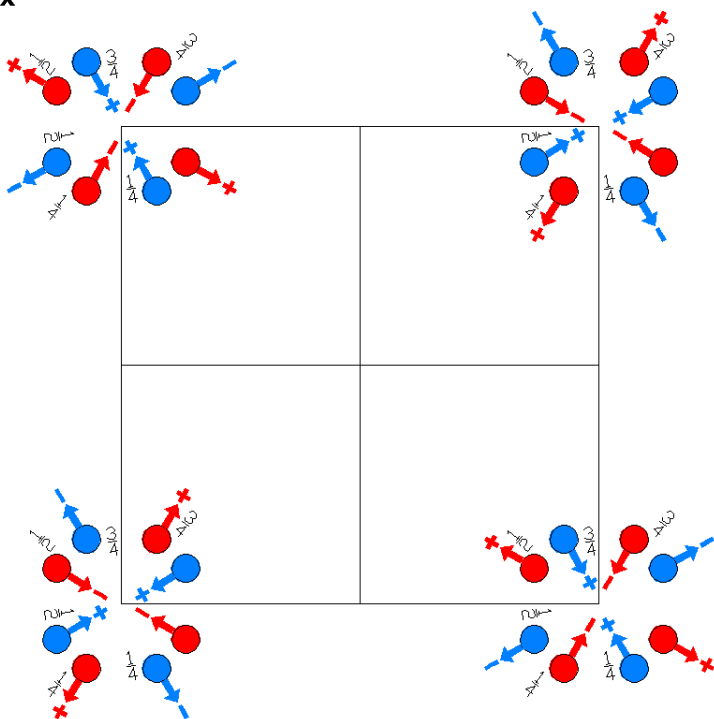
$P_P 4_3 '22'$

95.7.799

4221'

$P_P 4_3 '22'$

Tetragonal



Origin on 2 [0,1,0] at  $4_3'$  (1,2) 1

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (3) 4 <sup>+</sup> (0,0,3/4) 0,0,z<br>(4 <sub>z</sub>  0,0,3/4)' | (4) 4 <sup>-</sup> (0,0,1/4) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/4)' |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)         | (7) 2' x,x,1/8<br>(2 <sub>xy</sub>  0,0,1/4)'                    | (8) 2' x,x̄,3/8<br>(2 <sub>xy</sub>  0,0,3/4)'                                 |

For (1,0,0)' + set

- |  |  |   |  |
|--|--|---|--|
| (1) t' (1,0,0)<br>(1 1,0,0)'               | (2) 2' (0,0,1/2) 1/2,0,z<br>(2 <sub>z</sub>  1,0,1/2)' | (3) 4 <sup>+</sup> (0,0,3/4) 1/2,1/2,z<br>(4 <sub>z</sub>  1,0,3/4) | (4) 4 <sup>-</sup> (0,0,1/4) 1/2,-1/2,z<br>(4 <sub>z</sub> <sup>-1</sup>  1,0,1/4) |
| (5) 2' 1/2,y,0<br>(2 <sub>y</sub>  1,0,0)' | (6) 2' (1,0,0) x,0,1/4<br>(2 <sub>x</sub>  1,0,1/2)'   | (7) 2 x+1/2,x,1/8<br>(2 <sub>xy</sub>  1,0,1/4)                     | (8) 2 x+1/2,x̄,3/8<br>(2 <sub>xy</sub>  1,0,3/4)                                   |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
16 d 1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z+3/4$ [ $v, \bar{u}, \bar{w}$ ]	(4) $y, \bar{x}, z+1/4$ [ $v, \bar{u}, w$ ]
	(5) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(6) $x, \bar{y}, \bar{z}+1/2$ [ $u, \bar{v}, \bar{w}$ ]	(7) $y, x, \bar{z}+1/4$ [ $\bar{v}, \bar{u}, w$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+3/4$ [ $v, u, w$ ]
8 c ..2'	x,x,5/8 [u, $\bar{u}$ ,w]	$\bar{x}, \bar{x}, 1/8$ [ $\bar{u}, u, w$ ]	$\bar{x}, x, 3/8$ [ $\bar{u}, \bar{u}, w$ ]	x, $\bar{x}, 7/8$ [u,u, $\bar{w}$ ]
8 b .2'	1/2,y,0 [u,0,w]	1/2, $\bar{y}, 1/2$ [ $\bar{u}, 0, w$ ]	$\bar{y}, 1/2, 3/4$ [0, $\bar{u}, \bar{w}$ ]	y,1/2,1/4 [0,u, $\bar{w}$ ]
8 a .2.	0,y,0 [0,v,0]	0, $\bar{y}, 1/2$ [0, $\bar{v}, 0$ ]	$\bar{y}, 0, 3/4$ [v,0,0]	y,0,1/4 [ $\bar{v}, 0, 0$ ]

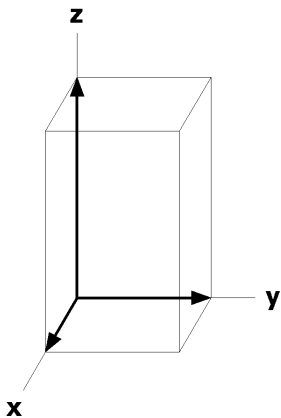
**Symmetry of Special Projections**

Along [0,0,1] p<sub>4</sub>-4m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,1/4

Along [1,1,0] p<sub>2b</sub>-2mg  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/8





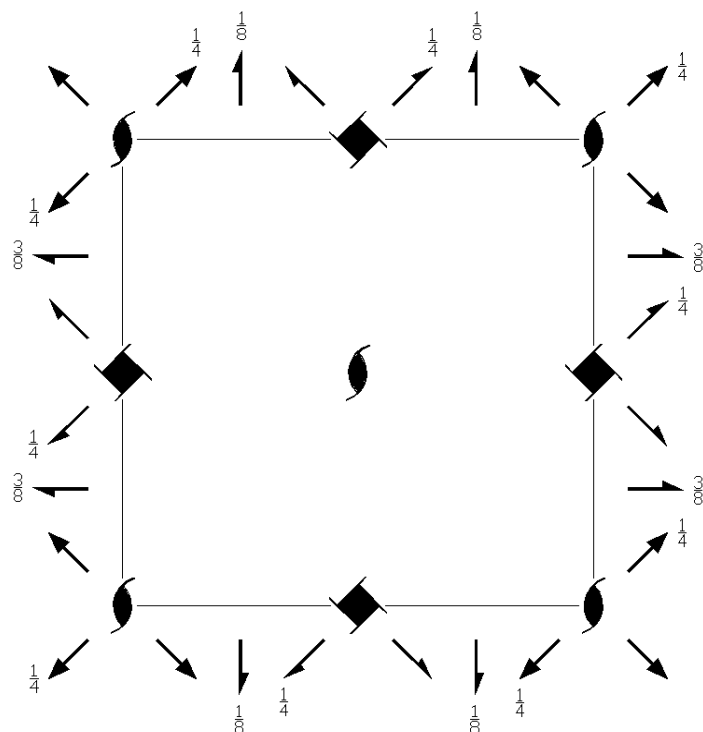
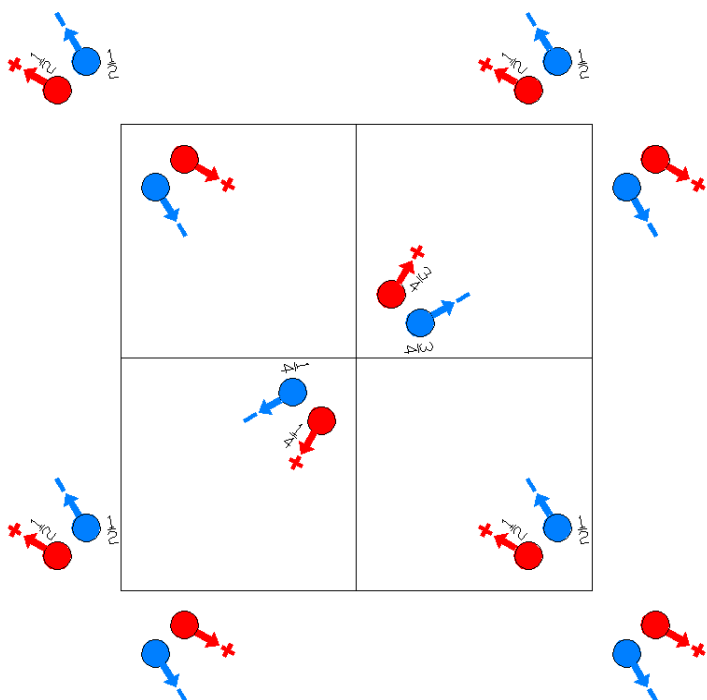
$P4_3 2_1 2$

422

Tetragonal

96.1.800

$P4_3 2_1 2$



Origin on 2  $[1,1,0]$  at 2, 1  $(1,2)$

Asymmetric unit  $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq 1/8$

### Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)         | (3) 4 <sup>+</sup> (0,0,3/4) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,3/4) | (4) 4 <sup>-</sup> (0,0,1/4) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/4) |
| (5) 2 (0,1/2,0) 1/4,y,3/8<br>(2 <sub>y</sub>  1/2,1/2,3/4) | (6) 2 (1/2,0,0) x,1/4,1/8<br>(2 <sub>x</sub>  1/2,1/2,1/4) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                               | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

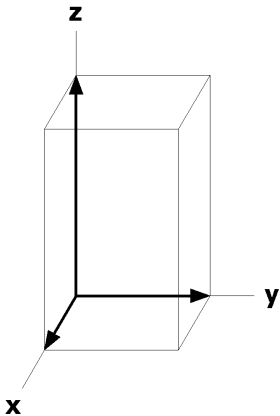
8	b	1	(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}+1/2, x+1/2, z+3/4$ [ $\bar{v}, u, w$ ]	(4) $y+1/2, \bar{x}+1/2, z+1/4$ [ $v, \bar{u}, w$ ]		
			(5) $\bar{x}+1/2, y+1/2, \bar{z}+3/4$ [ $\bar{u}, v, \bar{w}$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+1/4$ [ $u, \bar{v}, \bar{w}$ ]		
			(7) $y, x, \bar{z}$ [ $v, u, \bar{w}$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
4	a	.2	$x, x, 0$ [ $u, u, 0$ ]	$\bar{x}, \bar{x}, 1/2$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}+1/2, x+1/2, 3/4$ [ $\bar{u}, u, 0$ ]	$x+1/2, \bar{x}+1/2, 1/4$ [ $u, \bar{u}, 0$ ]

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4g'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 1/2, z$

Along  $[1,0,0]$   $p2'gg'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $x, 1/4, 1/8$

Along  $[1,1,0]$   $p2m'g'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x, x, 0$



$P4_3 2_1 21'$

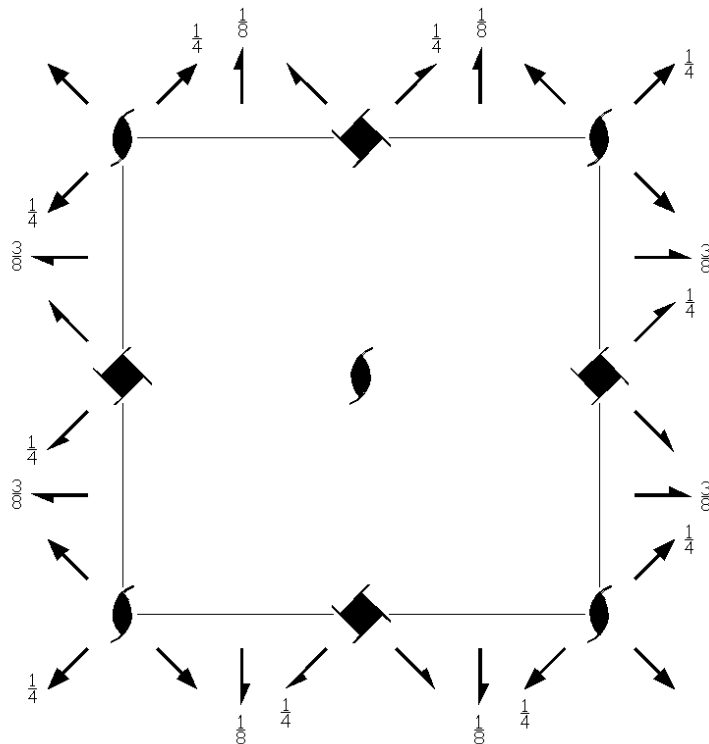
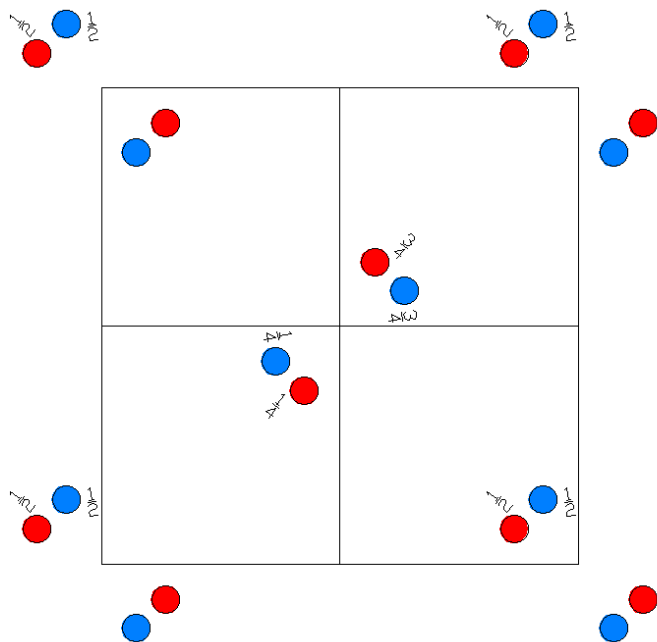
$4221'$

Tetragonal

96.2.801

$P4_3 2_1 21'$

$1'$



Origin on  $2 [1,1,0]1'$  at  $2_1 (1,2)1'$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

**Symmetry Operations**

For  $1 + \text{set}$

- |  |  |  |  |
|--|--|--|--|
| (1) $1$<br>( $1   0,0,0$ )                               | (2) $2 (0,0,1/2) \ 0,0,z$<br>( $2_z   0,0,1/2$ )         | (3) $4^+ (0,0,3/4) \ 0,1/2,z$<br>( $4_z^+   1/2,1/2,3/4$ ) | (4) $4^- (0,0,1/4) \ 1/2,0,z$<br>( $4_z^-   1/2,1/2,1/4$ ) |
| (5) $2 (0,1/2,0) \ 1/4,y,3/8$<br>( $2_y   1/2,1/2,3/4$ ) | (6) $2 (1/2,0,0) \ x,1/4,1/8$<br>( $2_x   1/2,1/2,1/4$ ) | (7) $2 \ x,x,0$<br>( $2_{xy}   0,0,0$ )                    | (8) $2 \ x,\bar{x},1/4$<br>( $2_{\bar{xy}}   0,0,1/2$ )    |

For  $1' + \text{set}$

- |   |   |   |   |
|---|---|---|---|
| (1) $1'$<br>( $1   0,0,0$ )                               | (2) $2' (0,0,1/2) \ 0,0,z$<br>( $2_z   0,0,1/2$ )         | (3) $4^{+'} (0,0,3/4) \ 0,1/2,z$<br>( $4_z^+   1/2,1/2,3/4$ ) | (4) $4^{-'} (0,0,1/4) \ 1/2,0,z$<br>( $4_z^-   1/2,1/2,1/4$ ) |
| (5) $2' (0,1/2,0) \ 1/4,y,3/8$<br>( $2_y   1/2,1/2,3/4$ ) | (6) $2' (1/2,0,0) \ x,1/4,1/8$<br>( $2_x   1/2,1/2,1/4$ ) | (7) $2' \ x,x,0$<br>( $2_{xy}   0,0,0$ )                      | (8) $2' \ x,\bar{x},1/4$<br>( $2_{\bar{xy}}   0,0,1/2$ )      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		1 +		1' +	
8	b 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z+1/2$ [0,0,0]	(3) $\bar{y}+1/2,x+1/2,z+3/4$ [0,0,0]	(4) $y+1/2,\bar{x}+1/2,z+1/4$ [0,0,0]
		(5) $\bar{x}+1/2,y+1/2,\bar{z}+3/4$ [0,0,0]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/4$ [0,0,0]	(7) $y,x,\bar{z}$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [0,0,0]
4	a ..21'	x,x,0 [0,0,0]	$\bar{x},\bar{x},1/2$ [0,0,0]	$\bar{x}+1/2,x+1/2,3/4$ [0,0,0]	$x+1/2,\bar{x}+1/2,1/4$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p4gm1'

$\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$

Origin at 0,1/2,z

Along [1,0,0] p2gg1'

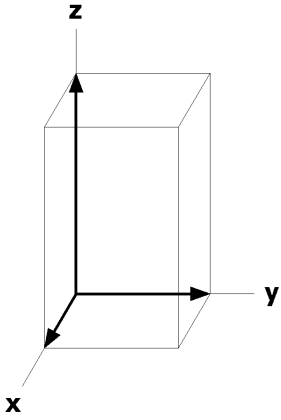
$\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$

Origin at x,1/4,1/8

Along [1,1,0] p2mg1'

$\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$

Origin at x,x,0



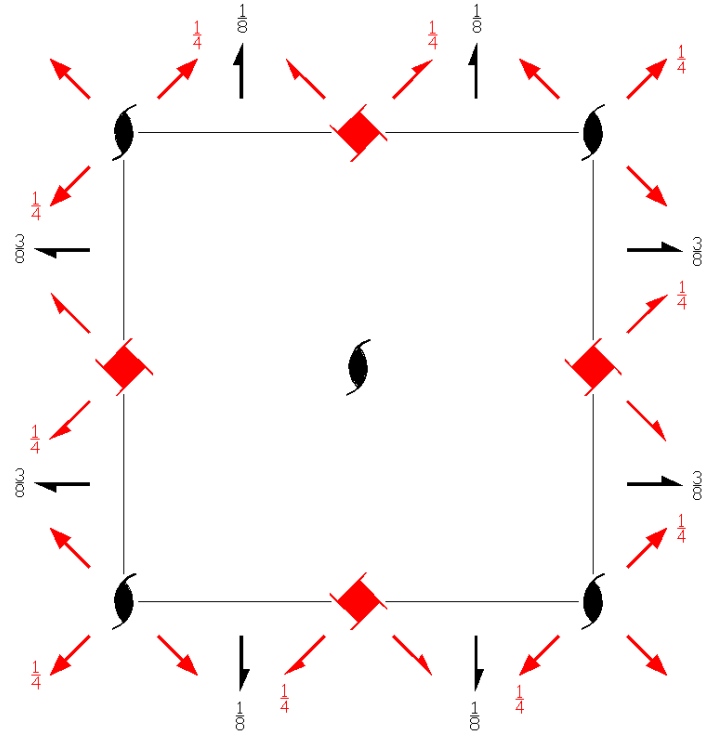
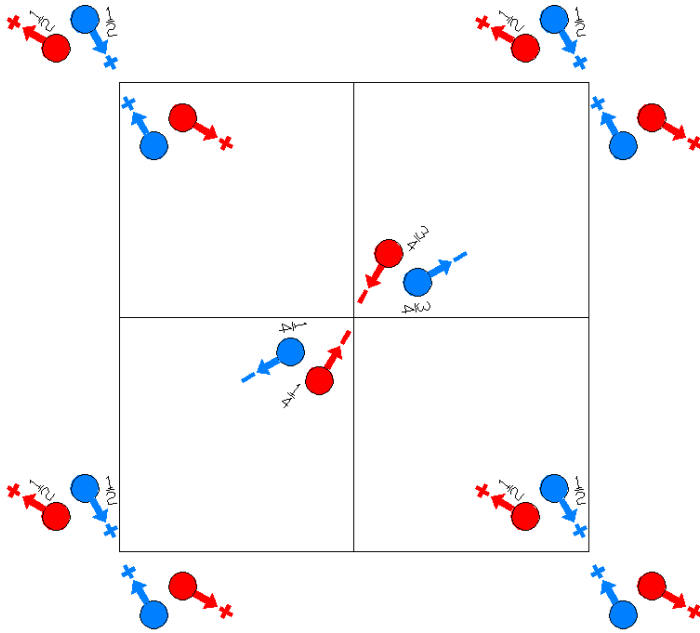
$P4_3'2_12'$

96.3.802

$4'22'$

$P4_3'2_12'$

Tetragonal



Origin on  $2'$   $[1,1,0]$  at  $2_1$   $1$   $(1,2')$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)         | (3) 4 <sup>+</sup> (0,0,3/4) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,3/4)' | (4) 4 <sup>-</sup> (0,0,1/4) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/4)' |
| (5) 2 (0,1/2,0) 1/4,y,3/8<br>(2 <sub>y</sub>  1/2,1/2,3/4) | (6) 2 (1/2,0,0) x,1/4,1/8<br>(2 <sub>x</sub>  1/2,1/2,1/4) | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                              | (8) 2' x,x̄,1/4<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,1/2)'                          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

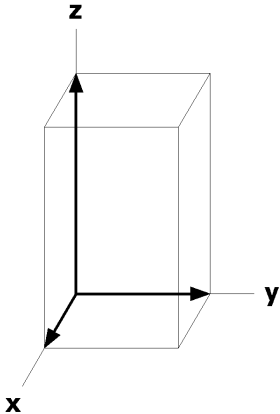
8	b	1	(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}+1/2, x+1/2, z+3/4$ [ $v, \bar{u}, \bar{w}$ ]	(4) $y+1/2, \bar{x}+1/2, z+1/4$ [ $\bar{v}, u, \bar{w}$ ]		
			(5) $\bar{x}+1/2, y+1/2, \bar{z}+3/4$ [ $\bar{u}, v, \bar{w}$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+1/4$ [ $u, \bar{v}, \bar{w}$ ]		
			(7) $y, x, \bar{z}$ [ $\bar{v}, \bar{u}, w$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+1/2$ [ $v, u, w$ ]		
4	a	..2'	$x, x, 0$ [ $u, \bar{u}, w$ ]	$\bar{x}, \bar{x}, 1/2$ [ $\bar{u}, u, w$ ]	$\bar{x}+1/2, x+1/2, 3/4$ [ $\bar{u}, \bar{u}, \bar{w}$ ]	$x+1/2, \bar{x}+1/2, 1/4$ [ $u, u, \bar{w}$ ]

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4'gm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 1/2, z$

Along  $[1,0,0]$   $p2g'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 1/4, 1/8$

Along  $[1,1,0]$   $p2m'g'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x, x, 0$



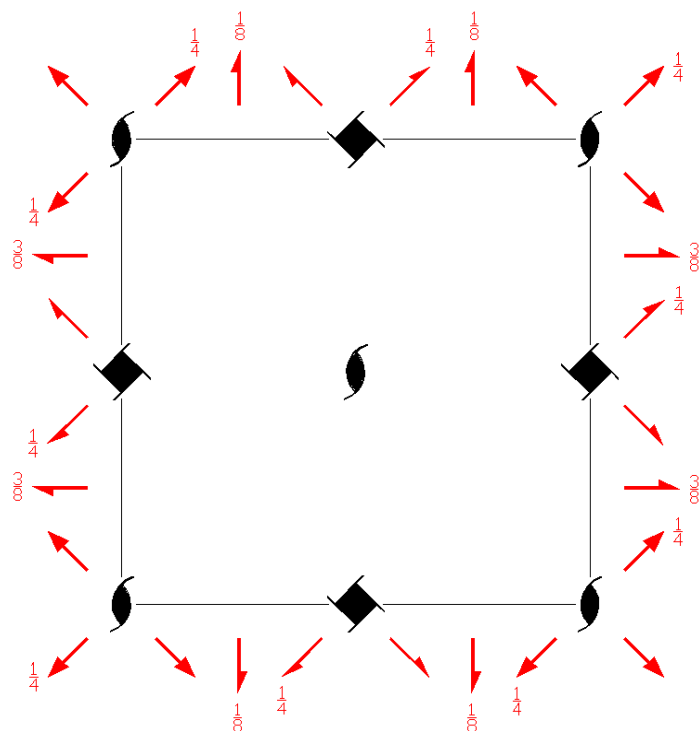
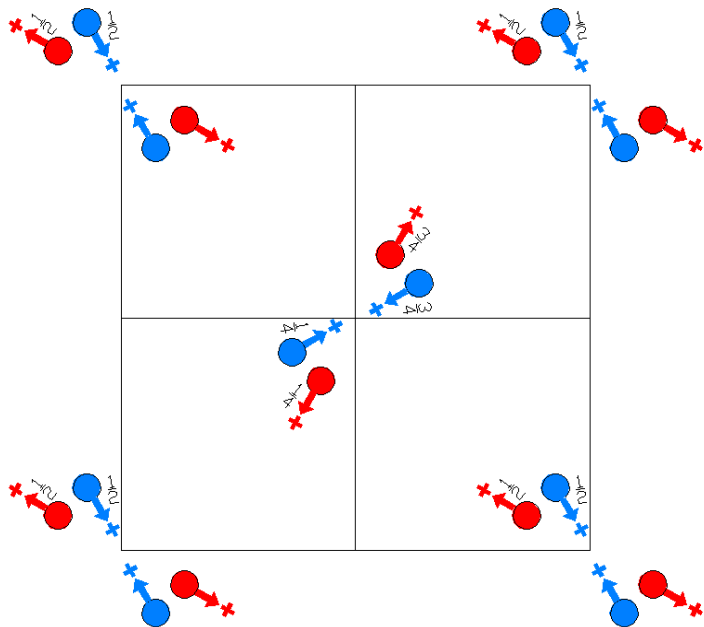
$P4_3 2_1 '2'$

42' $'2'$

Tetragonal

96.4.803

$P4_3 2_1 '2'$



Origin on  $2'$   $[1,1,0]$  at  $2_1$   $1$   $(1,2')$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)           | (3) 4 <sup>+</sup> (0,0,3/4) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,3/4) | (4) 4 <sup>-</sup> (0,0,1/4) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/4) |
| (5) 2' (0,1/2,0) 1/4,y,3/8<br>(2 <sub>y</sub>  1/2,1/2,3/4)' | (6) 2' (1/2,0,0) x,1/4,1/8<br>(2 <sub>x</sub>  1/2,1/2,1/4)' | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                             | (8) 2' x,x̄,1/4<br>(2 <sub>xy</sub> ̄ 0,0,1/2)'                                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

8	b	1	(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}+1/2, x+1/2, z+3/4$ [ $\bar{v}, u, w$ ]	(4) $y+1/2, \bar{x}+1/2, z+1/4$ [ $v, \bar{u}, w$ ]		
			(5) $\bar{x}+1/2, y+1/2, \bar{z}+3/4$ [ $u, \bar{v}, w$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+1/4$ [ $\bar{u}, v, w$ ]		
			(7) $y, x, \bar{z}$ [ $\bar{v}, \bar{u}, w$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+1/2$ [ $v, u, w$ ]		
4	a	..2'	$x, x, 0$ [ $u, \bar{u}, w$ ]	$\bar{x}, \bar{x}, 1/2$ [ $\bar{u}, u, w$ ]	$\bar{x}+1/2, x+1/2, 3/4$ [ $u, u, w$ ]	$x+1/2, \bar{x}+1/2, 1/4$ [ $\bar{u}, \bar{u}, w$ ]

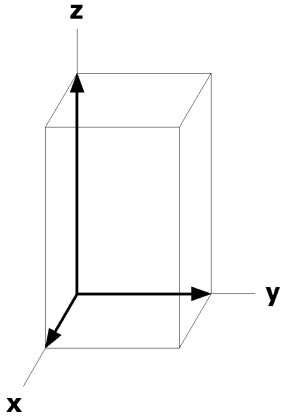
**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4g'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 1/2, z$

Along  $[1,0,0]$   $p2g'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 1/4, 1/8$

Along  $[1,1,0]$   $p2'mg'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x, x, 0$





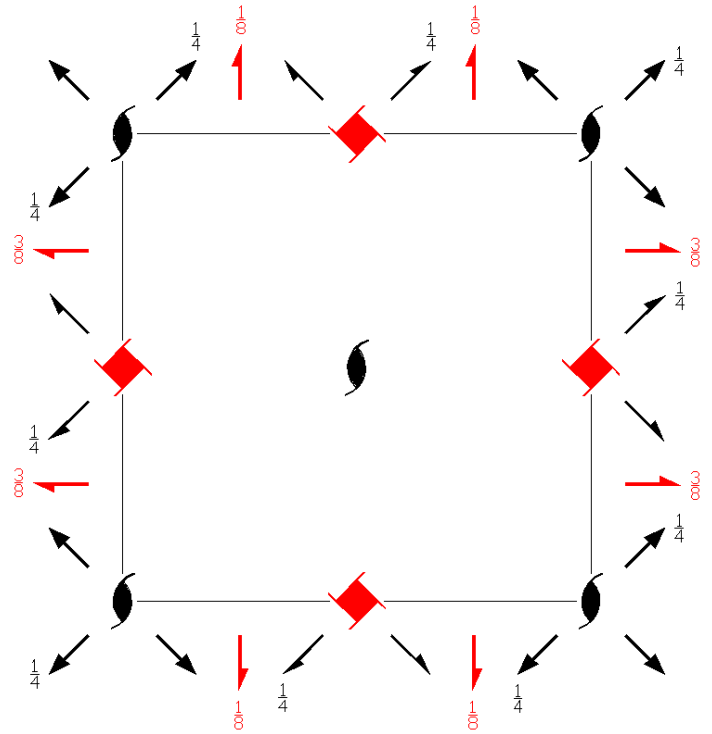
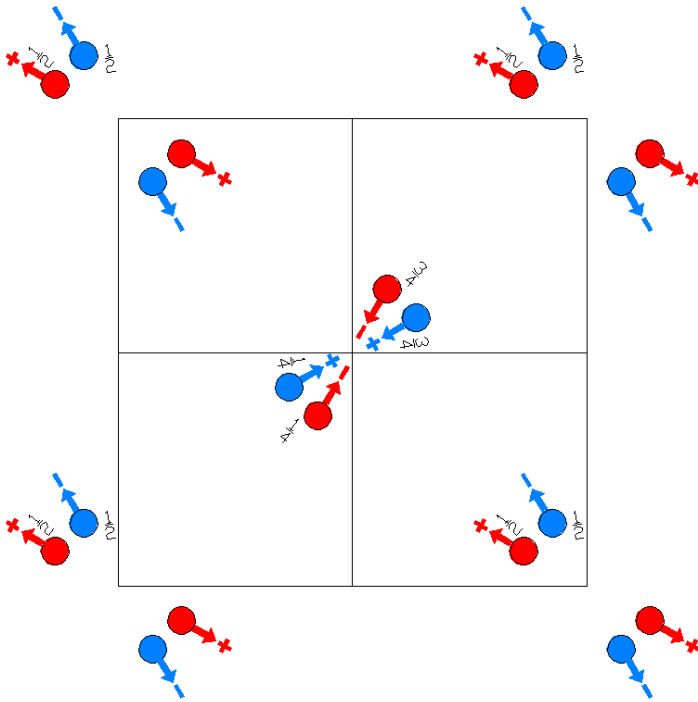
$P4_3'2_1'2$

96.5.804

$4'2'2$

$P4_3'2_1'2$

Tetragonal



Origin on  $2 [1,1,0]$  at  $2_1 1 (1,2)$

Asymmetric unit  $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq 1/8$

### Symmetry Operations

- |  |  |  |   |
|--|--|--|---|
| (1) $1$<br>( $1   0,0,0$ )                                     | (2) $2 (0,0,1/2) \quad 0,0,z$<br>( $2_z   0,0,1/2$ )           | (3) $4^{+'} (0,0,3/4) \quad 0,1/2,z$<br>( $4_z   1/2,1/2,3/4$ )' | (4) $4^{-'} (0,0,1/4) \quad 1/2,0,z$<br>( $4_z^{-1}   1/2,1/2,1/4$ )' |
| (5) $2' (0,1/2,0) \quad 1/4,y,3/8$<br>( $2_y   1/2,1/2,3/4$ )' | (6) $2' (1/2,0,0) \quad x,1/4,1/8$<br>( $2_x   1/2,1/2,1/4$ )' | (7) $2 \quad x,x,0$<br>( $2_{xy}   0,0,0$ )                      | (8) $2 \quad x,\bar{x},1/4$<br>( $2_{\bar{xy}}   0,0,1/2$ )           |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

8	b	1	(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}+1/2, x+1/2, z+3/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(4) $y+1/2, \bar{x}+1/2, z+1/4$ [ $\bar{v}, u, \bar{w}$ ]		
			(5) $\bar{x}+1/2, y+1/2, \bar{z}+3/4$ [ $u, \bar{v}, w$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+1/4$ [ $\bar{u}, v, w$ ]		
			(7) $y, x, \bar{z}$ [ $v, u, \bar{w}$ ]	(8) $\bar{y}, \bar{x}, \bar{z}+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
4	a	.2	$x, x, 0$ [ $u, u, 0$ ]	$\bar{x}, \bar{x}, 1/2$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}+1/2, x+1/2, 3/4$ [ $u, \bar{u}, 0$ ]	$x+1/2, \bar{x}+1/2, 1/4$ [ $\bar{u}, u, 0$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4'g'm

$\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$

Origin at 0,1/2,z

Along [1,0,0] p2'gg'

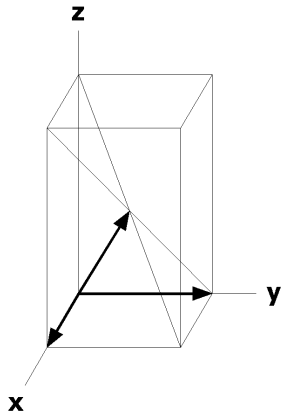
$\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$

Origin at x,1/4,1/8

Along [1,1,0] p2m'g'

$\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$

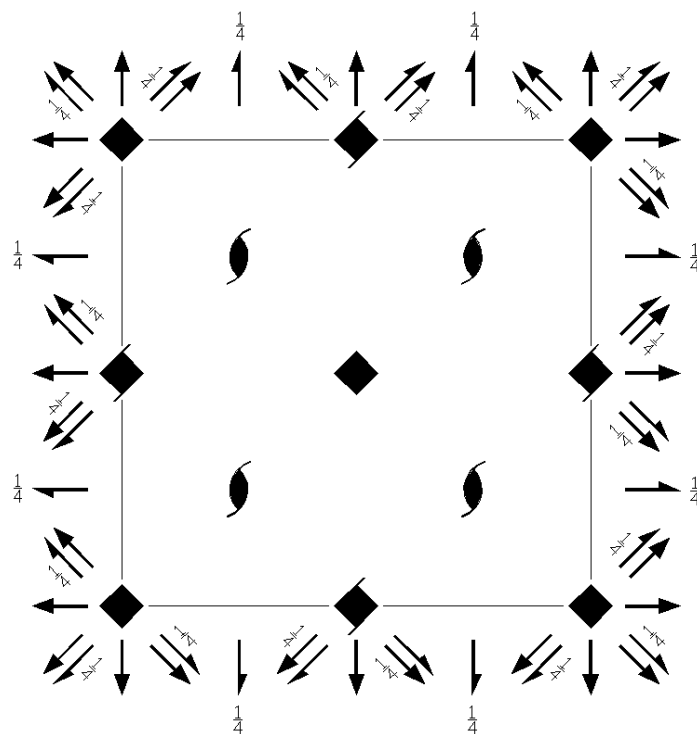
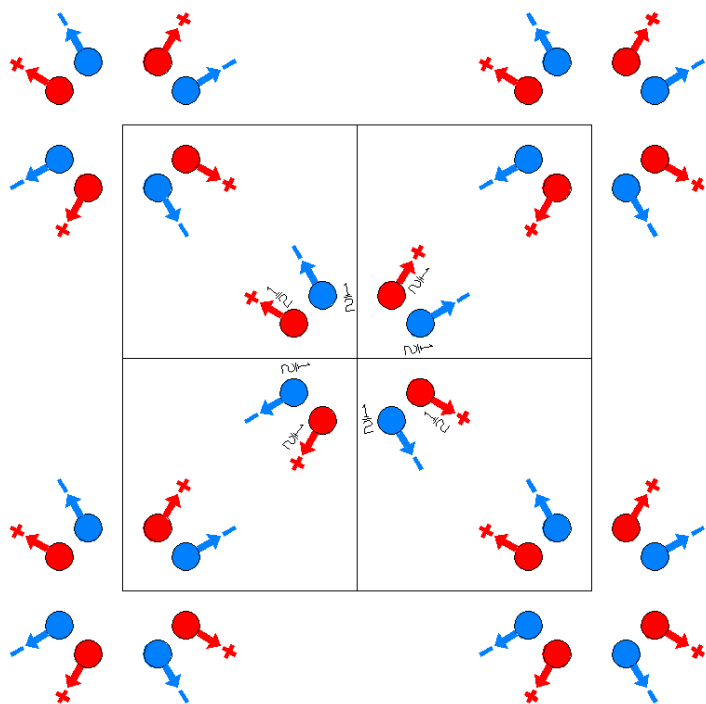
Origin at x,x,0



I422  
97.1.805

422  
I422

Tetragonal



Origin on 422

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)     |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                          | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0) |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                     | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub> <sup>+</sup>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-</sup>  1/2,1/2,1/2) |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)                        | (8) 2 x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

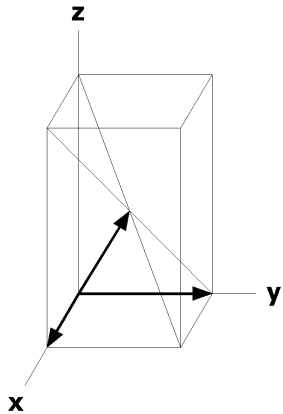
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
16	k	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ] (7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	j	.2	x,x+1/2,1/4 [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},u,0$ ]	x+1/2, $\bar{x},1/4$ [u, $\bar{u},0$ ]
8	i	.2	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,1/2 [0,u,0]	0, $\bar{x},1/2$ [0, $\bar{u},0$ ]
8	h	.2	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0,u,0]	0, $\bar{x},0$ [0, $\bar{u},0$ ]
8	g	.2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]	x, $\bar{x},0$ [u, $\bar{u},0$ ]
8	f	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4	e	4..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4	d	2.22	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]		
4	c	222.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
2	b	422	0,0,1/2 [0,0,0]			
2	a	422	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

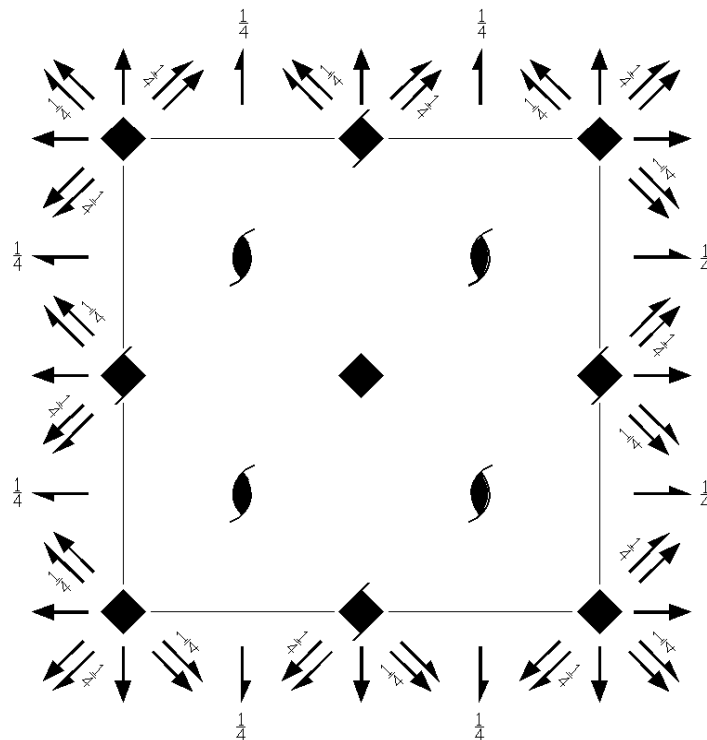
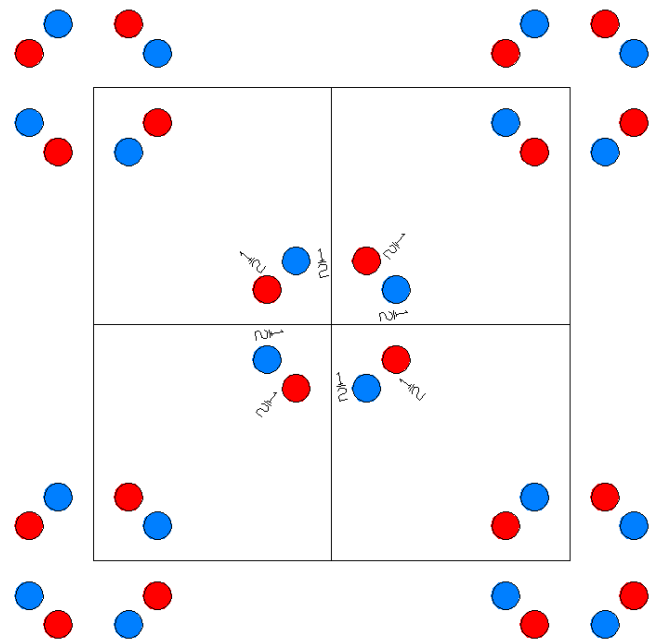


I4221'  
97.2.806

4221'  
I4221'

Tetragonal

1'



Origin on 4221'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)     |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                          | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0) |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                     | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub> <sup>+</sup>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-</sup>  1/2,1/2,1/2) |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)                        | (8) 2 x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)   |

## For (0,0,0)' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)'	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(5) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(6) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'	(7) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) 2' x, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  0,0,0)'

## For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (1 1/2,1/2,1/2)'	(2) 2' (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>  1/2,1/2,1/2)'	(3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)'	(4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'
(5) 2' (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>  1/2,1/2,1/2)'	(6) 2' (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>  1/2,1/2,1/2)'	(7) 2' (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(8) 2' x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

**Positions**

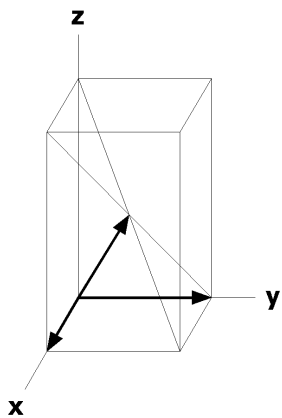
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'		
16	k	11'	(1) x,y,z [0,0,0] (5) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0] (6) x, $\bar{y},\bar{z}$ [0,0,0]	(3) $\bar{y},x,z$ [0,0,0] (7) y,x, $\bar{z}$ [0,0,0]	(4) y, $\bar{x},z$ [0,0,0] (8) $\bar{y},\bar{x},\bar{z}$ [0,0,0]
8	j	..21'	x,x+1/2,1/4 [0,0,0]	$\bar{x},\bar{x}+1/2,1/4$ [0,0,0]	$\bar{x}+1/2,x,1/4$ [0,0,0]	x+1/2, $\bar{x},1/4$ [0,0,0]
8	i	.2.1'	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]	0,x,1/2 [0,0,0]	0, $\bar{x},1/2$ [0,0,0]
8	h	.2.1'	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x},0$ [0,0,0]
8	g	..21'	x,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x},x,0$ [0,0,0]	x, $\bar{x},0$ [0,0,0]
8	f	2..1'	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]
4	e	4..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4	d	2.221'	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]		
4	c	222.1'	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
2	b	4221'	0,0,1/2 [0,0,0]			
2	a	4221'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



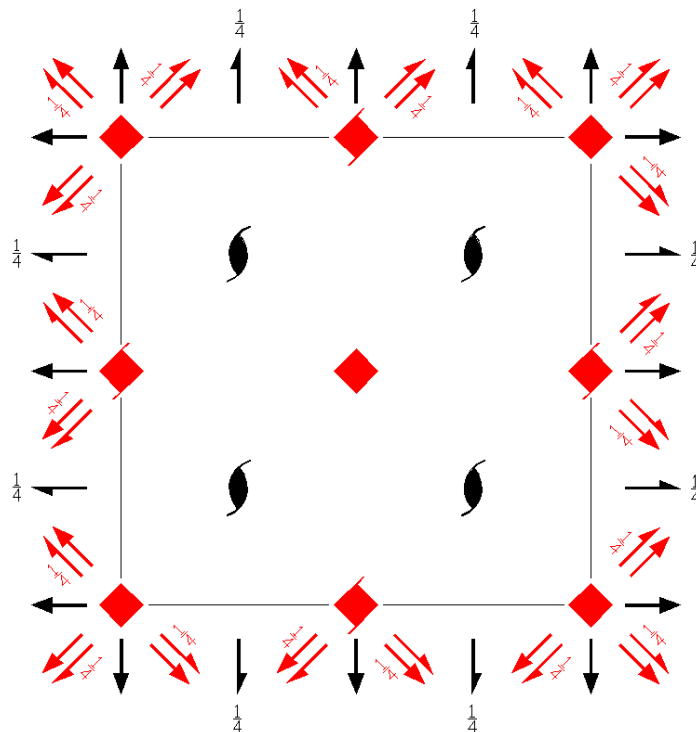
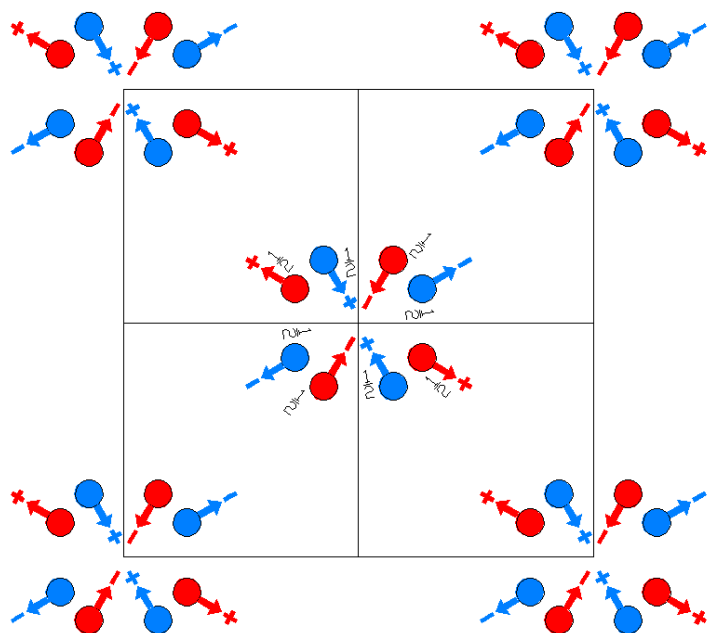
14'22'

97.3.807

4'22'

14'22'

Tetragonal



Origin on 4'22'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'            | (8) 2' x,x̄,0<br>(2 <sub>xy</sub> ̄ 0,0,0)'                        |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                     | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'          | (8) 2' x,x̄+1/2,1/4<br>(2 <sub>xy</sub> ̄ 1/2,1/2,1/2)'                              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(1/2,1/2,1/2) +			
16	k	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ] (7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	j	..2'	x,x+1/2,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,1/4$ [u,u, $\bar{w}$ ]	x+1/2, $\bar{x},1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]		
8	i	.2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,1/2 [0, $\bar{u},0$ ]	0, $\bar{x},1/2$ [0,u,0]		
8	h	.2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0, $\bar{u},0$ ]	0, $\bar{x},0$ [0,u,0]		
8	g	..2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [u, $\bar{u},w$ ]	$\bar{x},x,0$ [u,u, $\bar{w}$ ]	x, $\bar{x},0$ [ $\bar{u},\bar{u},\bar{w}$ ]		
8	f	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]		
4	e	4'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]				
4	d	2.2'2'	0,1/2,1/4 [0,0,w]	1/2,0,1/4 [0,0, $\bar{w}$ ]				
4	c	222.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]				
2	b	4'22'	0,0,1/2 [0,0,0]					
2	a	4'22'	0,0,0 [0,0,0]					

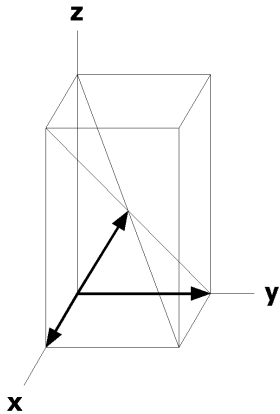
**Symmetry of Special Projections**

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0

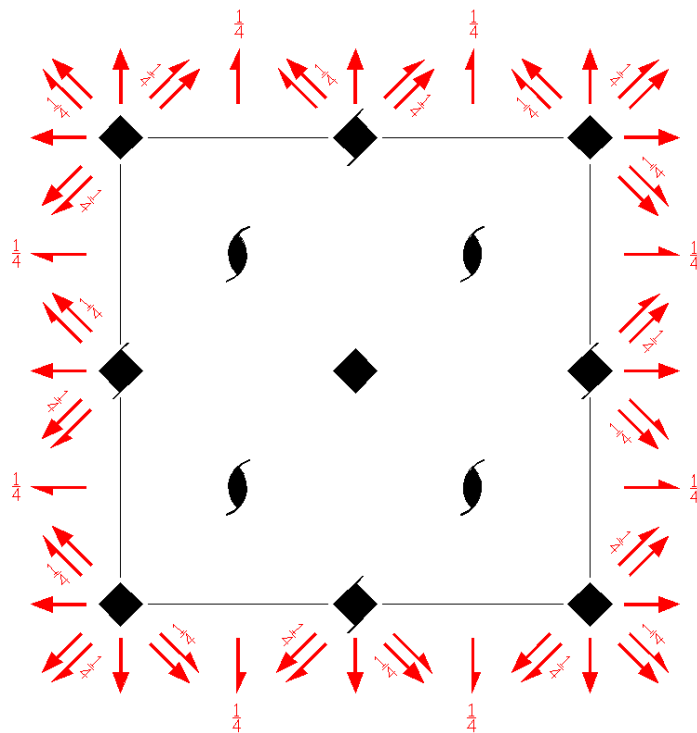
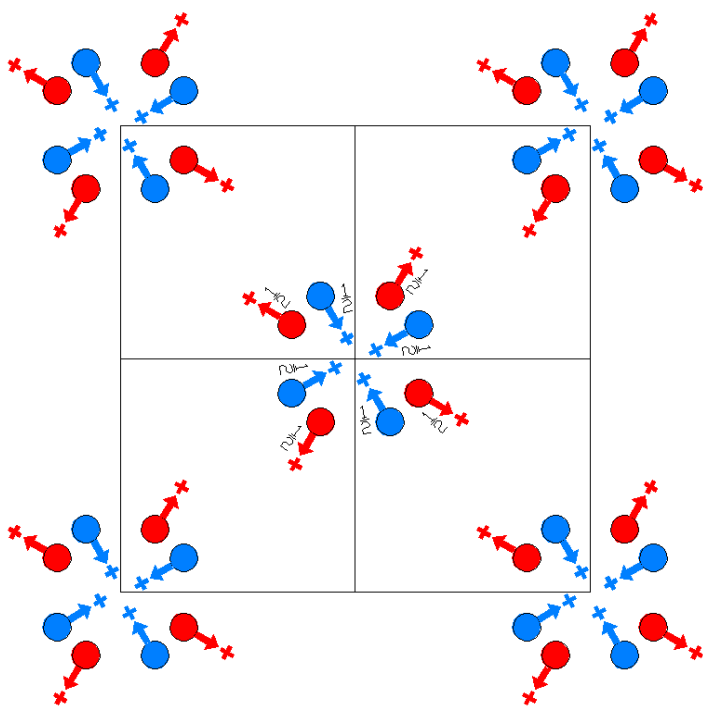




I42'2'  
97.4.808

42'2'  
I42'2'

Tetragonal



Origin on 42'2'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'           | (8) 2' x,x̄,0<br>(2 <sub>xy</sub>  0,0,0)'                        |

For (1/2,1/2,1/2) + set

- |  |  |   |   |
|--|--|---|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                       | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)   | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'         | (8) 2' x,x̄+1/2,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'                              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

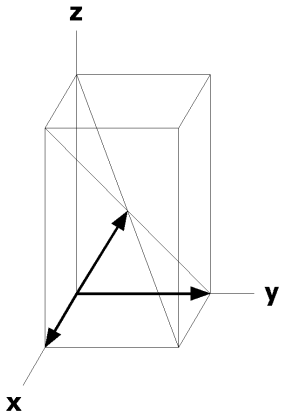
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
		(0,0,0) +	(1/2,1/2,1/2) +					
16 k 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]	(5) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]
8 j ..2'	x,x+1/2,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},\bar{u},w$ ]	x+1/2, $\bar{x},1/4$ [ $u,u,w$ ]				
8 i .2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	0,x,1/2 [ $\bar{v},0,w$ ]	0, $\bar{x},1/2$ [v,0,w]				
8 h .2'	x,0,0 [0,v,w]	$\bar{x},0,0$ [0, $\bar{v},w$ ]	0,x,0 [ $\bar{v},0,w$ ]	0, $\bar{x},0$ [v,0,w]				
8 g ..2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [ $u,\bar{u},w$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},0$ [ $u,u,w$ ]				
8 f 2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]				
4 e 4..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]						
4 d 2.2'2'	0,1/2,1/4 [0,0,w]	1/2,0,1/4 [0,0,w]						
4 c 22'2'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]						
2 b 42'2'	0,0,1/2 [0,0,w]							
2 a 42'2'	0,0,0 [0,0,w]							

**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



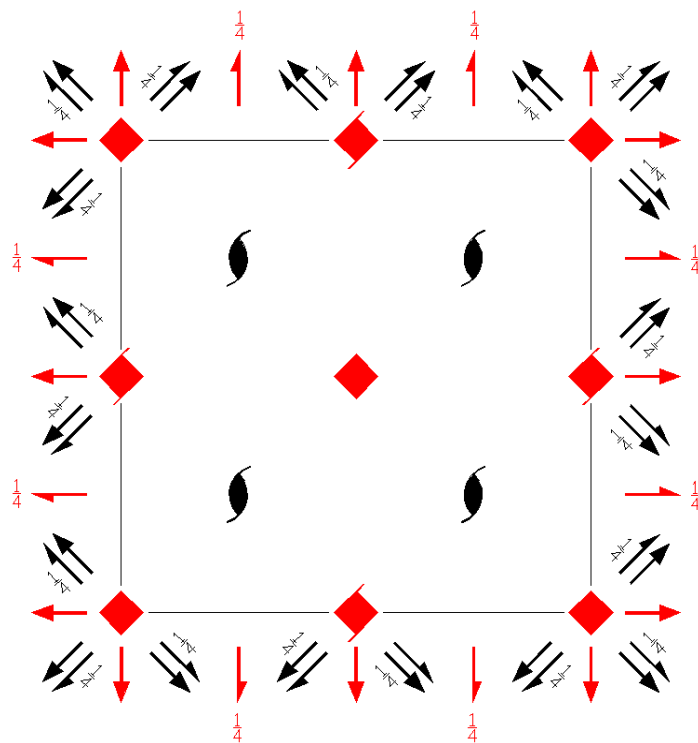
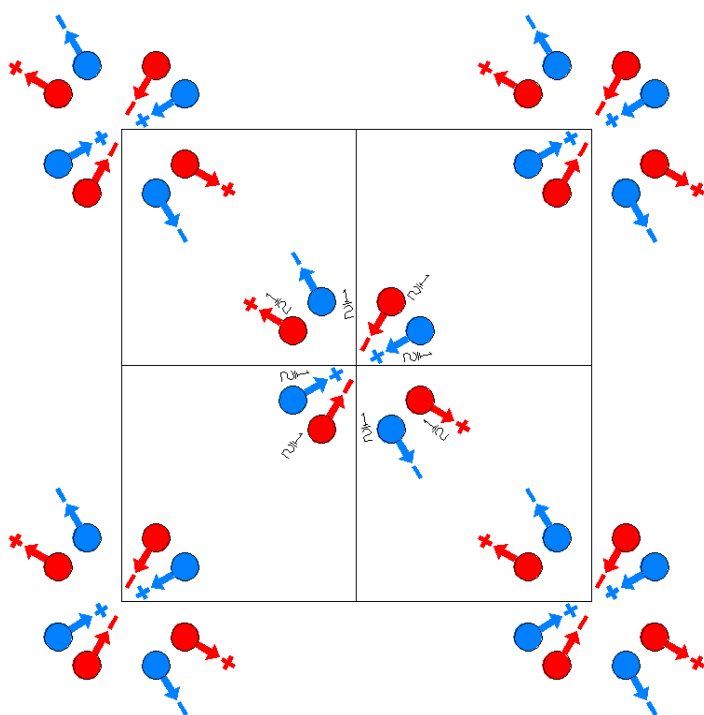
14'2'2

97.5.809

4'2'2

14'2'2

Tetragonal



Origin on 4'2'2

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> ' 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)' | (4) 4 <sup>-</sup> ' 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'   |
| (5) 2' 0,y,0<br>(2 <sub>y</sub> ' 0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub> ' 0,0,0)' | (7) 2 x,x,0<br>(2 <sub>xy</sub> ' 0,0,0)                            | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub> ' 0,0,0) |

For (1/2,1/2,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                        | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)    | (3) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub> <sup>+</sup>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-</sup>  1/2,1/2,1/2)' |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub> ' 1/2,1/2,1/2)' | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub> ' 1/2,1/2,1/2)' | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub> ' 1/2,1/2,1/2)                          | (8) 2 x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub> ' 1/2,1/2,1/2)     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

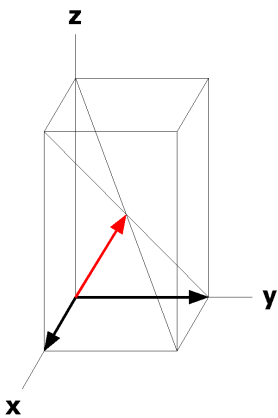
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(1/2,1/2,1/2) +			
16	k	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u, $\bar{v}$ ,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v}$ ,w] (6) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(3) $\bar{y},x,z$ [v, $\bar{u},\bar{w}$ ] (7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	j	..2	x,x+1/2,1/4 [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,1/4$ [u, $\bar{u},0$ ]	x+1/2, $\bar{x},1/4$ [ $\bar{u},u,0$ ]		
8	i	.2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v}$ ,w]	0,x,1/2 [v,0, $\bar{w}$ ]	0, $\bar{x},1/2$ [ $\bar{v},0,\bar{w}$ ]		
8	h	.2'	x,0,0 [0,v,w]	$\bar{x},0,0$ [0, $\bar{v}$ ,w]	0,x,0 [v,0, $\bar{w}$ ]	0, $\bar{x},0$ [ $\bar{v},0,\bar{w}$ ]		
8	g	..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [u, $\bar{u},0$ ]	x, $\bar{x},0$ [ $\bar{u},u,0$ ]		
8	f	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4	e	4'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]				
4	d	2.22	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]				
4	c	22'2'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]				
2	b	4'2'2	0,0,1/2 [0,0,0]					
2	a	4'2'2	0,0,0 [0,0,0]					

**Symmetry of Special Projections**

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

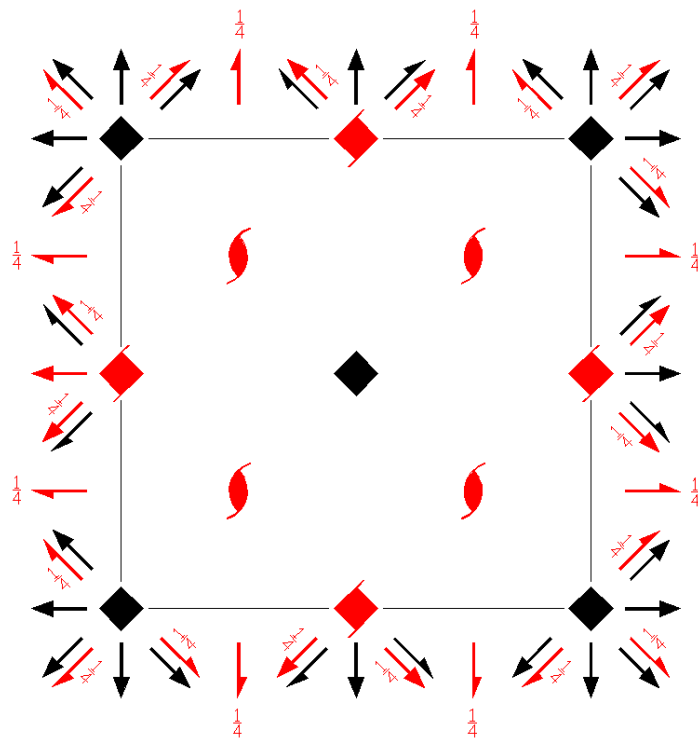
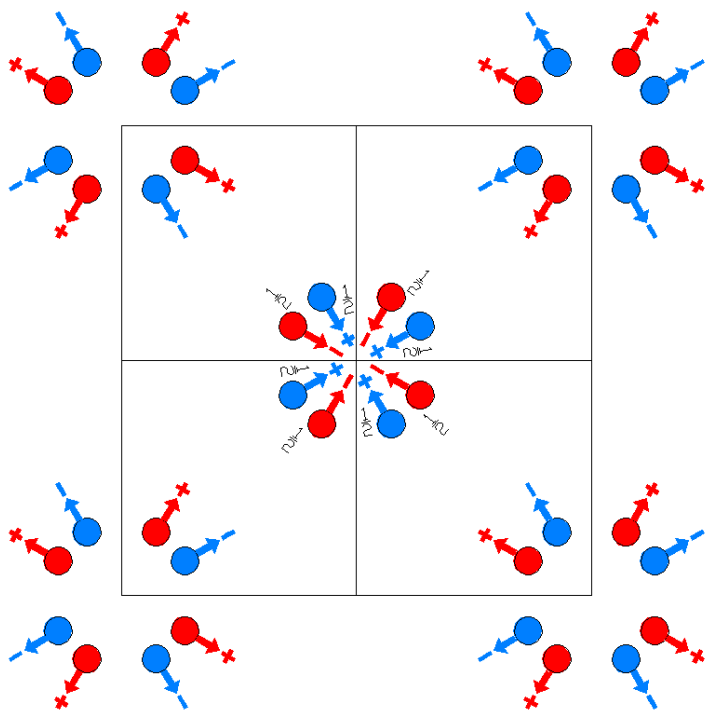
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I_p 422$   
97.6.810

$4221'$   
 $I_p 422$

Tetragonal



Origin on 422

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)    |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)             | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0) |

For (1/2,1/2,1/2)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'                     | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'            | (8) 2' x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)'     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

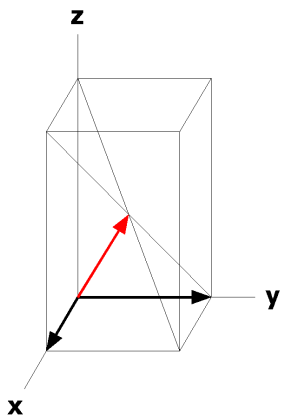
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1/2,1/2,1/2)' +		
16	k	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ] (7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	j	..2'	x,x+1/2,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [u, $\bar{u},w$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},\bar{u},w$ ]	x+1/2, $\bar{x},1/4$ [u,u,w]
8	i	.2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,1/2 [0,u,0]	0, $\bar{x},1/2$ [0, $\bar{u},0$ ]
8	h	.2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0,u,0]	0, $\bar{x},0$ [0, $\bar{u},0$ ]
8	g	..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]	x, $\bar{x},0$ [u, $\bar{u},0$ ]
8	f	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4	e	4..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4	d	2.2'2'	0,1/2,1/4 [0,0,w]	1/2,0,1/4 [0,0,w]		
4	c	222.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
2	b	422	0,0,1/2 [0,0,0]			
2	a	422	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $p_p \cdot 4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

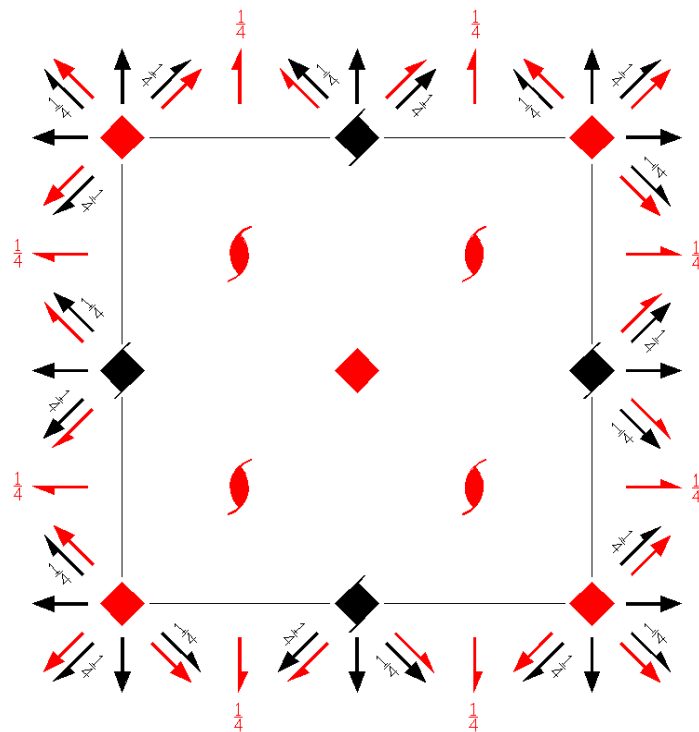
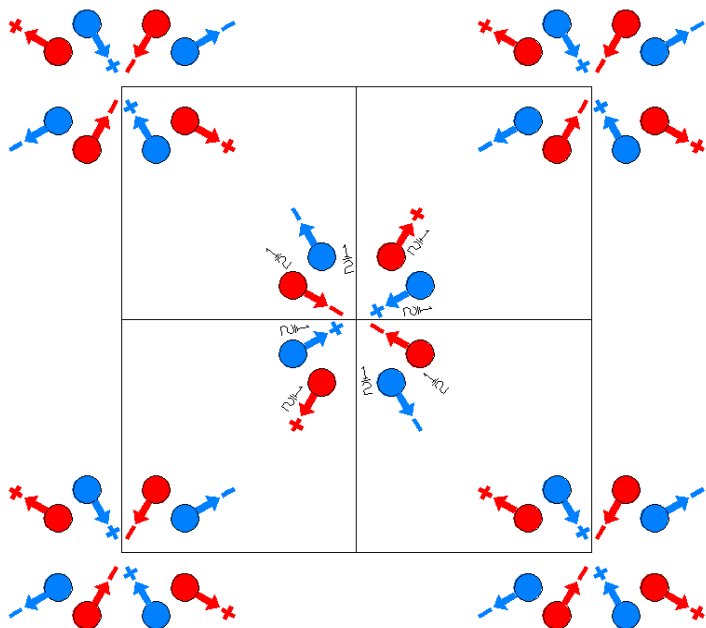
Along [1,1,0]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$I_p 4'22'$   
97.7.811

$4221'$   
 $I_p 4'22'$

Tetragonal



Origin on  $4'22'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For  $(0,0,0)$  + set

- |                                  |                                  |                                       |   |
|----------------------------------|----------------------------------|---------------------------------------|---|
| (1) 1<br>(1 0,0,0)               | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $4^+ 0,0,z$<br>( $4_z^+$  0,0,0)' | (4) $4^- 0,0,z$<br>( $4_z^-$  0,0,0)'             |
| (5) 2 $0,y,0$<br>( $2_y$  0,0,0) | (6) 2 $x,0,0$<br>( $2_x$  0,0,0) | (7) $2' x,x,0$<br>( $2_{xy}$  0,0,0)' | (8) $2' x,\bar{x},0$<br>( $2_{\bar{xy}}$  0,0,0)' |

For  $(1/2,1/2,1/2)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t' (1/2,1/2,1/2)$<br>(1  $1/2,1/2,1/2$ )'             | (2) $2' (0,0,1/2) 1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1/2$ )' | (3) $4^+ (0,0,1/2) 0,1/2,z$<br>( $4_z^+$   $1/2,1/2,1/2$ )'  | (4) $4^- (0,0,1/2) 1/2,0,z$<br>( $4_z^-$   $1/2,1/2,1/2$ )'      |
| (5) $2' (0,1/2,0) 1/4,y,1/4$<br>( $2_y$   $1/2,1/2,1/2$ )' | (6) $2' (1/2,0,0) x,1/4,1/4$<br>( $2_x$   $1/2,1/2,1/2$ )' | (7) 2 $(1/2,1/2,0) x,x,1/4$<br>( $2_{xy}$   $1/2,1/2,1/2$ )' | (8) 2 $x,\bar{x}+1/2,1/4$<br>( $2_{\bar{xy}}$   $1/2,1/2,1/2$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1/2,1/2,1/2)' +		
16	k	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ] (7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},w$ ]
8	j	.2	x,x+1/2,1/4 [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,1/4$ [u, $\bar{u},0$ ]	x+1/2, $\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]
8	i	.2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,1/2 [0, $\bar{u},0$ ]	0, $\bar{x},1/2$ [0,u,0]
8	h	.2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0, $\bar{u},0$ ]	0, $\bar{x},0$ [0,u,0]
8	g	.2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [u, $\bar{u},w$ ]	$\bar{x},x,0$ [u,u, $\bar{w}$ ]	x, $\bar{x},0$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	f	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]
4	e	4'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4	d	2.22	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]		
4	c	222.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
2	b	4'22'	0,0,1/2 [0,0,0]			
2	a	4'22'	0,0,0 [0,0,0]			

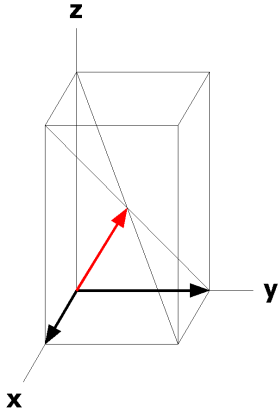
**Symmetry of Special Projections**

Along [0,0,1]  $p_p \cdot 4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,1/2,z

Along [1,0,0]  $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4





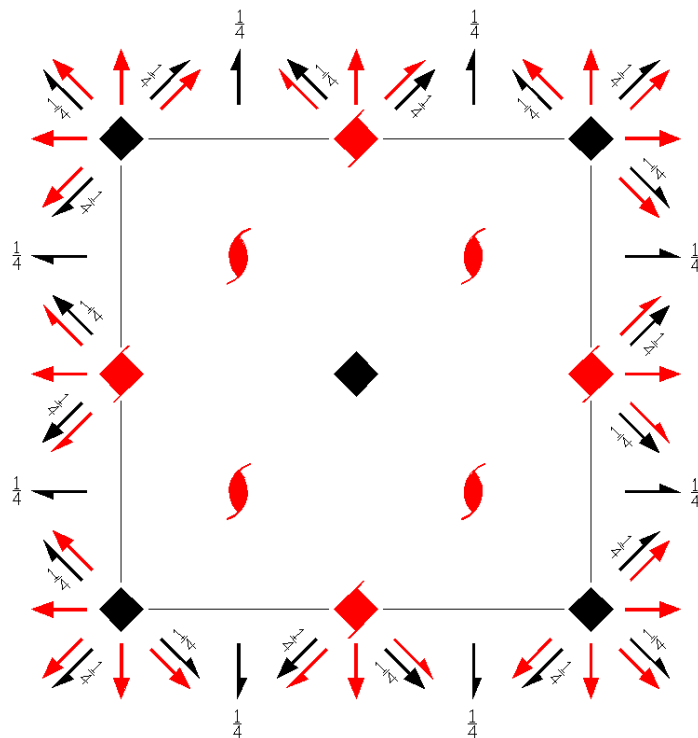
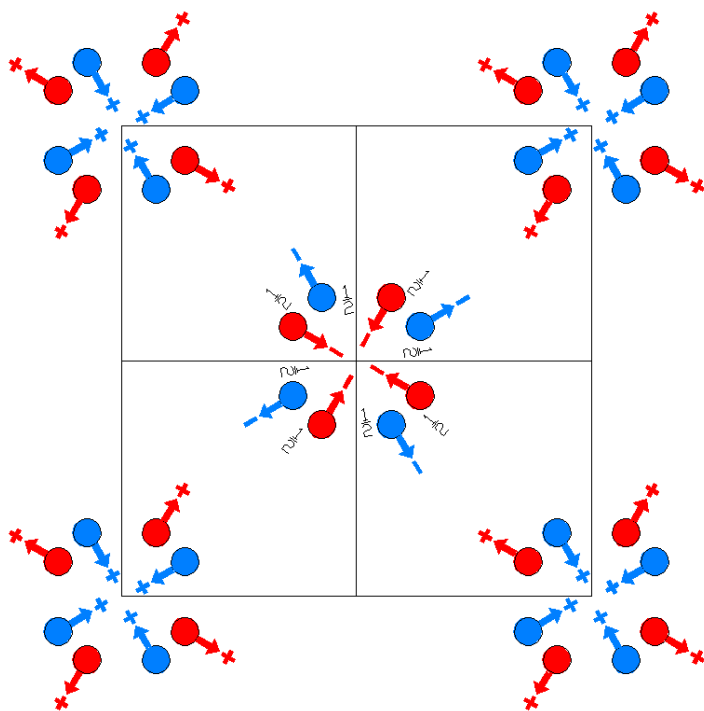
$I_p 42'2'$

97.8.812

$4221'$

$I_p 42'2'$

Tetragonal



Origin on  $42'2'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)      |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'           | (8) 2' x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)' |

For  $(1/2,1/2,1/2)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'                   | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)   | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)            | (8) 2 x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)     |

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(1/2,1/2,1/2)$ ; (2); (3); (5).

### Positions

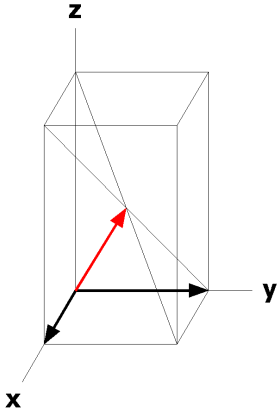
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
		(0,0,0) +	(1/2,1/2,1/2)' +					
16 k 1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $\bar{y},x,z [\bar{v},u,w]$	(4) $y,\bar{x},z [v,\bar{u},w]$	(5) $\bar{x},y,\bar{z} [u,\bar{v},w]$	(6) $x,\bar{y},\bar{z} [\bar{u},v,w]$	(7) $y,x,\bar{z} [\bar{v},\bar{u},w]$	(8) $\bar{y},\bar{x},\bar{z} [v,u,w]$
8 j ..2	$x,x+1/2,1/4 [u,u,0]$	$\bar{x},\bar{x}+1/2,1/4 [\bar{u},\bar{u},0]$	$\bar{x}+1/2,x,1/4 [\bar{u},u,0]$	$x+1/2,\bar{x},1/4 [u,\bar{u},0]$				
8 i .2'	$x,0,1/2 [0,v,w]$	$\bar{x},0,1/2 [0,\bar{v},w]$	$0,x,1/2 [\bar{v},0,w]$	$0,\bar{x},1/2 [v,0,w]$				
8 h .2'	$x,0,0 [0,v,w]$	$\bar{x},0,0 [0,\bar{v},w]$	$0,x,0 [\bar{v},0,w]$	$0,\bar{x},0 [v,0,w]$				
8 g ..2'	$x,x,0 [\bar{u},u,w]$	$\bar{x},\bar{x},0 [u,\bar{u},w]$	$\bar{x},x,0 [\bar{u},\bar{u},w]$	$x,\bar{x},0 [u,u,w]$				
8 f 2..	$0,1/2,z [0,0,w]$	$1/2,0,z [0,0,w]$	$0,1/2,\bar{z} [0,0,w]$	$1/2,0,\bar{z} [0,0,w]$				
4 e 4..	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,w]$						
4 d 2.22	$0,1/2,1/4 [0,0,0]$	$1/2,0,1/4 [0,0,0]$						
4 c 22'2'	$0,1/2,0 [0,0,w]$	$1/2,0,0 [0,0,w]$						
2 b 42'2'	$0,0,1/2 [0,0,w]$							
2 a 42'2'	$0,0,0 [0,0,w]$							

### Symmetry of Special Projections

Along  $[0,0,1]$   $p_p 4mm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c_p 2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p_{2a} 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,1/4$



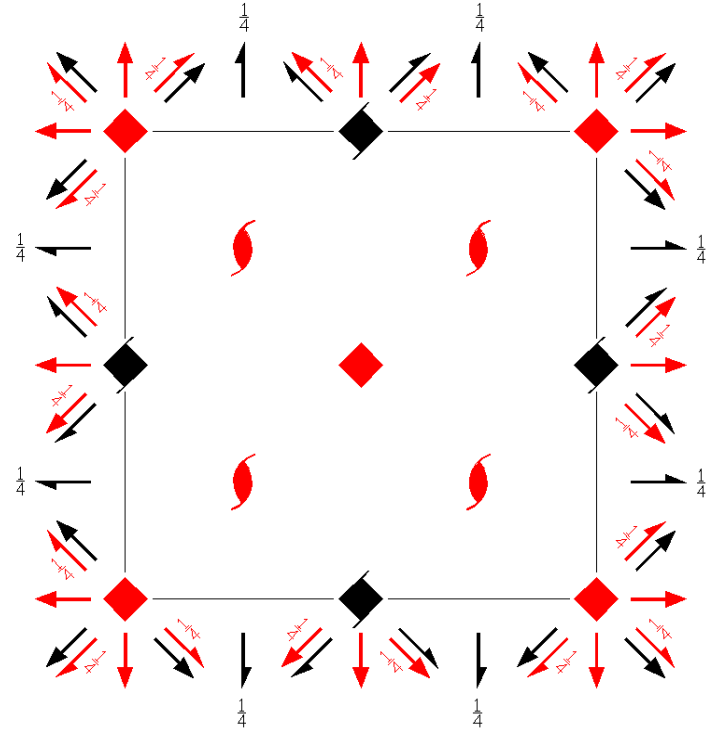
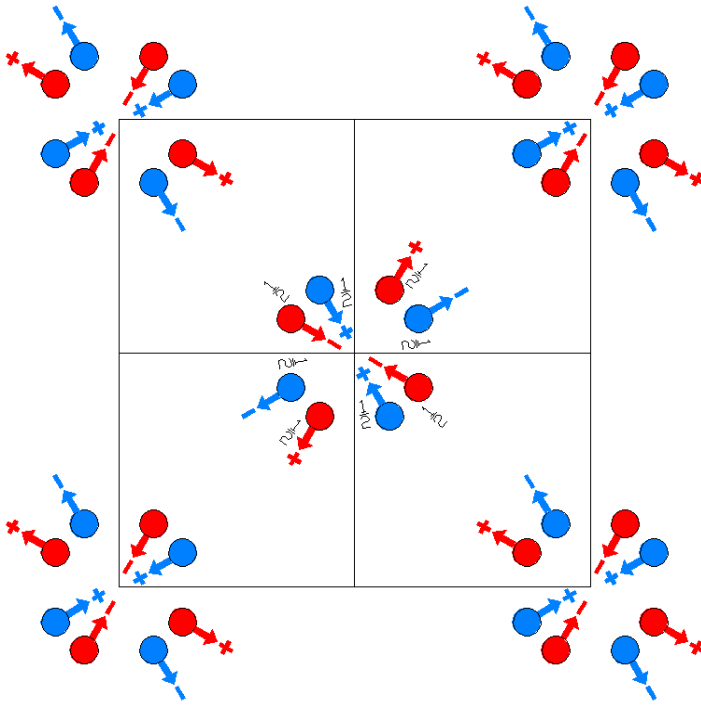
$I_p 4'2'2'$

97.9.813

$4221'$

$I_p 4'2'2'$

Tetragonal



Origin on  $4'2'2'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For  $(0,0,0)$  + set

- |                                    |                                    |                                       |   |
|------------------------------------|------------------------------------|---------------------------------------|---|
| (1) 1<br>(1 0,0,0)                 | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)   | (3) $4^+ 0,0,z$<br>( $4_z^+$  0,0,0)' | (4) $4^- 0,0,z$<br>( $4_z^-$  0,0,0)'           |
| (5) $2' 0,y,0$<br>( $2_y$  0,0,0)' | (6) $2' x,0,0$<br>( $2_x$  0,0,0)' | (7) 2 $x,x,0$<br>( $2_{xy}$  0,0,0)   | (8) 2 $x,\bar{x},0$<br>( $2_{\bar{xy}}$  0,0,0) |

For  $(1/2,1/2,1/2)$  + set

- |   |  |   |   |
|---|--|---|---|
| (1) $t' (1/2,1/2,1/2)$<br>(1  $1/2,1/2,1/2$ )'            | (2) $2' (0,0,1/2) 1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1/2$ )' | (3) $4^+ (0,0,1/2) 0,1/2,z$<br>( $4_z^+$   $1/2,1/2,1/2$ )'   | (4) $4^- (0,0,1/2) 1/2,0,z$<br>( $4_z^-$   $1/2,1/2,1/2$ )'       |
| (5) 2 $(0,1/2,0) 1/4,y,1/4$<br>( $2_y$   $1/2,1/2,1/2$ )' | (6) 2 $(1/2,0,0) x,1/4,1/4$<br>( $2_x$   $1/2,1/2,1/2$ )'  | (7) $2' (1/2,1/2,0) x,x,1/4$<br>( $2_{xy}$   $1/2,1/2,1/2$ )' | (8) $2' x,\bar{x}+1/2,1/4$<br>( $2_{\bar{xy}}$   $1/2,1/2,1/2$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

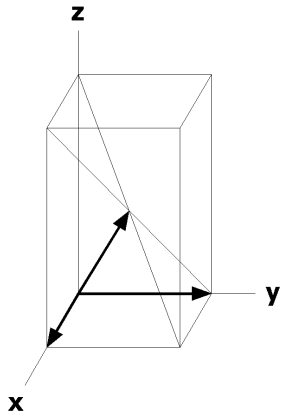
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1/2,1/2,1/2)' +		
16	k	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u, $\bar{v}$ ,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v}$ ,w] (6) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(3) $\bar{y},x,z$ [v, $\bar{u},\bar{w}$ ] (7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	j	..2'	x,x+1/2,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [u, $\bar{u},w$ ]	$\bar{x}+1/2,x,1/4$ [u,u, $\bar{w}$ ]	x+1/2, $\bar{x},1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	i	.2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	0,x,1/2 [v,0, $\bar{w}$ ]	0, $\bar{x},1/2$ [ $\bar{v},0,\bar{w}$ ]
8	h	.2'	x,0,0 [0,v,w]	$\bar{x},0,0$ [0, $\bar{v},w$ ]	0,x,0 [v,0, $\bar{w}$ ]	0, $\bar{x},0$ [ $\bar{v},0,\bar{w}$ ]
8	g	..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [u, $\bar{u},0$ ]	x, $\bar{x},0$ [ $\bar{u},u,0$ ]
8	f	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4	e	4'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4	d	2.2'2'	0,1/2,1/4 [0,0,w]	1/2,0,1/4 [0,0, $\bar{w}$ ]		
4	c	22'2'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]		
2	b	4'2'2	0,0,1/2 [0,0,0]			
2	a	4'2'2	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $p_p \cdot 4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,1/2,z

Along [1,0,0]  $c_p \cdot 2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

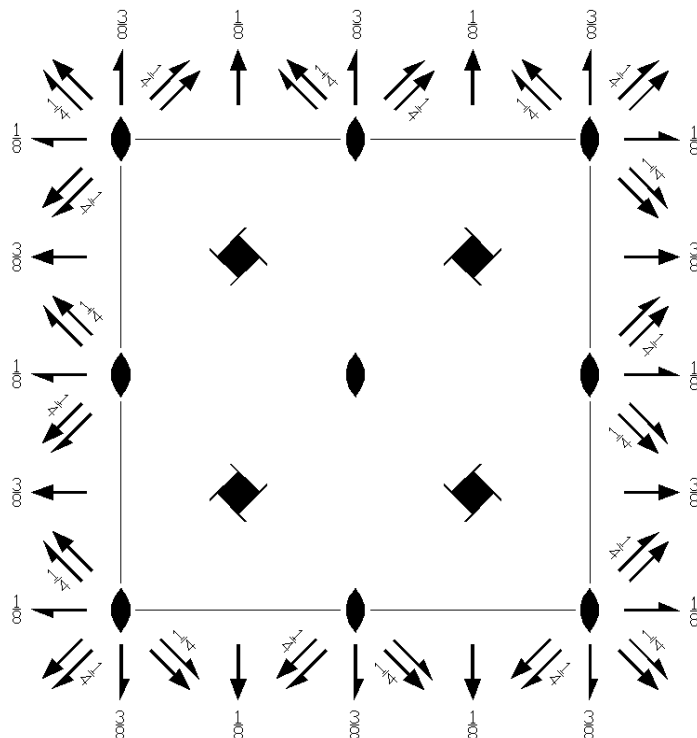
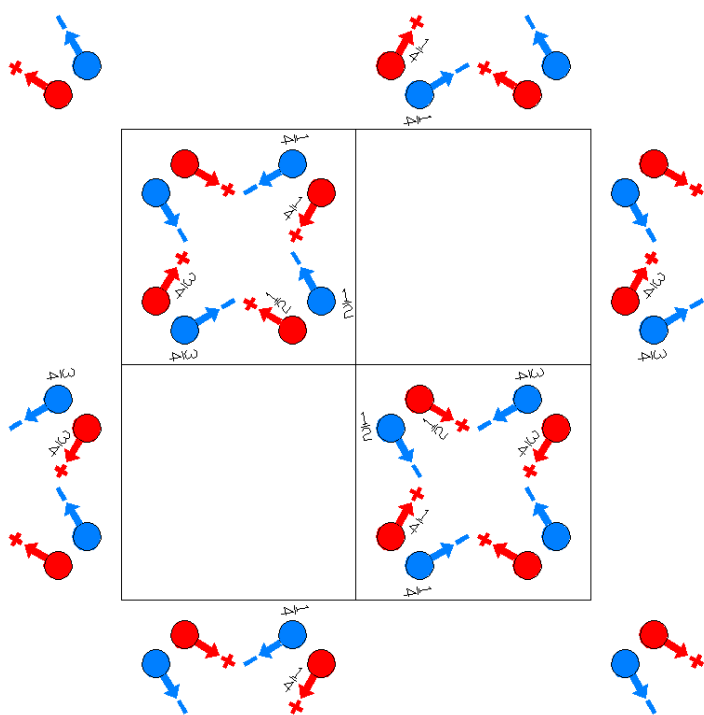
Along [1,1,0]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$I4_122$   
98.1.814

422  
 $I4_122$

Tetragonal



Origin at 222 at 212

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)         | (3) 4 <sup>+</sup> (0,0,1/4) -1/4,1/4,z<br>(4 <sub>z</sub>  0,1/2,1/4) | (4) 4 <sup>-</sup> (0,0,1/4) 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4) |
| (5) 2 (0,1/2,0) 0,y,1/8<br>(2 <sub>y</sub>  0,1/2,1/4) | (6) 2 x,1/4,1/8<br>(2 <sub>x</sub>  0,1/2,1/4) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                | (8) 2 x,x̄,0<br>(2 <sub>xy</sub>  0,0,0)  |

For (1/2,1/2,1/2) + set

- |  |  |   |  |
|--|--|---|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)         | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,3/4) 1/4,1/4,z<br>(4 <sub>z</sub>  1/2,0,3/4) | (4) 4 <sup>-</sup> (0,0,3/4) 1/4,-1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,0,3/4) |
| (5) 2 1/4,y,3/8<br>(2 <sub>y</sub>  1/2,0,3/4) | (6) 2 (1/2,0,0) x,0,3/8<br>(2 <sub>x</sub>  1/2,0,3/4)     | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)           | (8) 2 x,x̄+1/2,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)                                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

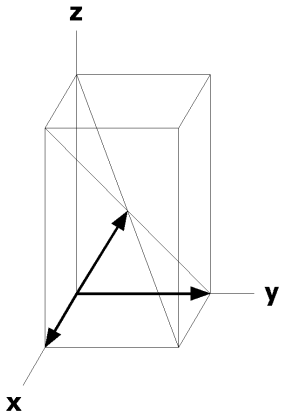
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1/2,1/2,1/2) +		
16	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	f	.2.	$x,1/4,1/8$ [u,0,0]	$\bar{x},3/4,1/8$ [ $\bar{u},0,0$ ]	$1/4,x,7/8$ [0,u,0]	$3/4,\bar{x},7/8$ [0, $\bar{u},0$ ]
8	e	..2	$\bar{x},x,0$ [ $\bar{u},u,0$ ]	$x,\bar{x},0$ [ $u,\bar{u},0$ ]	$x,x+1/2,1/4$ [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]
8	d	..2	$x,x,0$ [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,1/4$ [ $\bar{u},u,0$ ]	$x,\bar{x}+1/2,1/4$ [ $u,\bar{u},0$ ]
8	c	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/4 [0,0,w]	0,1/2, $\bar{z}+1/4$ [0,0, $\bar{w}$ ]
4	b	2.22	0,0,1/2 [0,0,0]	0,1/2,3/4 [0,0,0]		
4	a	2.22	0,0,0 [0,0,0]	0,1/2,1/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I4_1 221'$

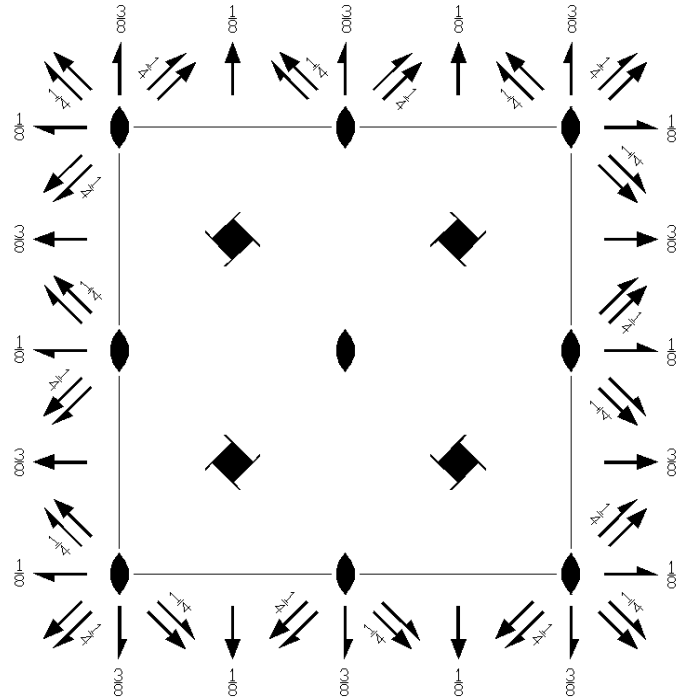
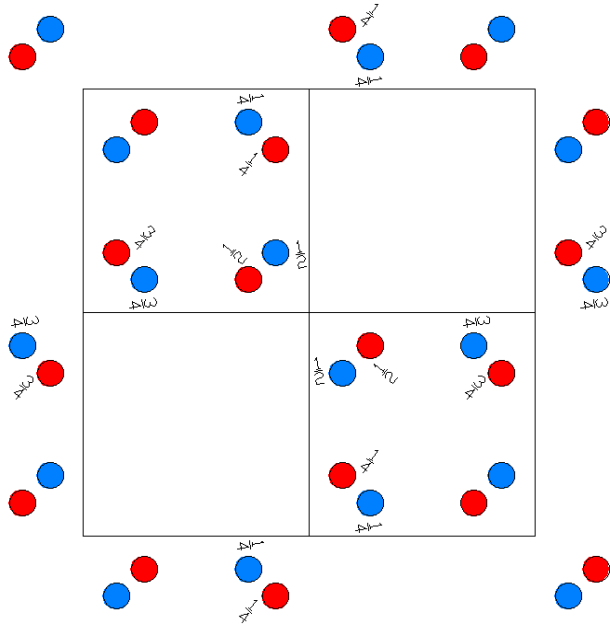
98.2.815

$4221'$

$I4_1 221'$

Tetragonal

1'



Origin at  $2221'$  at  $2121'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/8$

Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                               | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)         | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>( $4_z$  0,1/2,1/4) | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>( $4_z^{-1}$  0,1/2,1/4) |
| (5) 2 $(0,1/2,0) 0,y,1/8$<br>( $2_y$  0,1/2,1/4) | (6) 2 $x,1/4,1/8$<br>( $2_x$  0,1/2,1/4) | (7) 2 $x,x,0$<br>( $2_{xy}$  0,0,0)                     | (8) 2 $x,\bar{x},0$<br>( $2_{\bar{xy}}$  0,0,0)             |

For  $(1/2,1/2,1/2)$  + set

- |  |  |   |  |
|--|--|---|--|
| (1) $t$ $(1/2,1/2,1/2)$<br>(1 1/2,1/2,1/2) | (2) 2 $(0,0,1/2) 1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2) | (3) $4^+$ $(0,0,3/4) 1/4,1/4,z$<br>( $4_z$  1/2,0,3/4)  | (4) $4^-$ $(0,0,3/4) 1/4,-1/4,z$<br>( $4_z^{-1}$  1/2,0,3/4) |
| (5) 2 $1/4,y,3/8$<br>( $2_y$  1/2,0,3/4)   | (6) 2 $(1/2,0,0) x,0,3/8$<br>( $2_x$  1/2,0,3/4)     | (7) 2 $(1/2,1/2,0) x,x,1/4$<br>( $2_{xy}$  1/2,1/2,1/2) | (8) 2 $x,\bar{x}+1/2,1/4$<br>( $2_{\bar{xy}}$  1/2,1/2,1/2)  |

## For (0,0,0)' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> ' (0,0,1/4) -1/4,1/4,z (4 <sub>z</sub>  0,1/2,1/4)'	(4) 4 <sup>-</sup> ' (0,0,1/4) 1/4,1/4,z (4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4)'
(5) 2' (0,1/2,0) 0,y,1/8 (2 <sub>y</sub>  0,1/2,1/4)'	(6) 2' x,1/4,1/8 (2 <sub>x</sub>  0,1/2,1/4)'	(7) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) 2' x, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  0,0,0)'

## For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (1 1/2,1/2,1/2)'	(2) 2' (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>  1/2,1/2,1/2)'	(3) 4 <sup>+</sup> ' (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>  1/2,0,3/4)'	(4) 4 <sup>-</sup> ' (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>  1/2,0,3/4)'
(5) 2' 1/4,y,3/8 (2 <sub>y</sub>  1/2,0,3/4)'	(6) 2' (1/2,0,0) x,0,3/8 (2 <sub>x</sub>  1/2,0,3/4)'	(7) 2' (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(8) 2' x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1/2,1/2,1/2) +		
16	g	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]		
			(3) $\bar{y},x+1/2,z+1/4$ [0,0,0]	(4) $y,\bar{x}+1/2,z+1/4$ [0,0,0]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [0,0,0]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [0,0,0]		
			(7) y,x, $\bar{z}$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}$ [0,0,0]		
8	f	.2.1'	x,1/4,1/8 [0,0,0]	$\bar{x},3/4,1/8$ [0,0,0]	1/4,x,7/8 [0,0,0]	3/4, $\bar{x}$ ,7/8 [0,0,0]
8	e	..21'	$\bar{x},x,0$ [0,0,0]	x, $\bar{x},0$ [0,0,0]	x,x+1/2,1/4 [0,0,0]	$\bar{x},\bar{x}+1/2,1/4$ [0,0,0]
8	d	..21'	x,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x},x+1/2,1/4$ [0,0,0]	x, $\bar{x}+1/2,1/4$ [0,0,0]
8	c	2..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,1/2,z+1/4 [0,0,0]	0,1/2, $\bar{z}+1/4$ [0,0,0]
4	b	2.221'	0,0,1/2 [0,0,0]	0,1/2,3/4 [0,0,0]		
4	a	2.221'	0,0,0 [0,0,0]	0,1/2,1/4 [0,0,0]		

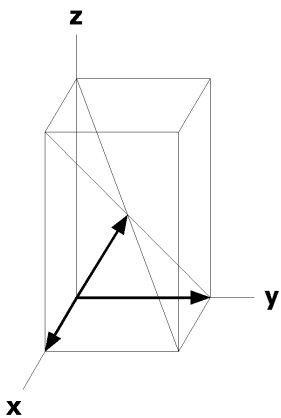
**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

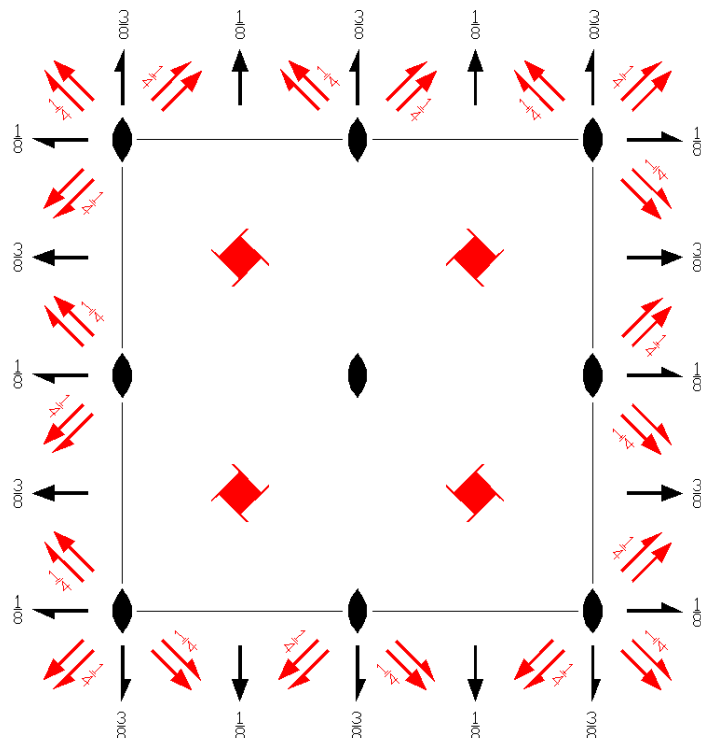
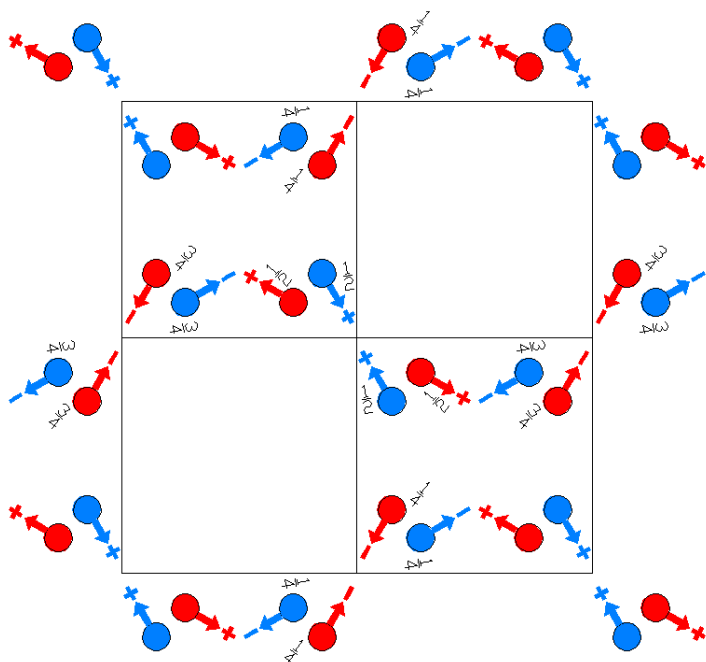




$I4_1'22'$   
98.3.816

$4'22'$   
 $I4_1'22'$

Tetragonal



Origin at  $22'2'$  at  $212'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                               | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)         | (3) $4^+ 1$ $(0,0,1/4) -1/4,1/4,z$<br>( $4_z^+$  0,1/2,1/4)' | (4) $4^- 1$ $(0,0,1/4) 1/4,1/4,z$<br>( $4_z^-$  0,1/2,1/4)' |
| (5) 2 $(0,1/2,0) 0,y,1/8$<br>( $2_y$  0,1/2,1/4) | (6) 2 $x,1/4,1/8$<br>( $2_x$  0,1/2,1/4) | (7) $2'$ $x,x,0$<br>( $2_{xy}$  0,0,0)'                      | (8) $2'$ $x,\bar{x},0$<br>( $2_{\bar{xy}}$  0,0,0)'         |

For  $(1/2,1/2,1/2)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t$ $(1/2,1/2,1/2)$<br>(1 1/2,1/2,1/2) | (2) 2 $(0,0,1/2) 1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2) | (3) $4^+ 1$ $(0,0,3/4) 1/4,1/4,z$<br>( $4_z^+$  1/2,0,3/4)' | (4) $4^- 1$ $(0,0,3/4) 1/4,-1/4,z$<br>( $4_z^-$  1/2,0,3/4)'    |
| (5) 2 $1/4,y,3/8$<br>( $2_y$  1/2,0,3/4)   | (6) 2 $(1/2,0,0) x,0,3/8$<br>( $2_x$  1/2,0,3/4)     | (7) $2'$ $(1/2,1/2,0) x,x,1/4$<br>( $2_{xy}$  1/2,1/2,1/2)' | (8) $2'$ $x,\bar{x}+1/2,1/4$<br>( $2_{\bar{xy}}$  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

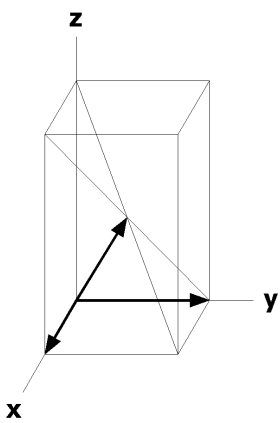
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
				(0,0,0) +	(1/2,1/2,1/2) +	
16	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]		
8	f	.2.	$x,1/4,1/8$ [u,0,0]	$\bar{x},3/4,1/8$ [ $\bar{u},0,0$ ]	$1/4,x,7/8$ [0, $\bar{u}$ ,0]	$3/4,\bar{x},7/8$ [0,u,0]
8	e	..2'	$\bar{x},x,0$ [u,u,w]	$x,\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	$x,x+1/2,1/4$ [ $\bar{u},u,\bar{w}$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $u,\bar{u},\bar{w}$ ]
8	d	..2'	$x,x,0$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [ $u,\bar{u},w$ ]	$\bar{x},x+1/2,1/4$ [ $u,u,\bar{w}$ ]	$x,\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	c	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,1/2,z+1/4 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/4$ [0,0, $\bar{w}$ ]
4	b	2.2'2'	0,0,1/2 [0,0,w]	0,1/2,3/4 [0,0, $\bar{w}$ ]		
4	a	2.2'2'	0,0,0 [0,0,w]	0,1/2,1/4 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p4'm'm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



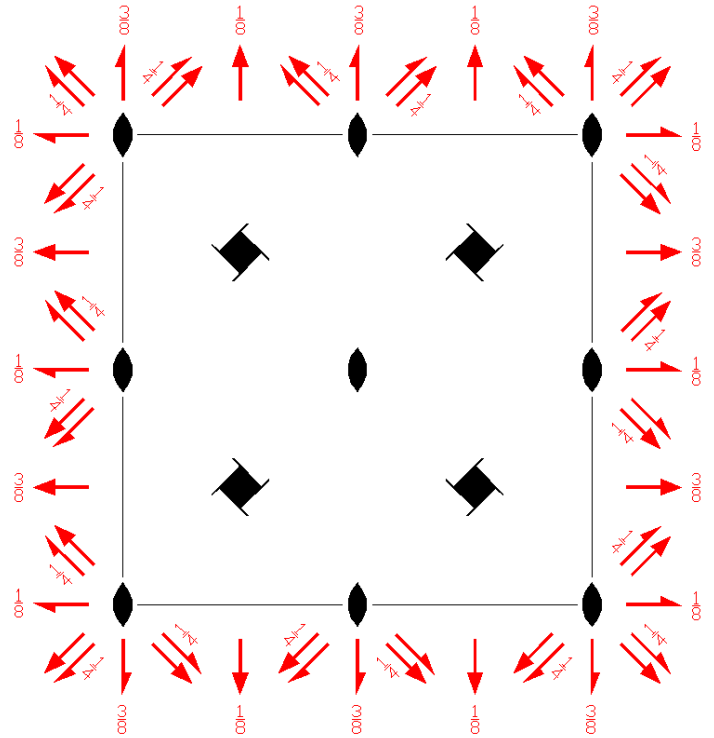
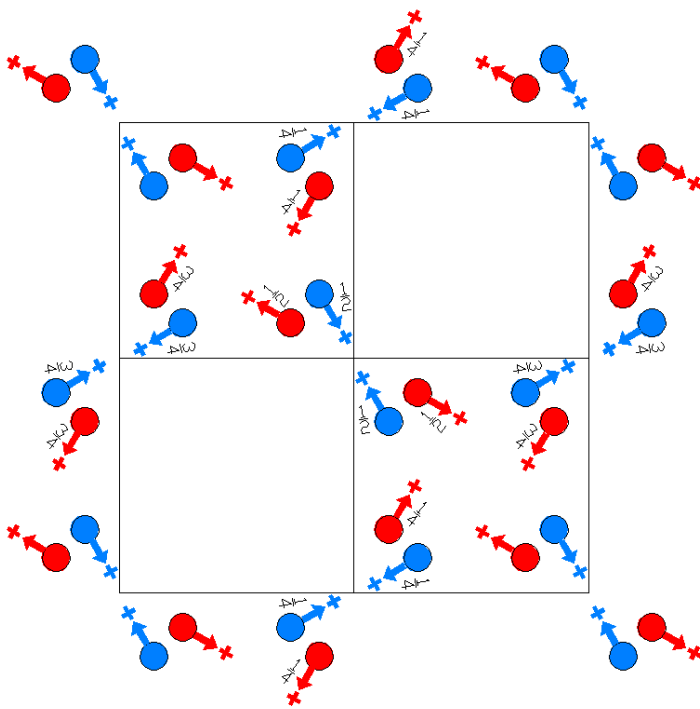
$I4_1 2' 2'$

98.4.817

$42' 2'$

$I4_1 2' 2'$

Tetragonal



Origin at  $22' 2'$  at  $212'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/8$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)             | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>( $4_z$  0,1/2,1/4) | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>( $4_z^{-1}$  0,1/2,1/4) |
| (5) $2'$ $(0,1/2,0) 0,y,1/8$<br>( $2_y$  0,1/2,1/4)' | (6) $2'$ $x,1/4,1/8$<br>( $2_x$  0,1/2,1/4)' | (7) $2'$ $x,x,0$<br>( $2_{xy}$  0,0,0)'                 | (8) $2'$ $x,\bar{x},0$<br>( $2_{\bar{xy}}$  0,0,0)'         |

For  $(1/2,1/2,1/2)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) t $(1/2,1/2,1/2)$<br>(1 1/2,1/2,1/2)     | (2) 2 $(0,0,1/2) 1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2) | (3) $4^+$ $(0,0,3/4) 1/4,1/4,z$<br>( $4_z$  1/2,0,3/4)      | (4) $4^-$ $(0,0,3/4) 1/4,-1/4,z$<br>( $4_z^{-1}$  1/2,0,3/4)    |
| (5) $2'$ $1/4,y,3/8$<br>( $2_y$  1/2,0,3/4)' | (6) $2'$ $(1/2,0,0) x,0,3/8$<br>( $2_x$  1/2,0,3/4)' | (7) $2'$ $(1/2,1/2,0) x,x,1/4$<br>( $2_{xy}$  1/2,1/2,1/2)' | (8) $2'$ $x,\bar{x}+1/2,1/4$<br>( $2_{\bar{xy}}$  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

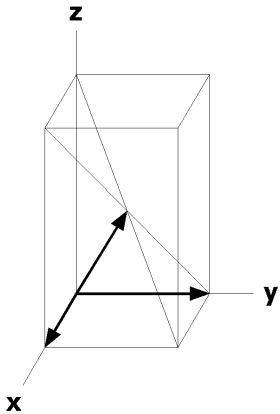
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
				(0,0,0) +	(1/2,1/2,1/2) +	
16	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},v,w$ ]		
			(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]		
8	f	.2'	$x,1/4,1/8$ [0,v,w]	$\bar{x},3/4,1/8$ [0, $\bar{v},w$ ]	$1/4,x,7/8$ [ $\bar{v},0,w$ ]	$3/4,\bar{x},7/8$ [ $v,0,w$ ]
8	e	..2'	$\bar{x},x,0$ [u,u,w]	$x,\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	$x,x+1/2,1/4$ [u, $\bar{u},w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},u,w$ ]
8	d	..2'	$x,x,0$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [u, $\bar{u},w$ ]	$\bar{x},x+1/2,1/4$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x}+1/2,1/4$ [u,u,w]
8	c	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,1/2,z+1/4 [0,0,w]	0,1/2, $\bar{z}+1/4$ [0,0,w]
4	b	2.2'2'	0,0,1/2 [0,0,w]	0,1/2,3/4 [0,0,w]		
4	a	2.2'2'	0,0,0 [0,0,w]	0,1/2,1/4 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,3/8

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



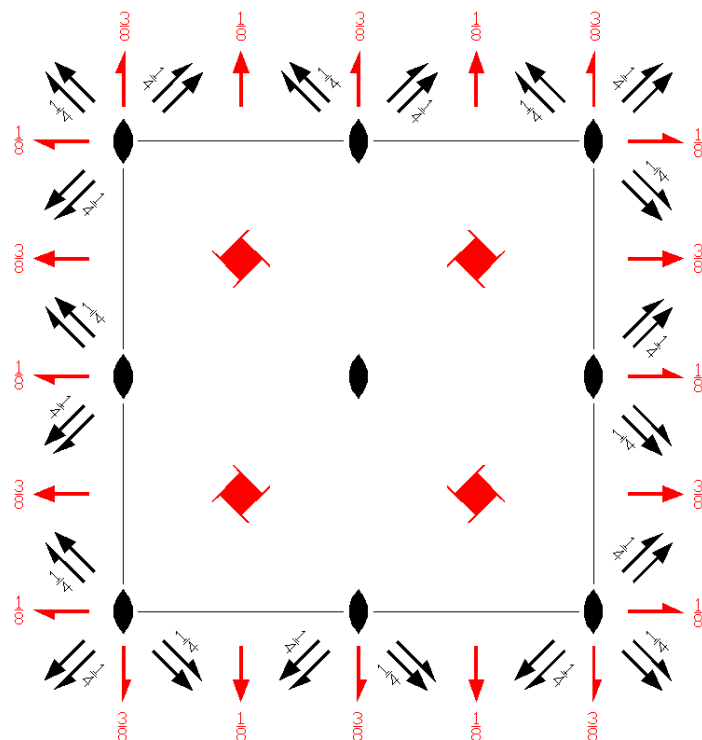
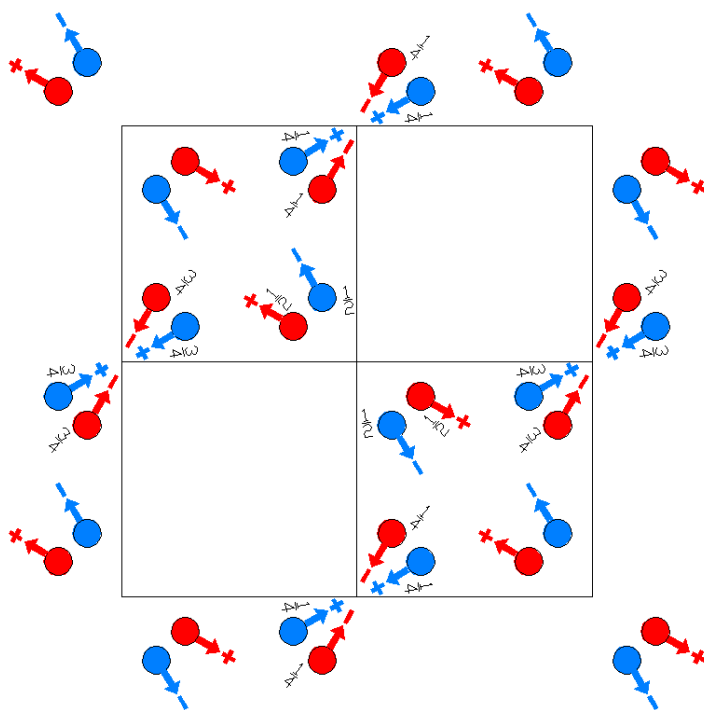
$I4_1'2'2'$

98.5.818

$4'2'2'$

$I4_1'2'2'$

Tetragonal



Origin at 222 at 212

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8$

### Symmetry Operations

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)           | (3) 4 <sup>+</sup> (0,0,1/4) -1/4,1/4,z<br>(4 <sub>z</sub>  0,1/2,1/4)' | (4) 4 <sup>-</sup> (0,0,1/4) 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4)' |
| (5) 2' (0,1/2,0) 0,y,1/8<br>(2 <sub>y</sub>  0,1/2,1/4)' | (6) 2' x,1/4,1/8<br>(2 <sub>x</sub>  0,1/2,1/4)' | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                 | (8) 2 x,x̄,0<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,0)                               |

For (1/2,1/2,1/2) + set

- |  |  |  |   |
|--|--|--|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)           | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,3/4) 1/4,1/4,z<br>(4 <sub>z</sub>  1/2,0,3/4)' | (4) 4 <sup>-</sup> (0,0,3/4) 1/4,-1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,0,3/4)' |
| (5) 2' 1/4,y,3/8<br>(2 <sub>y</sub>  1/2,0,3/4)' | (6) 2' (1/2,0,0) x,0,3/8<br>(2 <sub>x</sub>  1/2,0,3/4)'   | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)            | (8) 2 x,x̄+1/2,1/4<br>(2 <sub>xy</sub> <sup>-1</sup>  1/2,1/2,1/2)                    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

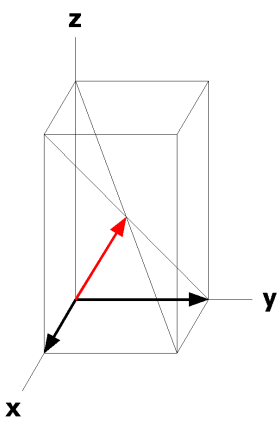
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
				(0,0,0) +	(1/2,1/2,1/2) +	
16	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},v,w$ ]		
			(7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	f	.2'	$x,1/4,1/8$ [0,v,w]	$\bar{x},3/4,1/8$ [0, $\bar{v}$ ,w]	$1/4,x,7/8$ [v,0, $\bar{w}$ ]	$3/4,\bar{x},7/8$ [ $\bar{v},0,\bar{w}$ ]
8	e	..2	$\bar{x},x,0$ [ $\bar{u},u,0$ ]	$x,\bar{x},0$ [ $u,\bar{u},0$ ]	$x,x+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $u,u,0$ ]
8	d	..2	$x,x,0$ [ $u,u,0$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,1/4$ [ $u,\bar{u},0$ ]	$x,\bar{x}+1/2,1/4$ [ $\bar{u},u,0$ ]
8	c	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/4 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/4$ [0,0,w]
4	b	2.22	0,0,1/2 [0,0,0]	0,1/2,3/4 [0,0,0]		
4	a	2.22	0,0,0 [0,0,0]	0,1/2,1/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4'm'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,3/8

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



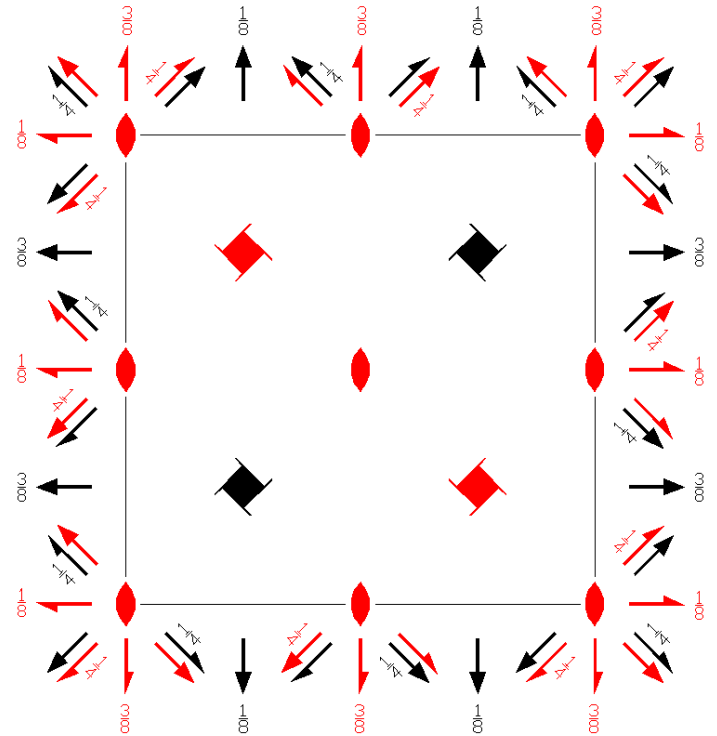
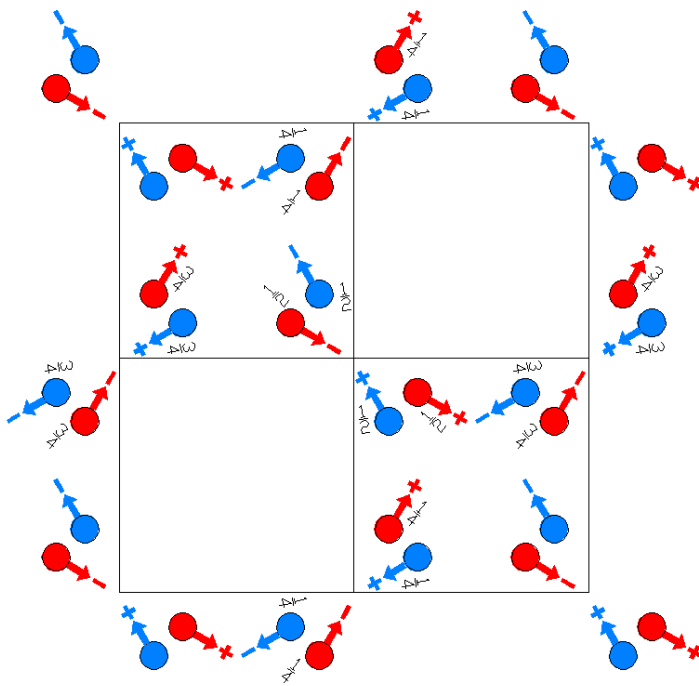
$I_P 4_1 22$

$4221'$

Tetragonal

98.6.819

$I_P 4_1 22$



Origin at  $2'2'2$  at  $2'1(2',2)$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/8$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                                 | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)'       | (3) $4^+$ (0,0,1/4) -1/4,1/4,z<br>( $4_z$  0,1/2,1/4) | (4) $4^-$ (0,0,1/4) 1/4,1/4,z<br>( $4_z^{-1}$  0,1/2,1/4)' |
| (5) $2'$ (0,1/2,0) 0,y,1/8<br>( $2_y$  0,1/2,1/4)' | (6) $2$ x,1/4,1/8<br>( $2_x$  0,1/2,1/4) | (7) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)'                 | (8) $2$ x, $\bar{x}$ ,0<br>( $2_{\bar{xy}}$  0,0,0)        |

For  $(1/2,1/2,1/2)'$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t'$ (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)' | (2) $2$ (0,0,1/2) 1/4,1/4,z<br>( $2_z$  1/2,1/2,1/2) | (3) $4^+$ (0,0,3/4) 1/4,1/4,z<br>( $4_z$  1/2,0,3/4)'   | (4) $4^-$ (0,0,3/4) 1/4,-1/4,z<br>( $4_z^{-1}$  1/2,0,3/4)        |
| (5) $2$ 1/4,y,3/8<br>( $2_y$  1/2,0,3/4)   | (6) $2'$ (1/2,0,0) x,0,3/8<br>( $2_x$  1/2,0,3/4)'   | (7) $2$ (1/2,1/2,0) x,x,1/4<br>( $2_{xy}$  1/2,1/2,1/2) | (8) $2'$ x, $\bar{x}$ +1/2,1/4<br>( $2_{\bar{xy}}$  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
				(0,0,0) +	(1/2,1/2,1/2)' +	
16	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]		
			(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [u, $\bar{v},w$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [u, $\bar{v},\bar{w}$ ]		
			(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	f	.2.	$x,1/4,1/8$ [u,0,0]	$\bar{x},3/4,1/8$ [u,0,0]	$1/4,x,7/8$ [0, $\bar{u},0$ ]	$3/4,\bar{x},7/8$ [0, $\bar{u},0$ ]
8	e	..2	$\bar{x},x,0$ [ $\bar{u},u,0$ ]	$x,\bar{x},0$ [ $\bar{u},u,0$ ]	$x,x+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]
8	d	..2'	$x,x,0$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},u,\bar{w}$ ]	$\bar{x},x+1/2,1/4$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	c	2'..	0,0,z [u,v,0]	0,0, $\bar{z}$ [ $\bar{v},\bar{u},0$ ]	0,1/2,z+1/4 [ $\bar{v},u,0$ ]	0,1/2, $\bar{z}+1/4$ [u, $\bar{v},0$ ]
4	b	2'.2'2	0,0,1/2 [ $\bar{u},u,0$ ]	0,1/2,3/4 [ $\bar{u},\bar{u},0$ ]		
4	a	2'.2'2	0,0,0 [ $\bar{u},u,0$ ]	0,1/2,1/4 [ $\bar{u},\bar{u},0$ ]		

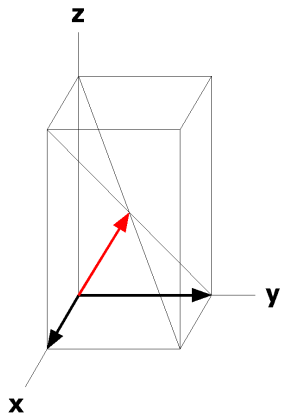
**Symmetry of Special Projections**

Along [0,0,1]  $p_p$ , 4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,-1/4,z

Along [1,0,0]  $c_p$ , 2'mm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

Along [1,1,0]  $p_{2a}$ , 2mm  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4





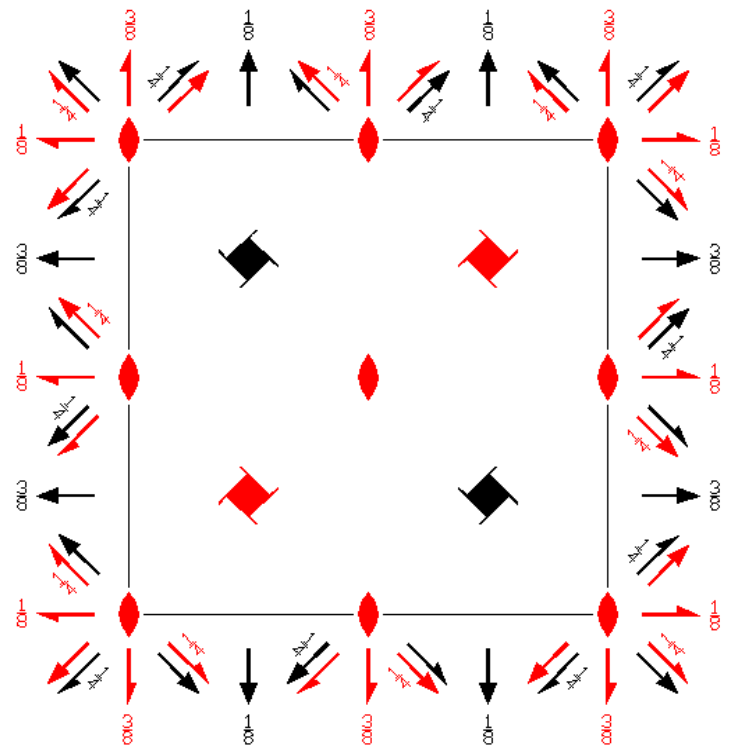
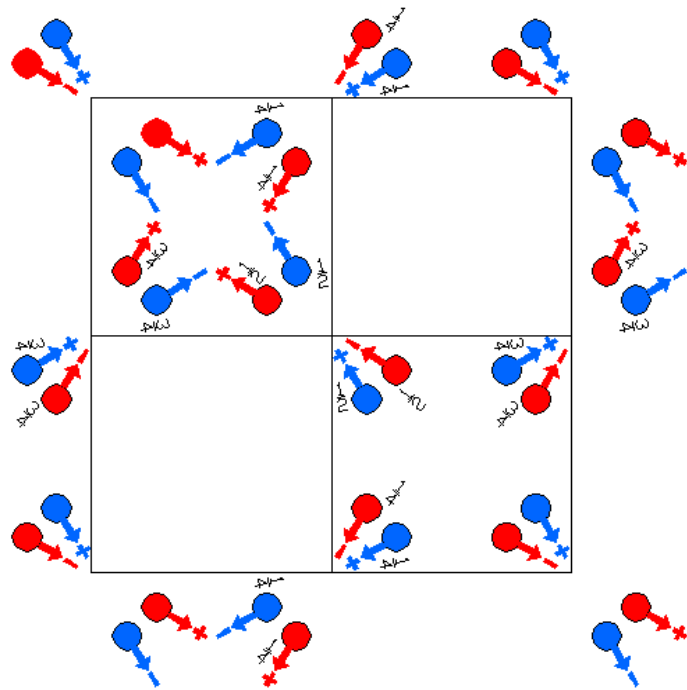
$I_p 4_1'22'$

98.7.820

4221'

$I_p 4_1'22'$

Tetragonal



Origin at  $2'22'$  at  $2'1(2,2')$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/8$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                                 | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)'       | (3) $4^+$ (0,0,1/4) -1/4,1/4,z<br>( $4_z$  0,1/2,1/4)' | (4) $4^-$ (0,0,1/4) 1/4,1/4,z<br>( $4_z^{-1}$  0,1/2,1/4) |
| (5) $2'$ (0,1/2,0) 0,y,1/8<br>( $2_y$  0,1/2,1/4)' | (6) $2$ x,1/4,1/8<br>( $2_x$  0,1/2,1/4) | (7) $2$ x,x,0<br>( $2_{xy}$  0,0,0)                    | (8) $2'$ x, $\bar{x}$ ,0<br>( $2_{\bar{xy}}$  0,0,0)'     |

For  $(1/2,1/2,1/2)'$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t'$ (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)' | (2) $2$ (0,0,1/2) 1/4,1/4,z<br>( $2_z$  1/2,1/2,1/2) | (3) $4^+$ (0,0,3/4) 1/4,1/4,z<br>( $4_z$  1/2,0,3/4)      | (4) $4^-$ (0,0,3/4) 1/4,-1/4,z<br>( $4_z^{-1}$  1/2,0,3/4)'     |
| (5) $2$ 1/4,y,3/8<br>( $2_y$  1/2,0,3/4)   | (6) $2'$ (1/2,0,0) x,0,3/8<br>( $2_x$  1/2,0,3/4)'   | (7) $2'$ (1/2,1/2,0) x,x,1/4<br>( $2_{xy}$  1/2,1/2,1/2)' | (8) $2$ x, $\bar{x}$ +1/2,1/4<br>( $2_{\bar{xy}}$  1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

### Positions

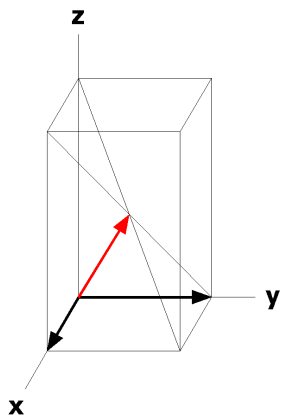
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
				(0,0,0) +	(1/2,1/2,1/2)' +	
16	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]		
			(3) $\bar{y},x+1/2,z+1/4$ [v, $\bar{u},\bar{w}$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [v, $\bar{u},w$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [u, $\bar{v},w$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [u, $\bar{v},\bar{w}$ ]		
			(7) $y,x,\bar{z}$ [v,u, $\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [v,u,w]		
8	f	.2.	$x,1/4,1/8$ [u,0,0]	$\bar{x},3/4,1/8$ [u,0,0]	$1/4,x,7/8$ [0,u,0]	$3/4,\bar{x},7/8$ [0,u,0]
8	e	..2'	$\bar{x},x,0$ [u,u,w]	$x,\bar{x},0$ [u,u, $\bar{w}$ ]	$x,x+1/2,1/4$ [u, $\bar{u},w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [u, $\bar{u},\bar{w}$ ]
8	d	..2	$x,x,0$ [u,u,0]	$\bar{x},\bar{x},0$ [u,u,0]	$\bar{x},x+1/2,1/4$ [u, $\bar{u},0$ ]	$x,\bar{x}+1/2,1/4$ [u, $\bar{u},0$ ]
8	c	2'..	$0,0,z$ [u,v,0]	$0,0,\bar{z}$ [v,u,0]	$0,1/2,z+1/4$ [v, $\bar{u},0$ ]	$0,1/2,\bar{z}+1/4$ [u, $\bar{v},0$ ]
4	b	2'.22'	$0,0,1/2$ [u,u,0]	$0,1/2,3/4$ [u, $\bar{u},0$ ]		
4	a	2'.22'	$0,0,0$ [u,u,0]	$0,1/2,1/4$ [u, $\bar{u},0$ ]		

### Symmetry of Special Projections

Along [0,0,1]  $p_p$ , 4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0]  $c_p$ , 2mm  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

Along [1,1,0]  $p_{2a}$ , 2mm  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



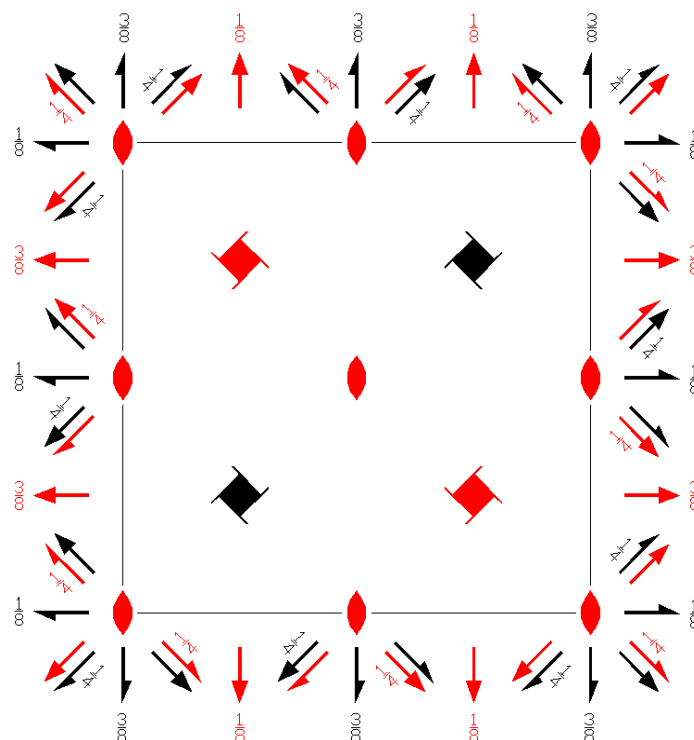
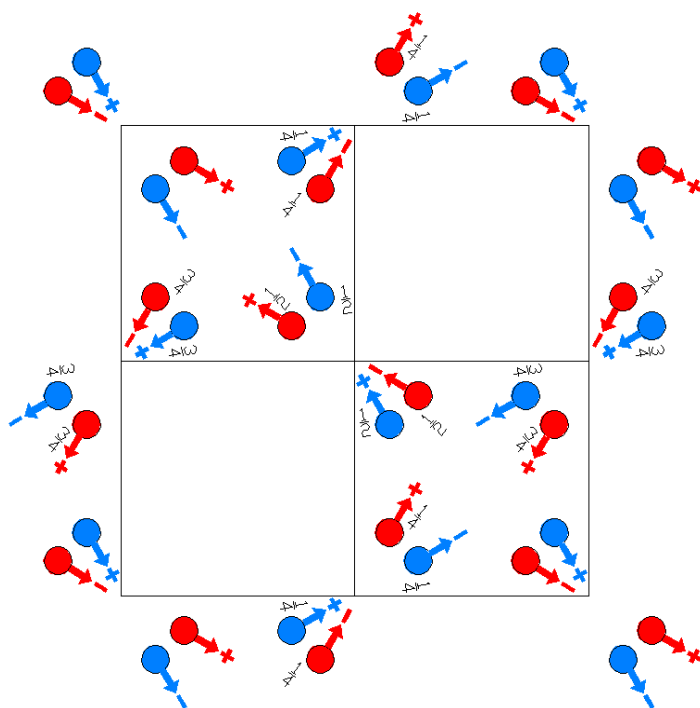
$I_P 4_1 2' 2'$

98.8.821

4221'

$I_P 4_1 2' 2'$

Tetragonal



Origin at 2'22' at 2'1(2,2')

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'         | (3) 4 <sup>+</sup> (0,0,1/4) -1/4,1/4,z<br>(4 <sub>z</sub>  0,1/2,1/4) | (4) 4 <sup>-</sup> (0,0,1/4) 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4)' |
| (5) 2 (0,1/2,0) 0,y,1/8<br>(2 <sub>y</sub>  0,1/2,1/4) | (6) 2' x,1/4,1/8<br>(2 <sub>x</sub>  0,1/2,1/4)' | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                | (8) 2' x,x̄,0<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,0)'                              |

For (1/2,1/2,1/2)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'         | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,3/4) 1/4,1/4,z<br>(4 <sub>z</sub>  1/2,0,3/4)' | (4) 4 <sup>-</sup> (0,0,3/4) 1/4,-1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,0,3/4) |
| (5) 2' 1/4,y,3/8<br>(2 <sub>y</sub>  1/2,0,3/4)' | (6) 2 (1/2,0,0) x,0,3/8<br>(2 <sub>x</sub>  1/2,0,3/4)     | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'          | (8) 2 x,x̄+1/2,1/4<br>(2 <sub>xy</sub> <sup>-</sup>  1/2,1/2,1/2)                    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

### Positions

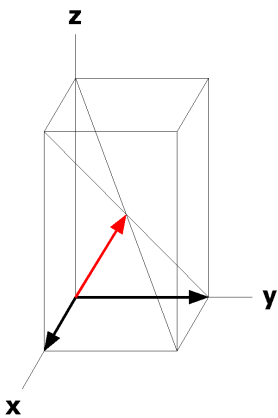
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
				(0,0,0) +	(1/2,1/2,1/2)' +	
16	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]		
			(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v}$ ,u,w]	(4) $y,\bar{x}+1/2,z+1/4$ [ $\bar{v}$ ,u, $\bar{w}$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u}$ ,v,w]		
			(7) $y,x,\bar{z}$ [v,u, $\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [v,u,w]		
8	f	.2'	x,1/4,1/8 [0,v,w]	$\bar{x},3/4,1/8$ [0,v, $\bar{w}$ ]	1/4,x,7/8 [v,0, $\bar{w}$ ]	3/4, $\bar{x}$ ,7/8 [v,0,w]
8	e	..2'	$\bar{x},x,0$ [u,u,w]	$x,\bar{x},0$ [u,u, $\bar{w}$ ]	x,x+1/2,1/4 [ $\bar{u}$ ,u, $\bar{w}$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u}$ ,u,w]
8	d	..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [u,u,0]	$\bar{x},x+1/2,1/4$ [ $\bar{u}$ ,u,0]	x, $\bar{x}+1/2,1/4$ [ $\bar{u}$ ,u,0]
8	c	2'..	0,0,z [u,v,0]	0,0, $\bar{z}$ [v,u,0]	0,1/2,z+1/4 [ $\bar{v}$ ,u,0]	0,1/2, $\bar{z}+1/4$ [ $\bar{u}$ ,v,0]
4	b	2'.22'	0,0,1/2 [u,u,0]	0,1/2,3/4 [ $\bar{u}$ ,u,0]		
4	a	2'.22'	0,0,0 [u,u,0]	0,1/2,1/4 [ $\bar{u}$ ,u,0]		

### Symmetry of Special Projections

Along [0,0,1]  $p_p, 4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,-1/4,z

Along [1,0,0]  $c_p, 2mm$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,3/8

Along [1,1,0]  $p_{2a}, 2mm$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



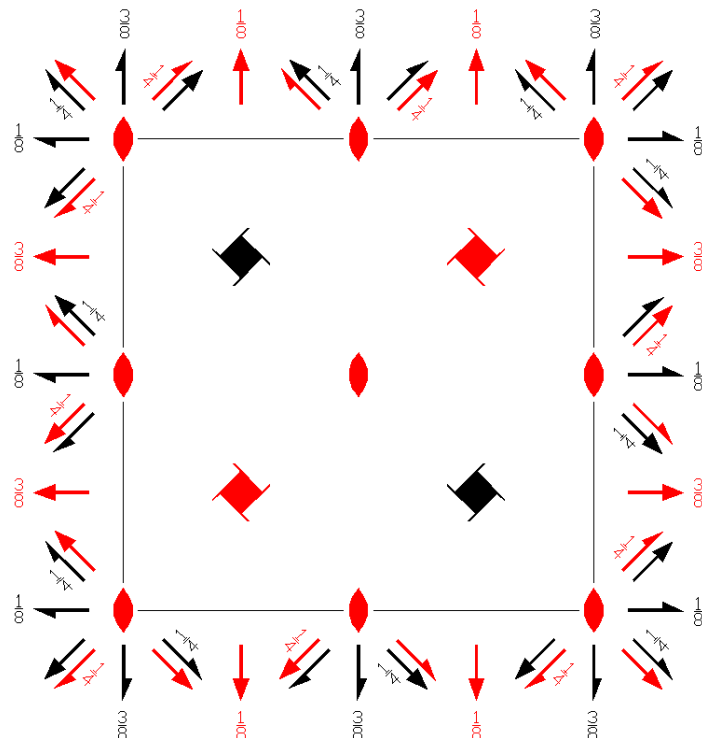
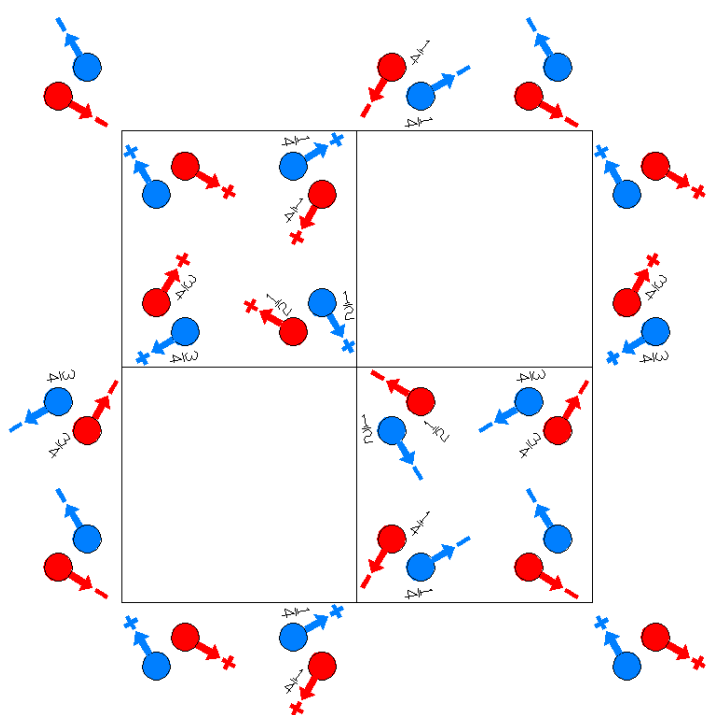
$I_p 4_1' 2' 2'$

98.9.822

4221'

$I_p 4_1' 2' 2'$

Tetragonal



Origin at  $2' 2' 2'$  at  $2' 1'(2', 2)$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/8$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                               | (2) $2'$ 0,0,z<br>( $2_z$  0,0,0)'         | (3) $4^+$ (0,0,1/4) -1/4,1/4,z<br>( $4_z$  0,1/2,1/4)' | (4) $4^-$ (0,0,1/4) 1/4,1/4,z<br>( $4_z^{-1}$  0,1/2,1/4) |
| (5) $2$ (0,1/2,0) 0,y,1/8<br>( $2_y$  0,1/2,1/4) | (6) $2'$ x,1/4,1/8<br>( $2_x$  0,1/2,1/4)' | (7) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)'                  | (8) $2$ x, $\bar{x}$ ,0<br>( $2_{\bar{xy}}$  0,0,0)       |

For (1/2,1/2,1/2)' + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t'$ (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)' | (2) $2$ (0,0,1/2) 1/4,1/4,z<br>( $2_z$  1/2,1/2,1/2) | (3) $4^+$ (0,0,3/4) 1/4,1/4,z<br>( $4_z$  1/2,0,3/4)    | (4) $4^-$ (0,0,3/4) 1/4,-1/4,z<br>( $4_z^{-1}$  1/2,0,3/4)'       |
| (5) $2'$ 1/4,y,3/8<br>( $2_y$  1/2,0,3/4)' | (6) $2$ (1/2,0,0) x,0,3/8<br>( $2_x$  1/2,0,3/4)     | (7) $2$ (1/2,1/2,0) x,x,1/4<br>( $2_{xy}$  1/2,1/2,1/2) | (8) $2'$ x, $\bar{x}$ +1/2,1/4<br>( $2_{\bar{xy}}$  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

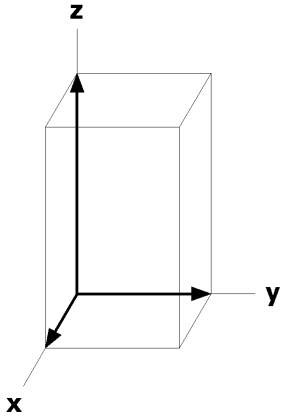
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
				(0,0,0) +	(1/2,1/2,1/2)' +	
16	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]		
			(3) $\bar{y}, x+1/2, z+1/4$ [v, $\bar{u}, \bar{w}$ ]	(4) $y, \bar{x}+1/2, z+1/4$ [v, $\bar{u}, w$ ]		
			(5) $\bar{x}, y+1/2, \bar{z}+1/4$ [ $\bar{u}, v, \bar{w}$ ]	(6) $x, \bar{y}+1/2, \bar{z}+1/4$ [ $\bar{u}, v, w$ ]		
			(7) $y, x, \bar{z}$ [ $\bar{v}, \bar{u}, w$ ]	(8) $\bar{y}, \bar{x}, \bar{z}$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
8	f	.2'	x,1/4,1/8 [0,v,w]	$\bar{x}, 3/4, 1/8$ [0,v, $\bar{w}$ ]	1/4,x,7/8 [ $\bar{v}, 0, w$ ]	3/4, $\bar{x}, 7/8$ [ $\bar{v}, 0, \bar{w}$ ]
8	e	..2	$\bar{x}, x, 0$ [ $\bar{u}, u, 0$ ]	$x, \bar{x}, 0$ [ $\bar{u}, u, 0$ ]	x,x+1/2,1/4 [u,u,0]	$\bar{x}, \bar{x}+1/2, 1/4$ [u,u,0]
8	d	..2'	x,x,0 [ $\bar{u}, u, w$ ]	$\bar{x}, \bar{x}, 0$ [ $\bar{u}, u, \bar{w}$ ]	$\bar{x}, x+1/2, 1/4$ [u,u, $\bar{w}$ ]	$x, \bar{x}+1/2, 1/4$ [u,u,w]
8	c	2'..	0,0,z [u,v,0]	0,0, $\bar{z}$ [ $\bar{v}, \bar{u}, 0$ ]	0,1/2,z+1/4 [v, $\bar{u}, 0$ ]	0,1/2, $\bar{z}+1/4$ [ $\bar{u}, v, 0$ ]
4	b	2'.2'2	0,0,1/2 [ $\bar{u}, u, 0$ ]	0,1/2,3/4 [u,u,0]		
4	a	2'.2'2	0,0,0 [ $\bar{u}, u, 0$ ]	0,1/2,1/4 [u,u,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_p$ , 4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0]  $c_p$ , 2'mm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

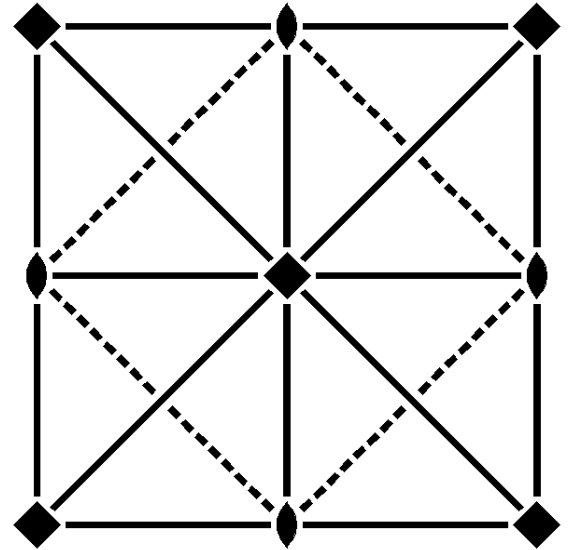
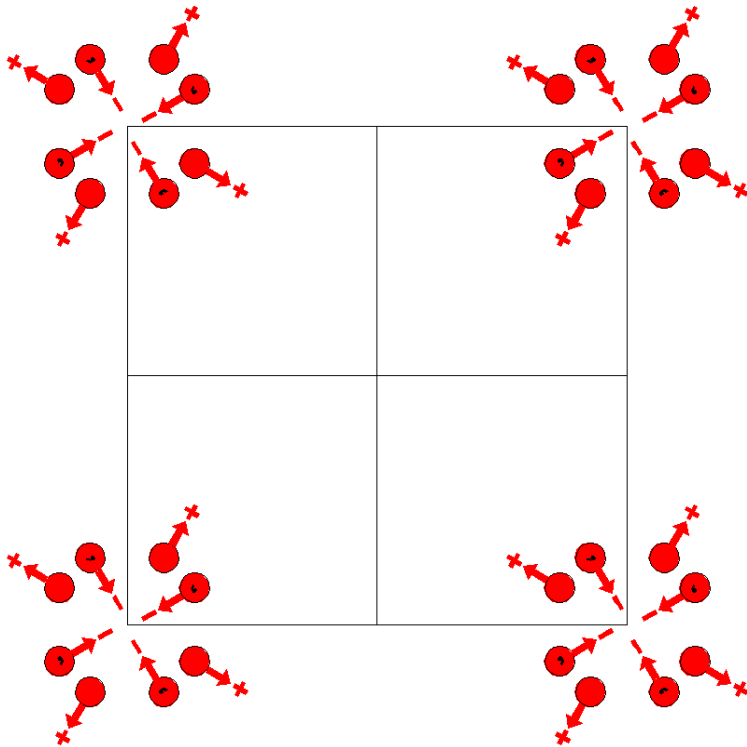
Along [1,1,0]  $p_{2a}$ , 2mm  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



P4mm  
99.1.823

4mm  
P4mm

Tetragonal



Origin on 4mm

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y$

Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (6) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (7) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)            | (8) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                           |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]
			(5) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(7) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(8) $y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]
4	f	.m.	$x,1/2,z$ [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v}$ ,0]	$1/2,x,z$ [ $\bar{v},0,0$ ]	$1/2,\bar{x},z$ [v,0,0]
4	e	.m.	$x,0,z$ [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]	$0,x,z$ [ $\bar{v},0,0$ ]	$0,\bar{x},z$ [v,0,0]
4	d	..m	$x,x,z$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]	$\bar{x},x,z$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},z$ [ $u,u,0$ ]
2	c	2mm.	$1/2,0,z$ [0,0,0]	$0,1/2,z$ [0,0,0]		
1	b	4mm	$1/2,1/2,z$ [0,0,0]			
1	a	4mm	$0,0,z$ [0,0,0]			

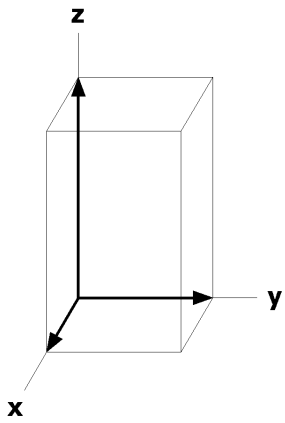
**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0





P4mm1'

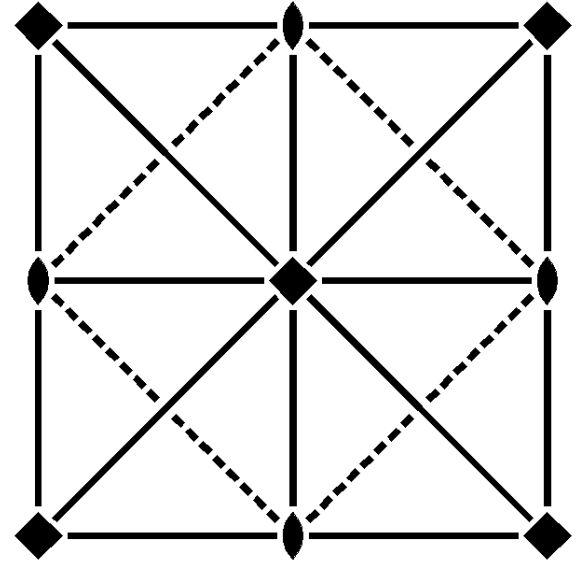
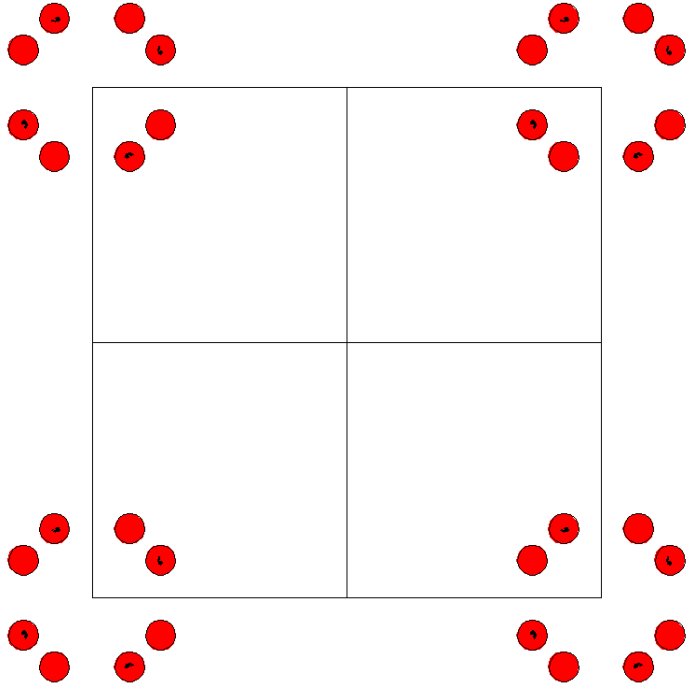
99.2.824

4mm1'

P4mm1'

Tetragonal

1'



Origin on 4mm1'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

Symmetry Operations

For 1 + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0) |
| (5) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (6) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (7) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                         | (8) m x,x,z<br>(m <sub>xy</sub> <sup>-</sup>  0,0,0)             |

For 1' + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1'<br>(1 0,0,0)'                     | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)' |
| (5) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (6) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (7) m' x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'                        | (8) m' x,x,z<br>(m <sub>xy</sub> <sup>-</sup>  0,0,0)'            |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

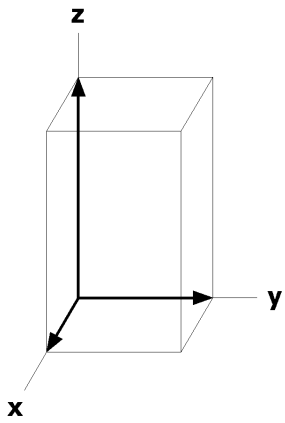
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
8 g 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z$ [0,0,0]	(4) $y,\bar{x},z$ [0,0,0]
	(5) $x,\bar{y},z$ [0,0,0]	(6) $\bar{x},y,z$ [0,0,0]	(7) $\bar{y},\bar{x},z$ [0,0,0]	(8) y,x,z [0,0,0]
4 f .m.1'	x,1/2,z [0,0,0]	$\bar{x},1/2,z$ [0,0,0]	1/2,x,z [0,0,0]	1/2, $\bar{x},z$ [0,0,0]
4 e .m.1'	x,0,z [0,0,0]	$\bar{x},0,z$ [0,0,0]	0,x,z [0,0,0]	0, $\bar{x},z$ [0,0,0]
4 d ..m1'	x,x,z [0,0,0]	$\bar{x},\bar{x},z$ [0,0,0]	$\bar{x},x,z$ [0,0,0]	x, $\bar{x},z$ [0,0,0]
2 c 2mm.1'	1/2,0,z [0,0,0]	0,1/2,z [0,0,0]		
1 b 4mm1'	1/2,1/2,z [0,0,0]			
1 a 4mm1'	0,0,z [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



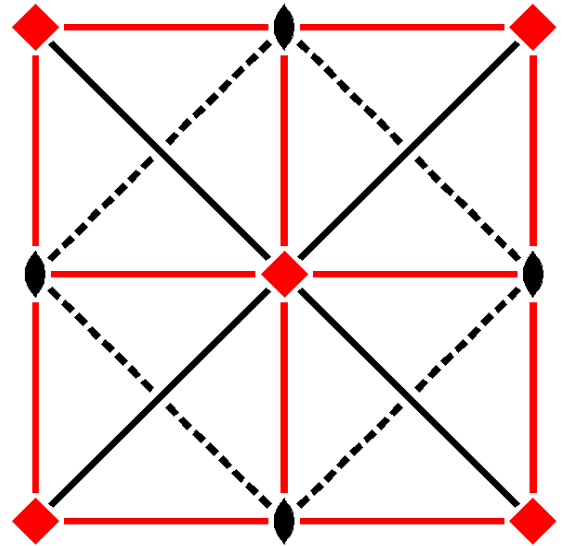
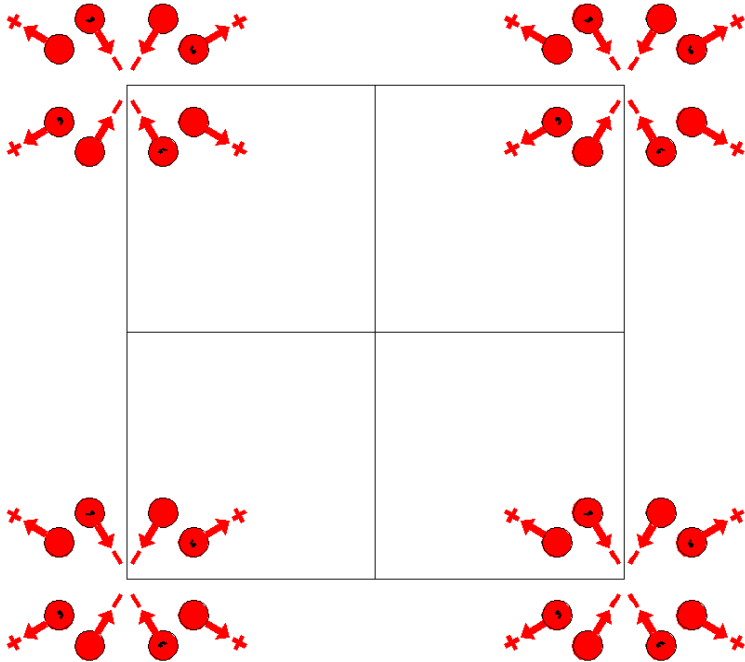
P4'm'm

99.3.825

4'm'm

P4'm'm

Tetragonal



Origin on 4'm'm

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 4<sup>+</sup> 0,0,z  
(4<sub>z</sub>|0,0,0)<sup>+</sup>

(4) 4<sup>-</sup> 0,0,z  
(4<sub>z</sub><sup>-1</sup>|0,0,0)<sup>-</sup>

(5) m' x,0,z  
(m<sub>y</sub>|0,0,0)<sup>-</sup>

(6) m' 0,y,z  
(m<sub>x</sub>|0,0,0)<sup>-</sup>

(7) m x,x̄,z  
(m<sub>xy</sub>|0,0,0)<sup>-</sup>

(8) m x,x,z  
(m<sub>xy</sub>|0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

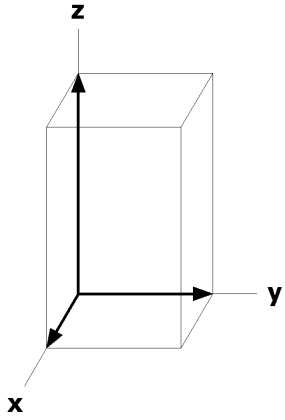
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	g	1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $\bar{y},x,z [v,\bar{u},\bar{w}]$	(4) $y,\bar{x},z [\bar{v},u,\bar{w}]$
			(5) $x,\bar{y},z [u,\bar{v},w]$	(6) $\bar{x},y,z [\bar{u},v,w]$	(7) $\bar{y},\bar{x},z [v,u,\bar{w}]$	(8) $y,x,z [\bar{v},\bar{u},\bar{w}]$
4	f	.m'	$x,1/2,z [u,0,w]$	$\bar{x},1/2,z [\bar{u},0,w]$	$1/2,x,z [0,\bar{u},\bar{w}]$	$1/2,\bar{x},z [0,u,\bar{w}]$
4	e	.m'	$x,0,z [u,0,w]$	$\bar{x},0,z [\bar{u},0,w]$	$0,x,z [0,\bar{u},\bar{w}]$	$0,\bar{x},z [0,u,\bar{w}]$
4	d	..m	$x,x,z [\bar{u},u,0]$	$\bar{x},\bar{x},z [u,\bar{u},0]$	$\bar{x},x,z [u,u,0]$	$x,\bar{x},z [\bar{u},\bar{u},0]$
2	c	2m'm'	$1/2,0,z [0,0,w]$	$0,1/2,z [0,0,\bar{w}]$		
1	b	4'm'm	$1/2,1/2,z [0,0,0]$			
1	a	4'm'm	$0,0,z [0,0,0]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4'm'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

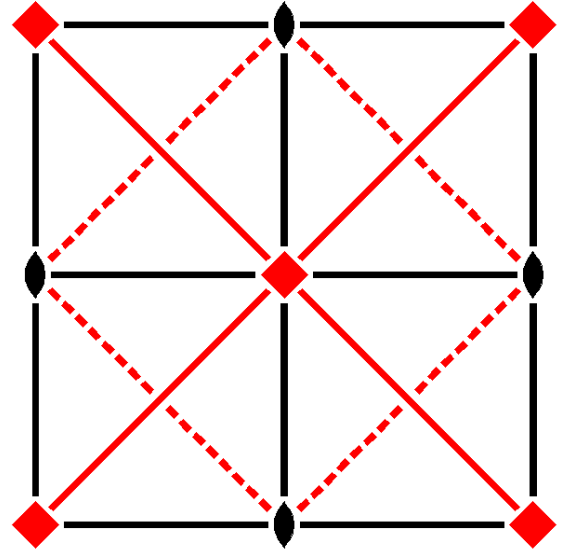
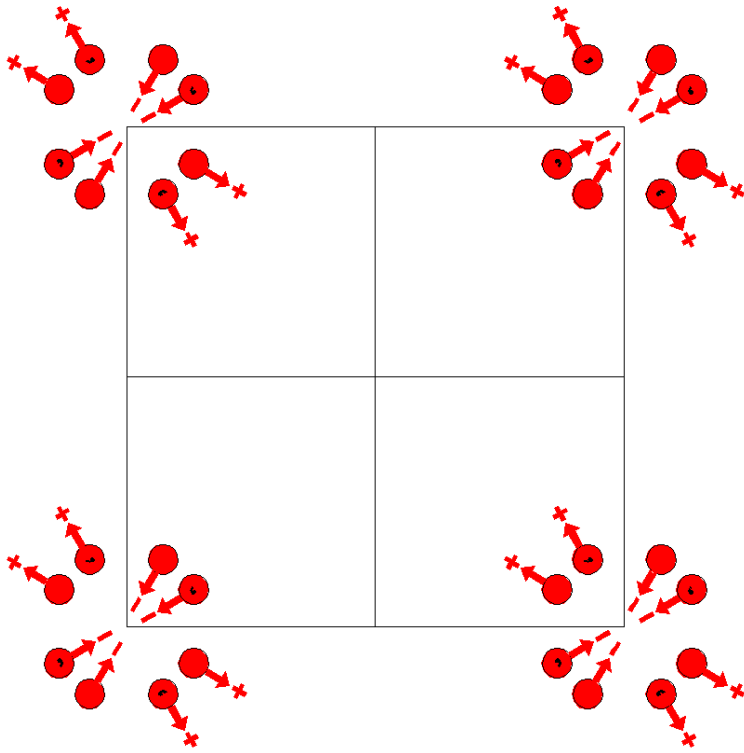
Along  $[1,1,0]$   $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$



P4'mm'  
99.4.826

4'mm'  
P4'mm'

Tetragonal



Origin on 4'mm'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 4<sup>+</sup> 0,0,z  
(4<sub>z</sub>|0,0,0)'

(4) 4<sup>-</sup> 0,0,z  
(4<sub>z</sub><sup>-1</sup>|0,0,0)'

(5) m x,0,z  
(m<sub>y</sub>|0,0,0)

(6) m 0,y,z  
(m<sub>x</sub>|0,0,0)

(7) m' x,x̄,z  
(m<sub>xy</sub>|0,0,0)'

(8) m' x,x,z  
(m<sub>xy</sub>|0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

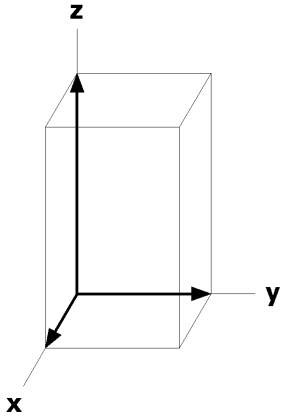
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $v,\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
			(5) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(7) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(8) $y,x,z$ [ $v,u,w$ ]
4	f	.m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v}$ ,0]	1/2,x,z [v,0,0]	1/2, $\bar{x},z$ [ $\bar{v}$ ,0,0]
4	e	.m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]	0,x,z [v,0,0]	0, $\bar{x},z$ [ $\bar{v}$ ,0,0]
4	d	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,z$ [ $u,\bar{u},\bar{w}$ ]	$x,\bar{x},z$ [ $\bar{u},u,\bar{w}$ ]
2	c	2mm.	1/2,0,z [0,0,0]	0,1/2,z [0,0,0]		
1	b	4'mm'	1/2,1/2,z [0,0,0]			
1	a	4'mm'	0,0,z [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

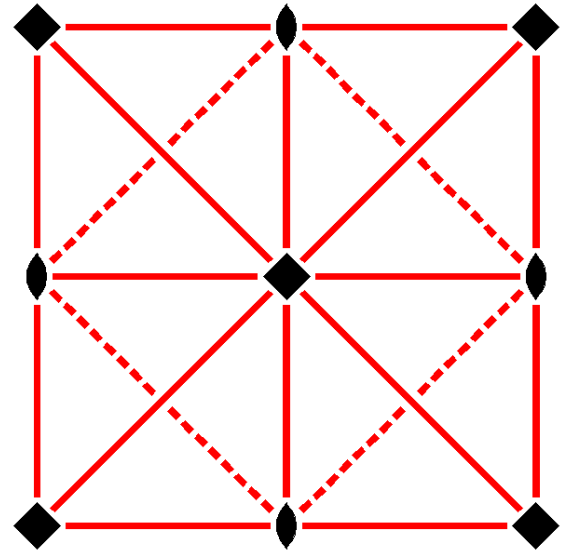
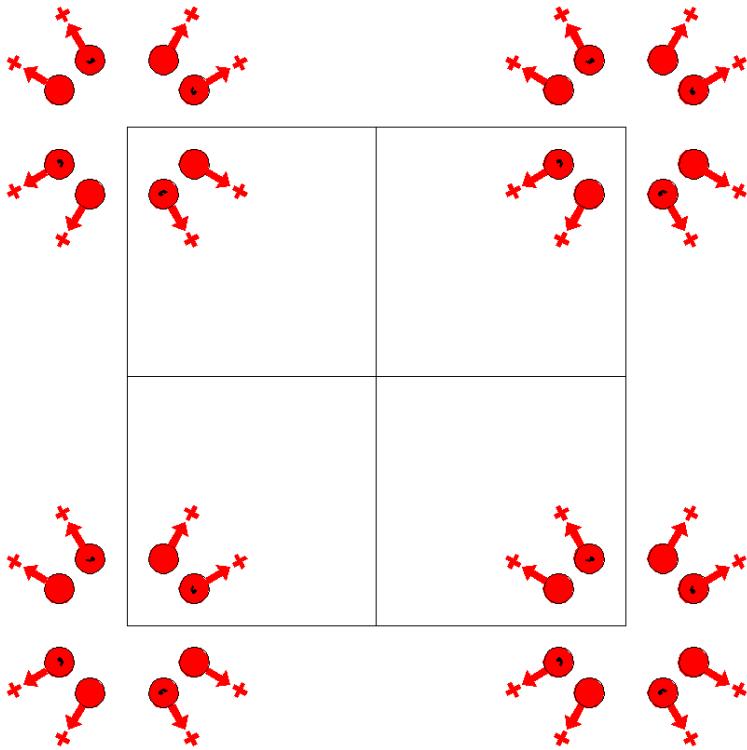
Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4m'm'  
99.5.827

4m'm'  
P4m'm'

Tetragonal



Origin on 4m'm'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$ ;  $x \leq y$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (6) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (7) m' x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'          | (8) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},w$ ]
			(5) x, $\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(6) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(7) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(8) y,x,z [v,u,w]
4	f	.m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ]	1/2,x,z [0,u,w]	1/2, $\bar{x},z$ [0, $\bar{u},w$ ]
4	e	.m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	0,x,z [0,u,w]	0, $\bar{x},z$ [0, $\bar{u},w$ ]
4	d	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,z$ [ $\bar{u},u,w$ ]	x, $\bar{x},z$ [u, $\bar{u},w$ ]
2	c	2m'm'	1/2,0,z [0,0,w]	0,1/2,z [0,0,w]		
1	b	4m'm'	1/2,1/2,z [0,0,w]			
1	a	4m'm'	0,0,z [0,0,w]			

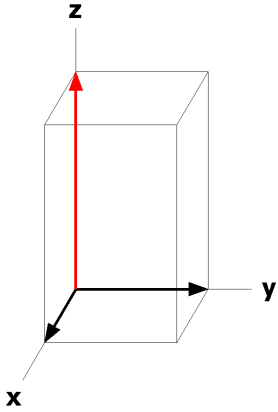
**Symmetry of Special Projections**

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0





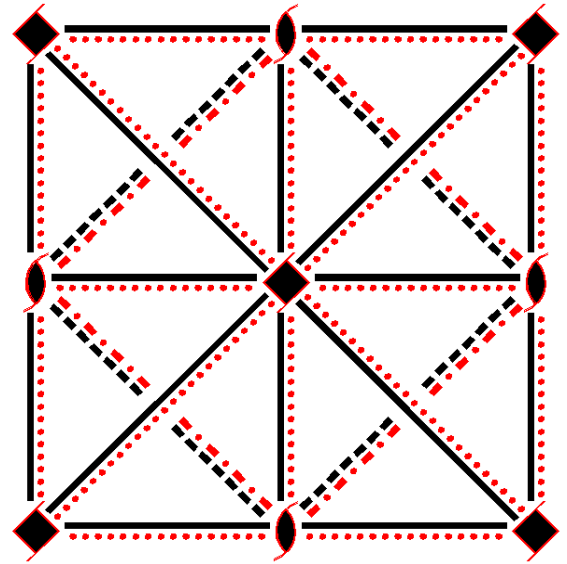
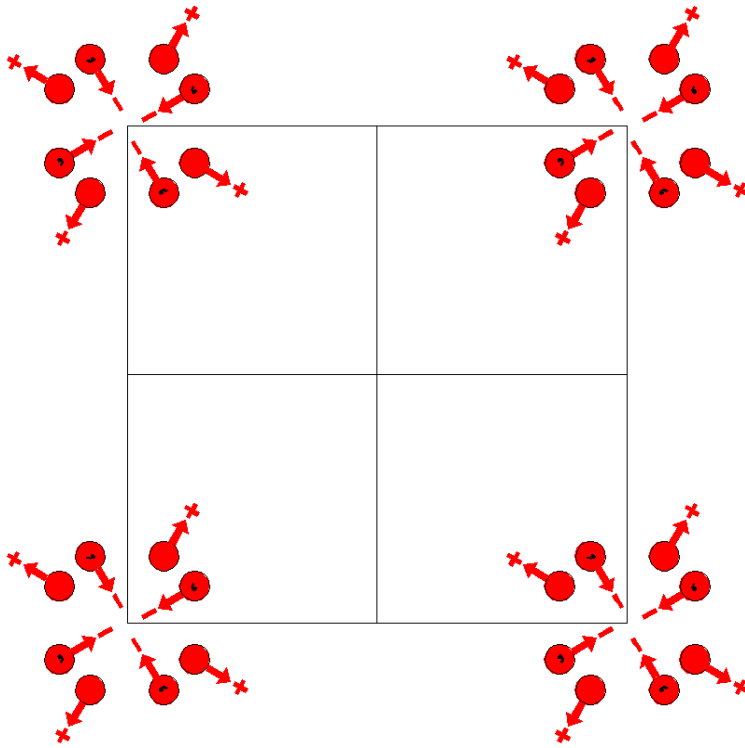
$P_{2c} 4mm$

99.6.828

$4mm1'$

$P_{2c} 4mm$

Tetragonal



Origin on  $4mm$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

Symmetry Operations

For  $(0,0,0)$  + set

- |                                  |                                  |   |   |
|----------------------------------|----------------------------------|---|---|
| (1) 1<br>(1 0,0,0)               | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $4^+$ $0,0,z$<br>( $4_z$  0,0,0)      | (4) $4^-$ $0,0,z$<br>( $4_z^{-1}$  0,0,0) |
| (5) m $x,0,z$<br>( $m_y$  0,0,0) | (6) m $0,y,z$<br>( $m_x$  0,0,0) | (7) m $x,\bar{x},z$<br>( $m_{xy}$  0,0,0) | (8) m $x,x,z$<br>( $m_{\bar{xy}}$  0,0,0) |

For  $(0,0,1)'$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t'$ $(0,0,1)$<br>(1 0,0,1)'               | (2) $2'$ $(0,0,1)$ $0,0,z$<br>( $2_z$  0,0,1)' | (3) $4^+$ $(0,0,1)$ $0,0,z$<br>( $4_z$  0,0,1)'         | (4) $4^-$ $(0,0,1)$ $0,0,z$<br>( $4_z^{-1}$  0,0,1)'    |
| (5) $c'$ $(0,0,1)$ $x,0,z$<br>( $m_y$  0,0,1)' | (6) $c'$ $(0,0,1)$ $0,y,z$<br>( $m_x$  0,0,1)' | (7) $c'$ $(0,0,1)$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,1)' | (8) $c'$ $(0,0,1)$ $x,x,z$<br>( $m_{\bar{xy}}$  0,0,1)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

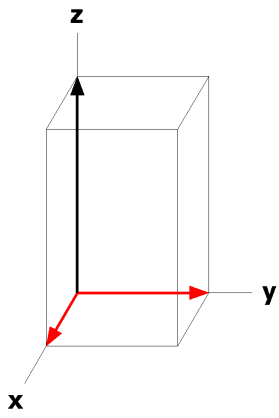
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(0,0,1)' +			
16	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},w$ ]		
			(5) x, $\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(7) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(8) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]		
8	f	.m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v}$ ,0]	1/2,x,z [ $\bar{v}$ ,0,0]	1/2, $\bar{x},z$ [v,0,0]		
8	e	.m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]	0,x,z [ $\bar{v}$ ,0,0]	0, $\bar{x},z$ [v,0,0]		
8	d	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]	$\bar{x},x,z$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},z$ [u,u,0]		
4	c	2mm.	1/2,0,z [0,0,0]	0,1/2,z [0,0,0]				
2	b	4mm	1/2,1/2,z [0,0,0]					
2	a	4mm	0,0,z [0,0,0]					

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



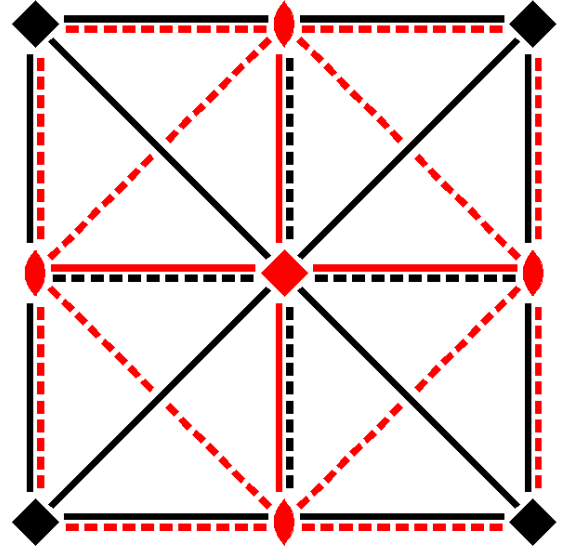
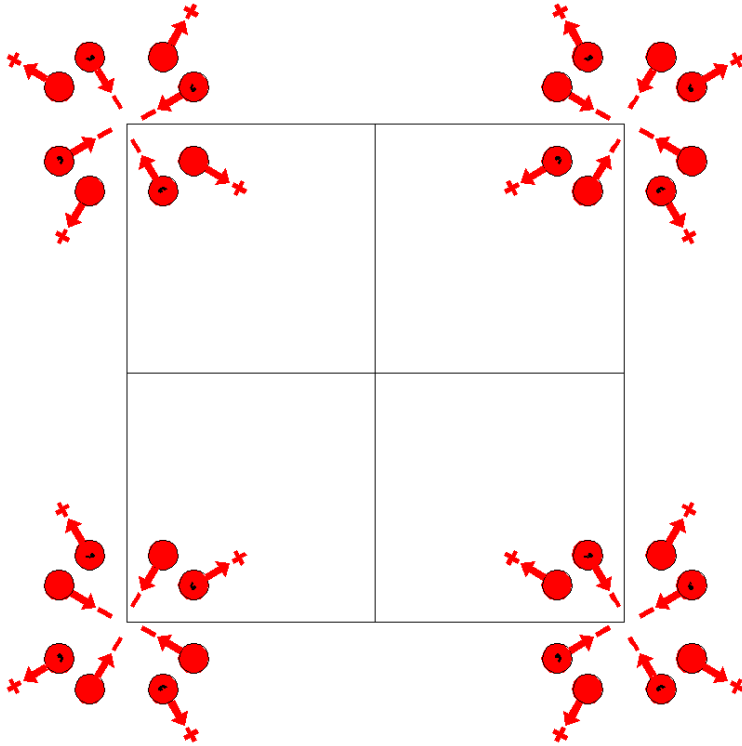
$P_P 4mm$

$4mm1'$

Tetragonal

99.7.829

$P_P 4mm$



Origin on  $4mm$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                                  |                                  |   |   |
|----------------------------------|----------------------------------|---|---|
| (1) 1<br>(1 0,0,0)               | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $4^+$ $0,0,z$<br>( $4_z^+$  0,0,0)    | (4) $4^-$ $0,0,z$<br>( $4_z^-$  0,0,0)    |
| (5) m $x,0,z$<br>( $m_y$  0,0,0) | (6) m $0,y,z$<br>( $m_x$  0,0,0) | (7) m $x,\bar{x},z$<br>( $m_{xy}$  0,0,0) | (8) m $x,x,z$<br>( $m_{\bar{xy}}$  0,0,0) |

For  $(1,0,0)'$  + set

- |  |  |  |   |
|--|--|--|---|
| (1) $t'$ $(1,0,0)$<br>(1 1,0,0)'               | (2) $2'$ $1/2,0,z$<br>( $2_z$  1,0,0)' | (3) $4^{+'}$ $1/2,1/2,z$<br>( $4_z^{+'}$  1,0,0)'                | (4) $4^{-'}$ $1/2,-1/2,z$<br>( $4_z^{-'}$  1,0,0)'              |
| (5) $a'$ $(1,0,0)$ $x,0,z$<br>( $m_y$  1,0,0)' | (6) $m'$ $1/2,y,z$<br>( $m_x$  1,0,0)' | (7) $g'$ $(1/2,-1/2,0)$ $x+1/2,\bar{x},z$<br>( $m_{xy}$  1,0,0)' | (8) $g'$ $(1/2,1/2,0)$ $x+1/2,x,z$<br>( $m_{\bar{xy}}$  1,0,0)' |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

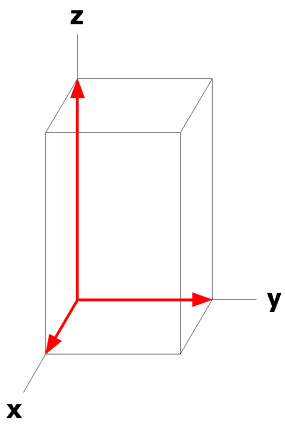
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(1,0,0)' +			
16	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},w$ ]		
			(5) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(7) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(8) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]		
8	f	.m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [u,0, $\bar{w}$ ]	1/2,x,z [0, $\bar{u},\bar{w}$ ]	1/2, $\bar{x},z$ [0, $\bar{u},w$ ]		
8	e	.m	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	0,x,z [ $\bar{v},0,0$ ]	0, $\bar{x},z$ [v,0,0]		
8	d	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [u, $\bar{u},0$ ]	$\bar{x},x,z$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},z$ [u,u,0]		
4	c	2'm'm.	1/2,0,z [0,v,0]	0,1/2,z [ $\bar{v},0,0$ ]				
2	b	4'm'm	1/2,1/2,z [0,0,0]					
2	a	4mm	0,0,z [0,0,0]					

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub>\*4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

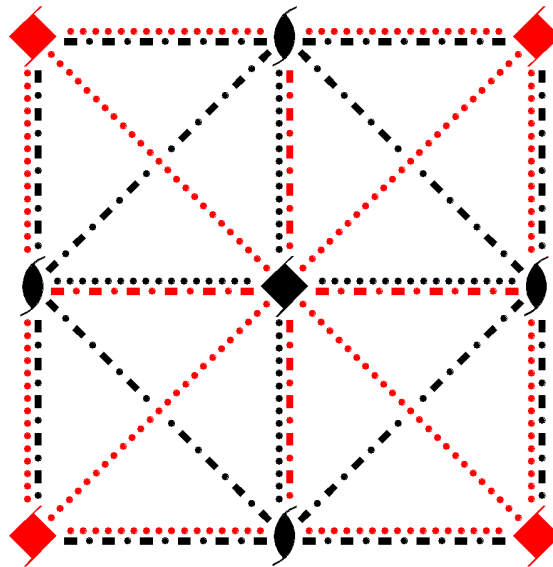
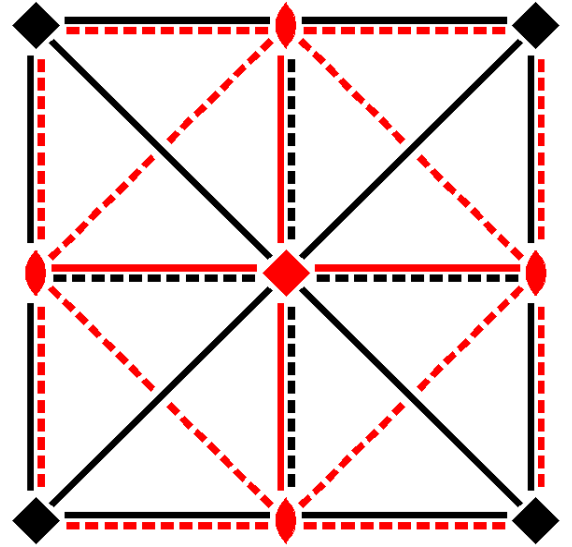
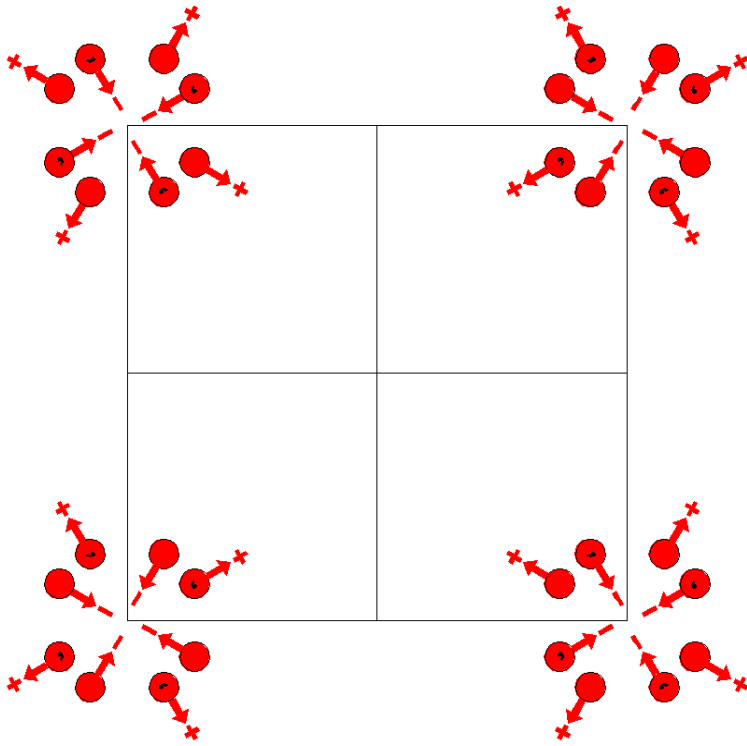
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_14mm$   
99.8.830

$4mm1'$   
 $P_14mm$

Tetragonal



Origin on 4mm

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y$ 

## Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)
(5) m x,0,z (m <sub>y</sub>  0,0,0)	(6) m 0,y,z (m <sub>x</sub>  0,0,0)	(7) m x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)	(8) m x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,0)

For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> ' 1/2,1/2,z (4 <sub>z</sub>  1,0,0)'	(4) 4 <sup>-</sup> ' 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,0)'
(5) a' (1,0,0) x,0,z (m <sub>y</sub>  1,0,0)'	(6) m' 1/2,y,z (m <sub>x</sub>  1,0,0)'	(7) g' (1/2,-1/2,0) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1,0,0)'	(8) g' (1/2,1/2,0) x+1/2,x,z (m <sub><math>\bar{xy}</math></sub>  1,0,0)'

Generators selected (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).

## Positions

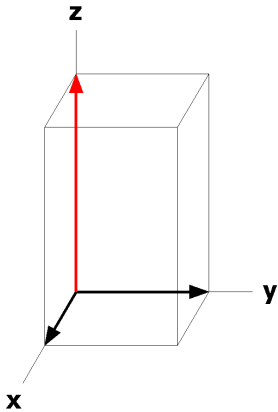
Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

			(0,0,0) +	(1,0,0)' +		
16	g	1	(1) x,y,z [u,v,w] (5) x, $\bar{y}$ ,z [ $\bar{u}$ ,v, $\bar{w}$ ]	(2) $\bar{x}$ , $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w] (6) $\bar{x}$ ,y,z [u, $\bar{v}$ , $\bar{w}$ ]	(3) $\bar{y}$ ,x,z [ $\bar{v}$ ,u,w] (7) $\bar{y}$ , $\bar{x}$ ,z [v,u, $\bar{w}$ ]	(4) y, $\bar{x}$ ,z [v, $\bar{u}$ ,w] (8) y,x,z [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]
8	f	.m'	x,1/2,z [u,0,w]	$\bar{x}$ ,1/2,z [u,0, $\bar{w}$ ]	1/2,x,z [0, $\bar{u}$ , $\bar{w}$ ]	1/2, $\bar{x}$ ,z [0, $\bar{u}$ ,w]
8	e	.m	x,0,z [0,v,0]	$\bar{x}$ ,0,z [0, $\bar{v}$ ,0]	0,x,z [ $\bar{v}$ ,0,0]	0, $\bar{x}$ ,z [v,0,0]
8	d	..m	x,x,z [ $\bar{u}$ ,u,0]	$\bar{x}$ , $\bar{x}$ ,z [u, $\bar{u}$ ,0]	$\bar{x}$ ,x,z [ $\bar{u}$ , $\bar{u}$ ,0]	x, $\bar{x}$ ,z [u,u,0]
4	c	2'm'm	1/2,0,z [0,v,0]	0,1/2,z [ $\bar{v}$ ,0,0]		
2	b	4'm'm	1/2,1/2,z [0,0,0]			
2	a	4mm	0,0,z [0,0,0]			

## Symmetry of Special Projections

Along [0,0,1] p4mm1'  
a\* = a b\* = b  
Origin at 0,0,zAlong [1,0,0] p1m11'  
a\* = b b\* = c  
Origin at x,0,0Along [1,1,0] p1m11'  
a\* = (-a + b)/2 b\* = c  
Origin at x,x,0



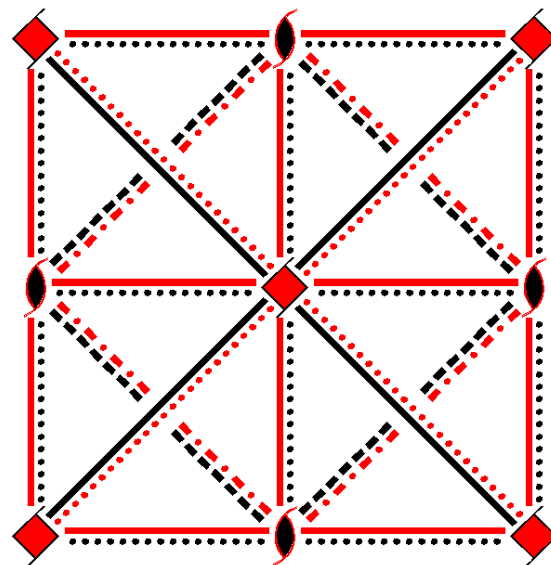
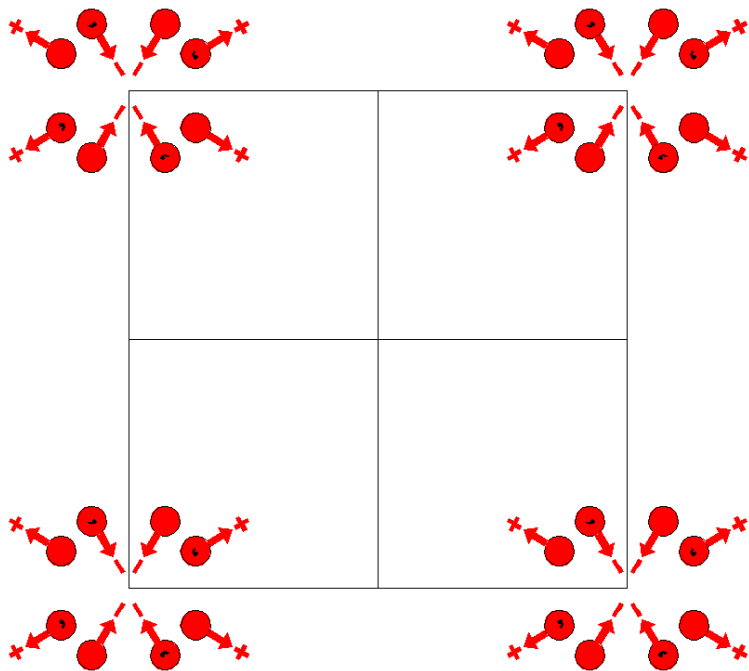
$P_{2c} 4'm'm$

$4mm1'$

Tetragonal

99.9.831

$P_{2c} 4'm'm$



Origin on  $4'm'm$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

For  $(0,0,0) +$  set

- |                                    |                                    |   |   |
|------------------------------------|------------------------------------|---|---|
| (1) 1<br>(1 0,0,0)                 | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)   | (3) $4^+ 0,0,z$<br>( $4_z$  0,0,0)'       | (4) $4^- 0,0,z$<br>( $4_z^{-1}$  0,0,0)'  |
| (5) $m' x,0,z$<br>( $m_y$  0,0,0)' | (6) $m' 0,y,z$<br>( $m_x$  0,0,0)' | (7) $m x,\bar{x},z$<br>( $m_{xy}$  0,0,0) | (8) $m x,x,z$<br>( $m_{\bar{xy}}$  0,0,0) |

For  $(0,0,1) +$  set

- |  |  |   |   |
|--|--|---|---|
| (1) $t' (0,0,1)$<br>(1 0,0,1)'           | (2) $2' (0,0,1) 0,0,z$<br>( $2_z$  0,0,1)' | (3) $4^+ (0,0,1) 0,0,z$<br>( $4_z$  0,0,1)          | (4) $4^- (0,0,1) 0,0,z$<br>( $4_z^{-1}$  0,0,1)     |
| (5) $c (0,0,1) x,0,z$<br>( $m_y$  0,0,1) | (6) $c (0,0,1) 0,y,z$<br>( $m_x$  0,0,1)   | (7) $c' (0,0,1) x,\bar{x},z$<br>( $m_{xy}$  0,0,1)' | (8) $c' (0,0,1) x,x,z$<br>( $m_{\bar{xy}}$  0,0,1)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(0,0,1)' +			
16	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $v,\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]		
			(5) x, $\bar{y},z$ [ $u,\bar{v},w$ ]	(6) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(7) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(8) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]		
8	f	.m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ]	1/2,x,z [0, $\bar{u},\bar{w}$ ]	1/2, $\bar{x},z$ [0,u, $\bar{w}$ ]		
8	e	.m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	0,x,z [0, $\bar{u},\bar{w}$ ]	0, $\bar{x},z$ [0,u, $\bar{w}$ ]		
8	d	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]	$\bar{x},x,z$ [u,u,0]	x, $\bar{x},z$ [ $\bar{u},\bar{u},0$ ]		
4	c	2m'm'	1/2,0,z [0,0,w]	0,1/2,z [0,0, $\bar{w}$ ]				
2	b	4'm'm	1/2,1/2,z [0,0,0]					
2	a	4'm'm	0,0,z [0,0,0]					

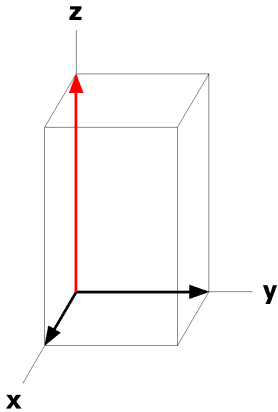
**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>'1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0





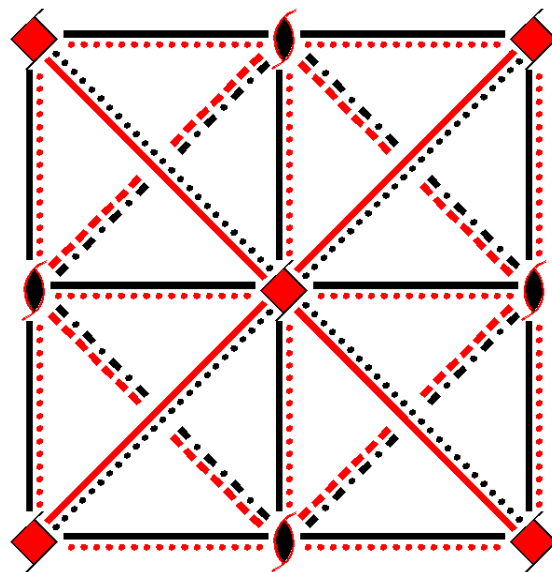
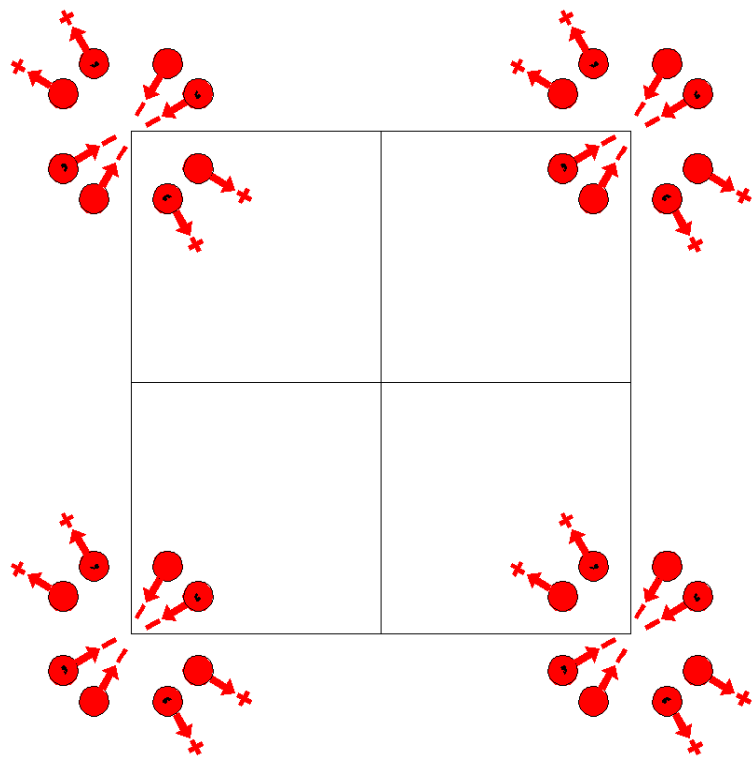
$P_{2c} 4'mm'$

$4mm1'$

Tetragonal

99.10.832

$P_{2c} 4'mm'$



Origin on  $4'mm'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                                  |                                  |   |   |
|----------------------------------|----------------------------------|---|---|
| (1) 1<br>(1 0,0,0)               | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $4^+ 0,0,z$<br>( $4_z$  0,0,0)'         | (4) $4^- 0,0,z$<br>( $4_z^{-1}$  0,0,0)'    |
| (5) m $x,0,z$<br>( $m_y$  0,0,0) | (6) m $0,y,z$<br>( $m_x$  0,0,0) | (7) m' $x,\bar{x},z$<br>( $m_{xy}$  0,0,0)' | (8) m' $x,x,z$<br>( $m_{\bar{xy}}$  0,0,0)' |

For  $(0,0,1)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) t' $(0,0,1)$<br>(1 0,0,1)'             | (2) 2' $(0,0,1) 0,0,z$<br>( $2_z$  0,0,1)' | (3) $4^+ (0,0,1) 0,0,z$<br>( $4_z$  0,0,1)        | (4) $4^- (0,0,1) 0,0,z$<br>( $4_z^{-1}$  0,0,1)   |
| (5) c' $(0,0,1) x,0,z$<br>( $m_y$  0,0,1)' | (6) c' $(0,0,1) 0,y,z$<br>( $m_x$  0,0,1)' | (7) c $(0,0,1) x,\bar{x},z$<br>( $m_{xy}$  0,0,1) | (8) c $(0,0,1) x,x,z$<br>( $m_{\bar{xy}}$  0,0,1) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

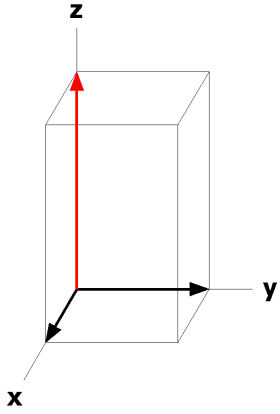
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates						
		(0,0,0) +	(0,0,1)' +				
16 g 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]			
	(5) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(7) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(8) $y,x,z$ [ $v,u,w$ ]			
8 f .m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v}$ ,0]	1/2,x,z [v,0,0]	1/2, $\bar{x},z$ [ $\bar{v}$ ,0,0]			
8 e .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]	0,x,z [v,0,0]	0, $\bar{x},z$ [ $\bar{v}$ ,0,0]			
8 d ..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,z$ [ $u,\bar{u},\bar{w}$ ]	$x,\bar{x},z$ [ $\bar{u},u,\bar{w}$ ]			
4 c 2mm.	1/2,0,z [0,0,0]	0,1/2,z [0,0,0]					
2 b 4'mm'	1/2,1/2,z [0,0,0]						
2 a 4'mm'	0,0,z [0,0,0]						

**Symmetry of Special Projections**

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p_{2b}1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



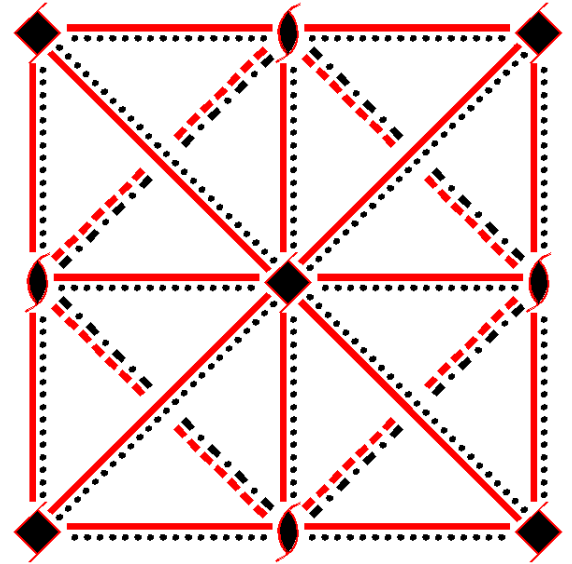
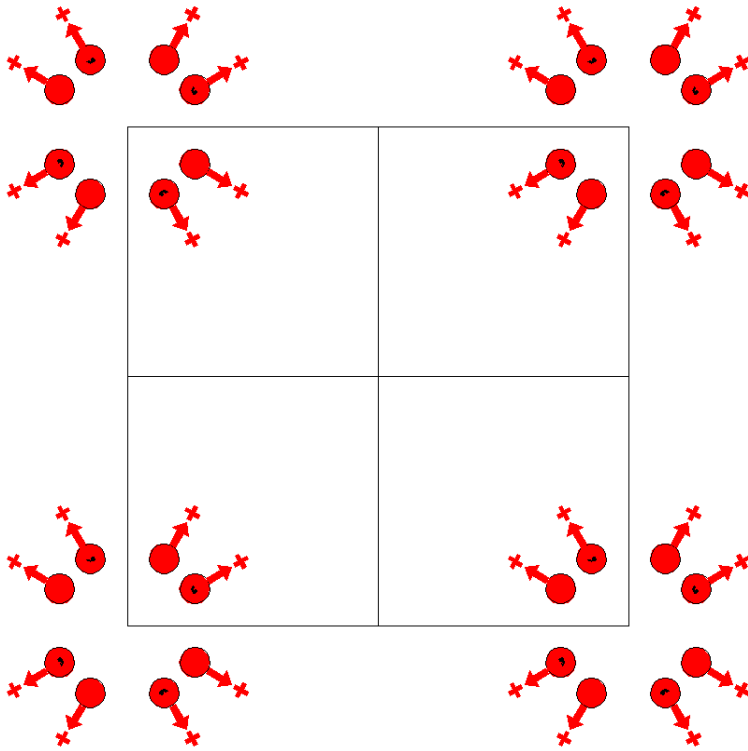
$P_{2c} 4m'm'$

$4mm1'$

Tetragonal

99.11.833

$P_{2c} 4m'm'$



Origin on  $4m'm'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

For  $(0,0,0) +$  set

- |                                      |                                      |   |   |
|--------------------------------------|--------------------------------------|---|---|
| (1) 1<br>(1 0,0,0)                   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)     | (3) $4^+$ $0,0,z$<br>( $4_z^+$  0,0,0)        | (4) $4^-$ $0,0,z$<br>( $4_z^-$  0,0,0)        |
| (5) $m'$ $x,0,z$<br>( $m_y$  0,0,0)' | (6) $m'$ $0,y,z$<br>( $m_x$  0,0,0)' | (7) $m'$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,0)' | (8) $m'$ $x,x,z$<br>( $m_{\bar{xy}}$  0,0,0)' |

For  $(0,0,1) +$  set

- |  |  |   |   |
|--|--|---|---|
| (1) $t'$ $(0,0,1)$<br>(1 0,0,1)'           | (2) $2'$ $(0,0,1) 0,0,z$<br>( $2_z$  0,0,1)' | (3) $4^+$ $(0,0,1) 0,0,z$<br>( $4_z^+$  0,0,1)'     | (4) $4^-$ $(0,0,1) 0,0,z$<br>( $4_z^-$  0,0,1)'     |
| (5) $c$ $(0,0,1) x,0,z$<br>( $m_y$  0,0,1) | (6) $c$ $(0,0,1) 0,y,z$<br>( $m_x$  0,0,1)   | (7) $c$ $(0,0,1) x,\bar{x},z$<br>( $m_{xy}$  0,0,1) | (8) $c$ $(0,0,1) x,x,z$<br>( $m_{\bar{xy}}$  0,0,1) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

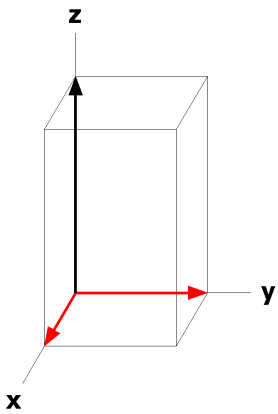
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(0,0,1)' +			
16	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},w$ ]		
			(5) x, $\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(6) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(7) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(8) y,x,z [v,u,w]		
8	f	.m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ]	1/2,x,z [0,u,w]	1/2, $\bar{x},z$ [0, $\bar{u},w$ ]		
8	e	.m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	0,x,z [0,u,w]	0, $\bar{x},z$ [0, $\bar{u},w$ ]		
8	d	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,z$ [ $\bar{u},u,w$ ]	x, $\bar{x},z$ [u, $\bar{u},w$ ]		
4	c	2m'm'	1/2,0,z [0,0,w]	0,1/2,z [0,0,w]				
2	b	4m'm'	1/2,1/2,z [0,0,w]					
2	a	4m'm'	0,0,z [0,0,w]					

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

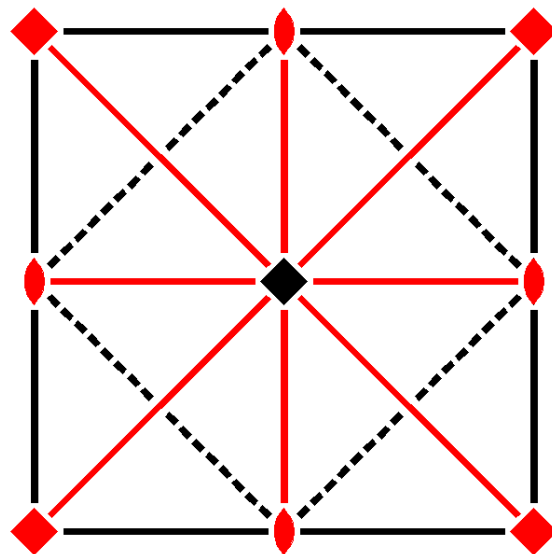
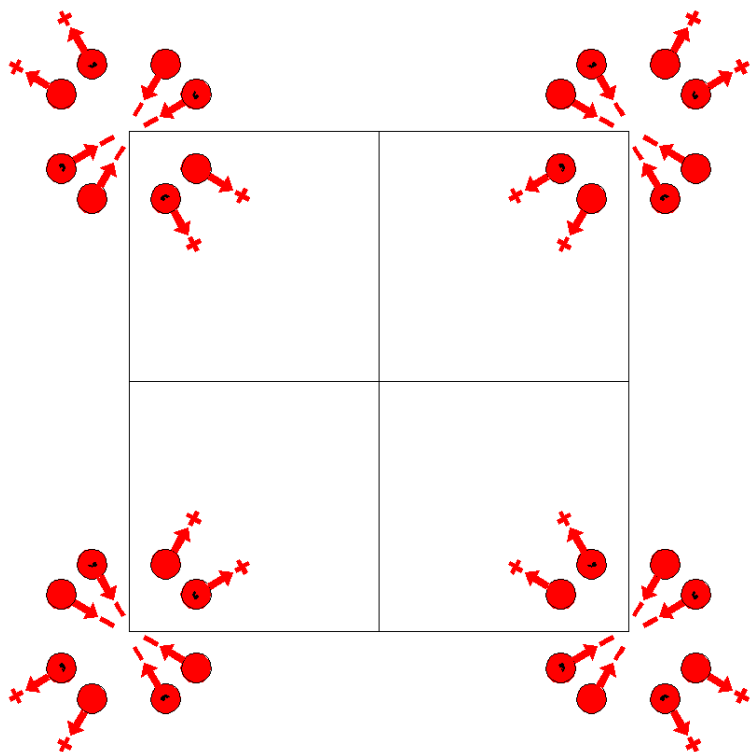
Along [1,1,0] p<sub>2b</sub>1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_4 4'mm'$   
99.12.834

$4mm1'$   
 $P_4 4'mm'$

Tetragonal



Origin on  $4'mm'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                                  |                                  |   |   |
|----------------------------------|----------------------------------|---|---|
| (1) 1<br>(1 0,0,0)               | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $4^+ 0,0,z$<br>( $4_z$  0,0,0)'         | (4) $4^- 0,0,z$<br>( $4_z^{-1}$  0,0,0)'    |
| (5) m $x,0,z$<br>( $m_y$  0,0,0) | (6) m $0,y,z$<br>( $m_x$  0,0,0) | (7) m' $x,\bar{x},z$<br>( $m_{xy}$  0,0,0)' | (8) m' $x,x,z$<br>( $m_{\bar{xy}}$  0,0,0)' |

For  $(1,0,0)$  + set

- |  |                                      |  |   |
|--|--------------------------------------|--|---|
| (1) t' $(1,0,0)$<br>(1 1,0,0)'             | (2) $2' 1/2,0,z$<br>( $2_x$  1,0,0)' | (3) $4^+ 1/2,1/2,z$<br>( $4_z$  1,0,0)                     | (4) $4^- 1/2,-1/2,z$<br>( $4_z^{-1}$  1,0,0)              |
| (5) a' $(1,0,0) x,0,z$<br>( $m_y$  1,0,0)' | (6) m' $1/2,y,z$<br>( $m_x$  1,0,0)' | (7) g $(1/2,-1/2,0) x+1/2,\bar{x},z$<br>( $m_{xy}$  1,0,0) | (8) g $(1/2,1/2,0) x+1/2,x,z$<br>( $m_{\bar{xy}}$  1,0,0) |

**Generators selected** (1);  $t'(1,0,0)$ ;  $t'(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3); (5).

**Positions**

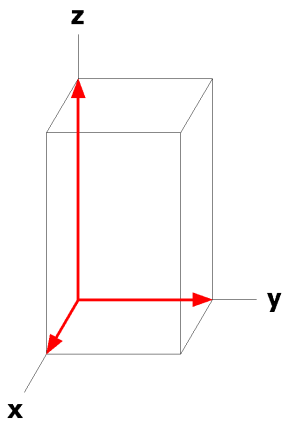
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(1,0,0)' +			
16	g	1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $\bar{y},x,z [v,\bar{u},\bar{w}]$	(4) $y,\bar{x},z [\bar{v},u,\bar{w}]$		
			(5) $x,\bar{y},z [\bar{u},v,\bar{w}]$	(6) $\bar{x},y,z [u,\bar{v},\bar{w}]$	(7) $\bar{y},\bar{x},z [\bar{v},\bar{u},w]$	(8) $y,x,z [v,u,w]$		
8	f	.m'	$x,1/2,z [u,0,w]$	$\bar{x},1/2,z [u,0,\bar{w}]$	$1/2,x,z [0,u,w]$	$1/2,\bar{x},z [0,u,\bar{w}]$		
8	e	.m.	$x,0,z [0,v,0]$	$\bar{x},0,z [0,\bar{v},0]$	$0,x,z [v,0,0]$	$0,\bar{x},z [\bar{v},0,0]$		
8	d	..m'	$x,x,z [u,u,w]$	$\bar{x},\bar{x},z [\bar{u},\bar{u},w]$	$\bar{x},x,z [u,\bar{u},\bar{w}]$	$x,\bar{x},z [\bar{u},u,\bar{w}]$		
4	c	2'm'm.	$1/2,0,z [0,v,0]$	$0,1/2,z [v,0,0]$				
2	b	4m'm'	$1/2,1/2,z [0,0,w]$					
2	a	4'mm'	$0,0,z [0,0,0]$					

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_4 4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $1/2,1/2,z$

Along  $[1,0,0]$   $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

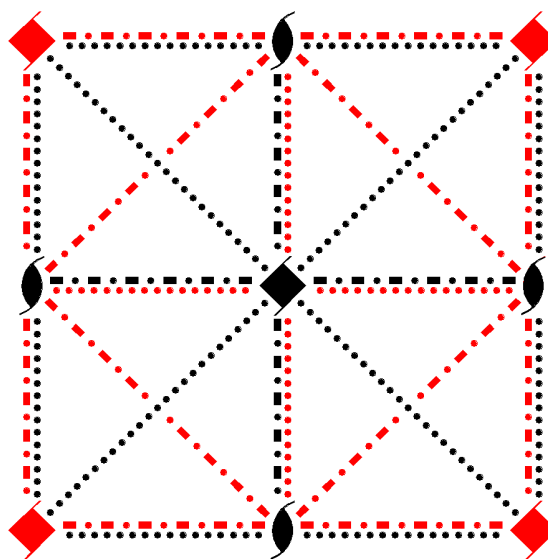
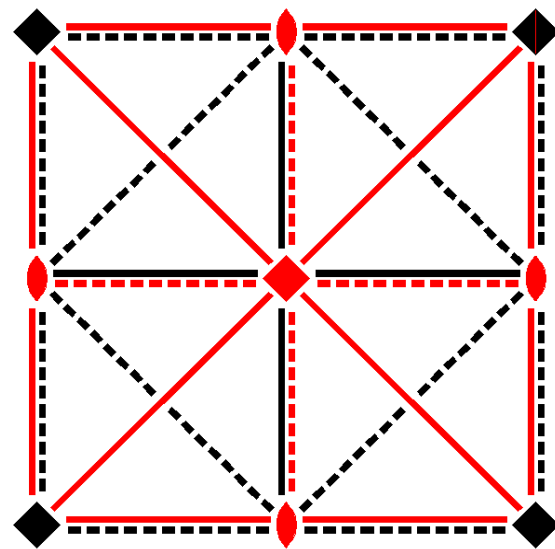
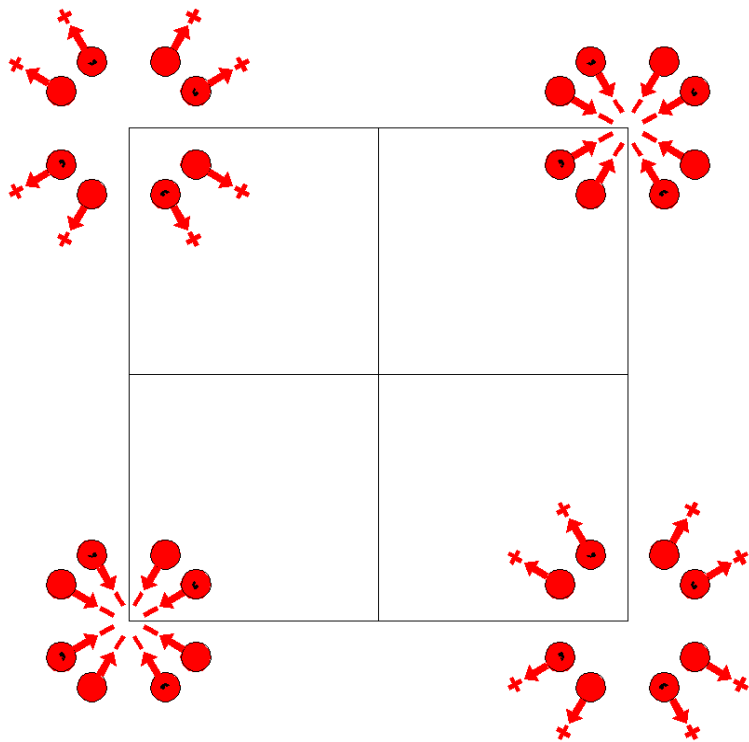
Along  $[1,1,0]$   $p_2 1m1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x-1/4,x+1/4,0$



$P_14m'm'$   
99.13.835

$4mm1'$   
 $P_14m'm'$

Tetragonal



Origin on 4mm

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y$ 

## Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)
(5) m' x,0,z (m <sub>y</sub>  0,0,0)'	(6) m' 0,y,z (m <sub>x</sub>  0,0,0)'	(7) m' x,x̄,z (m <sub>xy</sub>  0,0,0)'	(8) m' x,x,z (m <sub>xy</sub>  0,0,0)'

For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> ' 1/2,1/2,z (4 <sub>z</sub>  1,0,0)'	(4) 4 <sup>-</sup> ' 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,0)'
(5) a (1,0,0) x,0,z (m <sub>y</sub>  1,0,0)	(6) m 1/2,y,z (m <sub>x</sub>  1,0,0)	(7) g (1/2,-1/2,0) x+1/2,x̄,z (m <sub>xy</sub>  1,0,0)	(8) g (1/2,1/2,0) x+1/2,x,z (m <sub>xy</sub>  1,0,0)

Generators selected (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).

## Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
		(0,0,0) +	(1,0,0)' +					
16 g 1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w]	(3) ȳ,x,z [v̄,u,w]	(4) y,x̄,z [v,ū,w]	(5) x,ȳ,z [u,v̄,w]	(6) x̄,y,z [ū,v,w]	(7) ȳ,x̄,z [v̄,ū,w]	(8) y,x,z [v,u,w]
	8 f .m.	x,1/2,z [0,v,0]	x̄,1/2,z [0,v,0]	1/2,x,z [v,0,0]	1/2,x̄,z [v,0,0]			
8 e .m'	x,0,z [u,0,w]	x̄,0,z [ū,0,w]	0,x,z [0,u,w]	0,x̄,z [0,ū,w]				
8 d ..m'	x,x,z [u,u,w]	x̄,x̄,z [ū,ū,w]	x̄,x,z [ū,u,w]	x,x̄,z [u,ū,w]				
4 c 2'mm'	1/2,0,z [u,0,0]	0,1/2,z [0,u,0]						
2 b 4'm'm	1/2,1/2,z [0,0,0]							
2 a 4m'm'	0,0,z [0,0,w]							

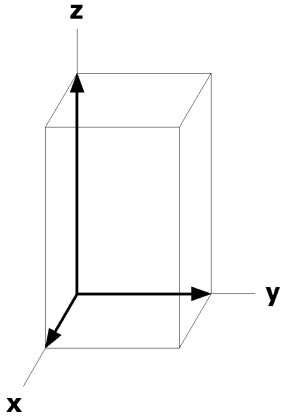
## Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p<sub>c</sub>1m1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}$   
 Origin at x-1/4,x+1/4,0

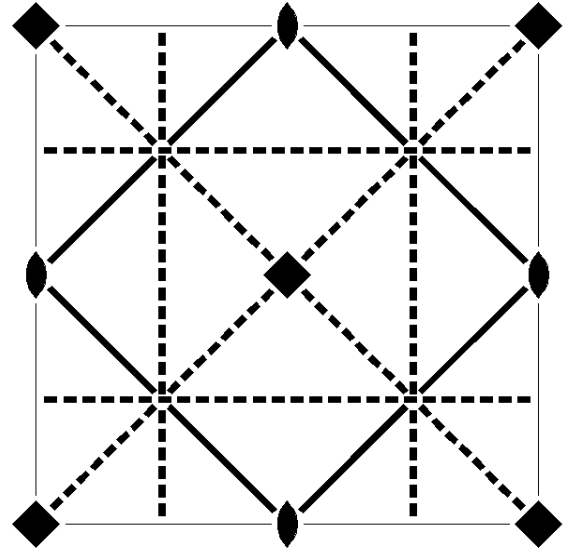
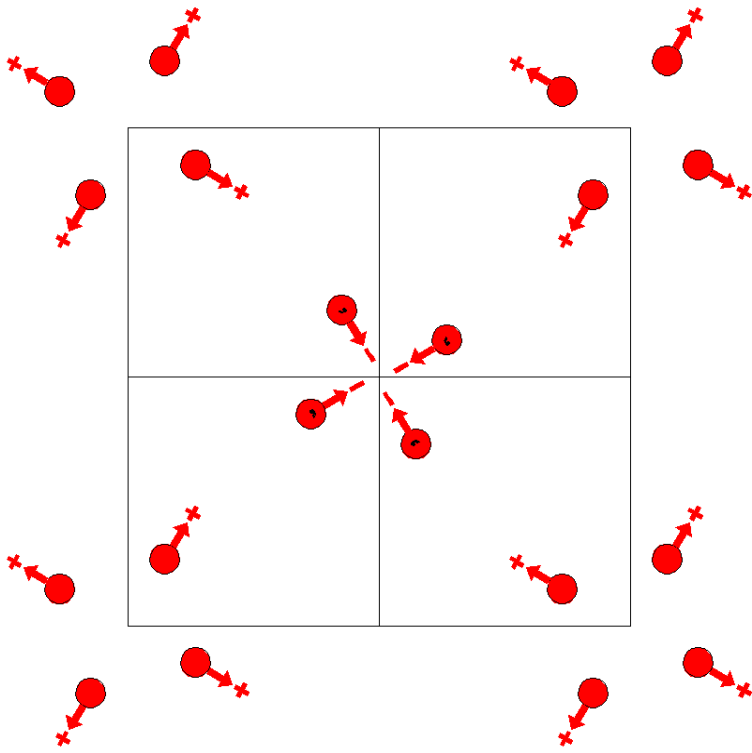




P4bm  
100.1.836

4mm  
P4bm

Tetragonal



Origin on 41g

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$ ;  $y \leq 1/2 - x$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (6) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (7) m x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)    | (8) g (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)           |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

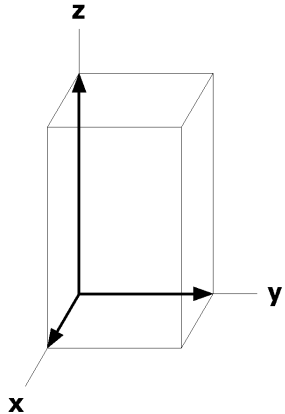
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
8	d	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$		
			(3) $\bar{y}, x, z [\bar{v}, u, w]$	(4) $y, \bar{x}, z [v, \bar{u}, w]$		
			(5) $x+1/2, \bar{y}+1/2, z [\bar{u}, v, \bar{w}]$	(6) $\bar{x}+1/2, y+1/2, z [u, \bar{v}, \bar{w}]$		
			(7) $\bar{y}+1/2, \bar{x}+1/2, z [v, u, \bar{w}]$	(8) $y+1/2, x+1/2, z [\bar{v}, \bar{u}, \bar{w}]$		
4	c	..m	$x, x+1/2, z [\bar{u}, u, 0]$	$\bar{x}, \bar{x}+1/2, z [u, \bar{u}, 0]$	$\bar{x}+1/2, x, z [\bar{u}, \bar{u}, 0]$	$x+1/2, \bar{x}, z [u, u, 0]$
2	b	2.mm	$1/2, 0, z [0, 0, 0]$	$0, 1/2, z [0, 0, 0]$		
2	a	4..	$0, 0, z [0, 0, w]$	$1/2, 1/2, z [0, 0, \bar{w}]$		

**Symmetry of Special Projections**

Along  $[0, 0, 1]$  p4gm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$   $p_{2a}1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 1/4, 0$

Along  $[1, 1, 0]$  p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 0$



P4bm1'

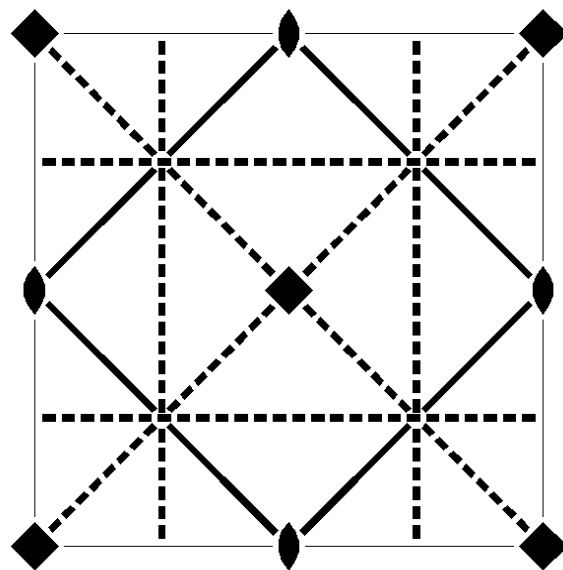
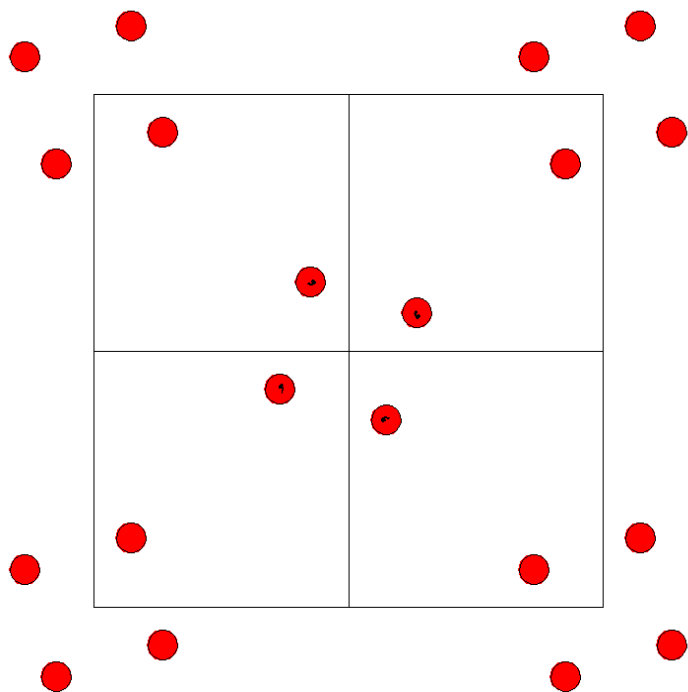
4mm1'

Tetragonal

100.2.837

P4bm1'

1'



Origin on 41g1'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2 - x$

Symmetry Operations

For 1 + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (6) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (7) m x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)    | (8) g (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)           |

For 1' + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1'<br>(1 0,0,0)'                                     | (2) 2' <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)'    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (5) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (6) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' | (7) m' x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)'   | (8) g' (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)'          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

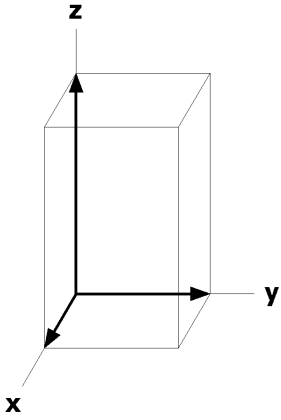
			1 +	1' +		
8	d	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]		
			(3) $\bar{y},x,z$ [0,0,0]	(4) y, $\bar{x},z$ [0,0,0]		
			(5) x+1/2, $\bar{y}$ +1/2,z [0,0,0]	(6) $\bar{x}$ +1/2,y+1/2,z [0,0,0]		
			(7) $\bar{y}$ +1/2, $\bar{x}$ +1/2,z [0,0,0]	(8) y+1/2,x+1/2,z [0,0,0]		
4	c	..m1'	x,x+1/2,z [0,0,0]	$\bar{x},\bar{x}$ +1/2,z [0,0,0]	$\bar{x}$ +1/2,x,z [0,0,0]	x+1/2, $\bar{x},z$ [0,0,0]
2	b	2.mm1'	1/2,0,z [0,0,0]	0,1/2,z [0,0,0]		
2	a	4..1'	0,0,z [0,0,0]	1/2,1/2,z [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

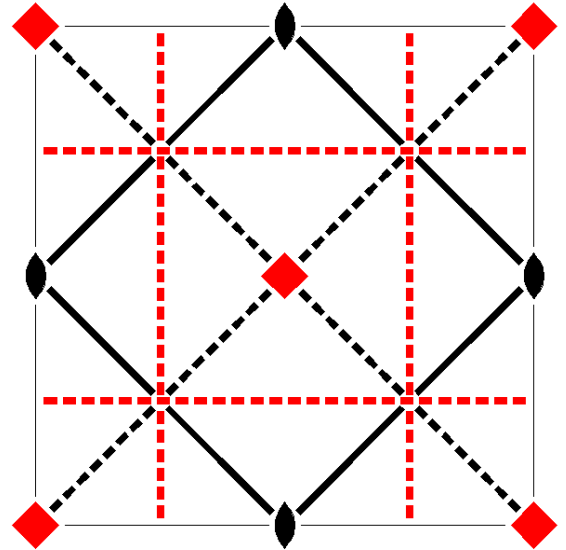
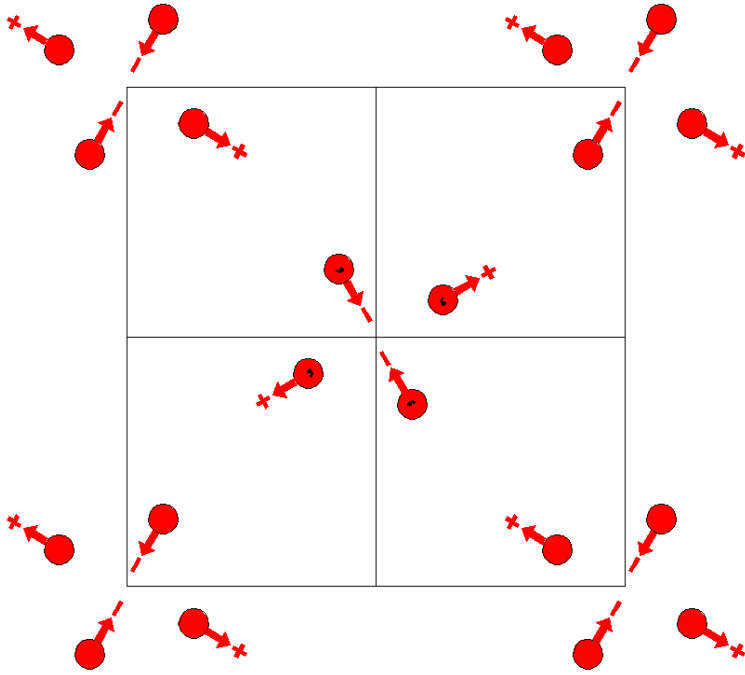
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4'b'm  
100.3.838

4'm'm  
P4'b'm

Tetragonal



Origin on 4'1g

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2 - x$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 4<sup>+</sup> 0,0,z  
(4<sub>z</sub><sup>+</sup>|0,0,0)'

(4) 4<sup>-</sup> 0,0,z  
(4<sub>z</sub><sup>-</sup>|0,0,0)'

(5) a' (1/2,0,0) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,0)'

(6) b' (0,1/2,0) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,0)'

(7) m x+1/2,x̄,z  
(m<sub>xy</sub>|1/2,1/2,0)

(8) g (1/2,1/2,0) x,x,z  
(m<sub>xy</sub>|1/2,1/2,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

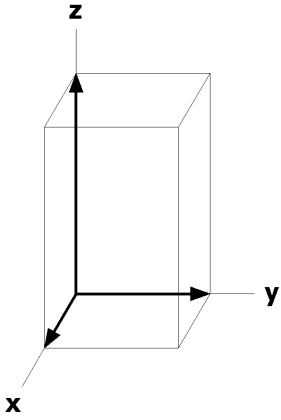
8	d	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$		
			(3) $\bar{y}, x, z [v, \bar{u}, \bar{w}]$	(4) $y, \bar{x}, z [\bar{v}, u, \bar{w}]$		
			(5) $x+1/2, \bar{y}+1/2, z [u, \bar{v}, w]$	(6) $\bar{x}+1/2, y+1/2, z [\bar{u}, v, w]$		
			(7) $\bar{y}+1/2, \bar{x}+1/2, z [v, u, \bar{w}]$	(8) $y+1/2, x+1/2, z [\bar{v}, \bar{u}, \bar{w}]$		
4	c	..m	$x, x+1/2, z [\bar{u}, u, 0]$	$\bar{x}, \bar{x}+1/2, z [u, \bar{u}, 0]$	$\bar{x}+1/2, x, z [u, u, 0]$	$x+1/2, \bar{x}, z [\bar{u}, \bar{u}, 0]$
2	b	2.mm	$1/2, 0, z [0, 0, 0]$	$0, 1/2, z [0, 0, 0]$		
2	a	4'..	$0, 0, z [0, 0, 0]$	$1/2, 1/2, z [0, 0, 0]$		

**Symmetry of Special Projections**

Along  $[0, 0, 1]$   $p4'g'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$   $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 0, 0$

Along  $[1, 1, 0]$   $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 0$



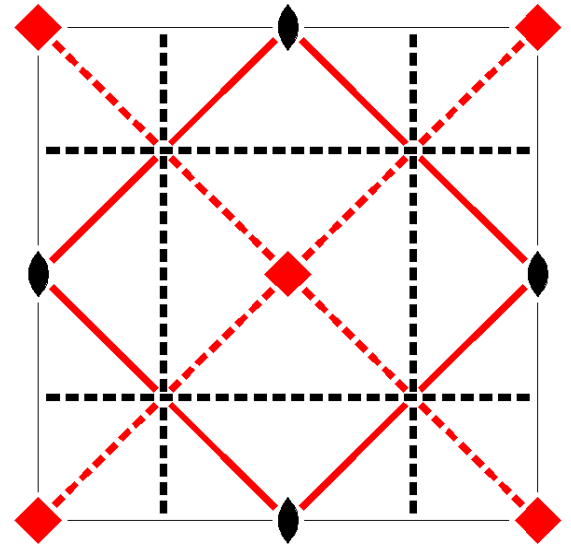
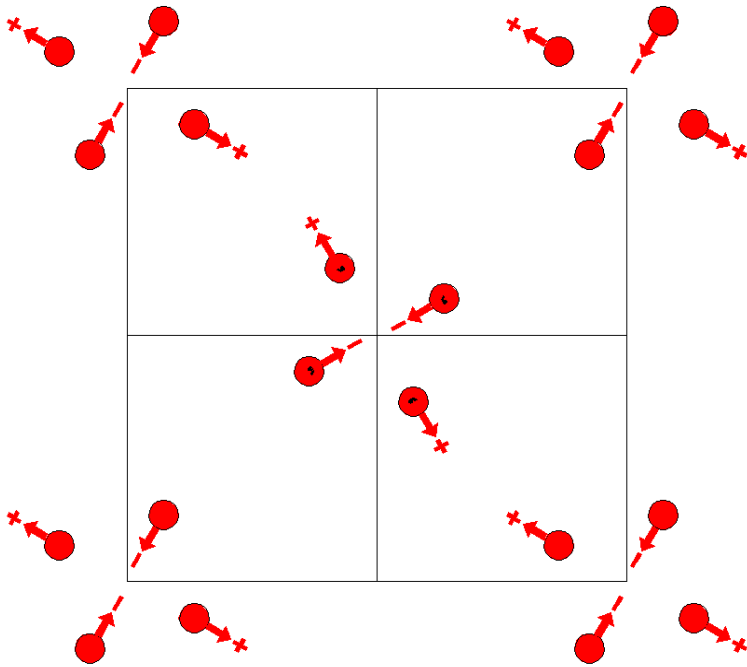
P4'bm'

100.4.839

4'mm'

P4'bm'

Tetragonal



Origin on 4'1g'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$ ;  $y \leq 1/2 - x$

Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (5) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (6) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (7) m' x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)'   | (8) g' (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)'          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

8	d	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$		
			(3) $\bar{y}, x, z [v, \bar{u}, \bar{w}]$	(4) $y, \bar{x}, z [\bar{v}, u, \bar{w}]$		
			(5) $x+1/2, \bar{y}+1/2, z [\bar{u}, v, \bar{w}]$	(6) $\bar{x}+1/2, y+1/2, z [u, \bar{v}, \bar{w}]$		
			(7) $\bar{y}+1/2, \bar{x}+1/2, z [v, \bar{u}, w]$	(8) $y+1/2, x+1/2, z [v, u, w]$		
4	c	..m'	$x, x+1/2, z [u, u, w]$	$\bar{x}, \bar{x}+1/2, z [\bar{u}, \bar{u}, w]$	$\bar{x}+1/2, x, z [u, \bar{u}, \bar{w}]$	$x+1/2, \bar{x}, z [\bar{u}, u, \bar{w}]$
2	b	2.m'm'	$1/2, 0, z [0, 0, w]$	$0, 1/2, z [0, 0, \bar{w}]$		
2	a	4'..	$0, 0, z [0, 0, 0]$	$1/2, 1/2, z [0, 0, 0]$		

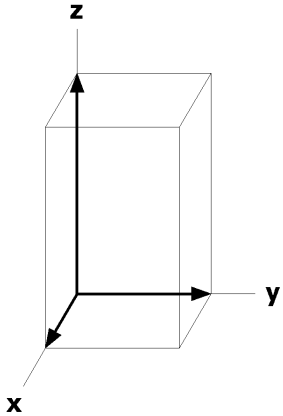
**Symmetry of Special Projections**

Along [0,0,1]  $p4'gm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 1/4, 0$

Along [1,1,0]  $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 0$

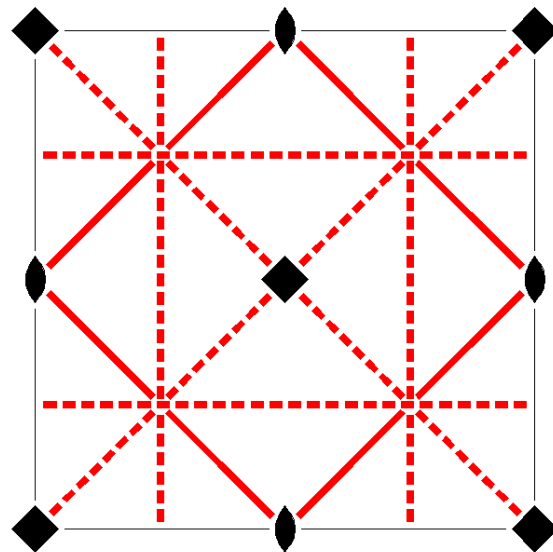
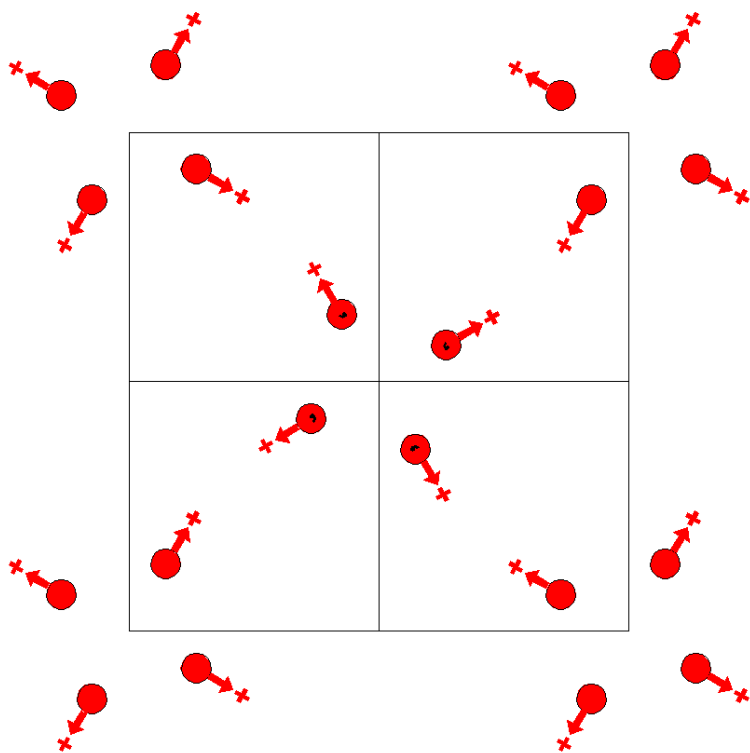




P4b'm'  
100.5.840

4m'm'  
P4b'm'

Tetragonal



Origin on 41g'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$ ;  $y \leq 1/2 - x$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)      | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (6) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' | (7) m' x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)'  | (8) g' (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)'         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

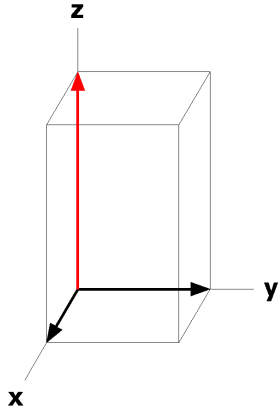
8	d	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$		
			(3) $\bar{y}, x, z [\bar{v}, u, w]$	(4) $y, \bar{x}, z [v, \bar{u}, w]$		
			(5) $x+1/2, \bar{y}+1/2, z [u, \bar{v}, w]$	(6) $\bar{x}+1/2, y+1/2, z [\bar{u}, v, w]$		
			(7) $\bar{y}+1/2, \bar{x}+1/2, z [\bar{v}, \bar{u}, w]$	(8) $y+1/2, x+1/2, z [v, u, w]$		
4	c	..m'	$x, x+1/2, z [u, u, w]$	$\bar{x}, \bar{x}+1/2, z [\bar{u}, \bar{u}, w]$	$\bar{x}+1/2, x, z [\bar{u}, u, w]$	$x+1/2, \bar{x}, z [u, \bar{u}, w]$
2	b	2.m'm'	$1/2, 0, z [0, 0, w]$	$0, 1/2, z [0, 0, w]$		
2	a	4..	$0, 0, z [0, 0, w]$	$1/2, 1/2, z [0, 0, w]$		

**Symmetry of Special Projections**

Along [0,0,1] p4g'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



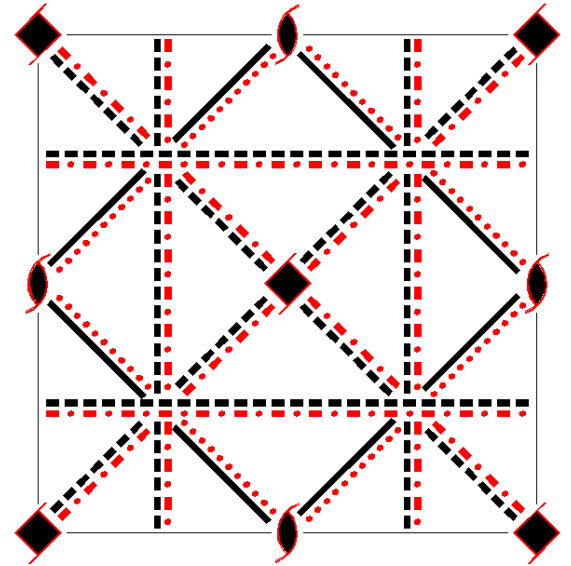
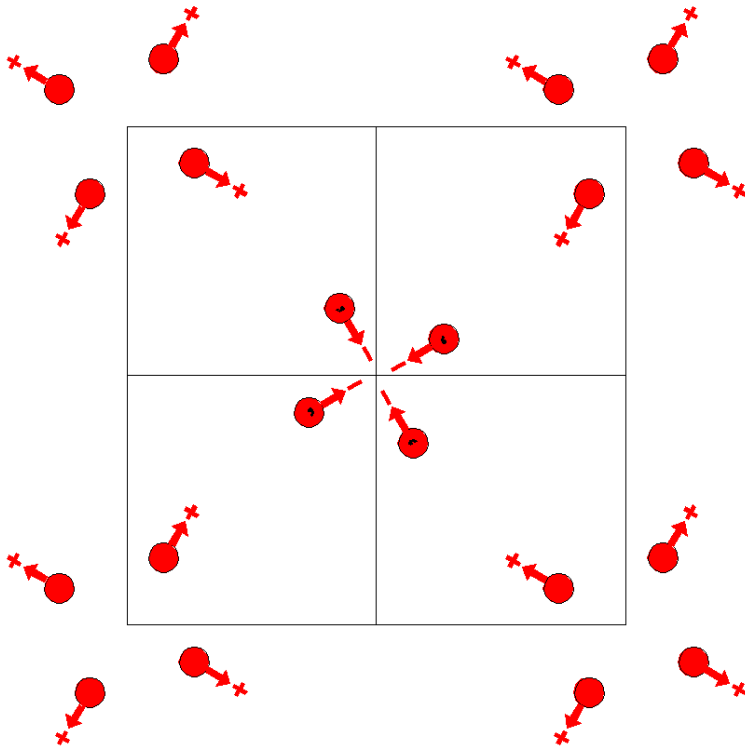
$P_{2c} 4bm$

$4mm1'$

Tetragonal

100.6.841

$P_{2c} 4bm$



Origin on  $41g$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2 - x$

Symmetry Operations

For  $(0,0,0) +$  set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                       | (3) $4^+$ $0,0,z$<br>( $4_z$  0,0,0)                  | (4) $4^-$ $0,0,z$<br>( $4_z^{-1}$  0,0,0)                       |
| (5) a $(1/2,0,0)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,0$ ) | (6) b $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ ) | (7) m $x+1/2,\bar{x},z$<br>( $m_{xy}$   $1/2,1/2,0$ ) | (8) g $(1/2,1/2,0)$ $x,x,z$<br>( $m_{\bar{xy}}$   $1/2,1/2,0$ ) |

For  $(0,0,1) +$  set

- |  |  |   |   |
|--|--|---|---|
| (1) $t'$ $(0,0,1)$<br>(1 0,0,1)'                           | (2) $2'$ $(0,0,1)$ $0,0,z$<br>( $2_z$  0,0,1)'             | (3) $4^{+'}$ $(0,0,1)$ $0,0,z$<br>( $4_z$  0,0,1)'                  | (4) $4^{-'}$ $(0,0,1)$ $0,0,z$<br>( $4_z^{-1}$  0,0,1)'             |
| (5) $n'$ $(1/2,0,1)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,1$ )' | (6) $n'$ $(0,1/2,1)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,1$ )' | (7) $c'$ $(0,0,1)$ $x+1/2,\bar{x},z$<br>( $m_{xy}$   $1/2,1/2,1$ )' | (8) $n'$ $(1/2,1/2,1)$ $x,x,z$<br>( $m_{\bar{xy}}$   $1/2,1/2,1$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

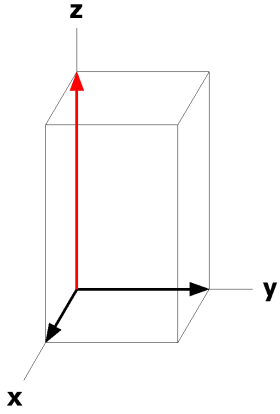
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
				(0,0,0) +	(0,0,1)' +	
16	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}, x, z$ [ $\bar{v}, u, w$ ]	(4) y, $\bar{x}, z$ [v, $\bar{u}, w$ ]		
			(5) x+1/2, $\bar{y}+1/2, z$ [ $\bar{u}, v, \bar{w}$ ]	(6) $\bar{x}+1/2, y+1/2, z$ [u, $\bar{v}, \bar{w}$ ]		
			(7) $\bar{y}+1/2, \bar{x}+1/2, z$ [v, u, $\bar{w}$ ]	(8) y+1/2, x+1/2, z [ $\bar{v}, \bar{u}, \bar{w}$ ]		
8	c	..m	x, x+1/2, z [ $\bar{u}, u, 0$ ]	$\bar{x}, \bar{x}+1/2, z$ [u, $\bar{u}, 0$ ]	$\bar{x}+1/2, x, z$ [ $\bar{u}, \bar{u}, 0$ ]	x+1/2, $\bar{x}, z$ [u, u, 0]
4	b	2.mm	1/2, 0, z [0, 0, 0]	0, 1/2, z [0, 0, 0]		
4	a	4..	0, 0, z [0, 0, w]	1/2, 1/2, z [0, 0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>c</sub>1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x, 1/4, 0

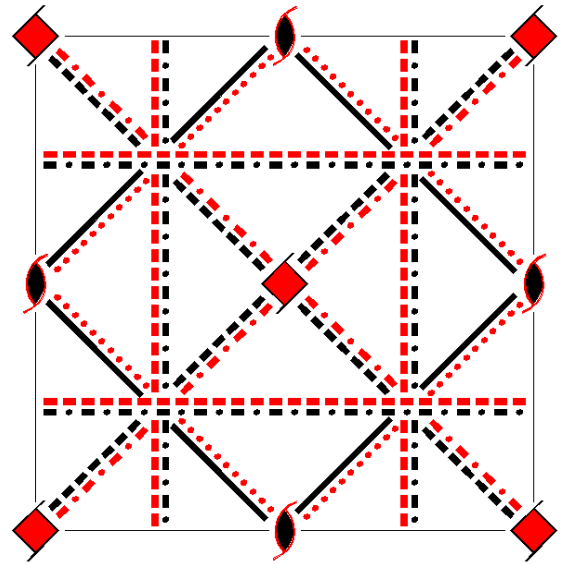
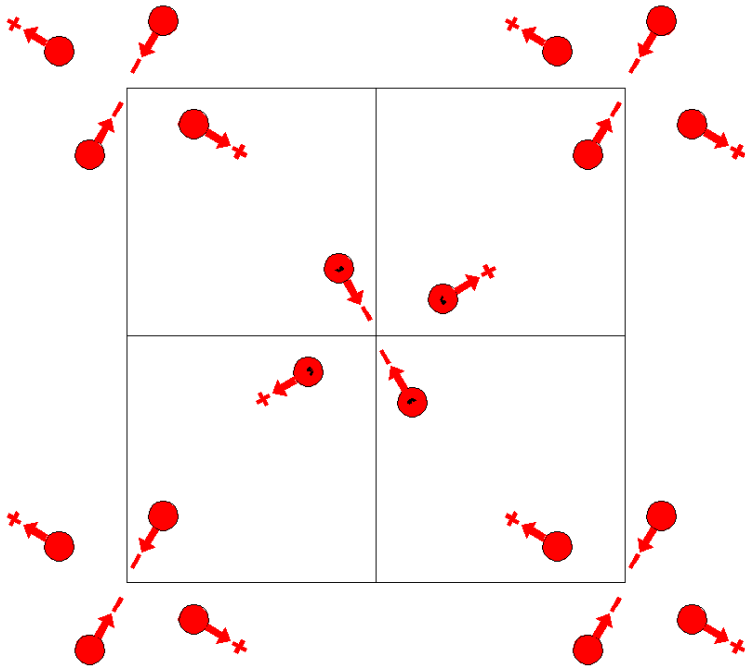
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x, x, 0



$P_{2c} 4'b'm$   
100.7.842

$4mm1'$   
 $P_{2c} 4'b'm$

Tetragonal



Origin on  $4'1g$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2 - x$

Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                   | (3) $4^+ 0,0,z$<br>( $4_z$  0,0,0)'               | (4) $4^- 0,0,z$<br>( $4_z^{-1}$  0,0,0)'                  |
| (5) $a' (1/2,0,0) x,1/4,z$<br>( $m_y$  1/2,1/2,0)' | (6) $b' (0,1/2,0) 1/4,y,z$<br>( $m_x$  1/2,1/2,0)' | (7) $m x+1/2,\bar{x},z$<br>( $m_{xy}$  1/2,1/2,0) | (8) $g (1/2,1/2,0) x,x,z$<br>( $m_{\bar{xy}}$  1/2,1/2,0) |

For  $(0,0,1)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t' (0,0,1)$<br>(1 0,0,1)'                   | (2) $2' (0,0,1) 0,0,z$<br>( $2_z$  0,0,1)'       | (3) $4^+ (0,0,1) 0,0,z$<br>( $4_z$  0,0,1)                  | (4) $4^- (0,0,1) 0,0,z$<br>( $4_z^{-1}$  0,0,1)             |
| (5) $n (1/2,0,1) x,1/4,z$<br>( $m_y$  1/2,1/2,1) | (6) $n (0,1/2,1) 1/4,y,z$<br>( $m_x$  1/2,1/2,1) | (7) $c' (0,0,1) x+1/2,\bar{x},z$<br>( $m_{xy}$  1/2,1/2,1)' | (8) $n' (1/2,1/2,1) x,x,z$<br>( $m_{\bar{xy}}$  1/2,1/2,1)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (0,0,1)' +

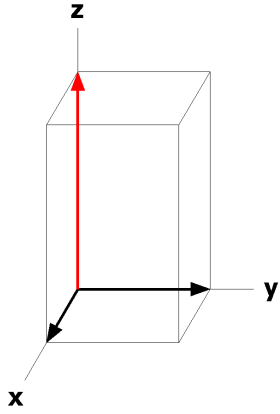
16	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}, x, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(4) y, $\bar{x}$ ,z [ $\bar{v}, u, \bar{w}$ ]		
			(5) x+1/2, $\bar{y}$ +1/2,z [u, $\bar{v}$ ,w]	(6) $\bar{x}$ +1/2,y+1/2,z [ $\bar{u}, v, w$ ]		
			(7) $\bar{y}$ +1/2, $\bar{x}$ +1/2,z [v,u, $\bar{w}$ ]	(8) y+1/2,x+1/2,z [ $\bar{v}, \bar{u}, \bar{w}$ ]		
8	c	..m	x,x+1/2,z [ $\bar{u}, u, 0$ ]	$\bar{x}, \bar{x}$ +1/2,z [u, $\bar{u}, 0$ ]	$\bar{x}$ +1/2,x,z [u,u,0]	x+1/2, $\bar{x}$ ,z [ $\bar{u}, \bar{u}, 0$ ]
4	b	2.mm	1/2,0,z [0,0,0]	0,1/2,z [0,0,0]		
4	a	4'..	0,0,z [0,0,0]	1/2,1/2,z [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
a\* = a b\* = b  
Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>1m1'  
a\* = b/2 b\* = c  
Origin at x,0,0

Along [1,1,0] p1m11'  
a\* = (-a + b)/2 b\* = c  
Origin at x,x,0



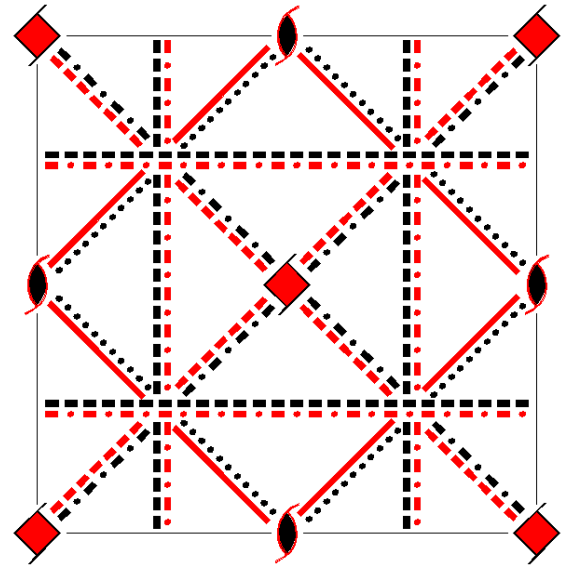
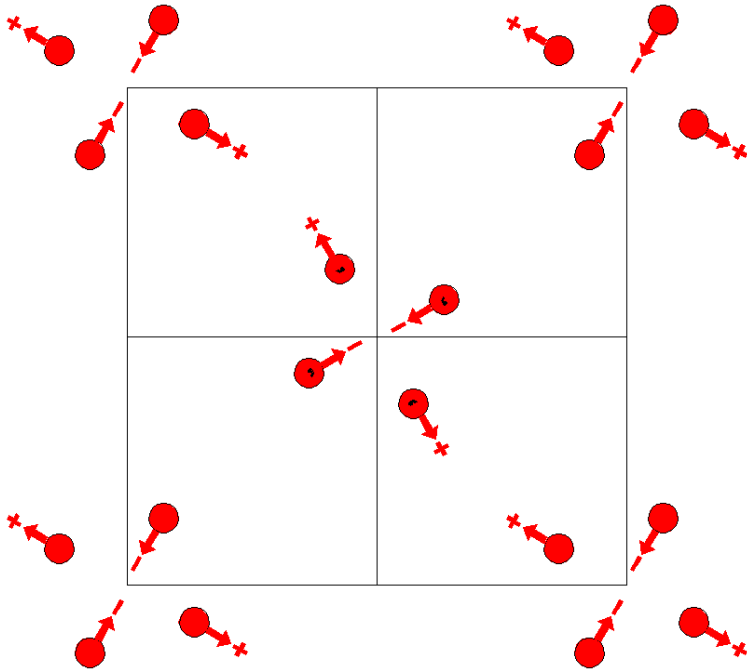
$P_{2c} 4'bm'$

100.8.843

$4mm1'$

$P_{2c} 4'bm'$

Tetragonal



Origin on  $4'1g'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2-x$

Symmetry Operations

For  $(0,0,0) +$  set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                     | (3) $4^+ 0,0,z$<br>( $4_z$  0,0,0)'                     | (4) $4^- 0,0,z$<br>( $4_z^{-1}$  0,0,0)'                        |
| (5) a $(1/2,0,0) x,1/4,z$<br>( $m_y$   $1/2,1/2,0$ ) | (6) b $(0,1/2,0) 1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ ) | (7) $m' x+1/2,\bar{x},z$<br>( $m_{xy}$   $1/2,1/2,0$ )' | (8) $g' (1/2,1/2,0) x,x,z$<br>( $m_{\bar{xy}}$   $1/2,1/2,0$ )' |

For  $(0,0,1) +$  set

- |  |  |   |   |
|--|--|---|---|
| (1) $t' (0,0,1)$<br>(1 0,0,1)'                         | (2) $2' (0,0,1) 0,0,z$<br>( $2_z$  0,0,1)'             | (3) $4^+ (0,0,1) 0,0,z$<br>( $4_z$  0,0,1)                    | (4) $4^- (0,0,1) 0,0,z$<br>( $4_z^{-1}$  0,0,1)               |
| (5) $n' (1/2,0,1) x,1/4,z$<br>( $m_y$   $1/2,1/2,1$ )' | (6) $n' (0,1/2,1) 1/4,y,z$<br>( $m_x$   $1/2,1/2,1$ )' | (7) c $(0,0,1) x+1/2,\bar{x},z$<br>( $m_{xy}$   $1/2,1/2,1$ ) | (8) n $(1/2,1/2,1) x,x,z$<br>( $m_{\bar{xy}}$   $1/2,1/2,1$ ) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
				(0,0,0) +	(0,0,1)' +	
16	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}, x, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(4) y, $\bar{x}, z$ [ $\bar{v}, u, \bar{w}$ ]		
			(5) x+1/2, $\bar{y}+1/2, z$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(6) $\bar{x}+1/2, y+1/2, z$ [ $u, \bar{v}, \bar{w}$ ]		
			(7) $\bar{y}+1/2, \bar{x}+1/2, z$ [ $\bar{v}, \bar{u}, w$ ]	(8) y+1/2, x+1/2, z [v, u, w]		
8	c	..m'	x, x+1/2, z [u, u, w]	$\bar{x}, \bar{x}+1/2, z$ [ $\bar{u}, \bar{u}, w$ ]	$\bar{x}+1/2, x, z$ [ $u, \bar{u}, \bar{w}$ ]	x+1/2, $\bar{x}, z$ [ $\bar{u}, u, \bar{w}$ ]
4	b	2.m'm'	1/2, 0, z [0, 0, w]	0, 1/2, z [0, 0, $\bar{w}$ ]		
4	a	4'..	0, 0, z [0, 0, 0]	1/2, 1/2, z [0, 0, 0]		

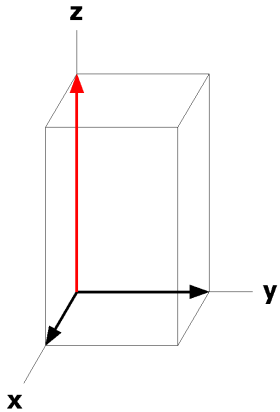
**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>c</sub>·1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x, 1/4, 0

Along [1,1,0] p<sub>2b</sub>·1m1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x, x, 0





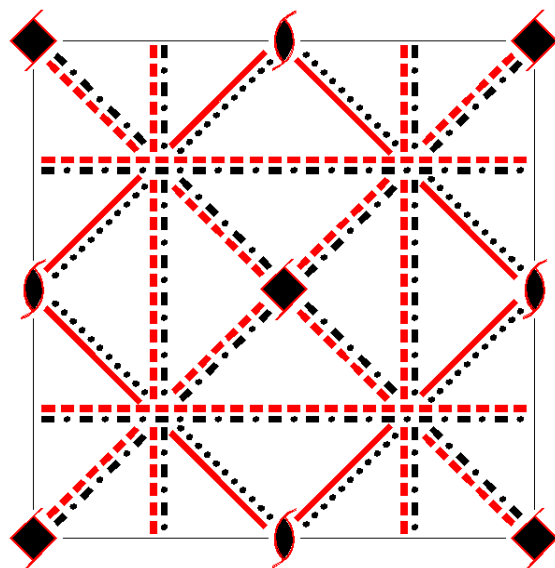
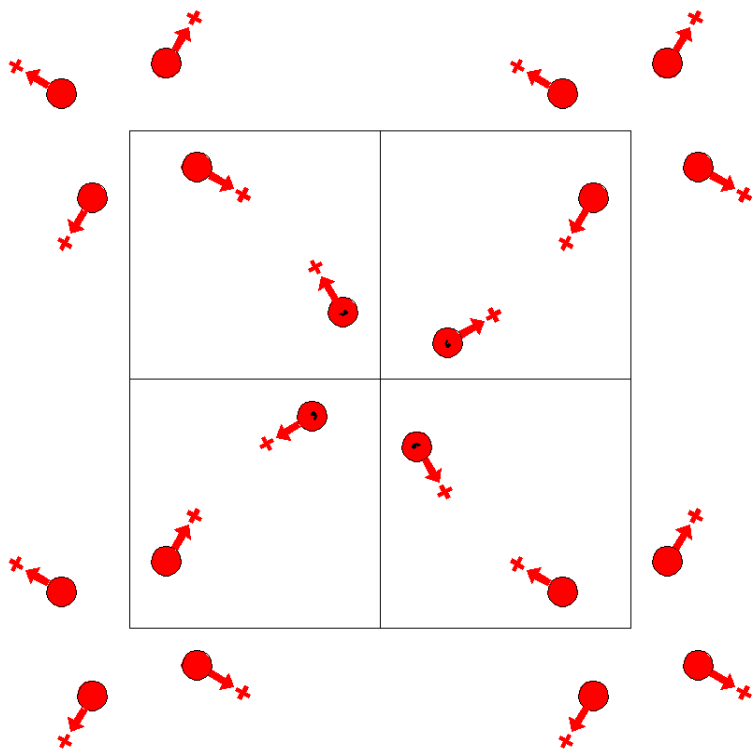
$P_{2c} 4b'm'$

100.9.844

$4mm1'$

$P_{2c} 4b'm'$

Tetragonal



Origin on  $41g'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2-x$

**Symmetry Operations**

For  $(0,0,0) +$  set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                           | (3) $4^+$ $0,0,z$<br>( $4_z$  0,0,0)                      | (4) $4^-$ $0,0,z$<br>( $4_z^{-1}$  0,0,0)                           |
| (5) $a'$ $(1/2,0,0) \ x,1/4,z$<br>( $m_y$   $1/2,1/2,0$ )' | (6) $b'$ $(0,1/2,0) \ 1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' | (7) $m'$ $x+1/2,\bar{x},z$<br>( $m_{xy}$   $1/2,1/2,0$ )' | (8) $g'$ $(1/2,1/2,0) \ x,x,z$<br>( $m_{\bar{xy}}$   $1/2,1/2,0$ )' |

For  $(0,0,1) +$  set

- |   |   |  |  |
|---|---|--|--|
| (1) $t'$ $(0,0,1)$<br>(1 0,0,1)'                          | (2) $2'$ $(0,0,1) \ 0,0,z$<br>( $2_z$  0,0,1)'            | (3) $4^{+ '}$ $(0,0,1) \ 0,0,z$<br>( $4_z$  0,0,1)'                | (4) $4^{- '}$ $(0,0,1) \ 0,0,z$<br>( $4_z^{-1}$  0,0,1)'           |
| (5) $n$ $(1/2,0,1) \ x,1/4,z$<br>( $m_y$   $1/2,1/2,1$ )' | (6) $n$ $(0,1/2,1) \ 1/4,y,z$<br>( $m_x$   $1/2,1/2,1$ )' | (7) $c$ $(0,0,1) \ x+1/2,\bar{x},z$<br>( $m_{xy}$   $1/2,1/2,1$ )' | (8) $n$ $(1/2,1/2,1) \ x,x,z$<br>( $m_{\bar{xy}}$   $1/2,1/2,1$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

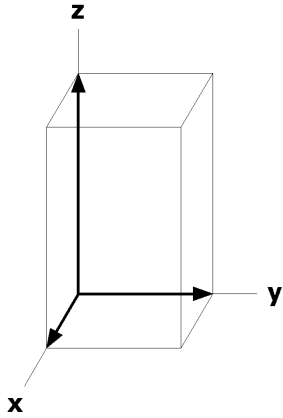
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
				(0,0,0) +	(0,0,1)' +	
16	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}, x, z$ [ $\bar{v}, u, w$ ]	(4) y, $\bar{x}, z$ [v, $\bar{u}, w$ ]		
			(5) x+1/2, $\bar{y}+1/2, z$ [u, $\bar{v}, w$ ]	(6) $\bar{x}+1/2, y+1/2, z$ [ $\bar{u}, v, w$ ]		
			(7) $\bar{y}+1/2, \bar{x}+1/2, z$ [ $\bar{v}, \bar{u}, w$ ]	(8) y+1/2, x+1/2, z [v, u, w]		
8	c	..m'	x, x+1/2, z [u, u, w]	$\bar{x}, \bar{x}+1/2, z$ [ $\bar{u}, \bar{u}, w$ ]	$\bar{x}+1/2, x, z$ [ $\bar{u}, u, w$ ]	x+1/2, $\bar{x}, z$ [u, $\bar{u}, w$ ]
4	b	2.m'm'	1/2, 0, z [0, 0, w]	0, 1/2, z [0, 0, w]		
4	a	4..	0, 0, z [0, 0, w]	1/2, 1/2, z [0, 0, w]		

**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>.1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

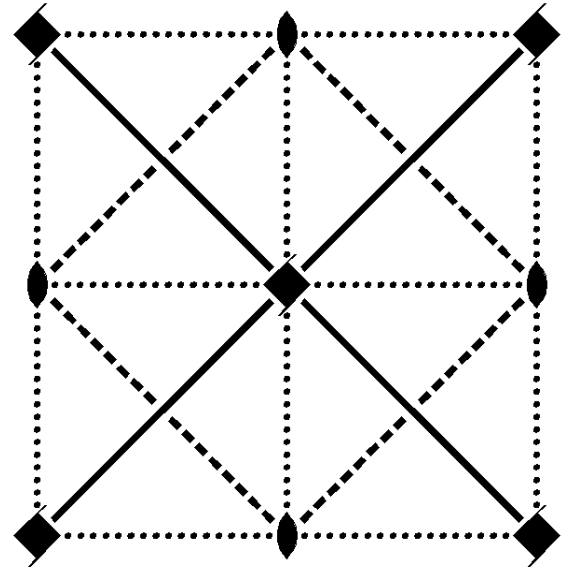
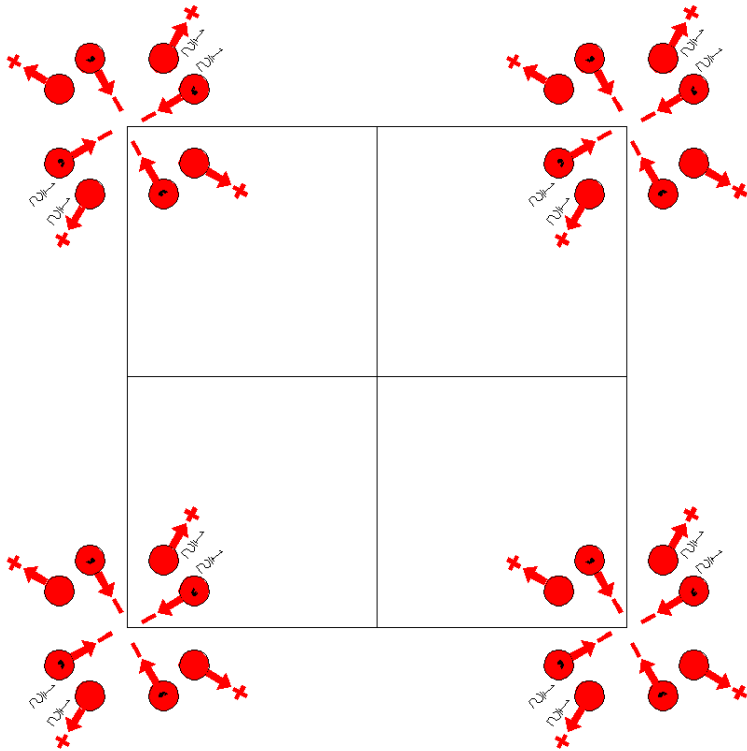
Along [1,1,0] p<sub>2b</sub>.1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P4_2 cm$   
101.1.845

4mm  
 $P4_2 cm$

Tetragonal



Origin on  $2mm$  on  $4_2 cm$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                         | (2) $2_{0,0,z}$<br>( $2_z$  0,0,0)         | (3) $4^+_{(0,0,1/2)}$ 0,0,z<br>( $4_z$  0,0,1/2) | (4) $4^-_{(0,0,1/2)}$ 0,0,z<br>( $4_z^{-1}$  0,0,1/2) |
| (5) c (0,0,1/2) x,0,z<br>( $m_y$  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>( $m_x$  0,0,1/2) | (7) m $x,\bar{x},z$<br>( $m_{xy}$  0,0,0)        | (8) m x,x,z<br>( $m_{\bar{xy}}$  0,0,0)               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

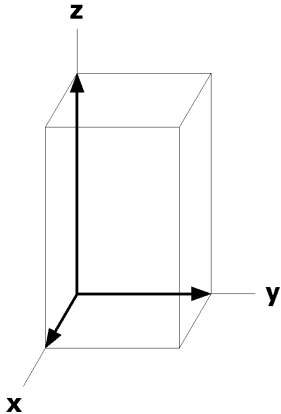
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	e	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{y}, x, z+1/2 [\bar{v}, u, w]$	(4) $y, \bar{x}, z+1/2 [v, \bar{u}, w]$
			(5) $x, \bar{y}, z+1/2 [\bar{u}, v, \bar{w}]$	(6) $\bar{x}, y, z+1/2 [u, \bar{v}, \bar{w}]$	(7) $\bar{y}, \bar{x}, z [v, u, \bar{w}]$	(8) $y, x, z [\bar{v}, \bar{u}, \bar{w}]$
4	d	..m	$x, x, z [\bar{u}, u, 0]$	$\bar{x}, \bar{x}, z [u, \bar{u}, 0]$	$\bar{x}, x, z+1/2 [\bar{u}, \bar{u}, 0]$	$x, \bar{x}, z+1/2 [u, u, 0]$
4	c	2..	$0, 1/2, z [0, 0, w]$	$1/2, 0, z+1/2 [0, 0, w]$	$0, 1/2, z+1/2 [0, 0, \bar{w}]$	$1/2, 0, z [0, 0, \bar{w}]$
2	b	2.mm	$1/2, 1/2, z [0, 0, 0]$	$1/2, 1/2, z+1/2 [0, 0, 0]$		
2	a	2.mm	$0, 0, z [0, 0, 0]$	$0, 0, z+1/2 [0, 0, 0]$		

**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P4_2cm1'$

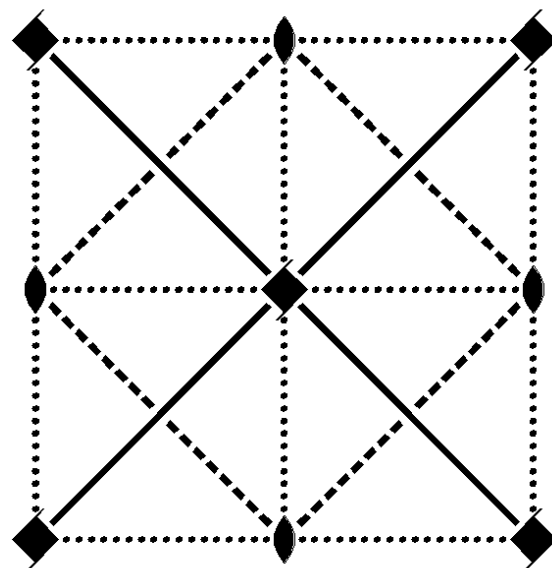
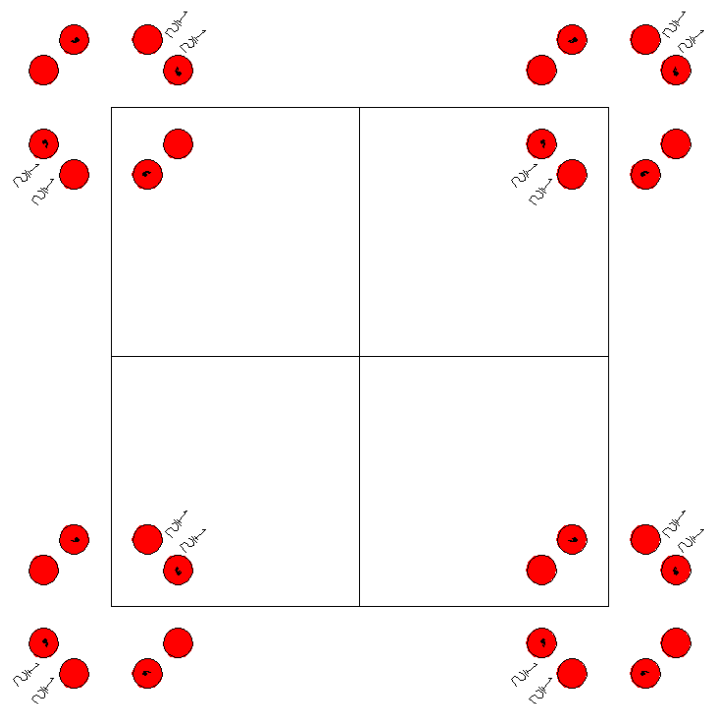
101.2.846

$4mm1'$

$P4_2cm1'$

Tetragonal

1'



Origin on  $2mm1'$  on  $4_2cm1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

Symmetry Operations

For 1 + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)  | (7) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                        | (8) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                                       |

For 1' + set

- |  |   |  |  |
|--|---|--|--|
| (1) 1'<br>(1 0,0,0)'                                 | (2) 2' <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (3) 4 <sup>+</sup> ' (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)' | (4) 4 <sup>-</sup> ' (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)'  | (7) m' <sub>x</sub> x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'            | (8) m' <sub>x</sub> x,x,z<br>(m <sub>xy</sub>  0,0,0)'                           |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

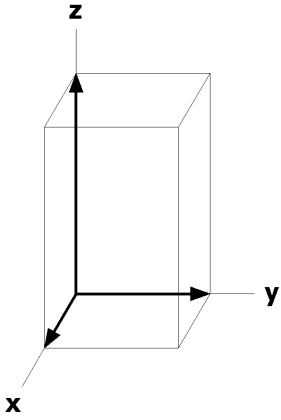
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
	1 +				1' +			
8 e 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z+1/2$ [0,0,0]	(4) $y,\bar{x},z+1/2$ [0,0,0]	(5) x, $\bar{y},z+1/2$ [0,0,0]	(6) $\bar{x},y,z+1/2$ [0,0,0]	(7) $\bar{y},\bar{x},z$ [0,0,0]	(8) y,x,z [0,0,0]
4 d ..m1'	x,x,z [0,0,0]	$\bar{x},\bar{x},z$ [0,0,0]	$\bar{x},x,z+1/2$ [0,0,0]	x, $\bar{x},z+1/2$ [0,0,0]				
4 c 2..1'	0,1/2,z [0,0,0]	1/2,0,z+1/2 [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0,z [0,0,0]				
2 b 2.mm1'	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]						
2 a 2.mm1'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]						

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



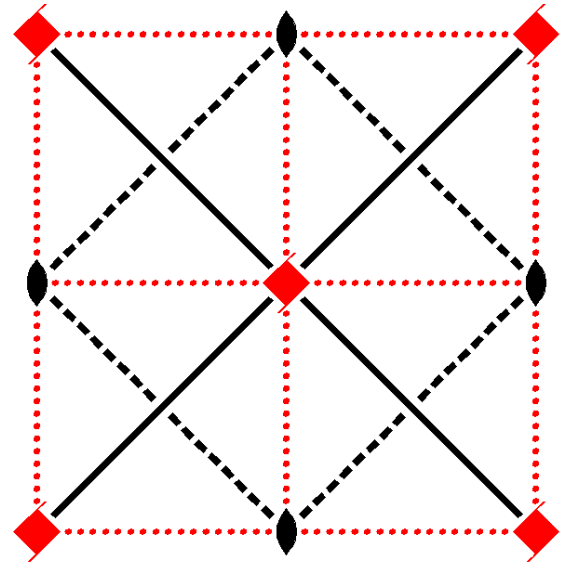
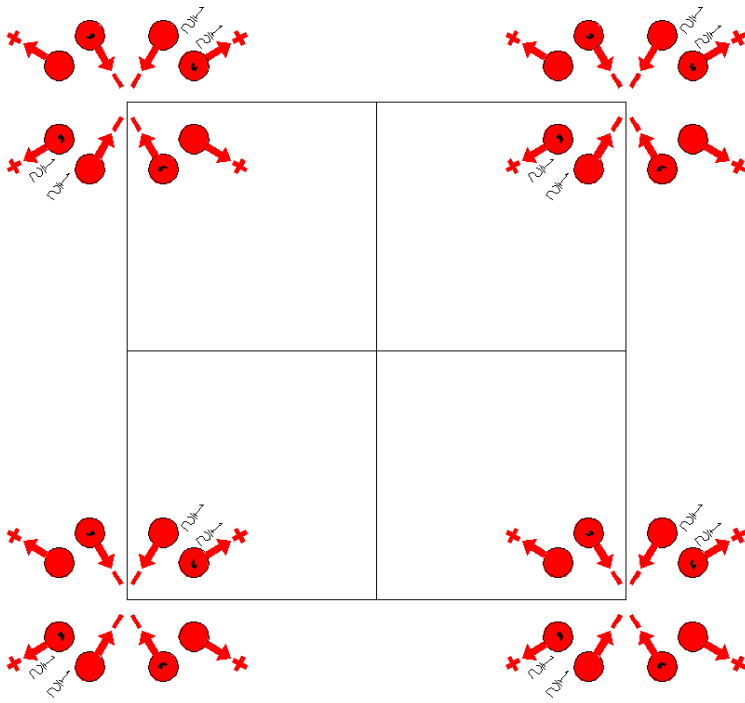
$P4_2'c'm$

101.3.847

$4'm'm$

$P4_2'c'm$

Tetragonal



Origin on  $2mm$  on  $4_2'c'm$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

### Symmetry Operations

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                             | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)               | (3) $4^+ ' (0,0,1/2) 0,0,z$<br>( $4_z$  0,0,1/2)' | (4) $4^- ' (0,0,1/2) 0,0,z$<br>( $4_z^{-1}$  0,0,1/2)' |
| (5) $c' (0,0,1/2) x,0,z$<br>( $m_y$  0,0,1/2)' | (6) $c' (0,0,1/2) 0,y,z$<br>( $m_x$  0,0,1/2)' | (7) $m x,\bar{x},z$<br>( $m_{xy}$  0,0,0)         | (8) $m x,x,z$<br>( $m_{\bar{xy}}$  0,0,0)              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	e	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $v,\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ]
			(5) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(6) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]	(7) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(8) $y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]
4	d	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]	$\bar{x},x,z+1/2$ [ $u,u,0$ ]	$x,\bar{x},z+1/2$ [ $\bar{u},\bar{u},0$ ]
4	c	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]
2	b	2.mm	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]		
2	a	2.mm	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]		

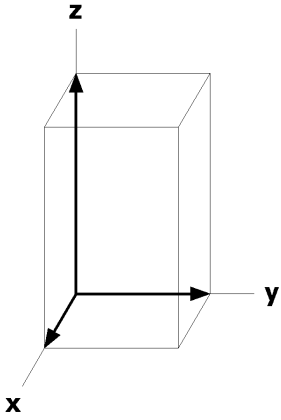
**Symmetry of Special Projections**

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0





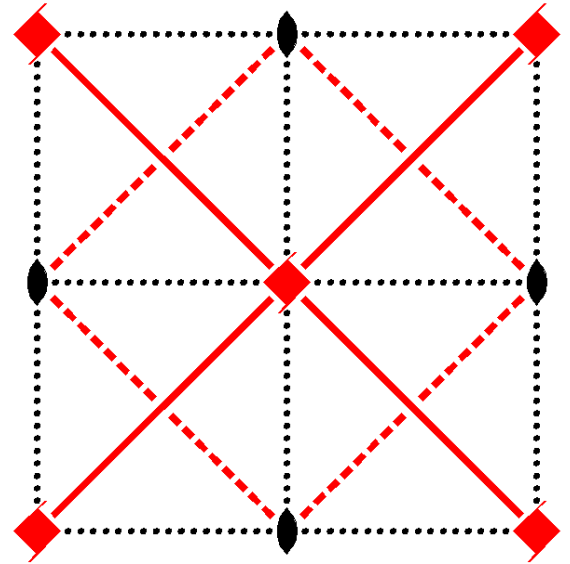
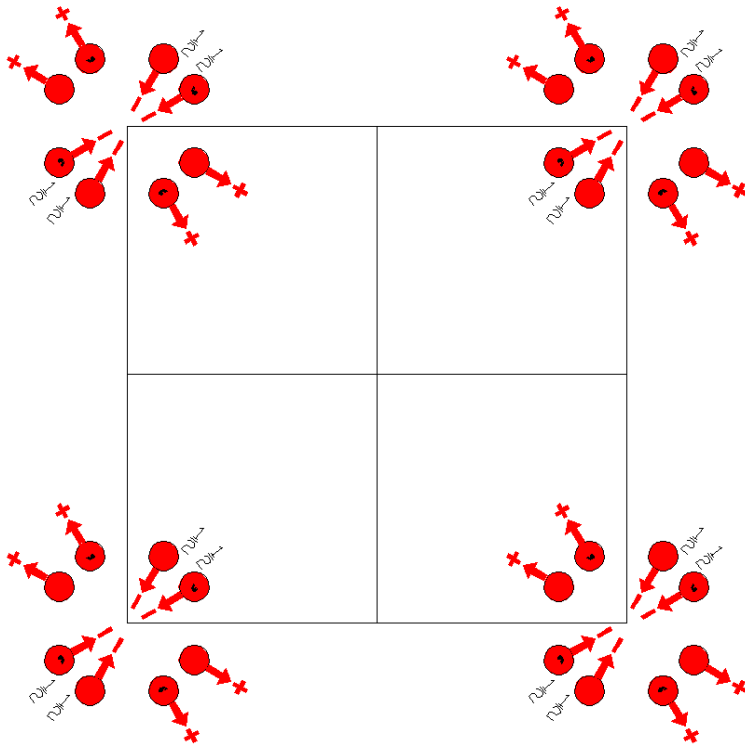
$P4_2'cm'$

101.4.848

$4'mm'$

$P4_2'cm'$

Tetragonal



Origin on  $2m'm'$  on  $4_2'cm'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)             | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (7) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                        | (8) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                                      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

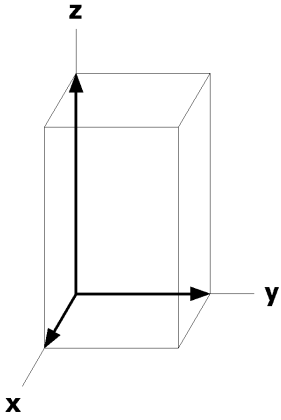
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	e	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ]
			(5) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(8) y,x,z [v,u,w]
4	d	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,z+1/2$ [ $u,\bar{u},\bar{w}$ ]	$x,\bar{x},z+1/2$ [ $\bar{u},u,\bar{w}$ ]
4	c	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0,z [0,0,w]
2	b	2.m'm'	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]		
2	a	2.m'm'	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>'1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



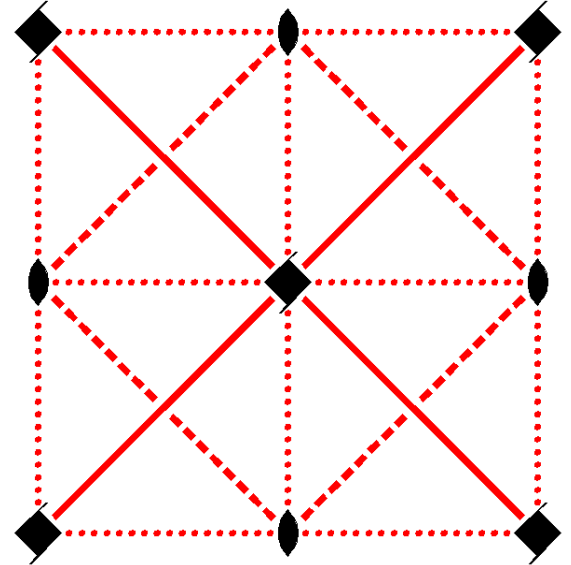
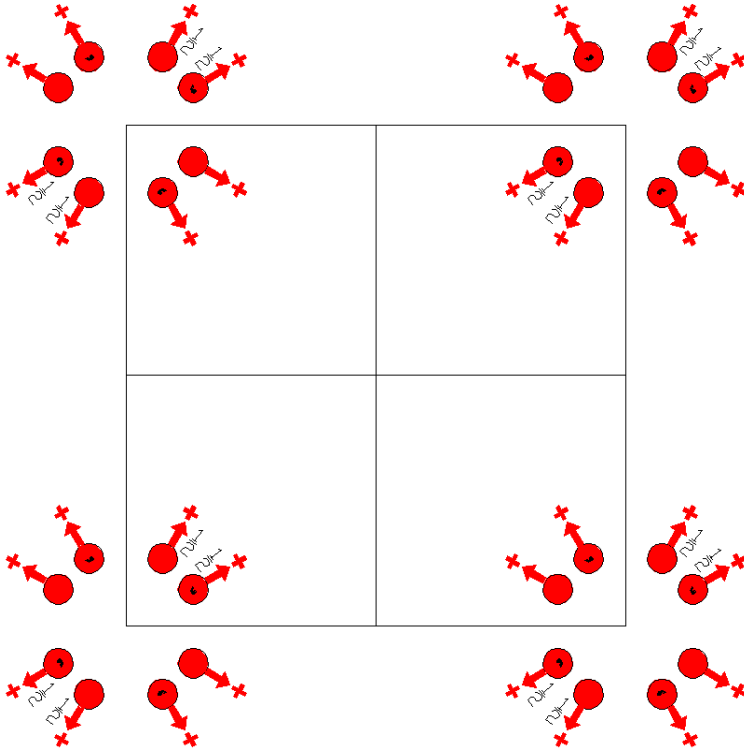
$P4_2 c'm'$

101.5.849

$4m'm'$

$P4_2 c'm'$

Tetragonal



Origin on  $2m'm'$  on  $4_2 c'm'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

### Symmetry Operations

(1) 1  
(1|0,0,0)

(2)  $2_{0,0,z}$   
( $2_z$ |0,0,0)

(3)  $4^+_{(0,0,1/2)}$  0,0,z  
( $4_z$ |0,0,1/2)

(4)  $4^-_{(0,0,1/2)}$  0,0,z  
( $4_z^{-1}$ |0,0,1/2)

(5)  $c'_{(0,0,1/2)}$  x,0,z  
( $m_y$ |0,0,1/2)'

(6)  $c'_{(0,0,1/2)}$  0,y,z  
( $m_x$ |0,0,1/2)'

(7)  $m'_{x,\bar{x},z}$   
( $m_{xy}$ |0,0,0)'

(8)  $m'_{x,x,z}$   
( $m_{\bar{xy}}$ |0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

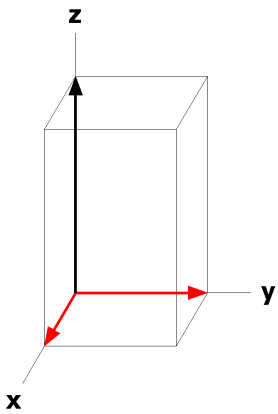
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	e	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]
			(5) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(6) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]	(7) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(8) y,x,z [v,u,w]
4	d	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,z+1/2$ [ $\bar{u},u,w$ ]	x, $\bar{x},z+1/2$ [u, $\bar{u},w$ ]
4	c	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0,z [0,0,w]
2	b	2.m'm'	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]		
2	a	2.m'm'	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



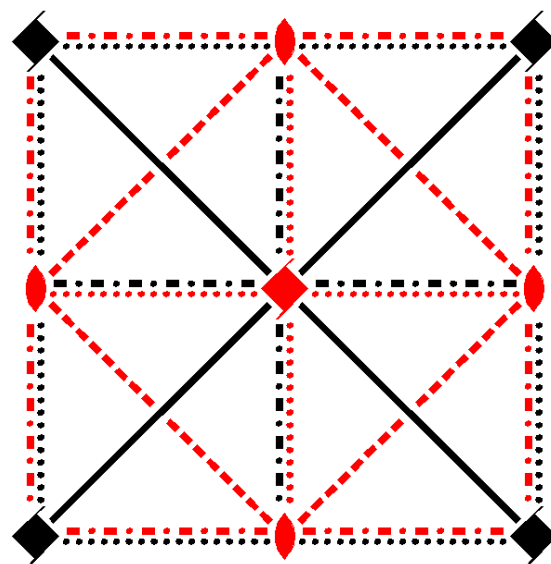
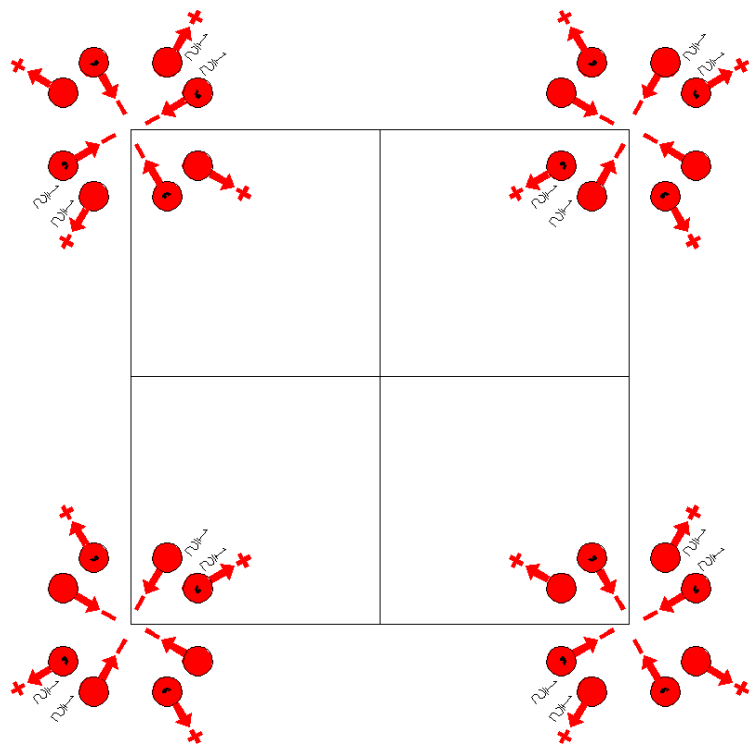
$P_P 4_2 cm$

$4mm1'$

Tetragonal

101.6.850

$P_P 4_2 cm$



Origin on  $2mm$  on  $4_2 cm$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)             | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (7) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                        | (8) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                                       |

For (1,0,0)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) t' (1,0,0)<br>(1 1,0,0)'                         | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'             | (3) 4 <sup>+</sup> (0,0,1/2) 1/2,1/2,z<br>(4 <sub>z</sub>  1,0,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,-1/2,z<br>(4 <sub>z</sub> <sup>-1</sup>  1,0,1/2)' |
| (5) n' (1,0,1/2) x,0,z<br>(m <sub>y</sub>  1,0,1/2)' | (6) c' (0,0,1/2) 1/2,y,z<br>(m <sub>x</sub>  1,0,1/2)' | (7) g' (1/2,-1/2,0) x+1/2,x̄,z<br>(m <sub>xy</sub>  1,0,0)'          | (8) g' (1/2,1/2,0) x+1/2,x,z<br>(m <sub>xy</sub>  1,0,0)'                           |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

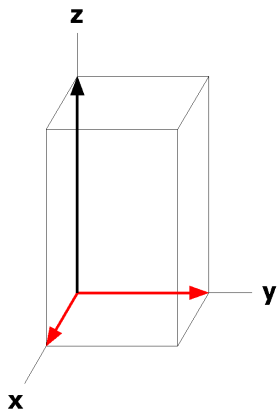
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(1,0,0)' +			
16 e 1	(1)	$x, y, z [u, v, w]$	(2)	$\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3)	$\bar{y}, x, z+1/2 [\bar{v}, u, w]$	(4)	$y, \bar{x}, z+1/2 [v, \bar{u}, w]$
	(5)	$x, \bar{y}, z+1/2 [\bar{u}, v, \bar{w}]$	(6)	$\bar{x}, y, z+1/2 [u, \bar{v}, \bar{w}]$	(7)	$\bar{y}, \bar{x}, z [v, u, \bar{w}]$	(8)	$y, x, z [\bar{v}, \bar{u}, \bar{w}]$
8 d ..m		$x, x, z [\bar{u}, u, 0]$		$\bar{x}, \bar{x}, z [u, \bar{u}, 0]$		$\bar{x}, x, z+1/2 [\bar{u}, \bar{u}, 0]$		$x, \bar{x}, z+1/2 [u, u, 0]$
8 c 2'..		$0, 1/2, z [u, v, 0]$		$1/2, 0, z+1/2 [v, \bar{u}, 0]$		$0, 1/2, z+1/2 [u, \bar{v}, 0]$		$1/2, 0, z [\bar{v}, \bar{u}, 0]$
4 b 2.mm		$1/2, 1/2, z [0, 0, 0]$		$1/2, 1/2, z+1/2 [0, 0, 0]$				
4 a 2.mm		$0, 0, z [0, 0, 0]$		$0, 0, z+1/2 [0, 0, 0]$				

**Symmetry of Special Projections**

Along [0,0,1]  $p_4, 4mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

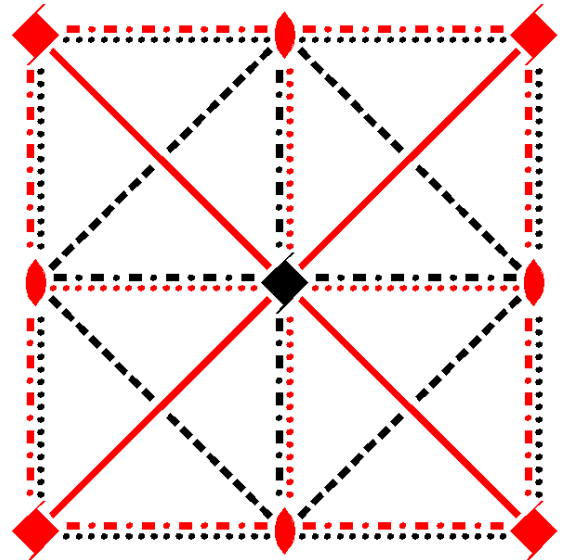
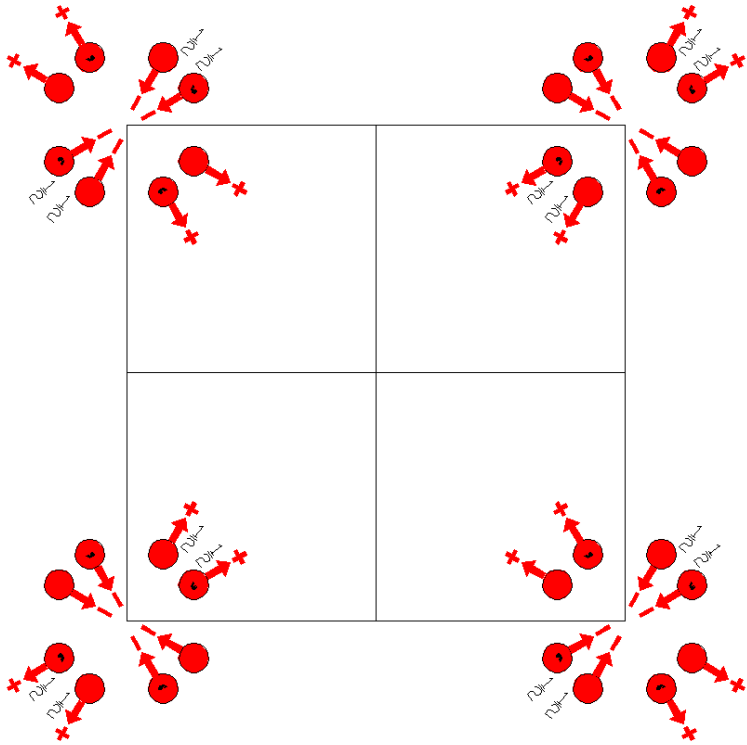
Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_P 4_2' cm'$   
101.7.851

$4mm1'$   
 $P_P 4_2' cm'$

Tetragonal



Origin on  $2m'm'$  on  $4_2' cm'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)             | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (7) m' x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'                       | (8) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                                      |

For (1,0,0)' + set

- |  |  |   |  |
|--|--|---|--|
| (1) t' (1,0,0)<br>(1 1,0,0)'                         | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'             | (3) 4 <sup>+</sup> (0,0,1/2) 1/2,1/2,z<br>(4 <sub>z</sub>  1,0,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,-1/2,z<br>(4 <sub>z</sub> <sup>-1</sup>  1,0,1/2) |
| (5) n' (1,0,1/2) x,0,z<br>(m <sub>y</sub>  1,0,1/2)' | (6) c' (0,0,1/2) 1/2,y,z<br>(m <sub>x</sub>  1,0,1/2)' | (7) g (1/2,-1/2,0) x+1/2,x̄,z<br>(m <sub>xy</sub>  1,0,0)           | (8) g (1/2,1/2,0) x+1/2,x,z<br>(m <sub>xy</sub>  1,0,0)                            |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(1,0,0)' +			
16 e 1	(1)	$x, y, z [u, v, w]$	(2)	$\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3)	$\bar{y}, x, z+1/2 [v, \bar{u}, \bar{w}]$	(4)	$y, \bar{x}, z+1/2 [\bar{v}, u, \bar{w}]$
	(5)	$x, \bar{y}, z+1/2 [\bar{u}, v, \bar{w}]$	(6)	$\bar{x}, y, z+1/2 [u, \bar{v}, \bar{w}]$	(7)	$\bar{y}, \bar{x}, z [v, \bar{u}, w]$	(8)	$y, x, z [v, u, w]$
8 d ..m'		$x, x, z [u, u, w]$		$\bar{x}, \bar{x}, z [\bar{u}, \bar{u}, w]$		$\bar{x}, x, z+1/2 [u, \bar{u}, \bar{w}]$		$x, \bar{x}, z+1/2 [\bar{u}, u, \bar{w}]$
8 c 2'..		$0, 1/2, z [u, v, 0]$		$1/2, 0, z+1/2 [\bar{v}, u, 0]$		$0, 1/2, z+1/2 [u, \bar{v}, 0]$		$1/2, 0, z [v, u, 0]$
4 b 2.m'm'		$1/2, 1/2, z [0, 0, w]$		$1/2, 1/2, z+1/2 [0, 0, \bar{w}]$				
4 a 2.m'm'		$0, 0, z [0, 0, w]$		$0, 0, z+1/2 [0, 0, \bar{w}]$				

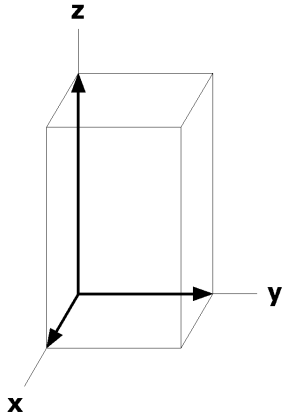
**Symmetry of Special Projections**

Along [0,0,1]  $p_4, 4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0]  $p_{2a} 1m1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x-1/4, x+1/4, 0$

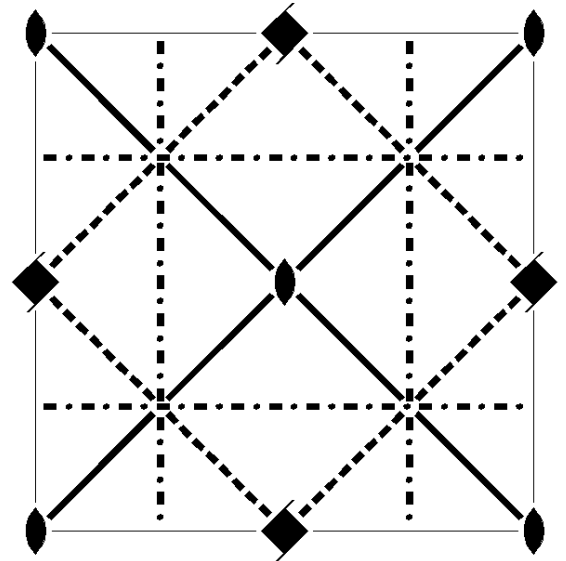
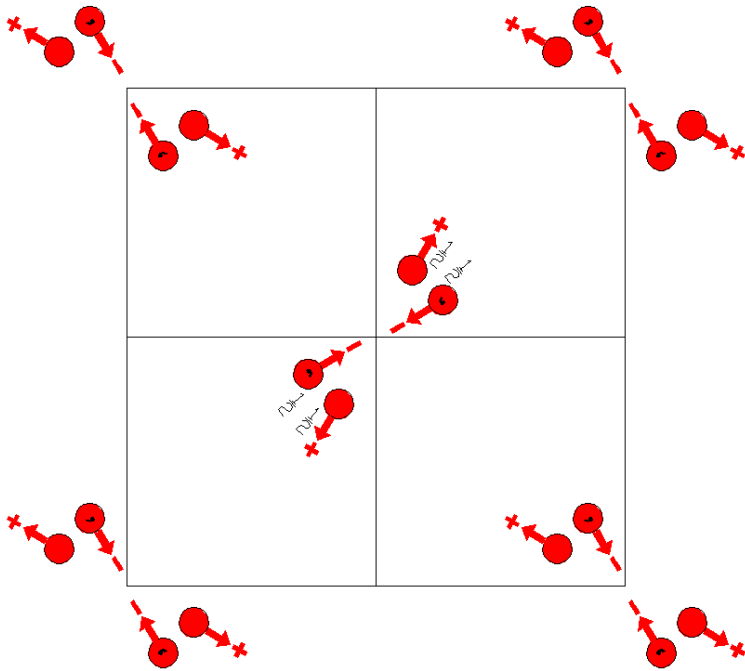




$P4_2nm$   
102.1.852

4mm  
 $P4_2nm$

Tetragonal



**Origin** on 2mm on 21m

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub> <sup>+</sup>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-</sup>  1/2,1/2,1/2) |
| (5) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (6) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (7) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)   | (8) m x,x,z<br>(m <sub>xy</sub>  0,0,0)  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

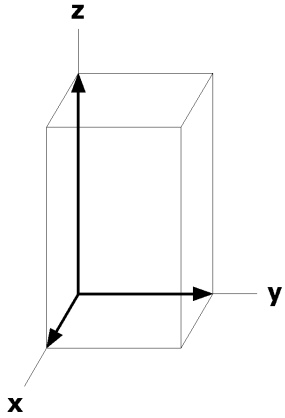
8	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}+1/2, x+1/2, z+1/2$ [ $\bar{v}, u, w$ ]	(4) $y+1/2, \bar{x}+1/2, z+1/2$ [ $v, \bar{u}, w$ ]		
			(5) $x+1/2, \bar{y}+1/2, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(6) $\bar{x}+1/2, y+1/2, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]		
			(7) $\bar{y}, \bar{x}, z$ [ $v, u, \bar{w}$ ]	(8) $y, x, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
4	c	..m	x,x,z [ $\bar{u}, u, 0$ ]	$\bar{x}, \bar{x}, z$ [ $u, \bar{u}, 0$ ]	$\bar{x}+1/2, x+1/2, z+1/2$ [ $\bar{u}, \bar{u}, 0$ ]	$x+1/2, \bar{x}+1/2, z+1/2$ [ $u, u, 0$ ]
4	b	2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	1/2,0,z [0,0, $\bar{w}$ ]
2	a	2.mm	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4gm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0]  $c_p \cdot 1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0

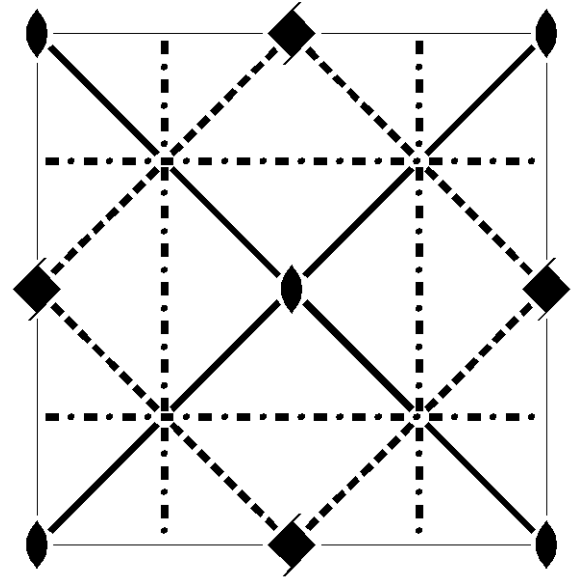
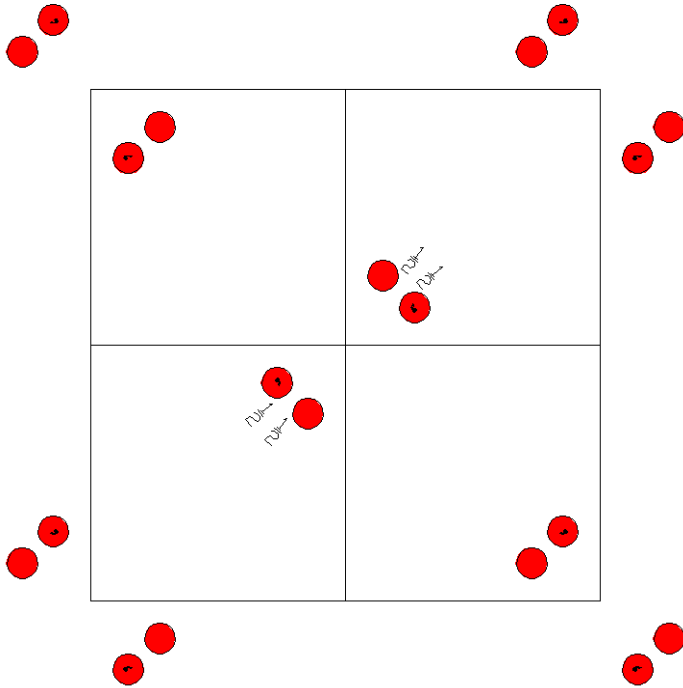


$P4_2nm1'$   
102.2.853

$4mm1'$   
 $P4_2nm1'$

Tetragonal

1'



Origin on  $2mm1'$  on  $21m1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

For 1 + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (6) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (7) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                              | (8) m x,x,z<br>(m <sub>xy</sub>  0,0,0)   |

For 1' + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1'<br>(1 0,0,0)'   | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                     | (3) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (6) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (7) m' x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'                               | (8) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

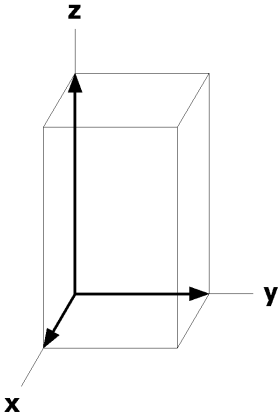
			Coordinates							
Multiplicity, Wyckoff letter, Site Symmetry.			1 +		1' +					
8	d	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y}+1/2,x+1/2,z+1/2$ [0,0,0]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [0,0,0]	(5) $x+1/2,\bar{y}+1/2,z+1/2$ [0,0,0]	(6) $\bar{x}+1/2,y+1/2,z+1/2$ [0,0,0]	(7) $\bar{y},\bar{x},z$ [0,0,0]	(8) y,x,z [0,0,0]
4	c	..m1'	x,x,z [0,0,0]	$\bar{x},\bar{x},z$ [0,0,0]	$\bar{x}+1/2,x+1/2,z+1/2$ [0,0,0]	$x+1/2,\bar{x}+1/2,z+1/2$ [0,0,0]				
4	b	2..1'	0,1/2,z [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0,z+1/2 [0,0,0]	1/2,0,z [0,0,0]				
2	a	2.mm1'	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]						

**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] c1m1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

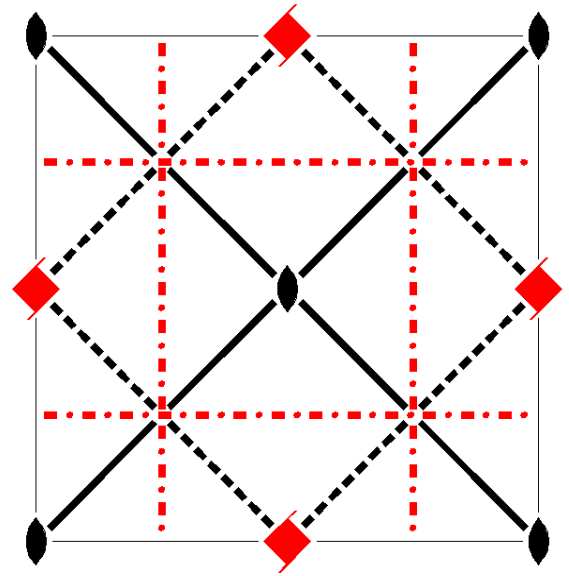
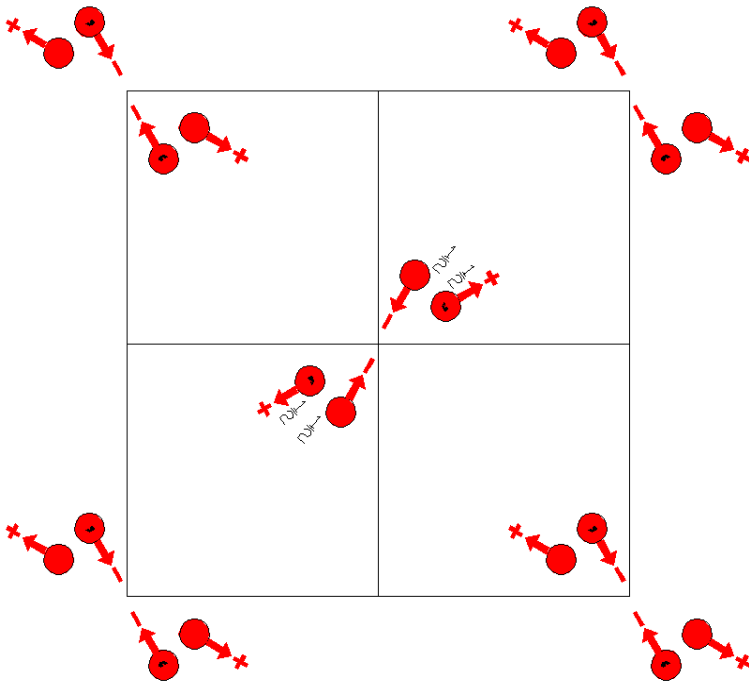
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P4_2'n'm$   
102.3.854

$4'm'm$   
 $P4_2'n'm$

Tetragonal



Origin on 2mm on 21m

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                       | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (6) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (7) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                               | (8) m x,x,z<br>(m <sub>xy</sub>  0,0,0)  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

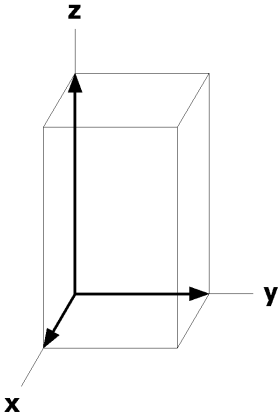
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(6) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]		
			(7) $\bar{y},\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]	(8) $y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]		
4	c	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,z+1/2$ [ $u,u,0$ ]	$x+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{u},\bar{u},0$ ]
4	b	2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]
2	a	2.mm	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4'g'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] c1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

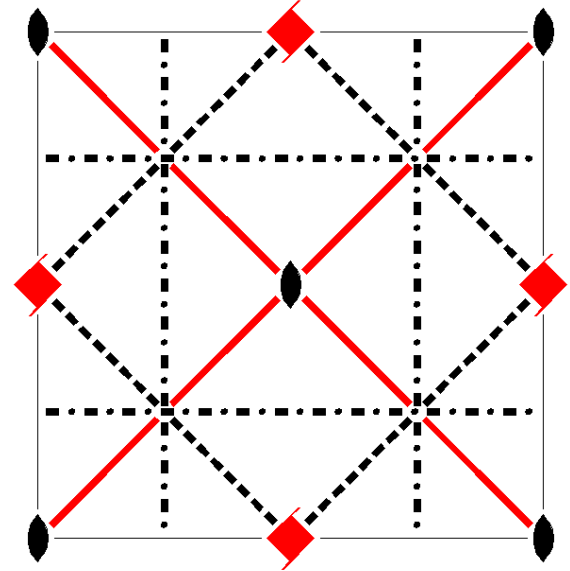
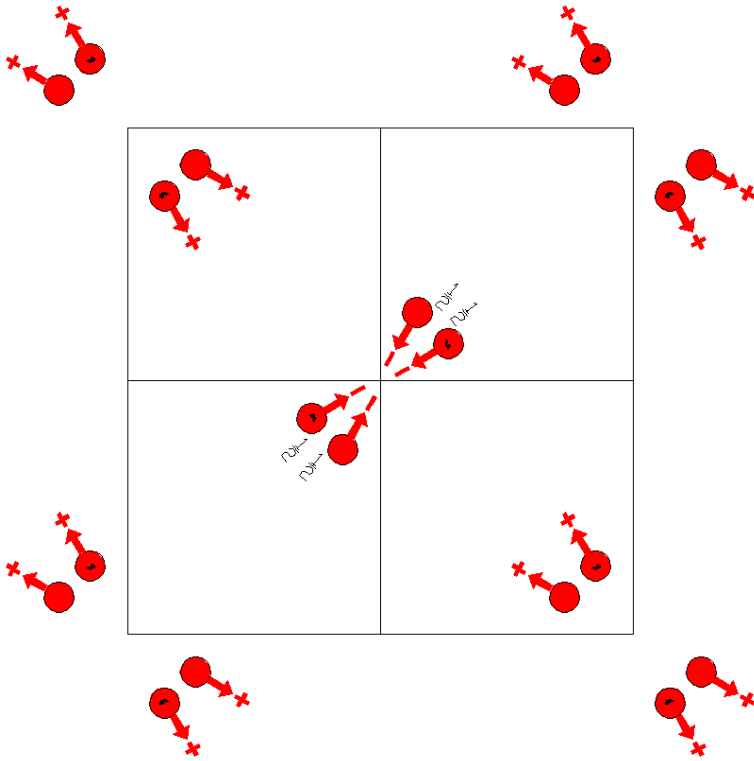
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P4_2'nm'$   
102.4.855

$4'mm'$   
 $P4_2'nm'$

Tetragonal



Origin on  $2m'm'$  on  $21m'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

### Symmetry Operations

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                         | (3) $4^+'$ $(0,0,1/2) 0,1/2,z$<br>( $4_z$   $1/2,1/2,1/2$ )' | (4) $4^-'$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1}$   $1/2,1/2,1/2$ )' |
| (5) n $(1/2,0,1/2) x,1/4,z$<br>( $m_y$   $1/2,1/2,1/2$ ) | (6) n $(0,1/2,1/2) 1/4,y,z$<br>( $m_x$   $1/2,1/2,1/2$ ) | (7) $m'$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,0)'                | (8) $m'$ $x,x,z$<br>( $m_{\bar{xy}}$  0,0,0)'                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}+1/2, x+1/2, z+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(4) $y+1/2, \bar{x}+1/2, z+1/2$ [ $\bar{v}, u, \bar{w}$ ]		
			(5) $x+1/2, \bar{y}+1/2, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(6) $\bar{x}+1/2, y+1/2, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]		
			(7) $\bar{y}, \bar{x}, z$ [ $\bar{v}, \bar{u}, w$ ]	(8) y,x,z [v,u,w]		
4	c	..m'	x,x,z [u,u,w]	$\bar{x}, \bar{x}, z$ [ $\bar{u}, \bar{u}, w$ ]	$\bar{x}+1/2, x+1/2, z+1/2$ [ $u, \bar{u}, \bar{w}$ ]	$x+1/2, \bar{x}+1/2, z+1/2$ [ $\bar{u}, u, \bar{w}$ ]
4	b	2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	1/2,0,z [0,0,w]
2	a	2.m'm'	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]		

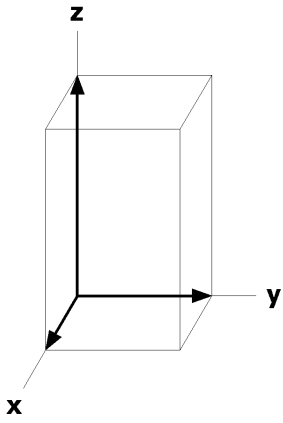
**Symmetry of Special Projections**

Along [0,0,1] p4'gm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] c<sub>p</sub>.1m'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0

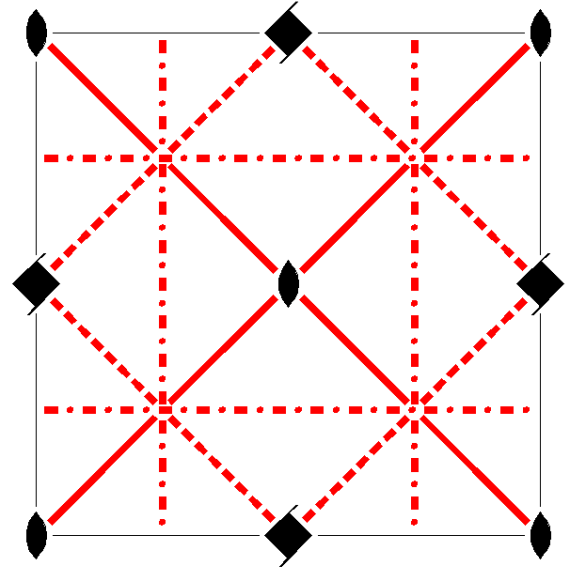
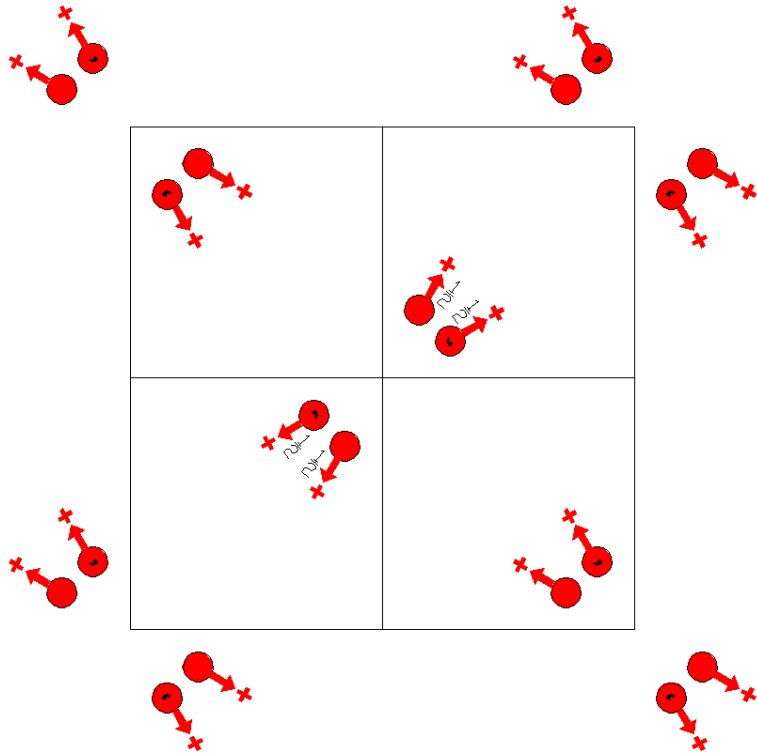




$P4_2 n'm'$   
102.5.856

$4m'm'$   
 $P4_2 n'm'$

Tetragonal



Origin on  $2m'm'$  on  $21m'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

### Symmetry Operations

(1) 1  
(1|0,0,0)

(2)  $2_{0,0,z}$   
( $2_z$ |0,0,0)

(3)  $4^+_{(0,0,1/2)}$   $0,1/2,z$   
( $4_z$ | $1/2,1/2,1/2$ )

(4)  $4^-_{(0,0,1/2)}$   $1/2,0,z$   
( $4_z^{-1}$ | $1/2,1/2,1/2$ )

(5)  $n'_{(1/2,0,1/2)}$   $x,1/4,z$   
( $m_y$ | $1/2,1/2,1/2$ )'

(6)  $n'_{(0,1/2,1/2)}$   $1/4,y,z$   
( $m_x$ | $1/2,1/2,1/2$ )'

(7)  $m'_{x,\bar{x},z}$   
( $m_{xy}$ |0,0,0)'

(8)  $m'_{x,x,z}$   
( $m_{\bar{xy}}$ |0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

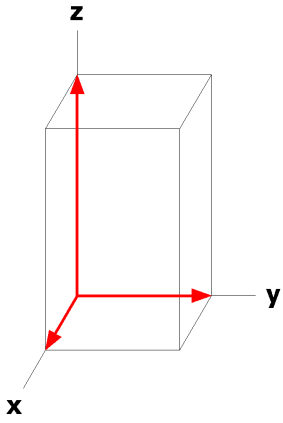
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}+1/2, x+1/2, z+1/2$ [ $\bar{v}, u, w$ ]	(4) $y+1/2, \bar{x}+1/2, z+1/2$ [ $v, \bar{u}, w$ ]		
			(5) $x+1/2, \bar{y}+1/2, z+1/2$ [ $u, \bar{v}, w$ ]	(6) $\bar{x}+1/2, y+1/2, z+1/2$ [ $\bar{u}, v, w$ ]		
			(7) $\bar{y}, \bar{x}, z$ [ $\bar{v}, \bar{u}, w$ ]	(8) y,x,z [v,u,w]		
4	c	..m'	x,x,z [u,u,w]	$\bar{x}, \bar{x}, z$ [ $\bar{u}, \bar{u}, w$ ]	$\bar{x}+1/2, x+1/2, z+1/2$ [ $\bar{u}, u, w$ ]	$x+1/2, \bar{x}+1/2, z+1/2$ [ $u, \bar{u}, w$ ]
4	b	2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0,z+1/2 [0,0,w]	1/2,0,z [0,0,w]
2	a	2.m'm'	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p4g'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0] c1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

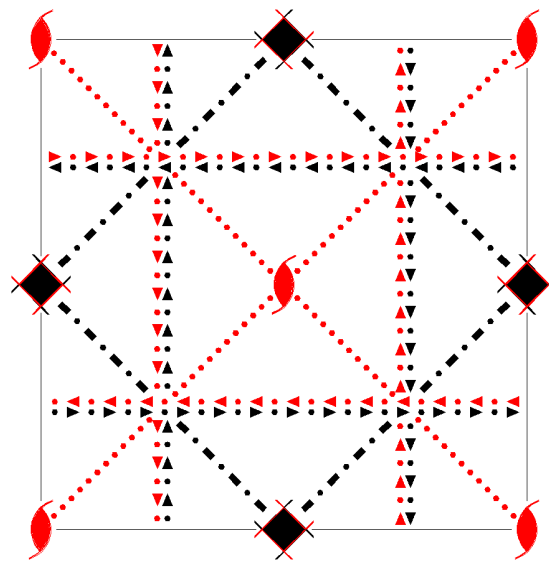
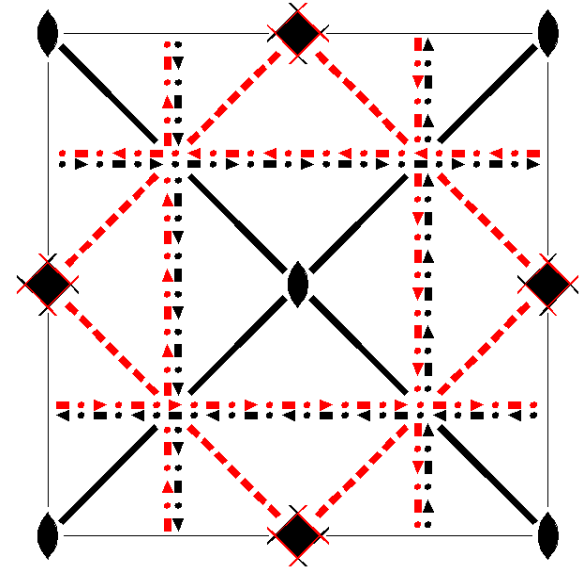
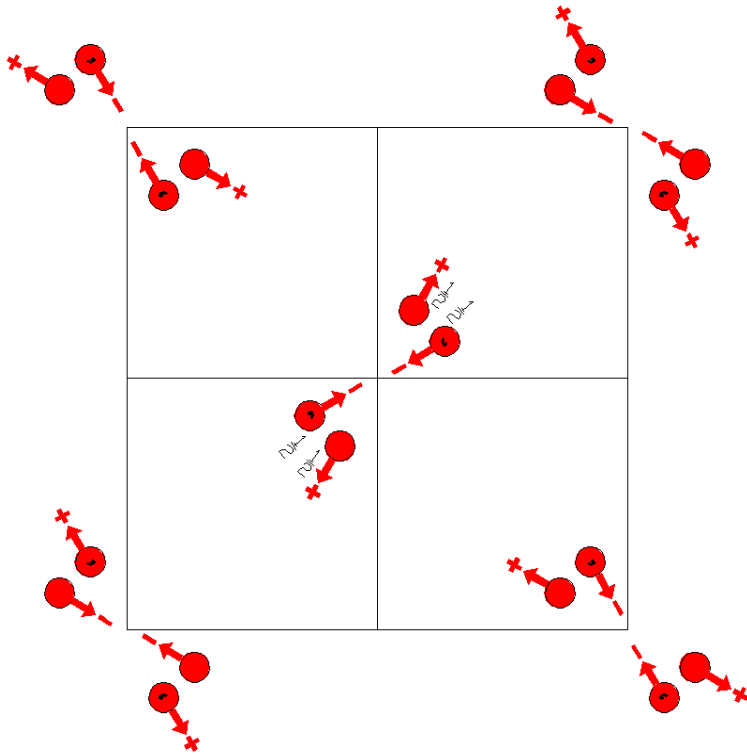
Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_14_2$  nm  
102.6.857

$4mm1'$   
 $P_14_2$  nm

Tetragonal



Origin on 2mm on 21m

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$ ;  $x \leq y$ 

## Symmetry Operations

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) n (1/2,0,1/2) x,1/2,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (6) n (0,1/2,1/2) 1/2,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (7) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                              | (8) m x,x,z<br>(m <sub>xy</sub>  0,0,0)   |

For (1,0,0)' + set

- |  |  |   |  |
|--|--|---|--|
| (1) t' (1,0,0)<br>(1 1,0,0)'                                 | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'                   | (3) 4 <sup>+</sup> ' (0,0,1/2) -1/2,0,z<br>(4 <sub>z</sub>  3/2,1/2,1/2)' | (4) 4 <sup>-</sup> ' (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub> <sup>-1</sup>  3/2,1/2,1/2)' |
| (5) n' (3/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  3/2,1/2,1/2)' | (6) n' (0,1/2,1/2) 3/4,y,z<br>(m <sub>x</sub>  3/2,1/2,1/2)' | (7) g' (1/2,-1/2,0) x+1/2,x̄,z<br>(m <sub>xy</sub>  1,0,0)'               | (8) g' (1/2,1/2,0) x+1/2,x,z<br>(m <sub>xy</sub>  1,0,0)'                              |

Generators selected (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).

## Positions

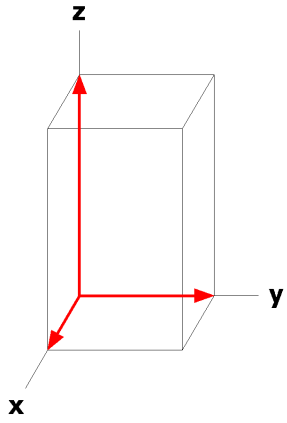
Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

			(0,0,0) +	(1,0,0)' +		
16	d	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w̄]		
			(3) ȳ+1/2,x+1/2,z+1/2 [v̄,u,w]	(4) y+1/2,x̄+1/2,z+1/2 [v,u,w]		
			(5) x+1/2,ȳ+1/2,z+1/2 [ū,v,w̄]	(6) x̄+1/2,y+1/2,z+1/2 [u,v̄,w̄]		
			(7) ȳ,x̄,z [v,u,w̄]	(8) y,x,z [v̄,ū,w̄]		
8	c	..m	x,x,z [ū,u,0]	x̄,x̄,z [ū,ū,0]	x̄+1/2,x+1/2,z+1/2 [ū,ū,0]	x+1/2,x̄+1/2,z+1/2 [u,u,0]
8	b	2'..	0,1/2,z [u,v,0]	0,1/2,z+1/2 [v̄,u,0]	1/2,0,z+1/2 [ū,v,0]	1/2,0,z [v̄,ū,0]
4	a	2.mm	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]		

## Symmetry of Special Projections

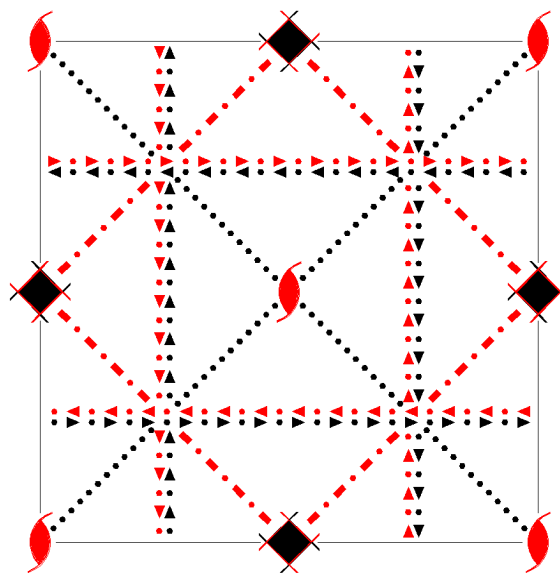
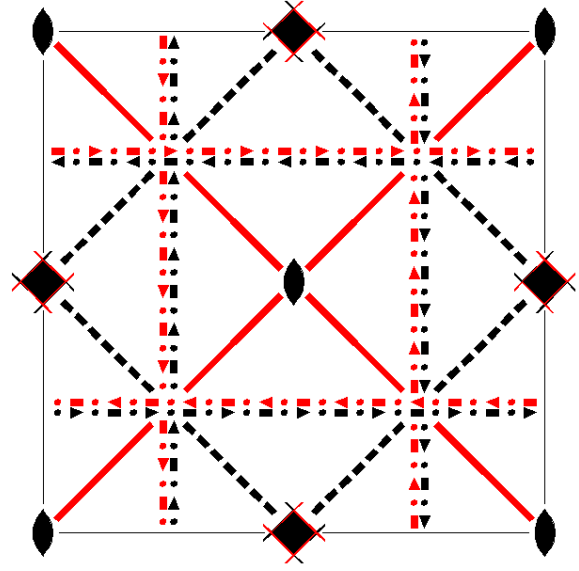
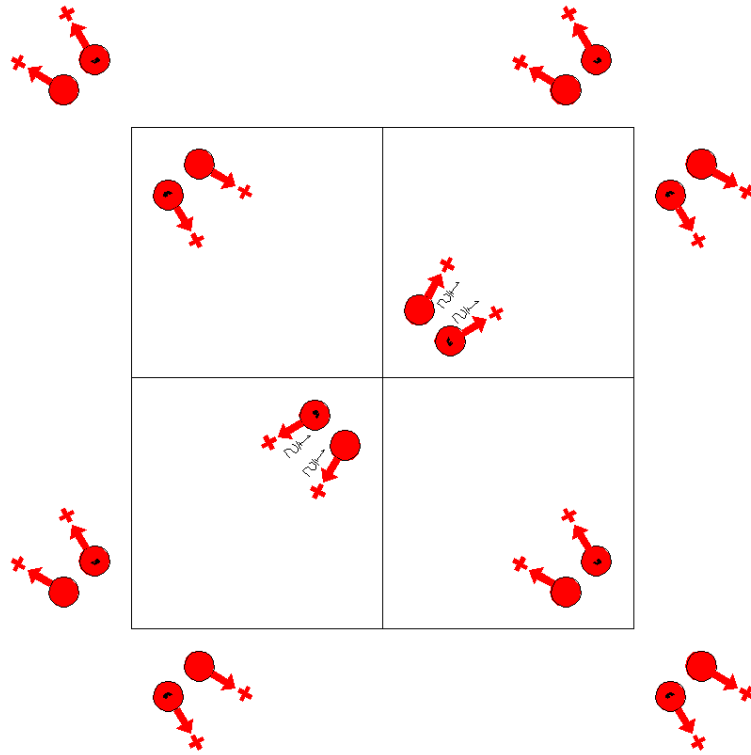
Along [0,0,1] p4gm1'  
a\* = a b\* = b  
Origin at 0,1/2,zAlong [1,0,0] c1m11'  
a\* = b b\* = c  
Origin at x,0,0Along [1,1,0] p1m11'  
a\* = (-a + b)/2 b\* = c  
Origin at x,x,0



$P_1 4_2 n' m'$   
102.7.858

$4mm1'$   
 $P_1 4_2 n' m'$

Tetragonal



Origin on 2m'm' on 21m'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$ ;  $x \leq y$ 

## Symmetry Operations

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)          | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) n' (1/2,0,1/2) x,1/2,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (6) n' (0,1/2,1/2) 1/2,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (7) m' x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'                            | (8) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'   |

For (1,0,0)' + set

- |  |  |   |  |
|--|--|---|--|
| (1) t' (1,0,0)<br>(1 1,0,0)'                               | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'                 | (3) 4 <sup>+</sup> ' (0,0,1/2) -1/2,0,z<br>(4 <sub>z</sub>  3/2,1/2,1/2)' | (4) 4 <sup>-</sup> ' (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub> <sup>-1</sup>  3/2,1/2,1/2)' |
| (5) n (3/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  3/2,1/2,1/2) | (6) n (0,1/2,1/2) 3/4,y,z<br>(m <sub>x</sub>  3/2,1/2,1/2) | (7) g (1/2,-1/2,0) x+1/2,x̄,z<br>(m <sub>xy</sub>  1,0,0)                 | (8) g (1/2,1/2,0) x+1/2,x,z<br>(m <sub>xy</sub>  1,0,0)                                |

Generators selected (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).

## Positions

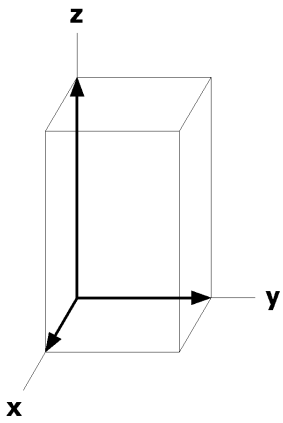
Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

			(0,0,0) +	(1,0,0)' +		
16	d	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w]		
			(3) ȳ+1/2,x+1/2,z+1/2 [v̄,u,w]	(4) y+1/2,x̄+1/2,z+1/2 [v,u,w]		
			(5) x+1/2,ȳ+1/2,z+1/2 [u,v̄,w]	(6) x̄+1/2,y+1/2,z+1/2 [ū,v,w]		
			(7) ȳ,x̄,z [v̄,ū,w]	(8) y,x,z [v,u,w]		
8	c	..m'	x,x,z [u,u,w]	x̄,x̄,z [ū,ū,w]	x̄+1/2,x+1/2,z+1/2 [ū,u,w]	x+1/2,x̄+1/2,z+1/2 [u,ū,w]
8	b	2'..	0,1/2,z [u,v,0]	0,1/2,z+1/2 [v̄,u,0]	1/2,0,z+1/2 [u,v̄,0]	1/2,0,z [v,u,0]
4	a	2.m'm'	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]		

## Symmetry of Special Projections

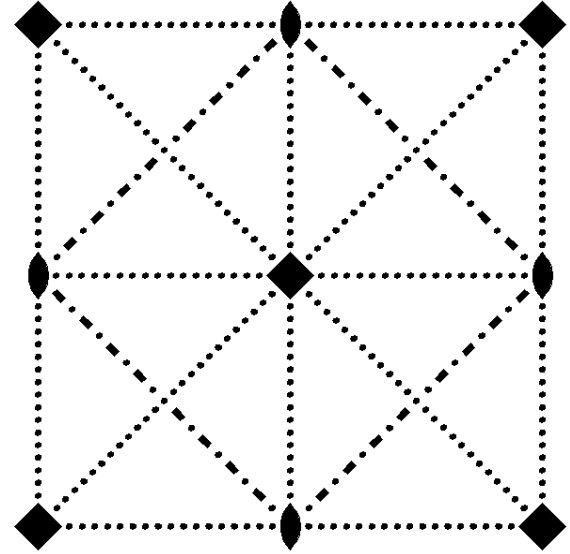
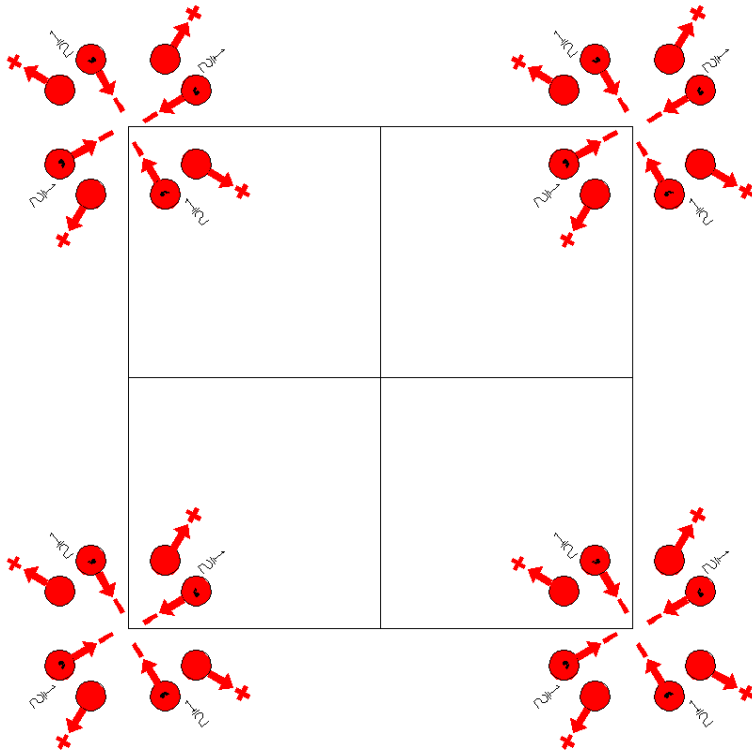
Along [0,0,1] p4gm1'  
a\* = a b\* = b  
Origin at 0,1/2,zAlong [1,0,0] c1m11'  
a\* = b b\* = c  
Origin at x,0,0Along [1,1,0] p<sub>c</sub>-1m1  
a\* = (-a + b)/2 b\* = c  
Origin at x,x,1/2



P4cc  
103.1.859

4mm  
P4cc

Tetragonal



**Origin** on 4cc

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)             | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0) |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (7) c (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2)    | (8) c (0,0,1/2) x,x,z<br>(m $\bar{xy}$  0,0,1/2)                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	d	1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $\bar{y},x,z [\bar{v},u,w]$	(4) $y,\bar{x},z [v,\bar{u},w]$
			(5) $x,\bar{y},z+1/2 [\bar{u},v,\bar{w}]$	(6) $\bar{x},y,z+1/2 [u,\bar{v},\bar{w}]$	(7) $\bar{y},\bar{x},z+1/2 [v,u,\bar{w}]$	(8) $y,x,z+1/2 [\bar{v},\bar{u},\bar{w}]$
4	c	2..	$0,1/2,z [0,0,w]$	$1/2,0,z [0,0,w]$	$0,1/2,z+1/2 [0,0,\bar{w}]$	$1/2,0,z+1/2 [0,0,\bar{w}]$
2	b	4..	$1/2,1/2,z [0,0,w]$	$1/2,1/2,z+1/2 [0,0,\bar{w}]$		
2	a	4..	$0,0,z [0,0,w]$	$0,0,z+1/2 [0,0,\bar{w}]$		

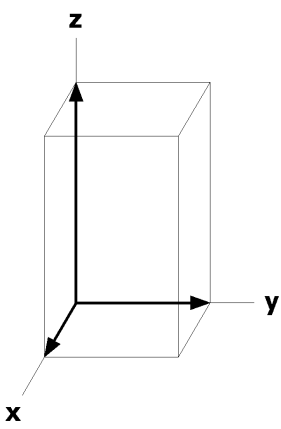
**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2b}1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p_{2b}1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$





P4cc1'

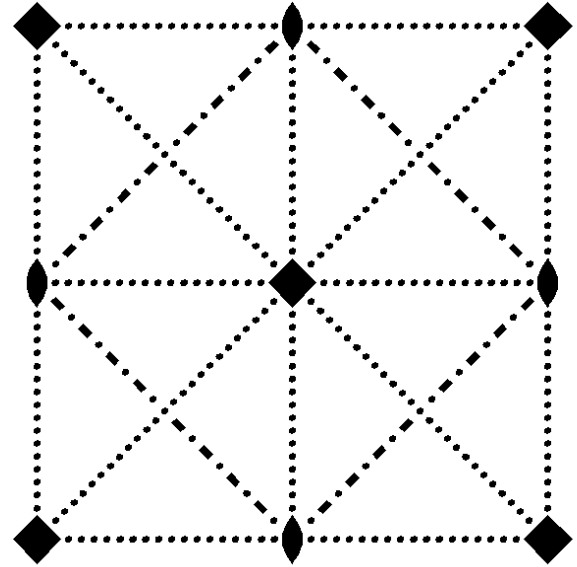
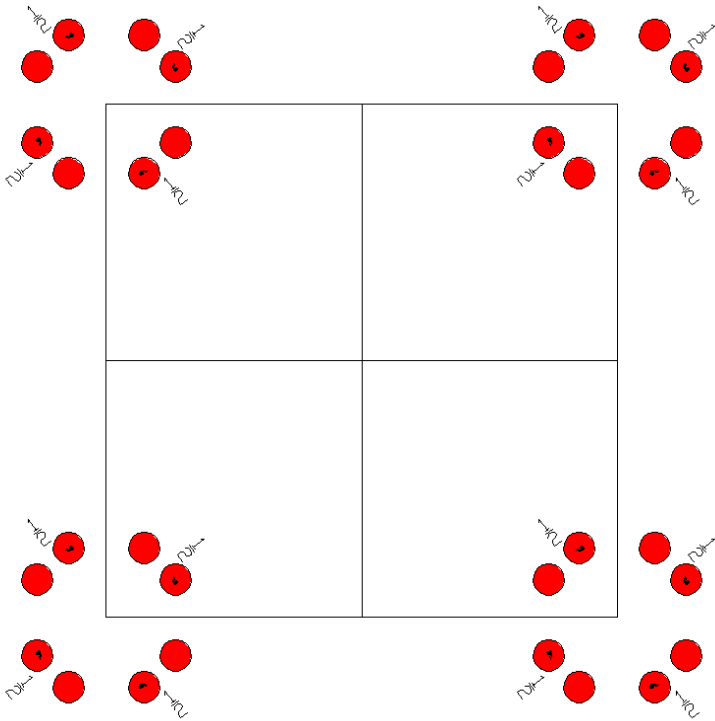
103.2.860

4mm1'

P4cc1'

Tetragonal

1'



Origin on 4cc1'

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

For 1 + set

- |  |   |  |  |
|--|---|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0) |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)  | (7) c (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)             | (8) c (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)              |

For 1' + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1'<br>(1 0,0,0)'                                 | (2) 2' <sub>z</sub> 0,0,z<br>(2' <sub>z</sub>  0,0,0)' | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)' |
| (5) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)'   | (7) c' (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)'            | (8) c' (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)'             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

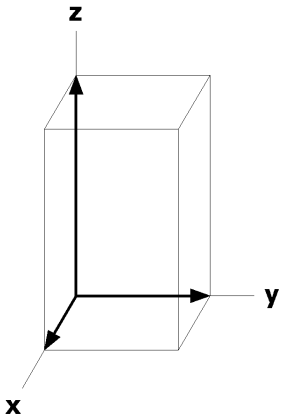
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
8 d 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z$ [0,0,0]	(4) $y,\bar{x},z$ [0,0,0]
	(5) $x,\bar{y},z+1/2$ [0,0,0]	(6) $\bar{x},y,z+1/2$ [0,0,0]	(7) $\bar{y},\bar{x},z+1/2$ [0,0,0]	(8) $y,x,z+1/2$ [0,0,0]
4 c 2..1'	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0,z+1/2 [0,0,0]
2 b 4..1'	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]		
2 a 4..1'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

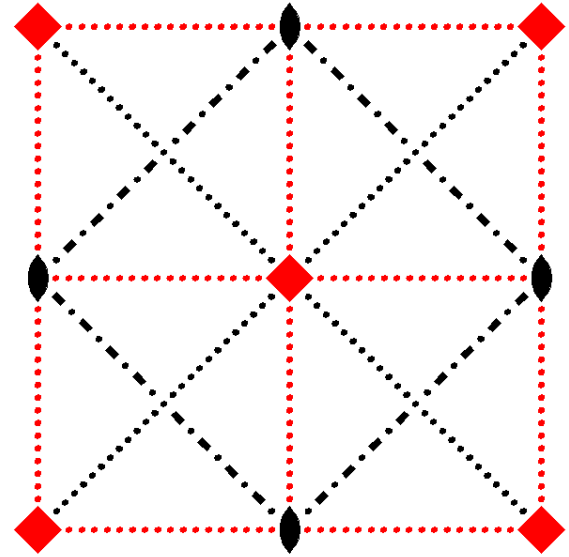
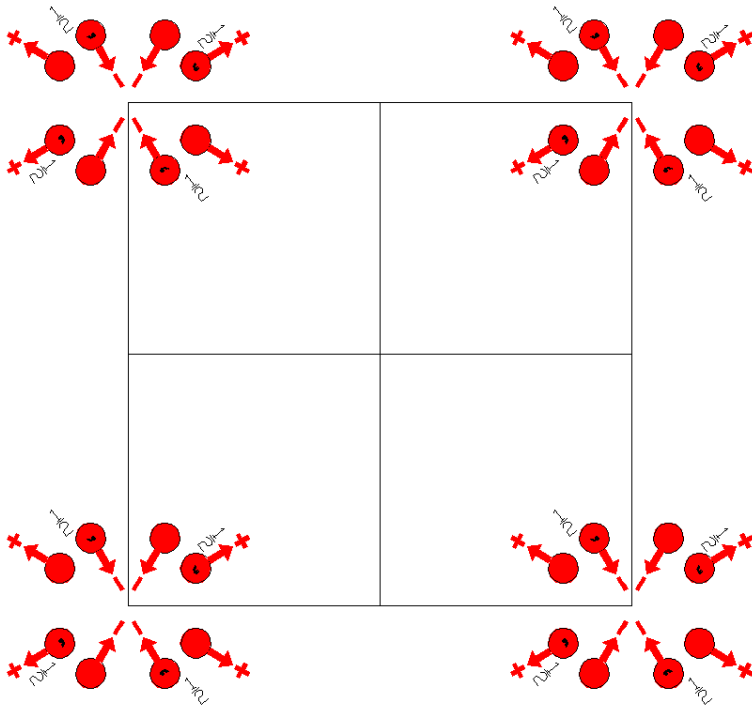
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



P4'c'c  
103.3.861

4'm'm  
P4'c'c

Tetragonal



Origin on 4'c'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)               | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (5) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' | (7) c (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2) | (8) c (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)                |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

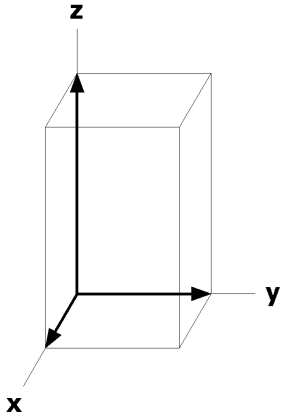
8	d	1	(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z$ [ $v, \bar{u}, \bar{w}$ ]	(4) $y, \bar{x}, z$ [ $\bar{v}, u, \bar{w}$ ]
			(5) $x, \bar{y}, z+1/2$ [ $u, \bar{v}, w$ ]	(6) $\bar{x}, y, z+1/2$ [ $\bar{u}, v, w$ ]	(7) $\bar{y}, \bar{x}, z+1/2$ [ $v, u, \bar{w}$ ]	(8) $y, x, z+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]
4	c	2..	$0, 1/2, z$ [ $0, 0, w$ ]	$1/2, 0, z$ [ $0, 0, \bar{w}$ ]	$0, 1/2, z+1/2$ [ $0, 0, w$ ]	$1/2, 0, z+1/2$ [ $0, 0, \bar{w}$ ]
2	b	4'..	$1/2, 1/2, z$ [ $0, 0, 0$ ]	$1/2, 1/2, z+1/2$ [ $0, 0, 0$ ]		
2	a	4'..	$0, 0, z$ [ $0, 0, 0$ ]	$0, 0, z+1/2$ [ $0, 0, 0$ ]		

**Symmetry of Special Projections**

Along  $[0, 0, 1]$   $p4'm'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$   $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, 0, 0$

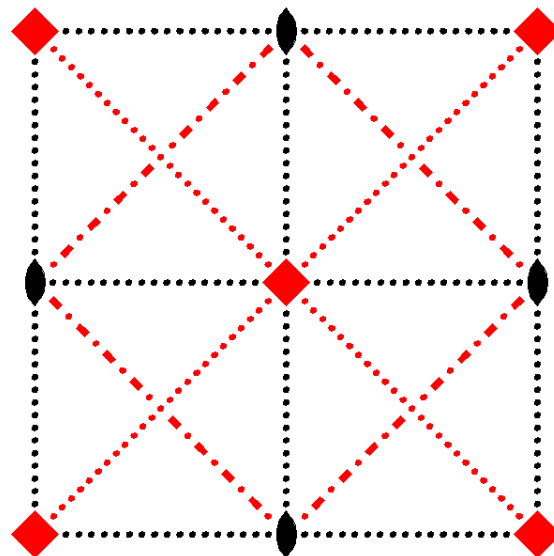
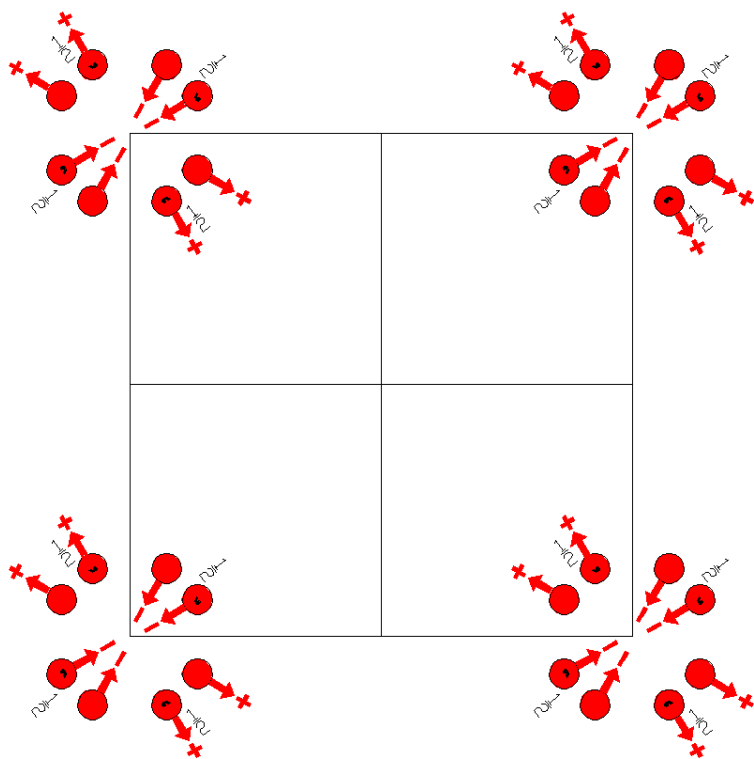
Along  $[1, 1, 0]$   $p_{2b}1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, x, 0$



P4'cc'  
103.4.862

4'mm'  
P4'cc'

Tetragonal



Origin on 4'cc'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> <sub>z</sub> 0,0,z<br>(4 <sub>z</sub>  0,0,0)' | (4) 4 <sup>-</sup> <sub>z</sub> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)  | (7) c' (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2)'   | (8) c' (0,0,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,1/2)'        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

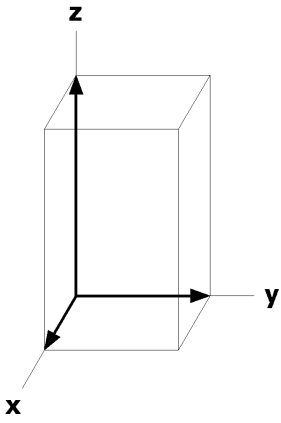
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	d	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(4) $y, \bar{x}, z$ [ $\bar{v}, u, \bar{w}$ ]
			(5) $x, \bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(6) $\bar{x}, y, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]	(7) $\bar{y}, \bar{x}, z+1/2$ [ $\bar{v}, \bar{u}, w$ ]	(8) $y, x, z+1/2$ [ $v, u, w$ ]
4	c	2..	$0, 1/2, z$ [0,0,w]	$1/2, 0, z$ [0,0, $\bar{w}$ ]	$0, 1/2, z+1/2$ [0,0, $\bar{w}$ ]	$1/2, 0, z+1/2$ [0,0,w]
2	b	4'..	$1/2, 1/2, z$ [0,0,0]	$1/2, 1/2, z+1/2$ [0,0,0]		
2	a	4'..	$0, 0, z$ [0,0,0]	$0, 0, z+1/2$ [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1]  $p4'mm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b}1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

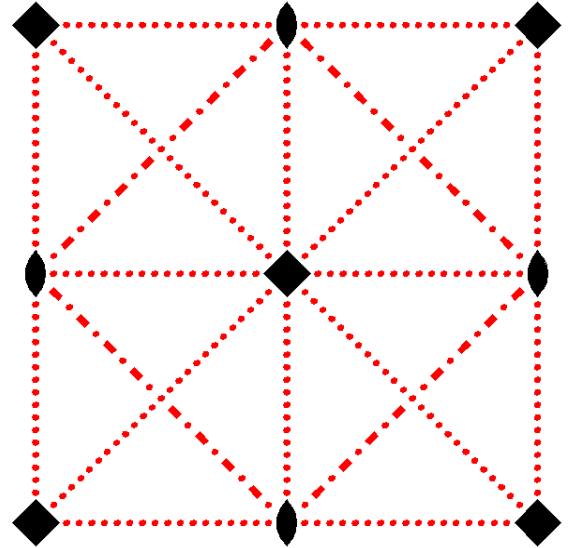
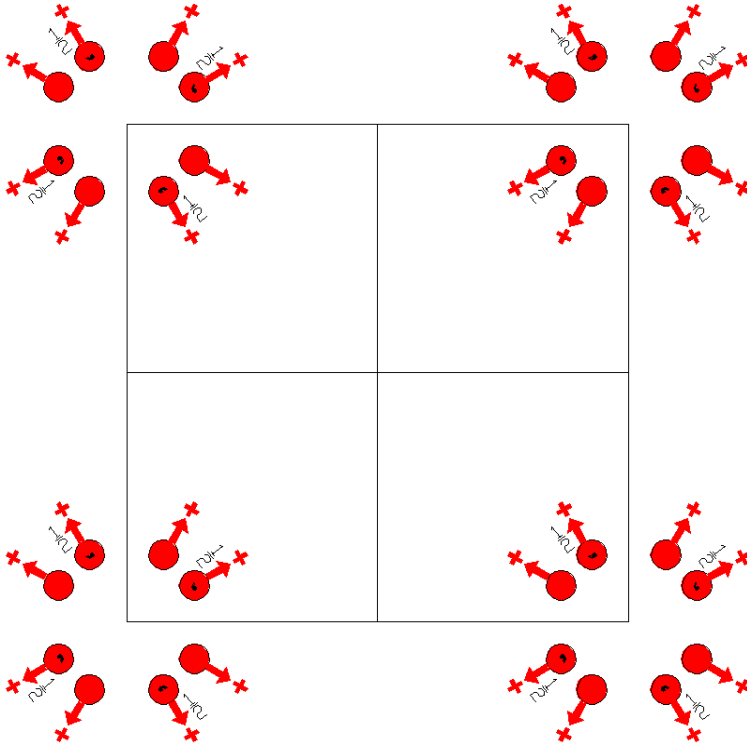
Along [1,1,0]  $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



P4c'c'  
103.5.863

4m'm'  
P4c'c'

Tetragonal



Origin on 4c'c'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                   | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)             | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' | (7) c' (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2)' | (8) c' (0,0,1/2) x,x,z<br>(m $\bar{xy}$  0,0,1/2)'                |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	d	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z$ [ $\bar{v}, u, w$ ]	(4) $y, \bar{x}, z$ [ $v, \bar{u}, w$ ]
			(5) $x, \bar{y}, z+1/2$ [ $u, \bar{v}, w$ ]	(6) $\bar{x}, y, z+1/2$ [ $\bar{u}, v, w$ ]	(7) $\bar{y}, \bar{x}, z+1/2$ [ $\bar{v}, \bar{u}, w$ ]	(8) $y, x, z+1/2$ [ $v, u, w$ ]
4	c	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0,z+1/2 [0,0,w]
2	b	4..	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]		
2	a	4..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]		

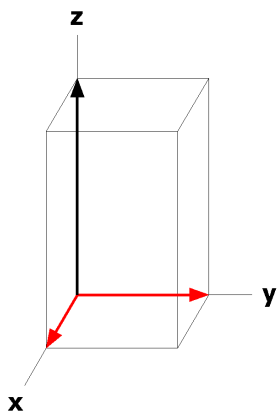
**Symmetry of Special Projections**

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0





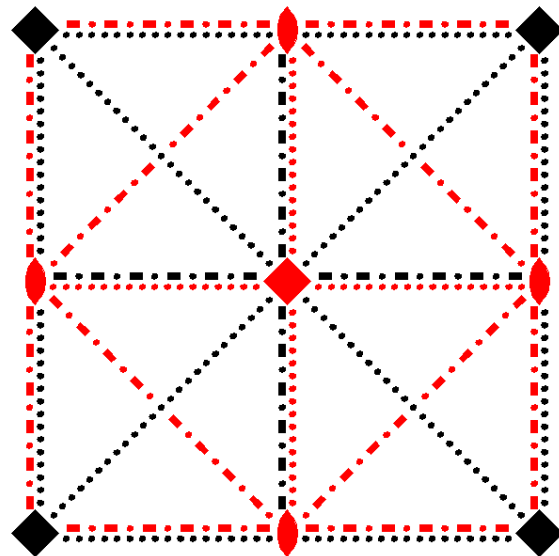
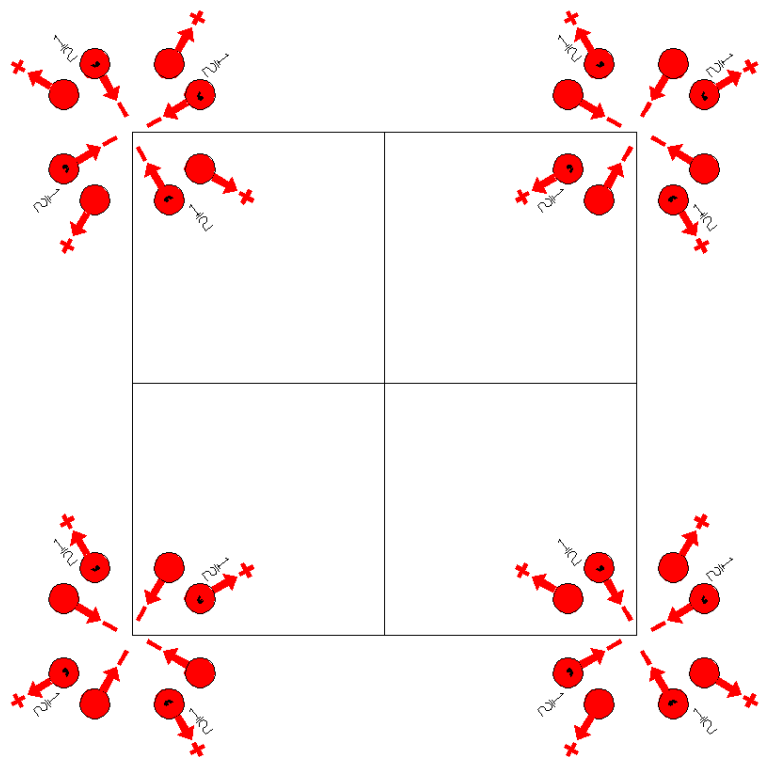
$P_P 4cc$

$4mm1'$

Tetragonal

103.6.864

$P_P 4cc$



Origin on 4cc

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                             | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)               | (3) $4^+$ $0,0,z$<br>( $4_z^+$  0,0,0)                  | (4) $4^-$ $0,0,z$<br>( $4_z^-$  0,0,0)                  |
| (5) c $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2) | (6) c $(0,0,1/2)$ $0,y,z$<br>( $m_x$  0,0,1/2) | (7) c $(0,0,1/2)$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2) | (8) c $(0,0,1/2)$ $x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2) |

For (1,0,0)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) $t'$ (1,0,0)<br>(1 1,0,0)'                   | (2) $2'$ $1/2,0,z$<br>( $2_z$  1,0,0)'             | (3) $4^+$ $1/2,1/2,z$<br>( $4_z^+$  1,0,0)'                        | (4) $4^-$ $1/2,-1/2,z$<br>( $4_z^-$  1,0,0)'                      |
| (5) $n'$ (1,0,1/2) $x,0,z$<br>( $m_y$  1,0,1/2)' | (6) $c'$ (0,0,1/2) $1/2,y,z$<br>( $m_x$  1,0,1/2)' | (7) $n'$ (1/2,-1/2,1/2) $x+1/2,\bar{x},z$<br>( $m_{xy}$  1,0,1/2)' | (8) $n'$ (1/2,1/2,1/2) $x+1/2,x,z$<br>( $m_{\bar{xy}}$  1,0,1/2)' |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

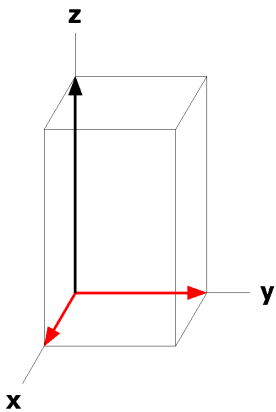
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(1,0,0)' +			
16 d 1	(1)	x,y,z [u,v,w]	(2)	$\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3)	$\bar{y}, x, z$ [ $\bar{v}, u, w$ ]	(4)	$y, \bar{x}, z$ [ $v, \bar{u}, w$ ]
	(5)	$x, \bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(6)	$\bar{x}, y, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]	(7)	$\bar{y}, \bar{x}, z+1/2$ [ $v, u, \bar{w}$ ]	(8)	$y, x, z+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]
8 c 2'..		0,1/2,z [u,v,0]		1/2,0,z [v, $\bar{u}$ ,0]		0,1/2,z+1/2 [u, $\bar{v}$ ,0]		1/2,0,z+1/2 [ $\bar{v}, \bar{u}$ ,0]
4 b 4'..		1/2,1/2,z [0,0,0]		1/2,1/2,z+1/2 [0,0,0]				
4 a 4..		0,0,z [0,0,w]		0,0,z+1/2 [0,0, $\bar{w}$ ]				

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub>-4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0] p<sub>c</sub>-1m1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x-1/4,x+1/4,0



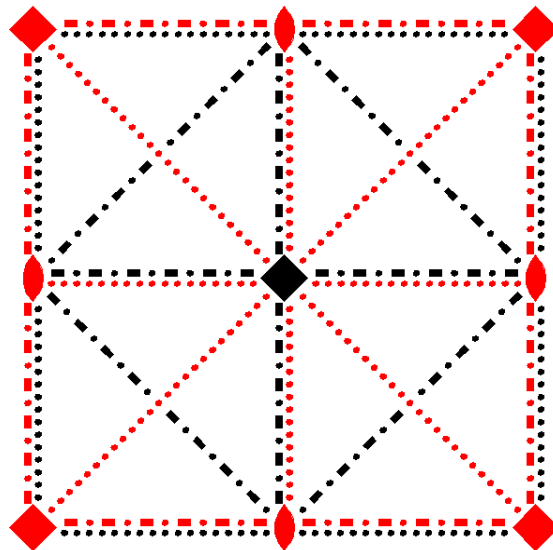
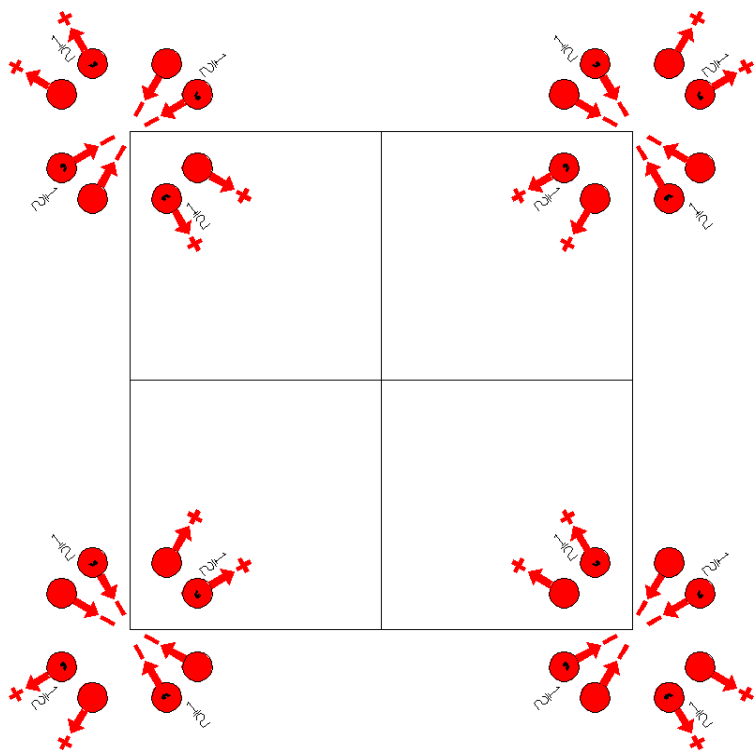
$P_P 4'cc'$

103.7.865

$4mm1'$

$P_P 4'cc'$

Tetragonal



Origin on  $4'cc'$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0)               | (3) 4 <sup>+</sup> $0,0,z$<br>(4 <sub>z</sub>  0,0,0)'          | (4) 4 <sup>-</sup> $0,0,z$<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (5) c $(0,0,1/2)$ $x,0,z$<br>(m <sub>y</sub>  0,0,1/2) | (6) c $(0,0,1/2)$ $0,y,z$<br>(m <sub>x</sub>  0,0,1/2) | (7) c' $(0,0,1/2)$ $x,\bar{x},z$<br>(m <sub>xy</sub>  0,0,1/2)' | (8) c' $(0,0,1/2)$ $x,x,z$<br>(m <sub>xy</sub>  0,0,1/2)'            |

For  $(1,0,0)$ ' + set

- |  |  |   |  |
|--|--|---|--|
| (1) t' $(1,0,0)$<br>(1 1,0,0)'                           | (2) 2' $1/2,0,z$<br>(2 <sub>z</sub>  1,0,0)'               | (3) 4 <sup>+</sup> $1/2,1/2,z$<br>(4 <sub>z</sub>  1,0,0) | (4) 4 <sup>-</sup> $1/2,-1/2,z$<br>(4 <sub>z</sub> <sup>-1</sup>  1,0,0) |
| (5) n' $(1,0,1/2)$ $x,0,z$<br>(m <sub>y</sub>  1,0,1/2)' | (6) c' $(0,0,1/2)$ $1/2,y,z$<br>(m <sub>x</sub>  1,0,1/2)' | (7) n $(1/2,-1/2,1/2)$ $x+1/2,\bar{x},z$                  | (8) n $(1/2,1/2,1/2)$ $x+1/2,x,z$<br>(m <sub>xy</sub>  1,0,1/2)          |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

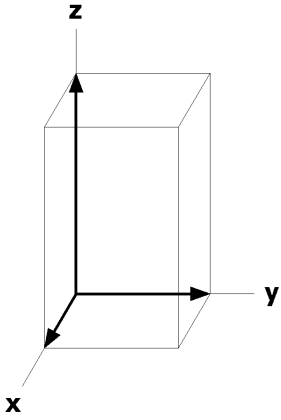
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(1,0,0)' +			
16 d 1	(1)	x,y,z [u,v,w]	(2)	$\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3)	$\bar{y}, x, z$ [ $\bar{v}, \bar{u}, w$ ]	(4)	$y, \bar{x}, z$ [ $\bar{v}, u, \bar{w}$ ]
	(5)	$x, \bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(6)	$\bar{x}, y, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]	(7)	$\bar{y}, \bar{x}, z+1/2$ [ $\bar{v}, \bar{u}, w$ ]	(8)	$y, x, z+1/2$ [ $v, u, w$ ]
8 c 2'..		0,1/2,z [u,v,0]		1/2,0,z [ $\bar{v}, u, 0$ ]		0,1/2,z+1/2 [u, $\bar{v}, 0$ ]		1/2,0,z+1/2 [v,u,0]
4 b 4..		1/2,1/2,z [0,0,w]		1/2,1/2,z+1/2 [0,0,w]				
4 a 4'..		0,0,z [0,0,0]		0,0,z+1/2 [0,0,0]				

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub>-4m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/2,1/2,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

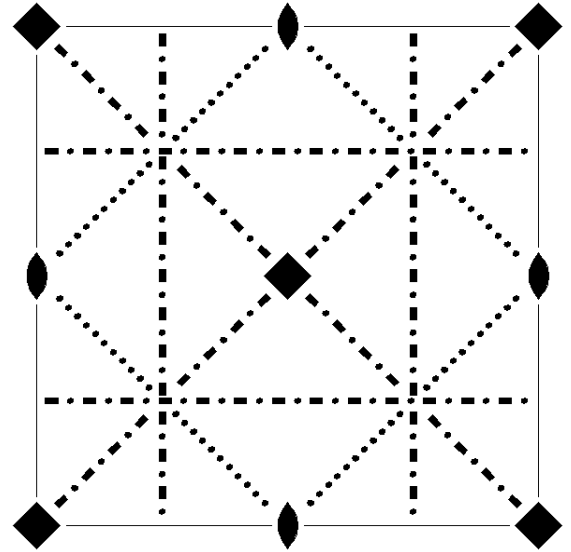
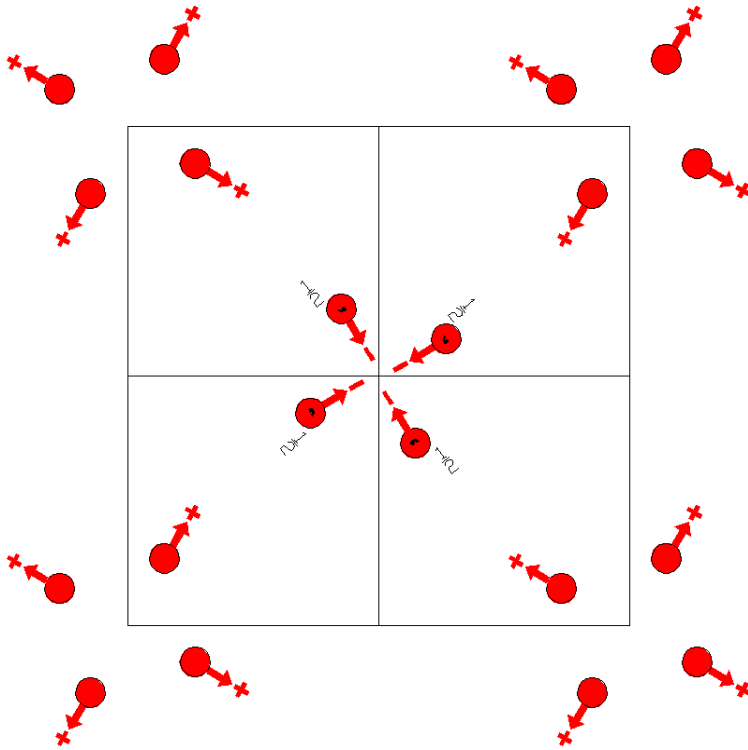
Along [1,1,0] p<sub>2a</sub>-1m1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x-1/4,x+1/4,0



P4nc  
104.1.866

4mm  
P4nc

Tetragonal



Origin on 41n

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0) |
| (5) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (6) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (7) c (0,0,1/2) x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)     | (8) n (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

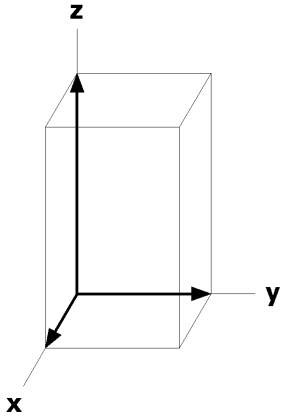
8	c	1	(1) $x, y, z$ [ $u, v, w$ ]		(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	
			(3) $\bar{y}, x, z$ [ $\bar{v}, u, w$ ]		(4) $y, \bar{x}, z$ [ $v, \bar{u}, w$ ]	
			(5) $x+1/2, \bar{y}+1/2, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]		(6) $\bar{x}+1/2, y+1/2, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]	
			(7) $\bar{y}+1/2, \bar{x}+1/2, z+1/2$ [ $v, u, \bar{w}$ ]		(8) $y+1/2, x+1/2, z+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	
4	b	2..	$0, 1/2, z$ [ $0, 0, w$ ]	$1/2, 0, z$ [ $0, 0, w$ ]	$1/2, 0, z+1/2$ [ $0, 0, \bar{w}$ ]	$0, 1/2, z+1/2$ [ $0, 0, \bar{w}$ ]
2	a	4..	$0, 0, z$ [ $0, 0, w$ ]	$1/2, 1/2, z+1/2$ [ $0, 0, \bar{w}$ ]		

**Symmetry of Special Projections**

Along  $[0, 0, 1]$   $p4gm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$   $c_p-1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 0, 0$

Along  $[1, 1, 0]$   $p_{2b}-1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, x, 0$

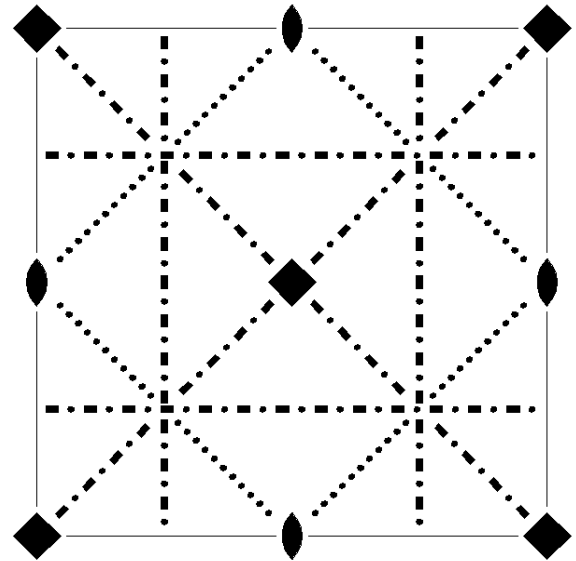
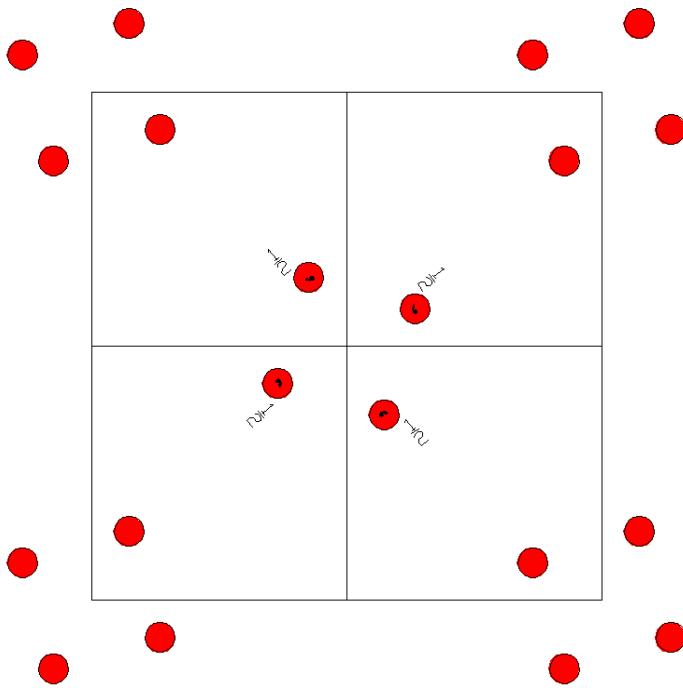


P4nc1'  
104.2.867

4mm1'  
P4nc1'

Tetragonal

1'



Origin on 41n1'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For 1 + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)        | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0) |
| (5) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (6) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (7) c (0,0,1/2) x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)     | (8) n (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)      |

For 1' + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1'<br>(1 0,0,0)'   | (2) 2' <sub>z</sub> 0,0,z<br>(2' <sub>z</sub>  0,0,0)'       | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)' |
| (5) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (6) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (7) c' (0,0,1/2) x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)'    | (8) n' (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)'     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates					
			1 +	1' +		
8 c 11'	(1)	x,y,z [0,0,0]		(2)	$\bar{x}, \bar{y}, z$ [0,0,0]	
	(3)	$\bar{y}, x, z$ [0,0,0]		(4)	$y, \bar{x}, z$ [0,0,0]	
	(5)	$x+1/2, \bar{y}+1/2, z+1/2$ [0,0,0]		(6)	$\bar{x}+1/2, y+1/2, z+1/2$ [0,0,0]	
	(7)	$\bar{y}+1/2, \bar{x}+1/2, z+1/2$ [0,0,0]		(8)	$y+1/2, x+1/2, z+1/2$ [0,0,0]	
4 b 2..1'		0,1/2,z [0,0,0]	1/2,0,z [0,0,0]		1/2,0,z+1/2 [0,0,0]	0,1/2,z+1/2 [0,0,0]
2 a 4..1'		0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]			

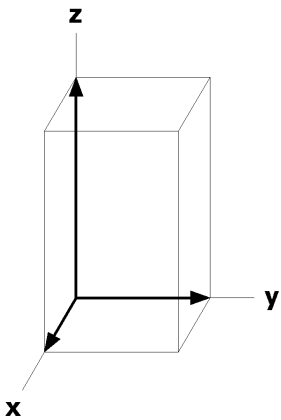
**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

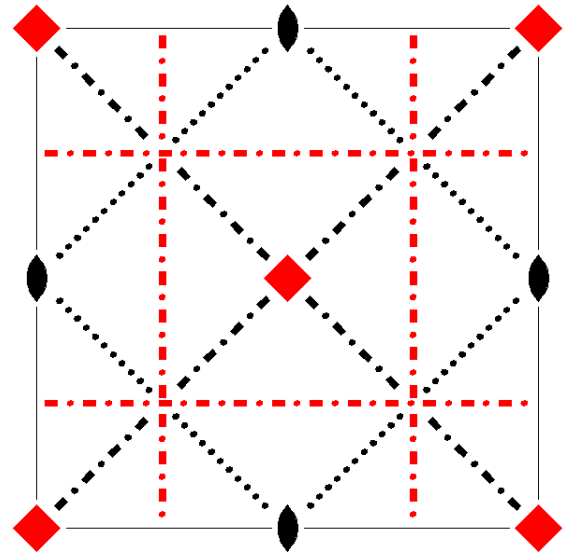
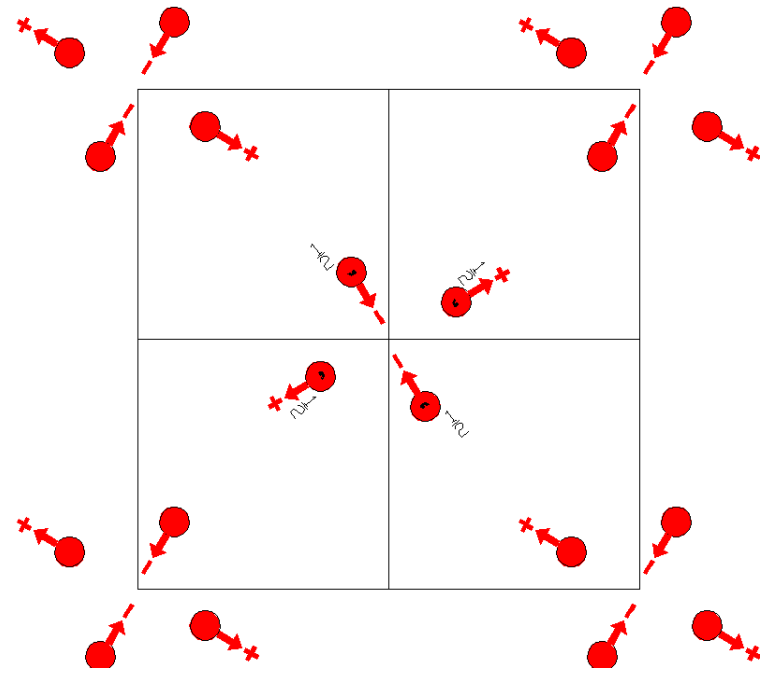




P4'n'c  
104.3.868

4'm'm  
P4'n'c

Tetragonal



Origin on 4'1n

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 4<sup>+</sup> 0,0,z  
(4<sub>z</sub>|0,0,0)'

(4) 4<sup>-</sup> 0,0,z  
(4<sub>z</sub><sup>-1</sup>|0,0,0)'

(5) n' (1/2,0,1/2) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,1/2)'

(6) n' (0,1/2,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,1/2)'

(7) c (0,0,1/2) x+1/2,x̄,z  
(m<sub>xy</sub>|1/2,1/2,1/2)

(8) n (1/2,1/2,1/2) x,x,z  
(m<sub>xy</sub>|1/2,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

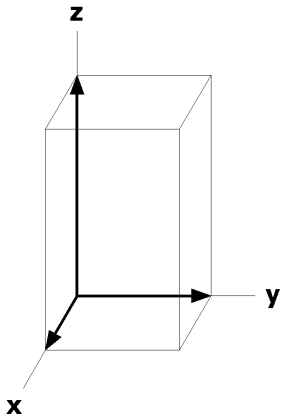
8	c	1	(1) $x, y, z$ [u,v,w]		(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	
			(3) $\bar{y}, x, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		(4) $y, \bar{x}, z$ [ $\bar{v}, u, \bar{w}$ ]	
			(5) $x+1/2, \bar{y}+1/2, z+1/2$ [u, $\bar{v}$ ,w]		(6) $\bar{x}+1/2, y+1/2, z+1/2$ [ $\bar{u}, v, w$ ]	
			(7) $\bar{y}+1/2, \bar{x}+1/2, z+1/2$ [ $\bar{v}, u, \bar{w}$ ]		(8) $y+1/2, x+1/2, z+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	
4	b	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
2	a	4'..	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4'g'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

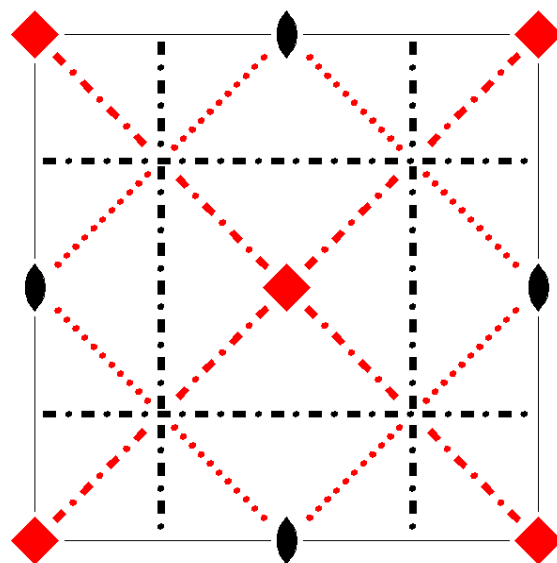
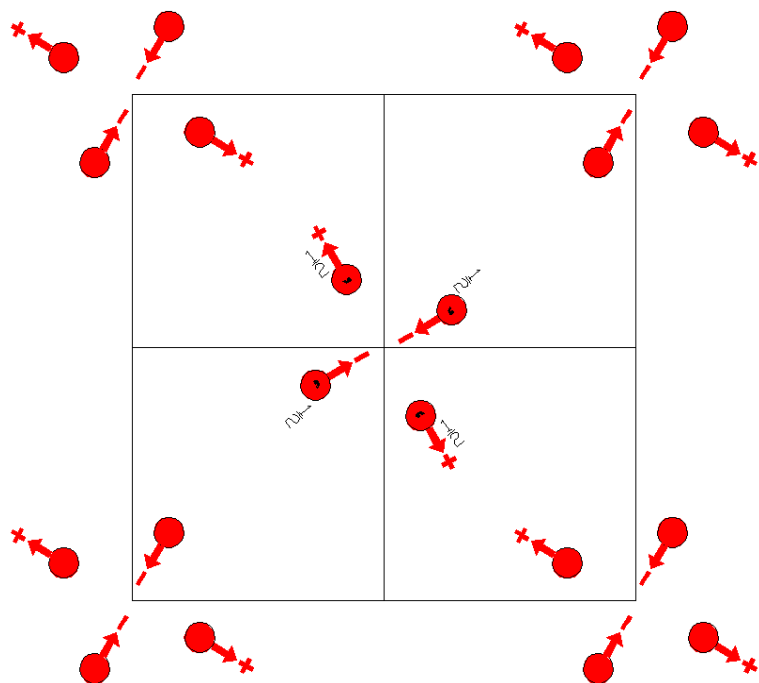
Along [1,1,0]  $p_{2b}1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



P4'nc'  
104.4.869

4'mm'  
P4'nc'

Tetragonal



Origin on 4'1n'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 4<sup>+</sup> 0,0,z  
(4<sub>z</sub><sup>+</sup>|0,0,0)'

(4) 4<sup>-</sup> 0,0,z  
(4<sub>z</sub><sup>-</sup>|0,0,0)'

(5) n (1/2,0,1/2) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,1/2)

(6) n (0,1/2,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,1/2)

(7) c' (0,0,1/2) x+1/2,x̄,z  
(m<sub>xy</sub>|1/2,1/2,1/2)'

(8) n' (1/2,1/2,1/2) x,x,z  
(m<sub>xy</sub>'|1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

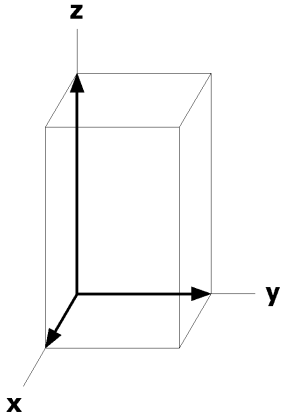
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	c	1	(1) x,y,z [u,v,w]		(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	
			(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]		(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]	
			(5) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]		(6) $\bar{x}+1/2,y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]	
			(7) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]		(8) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]	
4	b	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0,w]
2	a	4'..	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4'gm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c_p-1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

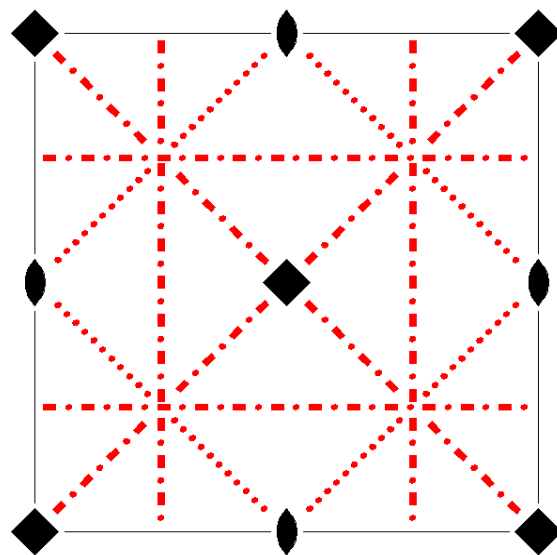
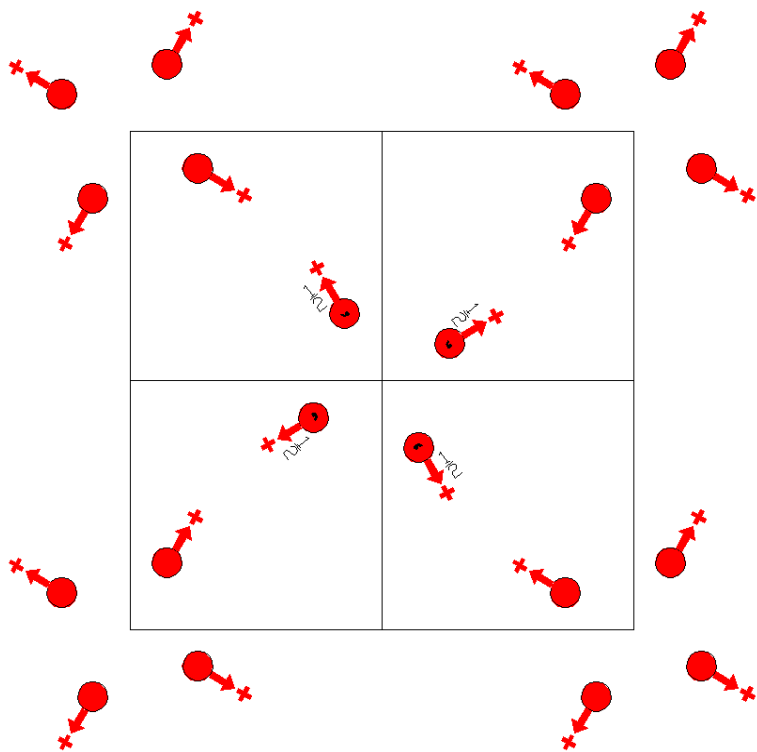
Along [1,1,0]  $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



P4n'c'  
104.5.870

4m'm'  
P4n'c'

Tetragonal



Origin on 41n'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)

(3) 4<sup>+</sup> 0,0,z  
(4<sub>z</sub><sup>+</sup>|0,0,0)

(4) 4<sup>-</sup> 0,0,z  
(4<sub>z</sub><sup>-</sup>|0,0,0)

(5) n' (1/2,0,1/2) x,1/4,z  
(m<sub>y</sub>|1/2,1/2,1/2)'

(6) n' (0,1/2,1/2) 1/4,y,z  
(m<sub>x</sub>|1/2,1/2,1/2)'

(7) c' (0,0,1/2) x+1/2,x̄,z  
(m<sub>xy</sub>|1/2,1/2,1/2)'

(8) n' (1/2,1/2,1/2) x,x,z  
(m<sub>xy</sub>|1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

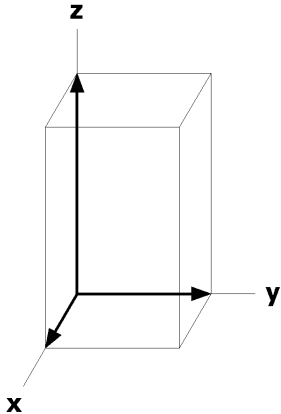
8	c	1	(1) $x, y, z$ [ $u, v, w$ ]		(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	
			(3) $\bar{y}, x, z$ [ $\bar{v}, u, w$ ]		(4) $y, \bar{x}, z$ [ $v, \bar{u}, w$ ]	
			(5) $x+1/2, \bar{y}+1/2, z+1/2$ [ $u, \bar{v}, w$ ]		(6) $\bar{x}+1/2, y+1/2, z+1/2$ [ $\bar{u}, v, w$ ]	
			(7) $\bar{y}+1/2, \bar{x}+1/2, z+1/2$ [ $\bar{v}, \bar{u}, w$ ]		(8) $y+1/2, x+1/2, z+1/2$ [ $v, u, w$ ]	
4	b	2..	$0, 1/2, z$ [ $0, 0, w$ ]	$1/2, 0, z$ [ $0, 0, w$ ]	$1/2, 0, z+1/2$ [ $0, 0, w$ ]	$0, 1/2, z+1/2$ [ $0, 0, w$ ]
2	a	4..	$0, 0, z$ [ $0, 0, w$ ]	$1/2, 1/2, z+1/2$ [ $0, 0, w$ ]		

**Symmetry of Special Projections**

Along  $[0, 0, 1]$   $p4g'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$   $c1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 0, 0$

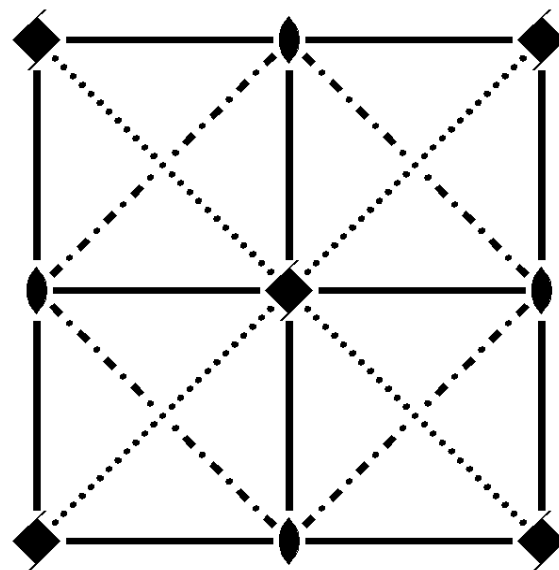
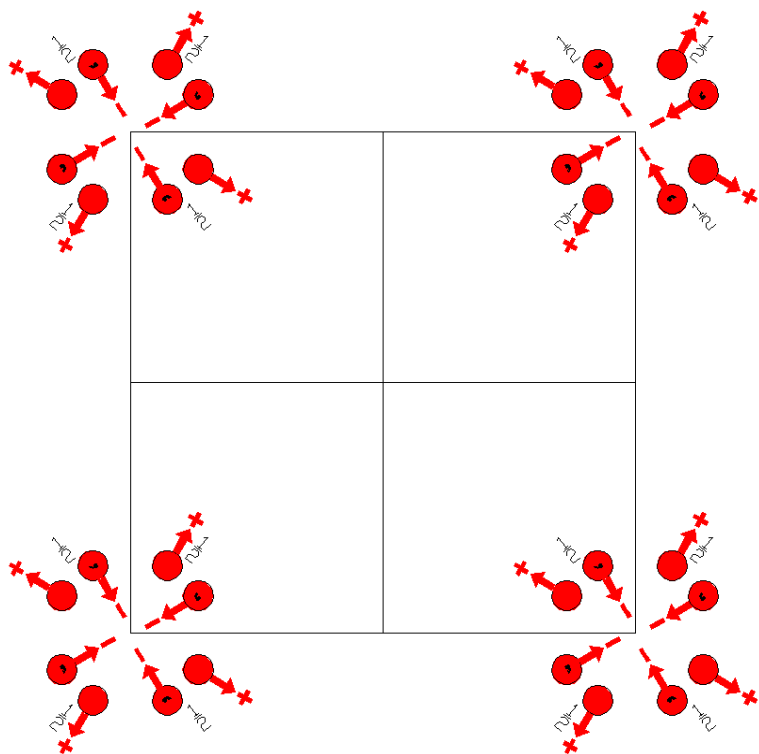
Along  $[1, 1, 0]$   $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, x, 0$



$P4_2mc$   
105.1.871

4mm  
 $P4_2mc$

Tetragonal



Origin on 2mm on  $4_2mc$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

- |                                  |                                  |   |   |
|----------------------------------|----------------------------------|---|---|
| (1) 1<br>(1 0,0,0)               | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $4^+$ (0,0,1/2) $0,0,z$<br>( $4_z$  0,0,1/2)      | (4) $4^-$ (0,0,1/2) $0,0,z$<br>( $4_z^{-1}$  0,0,1/2) |
| (5) m $x,0,z$<br>( $m_y$  0,0,0) | (6) m $0,y,z$<br>( $m_x$  0,0,0) | (7) c (0,0,1/2) $x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2) | (8) c (0,0,1/2) $x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	f	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]
			(5) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(7) $\bar{y},\bar{x},z+1/2$ [ $v,u,\bar{w}$ ]	(8) $y,x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
4	e	.m.	$x,1/2,z$ [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v}$ ,0]	$1/2,x,z+1/2$ [ $\bar{v},0,0$ ]	$1/2,\bar{x},z+1/2$ [ $v,0,0$ ]
4	d	.m.	$x,0,z$ [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]	$0,x,z+1/2$ [ $\bar{v},0,0$ ]	$0,\bar{x},z+1/2$ [ $v,0,0$ ]
2	c	2mm.	$0,1/2,z$ [0,0,0]	$1/2,0,z+1/2$ [0,0,0]		
2	b	2mm.	$1/2,1/2,z$ [0,0,0]	$1/2,1/2,z+1/2$ [0,0,0]		
2	a	2mm.	$0,0,z$ [0,0,0]	$0,0,z+1/2$ [0,0,0]		

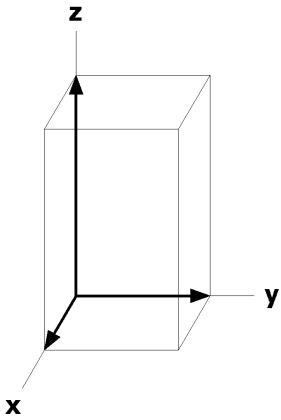
**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p<sub>2b</sub>1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



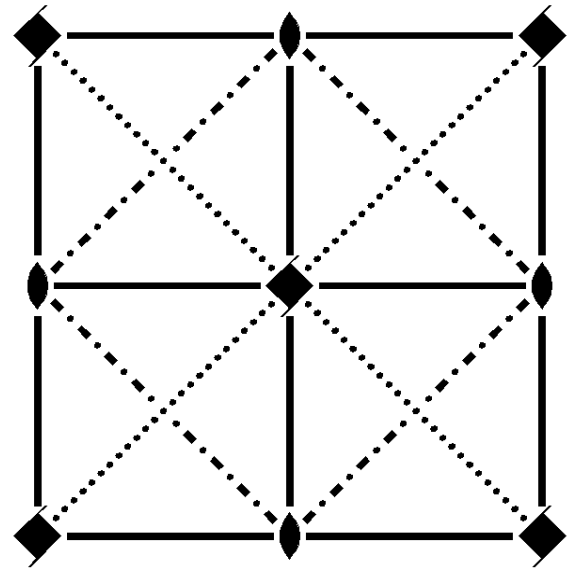
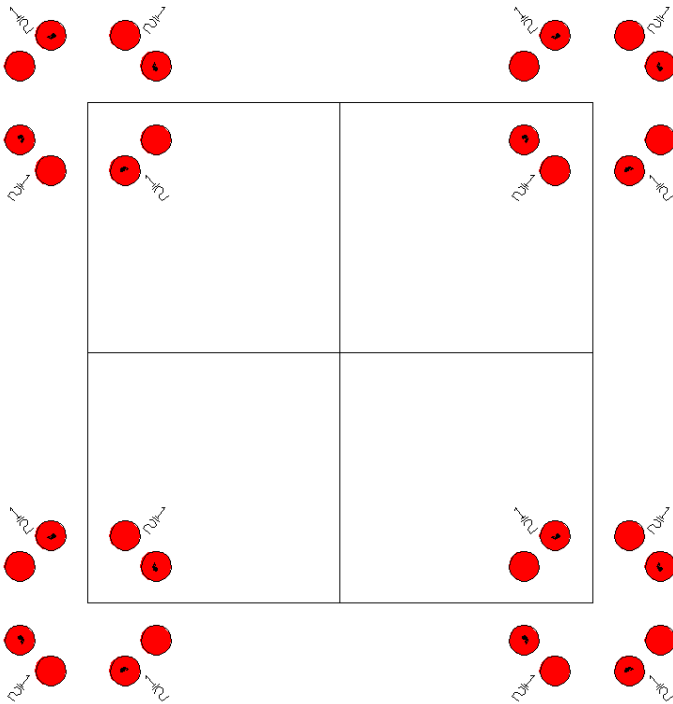


$P4_2mc1'$   
105.2.872

$4mm1'$   
 $P4_2mc1'$

Tetragonal

$1'$



Origin on  $2mm1'$  on  $4_2mc1'$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $1 +$  set

- |  |  |   |   |
|--|--|---|---|
| (1) $1$<br>( $1 0,0,0$ )               | (2) $2 \quad 0,0,z$<br>( $2_z 0,0,0$ ) | (3) $4^+ (0,0,1/2) \quad 0,0,z$<br>( $4_z^+ 0,0,1/2$ )      | (4) $4^- (0,0,1/2) \quad 0,0,z$<br>( $4_z^- 0,0,1/2$ )      |
| (5) $m \quad x,0,z$<br>( $m_y 0,0,0$ ) | (6) $m \quad 0,y,z$<br>( $m_x 0,0,0$ ) | (7) $c (0,0,1/2) \quad x,\bar{x},z$<br>( $m_{xy} 0,0,1/2$ ) | (8) $c (0,0,1/2) \quad x,x,z$<br>( $m_{\bar{xy}} 0,0,1/2$ ) |

For  $1' +$  set

- |  |  |   |   |
|--|--|---|---|
| (1) $1'$<br>( $1 0,0,0$ )'               | (2) $2' \quad 0,0,z$<br>( $2_z 0,0,0$ )' | (3) $4^{+'} (0,0,1/2) \quad 0,0,z$<br>( $4_z^+ 0,0,1/2$ )'    | (4) $4^{-'} (0,0,1/2) \quad 0,0,z$<br>( $4_z^- 0,0,1/2$ )'    |
| (5) $m' \quad x,0,z$<br>( $m_y 0,0,0$ )' | (6) $m' \quad 0,y,z$<br>( $m_x 0,0,0$ )' | (7) $c' (0,0,1/2) \quad x,\bar{x},z$<br>( $m_{xy} 0,0,1/2$ )' | (8) $c' (0,0,1/2) \quad x,x,z$<br>( $m_{\bar{xy}} 0,0,1/2$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

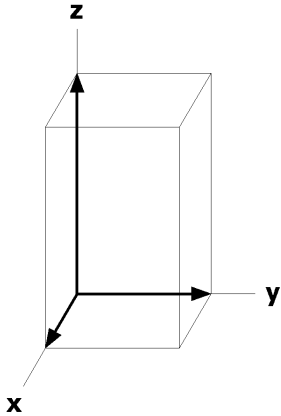
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates											
	1 +				1' +							
8 f 11'	(1)	x,y,z	[0,0,0]	(2)	$\bar{x},\bar{y},z$	[0,0,0]	(3)	$\bar{y},x,z+1/2$	[0,0,0]	(4)	$y,\bar{x},z+1/2$	[0,0,0]
	(5)	$x,\bar{y},z$	[0,0,0]	(6)	$\bar{x},y,z$	[0,0,0]	(7)	$\bar{y},\bar{x},z+1/2$	[0,0,0]	(8)	$y,x,z+1/2$	[0,0,0]
4 e .m.1'	x,1/2,z	[0,0,0]	$\bar{x},1/2,z$	[0,0,0]	1/2,x,z+1/2	[0,0,0]	1/2, $\bar{x},z+1/2$	[0,0,0]				
4 d .m.1'	x,0,z	[0,0,0]	$\bar{x},0,z$	[0,0,0]	0,x,z +1/2	[0,0,0]	0, $\bar{x},z+1/2$	[0,0,0]				
2 c 2mm.1'	0,1/2,z	[0,0,0]	1/2,0,z+1/2	[0,0,0]								
2 b 2mm.1'	1/2,1/2,z	[0,0,0]	1/2,1/2,z+1/2	[0,0,0]								
2 a 2mm.1'	0,0,z	[0,0,0]	0,0,z+1/2	[0,0,0]								

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

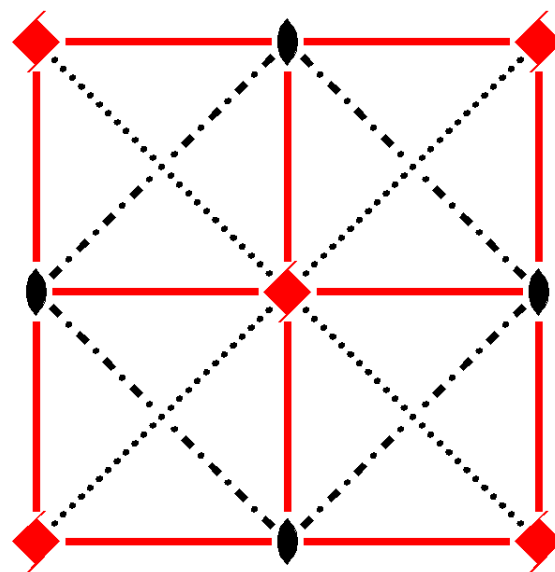
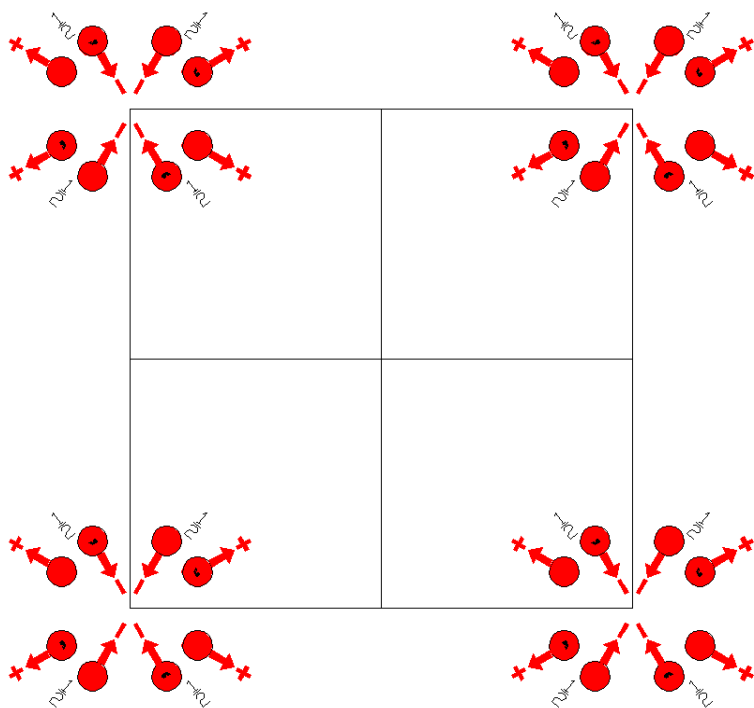
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P4_2'm'c$   
105.3.873

$4'm'm$   
 $P4_2'm'c$

Tetragonal



Origin on  $2m'm'$  on  $4_2'm'c$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

- |                                    |                                    |   |   |
|------------------------------------|------------------------------------|---|---|
| (1) 1<br>(1 0,0,0)                 | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)   | (3) $4^+ (0,0,1/2) 0,0,z$<br>( $4_z$  0,0,1/2)'       | (4) $4^- (0,0,1/2) 0,0,z$<br>( $4_z^{-1}$  0,0,1/2)'  |
| (5) $m' x,0,z$<br>( $m_y$  0,0,0)' | (6) $m' 0,y,z$<br>( $m_x$  0,0,0)' | (7) $c (0,0,1/2) x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2) | (8) $c (0,0,1/2) x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

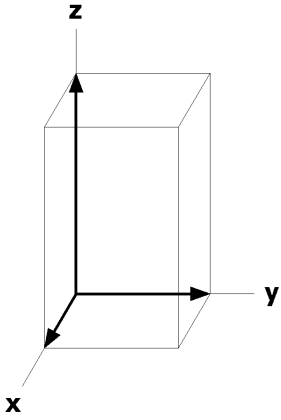
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	f	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{y}, x, z+1/2 [v, \bar{u}, \bar{w}]$	(4) $y, \bar{x}, z+1/2 [\bar{v}, u, \bar{w}]$
			(5) $x, \bar{y}, z [u, \bar{v}, w]$	(6) $\bar{x}, y, z [\bar{u}, v, w]$	(7) $\bar{y}, \bar{x}, z+1/2 [v, u, \bar{w}]$	(8) $y, x, z+1/2 [\bar{v}, \bar{u}, \bar{w}]$
4	e	.m'	$x, 1/2, z [u, 0, w]$	$\bar{x}, 1/2, z [\bar{u}, 0, w]$	$1/2, x, z+1/2 [0, \bar{u}, \bar{w}]$	$1/2, \bar{x}, z+1/2 [0, u, \bar{w}]$
4	d	.m'	$x, 0, z [u, 0, w]$	$\bar{x}, 0, z [\bar{u}, 0, w]$	$0, x, z+1/2 [0, \bar{u}, \bar{w}]$	$0, \bar{x}, z+1/2 [0, u, \bar{w}]$
2	c	2m'm'	$0, 1/2, z [0, 0, w]$	$1/2, 0, z+1/2 [0, 0, \bar{w}]$		
2	b	2m'm'	$1/2, 1/2, z [0, 0, w]$	$1/2, 1/2, z+1/2 [0, 0, \bar{w}]$		
2	a	2m'm'	$0, 0, z [0, 0, w]$	$0, 0, z+1/2 [0, 0, \bar{w}]$		

**Symmetry of Special Projections**

Along [0,0,1] p4'm'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

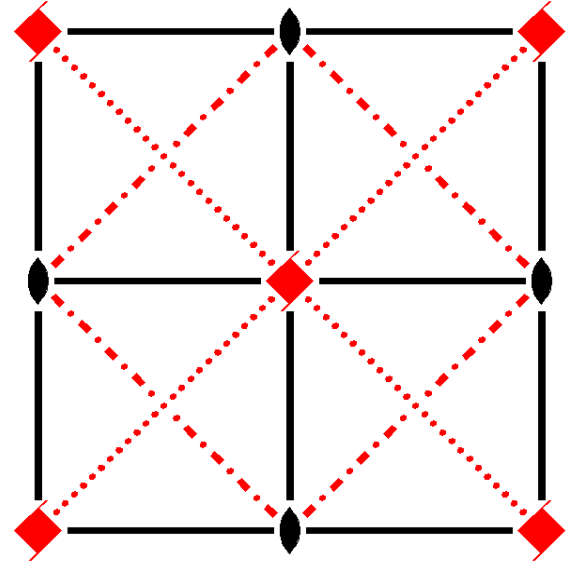
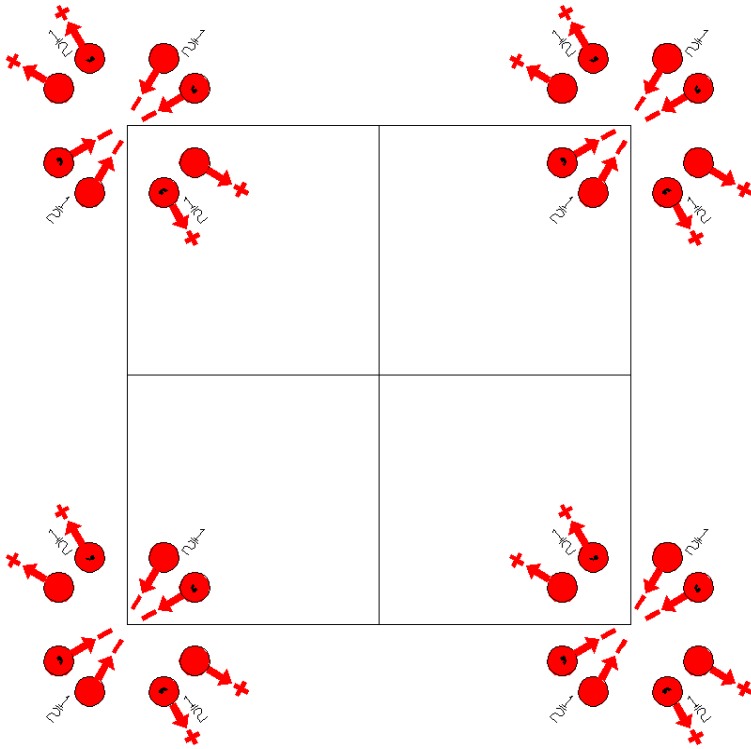
Along [1,1,0] p<sub>2b</sub>'1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P4_2' mc'$   
105.4.874

$4' mm'$   
 $P4_2' mc'$

Tetragonal



Origin on  $2mm$  on  $4_2' mc'$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

### Symmetry Operations

- |                                    |                                    |   |   |
|------------------------------------|------------------------------------|---|---|
| (1) 1<br>(1 0,0,0)                 | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)   | (3) $4^+ ' (0,0,1/2) \ 0,0,z$<br>( $4_z$  0,0,1/2)'       | (4) $4^- ' (0,0,1/2) \ 0,0,z$<br>( $4_z^{-1}$  0,0,1/2)'  |
| (5) $m \ x,0,z$<br>( $m_y$  0,0,0) | (6) $m \ 0,y,z$<br>( $m_x$  0,0,0) | (7) $c' (0,0,1/2) \ x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2)' | (8) $c' (0,0,1/2) \ x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

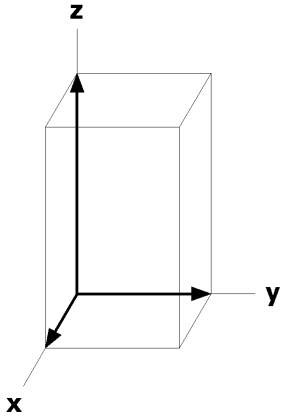
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	f	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ]
			(5) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(7) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $y,x,z+1/2$ [ $v,u,w$ ]
4	e	.m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v}$ ,0]	1/2,x,z+1/2 [v,0,0]	1/2, $\bar{x},z+1/2$ [ $\bar{v}$ ,0,0]
4	d	.m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]	0,x,z +1/2 [v,0,0]	0, $\bar{x},z+1/2$ [ $\bar{v}$ ,0,0]
2	c	2mm.	0,1/2,z [0,0,0]	1/2,0,z+1/2 [0,0,0]		
2	b	2mm.	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]		
2	a	2mm.	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

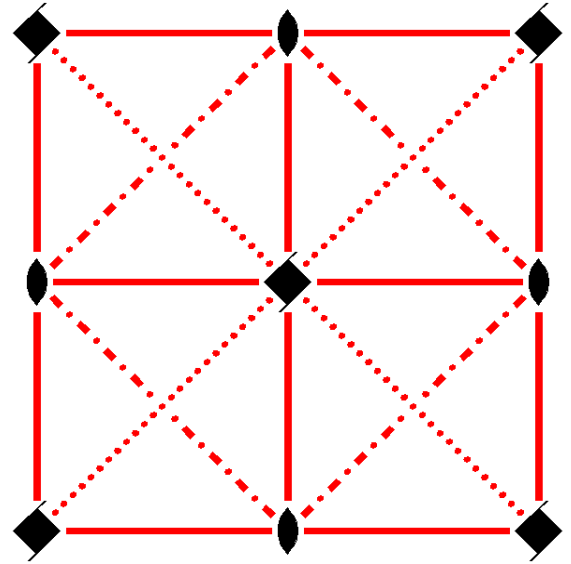
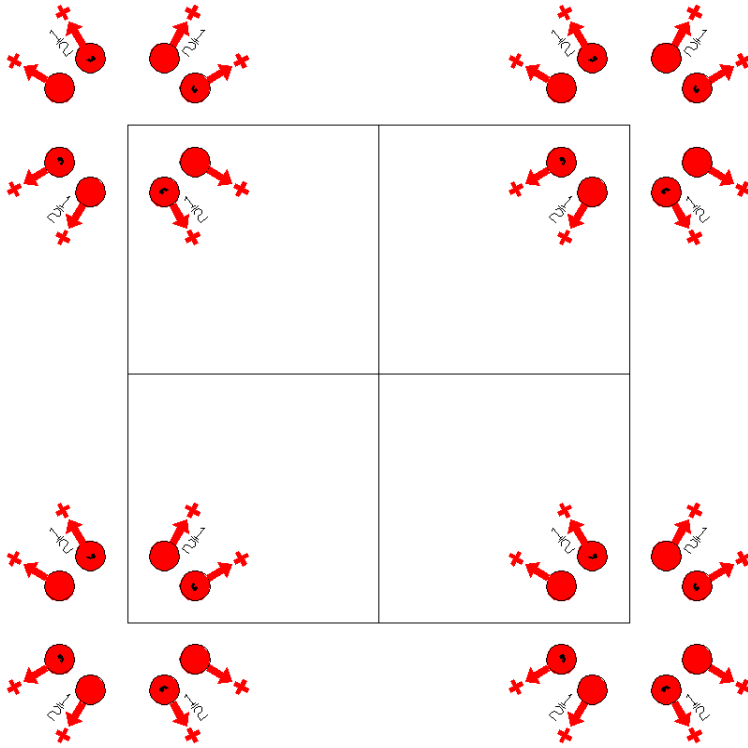
Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P4_2m'c'$   
105.5.875

$4m'm'$   
 $P4_2m'c'$

Tetragonal



Origin on  $2m'm'$  on  $4_2m'c'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

- |                                      |                                      |   |   |
|--------------------------------------|--------------------------------------|---|---|
| (1) 1<br>(1 0,0,0)                   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)     | (3) $4^+$ $(0,0,1/2)$ $0,0,z$<br>( $4_z$  0,0,1/2)          | (4) $4^-$ $(0,0,1/2)$ $0,0,z$<br>( $4_z^{-1}$  0,0,1/2)     |
| (5) $m'$ $x,0,z$<br>( $m_y$  0,0,0)' | (6) $m'$ $0,y,z$<br>( $m_x$  0,0,0)' | (7) $c'$ $(0,0,1/2)$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2)' | (8) $c'$ $(0,0,1/2)$ $x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	f	1	(1) x,y,z [u,v,w] (5) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ] (7) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ] (8) $y,x,z+1/2$ [ $v,u,w$ ]
4	e	.m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ]	1/2,x,z+1/2 [0,u,w]	1/2, $\bar{x},z+1/2$ [0, $\bar{u},w$ ]
4	d	.m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	0,x,z +1/2 [0,u,w]	0, $\bar{x},z+1/2$ [0, $\bar{u},w$ ]
2	c	2m'm'	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0,w]		
2	b	2m'm'	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]		
2	a	2m'm'	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]		

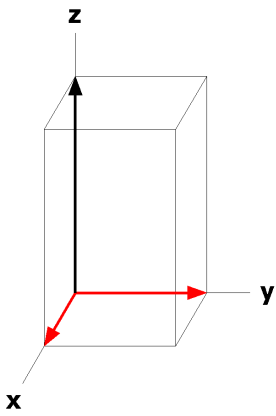
**Symmetry of Special Projections**

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

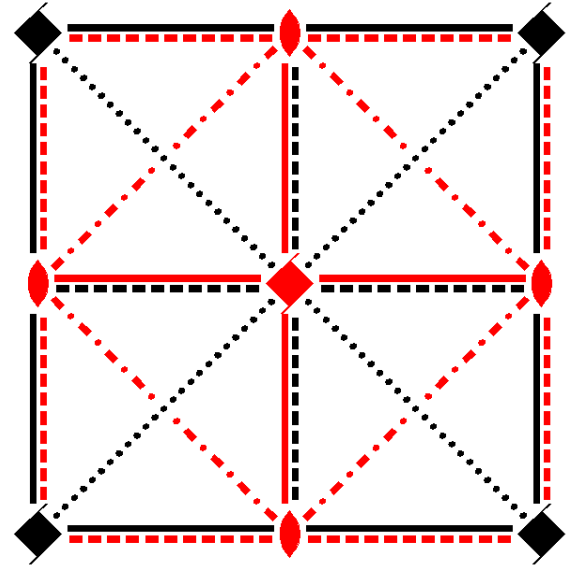
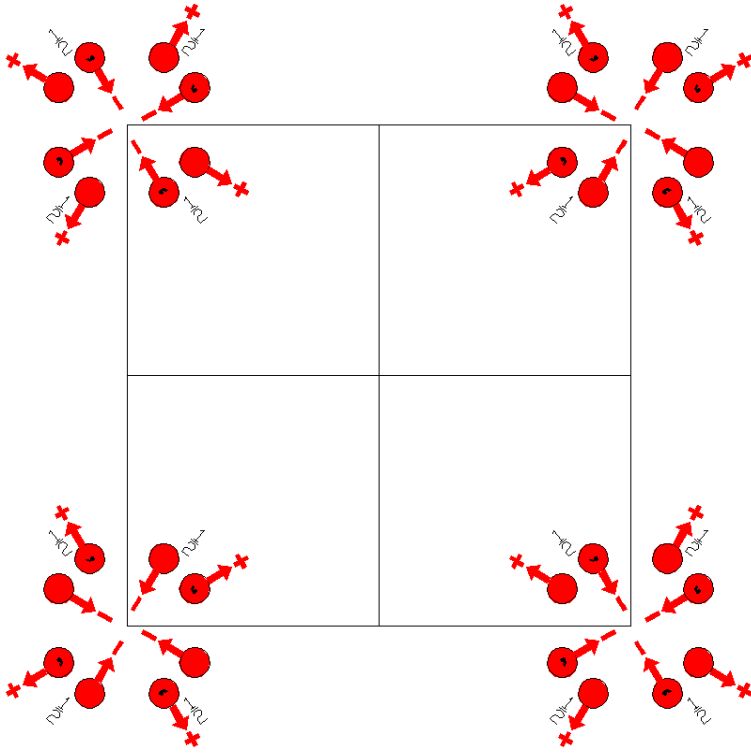




$P_P 4_2 mc$   
105.6.876

$4mm1'$   
 $P_P 4_2 mc$

Tetragonal



Origin on  $2mm$  on  $4_2 mc$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

For  $(0,0,0)$  + set

- |                                  |                                  |   |   |
|----------------------------------|----------------------------------|---|---|
| (1) 1<br>(1 0,0,0)               | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $4^+$ $(0,0,1/2) 0,0,z$<br>( $4_z$  0,0,1/2)      | (4) $4^-$ $(0,0,1/2) 0,0,z$<br>( $4_z^{-1}$  0,0,1/2) |
| (5) m $x,0,z$<br>( $m_y$  0,0,0) | (6) m $0,y,z$<br>( $m_x$  0,0,0) | (7) c $(0,0,1/2) x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2) | (8) c $(0,0,1/2) x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2) |

For  $(1,0,0)'$  + set

- |  |  |  |   |
|--|--|--|---|
| (1) $t'$ $(1,0,0)$<br>(1 1,0,0)'             | (2) $2'$ $1/2,0,z$<br>( $2_z$  1,0,0)' | (3) $4^{+ '}$ $(0,0,1/2) 1/2,1/2,z$<br>( $4_z$  1,0,1/2)'          | (4) $4^{- '}$ $(0,0,1/2) 1/2,-1/2,z$<br>( $4_z^{-1}$  1,0,1/2)'   |
| (5) $a'$ $(1,0,0) x,0,z$<br>( $m_y$  1,0,0)' | (6) $m'$ $1/2,y,z$<br>( $m_x$  1,0,0)' | (7) $n'$ $(1/2,-1/2,1/2) x+1/2,\bar{x},z$<br>( $m_{xy}$  1,0,1/2)' | (8) $n'$ $(1/2,1/2,1/2) x+1/2,x,z$<br>( $m_{\bar{xy}}$  1,0,1/2)' |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

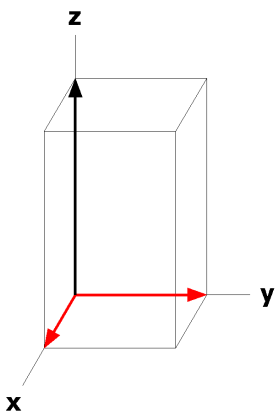
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1,0,0)' +		
16	f	1	(1) x,y,z [u,v,w] (5) x,y,z [ $\bar{u}$ ,v, $\bar{w}$ ]	(2) $\bar{x}$ , $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w]	(3) $\bar{y}$ ,x,z+1/2 [ $\bar{v}$ ,u,w]	(4) y, $\bar{x}$ ,z+1/2 [v, $\bar{u}$ ,w]
				(6) $\bar{x}$ ,y,z [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(7) $\bar{y}$ , $\bar{x}$ ,z+1/2 [v,u, $\bar{w}$ ]	(8) y,x,z+1/2 [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]
8	e	.m'	x,1/2,z [u,0,w]	$\bar{x}$ ,1/2,z [u,0, $\bar{w}$ ]	1/2,x,z+1/2 [0, $\bar{u}$ , $\bar{w}$ ]	1/2, $\bar{x}$ ,z+1/2 [0, $\bar{u}$ ,w]
8	d	.m	x,0,z [0,v,0]	$\bar{x}$ ,0,z [0, $\bar{v}$ ,0]	0,x,z+1/2 [ $\bar{v}$ ,0,0]	0, $\bar{x}$ ,z+1/2 [v,0,0]
4	c	2'mm'	0,1/2,z [u,0,0]	1/2,0,z+1/2 [0, $\bar{u}$ ,0]		
4	b	2m'm'	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]		
4	a	2mm	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub>4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p<sub>c</sub>1m1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x-1/4,x+1/4,0



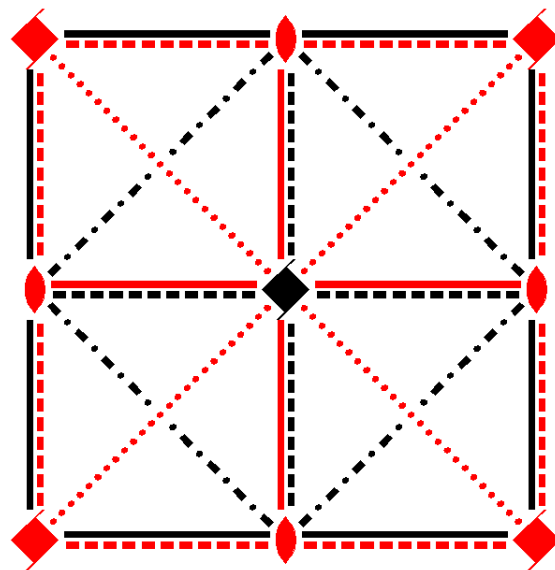
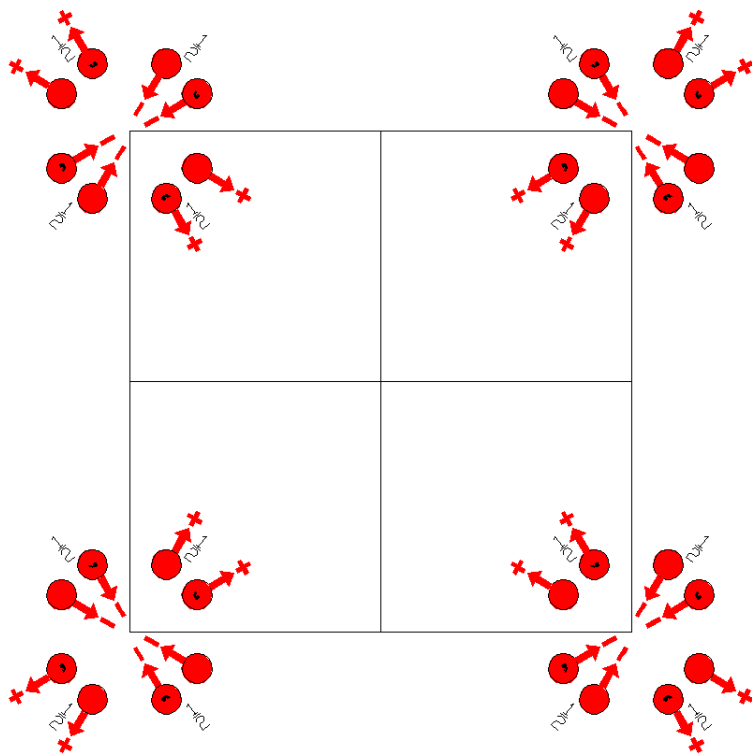
$P_P 4_2' mc'$

105.7.877

$4mm1'$

$P_P 4_2' mc'$

Tetragonal



Origin on  $2mm$  on  $4_2' mc'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                       | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> $(0,0,1/2)$ $0,0,z$<br>(4 <sub>z</sub>  0,0,1/2)' | (4) 4 <sup>-</sup> $(0,0,1/2)$ $0,0,z$<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) m $x,0,z$<br>(m <sub>y</sub>  0,0,0) | (6) m $0,y,z$<br>(m <sub>x</sub>  0,0,0) | (7) c' $(0,0,1/2)$ $x,\bar{x},z$<br>(m <sub>xy</sub>  0,0,1/2)'      | (8) c' $(0,0,1/2)$ $x,x,z$<br>(m <sub>xy</sub>  0,0,1/2)'                          |

For  $(1,0,0)$ ' + set

- |  |  |   |  |
|--|--|---|--|
| (1) t' $(1,0,0)$<br>(1 1,0,0)'                       | (2) 2' $1/2,0,z$<br>(2 <sub>z</sub>  1,0,0)' | (3) 4 <sup>+</sup> $(0,0,1/2)$ $1/2,1/2,z$<br>(4 <sub>z</sub>  1,0,1/2) | (4) 4 <sup>-</sup> $(0,0,1/2)$ $1/2,-1/2,z$<br>(4 <sub>z</sub> <sup>-1</sup>  1,0,1/2) |
| (5) a' $(1,0,0)$ $x,0,z$<br>(m <sub>y</sub>  1,0,0)' | (6) m' $1/2,y,z$<br>(m <sub>x</sub>  1,0,0)' | (7) n $(1/2,-1/2,1/2)$ $x+1/2,\bar{x},z$<br>(m <sub>xy</sub>  1,0,1/2)  | (8) n $(1/2,1/2,1/2)$ $x+1/2,x,z$<br>(m <sub>xy</sub>  1,0,1/2)                        |

**Generators selected** (1);  $t'(1,0,0)$ ;  $t'(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3); (5).

**Positions**

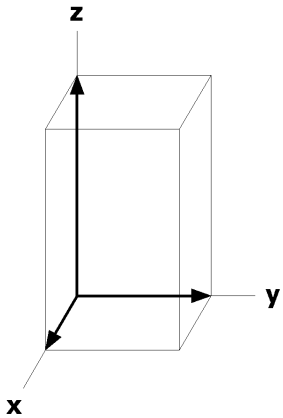
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1,0,0)' +		
16	f	1	(1) $x, y, z [u, v, w]$ (5) $x, \bar{y}, z [\bar{u}, v, \bar{w}]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$ (6) $\bar{x}, y, z [u, \bar{v}, \bar{w}]$	(3) $\bar{y}, x, z+1/2 [v, \bar{u}, \bar{w}]$ (7) $\bar{y}, \bar{x}, z+1/2 [\bar{v}, \bar{u}, w]$	(4) $y, \bar{x}, z+1/2 [\bar{v}, u, \bar{w}]$ (8) $y, x, z+1/2 [v, u, w]$
8	e	.m'	$x, 1/2, z [u, 0, w]$	$\bar{x}, 1/2, z [u, 0, \bar{w}]$	$1/2, x, z+1/2 [0, u, w]$	$1/2, \bar{x}, z+1/2 [0, u, \bar{w}]$
8	d	.m	$x, 0, z [0, v, 0]$	$\bar{x}, 0, z [0, \bar{v}, 0]$	$0, x, z+1/2 [v, 0, 0]$	$0, \bar{x}, z+1/2 [\bar{v}, 0, 0]$
4	c	2'mm'	$0, 1/2, z [u, 0, 0]$	$1/2, 0, z+1/2 [0, u, 0]$		
4	b	2m'm'	$1/2, 1/2, z [0, 0, w]$	$1/2, 1/2, z+1/2 [0, 0, w]$		
4	a	2mm	$0, 0, z [0, 0, 0]$	$0, 0, z+1/2 [0, 0, 0]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_p 4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

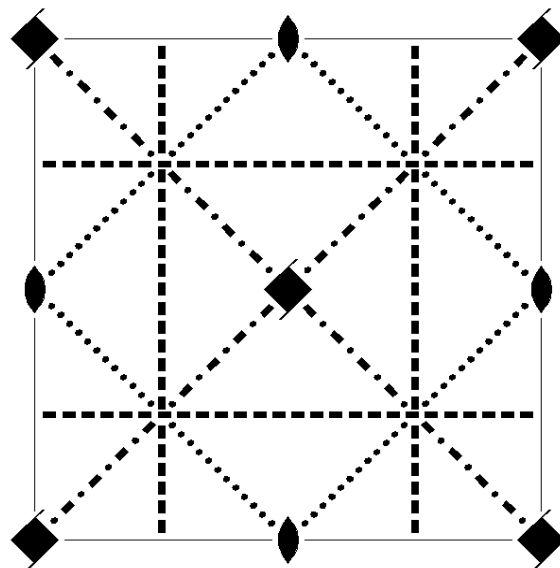
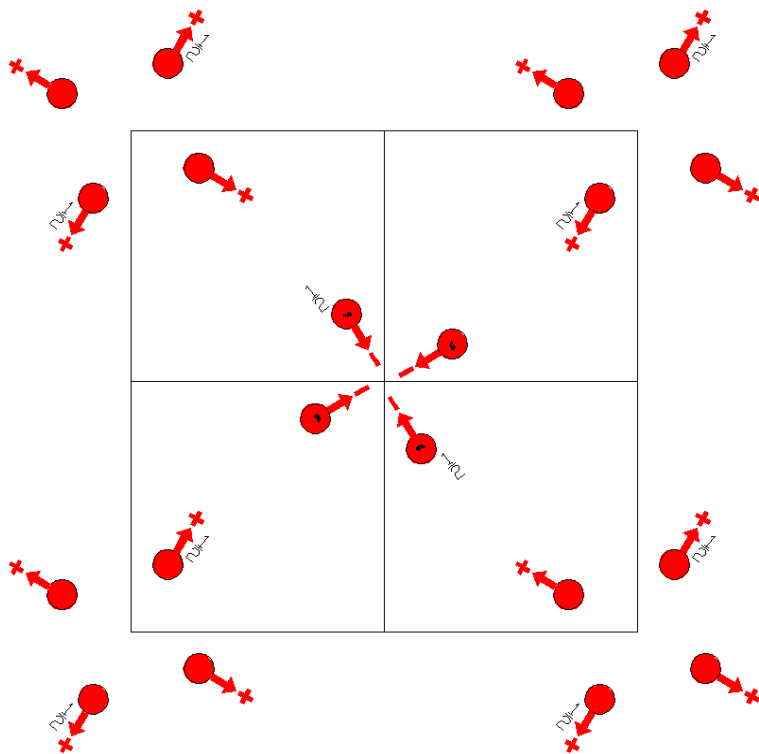
Along  $[1,1,0]$   $p_{2a} 1m1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x-1/4, x+1/4, 0$



P4<sub>2</sub>bc  
106.1.878

4mm  
P4<sub>2</sub>bc

Tetragonal



Origin on 2 on 4<sub>2</sub> 1n

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (5) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (6) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (7) c (0,0,1/2) x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)    | (8) n (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)                   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

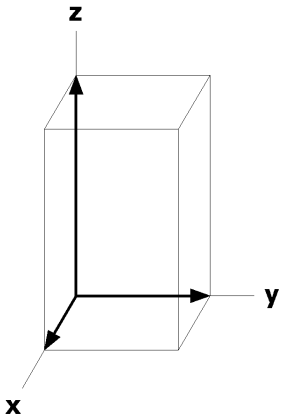
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	c	1	(1) x,y,z [u,v,w]		(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	
			(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]		(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]	
			(5) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]		(6) $\bar{x}+1/2,y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]	
			(7) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $v,u,\bar{w}$ ]		(8) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	
4	b	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
4	a	2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4gm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [1,1,0] p<sub>2b</sub>1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P4_2bc1'$

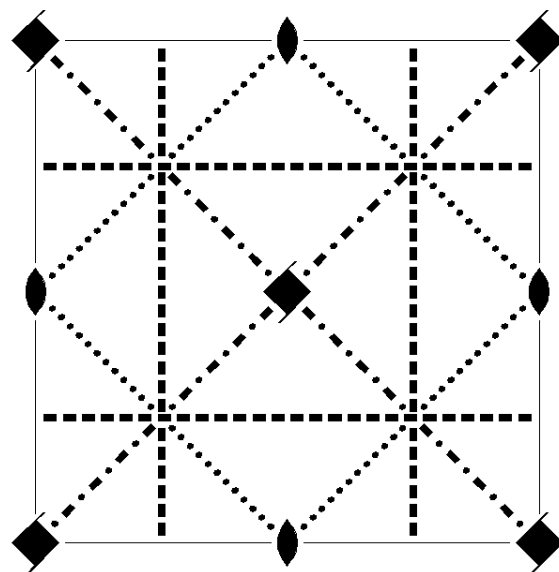
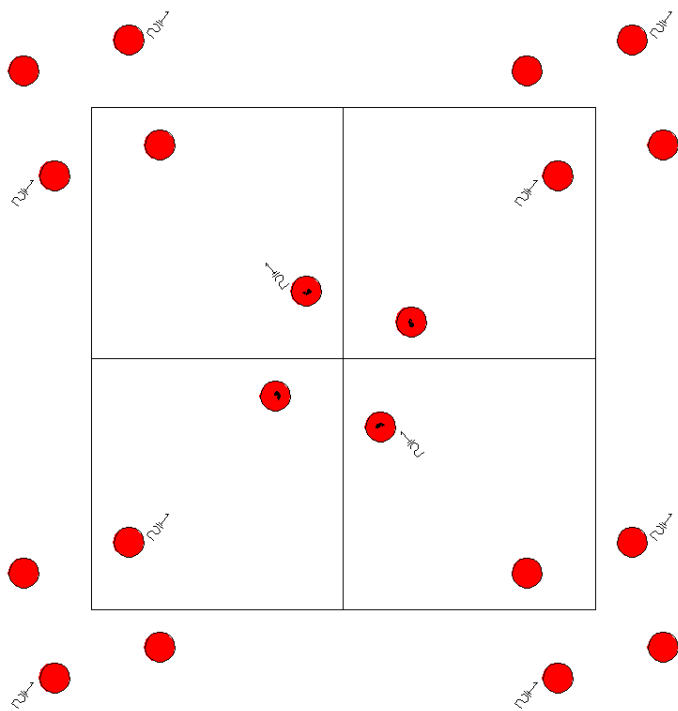
106.2.879

$4mm1'$

$P4_2bc1'$

Tetragonal

$1'$



Origin on  $21'$  on  $4_21n1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For  $1 + \text{set}$

- |  |  |   |   |
|--|--|---|---|
| (1) $1$<br>( $1 0,0,0$ )                           | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                 | (3) $4^+$ $(0,0,1/2) 0,0,z$<br>( $4_z 0,0,1/2$ )                | (4) $4^-$ $(0,0,1/2) 0,0,z$<br>( $4_z^{-1} 0,0,1/2$ )           |
| (5) $a$ $(1/2,0,0) x,1/4,z$<br>( $m_y 1/2,1/2,0$ ) | (6) $b$ $(0,1/2,0) 1/4,y,z$<br>( $m_x 1/2,1/2,0$ ) | (7) $c$ $(0,0,1/2) x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,1/2$ ) | (8) $n$ $(1/2,1/2,1/2) x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,1/2$ ) |

For  $1' + \text{set}$

- |  |  |   |   |
|--|--|---|---|
| (1) $1'$<br>( $1 0,0,0$ )'                           | (2) $2'$ $0,0,z$<br>( $2_z 0,0,0$ )'                 | (3) $4^{+'}$ $(0,0,1/2) 0,0,z$<br>( $4_z 0,0,1/2$ )'              | (4) $4^{-'}$ $(0,0,1/2) 0,0,z$<br>( $4_z^{-1} 0,0,1/2$ )'         |
| (5) $a'$ $(1/2,0,0) x,1/4,z$<br>( $m_y 1/2,1/2,0$ )' | (6) $b'$ $(0,1/2,0) 1/4,y,z$<br>( $m_x 1/2,1/2,0$ )' | (7) $c'$ $(0,0,1/2) x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,1/2$ )' | (8) $n'$ $(1/2,1/2,1/2) x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,1/2$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates					
			1 +	1' +		
8 c 11'	(1)	x,y,z [0,0,0]		(2)	$\bar{x}, \bar{y}, z$ [0,0,0]	
	(3)	$\bar{y}, x, z+1/2$ [0,0,0]		(4)	$y, \bar{x}, z+1/2$ [0,0,0]	
	(5)	$x+1/2, \bar{y}+1/2, z$ [0,0,0]		(6)	$\bar{x}+1/2, y+1/2, z$ [0,0,0]	
	(7)	$\bar{y}+1/2, \bar{x}+1/2, z+1/2$ [0,0,0]		(8)	$y+1/2, x+1/2, z+1/2$ [0,0,0]	
4 b 2..1'		0,1/2,z [0,0,0]	1/2,0,z+1/2 [0,0,0]	1/2,0,z [0,0,0]		0,1/2,z+1/2 [0,0,0]
4 a 2..1'		0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	

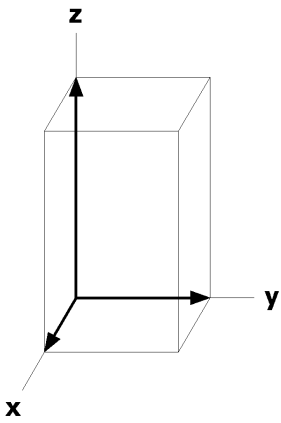
**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

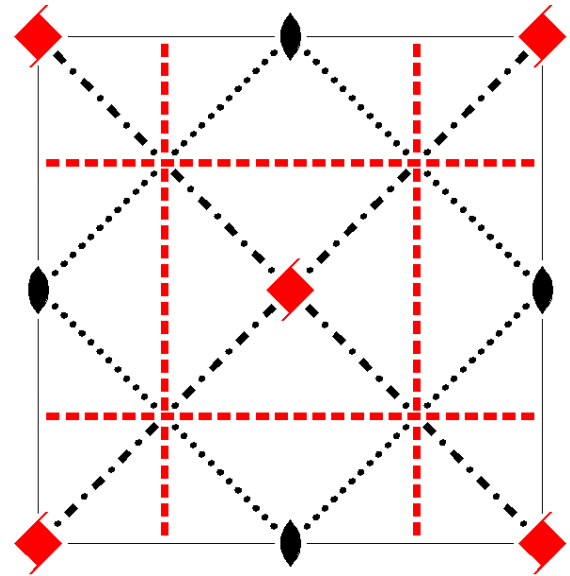
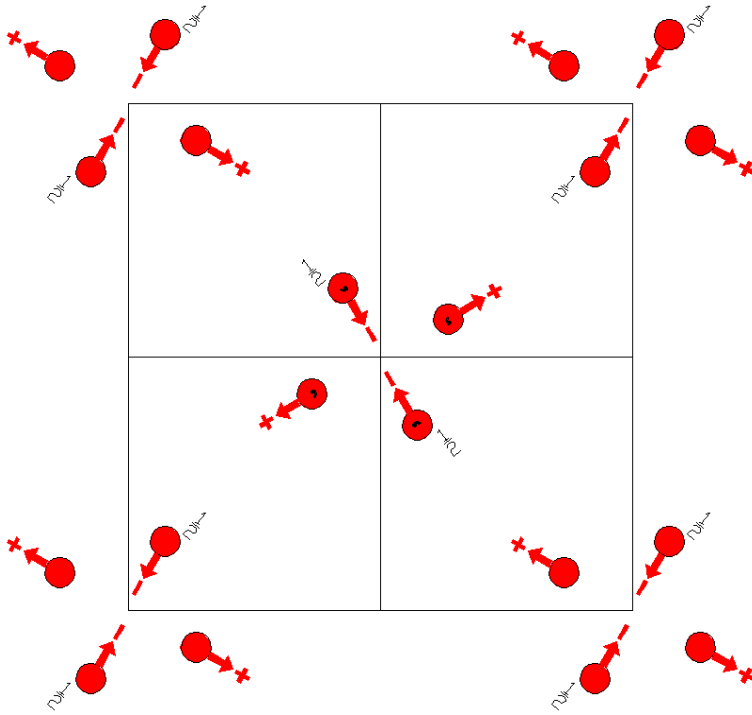




$P4_2'b'c$   
106.3.880

$4'm'm$   
 $P4_2'b'c$

Tetragonal



Origin on 2 on  $4_2'$  1n

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $4^+$   $(0,0,1/2)$   $0,0,z$   
( $4_z$ | $0,0,1/2$ )'

(4)  $4^-$   $(0,0,1/2)$   $0,0,z$   
( $4_z^{-1}$ | $0,0,1/2$ )'

(5)  $a'$   $(1/2,0,0)$   $x,1/4,z$   
( $m_y$ | $1/2,1/2,0$ )'

(6)  $b'$   $(0,1/2,0)$   $1/4,y,z$   
( $m_x$ | $1/2,1/2,0$ )'

(7)  $c$   $(0,0,1/2)$   $x+1/2,\bar{x},z$   
( $m_{xy}$ | $1/2,1/2,1/2$ )'

(8)  $n$   $(1/2,1/2,1/2)$   $x,x,z$   
( $m_{\bar{xy}}$ | $1/2,1/2,1/2$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

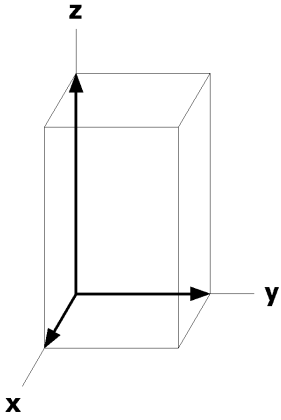
8	c	1	(1) x,y,z [u,v,w]		(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	
			(3) $\bar{y},x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]		(4) $y,\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ]	
			(5) $x+1/2,\bar{y}+1/2,z$ [ $u,\bar{v},w$ ]		(6) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]	
			(7) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $v,u,\bar{w}$ ]		(8) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	
4	b	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	1/2,0,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]
4	a	2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4'g'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

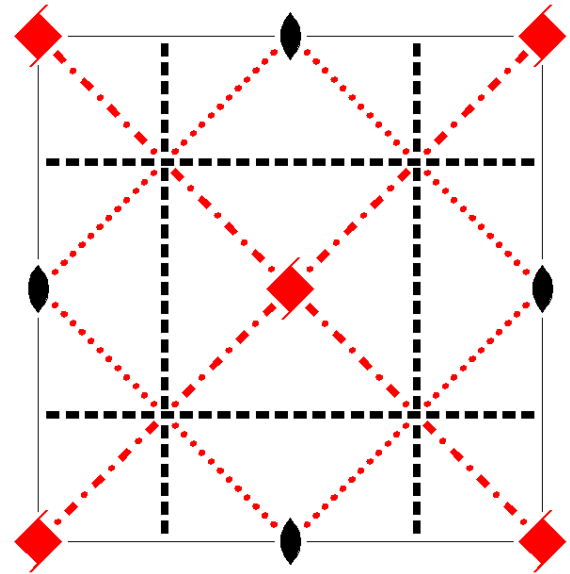
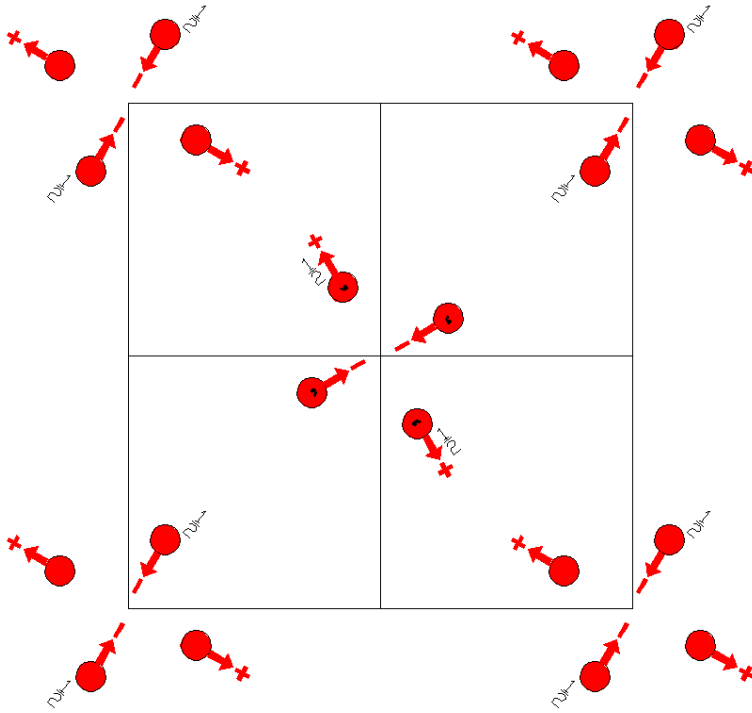
Along [1,1,0] p<sub>2b</sub>-1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P4_2'bc'$   
106.4.881

$4'mm'$   
 $P4_2'bc'$

Tetragonal



Origin on 2 on  $4_2'1n'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                               | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                 | (3) $4^+$ $(0,0,1/2) 0,0,z$<br>( $4_z$  0,0,1/2)'                 | (4) $4^-$ $(0,0,1/2) 0,0,z$<br>( $4_z^{-1}$  0,0,1/2)'            |
| (5) a $(1/2,0,0) x,1/4,z$<br>( $m_y$  1/2,1/2,0) | (6) b $(0,1/2,0) 1/4,y,z$<br>( $m_x$  1/2,1/2,0) | (7) $c'$ $(0,0,1/2) x+1/2,\bar{x},z$<br>( $m_{xy}$  1/2,1/2,1/2)' | (8) $n'$ $(1/2,1/2,1/2) x,x,z$<br>( $m_{\bar{xy}}$  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

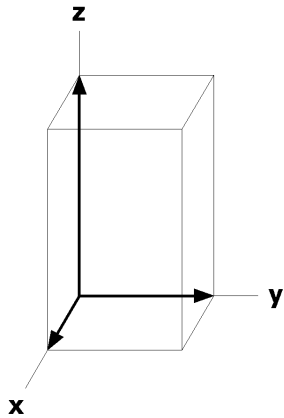
8	c	1	(1) x,y,z [u,v,w]		(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	
			(3) $\bar{y}, x, z+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		(4) $y, \bar{x}, z+1/2$ [ $\bar{v}, u, \bar{w}$ ]	
			(5) $x+1/2, \bar{y}+1/2, z$ [ $\bar{u}, v, \bar{w}$ ]		(6) $\bar{x}+1/2, y+1/2, z$ [ $u, \bar{v}, \bar{w}$ ]	
			(7) $\bar{y}+1/2, \bar{x}+1/2, z+1/2$ [ $\bar{v}, \bar{u}, w$ ]		(8) $y+1/2, x+1/2, z+1/2$ [ $v, u, w$ ]	
4	b	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0,w]
4	a	2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2,z [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0,w]

**Symmetry of Special Projections**

Along [0,0,1] p4'gm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

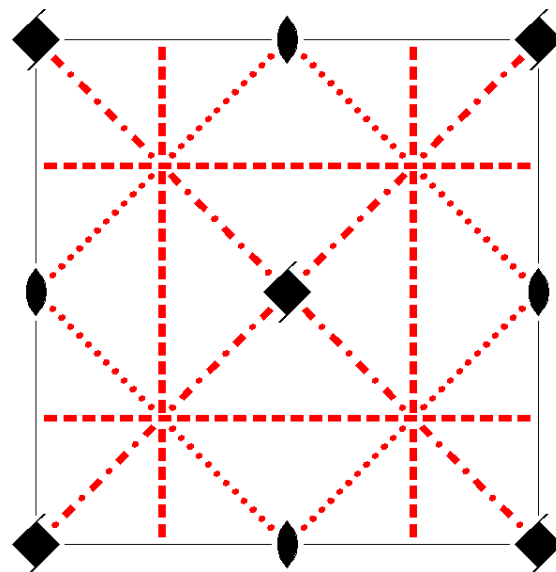
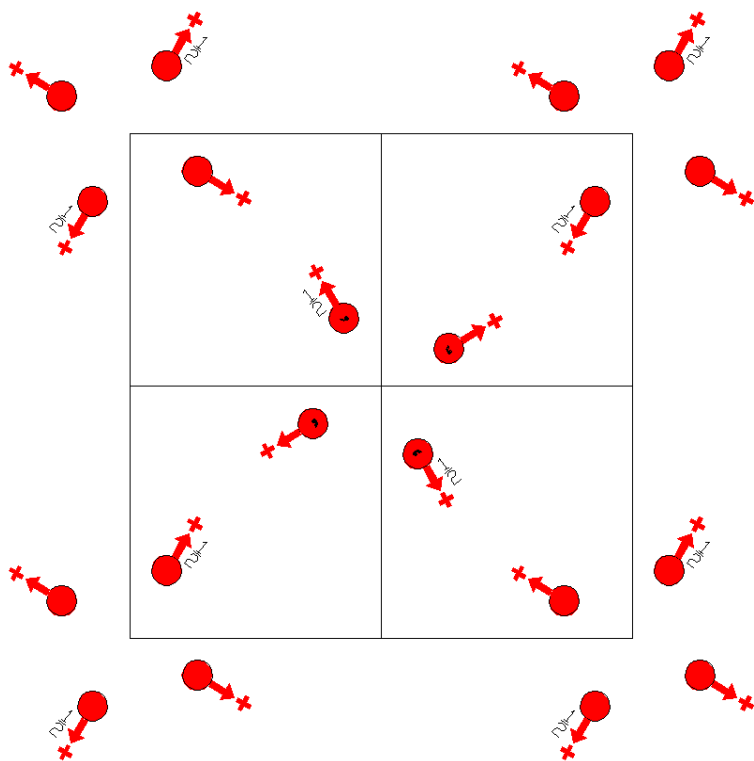
Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P4_2 b'c'$   
106.5.882

$4m'm'$   
 $P4_2 b'c'$

Tetragonal



Origin on 2 on  $4_2 1n'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                     | (3) $4^+$ $(0,0,1/2) 0,0,z$<br>( $4_z$  0,0,1/2)                  | (4) $4^-$ $(0,0,1/2) 0,0,z$<br>( $4_z^{-1}$  0,0,1/2)             |
| (5) $a'$ $(1/2,0,0) x,1/4,z$<br>( $m_y$  1/2,1/2,0)' | (6) $b'$ $(0,1/2,0) 1/4,y,z$<br>( $m_x$  1/2,1/2,0)' | (7) $c'$ $(0,0,1/2) x+1/2,\bar{x},z$<br>( $m_{xy}$  1/2,1/2,1/2)' | (8) $n'$ $(1/2,1/2,1/2) x,x,z$<br>( $m_{\bar{xy}}$  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

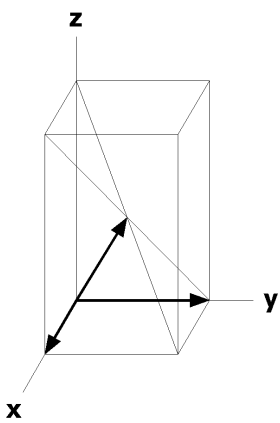
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
8	c	1	(1) x,y,z [u,v,w]		(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	
			(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]		(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]	
			(5) $x+1/2,\bar{y}+1/2,z$ [ $u,\bar{v},w$ ]		(6) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]	
			(7) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]		(8) $y+1/2,x+1/2,z+1/2$ [ $v,u,w$ ]	
4	b	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0,w]	1/2,0,z [0,0,w]	0,1/2,z+1/2 [0,0,w]
4	a	2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]

**Symmetry of Special Projections**

Along [0,0,1] p4g'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

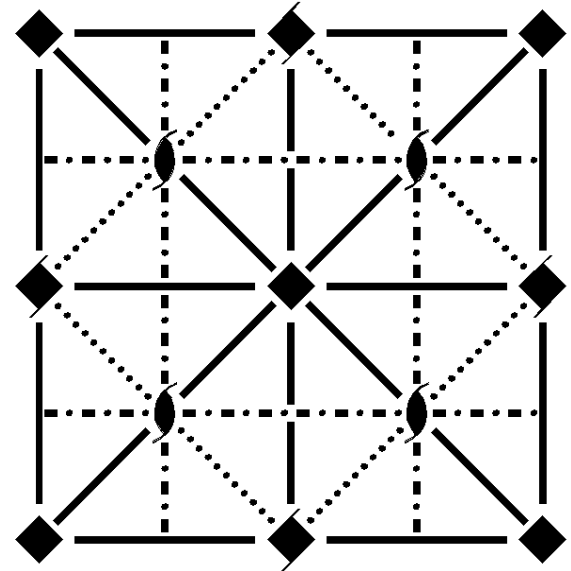
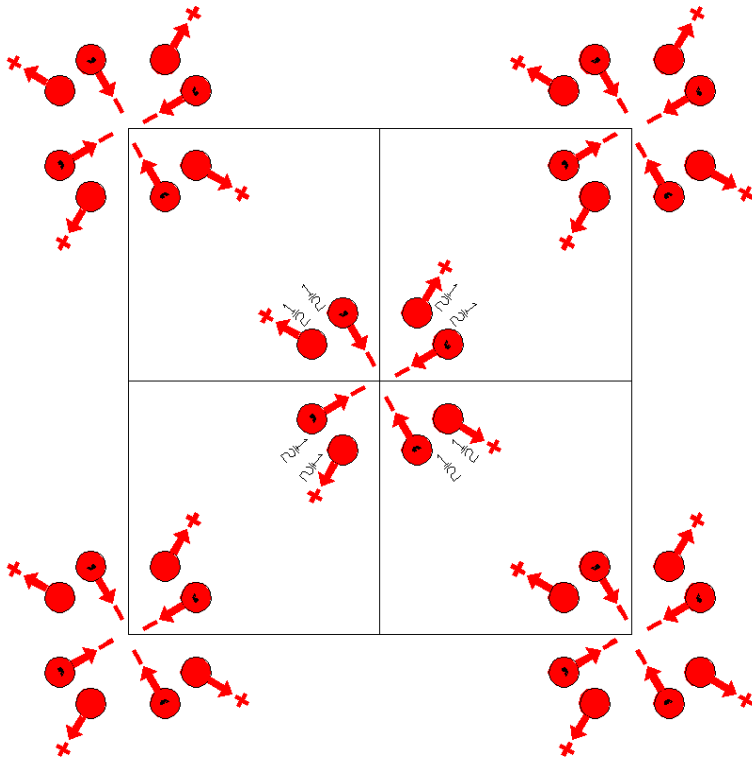
Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



I4mm  
107.1.883

4mm  
I4mm

Tetragonal



Origin on 4mm

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0) |
| (5) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (6) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (7) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                         | (8) m x,x,z<br>(m <sub>xȳ</sub>  0,0,0)                         |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                     | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub> <sup>+</sup>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-</sup>  1/2,1/2,1/2) |
| (5) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (6) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (7) c (0,0,1/2) x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)                       | (8) n (1/2,1/2,1/2) x,x,z<br>(m <sub>xȳ</sub>  1/2,1/2,1/2)                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(1/2,1/2,1/2) +			
16 e 1	(1)	x,y,z [u,v,w]	(2)	$\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3)	$\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4)	$y,\bar{x},z$ [ $v,\bar{u},w$ ]
	(5)	$x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(6)	$\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(7)	$\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(8)	$y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]
8 d .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]	0,x,z [ $\bar{v}$ ,0,0]	0, $\bar{x},z$ [v,0,0]				
8 c ..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]	$\bar{x},x,z$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},z$ [u,u,0]				
4 b 2mm.	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]						
2 a 4mm	0,0,z [0,0,0]							

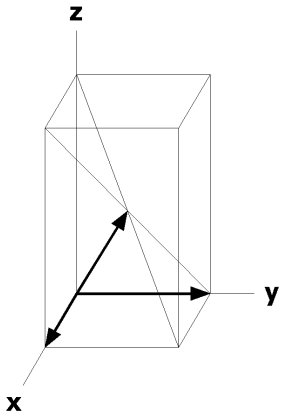
**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



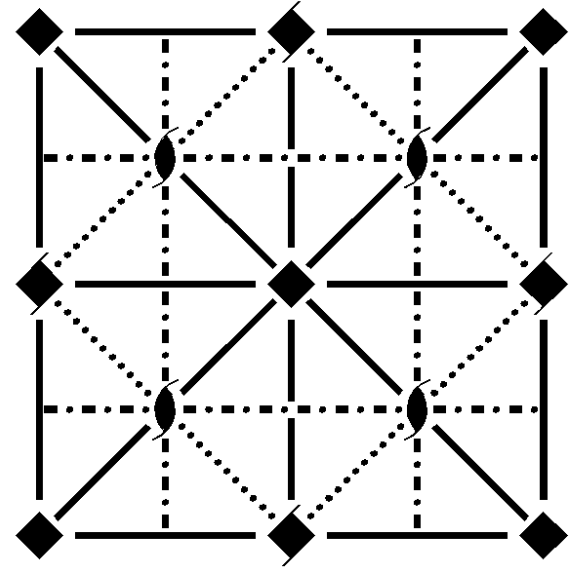
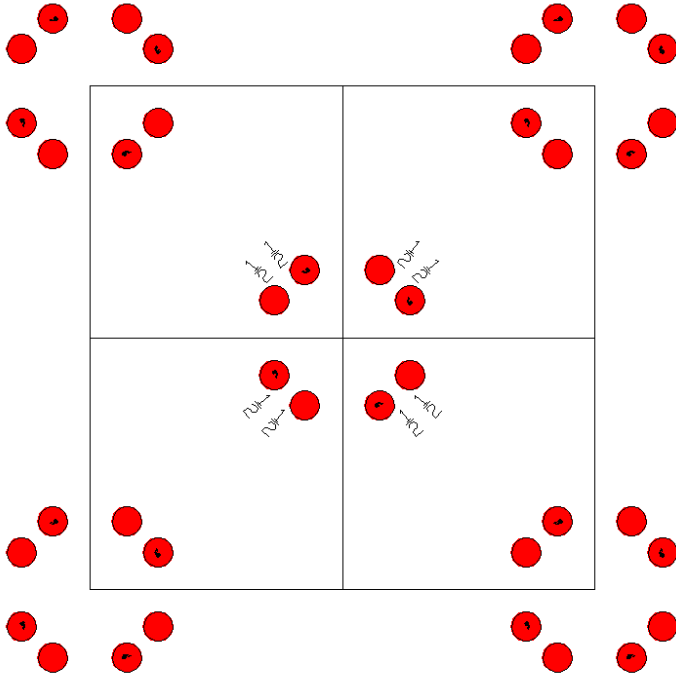


I4mm1'  
107.2.884

4mm1'  
I4mm1'

Tetragonal

1'



Origin on 4mm1'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0) |
| (5) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (6) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (7) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                         | (8) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                          |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                     | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub> <sup>+</sup>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-</sup>  1/2,1/2,1/2) |
| (5) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (6) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (7) c (0,0,1/2) x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)                       | (8) n (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)                        |

## For (0,0,0)' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)'	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(5) m' x,0,z (m <sub>y</sub>  0,0,0)'	(6) m' 0,y,z (m <sub>x</sub>  0,0,0)'	(7) m' x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)'	(8) m' x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,0)'

## For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (1 1/2,1/2,1/2)'	(2) 2' (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>  1/2,1/2,1/2)'	(3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)'	(4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'
(5) n' (1/2,0,1/2) x,1/4,z (m <sub>y</sub>  1/2,1/2,1/2)'	(6) n' (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1/2)'	(7) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,1/2)'	(8) n' (1/2,1/2,1/2) x,x,z (m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

(0,0,0) + (1/2,1/2,1/2) +  
(0,0,0)' + (1/2,1/2,1/2)'

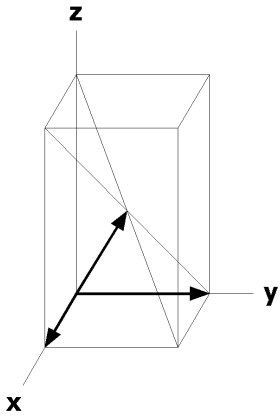
16	e	11'	(1) x,y,z [0,0,0] (5) x, $\bar{y}$ ,z [0,0,0]	(2) $\bar{x}$ , $\bar{y}$ ,z [0,0,0] (6) $\bar{x}$ ,y,z [0,0,0]	(3) $\bar{y}$ ,x,z [0,0,0] (7) $\bar{y}$ , $\bar{x}$ ,z [0,0,0]	(4) y, $\bar{x}$ ,z [0,0,0] (8) y,x,z [0,0,0]
8	d	.m.1'	x,0,z [0,0,0]	$\bar{x}$ ,0,z [0,0,0]	0,x,z [0,0,0]	0, $\bar{x}$ ,z [0,0,0]
8	c	..m1'	x,x,z [0,0,0]	$\bar{x}$ , $\bar{x}$ ,z [0,0,0]	$\bar{x}$ ,x,z [0,0,0]	x, $\bar{x}$ ,z [0,0,0]
4	b	2mm.1'	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]		
2	a	4mm1'	0,0,z [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,0,0

Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,x,0



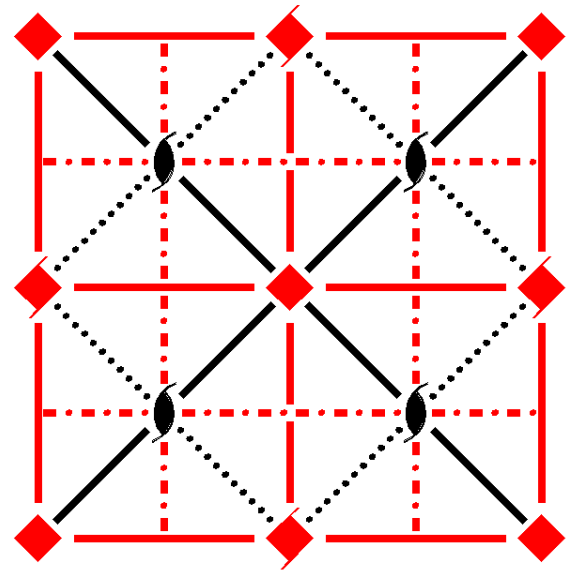
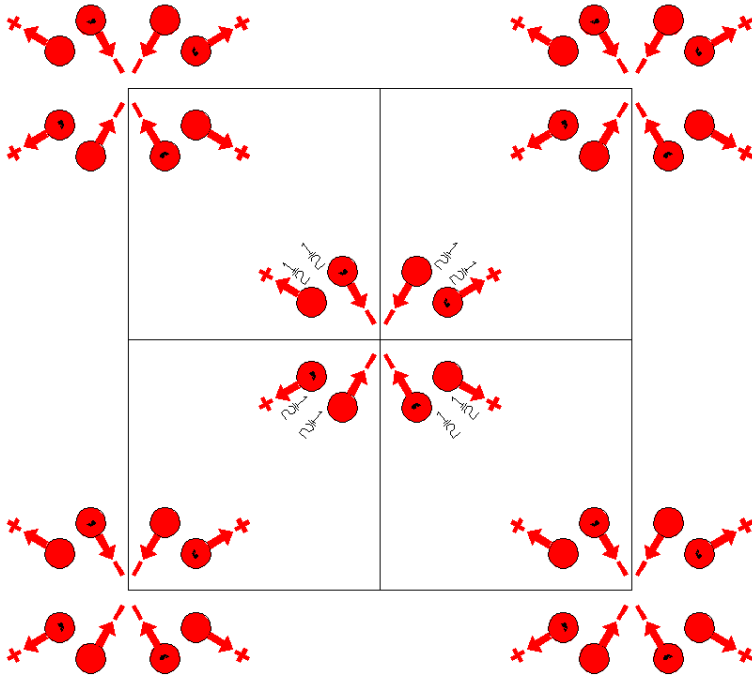
4m'm

107.3.885

4m'm

4m'm

Tetragonal



Origin on 4m'm

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (5) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (6) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (7) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)             | (8) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                            |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                       | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)   | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (6) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (7) c (0,0,1/2) x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)           | (8) n (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)                          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

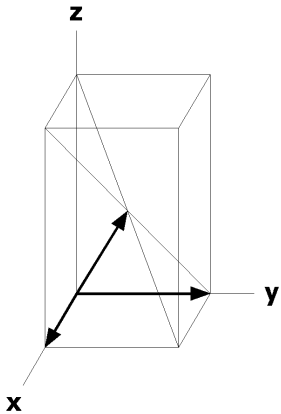
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(1/2,1/2,1/2) +			
16 e 1	(1)	x,y,z [u,v,w]	(2)	$\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3)	$\bar{y},x,z$ [ $v,\bar{u},\bar{w}$ ]	(4)	$y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
	(5)	$x,\bar{y},z$ [ $u,\bar{v},w$ ]	(6)	$\bar{x},y,z$ [ $\bar{u},v,w$ ]	(7)	$\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(8)	$y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]
8 d .m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	0,x,z [0, $\bar{u},\bar{w}$ ]	0, $\bar{x},z$ [0,u, $\bar{w}$ ]				
8 c ..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]	$\bar{x},x,z$ [u,u,0]	x, $\bar{x},z$ [ $\bar{u},\bar{u},0$ ]				
4 b 2m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]						
2 a 4'm'm	0,0,z [0,0,0]							

**Symmetry of Special Projections**

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



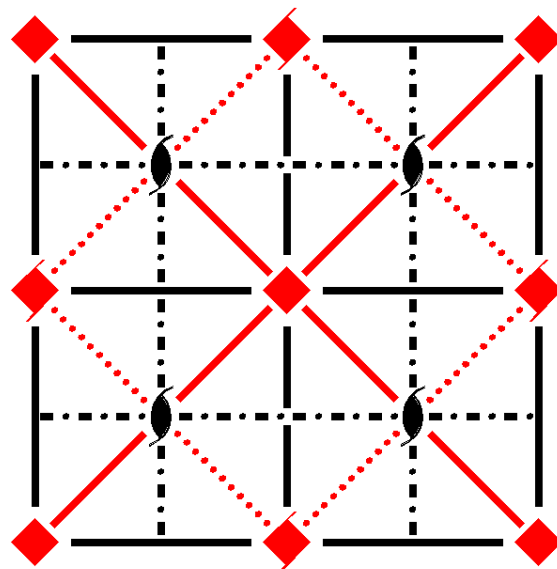
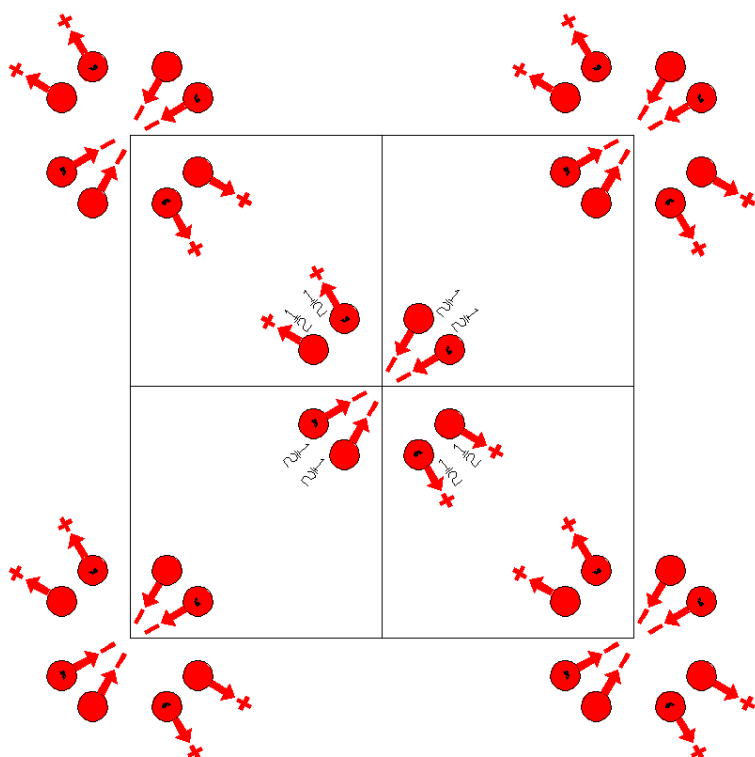
4'mm'

107.4.886

4'mm'

4'mm'

Tetragonal



Origin on 4'mm'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (5) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (6) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (7) m' x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'           | (8) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                          |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                     | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (6) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (7) c' (0,0,1/2) x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)'         | (8) n' (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)'                        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

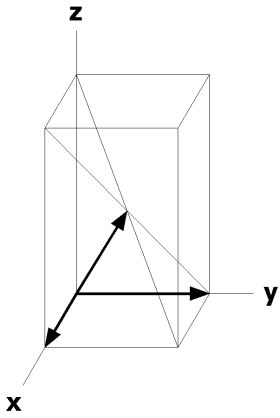
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(1/2,1/2,1/2) +			
16 e 1	(1)	x,y,z [u,v,w]	(2)	$\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3)	$\bar{y}, x, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(4)	$y, \bar{x}, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]
	(5)	$x, \bar{y}, z$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(6)	$\bar{x}, y, z$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(7)	$\bar{y}, \bar{x}, z$ [ $\bar{v}, \bar{u}, w$ ]	(8)	$y, x, z$ [ $\bar{v}, u, w$ ]
8 d .m.	x,0,z [0,v,0]	$\bar{x}, 0, z$ [ $0, \bar{v}, 0$ ]	0,x,z [v,0,0]	$0, \bar{x}, z$ [ $\bar{v}, 0, 0$ ]				
8 c ..m'	x,x,z [u,u,w]	$\bar{x}, \bar{x}, z$ [ $\bar{u}, \bar{u}, w$ ]	$\bar{x}, x, z$ [ $\bar{u}, u, \bar{w}$ ]	$x, \bar{x}, z$ [ $\bar{u}, \bar{u}, \bar{w}$ ]				
4 b 2mm.	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]						
2 a 4'mm'	0,0,z [0,0,0]							

**Symmetry of Special Projections**

Along [0,0,1] p4'm'm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



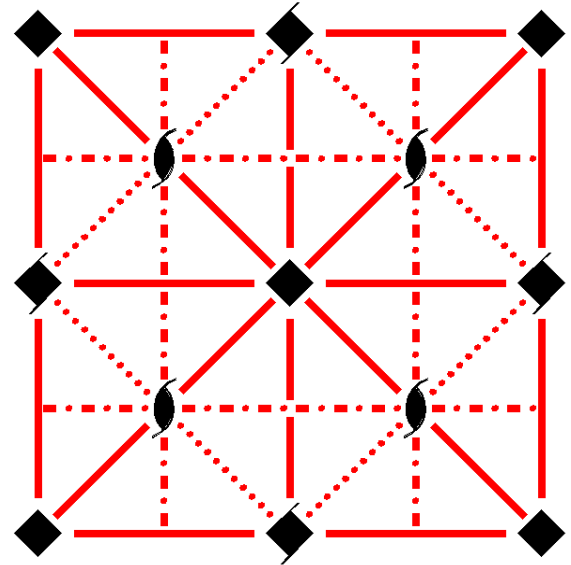
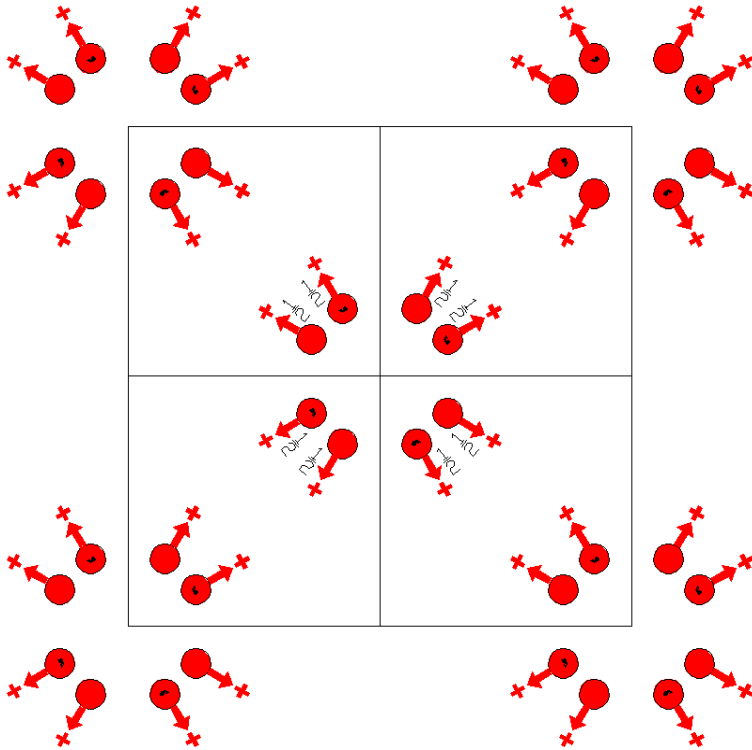
14m'm'

107.5.887

4m'm'

14m'm'

Tetragonal



Origin on 4m'm'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

### Symmetry Operations

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (6) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (7) m' x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'          | (8) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                         |

For (1/2,1/2,1/2) + set

- |  |  |   |   |
|--|--|---|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                       | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)   | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (6) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (7) c' (0,0,1/2) x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)'        | (8) n' (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)'                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(1/2,1/2,1/2) +			
16 e 1	(1)	x,y,z [u,v,w]	(2)	$\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3)	$\bar{y}, x, z$ [ $\bar{v}, u, w$ ]	(4)	$y, \bar{x}, z$ [ $v, \bar{u}, w$ ]
	(5)	$x, \bar{y}, z$ [ $u, \bar{v}, w$ ]	(6)	$\bar{x}, y, z$ [ $\bar{u}, v, w$ ]	(7)	$\bar{y}, \bar{x}, z$ [ $\bar{v}, \bar{u}, w$ ]	(8)	$y, x, z$ [ $v, u, w$ ]
8 d .m'	x,0,z [u,0,w]	$\bar{x}, 0, z$ [ $\bar{u}, 0, w$ ]	0,x,z [0,u,w]	$0, \bar{x}, z$ [ $0, \bar{u}, w$ ]				
8 c ..m'	x,x,z [u,u,w]	$\bar{x}, \bar{x}, z$ [ $\bar{u}, \bar{u}, w$ ]	$\bar{x}, x, z$ [ $\bar{u}, u, w$ ]	$x, \bar{x}, z$ [ $u, \bar{u}, w$ ]				
4 b 2m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]						
2 a 4m'm'	0,0,z [0,0,w]							

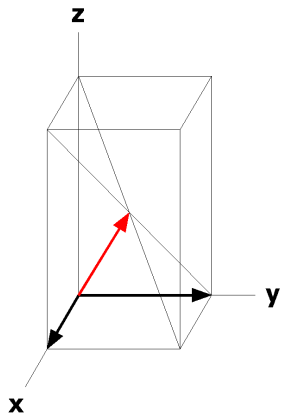
**Symmetry of Special Projections**

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0





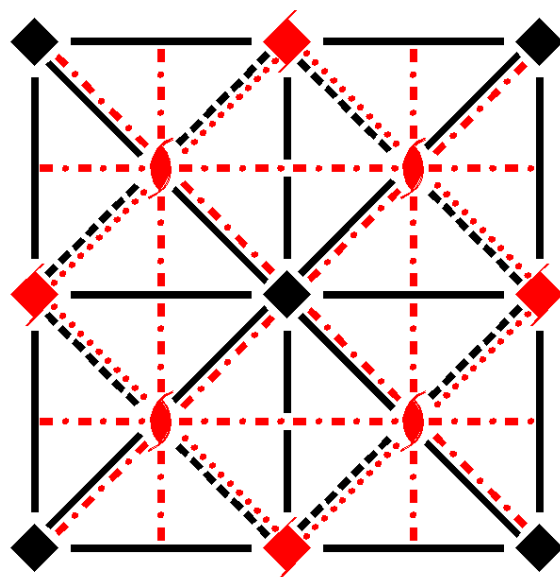
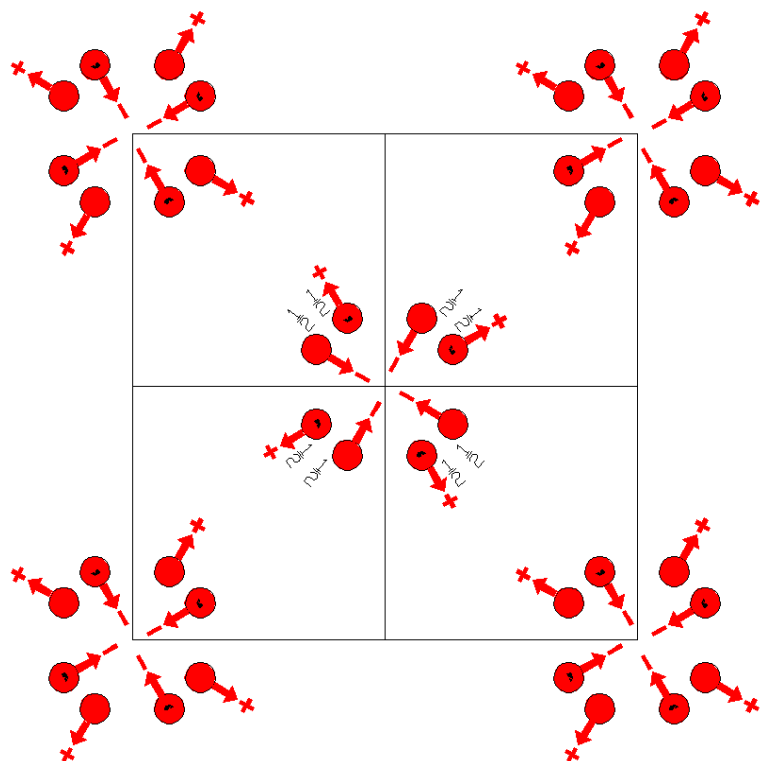
$I_p 4mm$

$4mm1'$

Tetragonal

107.6.888

$I_p 4mm$



Origin on  $4mm$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |                                  |                                  |   |   |
|----------------------------------|----------------------------------|---|---|
| (1) 1<br>(1 0,0,0)               | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $4^+$ $0,0,z$<br>( $4_z$  0,0,0)      | (4) $4^-$ $0,0,z$<br>( $4_z^{-1}$  0,0,0) |
| (5) m $x,0,z$<br>( $m_y$  0,0,0) | (6) m $0,y,z$<br>( $m_x$  0,0,0) | (7) m $x,\bar{x},z$<br>( $m_{xy}$  0,0,0) | (8) m $x,x,z$<br>( $m_{\bar{xy}}$  0,0,0) |

For  $(1/2,1/2,1/2)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t'$ $(1/2,1/2,1/2)$<br>(1  $1/2,1/2,1/2$ )'               | (2) $2'$ $(0,0,1/2) \ 1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1/2$ )' | (3) $4^+'$ $(0,0,1/2) \ 0,1/2,z$<br>( $4_z$   $1/2,1/2,1/2$ )'          | (4) $4^-'$ $(0,0,1/2) \ 1/2,0,z$<br>( $4_z^{-1}$   $1/2,1/2,1/2$ )'     |
| (5) $n'$ $(1/2,0,1/2) \ x,1/4,z$<br>( $m_y$   $1/2,1/2,1/2$ )' | (6) $n'$ $(0,1/2,1/2) \ 1/4,y,z$<br>( $m_x$   $1/2,1/2,1/2$ )' | (7) $c'$ $(0,0,1/2) \ x+1/2,\bar{x},z$<br>( $m_{xy}$   $1/2,1/2,1/2$ )' | (8) $n'$ $(1/2,1/2,1/2) \ x,x,z$<br>( $m_{\bar{xy}}$   $1/2,1/2,1/2$ )' |

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(1/2,1/2,1/2)$ ; (2); (3); (5).

**Positions**

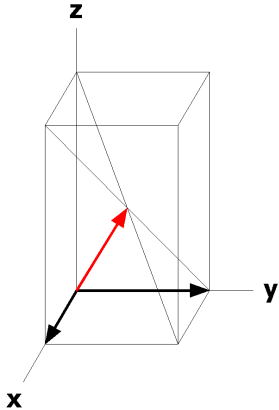
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates						
		(0,0,0) +	(1/2,1/2,1/2)' +				
16 e 1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $\bar{v},\bar{u},w$ ]			
	(5) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(7) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(8) $y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]			
8 d .m.	$x,0,z$ [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]	$0,x,z$ [ $\bar{v},0,0$ ]	$0,\bar{x},z$ [v,0,0]			
8 c ..m	$x,x,z$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]	$\bar{x},x,z$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},z$ [ $u,u,0$ ]			
4 b 2mm.	$0,1/2,z$ [0,0,0]	$1/2,0,z$ [0,0,0]					
2 a 4mm	$0,0,z$ [0,0,0]						

**Symmetry of Special Projections**

Along [0,0,1]  $p_4$ , 4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



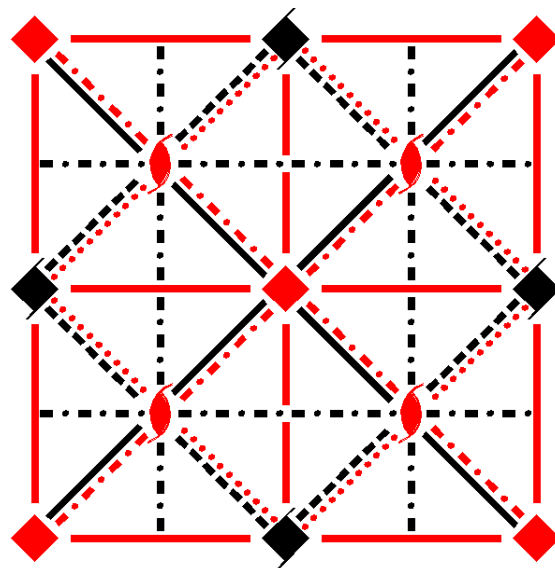
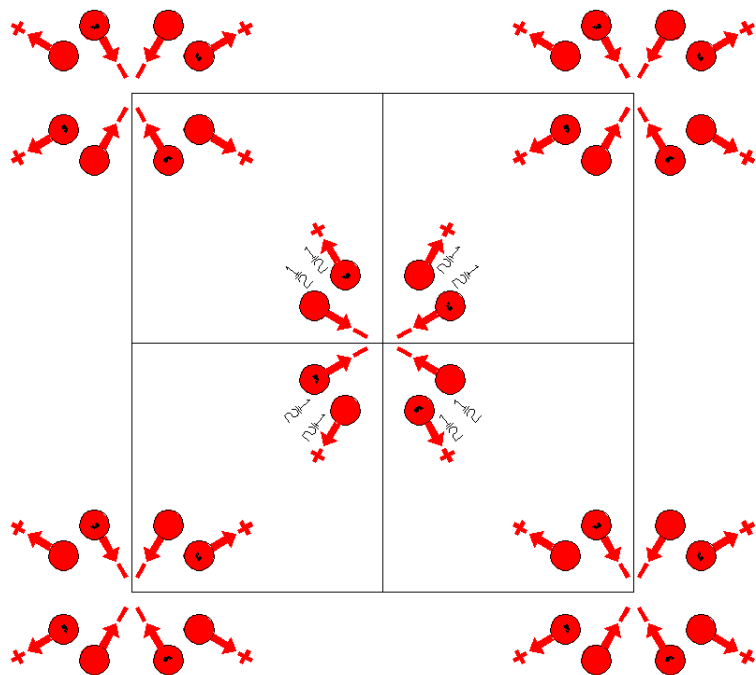
$I_p 4'm'm$

$4mm1'$

Tetragonal

107.7.889

$I_p 4'm'm$



Origin on  $4'm'm$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

Symmetry Operations

For  $(0,0,0)$  + set

- |                                    |                                    |   |   |
|------------------------------------|------------------------------------|---|---|
| (1) 1<br>(1 0,0,0)                 | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)   | (3) $4^+ 0,0,z$<br>( $4_z$  0,0,0)'       | (4) $4^- 0,0,z$<br>( $4_z^{-1}$  0,0,0)'  |
| (5) $m' x,0,z$<br>( $m_y$  0,0,0)' | (6) $m' 0,y,z$<br>( $m_x$  0,0,0)' | (7) $m x,\bar{x},z$<br>( $m_{xy}$  0,0,0) | (8) $m x,x,z$<br>( $m_{\bar{xy}}$  0,0,0) |

For  $(1/2,1/2,1/2)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t' (1/2,1/2,1/2)$<br>(1 1/2,1/2,1/2)'           | (2) $2' (0,0,1/2) 1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2)' | (3) $4^+ (0,0,1/2) 0,1/2,z$<br>( $4_z$  1/2,1/2,1/2)            | (4) $4^- (0,0,1/2) 1/2,0,z$<br>( $4_z^{-1}$  1/2,1/2,1/2)       |
| (5) $n (1/2,0,1/2) x,1/4,z$<br>( $m_y$  1/2,1/2,1/2) | (6) $n (0,1/2,1/2) 1/4,y,z$<br>( $m_x$  1/2,1/2,1/2)   | (7) $c' (0,0,1/2) x+1/2,\bar{x},z$<br>( $m_{xy}$  1/2,1/2,1/2)' | (8) $n' (1/2,1/2,1/2) x,x,z$<br>( $m_{\bar{xy}}$  1/2,1/2,1/2)' |

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(1/2,1/2,1/2)$ ; (2); (3); (5).

**Positions**

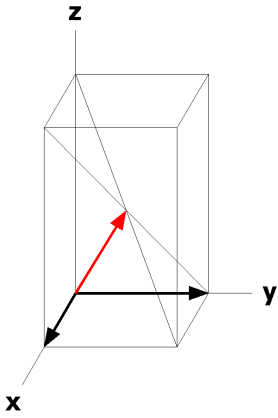
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates											
			(0,0,0) +		$(1/2,1/2,1/2)'$ +							
16 e 1	(1)	$x,y,z$	$[u,v,w]$	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y},x,z$	$[v,\bar{u},\bar{w}]$	(4)	$y,\bar{x},z$	$[\bar{v},u,\bar{w}]$
	(5)	$x,\bar{y},z$	$[u,\bar{v},w]$	(6)	$\bar{x},y,z$	$[\bar{u},v,w]$	(7)	$\bar{y},\bar{x},z$	$[v,u,\bar{w}]$	(8)	$y,x,z$	$[\bar{v},\bar{u},\bar{w}]$
8 d .m'		$x,0,z$	$[u,0,w]$		$\bar{x},0,z$	$[\bar{u},0,w]$		$0,x,z$	$[0,\bar{u},\bar{w}]$		$0,\bar{x},z$	$[0,u,\bar{w}]$
8 c ..m		$x,x,z$	$[\bar{u},u,0]$		$\bar{x},\bar{x},z$	$[u,\bar{u},0]$		$\bar{x},x,z$	$[u,u,0]$		$x,\bar{x},z$	$[\bar{u},\bar{u},0]$
4 b $2m'm'$		$0,1/2,z$	$[0,0,w]$		$1/2,0,z$	$[0,0,\bar{w}]$						
2 a $4'm'm$		$0,0,z$	$[0,0,0]$									

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_p, 4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,1/2,z$

Along  $[1,0,0]$   $c_p, 1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



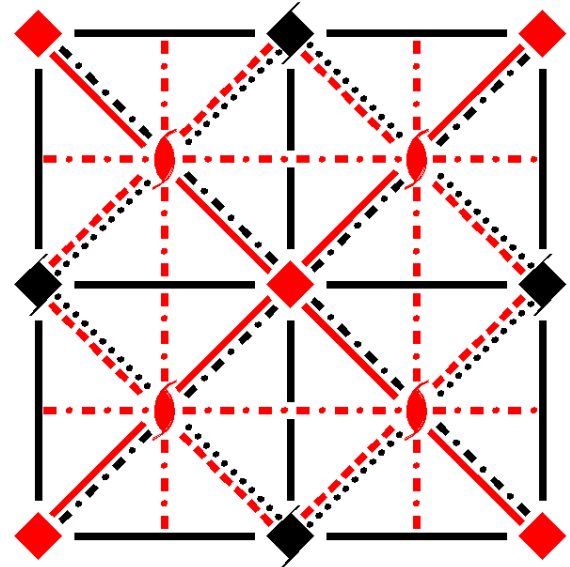
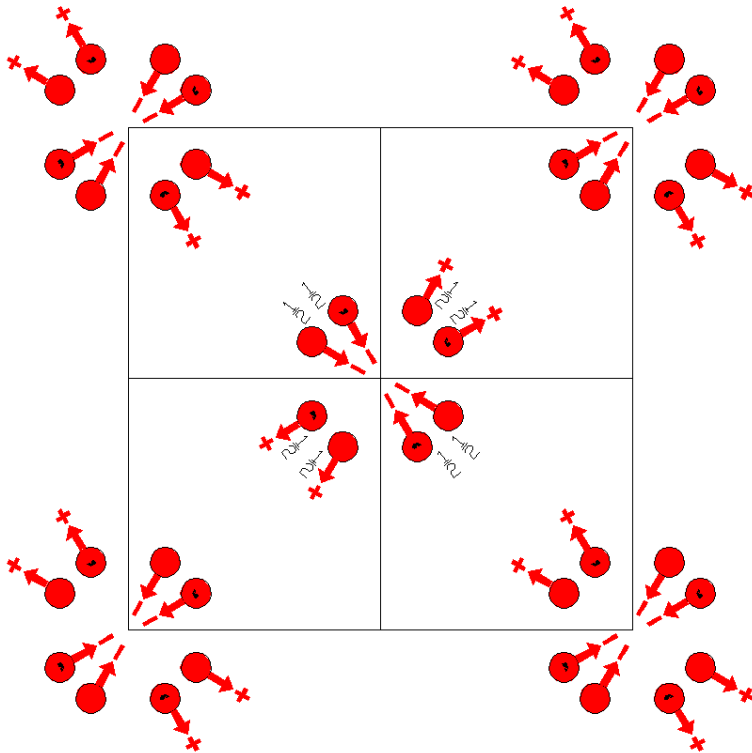
$I_p 4'mm'$

$4mm1'$

Tetragonal

107.8.890

$I_p 4'mm'$



Origin on  $4'mm'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

Symmetry Operations

For  $(0,0,0)$  + set

- |                                  |                                  |   |   |
|----------------------------------|----------------------------------|---|---|
| (1) 1<br>(1 0,0,0)               | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $4^+ 0,0,z$<br>( $4_z$  0,0,0)'         | (4) $4^- 0,0,z$<br>( $4_z^{-1}$  0,0,0)'    |
| (5) m $x,0,z$<br>( $m_y$  0,0,0) | (6) m $0,y,z$<br>( $m_x$  0,0,0) | (7) $m' x,\bar{x},z$<br>( $m_{xy}$  0,0,0)' | (8) $m' x,x,z$<br>( $m_{\bar{xy}}$  0,0,0)' |

For  $(1/2,1/2,1/2)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t' (1/2,1/2,1/2)$<br>(1  $1/2,1/2,1/2$ )'               | (2) $2' (0,0,1/2) \ 1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1/2$ )' | (3) $4^+ (0,0,1/2) \ 0,1/2,z$<br>( $4_z$   $1/2,1/2,1/2$ )'          | (4) $4^- (0,0,1/2) \ 1/2,0,z$<br>( $4_z^{-1}$   $1/2,1/2,1/2$ )'     |
| (5) $n' (1/2,0,1/2) \ x,1/4,z$<br>( $m_y$   $1/2,1/2,1/2$ )' | (6) $n' (0,1/2,1/2) \ 1/4,y,z$<br>( $m_x$   $1/2,1/2,1/2$ )' | (7) c $(0,0,1/2) \ x+1/2,\bar{x},z$<br>( $m_{xy}$   $1/2,1/2,1/2$ )' | (8) n $(1/2,1/2,1/2) \ x,x,z$<br>( $m_{\bar{xy}}$   $1/2,1/2,1/2$ )' |

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(1/2,1/2,1/2)$ ; (2); (3); (5).

**Positions**

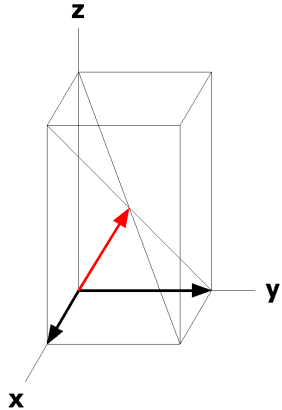
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +	(1/2,1/2,1/2)' +				
16 e 1	(1)	$x,y,z$ [u,v,w]	(2)	$\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3)	$\bar{y},x,z$ [ $v,\bar{u},\bar{w}$ ]	(4)	$y,\bar{x},z$ [ $v,\bar{u},\bar{w}$ ]
	(5)	$x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(6)	$\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(7)	$\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(8)	$y,x,z$ [ $v,u,w$ ]
8 d .m.		$x,0,z$ [0,v,0]		$\bar{x},0,z$ [0, $\bar{v}$ ,0]		$0,x,z$ [v,0,0]		$0,\bar{x},z$ [ $\bar{v}$ ,0,0]
8 c ..m'		$x,x,z$ [u,u,w]		$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]		$\bar{x},x,z$ [ $u,\bar{u},\bar{w}$ ]		$x,\bar{x},z$ [ $\bar{u},u,\bar{w}$ ]
4 b 2mm.		$0,1/2,z$ [0,0,0]		$1/2,0,z$ [0,0,0]				
2 a 4'mm'		$0,0,z$ [0,0,0]						

**Symmetry of Special Projections**

Along [0,0,1]  $p_4$ , 4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,1/2,z

Along [1,0,0]  $c1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p_{2b}$ , 1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



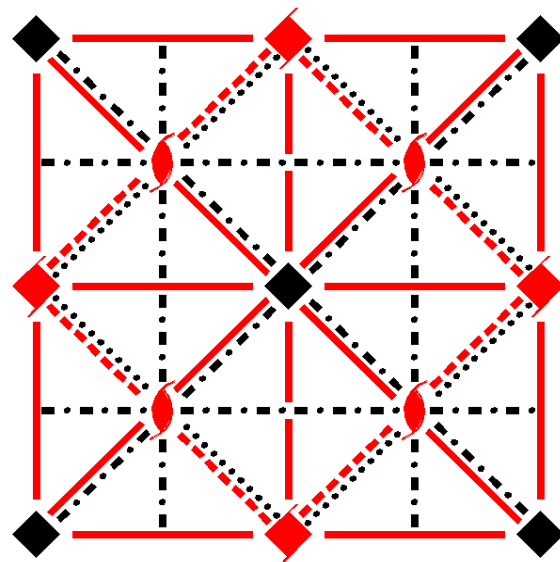
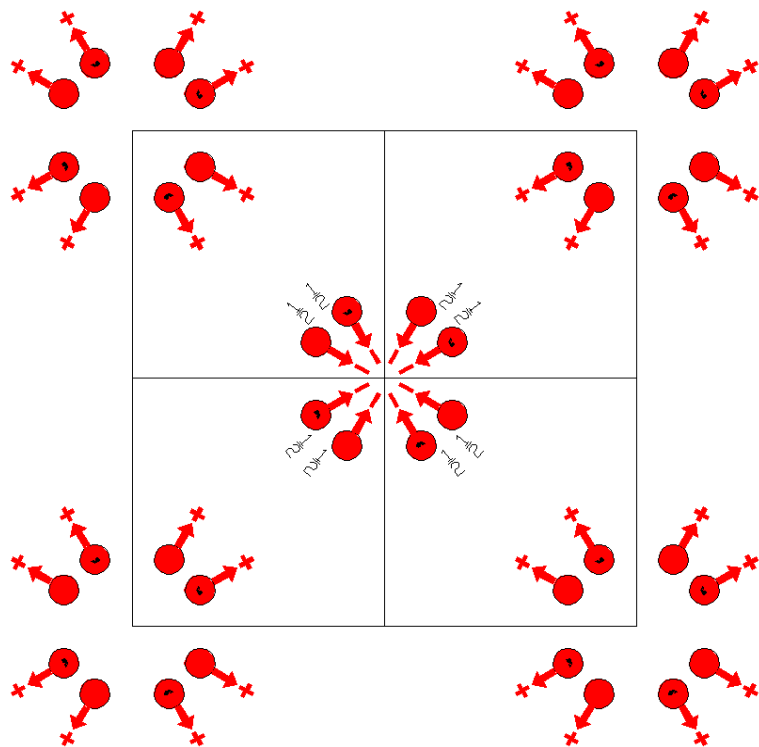
$I_p 4m'm'$

$4mm1'$

Tetragonal

107.9.891

$I_p 4m'm'$



Origin on  $4m'm'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

Symmetry Operations

For  $(0,0,0)$  + set

- |                                      |                                      |   |   |
|--------------------------------------|--------------------------------------|---|---|
| (1) 1<br>(1 0,0,0)                   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)     | (3) $4^+$ $0,0,z$<br>( $4_z$  0,0,0)          | (4) $4^-$ $0,0,z$<br>( $4_z^{-1}$  0,0,0)     |
| (5) $m'$ $x,0,z$<br>( $m_y$  0,0,0)' | (6) $m'$ $0,y,z$<br>( $m_x$  0,0,0)' | (7) $m'$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,0)' | (8) $m'$ $x,x,z$<br>( $m_{\bar{xy}}$  0,0,0)' |

For  $(1/2,1/2,1/2)$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t'$ $(1/2,1/2,1/2)$<br>(1  $1/2,1/2,1/2$ )'              | (2) $2'$ $(0,0,1/2) \ 1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1/2$ )' | (3) $4^{+}$ $(0,0,1/2) \ 0,1/2,z$<br>( $4_z$   $1/2,1/2,1/2$ )'        | (4) $4^{-}$ $(0,0,1/2) \ 1/2,0,z$<br>( $4_z^{-1}$   $1/2,1/2,1/2$ )'   |
| (5) $n$ $(1/2,0,1/2) \ x,1/4,z$<br>( $m_y$   $1/2,1/2,1/2$ )' | (6) $n$ $(0,1/2,1/2) \ 1/4,y,z$<br>( $m_x$   $1/2,1/2,1/2$ )'  | (7) $c$ $(0,0,1/2) \ x+1/2,\bar{x},z$<br>( $m_{xy}$   $1/2,1/2,1/2$ )' | (8) $n$ $(1/2,1/2,1/2) \ x,x,z$<br>( $m_{\bar{xy}}$   $1/2,1/2,1/2$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1/2,1/2,1/2)' +		
16	e	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ] (7) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ] (8) $y,x,z$ [ $v,u,w$ ]
8	d	.m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	0,x,z [0,u,w]	0, $\bar{x},z$ [0, $\bar{u},w$ ]
8	c	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,z$ [ $\bar{u},u,w$ ]	x, $\bar{x},z$ [ $u,\bar{u},w$ ]
4	b	2m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]		
2	a	4m'm'	0,0,z [0,0,w]			

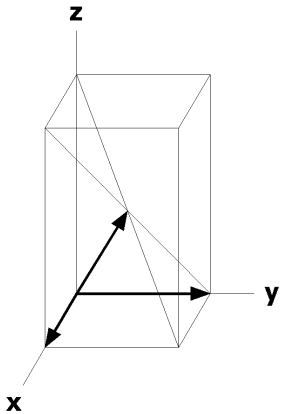
**Symmetry of Special Projections**

Along [0,0,1]  $p_p, 4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c_p, 1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p_{2b}, 1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0





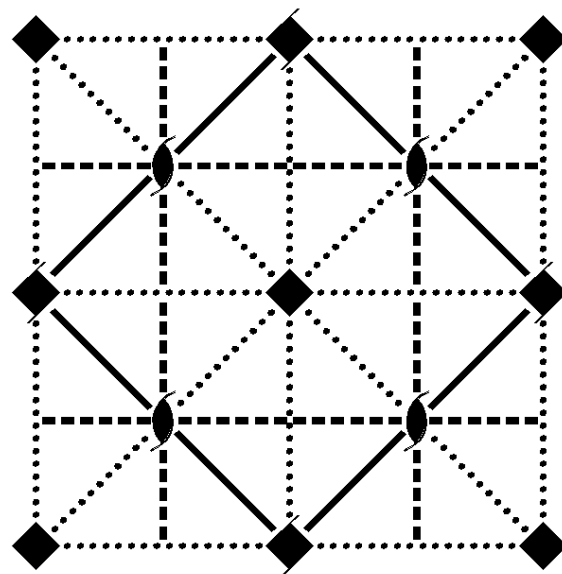
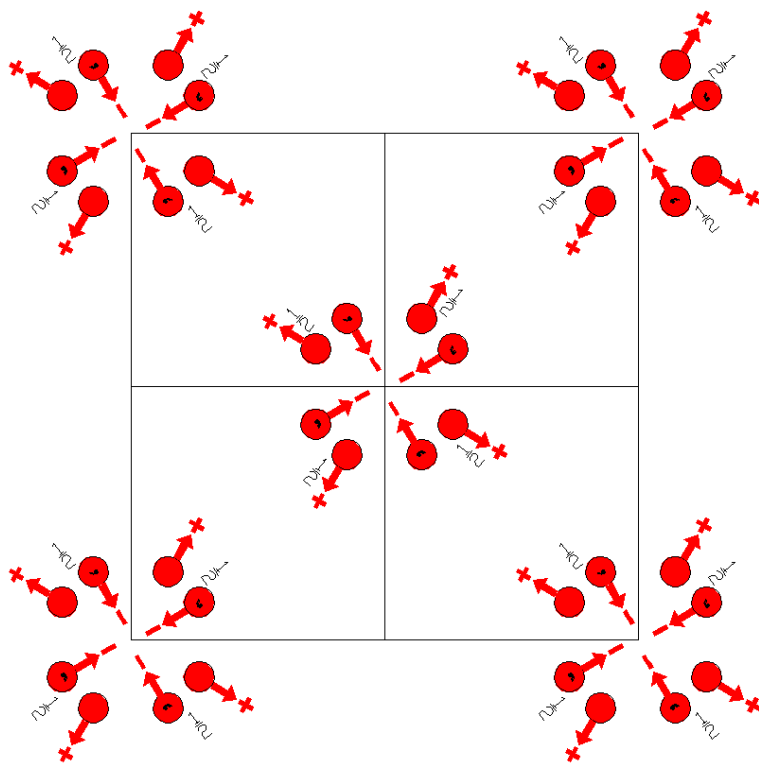
l4cm

4mm

Tetragonal

108.1.892

l4cm



Origin on 4cc

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2 - x$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (6) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (7) m x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)    | (8) g (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)           |

For (1/2,1/2,1/2) + set

- |  |  |   |   |
|--|--|---|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)             | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)         | (7) c (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)                  | (8) c (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)                                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

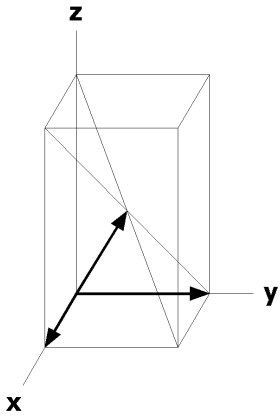
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1/2,1/2,1/2) +		
16	d	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]		
			(5) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x}+1/2,y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $v,u,\bar{w}$ ]	(8) $y+1/2,x+1/2,z$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	c	..m	$x,x+1/2,z$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}+1/2,z$ [ $u,\bar{u},0$ ]	$x+1/2,\bar{x},z$ [ $u,u,0$ ]	$\bar{x}+1/2,x,z$ [ $\bar{u},\bar{u},0$ ]
4	b	2.mm	$1/2,0,z$ [ $0,0,0$ ]	$0,1/2,z$ [ $0,0,0$ ]		
2	a	4..	$0,0,z$ [ $0,0,w$ ]	$1/2,1/2,z$ [ $0,0,\bar{w}$ ]		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a}1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,1/4,0$

Along  $[1,1,0]$   $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



$I4cm1'$

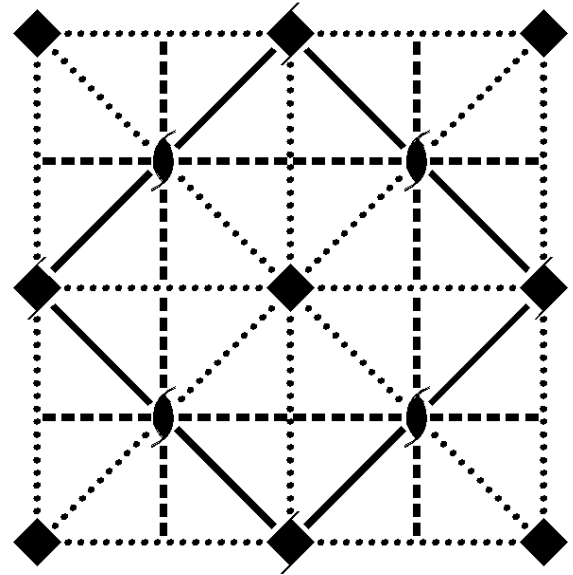
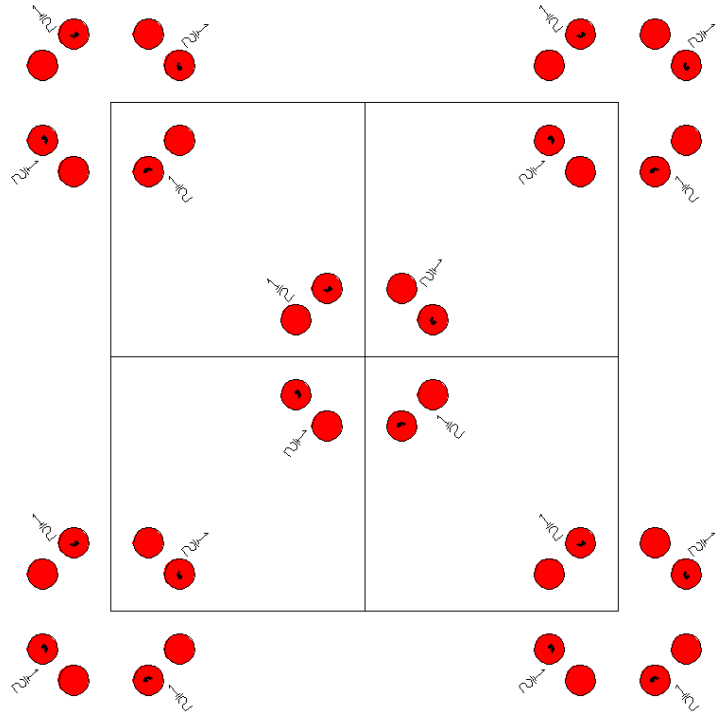
$4mm1'$

Tetragonal

108.2.893

$I4cm1'$

$1'$



Origin on  $4cc1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2 - x$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                       | (3) $4^+$ $0,0,z$<br>( $4_z$  0,0,0)                  | (4) $4^-$ $0,0,z$<br>( $4_z^{-1}$  0,0,0)                       |
| (5) a $(1/2,0,0)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,0$ ) | (6) b $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ ) | (7) m $x+1/2,\bar{x},z$<br>( $m_{xy}$   $1/2,1/2,0$ ) | (8) g $(1/2,1/2,0)$ $x,x,z$<br>( $m_{\bar{xy}}$   $1/2,1/2,0$ ) |

For  $(1/2,1/2,1/2)$  + set

- |  |  |  |   |
|--|--|--|---|
| (1) t $(1/2,1/2,1/2)$<br>(1  $1/2,1/2,1/2$ )       | (2) 2 $(0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1/2$ ) | (3) $4^+$ $(0,0,1/2)$ $0,1/2,z$<br>( $4_z$   $1/2,1/2,1/2$ ) | (4) $4^-$ $(0,0,1/2)$ $1/2,0,z$<br>( $4_z^{-1}$   $1/2,1/2,1/2$ ) |
| (5) c $(0,0,1/2)$ $x,0,z$<br>( $m_y$   $0,0,1/2$ ) | (6) c $(0,0,1/2)$ $0,y,z$<br>( $m_x$   $0,0,1/2$ )         | (7) c $(0,0,1/2)$ $x,\bar{x},z$<br>( $m_{xy}$   $0,0,1/2$ )  | (8) c $(0,0,1/2)$ $x,x,z$<br>( $m_{\bar{xy}}$   $0,0,1/2$ )       |

## For (0,0,0)' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> ' 0,0,z (4 <sub>z</sub>  0,0,0)'	(4) 4 <sup>-</sup> ' 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(5) a' (1/2,0,0) x,1/4,z (m <sub>y</sub>  1/2,1/2,0)'	(6) b' (0,1/2,0) 1/4,y,z (m <sub>x</sub>  1/2,1/2,0)'	(7) m' x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,0)'	(8) g' (1/2,1/2,0) x,x,z (m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)'

## For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (1 1/2,1/2,1/2)'	(2) 2' (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>  1/2,1/2,1/2)'	(3) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)'	(4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'
(5) c' (0,0,1/2) x,0,z (m <sub>y</sub>  0,0,1/2)'	(6) c' (0,0,1/2) 0,y,z (m <sub>x</sub>  0,0,1/2)'	(7) c' (0,0,1/2) x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,1/2)'	(8) c' (0,0,1/2) x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

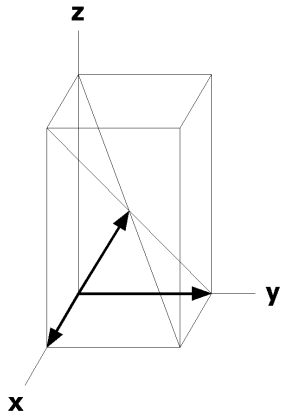
			(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'
16	d	11'	(1) x,y,z [0,0,0] (3) $\bar{y}$ ,x,z [0,0,0] (5) x+1/2, $\bar{y}$ +1/2,z [0,0,0] (7) $\bar{y}$ +1/2, $\bar{x}$ +1/2,z [0,0,0]	(2) $\bar{x}$ , $\bar{y}$ ,z [0,0,0] (4) y, $\bar{x}$ ,z [0,0,0] (6) $\bar{x}$ +1/2,y+1/2,z [0,0,0] (8) y+1/2,x+1/2,z [0,0,0]
8	c	..m1'	x,x+1/2,z [0,0,0]	$\bar{x}$ , $\bar{x}$ +1/2,z [0,0,0]    x+1/2, $\bar{x}$ ,z [0,0,0] $\bar{x}$ +1/2,x,z [0,0,0]
4	b	2.mm1'	1/2,0,z [0,0,0]	0,1/2,z [0,0,0]
4	a	4..1'	0,0,z [0,0,0]	1/2,1/2,z [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

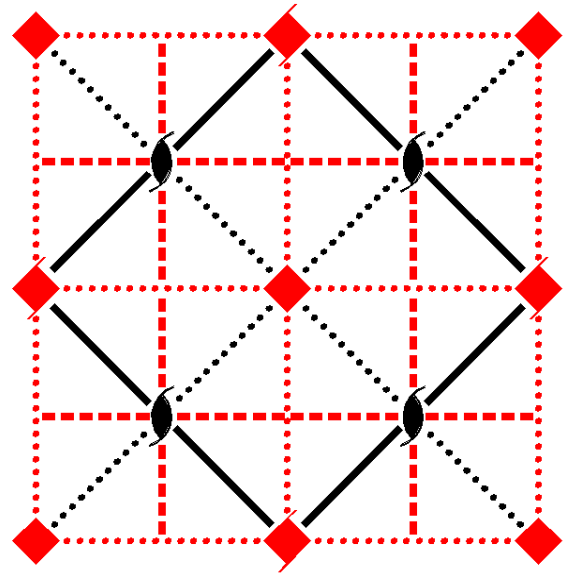
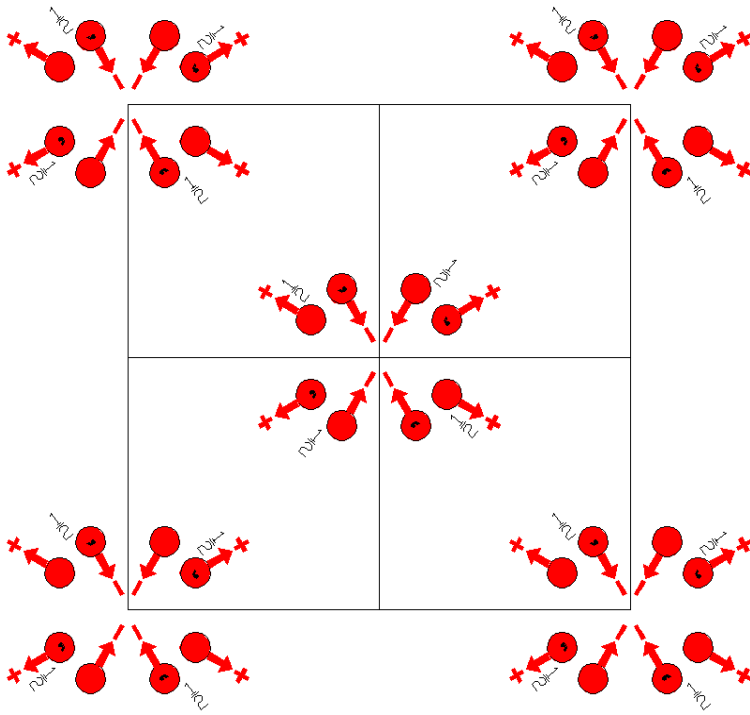
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



I4'c'm  
108.3.894

4'm'm  
I4'c'm

Tetragonal



Origin on 4'c'c

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2 - x$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                   | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (5) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (6) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' | (7) m x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)     | (8) g (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)            |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)               | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)'       | (7) c (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)                   | (8) c (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)                                  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

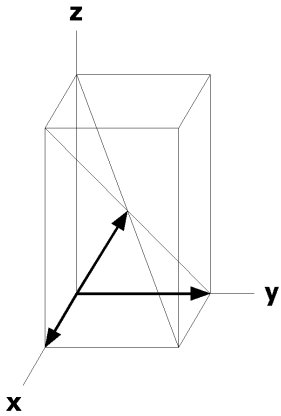
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1/2,1/2,1/2) +		
16	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},\bar{w}$ ]		
			(5) $x+1/2,\bar{y}+1/2,z$ [ $u,\bar{v},w$ ]	(6) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]		
			(7) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $v,u,\bar{w}$ ]	(8) $y+1/2,x+1/2,z$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	c	..m	$x,x+1/2,z$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}+1/2,z$ [ $u,\bar{u},0$ ]	$x+1/2,\bar{x},z$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,z$ [ $u,u,0$ ]
4	b	2.mm	$1/2,0,z$ [0,0,0]	$0,1/2,z$ [0,0,0]		
4	a	4'..	$0,0,z$ [0,0,0]	$1/2,1/2,z$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

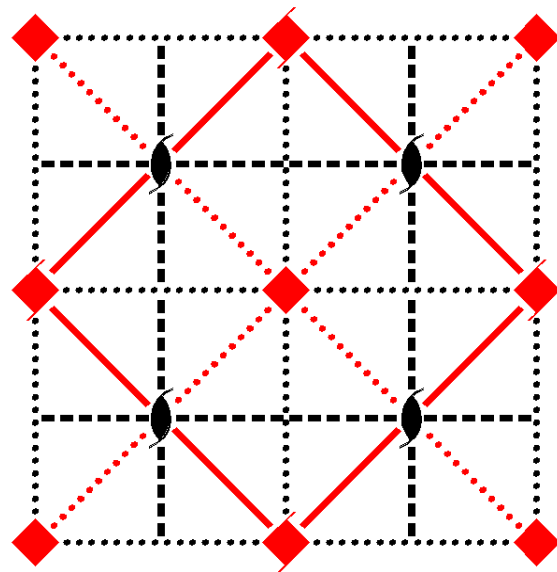
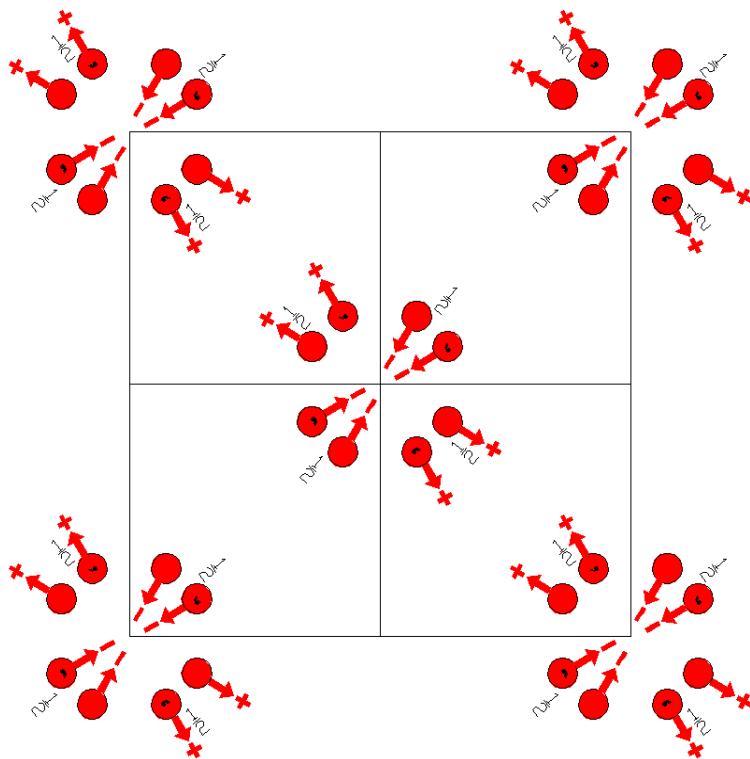
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



I4'cm'  
108.4.895

4'mm'  
I4'cm'

Tetragonal



Origin on 4'cc'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (5) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (6) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (7) m' x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)'   | (8) g' (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)'          |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)             | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)         | (7) c' (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)'                 | (8) c' (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)'                                |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1/2,1/2,1/2) +		
16	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(5) x+1/2, $\bar{y}$ +1/2,z [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $\bar{x}$ +1/2,y+1/2,z [ $\bar{u},\bar{v},\bar{w}$ ]		
			(7) $\bar{y}$ +1/2, $\bar{x}$ +1/2,z [ $\bar{v},\bar{u},\bar{w}$ ]	(8) y+1/2,x+1/2,z [v,u,w]		
8	c	..m'	x,x+1/2,z [u,u,w]	$\bar{x},\bar{x}$ +1/2,z [ $\bar{u},\bar{u},w$ ]	x+1/2, $\bar{x},z$ [ $\bar{u},\bar{u},\bar{w}$ ]	$\bar{x}$ +1/2,x,z [u, $\bar{u},\bar{w}$ ]
4	b	2.m'm'	1/2,0,z [0,0,w]	0,1/2,z [0,0, $\bar{w}$ ]		
2	a	4'..	0,0,z [0,0,0]	1/2,1/2,z [0,0,0]		

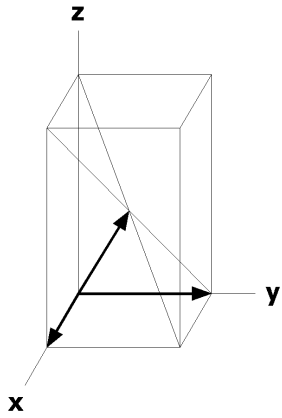
**Symmetry of Special Projections**

Along [0,0,1] p4'm'm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

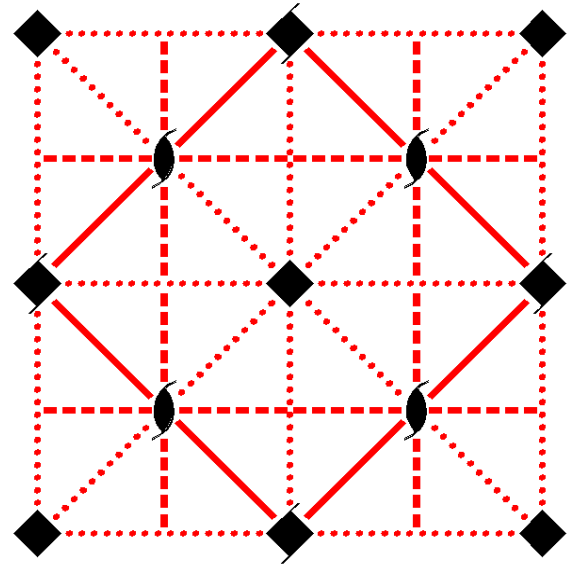
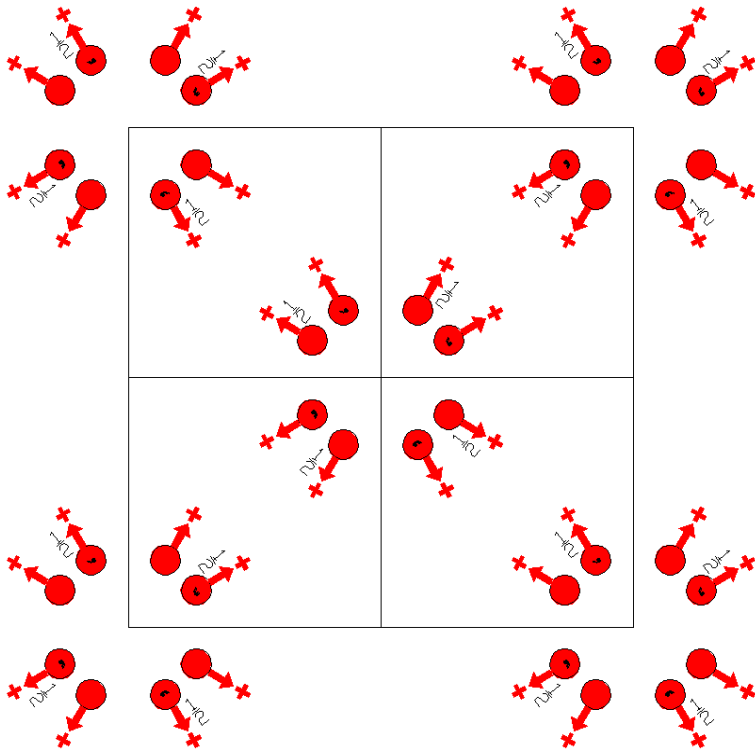




I4c'm'  
108.5.896

4m'm'  
I4c'm'

Tetragonal



Origin on 4c'c'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2 - x$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                   | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (6) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' | (7) m' x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)'  | (8) g' (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)'         |

For (1/2,1/2,1/2) + set

- |  |  |   |   |
|--|--|---|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)               | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)'       | (7) c' (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)'                | (8) c' (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)'                               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

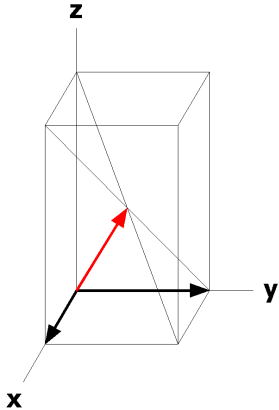
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1/2,1/2,1/2) +		
16	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ]		
			(5) x+1/2, $\bar{y}$ +1/2,z [u, $\bar{v},w$ ]	(6) $\bar{x}$ +1/2,y+1/2,z [ $\bar{u},v,w$ ]		
			(7) $\bar{y}$ +1/2, $\bar{x}$ +1/2,z [ $\bar{v},\bar{u},w$ ]	(8) y+1/2,x+1/2,z [v,u,w]		
8	c	..m'	x,x+1/2,z [u,u,w]	$\bar{x},\bar{x}$ +1/2,z [ $\bar{u},\bar{u},w$ ]	x+1/2, $\bar{x},z$ [u, $\bar{u},w$ ]	$\bar{x}$ +1/2,x,z [ $\bar{u},u,w$ ]
4	b	2.m'm'	1/2,0,z [0,0,w]	0,1/2,z [0,0,w]		
2	a	4..	0,0,z [0,0,w]	1/2,1/2,z [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



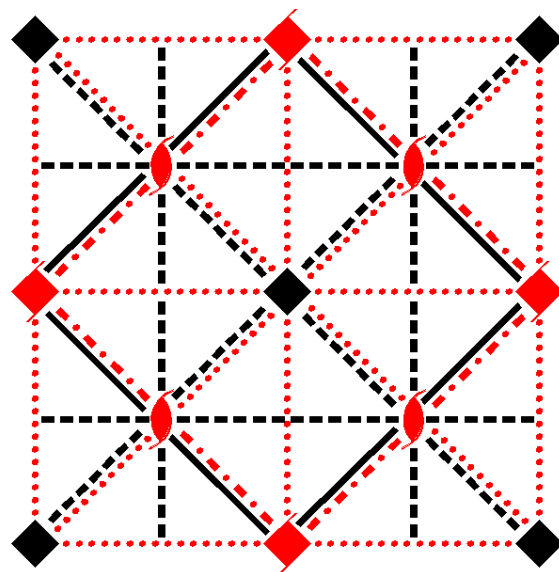
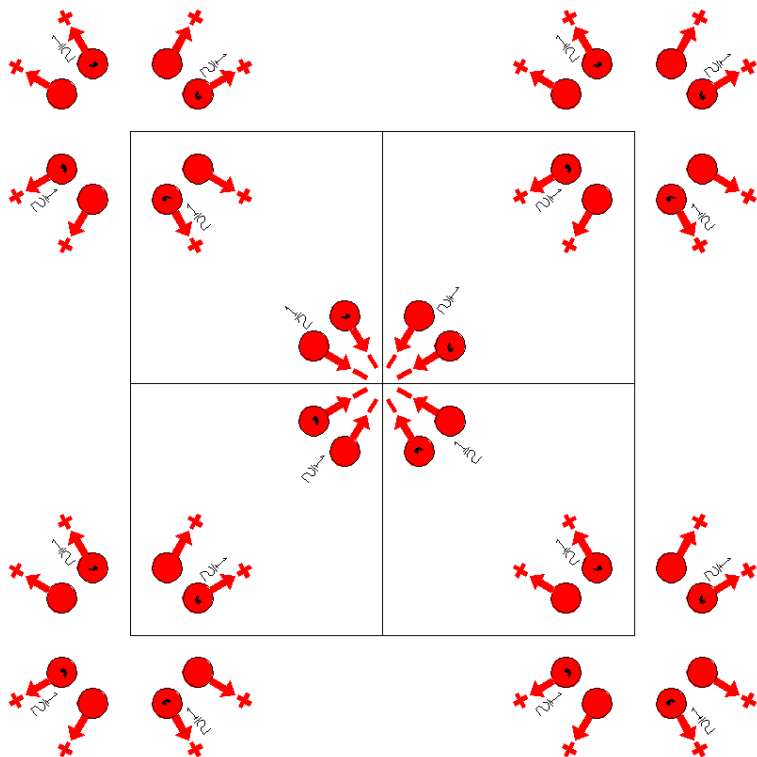
$I_p$  4cm

4mm1'

Tetragonal

108.6.897

$I_p$  4cm



Origin on 4c'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2 - x$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (6) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (7) m x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)    | (8) g (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)           |

For (1/2,1/2,1/2)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'             | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)'         | (7) c' (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)'                   | (8) c' (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)'                                  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

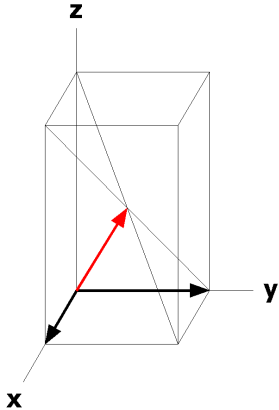
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
				(0,0,0) +	(1/2,1/2,1/2)' +	
16	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ]		
			(5) x+1/2, $\bar{y}$ +1/2,z [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x}$ +1/2,y+1/2,z [u, $\bar{v},\bar{w}$ ]		
			(7) $\bar{y}$ +1/2, $\bar{x}$ +1/2,z [v,u, $\bar{w}$ ]	(8) y+1/2,x+1/2,z [ $\bar{v},\bar{u},\bar{w}$ ]		
8	c	..m	x,x+1/2,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}$ +1/2,z [u, $\bar{u},0$ ]	x+1/2, $\bar{x},z$ [u,u,0]	$\bar{x}$ +1/2,x,z [ $\bar{u},\bar{u},0$ ]
4	b	2.mm	1/2,0,z [0,0,0]	0,1/2,z [0,0,0]		
2	a	4..	0,0,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub> 4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub> 1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,0

Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



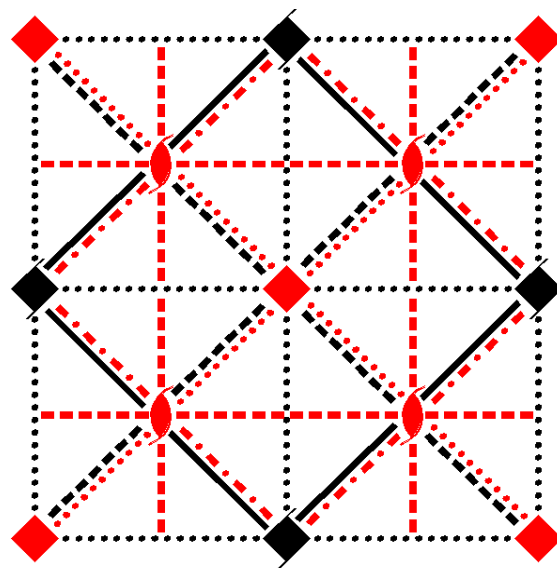
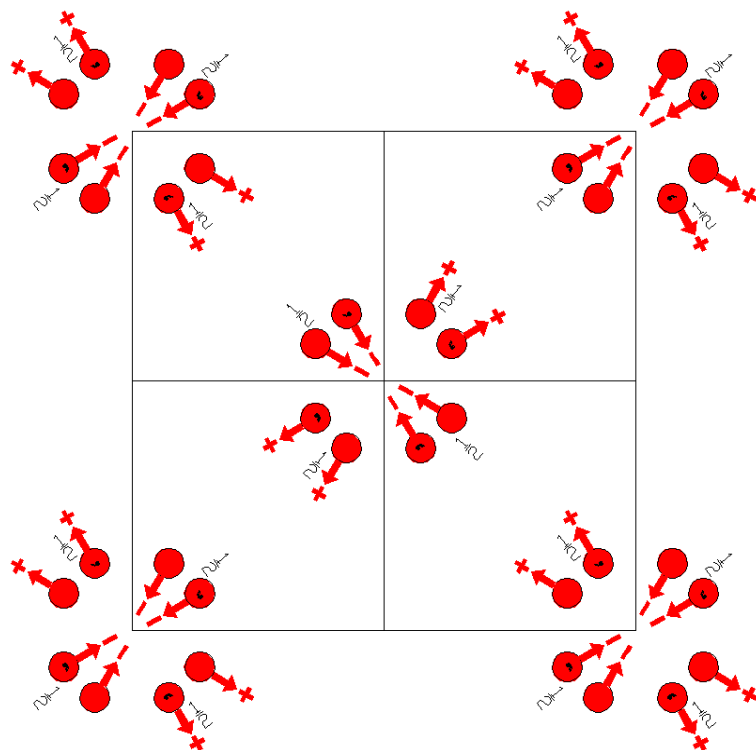
$I_p 4'c'm$

$4mm1'$

Tetragonal

108.7.898

$I_p 4'c'm$



Origin on  $4'cc'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2 - x$

Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                         | (3) $4^+ 0,0,z$<br>( $4_z$  0,0,0)'                     | (4) $4^- 0,0,z$<br>( $4_z^{-1}$  0,0,0)'                        |
| (5) $a' (1/2,0,0)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,0$ )' | (6) $b' (0,1/2,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' | (7) $m$ $x+1/2,\bar{x},z$<br>( $m_{xy}$   $1/2,1/2,0$ ) | (8) $g (1/2,1/2,0)$ $x,x,z$<br>( $m_{\bar{xy}}$   $1/2,1/2,0$ ) |

For  $(1/2,1/2,1/2)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t' (1/2,1/2,1/2)$<br>(1  $1/2,1/2,1/2$ )'     | (2) $2' (0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1/2$ )' | (3) $4^+ (0,0,1/2)$ $0,1/2,z$<br>( $4_z$   $1/2,1/2,1/2$ )    | (4) $4^- (0,0,1/2)$ $1/2,0,z$<br>( $4_z^{-1}$   $1/2,1/2,1/2$ ) |
| (5) $c (0,0,1/2)$ $x,0,z$<br>( $m_y$   $0,0,1/2$ ) | (6) $c (0,0,1/2)$ $0,y,z$<br>( $m_x$   $0,0,1/2$ )           | (7) $c' (0,0,1/2)$ $x,\bar{x},z$<br>( $m_{xy}$   $0,0,1/2$ )' | (8) $c' (0,0,1/2)$ $x,x,z$<br>( $m_{\bar{xy}}$   $0,0,1/2$ )'   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

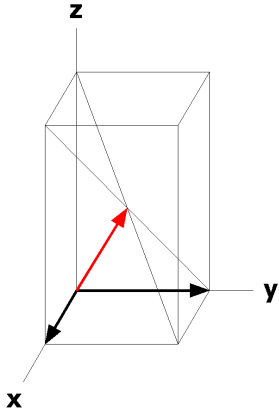
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
				(0,0,0) +	(1/2,1/2,1/2)' +	
16	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(5) x+1/2, $\bar{y}$ +1/2,z [u, $\bar{v},w$ ]	(6) $\bar{x}$ +1/2,y+1/2,z [ $\bar{u},\bar{v},w$ ]		
			(7) $\bar{y}$ +1/2, $\bar{x}$ +1/2,z [ $\bar{v},\bar{u},\bar{w}$ ]	(8) y+1/2,x+1/2,z [ $\bar{v},\bar{u},\bar{w}$ ]		
8	c	..m	x,x+1/2,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}$ +1/2,z [u, $\bar{u},0$ ]	x+1/2, $\bar{x},z$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}$ +1/2,x,z [u,u,0]
4	b	2.mm	1/2,0,z [0,0,0]	0,1/2,z [0,0,0]		
4	a	4'..	0,0,z [0,0,0]	1/2,1/2,z [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_p 4mm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,1/2,z

Along [1,0,0]  $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



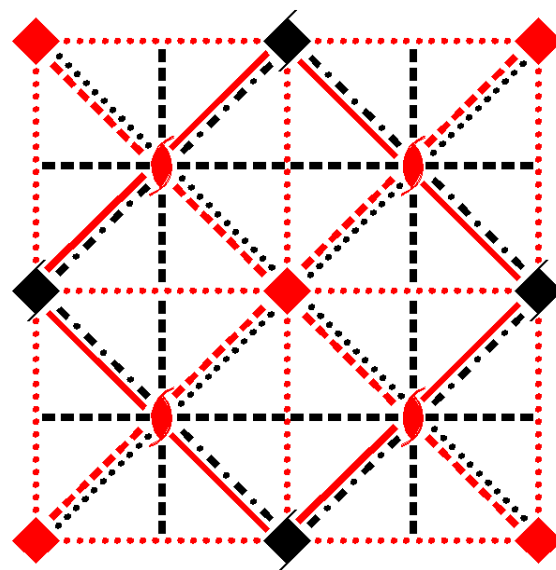
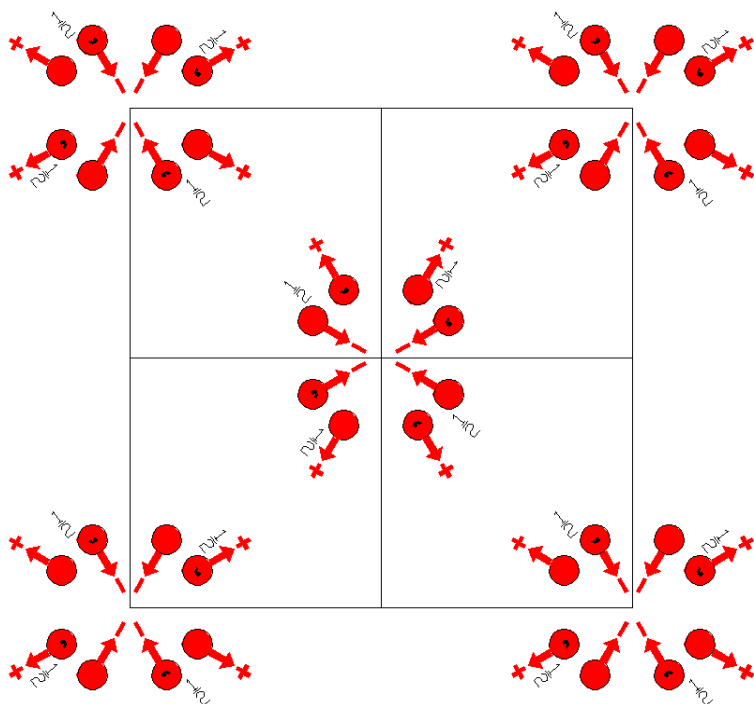
$I_p 4'cm'$

$4mm1'$

Tetragonal

108.8.899

$I_p 4'cm'$



Origin on  $4'c'c$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2 - x$

Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1   0,0,0)                                   | (2) 2 $0,0,z$<br>( $2_z$   0,0,0)                      | (3) $4^+ 0,0,z$<br>( $4_z$   0,0,0)'                    | (4) $4^- 0,0,z$<br>( $4_z^{-1}$   0,0,0)'                         |
| (5) a $(1/2,0,0)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,0$ ) | (6) b $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ ) | (7) $m' x+1/2,\bar{x},z$<br>( $m_{xy}$   $1/2,1/2,0$ )' | (8) $g' (1/2,1/2,0)$ $x,x,z$<br>( $m_{\bar{xy}}$   $1/2,1/2,0$ )' |

For  $(1/2,1/2,1/2)$  + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t' (1/2,1/2,1/2)$<br>(1   $1/2,1/2,1/2$ )'      | (2) $2' (0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1/2$ )' | (3) $4^+ (0,0,1/2)$ $0,1/2,z$<br>( $4_z$   $1/2,1/2,1/2$ )  | (4) $4^- (0,0,1/2)$ $1/2,0,z$<br>( $4_z^{-1}$   $1/2,1/2,1/2$ ) |
| (5) $c' (0,0,1/2)$ $x,0,z$<br>( $m_y$   $0,0,1/2$ )' | (6) $c' (0,0,1/2)$ $0,y,z$<br>( $m_x$   $0,0,1/2$ )'         | (7) $c (0,0,1/2)$ $x,\bar{x},z$<br>( $m_{xy}$   $0,0,1/2$ ) | (8) $c (0,0,1/2)$ $x,x,z$<br>( $m_{\bar{xy}}$   $0,0,1/2$ )     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
				(0,0,0) +	(1/2,1/2,1/2)' +	
16	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}, x, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(4) y, $\bar{x}, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
			(5) x+1/2, $\bar{y}$ +1/2, z [ $\bar{u}, \bar{v}, \bar{w}$ ]	(6) $\bar{x}$ +1/2, y+1/2, z [ $\bar{u}, \bar{v}, \bar{w}$ ]		
			(7) $\bar{y}$ +1/2, $\bar{x}$ +1/2, z [ $\bar{v}, \bar{u}, \bar{w}$ ]	(8) y+1/2, x+1/2, z [v,u,w]		
8	c	..m'	x, x+1/2, z [u,u,w]	$\bar{x}, \bar{x}$ +1/2, z [ $\bar{u}, \bar{u}, w$ ]	x+1/2, $\bar{x}, z$ [ $\bar{u}, \bar{u}, w$ ]	$\bar{x}$ +1/2, x, z [u, $\bar{u}, w$ ]
4	b	2.m'm'	1/2, 0, z [0,0,w]	0, 1/2, z [0,0, $\bar{w}$ ]		
2	a	4'..	0, 0, z [0,0,0]	1/2, 1/2, z [0,0,0]		

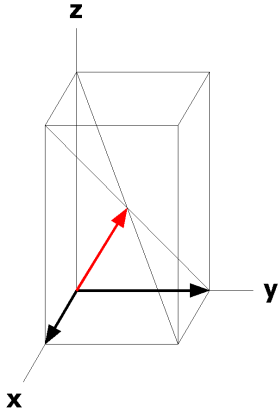
**Symmetry of Special Projections**

Along [0,0,1]  $p_p 4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0, 1/2, z

Along [1,0,0]  $p_{2a} 1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x, 1/4, 0

Along [1,1,0]  $p_{2b} 1m1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x, x, 0





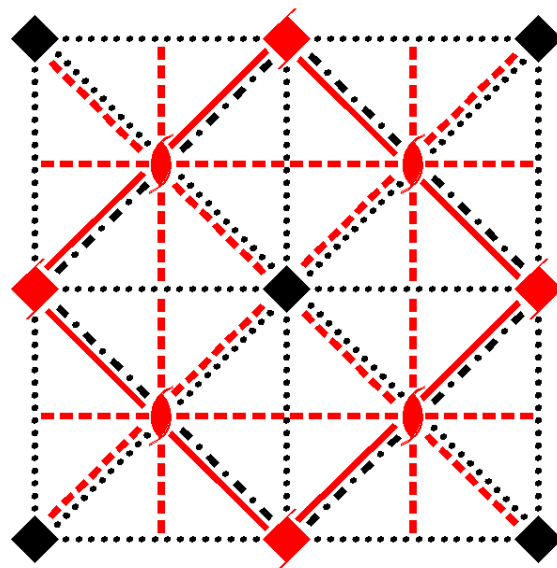
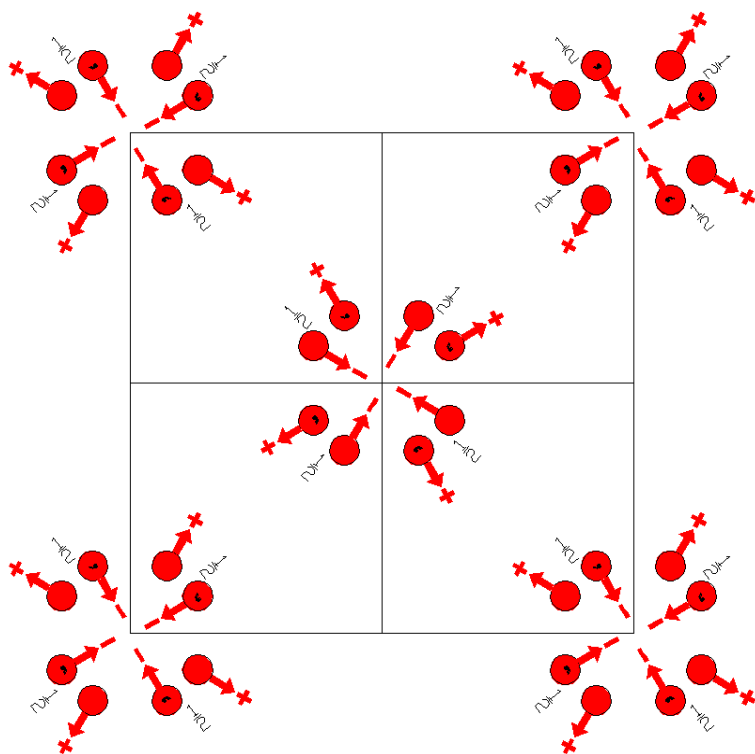
$I_p 4c'm'$

$4mm1'$

Tetragonal

108.9.900

$I_p 4c'm'$



Origin on 4cc

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2 - x$

Symmetry Operations

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                   | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (6) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' | (7) m' x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)'  | (8) g' (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)'         |

For (1/2,1/2,1/2)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'           | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)           | (7) c (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)                     | (8) c (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)                                    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

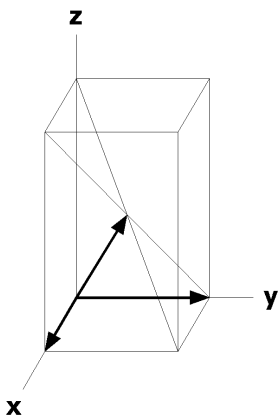
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
				(0,0,0) +	(1/2,1/2,1/2)' +	
16	d	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ]		
			(5) x+1/2, $\bar{y}$ +1/2,z [u, $\bar{v},w$ ]	(6) $\bar{x}$ +1/2,y+1/2,z [ $\bar{u},v,w$ ]		
			(7) $\bar{y}$ +1/2, $\bar{x}$ +1/2,z [ $\bar{v},\bar{u},w$ ]	(8) y+1/2,x+1/2,z [v,u,w]		
8	c	..m'	x,x+1/2,z [u,u,w]	$\bar{x},\bar{x}$ +1/2,z [ $\bar{u},\bar{u},w$ ]	x+1/2, $\bar{x},z$ [u, $\bar{u},w$ ]	$\bar{x}$ +1/2,x,z [ $\bar{u},u,w$ ]
4	b	2.m'm'	1/2,0,z [0,0,w]	0,1/2,z [0,0,w]		
2	a	4..	0,0,z [0,0,w]	1/2,1/2,z [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_p 4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

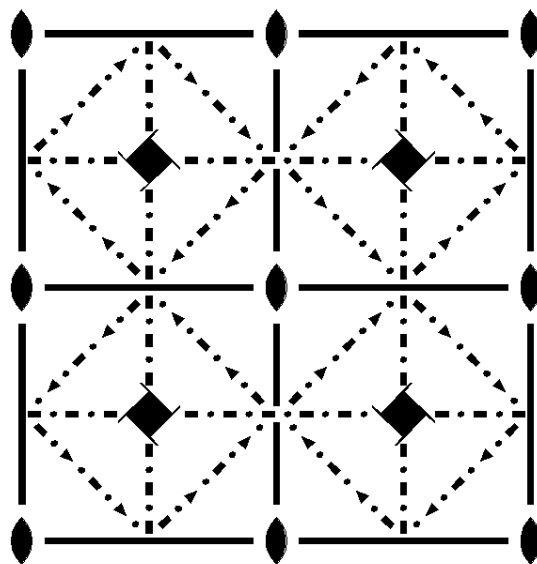
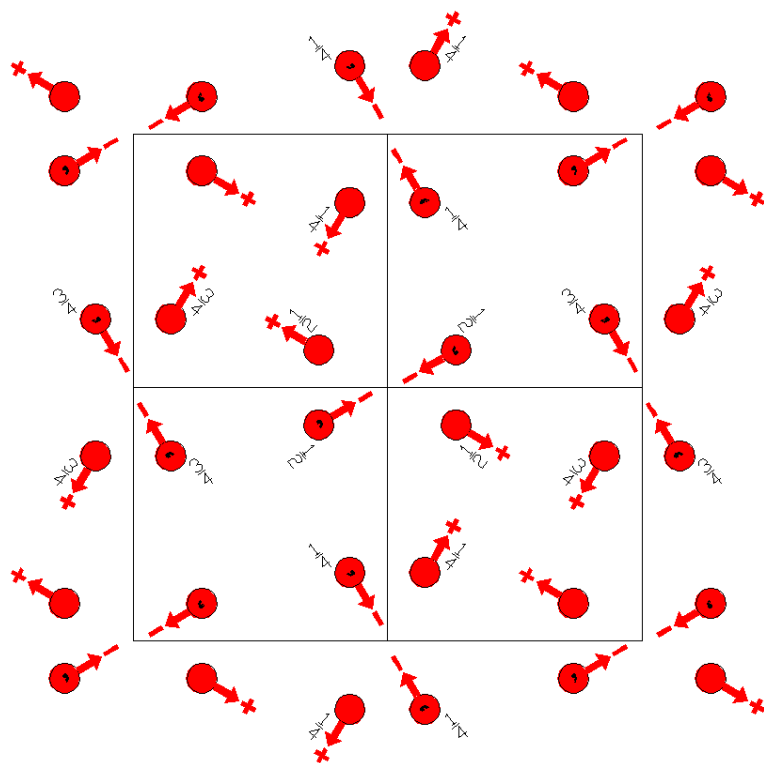
Along [1,1,0]  $p_{2b} 1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I4_1md$   
109.1.901

4mm  
 $I4_1md$

Tetragonal



Origin on 2mm on 2m1

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) 4 <sup>+</sup> (0,0,1/4) -1/4,1/4,z<br>(4 <sub>z</sub>  0,1/2,1/4) | (4) 4 <sup>-</sup> (0,0,1/4) 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4) |
| (5) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (6) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (7) d (-1/4,1/4,1/4) x+1/4,x̄,z<br>(m <sub>xy</sub>  0,1/2,1/4)        | (8) d (1/4,1/4,1/4) x-1/4,x,z<br>(m <sub>xy</sub>  0,1/2,1/4)                       |

For (1/2,1/2,1/2) + set

- |  |  |   |  |
|--|--|---|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                     | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,3/4) 1/4,1/4,z<br>(4 <sub>z</sub>  1/2,0,3/4) | (4) 4 <sup>-</sup> (0,0,3/4) 1/4,-1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,0,3/4) |
| (5) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (6) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (7) d (1/4,-1/4,3/4) x+1/4,x̄,z<br>(m <sub>xy</sub>  1/2,0,3/4)       | (8) d (1/4,1/4,3/4) x+1/4,x,z<br>(m <sub>xy</sub>  1/2,0,3/4)                        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

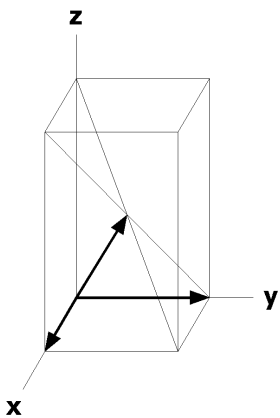
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1/2,1/2,1/2) +		
16	c	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}, x+1/2, z+1/4$ [ $\bar{v}, u, w$ ]	(4) $y, \bar{x}+1/2, z+1/4$ [ $v, \bar{u}, w$ ]		
			(5) $x, \bar{y}, z$ [ $\bar{u}, v, \bar{w}$ ]	(6) $\bar{x}, y, z$ [ $u, \bar{v}, \bar{w}$ ]		
			(7) $\bar{y}, \bar{x}+1/2, z+1/4$ [ $v, u, \bar{w}$ ]	(8) $y, x+1/2, z+1/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
8	b	.m.	0,y,z [0,v,0]	0, $\bar{y}$ ,z [0, $\bar{v}$ , 0]	$\bar{y}, 1/2, z+1/4$ [ $\bar{v}, 0, 0$ ]	y,1/2,z+1/4 [v,0,0]
4	a	2mm.	0,0,z [0,0,0]	0,1/2,z+1/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4gm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] c<sub>p</sub>-1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I4_1md1'$

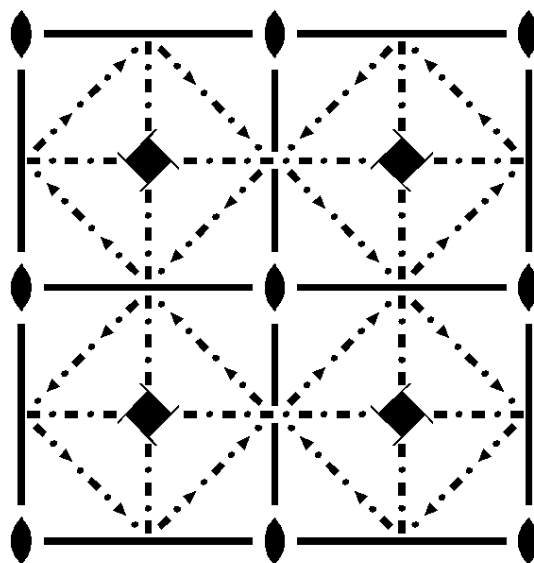
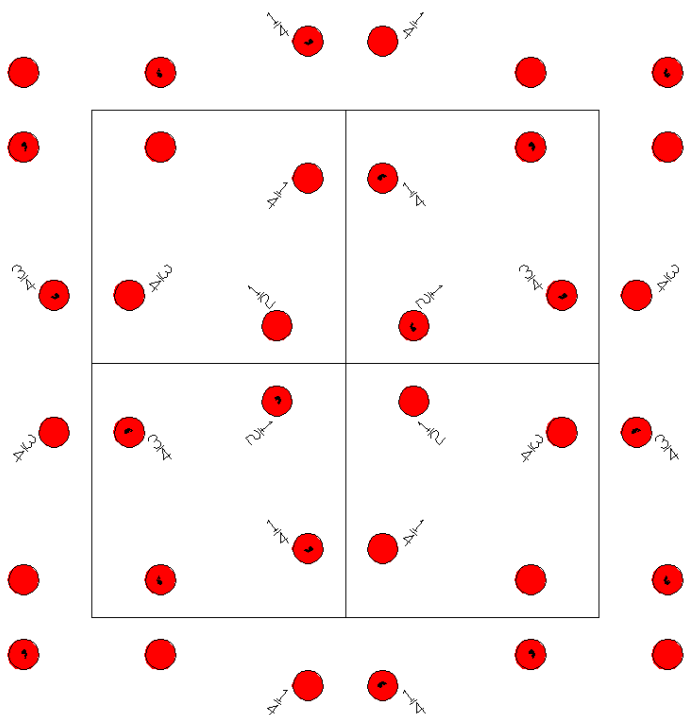
$4mm1'$

Tetragonal

109.2.902

$I4_1md1'$

$1'$



Origin on  $2mm1'$  on  $2m11'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |                                    |                                    |  |   |
|------------------------------------|------------------------------------|--|---|
| (1) $1$<br>( $1 0,0,0$ )           | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ ) | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>( $4_z 0,1/2,1/4$ )            | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>( $4_z^{-1} 0,1/2,1/4$ )       |
| (5) $m$ $x,0,z$<br>( $m_y 0,0,0$ ) | (6) $m$ $0,y,z$<br>( $m_x 0,0,0$ ) | (7) $d$ $(-1/4,1/4,1/4) x+1/4,\bar{x},z$<br>( $m_{xy} 0,1/2,1/4$ ) | (8) $d$ $(1/4,1/4,1/4) x-1/4,x,z$<br>( $m_{\bar{xy}} 0,1/2,1/4$ ) |

For (1/2,1/2,1/2) + set

- |  |  |  |   |
|--|--|--|---|
| (1) $t$ $(1/2,1/2,1/2)$<br>( $1 1/2,1/2,1/2$ )         | (2) $2$ $(0,0,1/2) 1/4,1/4,z$<br>( $2_z 1/2,1/2,1/2$ ) | (3) $4^+$ $(0,0,3/4) 1/4,1/4,z$<br>( $4_z 1/2,0,3/4$ )             | (4) $4^-$ $(0,0,3/4) 1/4,-1/4,z$<br>( $4_z^{-1} 1/2,0,3/4$ )      |
| (5) $n$ $(1/2,0,1/2) x,1/4,z$<br>( $m_y 1/2,1/2,1/2$ ) | (6) $n$ $(0,1/2,1/2) 1/4,y,z$<br>( $m_x 1/2,1/2,1/2$ ) | (7) $d$ $(1/4,-1/4,3/4) x+1/4,\bar{x},z$<br>( $m_{xy} 1/2,0,3/4$ ) | (8) $d$ $(1/4,1/4,3/4) x+1/4,x,z$<br>( $m_{\bar{xy}} 1/2,0,3/4$ ) |

## For (0,0,0)' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> ' (0,0,1/4) -1/4,1/4,z (4 <sub>z</sub>  0,1/2,1/4)'	(4) 4 <sup>-</sup> ' (0,0,1/4) 1/4,1/4,z (4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4)
(5) m' x,0,z (m <sub>y</sub>  0,0,0)'	(6) m' 0,y,z (m <sub>x</sub>  0,0,0)'	(7) d' (-1/4,1/4,1/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>  0,1/2,1/4)'	(8) d' (1/4,1/4,1/4) x-1/4,x,z (m $\bar{xy}$  0,1/2,1/4)'

## For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (1 1/2,1/2,1/2)'	(2) 2' (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>  1/2,1/2,1/2)'	(3) 4 <sup>+</sup> ' (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>  1/2,0,3/4)'	(4) 4 <sup>-</sup> ' (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>  1/2,0,3/4)'
(5) n' (1/2,0,1/2) x,1/4,z (m <sub>y</sub>  1/2,1/2,1/2)'	(6) n' (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1/2)'	(7) d' (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,0,3/4)'	(8) d' (1/4,1/4,3/4) x+1/4,x,z (m $\bar{xy}$  1/2,0,3/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

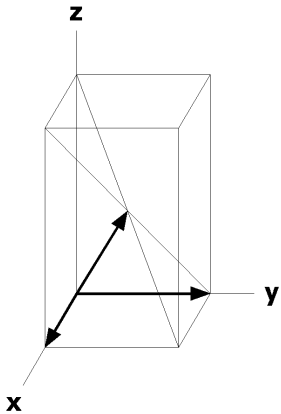
			(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'	
16	c	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	
			(3) $\bar{y},x+1/2,z+1/4$ [0,0,0]	(4) $y,\bar{x}+1/2,z+1/4$ [0,0,0]	
			(5) x, $\bar{y},z$ [0,0,0]	(6) $\bar{x},y,z$ [0,0,0]	
			(7) $\bar{y},\bar{x}+1/2,z+1/4$ [0,0,0]	(8) $y,x+1/2,z+1/4$ [0,0,0]	
8	b	.m.1'	0,y,z [0,0,0]	0, $\bar{y},z$ [0,0,0]	$\bar{y},1/2,z+1/4$ [0,0,0]
4	a	2mm.1'	0,0,z [0,0,0]	0,1/2,z+1/4 [0,0,0]	$y,1/2,z+1/4$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] c1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



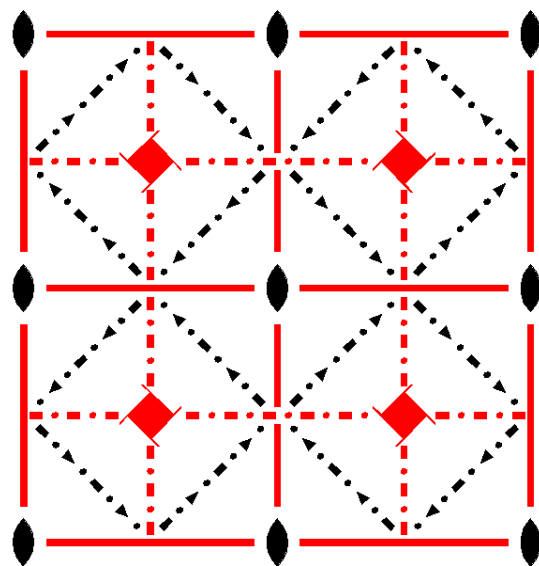
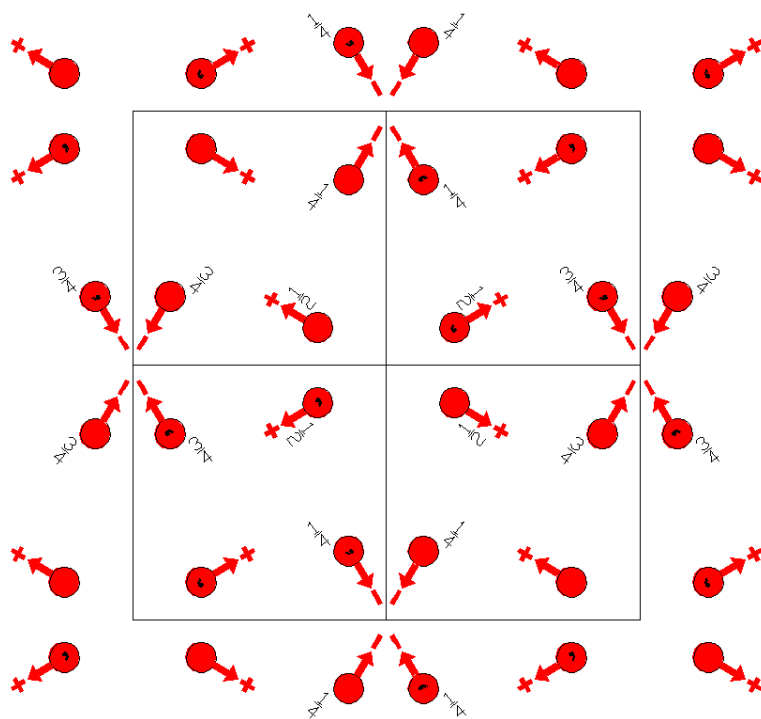
$I4_1'm'd$

109.3.903

$4'm'm$

$I4_1'm'd$

Tetragonal



Origin on  $2m'm'$  on  $2m'1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

For  $(0,0,0)$  + set

- |                                    |                                    |  |   |
|------------------------------------|------------------------------------|--|---|
| (1) 1<br>(1 0,0,0)                 | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)   | (3) $4^+ 1 (0,0,1/4) -1/4,1/4,z$<br>( $4_z$  0,1/2,1/4)'         | (4) $4^- 1 (0,0,1/4) 1/4,1/4,z$<br>( $4_z^{-1}$  0,1/2,1/4)'    |
| (5) $m' x,0,z$<br>( $m_y$  0,0,0)' | (6) $m' 0,y,z$<br>( $m_x$  0,0,0)' | (7) $d (-1/4,1/4,1/4) x+1/4,\bar{x},z$<br>( $m_{xy}$  0,1/2,1/4) | (8) $d (1/4,1/4,1/4) x-1/4,x,z$<br>( $m_{\bar{xy}}$  0,1/2,1/4) |

For  $(1/2,1/2,1/2)$  + set

- |  |  |  |   |
|--|--|--|---|
| (1) $t (1/2,1/2,1/2)$<br>(1 1/2,1/2,1/2)               | (2) 2 $(0,0,1/2) 1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2)   | (3) $4^+ 1 (0,0,3/4) 1/4,1/4,z$<br>( $4_z$  1/2,0,3/4)'          | (4) $4^- 1 (0,0,3/4) 1/4,-1/4,z$<br>( $4_z^{-1}$  1/2,0,3/4)'   |
| (5) $n' (1/2,0,1/2) x,1/4,z$<br>( $m_y$  1/2,1/2,1/2)' | (6) $n' (0,1/2,1/2) 1/4,y,z$<br>( $m_x$  1/2,1/2,1/2)' | (7) $d (1/4,-1/4,3/4) x+1/4,\bar{x},z$<br>( $m_{xy}$  1/2,0,3/4) | (8) $d (1/4,1/4,3/4) x+1/4,x,z$<br>( $m_{\bar{xy}}$  1/2,0,3/4) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
16	c	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}, x+1/2, z+1/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(4) $y, \bar{x}+1/2, z+1/4$ [ $\bar{v}, u, \bar{w}$ ]		
			(5) $x, \bar{y}, z$ [ $u, \bar{v}, w$ ]	(6) $\bar{x}, y, z$ [ $\bar{u}, v, w$ ]		
			(7) $\bar{y}, \bar{x}+1/2, z+1/4$ [ $\bar{v}, u, \bar{w}$ ]	(8) $y, x+1/2, z+1/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
8	b	.m'.	0,y,z [0,v,w]	0, $\bar{y}$ ,z [0, $\bar{v}$ ,w]	$\bar{y}, 1/2, z+1/4$ [v,0, $\bar{w}$ ]	y,1/2,z+1/4 [ $\bar{v}, 0, \bar{w}$ ]
4	a	2m'm'.	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0, $\bar{w}$ ]		

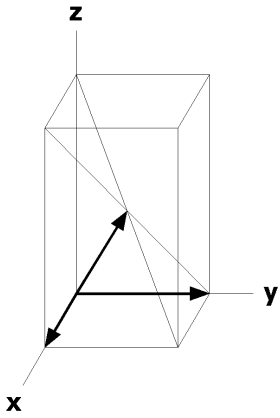
### Symmetry of Special Projections

Along [0,0,1] p4'gm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] c1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] c<sub>p</sub>-1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0





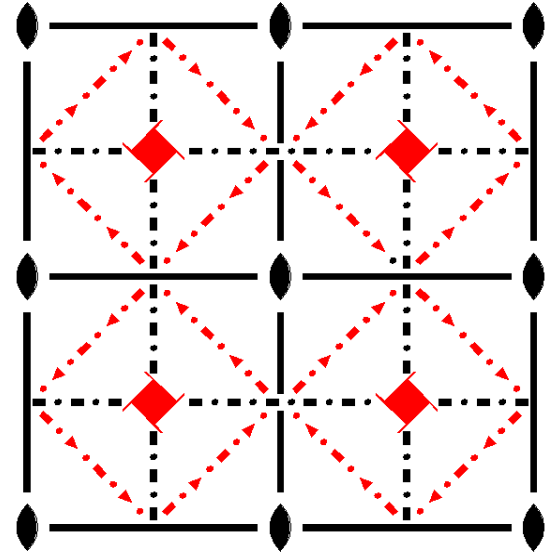
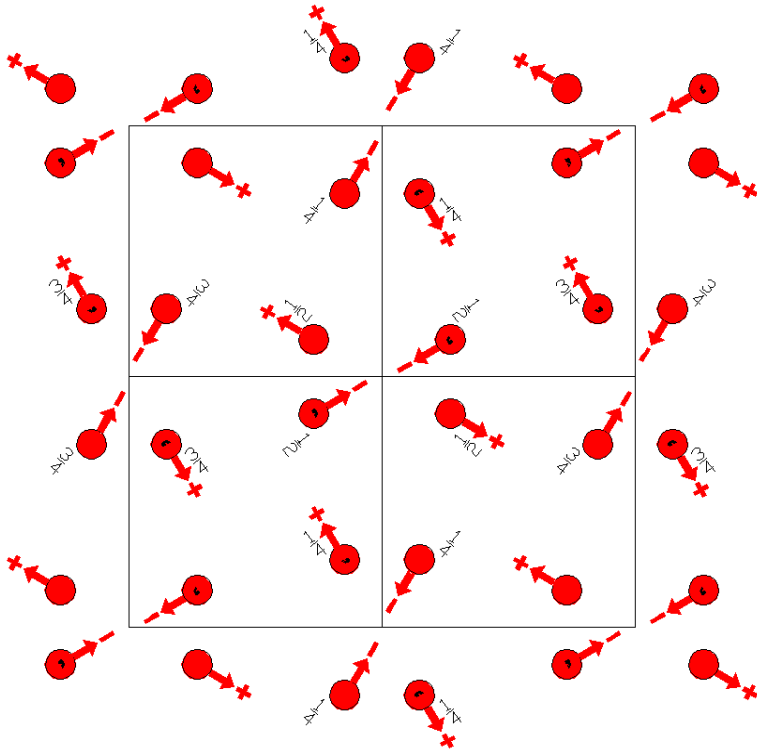
$I4_1'md'$

109.4.904

$4'mm'$

$I4_1'md'$

Tetragonal



Origin on  $2mm$  on  $2m1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For  $(0,0,0)$  + set

- |                                  |                                  |  |   |
|----------------------------------|----------------------------------|--|---|
| (1) 1<br>(1 0,0,0)               | (2) 2 $0,0,z$<br>( $2_z$  0,0,0) | (3) $4^+ ' (0,0,1/4) -1/4,1/4,z$<br>( $4_z$  0,1/2,1/4)'           | (4) $4^- ' (0,0,1/4) 1/4,1/4,z$<br>( $4_z^{-1}$  0,1/2,1/4)'      |
| (5) $m x,0,z$<br>( $m_y$  0,0,0) | (6) $m 0,y,z$<br>( $m_x$  0,0,0) | (7) $d' (-1/4,1/4,1/4) x+1/4,\bar{x},z$<br>( $m_{xy}$  0,1/2,1/4)' | (8) $d' (1/4,1/4,1/4) x-1/4,x,z$<br>( $m_{\bar{xy}}$  0,1/2,1/4)' |

For  $(1/2,1/2,1/2)$  + set

- |  |  |  |   |
|--|--|--|---|
| (1) $t (1/2,1/2,1/2)$<br>(1 1/2,1/2,1/2)             | (2) 2 $(0,0,1/2) 1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2) | (3) $4^+ ' (0,0,3/4) 1/4,1/4,z$<br>( $4_z$  1/2,0,3/4)'            | (4) $4^- ' (0,0,3/4) 1/4,-1/4,z$<br>( $4_z^{-1}$  1/2,0,3/4)'     |
| (5) $n (1/2,0,1/2) x,1/4,z$<br>( $m_y$  1/2,1/2,1/2) | (6) $n (0,1/2,1/2) 1/4,y,z$<br>( $m_x$  1/2,1/2,1/2) | (7) $d' (1/4,-1/4,3/4) x+1/4,\bar{x},z$<br>( $m_{xy}$  1/2,0,3/4)' | (8) $d' (1/4,1/4,3/4) x+1/4,x,z$<br>( $m_{\bar{xy}}$  1/2,0,3/4)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

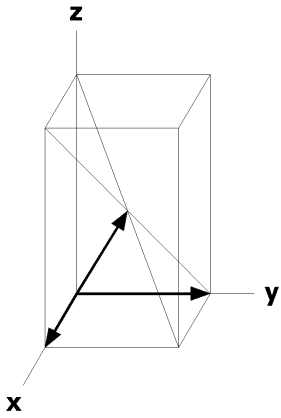
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1/2,1/2,1/2) +		
16	c	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}, x+1/2, z+1/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(4) $y, \bar{x}+1/2, z+1/4$ [ $\bar{v}, u, \bar{w}$ ]		
			(5) $x, \bar{y}, z$ [ $\bar{u}, v, \bar{w}$ ]	(6) $\bar{x}, y, z$ [ $u, \bar{v}, \bar{w}$ ]		
			(7) $\bar{y}, \bar{x}+1/2, z+1/4$ [ $\bar{v}, \bar{u}, w$ ]	(8) $y, x+1/2, z+1/4$ [ $v, u, w$ ]		
8	b	.m.	0,y,z [u,0,0]	0, $\bar{y}$ ,z [ $\bar{u}$ ,0,0]	$\bar{y}, 1/2, z+1/4$ [0, $\bar{u}$ ,0]	y,1/2,z+1/4 [0,u,0]
4	a	2mm.	0,0,z [0,0,0]	0,1/2,z+1/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4'g'm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] c1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



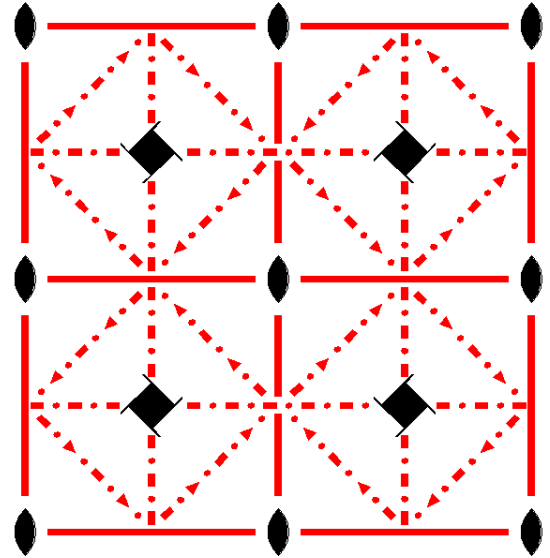
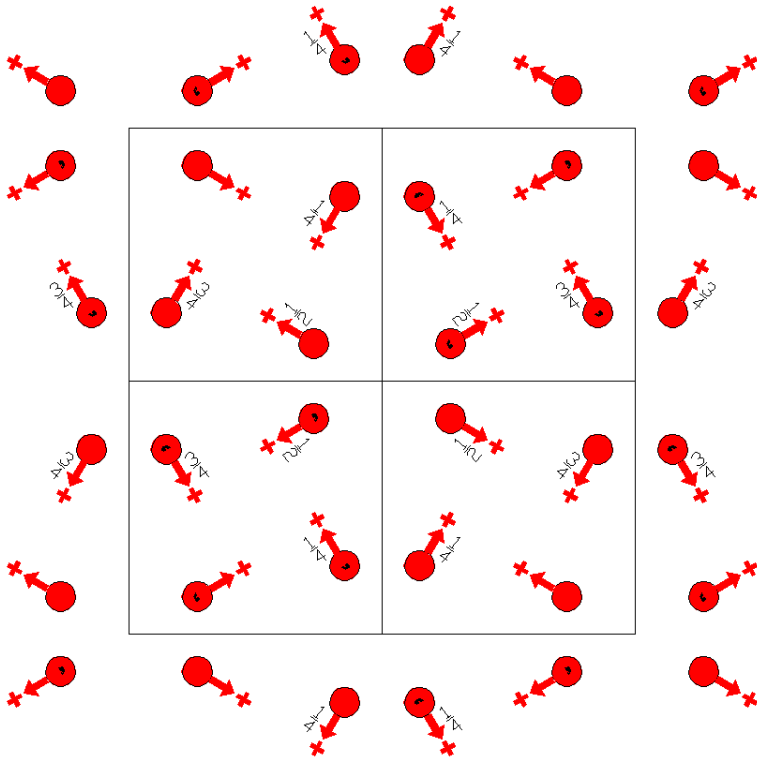
$I4_1m'd'$

109.5.905

$4m'm'$

$I4_1m'd'$

Tetragonal



Origin on  $2m'm'$  on  $2m'1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 4 <sup>+</sup> (0,0,1/4) -1/4,1/4,z<br>(4 <sub>z</sub>  0,1/2,1/4)     | (4) 4 <sup>-</sup> (0,0,1/4) 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4) |
| (5) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (6) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (7) d' (-1/4,1/4,1/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,1/2,1/4)' | (8) d' (1/4,1/4,1/4) x-1/4,x,z<br>(m <sub>xy</sub>  0,1/2,1/4)'                     |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                       | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)   | (3) 4 <sup>+</sup> (0,0,3/4) 1/4,1/4,z<br>(4 <sub>z</sub>  1/2,0,3/4)      | (4) 4 <sup>-</sup> (0,0,3/4) 1/4,-1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,0,3/4) |
| (5) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (6) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (7) d' (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,0,3/4)' | (8) d' (1/4,1/4,3/4) x+1/4,x,z<br>(m <sub>xy</sub>  1/2,0,3/4)'                      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

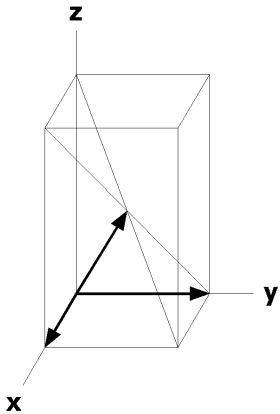
			(0,0,0) +	(1/2,1/2,1/2) +		
16	c	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}, x+1/2, z+1/4$ [ $\bar{v}, u, w$ ]	(4) $y, \bar{x}+1/2, z+1/4$ [v, $\bar{u}, w$ ]		
			(5) $x, \bar{y}, z$ [u, $\bar{v}, w$ ]	(6) $\bar{x}, y, z$ [ $\bar{u}, v, w$ ]		
			(7) $\bar{y}, \bar{x}+1/2, z+1/4$ [ $\bar{v}, \bar{u}, w$ ]	(8) $y, x+1/2, z+1/4$ [v,u,w]		
8	b	.m'	0,y,z [0,v,w]	0, $\bar{y}, z$ [0, $\bar{v}, w$ ]	$\bar{y}, 1/2, z+1/4$ [ $\bar{v}, 0, w$ ]	y,1/2,z+1/4 [v,0,w]
4	a	2m'm'	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p4g'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] c1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

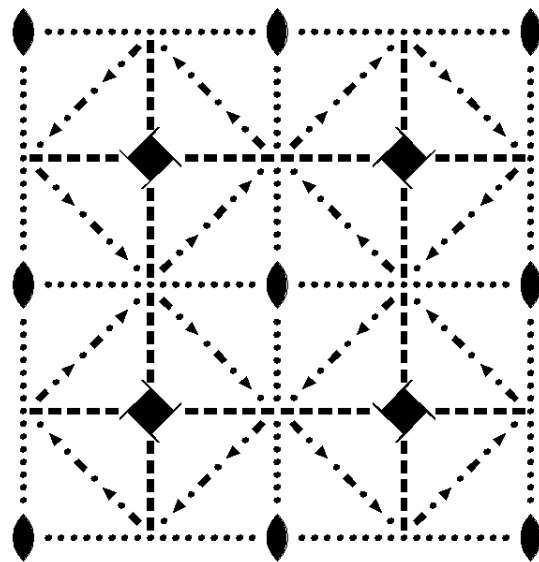
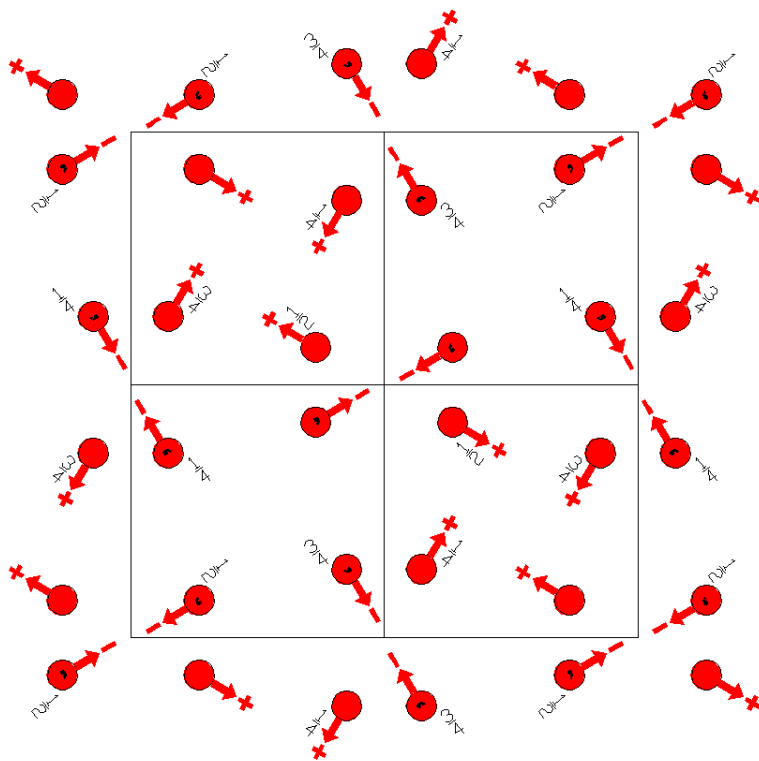
Along [1,1,0] c1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I4_1cd$   
110.1.906

4mm  
 $I4_1cd$

Tetragonal



Origin on  $2c_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)             | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>( $4_z$  0,1/2,1/4)          | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>( $4_z^{-1}$  0,1/2,1/4)     |
| (5) c $(0,0,1/2) x,0,z$<br>( $m_y$  0,0,1/2) | (6) c $(0,0,1/2) 0,y,z$<br>( $m_x$  0,0,1/2) | (7) d $(-1/4,1/4,3/4) x+1/4,\bar{x},z$<br>( $m_{xy}$  0,1/2,3/4) | (8) d $(1/4,1/4,3/4) x-1/4,x,z$<br>( $m_{\bar{xy}}$  0,1/2,3/4) |

For  $(1/2,1/2,1/2)$  + set

- |  |  |  |   |
|--|--|--|---|
| (1) t $(1/2,1/2,1/2)$<br>(1 1/2,1/2,1/2)         | (2) 2 $(0,0,1/2) 1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2) | (3) $4^+$ $(0,0,3/4) 1/4,1/4,z$<br>( $4_z$  1/2,0,3/4)           | (4) $4^-$ $(0,0,3/4) 1/4,-1/4,z$<br>( $4_z^{-1}$  1/2,0,3/4)    |
| (5) a $(1/2,0,0) x,1/4,z$<br>( $m_y$  1/2,1/2,0) | (6) b $(0,1/2,0) 1/4,y,z$<br>( $m_x$  1/2,1/2,0)     | (7) d $(1/4,-1/4,1/4) x+1/4,\bar{x},z$<br>( $m_{xy}$  1/2,0,1/4) | (8) d $(1/4,1/4,1/4) x+1/4,x,z$<br>( $m_{\bar{xy}}$  1/2,0,1/4) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

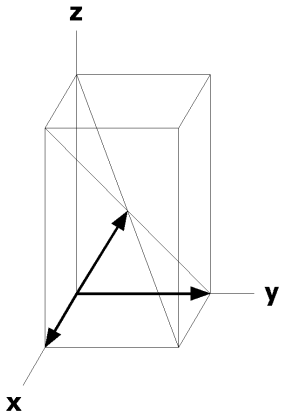
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1/2,1/2,1/2) +		
16	b	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}, x+1/2, z+1/4$ [ $\bar{v}, u, w$ ]	(4) $y, \bar{x}+1/2, z+1/4$ [ $v, \bar{u}, w$ ]		
			(5) $x, \bar{y}, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(6) $\bar{x}, y, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]		
			(7) $\bar{y}, \bar{x}+1/2, z+3/4$ [ $v, u, \bar{w}$ ]	(8) $y, x+1/2, z+3/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
8	a	2..	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2,z+3/4 [0,0, $\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4gm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] p<sub>2b</sub>\*1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0] c<sub>2</sub>\*1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I4_1cd1'$

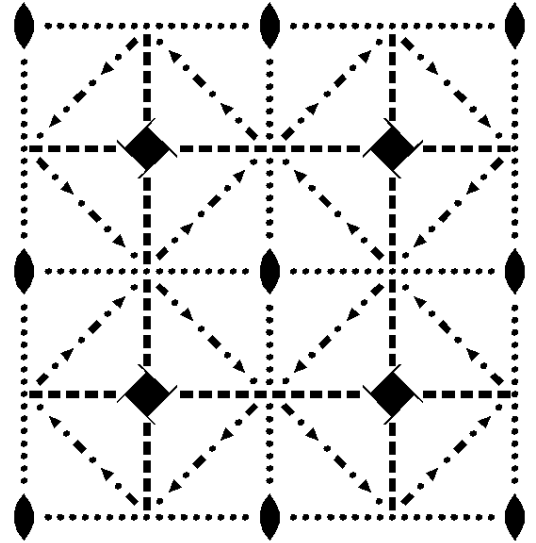
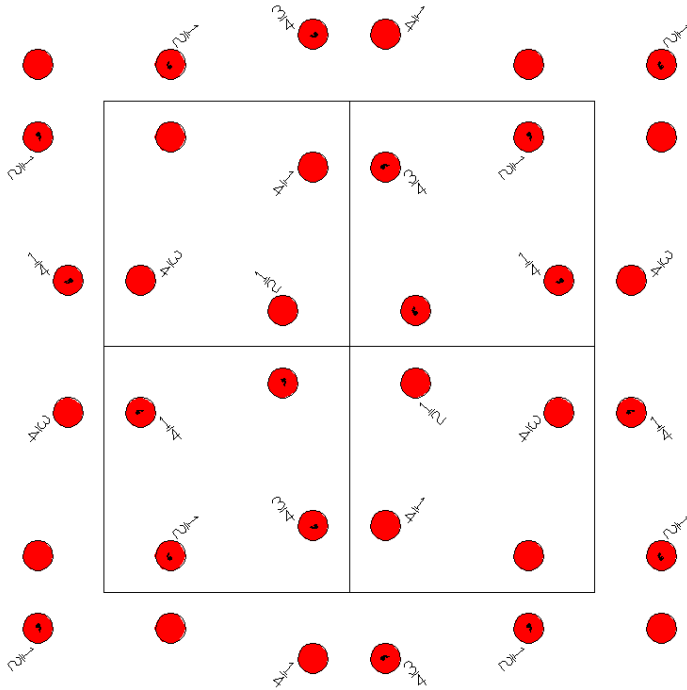
$4mm1'$

Tetragonal

110.2.907

$I4_1cd1'$

1'



Origin on  $2c11'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)             | (3) $4^+$ (0,0,1/4) $-1/4,1/4,z$<br>( $4_z$  0,1/2,1/4)            | (4) $4^-$ (0,0,1/4) $1/4,1/4,z$<br>( $4_z^{-1}$  0,1/2,1/4)       |
| (5) c (0,0,1/2) $x,0,z$<br>( $m_y$  0,0,1/2) | (6) c (0,0,1/2) $0,y,z$<br>( $m_x$  0,0,1/2) | (7) d $(-1/4,1/4,3/4)$ $x+1/4,\bar{x},z$<br>( $m_{xy}$  0,1/2,3/4) | (8) d $(1/4,1/4,3/4)$ $x-1/4,x,z$<br>( $m_{\bar{xy}}$  0,1/2,3/4) |

For (1/2,1/2,1/2) + set

- |  |  |  |   |
|--|--|--|---|
| (1) t $(1/2,1/2,1/2)$<br>(1 1/2,1/2,1/2)           | (2) 2 $(0,0,1/2)$ $1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2) | (3) $4^+$ (0,0,3/4) $1/4,1/4,z$<br>( $4_z$  1/2,0,3/4)             | (4) $4^-$ (0,0,3/4) $1/4,-1/4,z$<br>( $4_z^{-1}$  1/2,0,3/4)      |
| (5) a $(1/2,0,0)$ $x,1/4,z$<br>( $m_y$  1/2,1/2,0) | (6) b $(0,1/2,0)$ $1/4,y,z$<br>( $m_x$  1/2,1/2,0)     | (7) d $(1/4,-1/4,1/4)$ $x+1/4,\bar{x},z$<br>( $m_{xy}$  1/2,0,1/4) | (8) d $(1/4,1/4,1/4)$ $x+1/4,x,z$<br>( $m_{\bar{xy}}$  1/2,0,1/4) |

## For (0,0,0)' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> ' (0,0,1/4) -1/4,1/4,z (4 <sub>z</sub>  0,1/2,1/4)'	(4) 4 <sup>-</sup> ' (0,0,1/4) 1/4,1/4,z (4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4)'
(5) c' (0,0,1/2) x,0,z (m <sub>y</sub>  0,0,1/2)'	(6) c' (0,0,1/2) 0,y,z (m <sub>x</sub>  0,0,1/2)'	(7) d' (-1/4,1/4,3/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>  0,1/2,3/4)'	(8) d' (1/4,1/4,3/4) x-1/4,x,z (m $\bar{xy}$  0,1/2,3/4)'

## For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (1 1/2,1/2,1/2)'	(2) 2' (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>  1/2,1/2,1/2)'	(3) 4 <sup>+</sup> ' (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>  1/2,0,3/4)'	(4) 4 <sup>-</sup> ' (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>  1/2,0,3/4)'
(5) a' (1/2,0,0) x,1/4,z (m <sub>y</sub>  1/2,1/2,0)'	(6) b' (0,1/2,0) 1/4,y,z (m <sub>x</sub>  1/2,1/2,0)'	(7) d' (1/4,-1/4,1/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,0,1/4)'	(8) d' (1/4,1/4,1/4) x+1/4,x,z (m $\bar{xy}$  1/2,0,1/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

			(0,0,0) + (0,0,0)' +	(1/2,1/2,1/2) + (1/2,1/2,1/2)' +	
16	b	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	
			(3) $\bar{y},x+1/2,z+1/4$ [0,0,0]	(4) $y,\bar{x}+1/2,z+1/4$ [0,0,0]	
			(5) $x,\bar{y},z+1/2$ [0,0,0]	(6) $\bar{x},y,z+1/2$ [0,0,0]	
			(7) $\bar{y},\bar{x}+1/2,z+3/4$ [0,0,0]	(8) $y,x+1/2,z+3/4$ [0,0,0]	
8	a	2..1'	0,0,z [0,0,0]	0,1/2,z+1/4 [0,0,0]	0,0,z+1/2 [0,0,0]
					0,1/2,z+3/4 [0,0,0]

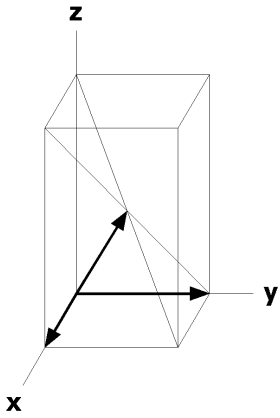
**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0] c1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

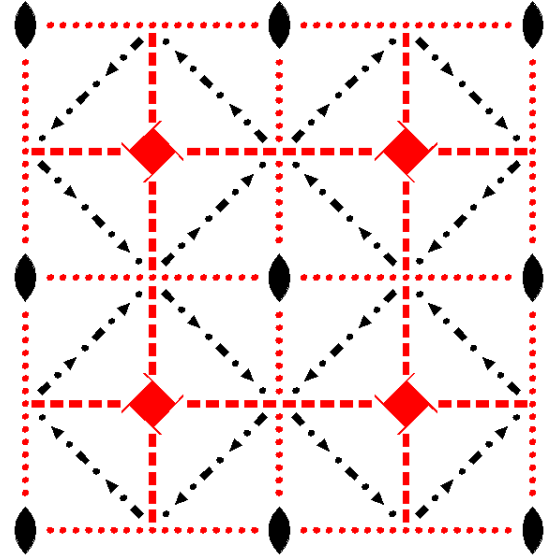
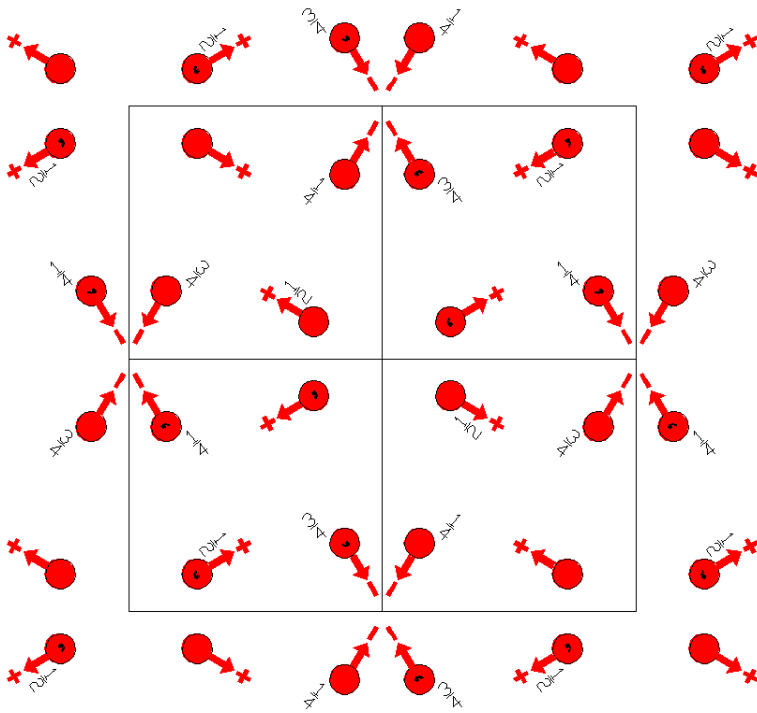




$I4_1'c'd$   
110.3.908

$4'm'm$   
 $I4_1'c'd$

Tetragonal



Origin on  $2c'1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                               | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                 | (3) $4^+ 1$ $(0,0,1/4) -1/4,1/4,z$<br>( $4_z$  0,1/2,1/4)'         | (4) $4^- 1$ $(0,0,1/4) 1/4,1/4,z$<br>( $4_z^{-1}$  0,1/2,1/4)'    |
| (5) $c'$ $(0,0,1/2) x,0,z$<br>( $m_y$  0,0,1/2)' | (6) $c'$ $(0,0,1/2) 0,y,z$<br>( $m_x$  0,0,1/2)' | (7) $d$ $(-1/4,1/4,3/4) x+1/4,\bar{x},z$<br>( $m_{xy}$  0,1/2,3/4) | (8) $d$ $(1/4,1/4,3/4) x-1/4,x,z$<br>( $m_{\bar{xy}}$  0,1/2,3/4) |

For  $(1/2,1/2,1/2)$  + set

- |  |  |  |   |
|--|--|--|---|
| (1) $t$ $(1/2,1/2,1/2)$<br>(1 1/2,1/2,1/2)           | (2) 2 $(0,0,1/2) 1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2) | (3) $4^+ 1$ $(0,0,3/4) 1/4,1/4,z$<br>( $4_z$  1/2,0,3/4)'          | (4) $4^- 1$ $(0,0,3/4) 1/4,-1/4,z$<br>( $4_z^{-1}$  1/2,0,3/4)'   |
| (5) $a'$ $(1/2,0,0) x,1/4,z$<br>( $m_y$  1/2,1/2,0)' | (6) $b'$ $(0,1/2,0) 1/4,y,z$<br>( $m_x$  1/2,1/2,0)' | (7) $d$ $(1/4,-1/4,1/4) x+1/4,\bar{x},z$<br>( $m_{xy}$  1/2,0,1/4) | (8) $d$ $(1/4,1/4,1/4) x+1/4,x,z$<br>( $m_{\bar{xy}}$  1/2,0,1/4) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

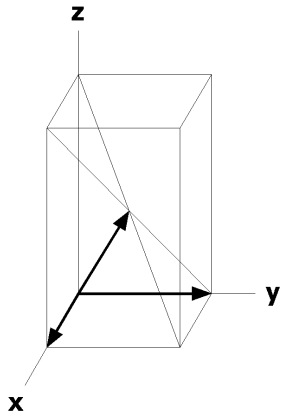
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1/2,1/2,1/2) +		
16	b	1	(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}, x+1/2, z+1/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(4) $y, \bar{x}+1/2, z+1/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
			(5) $x, \bar{y}, z+1/2$ [ $u, \bar{v}, w$ ]	(6) $\bar{x}, y, z+1/2$ [ $\bar{u}, v, w$ ]		
			(7) $\bar{y}, \bar{x}+1/2, z+3/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(8) $y, x+1/2, z+3/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
8	a	2..	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]	0,1/2,z+3/4 [0,0, $\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4'gm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] p1m'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

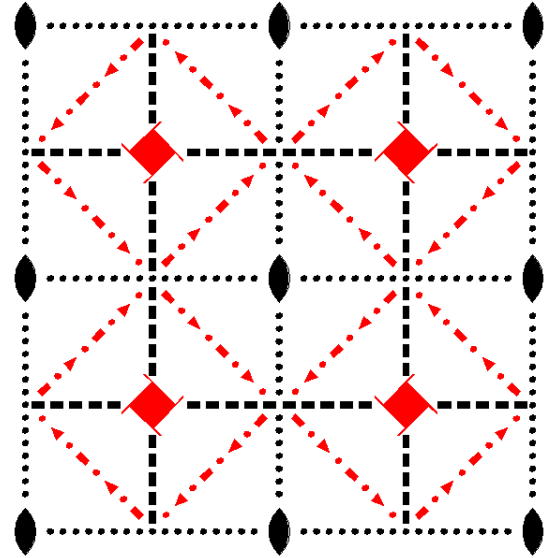
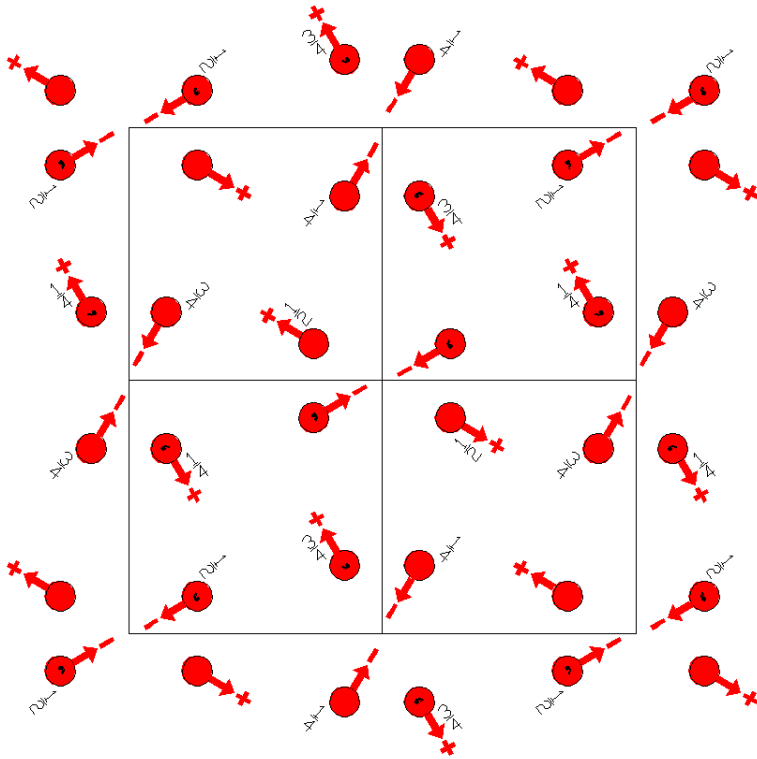
Along [1,1,0] c<sub>2v</sub>'1m'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I4_1'cd'$   
110.4.909

$4'mm'$   
 $I4_1'cd'$

Tetragonal



Origin on  $2c_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For  $(0,0,0)$  + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)             | (3) $4^+ (0,0,1/4) -1/4,1/4,z$<br>( $4_z$  0,1/2,1/4)'             | (4) $4^- (0,0,1/4) 1/4,1/4,z$<br>( $4_z^{-1}$  0,1/2,1/4)'        |
| (5) c $(0,0,1/2) x,0,z$<br>( $m_y$  0,0,1/2) | (6) c $(0,0,1/2) 0,y,z$<br>( $m_x$  0,0,1/2) | (7) $d' (-1/4,1/4,3/4) x+1/4,\bar{x},z$<br>( $m_{xy}$  0,1/2,3/4)' | (8) $d' (1/4,1/4,3/4) x-1/4,x,z$<br>( $m_{\bar{xy}}$  0,1/2,3/4)' |

For  $(1/2,1/2,1/2)$  + set

- |  |  |  |   |
|--|--|--|---|
| (1) t $(1/2,1/2,1/2)$<br>(1 1/2,1/2,1/2)         | (2) 2 $(0,0,1/2) 1/4,1/4,z$<br>( $2_z$  1/2,1/2,1/2) | (3) $4^+ (0,0,3/4) 1/4,1/4,z$<br>( $4_z$  1/2,0,3/4)'              | (4) $4^- (0,0,3/4) 1/4,-1/4,z$<br>( $4_z^{-1}$  1/2,0,3/4)'       |
| (5) a $(1/2,0,0) x,1/4,z$<br>( $m_y$  1/2,1/2,0) | (6) b $(0,1/2,0) 1/4,y,z$<br>( $m_x$  1/2,1/2,0)     | (7) $d' (1/4,-1/4,1/4) x+1/4,\bar{x},z$<br>( $m_{xy}$  1/2,0,1/4)' | (8) $d' (1/4,1/4,1/4) x+1/4,x,z$<br>( $m_{\bar{xy}}$  1/2,0,1/4)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

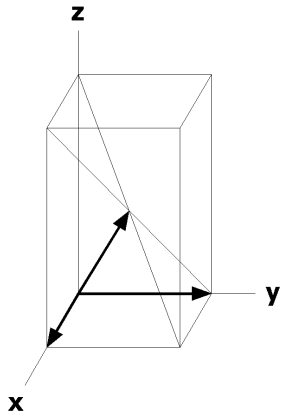
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1/2,1/2,1/2) +		
16	b	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$		
			(3) $\bar{y},x+1/2,z+1/4 [v,\bar{u},\bar{w}]$	(4) $y,\bar{x}+1/2,z+1/4 [\bar{v},u,\bar{w}]$		
			(5) $x,\bar{y},z+1/2 [\bar{u},v,\bar{w}]$	(6) $\bar{x},y,z+1/2 [u,\bar{v},\bar{w}]$		
			(7) $\bar{y},\bar{x}+1/2,z+3/4 [\bar{v},\bar{u},w]$	(8) $y,x+1/2,z+3/4 [v,u,w]$		
8	a	2..	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2,z+3/4 [0,0,w]

**Symmetry of Special Projections**

Along [0,0,1] p4'g'm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] p<sub>2b</sub>'1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

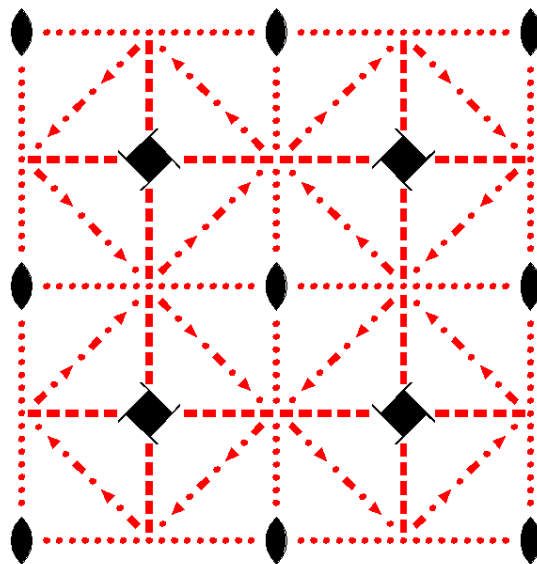
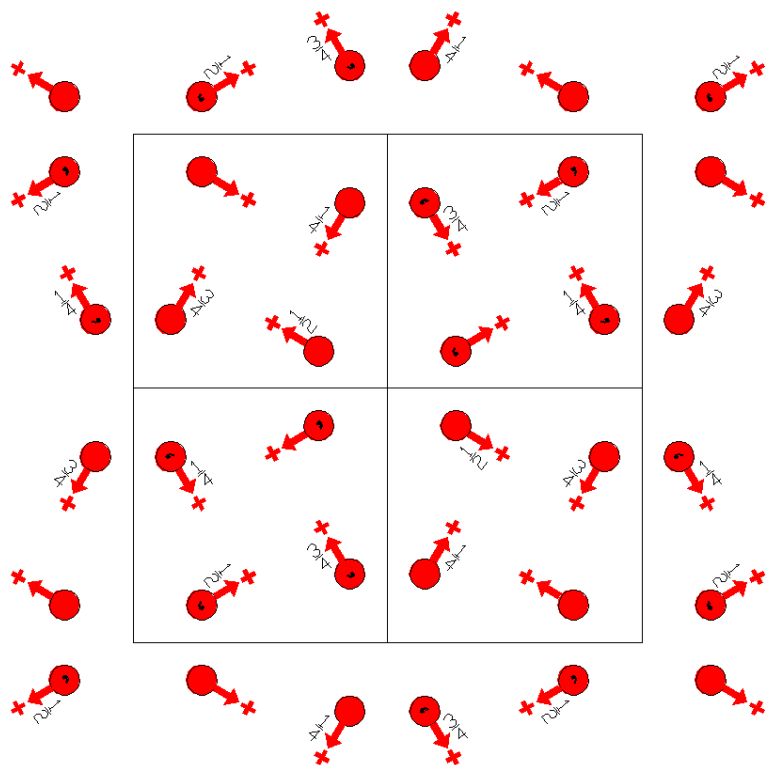
Along [1,1,0] c1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I4_1c'd'$   
110.5.910

$4m'm'$   
 $I4_1c'd'$

Tetragonal



Origin on  $2c'1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                                   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)               | (3) 4 <sup>+</sup> (0,0,1/4) -1/4,1/4,z<br>(4 <sub>z</sub>  0,1/2,1/4)     | (4) 4 <sup>-</sup> (0,0,1/4) 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4) |
| (5) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' | (7) d' (-1/4,1/4,3/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,1/2,3/4)' | (8) d' (1/4,1/4,3/4) x-1/4,x,z<br>(m <sub>xy</sub>  0,1/2,3/4)'                     |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                   | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,3/4) 1/4,1/4,z<br>(4 <sub>z</sub>  1/2,0,3/4)      | (4) 4 <sup>-</sup> (0,0,3/4) 1/4,-1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,0,3/4) |
| (5) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (6) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)'   | (7) d' (1/4,-1/4,1/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,0,1/4)' | (8) d' (1/4,1/4,1/4) x+1/4,x,z<br>(m <sub>xy</sub>  1/2,0,1/4)'                      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

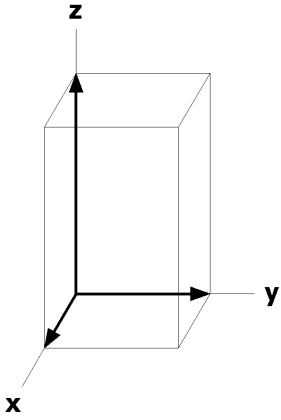
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
			(0,0,0) +	(1/2,1/2,1/2) +		
16	b	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$		
			(3) $\bar{y},x+1/2,z+1/4 [\bar{v},u,w]$	(4) $y,\bar{x}+1/2,z+1/4 [v,\bar{u},w]$		
			(5) $x,\bar{y},z+1/2 [u,\bar{v},w]$	(6) $\bar{x},y,z+1/2 [\bar{u},v,w]$		
			(7) $\bar{y},\bar{x}+1/2,z+3/4 [\bar{v},\bar{u},w]$	(8) $y,x+1/2,z+3/4 [v,u,w]$		
8	a	2..	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0,w]	0,0,z+1/2 [0,0,w]	0,1/2,z+3/4 [0,0,w]

**Symmetry of Special Projections**

Along [0,0,1] p4g'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,1/4,z

Along [1,0,0] p1m'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

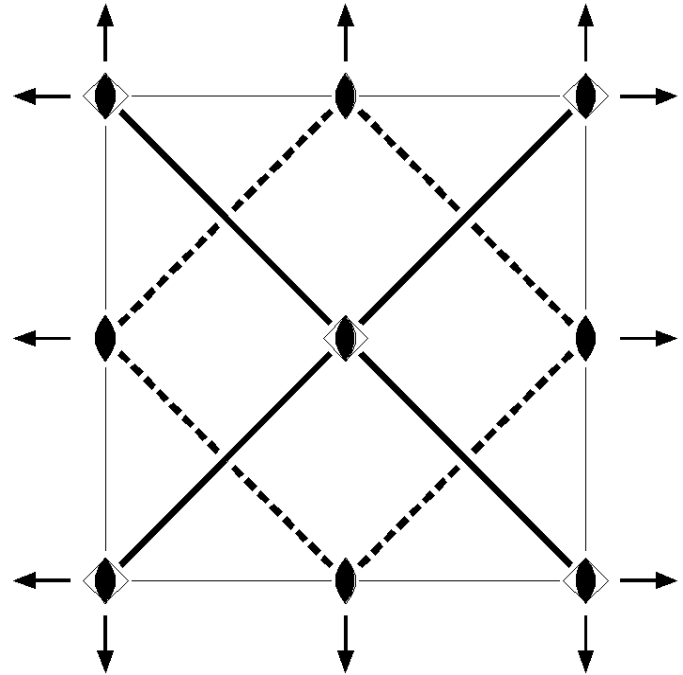
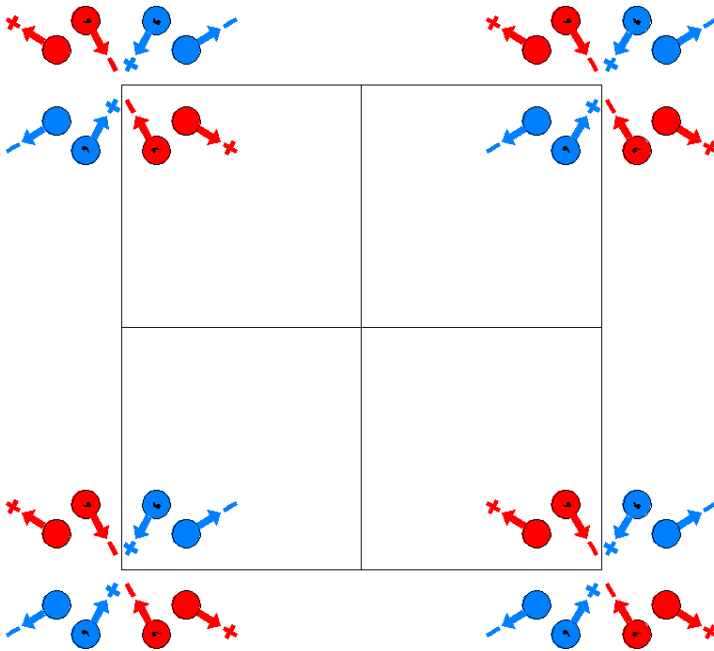
Along [1,1,0] c1m'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P\bar{4}2m$   
111.1.911

$\bar{4}2m$   
 $P\bar{4}2m$

Tetragonal



Origin on  $\bar{4}2m$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$ ;  $x \leq y$

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $\bar{4}^+$   $0,0,z$ ;  $0,0,0$   
( $\bar{4}_z$ |0,0,0)

(4)  $\bar{4}^-$   $0,0,z$ ;  $0,0,0$   
( $\bar{4}_z^{-1}$ |0,0,0)

(5) 2  $0,y,0$   
( $2_y$ |0,0,0)

(6) 2  $x,0,0$   
( $2_x$ |0,0,0)

(7)  $m$   $x,\bar{x},z$   
( $m_{xy}$ |0,0,0)

(8)  $m$   $x,x,z$   
( $m_{\bar{xy}}$ |0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

8	o	1	(1) x,y,z [u,v,w] (5) $\overline{x},\overline{y},\overline{z}$ [ $\overline{u},\overline{v},\overline{w}$ ]	(2) $\overline{x},\overline{y},z$ [ $\overline{u},\overline{v},w$ ] (6) x, $\overline{y},\overline{z}$ [u, $\overline{v},\overline{w}$ ]	(3) y, $\overline{x},\overline{z}$ [ $\overline{v},u,w$ ] (7) $\overline{y},\overline{x},z$ [v,u, $\overline{w}$ ]	(4) $\overline{y},x,\overline{z}$ [v, $\overline{u},w$ ] (8) y,x,z [ $\overline{v},\overline{u},\overline{w}$ ]
4	n	..m	x,x,z [ $\overline{u},u,0$ ]	$\overline{x},\overline{x},z$ [u, $\overline{u},0$ ]	x, $\overline{x},\overline{z}$ [ $\overline{u},\overline{u},0$ ]	$\overline{x},x,\overline{z}$ [u,u,0]
4	m	2..	0,1/2,z [0,0,w]	1/2,0, $\overline{z}$ [0,0,w]	0,1/2, $\overline{z}$ [0,0, $\overline{w}$ ]	1/2,0,z [0,0, $\overline{w}$ ]
4	l	.2.	x,1/2,0 [u,0,0]	$\overline{x},1/2,0$ [ $\overline{u},0,0$ ]	1/2, $\overline{x},0$ [0,u,0]	1/2,x,0 [0, $\overline{u},0$ ]
4	k	.2.	x,0,1/2 [u,0,0]	$\overline{x},0,1/2$ [ $\overline{u},0,0$ ]	0, $\overline{x},1/2$ [0,u,0]	0,x,1/2 [0, $\overline{u},0$ ]
4	j	.2.	x,1/2,1/2 [u,0,0]	$\overline{x},1/2,1/2$ [ $\overline{u},0,0$ ]	1/2, $\overline{x},1/2$ [0,u,0]	1/2,x,1/2 [0, $\overline{u},0$ ]
4	i	.2.	x,0,0 [u,0,0]	$\overline{x},0,0$ [ $\overline{u},0,0$ ]	0, $\overline{x},0$ [0,u,0]	0,x,0 [0, $\overline{u},0$ ]
2	h	2.mm	1/2,1/2,z [0,0,0]	1/2,1/2, $\overline{z}$ [0,0,0]		
2	g	2.mm	0,0,z [0,0,0]	0,0, $\overline{z}$ [0,0,0]		
2	f	222.	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	e	222.	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
1	d	$\overline{4}2m$	1/2,1/2,0 [0,0,0]			
1	c	$\overline{4}2m$	0,0,1/2 [0,0,0]			
1	b	$\overline{4}2m$	1/2,1/2,1/2 [0,0,0]			
1	a	$\overline{4}2m$	0,0,0 [0,0,0]			

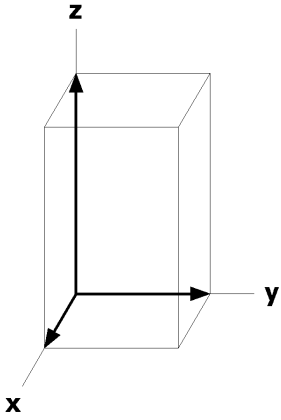
**Symmetry of Special Projections**

Along [0,0,1]  $p4'mm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,0,0

Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,x,0



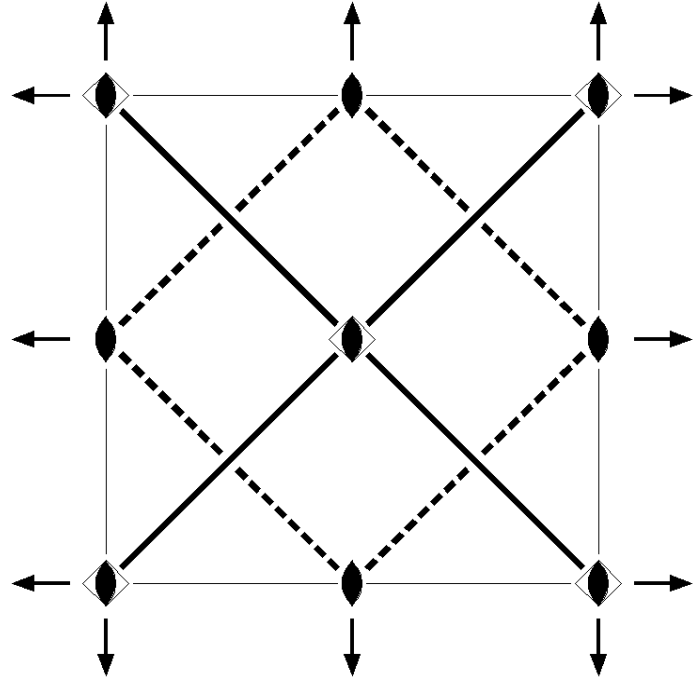
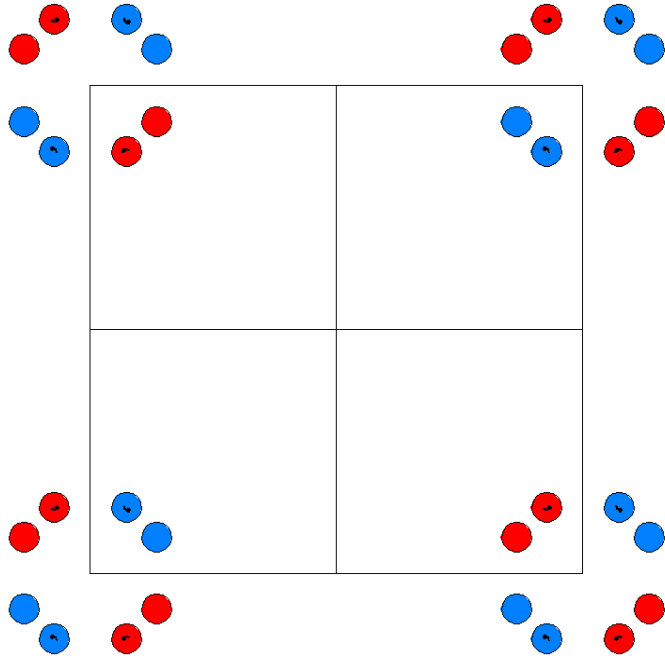


$P\bar{4}2m1'$   
111.2.912

$\bar{4}2m1'$   
 $P\bar{4}2m1'$

Tetragonal

1'



Origin on  $\bar{4}2m1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

For 1 + set

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                                | (2) 2 <sub>0,0,z</sub><br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ <sub>0,0,z</sub><br>( $\bar{4}_z^+$  0,0,0)           | (4) $\bar{4}^-$ <sub>0,0,z</sub><br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) 2 <sub>0,y,0</sub><br>(2 <sub>y</sub>  0,0,0) | (6) 2 <sub>x,0,0</sub><br>(2 <sub>x</sub>  0,0,0) | (7) m <sub>x,<math>\bar{x}</math>,z</sub><br>(m <sub>xy</sub>  0,0,0) | (8) m <sub>x,x,z</sub><br>(m <sub>xy</sub>  0,0,0)             |

For 1' + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1'<br>(1 0,0,0)'                                | (2) 2' <sub>0,0,z</sub><br>(2 <sub>z</sub>  0,0,0)' | (3) $\bar{4}^+$ ' <sub>0,0,z</sub><br>( $\bar{4}_z^+$  0,0,0)'          | (4) $\bar{4}^-$ ' <sub>0,0,z</sub><br>( $\bar{4}_z^{-1}$  0,0,0)' |
| (5) 2' <sub>0,y,0</sub><br>(2 <sub>y</sub>  0,0,0)' | (6) 2' <sub>x,0,0</sub><br>(2 <sub>x</sub>  0,0,0)' | (7) m' <sub>x,<math>\bar{x}</math>,z</sub><br>(m <sub>xy</sub>  0,0,0)' | (8) m' <sub>x,x,z</sub><br>(m <sub>xy</sub>  0,0,0)'              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

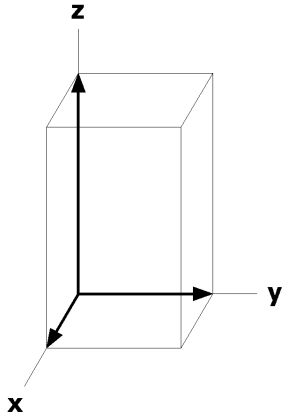
			Coordinates			
			1+		1' +	
8	o	11'	(1) x,y,z [0,0,0]	(2) $\overline{x},\overline{y},z$ [0,0,0]	(3) $y,\overline{x},\overline{z}$ [0,0,0]	(4) $\overline{y},x,\overline{z}$ [0,0,0]
			(5) $\overline{x},y,\overline{z}$ [0,0,0]	(6) $x,\overline{y},\overline{z}$ [0,0,0]	(7) $\overline{y},\overline{x},z$ [0,0,0]	(8) y,x,z [0,0,0]
4	n	..m1'	x,x,z [0,0,0]	$\overline{x},\overline{x},z$ [0,0,0]	$x,\overline{x},\overline{z}$ [0,0,0]	$\overline{x},x,\overline{z}$ [0,0,0]
4	m	2..1'	0,1/2,z [0,0,0]	1/2,0, $\overline{z}$ [0,0,0]	0,1/2, $\overline{z}$ [0,0,0]	1/2,0,z [0,0,0]
4	l	.2.1'	x,1/2,0 [0,0,0]	$\overline{x},1/2,0$ [0,0,0]	1/2, $\overline{x},0$ [0,0,0]	1/2,x,0 [0,0,0]
4	k	.2.1'	x,0,1/2 [0,0,0]	$\overline{x},0,1/2$ [0,0,0]	0, $\overline{x},1/2$ [0,0,0]	0,x,1/2 [0,0,0]
4	j	.2.1'	x,1/2,1/2 [0,0,0]	$\overline{x},1/2,1/2$ [0,0,0]	1/2, $\overline{x},1/2$ [0,0,0]	1/2,x,1/2 [0,0,0]
4	i	.2.1'	x,0,0 [0,0,0]	$\overline{x},0,0$ [0,0,0]	0, $\overline{x},0$ [0,0,0]	0,x,0 [0,0,0]
2	h	2.mm1'	1/2,1/2,z [0,0,0]	1/2,1/2, $\overline{z}$ [0,0,0]		
2	g	2.mm1'	0,0,z [0,0,0]	0,0, $\overline{z}$ [0,0,0]		
2	f	222.1'	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	e	222.1'	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
1	d	$\overline{4}2m1'$	1/2,1/2,0 [0,0,0]			
1	c	$\overline{4}2m1'$	0,0,1/2 [0,0,0]			
1	b	$\overline{4}2m1'$	1/2,1/2,1/2 [0,0,0]			
1	a	$\overline{4}2m1'$	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

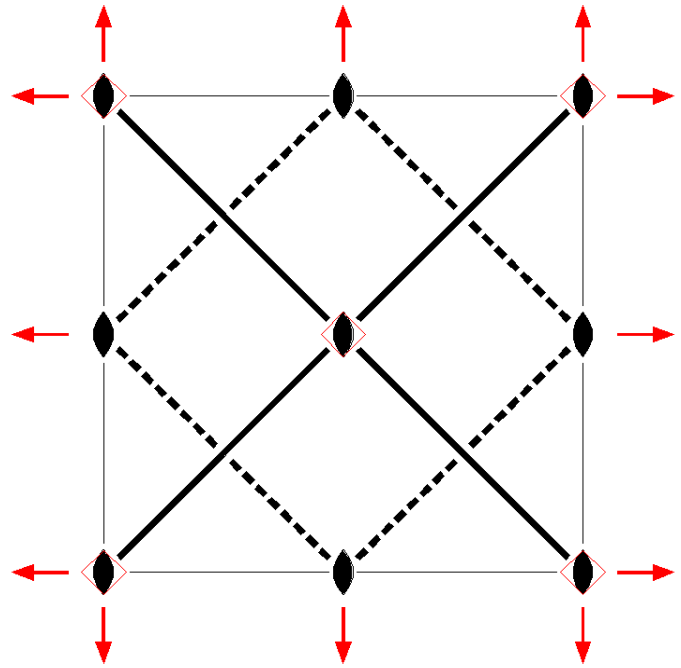
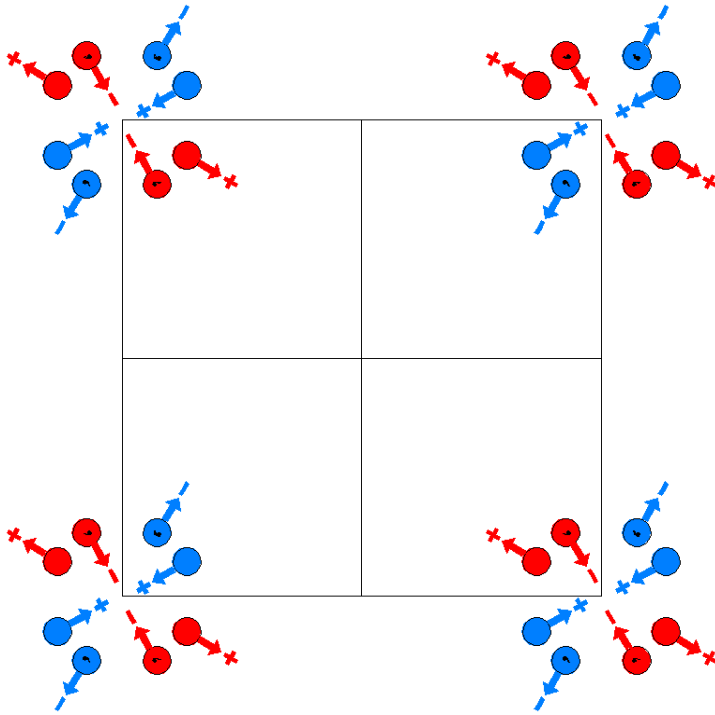
Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P\bar{4}'2'm$   
111.3.913

$\bar{4}'2'm$   
 $P\bar{4}'2'm$

Tetragonal



Origin on  $\bar{4}'2'm$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$ ;  $x \leq y$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)' |
| (5) 2' <sub>y</sub> 0,y,0<br>(2' <sub>y</sub>  0,0,0)' | (6) 2' <sub>x</sub> x,0,0<br>(2' <sub>x</sub>  0,0,0)' | (7) m <sub>xy</sub> x,x,z<br>(m <sub>xy</sub>  0,0,0)    | (8) m <sub>xy</sub> x,x,z<br>(m <sub>xy</sub>  0,0,0)    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

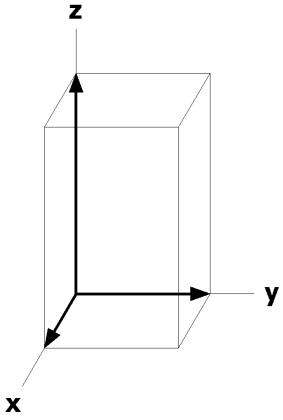
8	o	1	(1) x,y,z [u,v,w] (5) $\overline{x},\overline{y},\overline{z}$ [u,v,w]	(2) $\overline{x},\overline{y},z$ [ $\overline{u},\overline{v},w$ ] (6) x, $\overline{y},\overline{z}$ [ $\overline{u},v,w$ ]	(3) y, $\overline{x},\overline{z}$ [v, $\overline{u},\overline{w}$ ] (7) $\overline{y},\overline{x},z$ [v,u, $\overline{w}$ ]	(4) $\overline{y},x,\overline{z}$ [ $\overline{v},u,\overline{w}$ ] (8) y,x,z [ $\overline{v},\overline{u},\overline{w}$ ]
4	n	..m	x,x,z [u, $\overline{u},0$ ]	$\overline{x},\overline{x},z$ [ $\overline{u},u,0$ ]	x, $\overline{x},\overline{z}$ [ $\overline{u},\overline{u},0$ ]	$\overline{x},x,\overline{z}$ [u,u,0]
4	m	2..	0,1/2,z [0,0,w]	1/2,0, $\overline{z}$ [0,0, $\overline{w}$ ]	0,1/2, $\overline{z}$ [0,0,w]	1/2,0,z [0,0, $\overline{w}$ ]
4	l	.2'	x,1/2,0 [0,v,w]	$\overline{x},1/2,0$ [0, $\overline{v},w$ ]	1/2, $\overline{x},0$ [v,0, $\overline{w}$ ]	1/2,x,0 [ $\overline{v},0,\overline{w}$ ]
4	k	.2'	x,0,1/2 [0,v,w]	$\overline{x},0,1/2$ [0, $\overline{v},w$ ]	0, $\overline{x},1/2$ [v,0, $\overline{w}$ ]	0,x,1/2 [ $\overline{v},0,\overline{w}$ ]
4	j	.2'	x,1/2,1/2 [0,v,w]	$\overline{x},1/2,1/2$ [0, $\overline{v},w$ ]	1/2, $\overline{x},1/2$ [v,0, $\overline{w}$ ]	1/2,x,1/2 [ $\overline{v},0,\overline{w}$ ]
4	i	.2'	x,0,0 [0,v,w]	$\overline{x},0,0$ [0, $\overline{v},w$ ]	0, $\overline{x},0$ [v,0, $\overline{w}$ ]	0,x,0 [ $\overline{v},0,\overline{w}$ ]
2	h	2.mm	1/2,1/2,z [0,0,0]	1/2,1/2, $\overline{z}$ [0,0,0]		
2	g	2.mm	0,0,z [0,0,0]	0,0, $\overline{z}$ [0,0,0]		
2	f	22'2'	1/2,0,1/2 [0,0,w]	0,1/2,1/2 [0,0, $\overline{w}$ ]		
2	e	22'2'	1/2,0,0 [0,0,w]	0,1/2,0 [0,0, $\overline{w}$ ]		
1	d	$\overline{4}2'm$	1/2,1/2,0 [0,0,w]			
1	c	$\overline{4}2'm$	0,0,1/2 [0,0,w]			
1	b	$\overline{4}2'm$	1/2,1/2,1/2 [0,0,w]			
1	a	$\overline{4}2'm$	0,0,0 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1]  $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at x,0,0

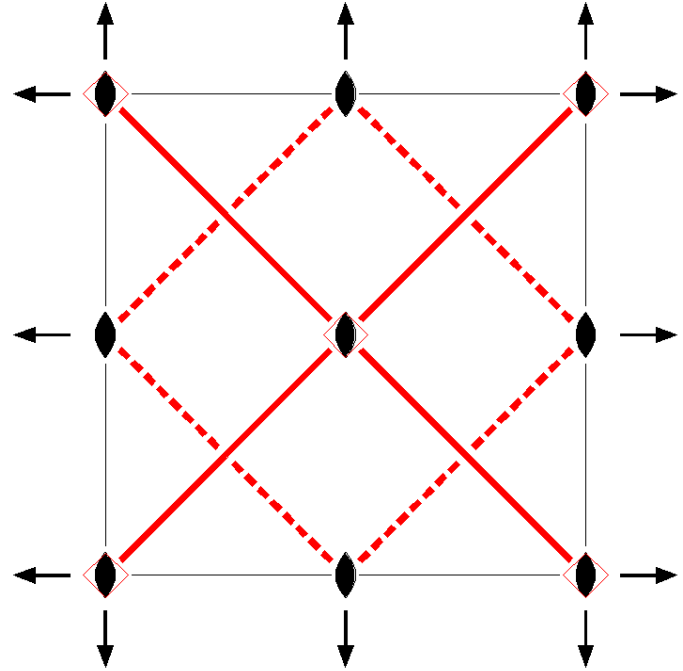
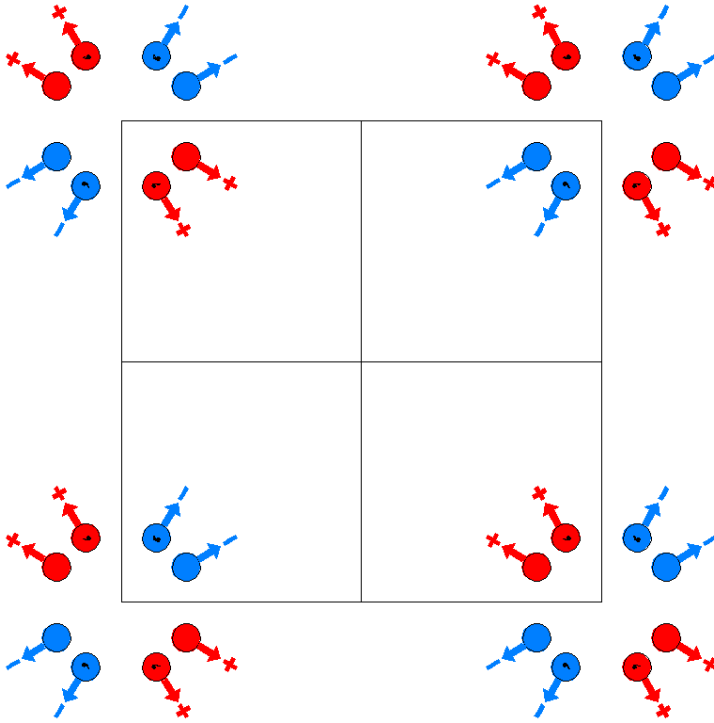
Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,x,0



$P\bar{4}'2m'$   
111.4.914

$\bar{4}'2m'$   
 $P\bar{4}'2m'$

Tetragonal



Origin on  $\bar{4}'2m'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$ ;  $x \leq y$

**Symmetry Operations**

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}'^+$ 0,0,z; 0,0,0<br>( $\bar{4}'_z$  0,0,0)' | (4) $\bar{4}'^-$ 0,0,z; 0,0,0<br>( $\bar{4}'_z^{-1}$  0,0,0)' |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) m' x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)'      | (8) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

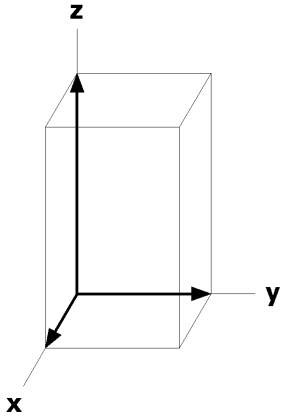
8	o	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(3) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ] (7) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ] (8) y,x,z [v,u,w]
4	n	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},\bar{z}$ [u, $\bar{u},\bar{w}$ ]	$\bar{x},x,\bar{z}$ [ $\bar{u},u,\bar{w}$ ]
4	m	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0,z [0,0,w]
4	l	.2.	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	1/2, $\bar{x},0$ [0, $\bar{u},0$ ]	1/2,x,0 [0,u,0]
4	k	.2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0, $\bar{x},1/2$ [0, $\bar{u},0$ ]	0,x,1/2 [0,u,0]
4	j	.2.	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	1/2, $\bar{x},1/2$ [0, $\bar{u},0$ ]	1/2,x,1/2 [0,u,0]
4	i	.2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0, $\bar{x},0$ [0, $\bar{u},0$ ]	0,x,0 [0,u,0]
2	h	2.m'm'	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	g	2.m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	f	222.	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
2	e	222.	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
1	d	$\overline{4}2m'$	1/2,1/2,0 [0,0,0]			
1	c	$\overline{4}2m'$	0,0,1/2 [0,0,0]			
1	b	$\overline{4}2m'$	1/2,1/2,1/2 [0,0,0]			
1	a	$\overline{4}2m'$	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,0,0

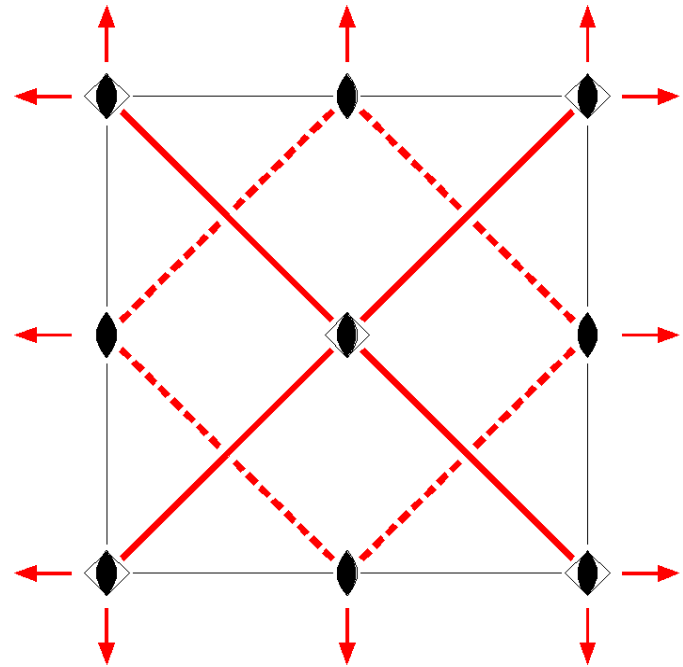
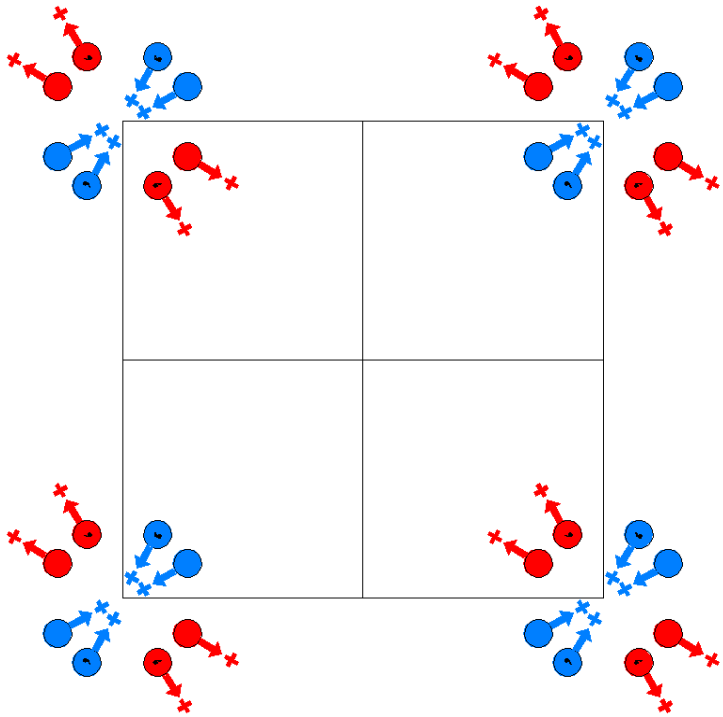
Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,x,0



$P\bar{4}2'm'$   
111.5.915

$\bar{4}2'm'$   
 $P\bar{4}2'm'$

Tetragonal



Origin on  $\bar{4}2'm'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' | (7) m' x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)'   | (8) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

8	o	1	(1) x,y,z [u,v,w] (5) $\overline{x},\overline{y},\overline{z}$ [u, $\overline{v}$ ,w]	(2) $\overline{x},\overline{y},z$ [ $\overline{u},\overline{v}$ ,w] (6) x, $\overline{y},\overline{z}$ [ $\overline{u},v$ ,w]	(3) y, $\overline{x},\overline{z}$ [ $\overline{v},u$ ,w] (7) $\overline{y},\overline{x},z$ [ $\overline{v},\overline{u}$ ,w]	(4) $\overline{y},x,\overline{z}$ [v, $\overline{u}$ ,w] (8) y,x,z [v,u,w]
4	n	..m'	x,x,z [u,u,w]	$\overline{x},\overline{x},z$ [ $\overline{u},\overline{u}$ ,w]	x, $\overline{x},\overline{z}$ [ $\overline{u},u$ ,w]	$\overline{x},x,\overline{z}$ [u, $\overline{u}$ ,w]
4	m	2..	0,1/2,z [0,0,w]	1/2,0, $\overline{z}$ [0,0,w]	0,1/2, $\overline{z}$ [0,0,w]	1/2,0,z [0,0,w]
4	l	.2'	x,1/2,0 [0,v,w]	$\overline{x},1/2,0$ [0, $\overline{v}$ ,w]	1/2, $\overline{x},0$ [ $\overline{v},0$ ,w]	1/2,x,0 [v,0,w]
4	k	.2'	x,0,1/2 [0,v,w]	$\overline{x},0,1/2$ [0, $\overline{v}$ ,w]	0, $\overline{x},1/2$ [ $\overline{v},0$ ,w]	0,x,1/2 [v,0,w]
4	j	.2'	x,1/2,1/2 [0,v,w]	$\overline{x},1/2,1/2$ [0, $\overline{v}$ ,w]	1/2, $\overline{x},1/2$ [ $\overline{v},0$ ,w]	1/2,x,1/2 [v,0,w]
4	i	.2'	x,0,0 [0,v,w]	$\overline{x},0,0$ [0, $\overline{v}$ ,w]	0, $\overline{x},0$ [ $\overline{v},0$ ,w]	0,x,0 [v,0,w]
2	h	2.m'm'	1/2,1/2,z [0,0,w]	1/2,1/2, $\overline{z}$ [0,0,w]		
2	g	2.m'm'	0,0,z [0,0,w]	0,0, $\overline{z}$ [0,0,w]		
2	f	22'2'	1/2,0,1/2 [0,0,w]	0,1/2,1/2 [0,0,w]		
2	e	22'2'	1/2,0,0 [0,0,w]	0,1/2,0 [0,0,w]		
1	d	$\overline{4}2'm'$	1/2,1/2,0 [0,0,w]			
1	c	$\overline{4}2'm'$	0,0,1/2 [0,0,w]			
1	b	$\overline{4}2'm'$	1/2,1/2,1/2 [0,0,w]			
1	a	$\overline{4}2'm'$	0,0,0 [0,0,w]			

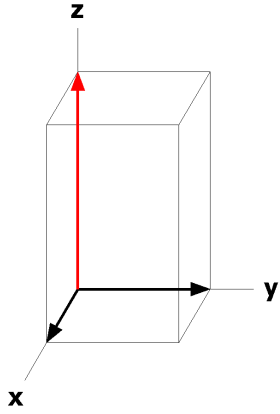
**Symmetry of Special Projections**

Along [0,0,1]  $p4'mm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at x,0,0

Along [1,1,0]  $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,x,0

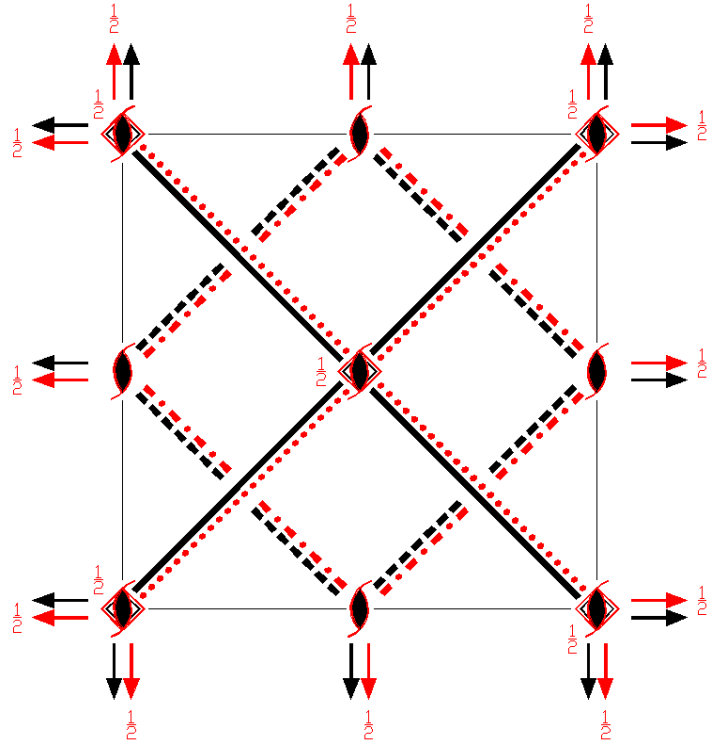
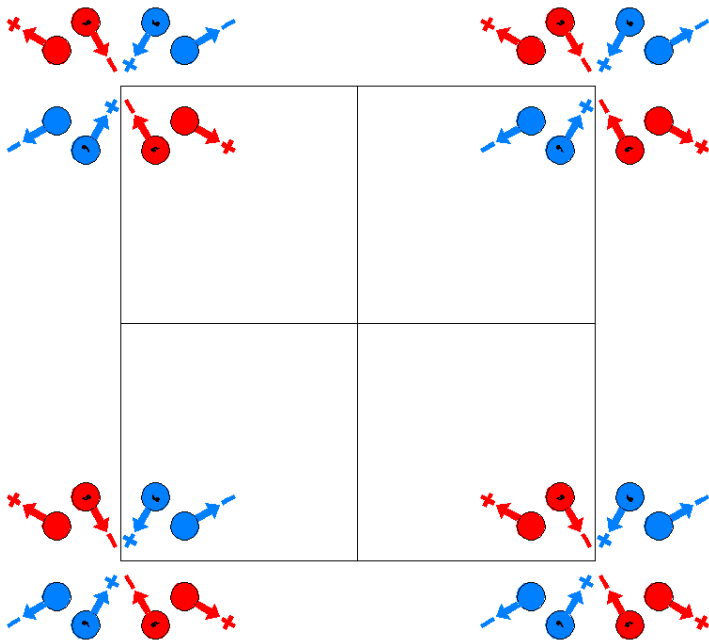




$P_{2c} \bar{4}2m$   
111.6.916

$\bar{4}2m1'$   
 $P_{2c} \bar{4}2m$

Tetragonal



Origin on  $\bar{4}2m$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

### Symmetry Operations

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                                | (2) 2 <sub>0,0,z</sub><br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ <sub>0,0,z</sub> ; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)   | (4) $\bar{4}^-$ <sub>0,0,z</sub> ; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)   |
| (5) 2 <sub>0,y,0</sub><br>(2 <sub>y</sub>  0,0,0) | (6) 2 <sub>x,0,0</sub><br>(2 <sub>x</sub>  0,0,0) | (7) m <sub>x,<math>\bar{x}</math>,z</sub><br>(m <sub>xy</sub>  0,0,0) | (8) m <sub>x,x,z</sub><br>(m <sub><math>\bar{xy}</math></sub>  0,0,0) |

For (0,0,1/2) + set

- |   |   |  |   |
|---|---|--|---|
| (1) t' <sub>(0,0,1)</sub><br>(1 0,0,1)'               | (2) 2' <sub>(0,0,1)</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,1)' | (3) $\bar{4}^+$ ' <sub>0,0,z</sub> ; 0,0,1/2<br>( $\bar{4}_z^+$  0,0,1)' | (4) $\bar{4}^-$ ' <sub>0,0,z</sub> ; 0,0,1/2<br>( $\bar{4}_z^-$  0,0,1)'        |
| (5) 2' <sub>0,y,1/2</sub><br>(2 <sub>y</sub>  0,0,1)' | (6) 2' <sub>x,0,1/2</sub><br>(2 <sub>x</sub>  0,0,1)'       | (7) c' <sub>(0,0,1)</sub> x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1)'   | (8) c' <sub>(0,0,1)</sub> x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,1)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

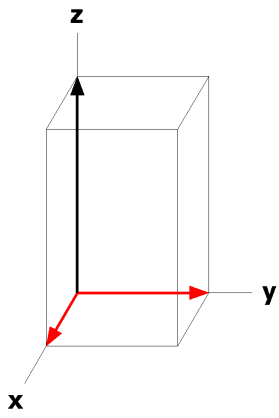
				(0,0,0)+	(0,0,1)' +	
16	o	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(3) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ] (7) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [v, $\bar{u},w$ ] (8) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
8	n	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [u, $\bar{u},0$ ]	x, $\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,\bar{z}$ [u,u,0]
8	m	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0,z [0,0, $\bar{w}$ ]
8	l	.2.	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	1/2, $\bar{x},0$ [0,u,0]	1/2,x,0 [0, $\bar{u},0$ ]
8	k	.2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	0, $\bar{x},1/2$ [v,0, $\bar{w}$ ]	0,x,1/2 [ $\bar{v},0,\bar{w}$ ]
8	j	.2'	x,1/2,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0, $\bar{v},w$ ]	1/2, $\bar{x},1/2$ [v,0, $\bar{w}$ ]	1/2,x,1/2 [ $\bar{v},0,\bar{w}$ ]
8	i	.2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0, $\bar{x},0$ [0,u,0]	0,x,0 [0, $\bar{u},0$ ]
4	h	2.mm	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
4	g	2.mm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4	f	22'2'	1/2,0,1/2 [0,0,w]	0,1/2,1/2 [0,0, $\bar{w}$ ]		
4	e	222.	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]		
2	d	$\bar{4}2m$	1/2,1/2,0 [0,0,0]			
2	c	$\bar{4}'2'm$	0,0,1/2 [0,0,0]			
2	b	$\bar{4}'2'm$	1/2,1/2,1/2 [0,0,0]			
2	a	$\bar{4}2m$	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a'} 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



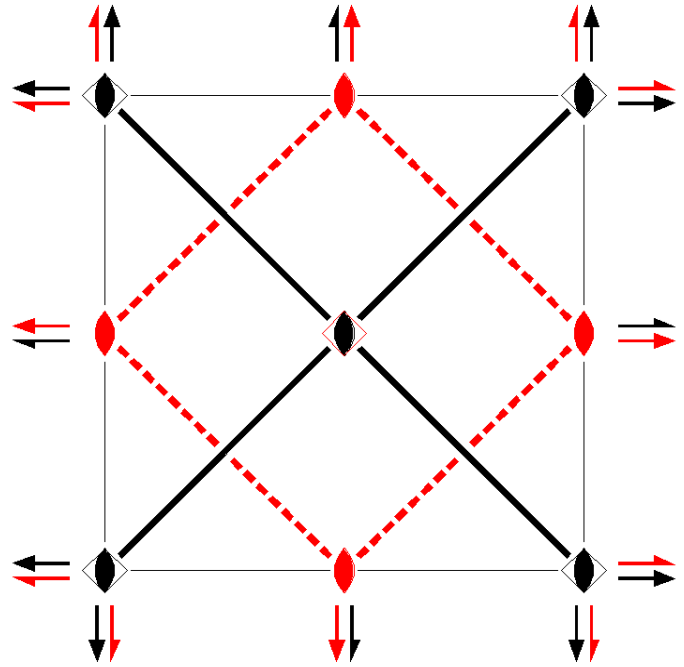
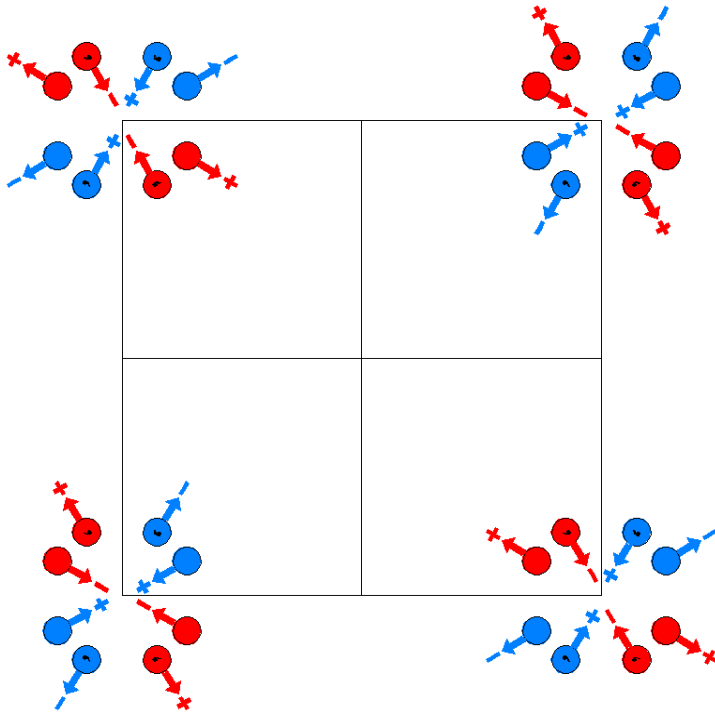
$P_p\bar{4}2m$

111.7.917

$\bar{4}2m1'$

$P_p\bar{4}2m$

Tetragonal



Origin on  $\bar{4}2m$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

Symmetry Operations

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) m x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)       | (8) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                 |

For (1,0,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1,0,0)<br>(1 1,0,0)'               | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'       | (3) $\bar{4}^+$ ' 1/2,-1/2,z; 1/2,-1/2,0<br>( $\bar{4}_z^+$  1,0,0)' | (4) $\bar{4}^-$ ' 1/2,1/2,z; 1/2,1/2,0<br>( $\bar{4}_z^-$  1,0,0)' |
| (5) 2' 1/2,y,0<br>(2 <sub>y</sub>  1,0,0)' | (6) 2' (1,0,0) x,0,0<br>(2 <sub>x</sub>  1,0,0)' | (7) g' (1/2,-1/2,0) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1,0,0)' | (8) g' (1/2,1/2,0) x+1/2,x,z<br>(m <sub>xy</sub>  1,0,0)'          |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

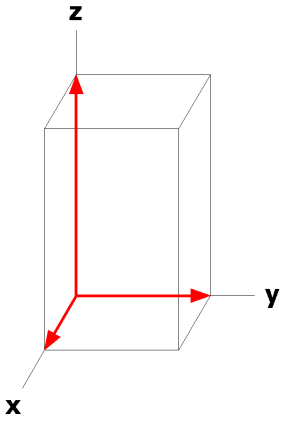
			(0,0,0) + (1,0,0)' +			
16	o	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ] (7) $\bar{y},\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ] (8) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
8	n	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,\bar{z}$ [ $\bar{u},u,0$ ]
8	m	2'..	0,1/2,z [u,v,0]	1/2,0, $\bar{z}$ [ $\bar{v},u,0$ ]	0,1/2, $\bar{z}$ [ $\bar{u},v,0$ ]	1/2,0,z [ $\bar{v},\bar{u},0$ ]
8	l	.2'	x,1/2,0 [0,v,w]	$\bar{x},1/2,0$ [0,v, $\bar{w}$ ]	1/2, $\bar{x},0$ [ $\bar{v},0,w$ ]	1/2,x,0 [ $\bar{v},0,\bar{w}$ ]
8	k	.2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0, $\bar{x},1/2$ [0,u,0]	0,x,1/2 [0, $\bar{u},0$ ]
8	j	.2'	x,1/2,1/2 [0,v,w]	$\bar{x},1/2,1/2$ [0,v, $\bar{w}$ ]	1/2, $\bar{x},1/2$ [ $\bar{v},0,w$ ]	1/2,x,1/2 [ $\bar{v},0,\bar{w}$ ]
8	i	.2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0, $\bar{x},0$ [0,u,0]	0,x,0 [0, $\bar{u},0$ ]
4	h	2.mm	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
4	g	2.mm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4	f	2'22'	1/2,0,1/2 [u,0,0]	0,1/2,1/2 [0, $\bar{u},0$ ]		
4	e	2'22'	1/2,0,0 [u,0,0]	0,1/2,0 [0, $\bar{u},0$ ]		
2	d	$\bar{4}'2'm$	1/2,1/2,0 [0,0,0]			
2	c	$\bar{4}2m$	0,0,1/2 [0,0,0]			
2	b	$\bar{4}'2'm$	1/2,1/2,1/2 [0,0,0]			
2	a	$\bar{4}2m$	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1]  $p_2, 4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/2,1/2,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

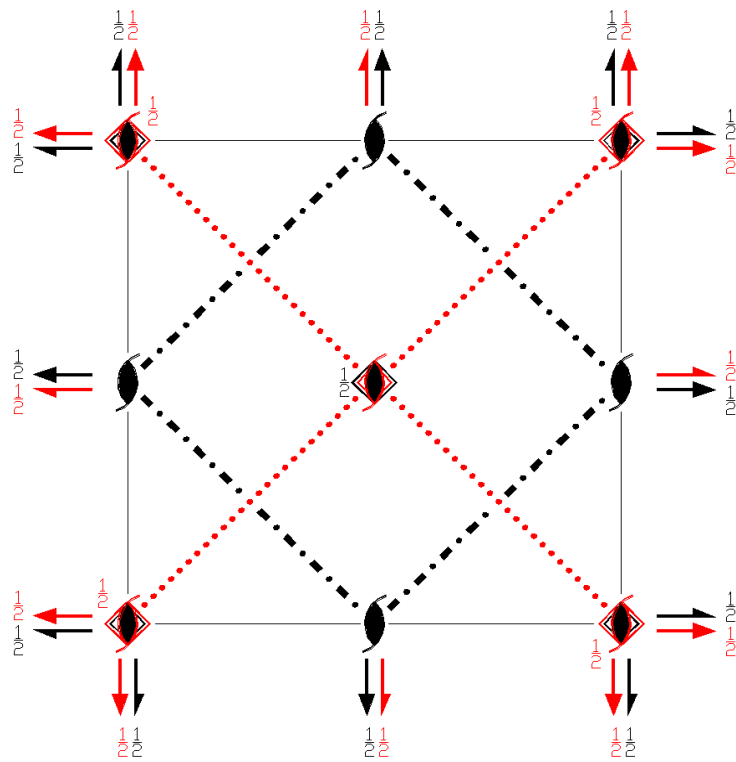
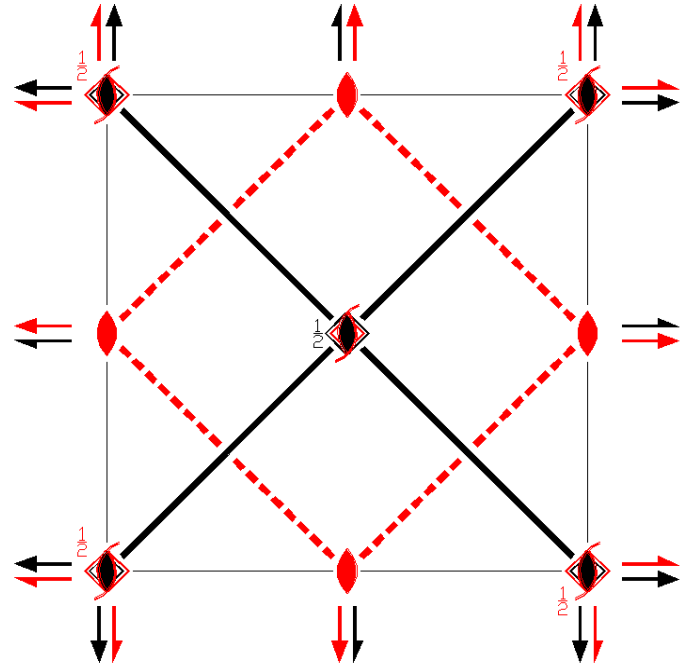
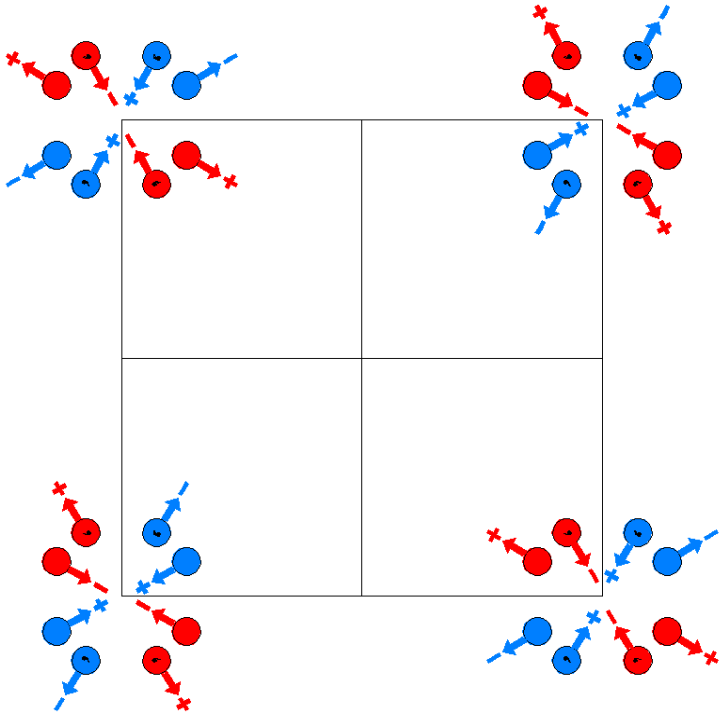
Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P\bar{4}2m$   
111.8.918

$\bar{4}2m1'$   
 $P\bar{4}2m$

Tetragonal



Origin on  $\bar{4}$ 2mAsymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$ ;  $x \leq y$ 

## Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 <sub>z</sub> 0,0,z (2 <sub>z</sub>  0,0,0)	(3) $\bar{4}_z^+$ 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)	(4) $\bar{4}_z^-$ 0,0,z; 0,0,0 ( $\bar{4}_z^{-1}$  0,0,0)
(5) 2 <sub>y</sub> 0,y,0 (2 <sub>y</sub>  0,0,0)	(6) 2 <sub>x</sub> x,0,0 (2 <sub>x</sub>  0,0,0)	(7) m <sub>xy</sub> x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)	(8) m <sub>xy</sub> x,x,z (m <sub>xy</sub>  0,0,0)

For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' <sub>z</sub> 1/2,0,z (2' <sub>z</sub>  1,0,0)'	(3) $\bar{4}_z^+$ 1/2,-1/2,z; 1/2,-1/2,0 ( $\bar{4}_z$  1,0,0)'	(4) $\bar{4}_z^-$ 1/2,1/2,z; 1/2,1/2,0 ( $\bar{4}_z^{-1}$  1,0,0)'
(5) 2' <sub>y</sub> 1/2,y,0 (2' <sub>y</sub>  1,0,0)'	(6) 2' <sub>x</sub> (1,0,0) x,0,0 (2' <sub>x</sub>  1,0,0)'	(7) g' <sub>xy</sub> (1/2,-1/2,0) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1,0,0)'	(8) g' <sub>xy</sub> (1/2,1/2,0) x+1/2,x,z (m <sub>xy</sub>  1,0,0)'

Generators selected (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

			(0,0,0) +		(1,0,0)' +	
16	o	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(3) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ] (7) $\bar{y},x,\bar{z}$ [v,u, $\bar{w}$ ]	(4) $\bar{y},x,z$ [v, $\bar{u},w$ ] (8) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
8	n	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [u, $\bar{u},0$ ]	x, $\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,\bar{z}$ [u,u,0]
8	m	2'..	0,1/2,z [u,v,0]	1/2,0, $\bar{z}$ [ $\bar{v},u,0$ ]	0,1/2, $\bar{z}$ [ $\bar{u},v,0$ ]	1/2,0,z [ $\bar{v},\bar{u},0$ ]
8	l	.2'	x,1/2,0 [0,v,w]	$\bar{x},1/2,0$ [0,v, $\bar{w}$ ]	1/2, $\bar{x},0$ [ $\bar{v},0,w$ ]	1/2,x,0 [ $\bar{v},0,\bar{w}$ ]
8	k	.2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	0, $\bar{x},1/2$ [v,0, $\bar{w}$ ]	0,x,1/2 [ $\bar{v},0,\bar{w}$ ]
8	j	.2.	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [u,0,0]]	1/2, $\bar{x},1/2$ [0, $\bar{u},0$ ]	1/2,x,1/2 [0, $\bar{u},0$ ]
8	i	.2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0, $\bar{x},0$ [0,u,0]	0,x,0 [0, $\bar{u},0$ ]
4	h	2.mm	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
4	g	2.mm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4	f	2'2'2.	1/2,0,1/2 [0,v,0]	0,1/2,1/2 [ $\bar{v},0,0$ ]		
4	e	2'22'.	1/2,0,0 [u,0,0]	0,1/2,0 [0, $\bar{u},0$ ]		
2	d	$\bar{4}$ '2'm	1/2,1/2,0 [0,0,0]			

2 c  $\bar{4}'2'm$  0,0,1/2 [0,0,0]

2 b  $\bar{4}2m$  1/2,1/2,1/2 [0,0,0]

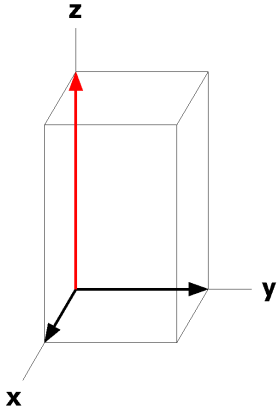
2 a  $\bar{4}2m$  0,0,0 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



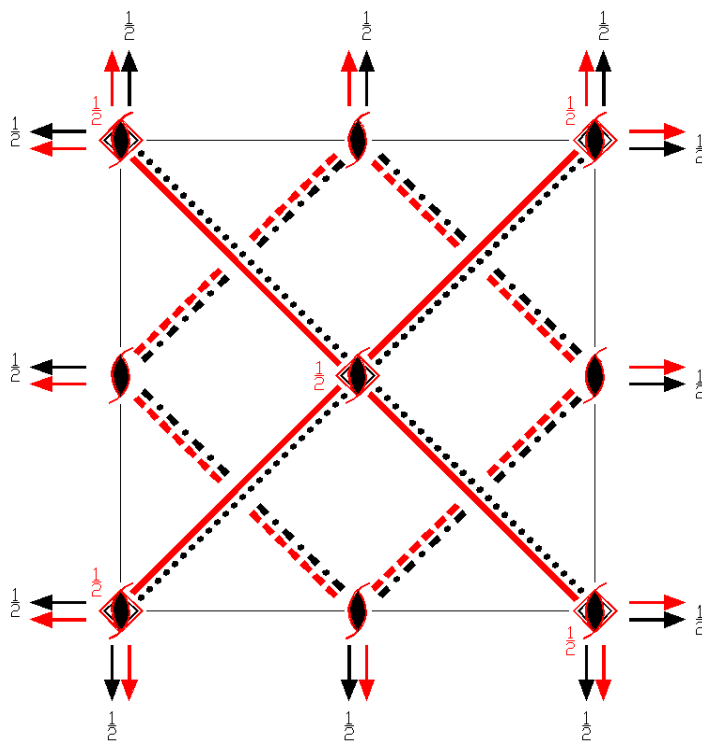
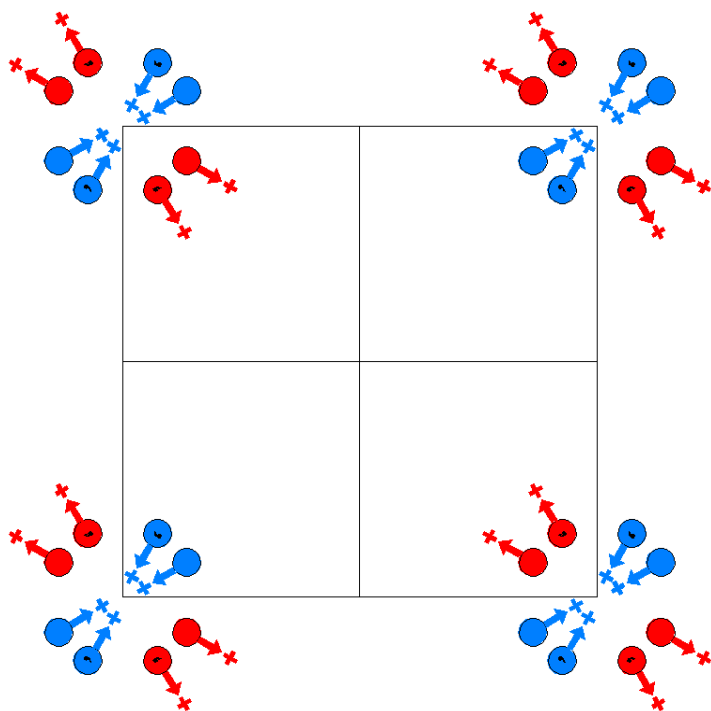
$P_{2c} \bar{4}2'm'$

111.9.919

$\bar{4}2m1'$

$P_{2c} \bar{4}2'm'$

Tetragonal



Origin on  $\bar{4}2'm'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0) |
| (5) 2' 0,y,0<br>(2 <sub>y</sub> ' 0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub> ' 0,0,0)' | (7) m' x, $\bar{x}$ ,z<br>(m <sub>xy</sub> ' 0,0,0)'    | (8) m' x,x,z<br>(m <sub>xy</sub> ' 0,0,0)'              |

For (0,0,1/2) + set

- |  |   |   |   |
|--|---|---|---|
| (1) t' (0,0,1)<br>(1 0,0,1)'             | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub> ' 0,0,1)' | (3) $\bar{4}^+$ ' 0,0,z; 0,0,1/2<br>( $\bar{4}_z^+$ ' 0,0,1)' | (4) $\bar{4}^-$ ' 0,0,z; 0,0,1/2<br>( $\bar{4}_z^-$ ' 0,0,1)' |
| (5) 2 0,y,1/2<br>(2 <sub>y</sub>  0,0,1) | (6) 2 x,0,1/2<br>(2 <sub>x</sub>  0,0,1)          | (7) c (0,0,1) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1)     | (8) c (0,0,1) x,x,z<br>(m <sub>xy</sub>  0,0,1)               |



**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

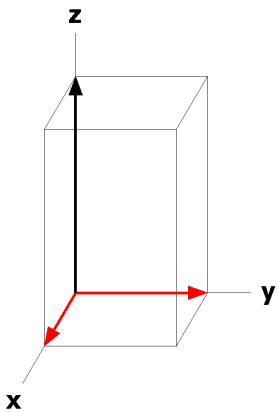
			(0,0,0)+ (0,0,1)' +			
16	o	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u, $\bar{v}$ ,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v}$ ,w] (6) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(3) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ] (7) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ] (8) y,x,z [v,u,w]
8	n	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},\bar{z}$ [ $\bar{u},u,w$ ]	$\bar{x},x,\bar{z}$ [u, $\bar{u},w$ ]
8	m	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0,z [0,0,w]
8	l	.2'	x,1/2,0 [0,v,w]	$\bar{x},1/2,0$ [0, $\bar{v}$ ,w]	1/2, $\bar{x},0$ [ $\bar{v},0,w$ ]	1/2,x,0 [v,0,w]
8	k	.2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0, $\bar{x},1/2$ [0, $\bar{u},0$ ]	0,x,1/2 [0,u,0]
8	j	.2.	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	1/2, $\bar{x},1/2$ [0, $\bar{u},0$ ]	1/2,x,1/2 [0,u,0]
8	i	.2'	x,0,0 [0,v,w]	$\bar{x},0,0$ [0, $\bar{v}$ ,w]	0, $\bar{x},0$ [ $\bar{v},0,w$ ]	0,x,0 [v,0,w]
4	h	2.m'm'	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
4	g	2.m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
4	f	222.	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]		
4	e	22'2'	1/2,0,0 [0,0,w]	0,1/2,0 [0,0,w]		
2	d	$\bar{4}2m$	1/2,1/2,0 [0,0,0]			
2	c	$\bar{4}'2m'$	0,0,1/2 [0,0,0]			
2	b	$\bar{4}'2m'$	1/2,1/2,1/2 [0,0,0]			
2	a	$\bar{4}2'm'$	0,0,0 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0]  $p_{2a} 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at x,1/2,0

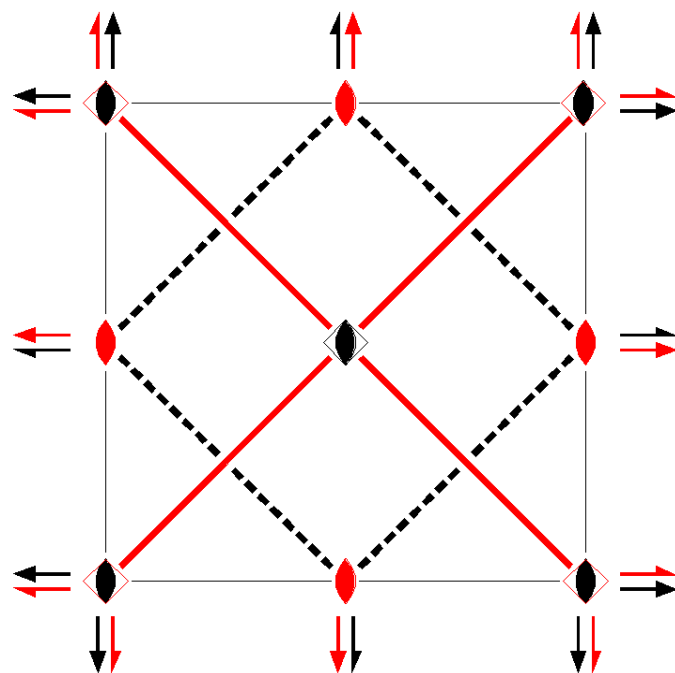
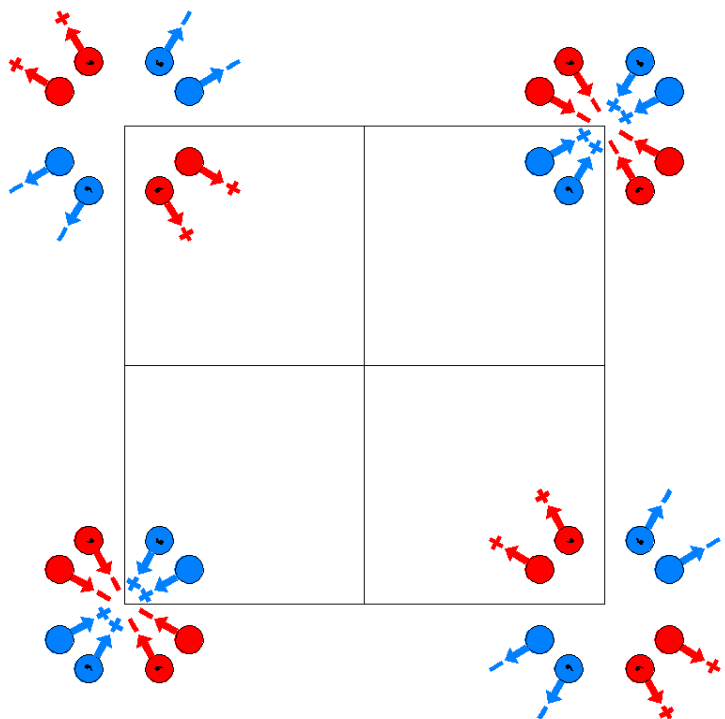
Along [1,1,0]  $p_{2b} 1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,x,0



$P\bar{4}2m'$   
111.10.920

$\bar{4}2m1'$   
 $P\bar{4}2m'$

Tetragonal



Origin on  $\bar{4}2m'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)'  |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) m' x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)'    | (8) m' x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,0)' |

For (1,0,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1,0,0)<br>(1 1,0,0)'               | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'       | (3) $\bar{4}^+$ 1/2,-1/2,z; 1/2,-1/2,0<br>( $\bar{4}_z$  1,0,0)    | (4) $\bar{4}^-$ 1/2,1/2,z; 1/2,1/2,0<br>( $\bar{4}_z^{-1}$  1,0,0)         |
| (5) 2' 1/2,y,0<br>(2 <sub>y</sub>  1,0,0)' | (6) 2' (1,0,0) x,0,0<br>(2 <sub>x</sub>  1,0,0)' | (7) g (1/2,-1/2,0) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1,0,0) | (8) g (1/2,1/2,0) x+1/2,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1,0,0) |

**Generators selected** (1);  $t'(1,0,0)$ ;  $t'(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3); (5).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

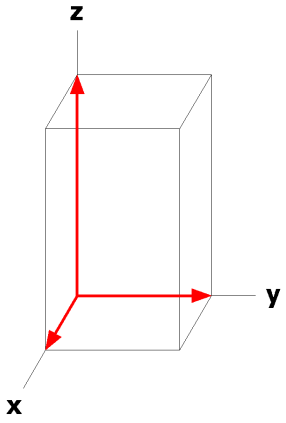
			(0,0,0) + (1,0,0)' +			
16	o	1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $y,\bar{x},\bar{z} [v,\bar{u},\bar{w}]$	(4) $\bar{y},x,\bar{z} [\bar{v},u,\bar{w}]$
			(5) $\bar{x},y,\bar{z} [\bar{u},v,\bar{w}]$	(6) $x,\bar{y},\bar{z} [u,\bar{v},\bar{w}]$	(7) $\bar{y},\bar{x},z [v,\bar{u},w]$	(8) $y,x,z [v,u,w]$
8	n	..m'	$x,x,z [u,u,w]$	$\bar{x},\bar{x},z [\bar{u},\bar{u},w]$	$x,\bar{x},\bar{z} [u,\bar{u},\bar{w}]$	$\bar{x},x,\bar{z} [\bar{u},u,\bar{w}]$
8	m	2'..	$0,1/2,z [u,v,0]$	$1/2,0,\bar{z} [v,\bar{u},0]$	$0,1/2,\bar{z} [\bar{u},v,0]$	$1/2,0,z [v,u,0]$
8	l	.2'	$x,1/2,0 [0,v,w]$	$\bar{x},1/2,0 [0,v,\bar{w}]$	$1/2,\bar{x},0 [v,0,\bar{w}]$	$1/2,x,0 [v,0,w]$
8	k	.2.	$x,0,1/2 [u,0,0]$	$\bar{x},0,1/2 [\bar{u},0,0]$	$0,\bar{x},1/2 [0,\bar{u},0]$	$0,x,1/2 [0,u,0]$
8	j	.2'	$x,1/2,1/2 [0,v,w]$	$\bar{x},1/2,1/2 [0,v,\bar{w}]$	$1/2,\bar{x},1/2 [v,0,\bar{w}]$	$1/2,x,1/2 [v,0,w]$
8	i	.2.	$x,0,0 [u,0,0]$	$\bar{x},0,0 [\bar{u},0,0]$	$0,\bar{x},0 [0,\bar{u},0]$	$0,x,0 [0,u,0]$
4	h	2.m'm'	$1/2,1/2,z [0,0,w]$	$1/2,1/2,\bar{z} [0,0,w]$		
4	g	2.m'm'	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,\bar{w}]$		
4	f	2'22'	$1/2,0,1/2 [u,0,0]$	$0,1/2,1/2 [0,u,0]$		
4	e	2'22'	$1/2,0,0 [u,0,0]$	$0,1/2,0 [0,u,0]$		
2	d	$\bar{4}2'm'$	$1/2,1/2,0 [0,0,w]$			
2	c	$\bar{4}'2m'$	$0,0,1/2 [0,0,0]$			
2	b	$\bar{4}2'm'$	$1/2,1/2,1/2 [0,0,w]$			
2	a	$\bar{4}'2m'$	$0,0,0 [0,0,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $p_4$ -4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

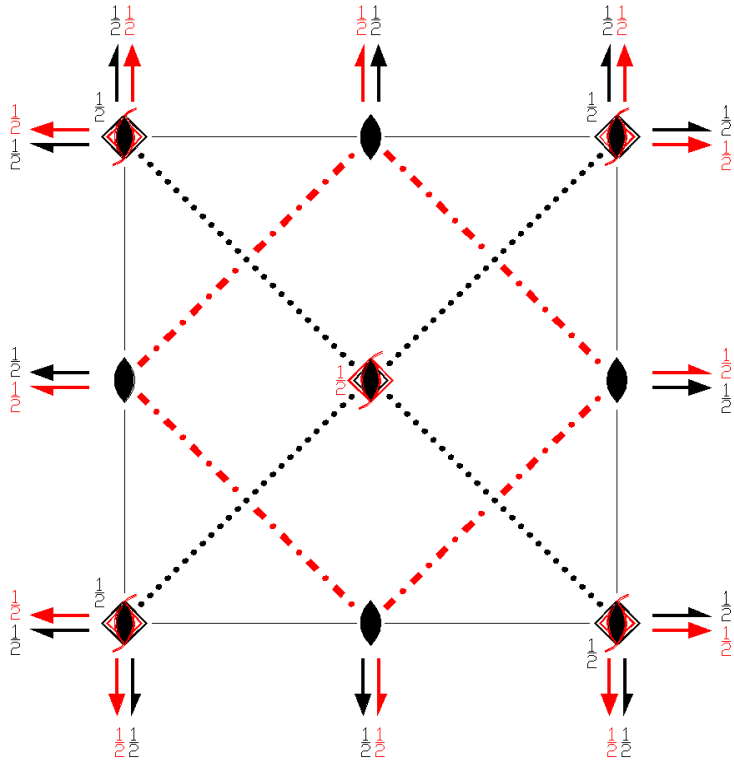
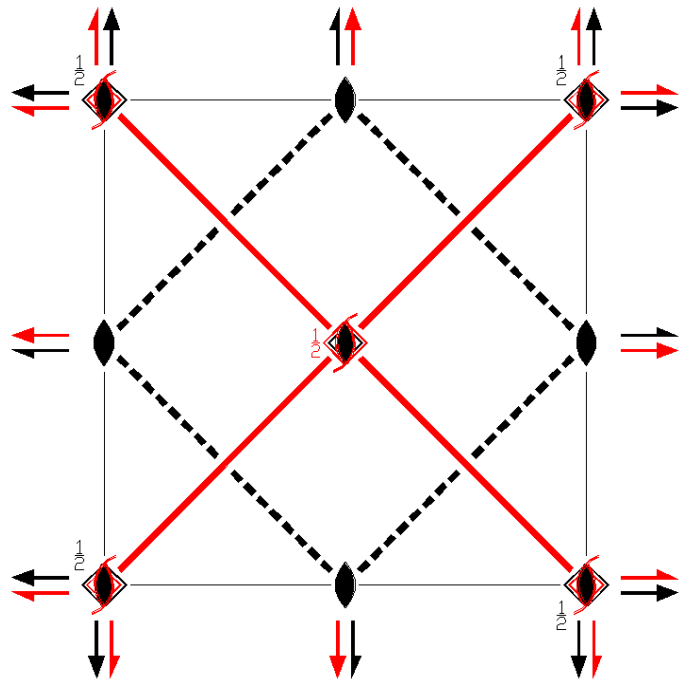
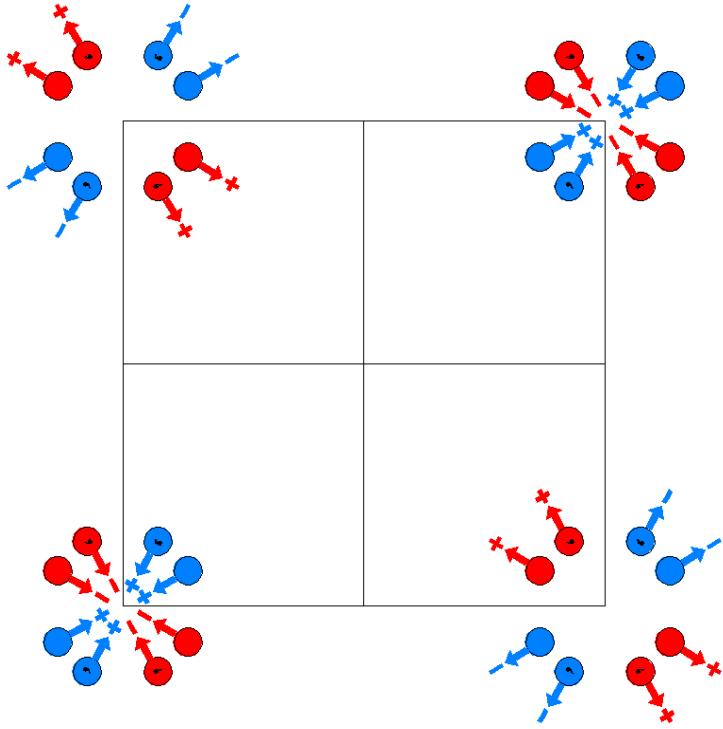
Along  $[1,1,0]$   $p_{2a}1m1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x-1/4,x+1/4,0$



$P\bar{4}'2m'$   
111.11.921

$\bar{4}2m1'$   
 $P\bar{4}'2m'$

Tetragonal



**Origin** on  $\bar{4}'2m'$ **Asymmetric unit**  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y$ **Symmetry Operations**

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'	(4) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z^{-1}$  0,0,0)'
(5) 2 0,y,0 (2 <sub>y</sub>  0,0,0)	(6) 2 x,0,0 (2 <sub>x</sub>  0,0,0)	(7) m' x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)'	(8) m' x,x,z (m <sub>xy</sub>  0,0,0)'

For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) $\bar{4}^+$ 1/2,-1/2,z; 1/2,-1/2,0 ( $\bar{4}_z$  1,0,0)	(4) $\bar{4}^-$ 1/2,1/2,z; 1/2,1/2,0 ( $\bar{4}_z^{-1}$  1,0,0)
(5) 2' 1/2,y,0 (2 <sub>y</sub>  1,0,0)'	(6) 2' (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)'	(7) g (1/2,-1/2,0) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1,0,0)	(8) g (1/2,1/2,0) x+1/2,x,z (m <sub>xy</sub>  1,0,0)

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).**Positions**Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

			(0,0,0) +		(1,0,0)' +	
16	o	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(3) y, $\bar{x},z$ [v, $\bar{u},\bar{w}$ ] (7) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,z$ [ $\bar{v},u,\bar{w}$ ] (8) y,x,z [v,u,w]
8	n	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},z$ [u, $\bar{u},\bar{w}$ ]	$\bar{x},x,z$ [ $\bar{u},u,\bar{w}$ ]
8	m	2'..	0,1/2,z [u,v,0]	1/2,0, $\bar{z}$ [v, $\bar{u},0$ ]	0,1/2, $\bar{z}$ [ $\bar{u},v,0$ ]	1/2,0,z [v,u,0]
8	l	.2'	x,1/2,0 [0,v,w]	$\bar{x},1/2,0$ [0,v, $\bar{w}$ ]	1/2, $\bar{x},0$ [v,0, $\bar{w}$ ]	1/2,x,0 [v,0,w]
8	k	.2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	0, $\bar{x},1/2$ [ $\bar{v},0,w$ ]	0,x,1/2 [v,0,w]
8	j	.2.	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [u,0,0]	1/2, $\bar{x},1/2$ [0,u,0]	1/2,x,1/2 [0,u,0]
8	i	.2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0, $\bar{x},0$ [0, $\bar{u},0$ ]	0,x,0 [0,u,0]
4	h	2.m'm'	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
4	g	2.m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
4	f	2'2'2.	1/2,0,1/2 [0,v,0]	0,1/2,1/2 [v,0,0]		
4	e	2'22'.	1/2,0,0 [u,0,0]	0,1/2,0 [0,u,0]		
2	d	$\bar{4}2'm'$	1/2,1/2,0 [0,0,w]			

2 c  $\bar{4}'2m'$  0,0,1/2 [0,0,w]

2 b  $\bar{4}'2m'$  1/2,1/2,1/2 [0,0,0]

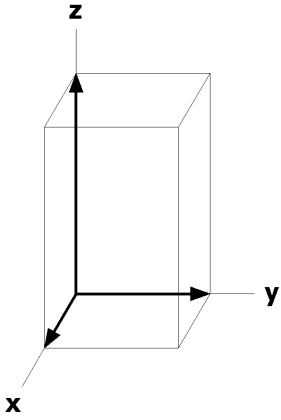
2 a  $\bar{4}'2m'$  0,0,0 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

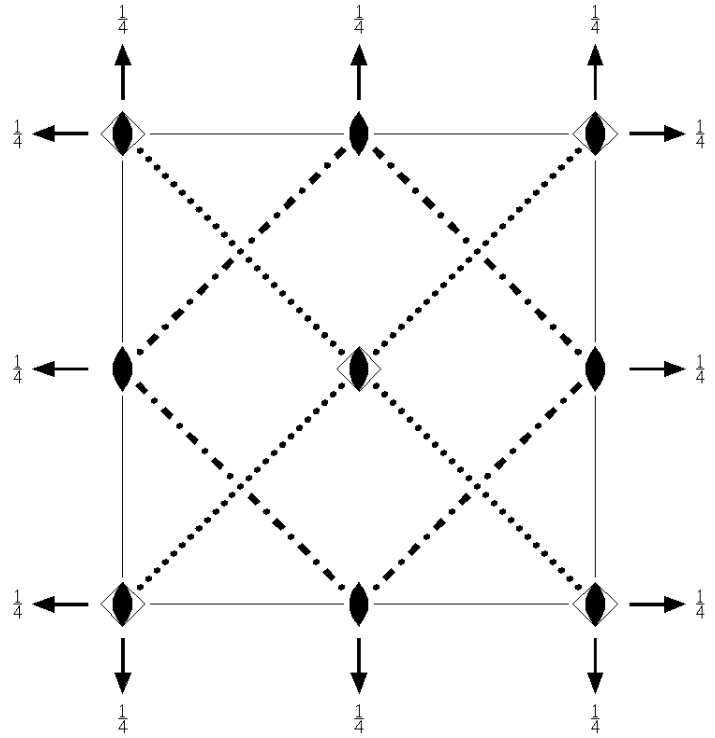
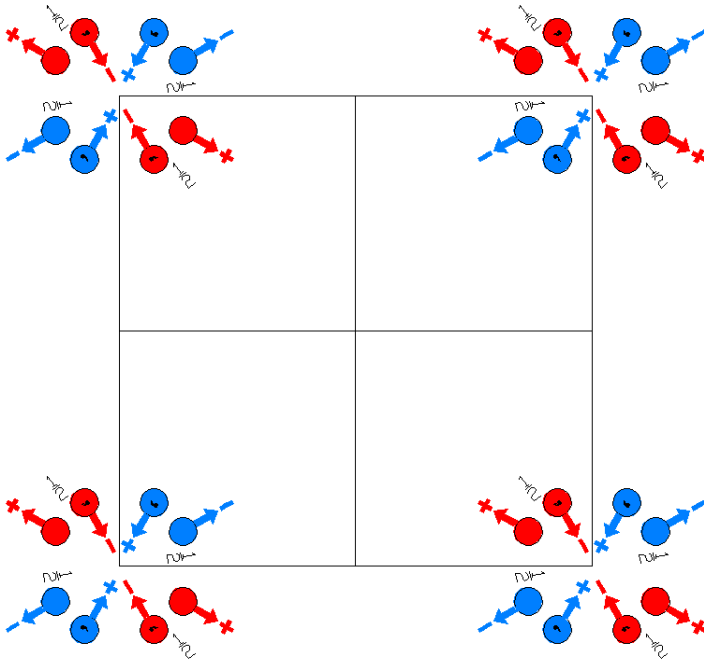
Along [1,1,0]  $p_2c'1m1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x-1/4, x+1/4, 0$



$P\bar{4}2c$   
112.1.922

$\bar{4}2m$   
 $P\bar{4}2c$

Tetragonal



Origin on  $\bar{4}1c$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$

### Symmetry Operations

- |                                      |                                      |  |   |
|--------------------------------------|--------------------------------------|--|---|
| (1) 1<br>(1 0,0,0)                   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)     | (3) $\bar{4}^+$ $0,0,z$ ; $0,0,0$<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ $0,0,z$ ; $0,0,0$<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) 2 $0,y,1/4$<br>( $2_y$  0,0,1/2) | (6) 2 $x,0,1/4$<br>( $2_x$  0,0,1/2) | (7) c $(0,0,1/2)$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2)    | (8) c $(0,0,1/2)$ $x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2)         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	n	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ]	(3) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ] (7) $\bar{y},\bar{x},z+1/2$ [v,u, $\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [v, $\bar{u},w$ ] (8) y,x,z+1/2 [ $\bar{v},\bar{u},\bar{w}$ ]
4	m	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]
4	l	2..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]
4	k	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]
4	j	.2.	0,y,1/4 [0,v,0]	0, $\bar{y}$ ,1/4 [0, $\bar{v}$ ,0]	y,0,3/4 [ $\bar{v}$ ,0,0]	$\bar{y}$ ,0,3/4 [v,0,0]
4	i	.2.	x,1/2,1/4 [u,0,0]	$\bar{x}$ ,1/2,1/4 [ $\bar{u}$ ,0,0]	1/2, $\bar{x}$ ,3/4 [0,u,0]	1/2,x,3/4 [0, $\bar{u}$ ,0]
4	h	.2.	1/2,y,1/4 [0,v,0]	1/2, $\bar{y}$ ,1/4 [0, $\bar{v}$ ,0]	y,1/2,3/4 [ $\bar{v}$ ,0,0]	$\bar{y}$ ,1/2,3/4 [v,0,0]
4	g	.2.	x,0,1/4 [u,0,0]	$\bar{x}$ ,0,1/4 [ $\bar{u}$ ,0,0]	0, $\bar{x}$ ,3/4 [0,u,0]	0,x,3/4 [0, $\bar{u}$ ,0]
2	f	$\bar{4}$ ..	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		
2	e	$\bar{4}$ ..	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		
2	d	222.	0,1/2,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]		
2	c	222.	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	b	222.	1/2,0,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]		
2	a	222.	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

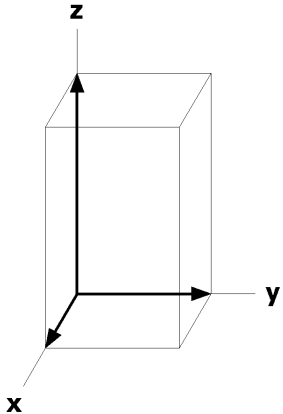
**Symmetry of Special Projections**

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,1/4

Along [1,1,0] p<sub>2b</sub>-1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



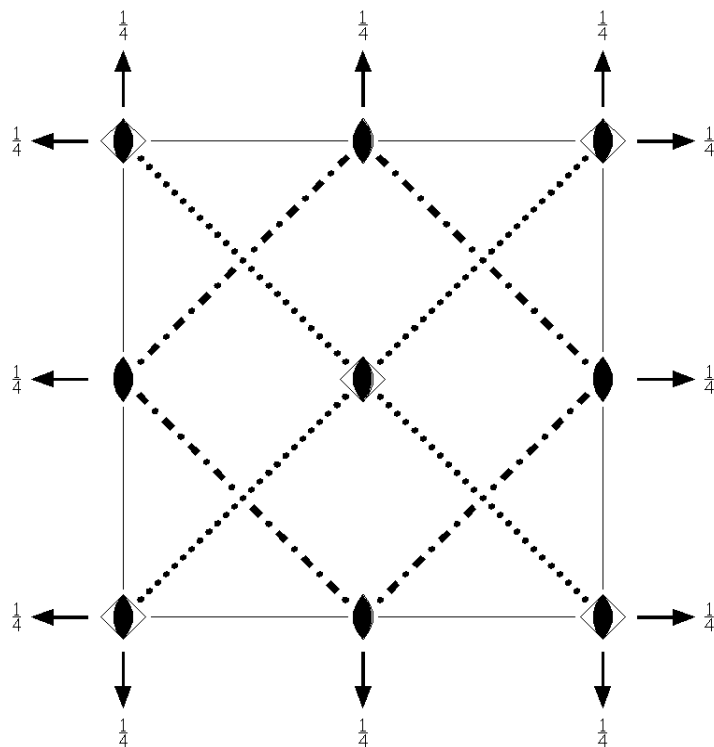
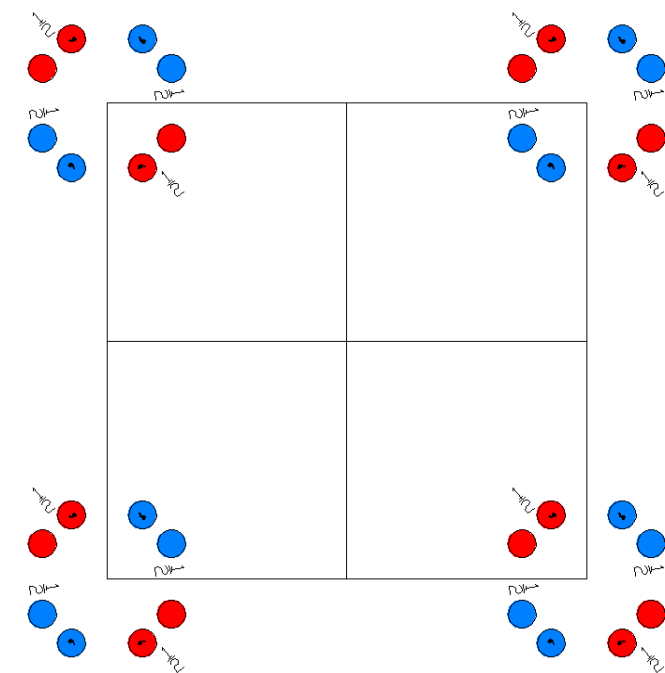


$P\bar{4}2c1'$   
112.2.923

$\bar{4}2m1'$   
 $P\bar{4}2c1'$

Tetragonal

1'



Origin on  $\bar{4}1c1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For 1 + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)     | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)         | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2) | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2) | (7) c (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2) | (8) c (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)        |

For 1' + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1'<br>(1 0,0,0)'                         | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'     | (3) $\bar{4}^+$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)'        | (4) $\bar{4}^-$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)' |
| (5) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)' | (6) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)' | (7) c' (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2)' | (8) c' (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)'         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

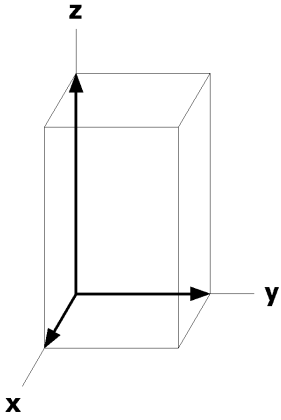
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates								
	1 +				1' +				
8 n 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) y, $\bar{x},\bar{z}$ [0,0,0]	(4) $\bar{y},x,\bar{z}$ [0,0,0]	(5) $\bar{x},y,\bar{z}+1/2$ [0,0,0]	(6) x, $\bar{y},\bar{z}+1/2$ [0,0,0]	(7) $\bar{y},\bar{x},z+1/2$ [0,0,0]	(8) y,x,z+1/2 [0,0,0]	
4 m 2..1'	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	0,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,0,z+1/2 [0,0,0]	4 l 2..1'	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,1/2,z+1/2 [0,0,0]
4 k 2..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0,z+1/2 [0,0,0]	4 j .2.1'	0,y,1/4 [0,0,0]	0, $\bar{y}$ ,1/4 [0,0,0]	y,0,3/4 [0,0,0]	$\bar{y}$ ,0,3/4 [0,0,0]
4 i .2.1'	x,1/2,1/4 [0,0,0]	$\bar{x}$ ,1/2,1/4 [0,0,0]	1/2, $\bar{x}$ ,3/4 [0,0,0]	1/2,x,3/4 [0,0,0]	4 h .2.1'	1/2,y,1/4 [0,0,0]	1/2, $\bar{y}$ ,1/4 [0,0,0]	y,1/2,3/4 [0,0,0]	$\bar{y}$ ,1/2,3/4 [0,0,0]
4 g .2.1'	x,0,1/4 [0,0,0]	$\bar{x}$ ,0,1/4 [0,0,0]	0, $\bar{x}$ ,3/4 [0,0,0]	0,x,3/4 [0,0,0]	2 f $\bar{4}..1'$	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2 e $\bar{4}..1'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]			2 d 222.1'	0,1/2,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]		
2 c 222.1'	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]			2 b 222.1'	1/2,0,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]		
2 a 222.1'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]							

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,1/4

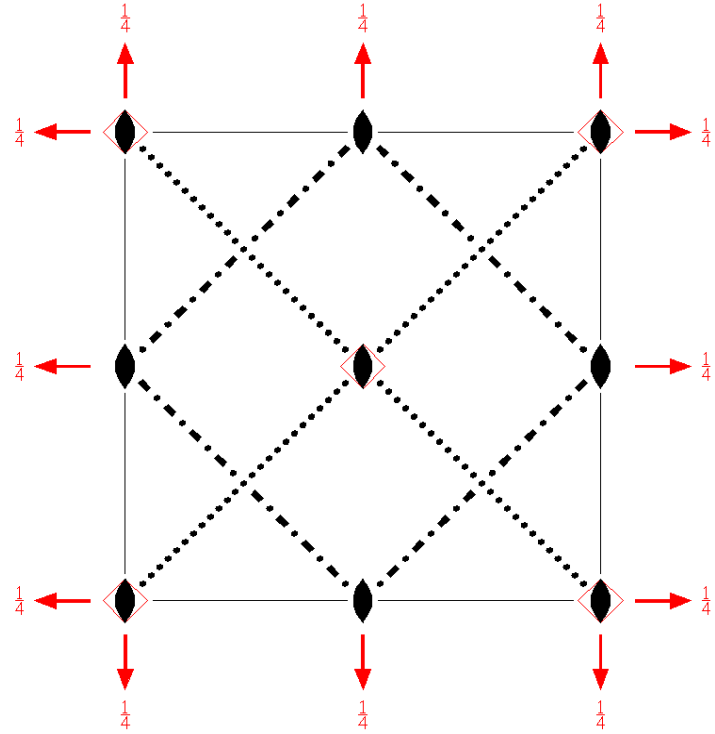
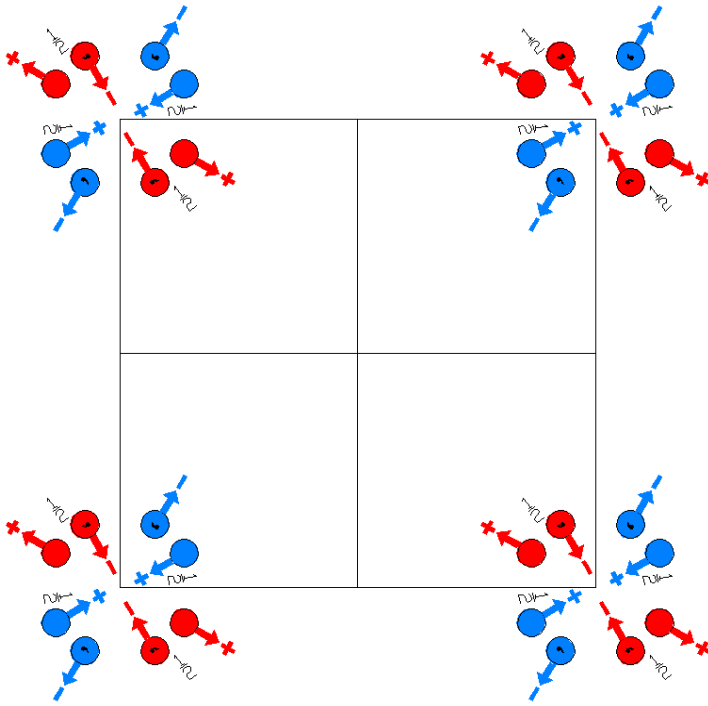
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P\bar{4}'2'c$   
112.3.924

$\bar{4}'2'm$   
 $P\bar{4}'2'c$

Tetragonal



Origin on  $\bar{4}'1c$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                                      | (2) 2 <sub>0,0,z</sub><br>(2 <sub>z</sub>  0,0,0)       | (3) $\bar{4}'^+$<br>( $\bar{4}'_z$  0,0,0)' | (4) $\bar{4}'^-$<br>( $\bar{4}'_z^{-1}$  0,0,0)' |
| (5) 2' <sub>0,y,1/4</sub><br>(2 <sub>y</sub>  0,0,1/2)' | (6) 2' <sub>x,0,1/4</sub><br>(2 <sub>x</sub>  0,0,1/2)' | (7) c<br>(m <sub>xy</sub>  0,0,1/2)         | (8) c<br>(m <sub>xy</sub>  0,0,1/2)              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

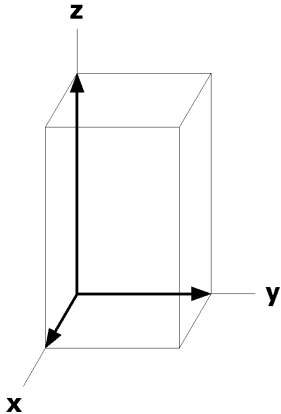
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	n	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(6) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) $\bar{y},\bar{x},z+1/2$ [v,u, $\bar{w}$ ]	(8) y,x,z+1/2 [ $\bar{v},\bar{u},\bar{w}$ ]
4	m	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]
4	l	2..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]
4	k	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]
4	j	.2'	0,y,1/4 [u,0,w]	0, $\bar{y}$ ,1/4 [ $\bar{u}$ ,0,w]	y,0,3/4 [0, $\bar{u},\bar{w}$ ]	$\bar{y}$ ,0,3/4 [0,u, $\bar{w}$ ]
4	i	.2'	x,1/2,1/4 [0,v,w]	$\bar{x}$ ,1/2,1/4 [0, $\bar{v},w$ ]	1/2, $\bar{x}$ ,3/4 [v,0, $\bar{w}$ ]	1/2,x,3/4 [ $\bar{v}$ ,0, $\bar{w}$ ]
4	h	.2'	1/2,y,1/4 [u,0,w]	1/2, $\bar{y}$ ,1/4 [ $\bar{u}$ ,0,w]	y,1/2,3/4 [0, $\bar{u},\bar{w}$ ]	$\bar{y}$ ,1/2,3/4 [0,u, $\bar{w}$ ]
4	g	.2'	x,0,1/4 [0,v,w]	$\bar{x}$ ,0,1/4 [0, $\bar{v},w$ ]	0, $\bar{x}$ ,3/4 [v,0, $\bar{w}$ ]	0,x,3/4 [ $\bar{v}$ ,0, $\bar{w}$ ]
2	f	$\bar{4}'..$	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	e	$\bar{4}'..$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
2	d	22'2'	0,1/2,1/4 [0,0,w]	1/2,0,3/4 [0,0, $\bar{w}$ ]		
2	c	22'2'	1/2,1/2,1/4 [0,0,w]	1/2,1/2,3/4 [0,0, $\bar{w}$ ]		
2	b	22'2'	1/2,0,1/4 [0,0,w]	0,1/2,3/4 [0,0, $\bar{w}$ ]		
2	a	22'2'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,1/4

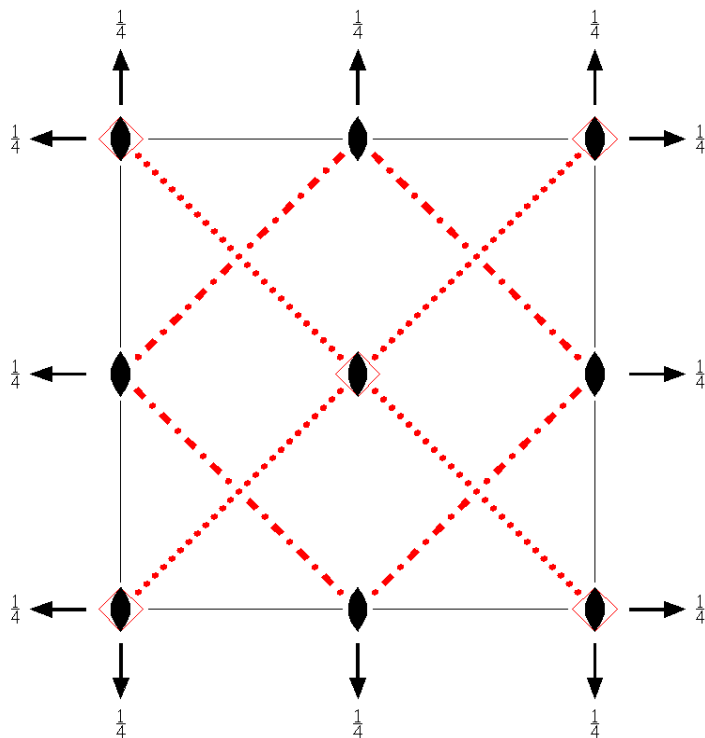
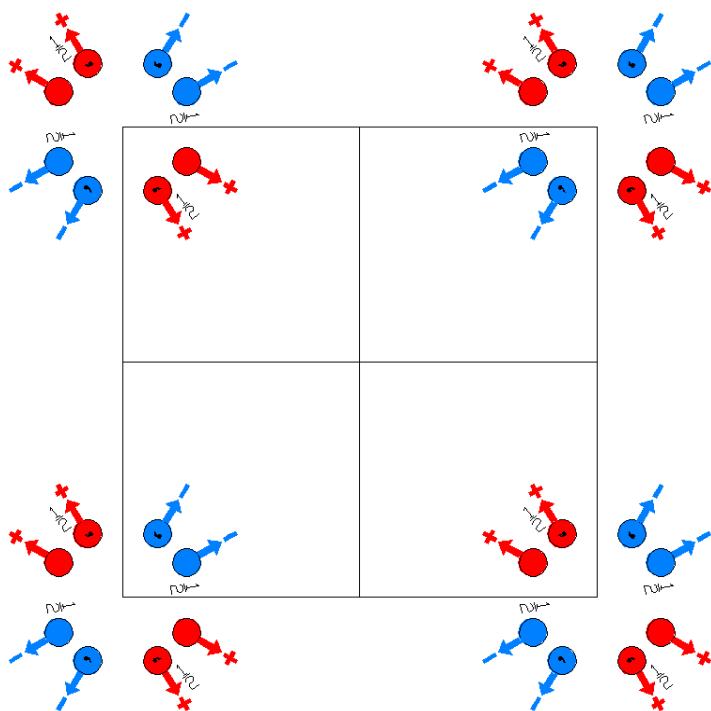
Along [1,1,0]  $p_{2b}1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P\bar{4}'2c'$   
112.4.925

$\bar{4}'2m'$   
 $P\bar{4}'2c'$

Tetragonal



Origin on  $\bar{4}'1c'$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)     | (3) $\bar{4}'^+$ 0,0,z; 0,0,0<br>( $\bar{4}'_z$  0,0,0)'        | (4) $\bar{4}'^-$ 0,0,z; 0,0,0<br>( $\bar{4}'_z^{-1}$  0,0,0)'            |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2) | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2) | (7) c' (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2)' | (8) c' (0,0,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

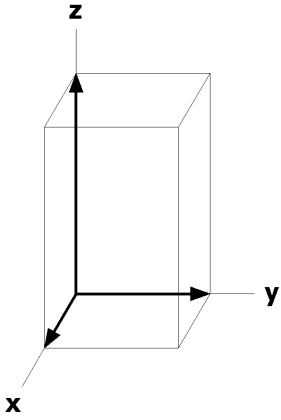
8	n	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $y,\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ]	(7) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $y,x,z+1/2$ [v,u,w]
4	m	2..	$0,1/2,z$ [0,0,w]	$1/2,0,\bar{z}$ [0,0, $\bar{w}$ ]	$0,1/2,\bar{z}+1/2$ [0,0, $\bar{w}$ ]	$1/2,0,z+1/2$ [0,0,w]
4	l	2..	$1/2,1/2,z$ [0,0,w]	$1/2,1/2,\bar{z}$ [0,0, $\bar{w}$ ]	$1/2,1/2,\bar{z}+1/2$ [0,0, $\bar{w}$ ]	$1/2,1/2,z+1/2$ [0,0,w]
4	k	2..	$0,0,z$ [0,0,w]	$0,0,\bar{z}$ [0,0, $\bar{w}$ ]	$0,0,\bar{z}+1/2$ [0,0, $\bar{w}$ ]	$0,0,z+1/2$ [0,0,w]
4	j	.2.	$0,y,1/4$ [0,v,0]	$0,\bar{y},1/4$ [0, $\bar{v},0$ ]	$y,0,3/4$ [v,0,0]	$\bar{y},0,3/4$ [ $\bar{v},0,0$ ]
4	i	.2.	$x,1/2,1/4$ [u,0,0]	$\bar{x},1/2,1/4$ [ $\bar{u},0,0$ ]	$1/2,\bar{x},3/4$ [0, $\bar{u},0$ ]	$1/2,x,3/4$ [0,u,0]
4	h	.2.	$1/2,y,1/4$ [0,v,0]	$1/2,\bar{y},1/4$ [0, $\bar{v},0$ ]	$y,1/2,3/4$ [v,0,0]	$\bar{y},1/2,3/4$ [ $\bar{v},0,0$ ]
4	g	.2.	$x,0,1/4$ [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	$0,\bar{x},3/4$ [0, $\bar{u},0$ ]	$0,x,3/4$ [0,u,0]
2	f	$\bar{4}'..$	$1/2,1/2,0$ [0,0,0]	$1/2,1/2,1/2$ [0,0,0]		
2	e	$\bar{4}'..$	$0,0,0$ [0,0,0]	$0,0,1/2$ [0,0,0]		
2	d	222.	$0,1/2,1/4$ [0,0,0]	$1/2,0,3/4$ [0,0,0]		
2	c	222.	$1/2,1/2,1/4$ [0,0,0]	$1/2,1/2,3/4$ [0,0,0]		
2	b	222.	$1/2,0,1/4$ [0,0,0]	$0,1/2,3/4$ [0,0,0]		
2	a	222.	$0,0,1/4$ [0,0,0]	$0,0,3/4$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4mm$   
 $\mathbf{a}^* = -\mathbf{b}$   $\mathbf{b}^* = \mathbf{a}$   
 Origin at 0,0,z

Along [1,0,0]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,1/4

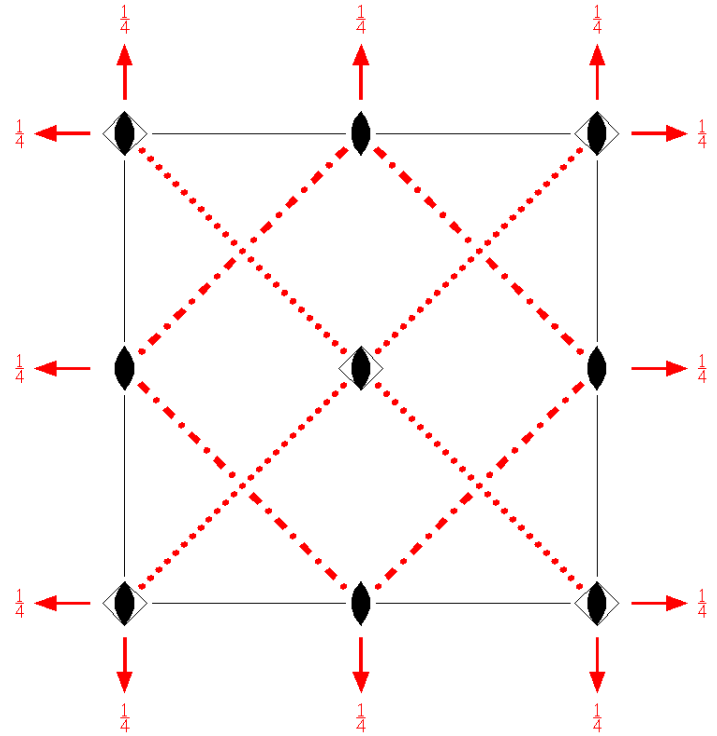
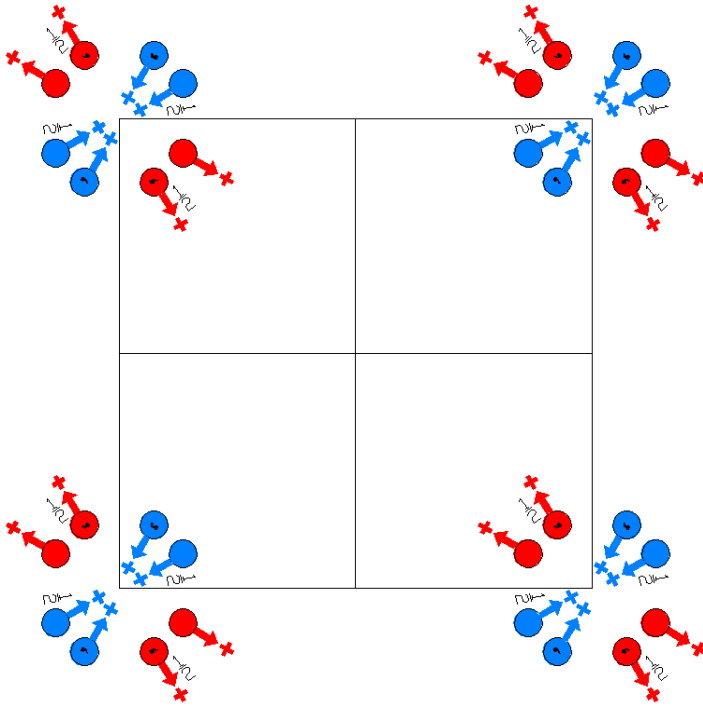
Along [1,1,0]  $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P\bar{4}2c'$   
112.5.926

$\bar{4}2'm'$   
 $P\bar{4}2c'$

Tetragonal



Origin on  $\bar{4}1c'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)       | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)           | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) 2' <sub>y</sub> 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)' | (6) 2' <sub>x</sub> x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)' | (7) c' (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2)' | (8) c' (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)'      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	n	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(6) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(7) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) y,x,z+1/2 [v,u,w]
4	m	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,0,z+1/2 [0,0,w]
4	l	2..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,1/2,z+1/2 [0,0,w]
4	k	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0,z+1/2 [0,0,w]
4	j	.2'	0,y,1/4 [u,0,w]	0, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	y,0,3/4 [0,u,w]	$\bar{y},0,3/4$ [0, $\bar{u},w$ ]
4	i	.2'	x,1/2,1/4 [0,v,w]	$\bar{x},1/2,1/4$ [0, $\bar{v},w$ ]	1/2, $\bar{x},3/4$ [ $\bar{v},0,w$ ]	1/2,x,3/4 [v,0,w]
4	h	.2'	1/2,y,1/4 [u,0,w]	1/2, $\bar{y},1/4$ [ $\bar{u},0,w$ ]	y,1/2,3/4 [0,u,w]	$\bar{y},1/2,3/4$ [0, $\bar{u},w$ ]
4	g	.2'	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	0, $\bar{x},3/4$ [ $\bar{v},0,w$ ]	0,x,3/4 [v,0,w]
2	f	$\bar{4}..$	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]		
2	e	$\bar{4}..$	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]		
2	d	22'2'	0,1/2,1/4 [0,0,w]	1/2,0,3/4 [0,0,w]		
2	c	22'2'	1/2,1/2,1/4 [0,0,w]	1/2,1/2,3/4 [0,0,w]		
2	b	22'2'	1/2,0,1/4 [0,0,w]	0,1/2,3/4 [0,0,w]		
2	a	22'2'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		

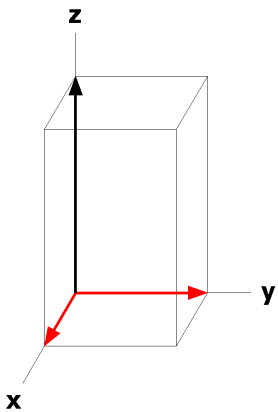
**Symmetry of Special Projections**

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,1/4

Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

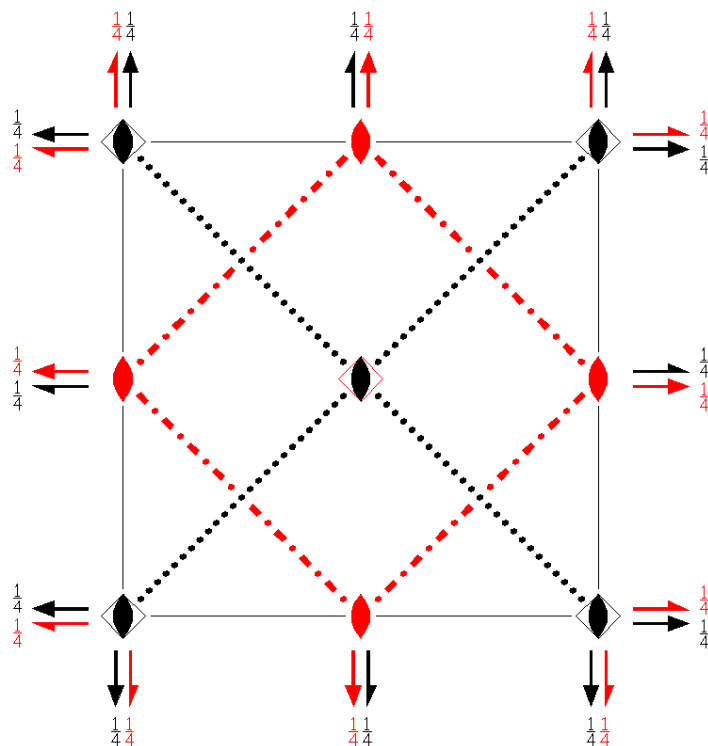
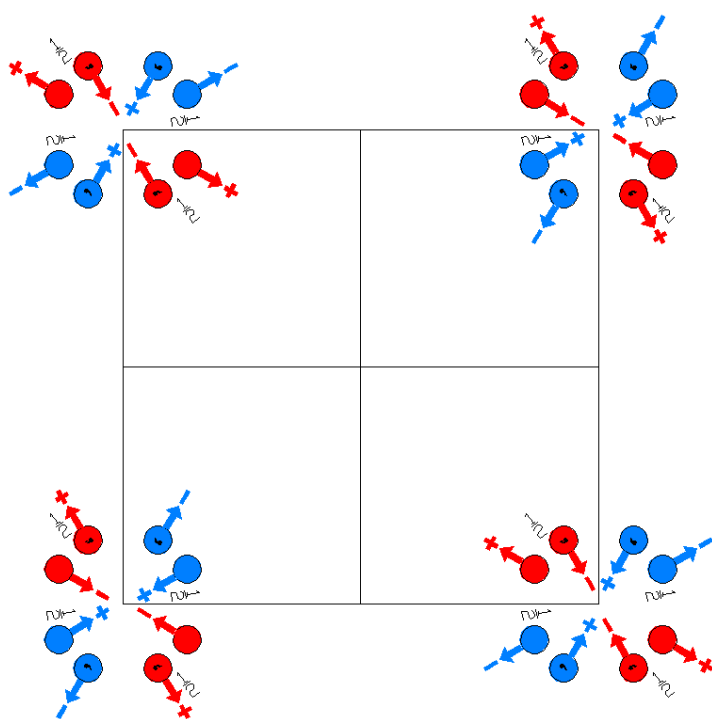




$P_p\bar{4}2c$   
112.6.927

$\bar{4}2m1'$   
 $P_p\bar{4}2c$

Tetragonal



Origin on  $\bar{4}1c$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)     | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)         | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2) | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2) | (7) c (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2) | (8) c (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)        |

For (1,0,0)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) t' (1,0,0)<br>(1 1,0,0)'                   | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'           | (3) $\bar{4}^+$ ' 1/2,-1/2,z; 1/2,-1/2,0<br>( $\bar{4}_z$  1,0,0)'   | (4) $\bar{4}^-$ ' 1/2,1/2,z; 1/2,1/2,0<br>( $\bar{4}_z^{-1}$  1,0,0)' |
| (5) 2' 1/2,y,1/4<br>(2 <sub>y</sub>  1,0,1/2)' | (6) 2' (1,0,0) x,0,1/4<br>(2 <sub>x</sub>  1,0,1/2)' | (7) n' (1/2,-1/2,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1,0,1/2)' | (8) n' (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1,0,1/2)'             |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

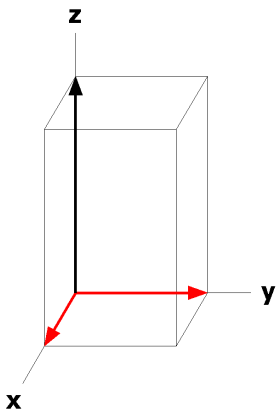
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(1,0,0)' +			
16 n 1	(1)	x,y,z [u,v,w]	(2)	$\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3)	y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4)	$\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]
	(5)	$\bar{x},\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6)	x, $\bar{y},\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7)	$\bar{y},\bar{x},z+1/2$ [ $v,u,\bar{w}$ ]	(8)	y,x,z+1/2 [ $\bar{v},\bar{u},\bar{w}$ ]
8 m 2'..		0,1/2,z [u,v,0]		1/2,0, $\bar{z}$ [ $\bar{v},u,0$ ]		0,1/2, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]		1/2,0,z+1/2 [ $\bar{v},\bar{u},0$ ]
8 l 2..		1/2,1/2,z [0,0,w]		1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		1/2,1/2, $\bar{z}+1/2$ [0,0,w]		1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]
8 k 2..		0,0,z [0,0,w]		0,0, $\bar{z}$ [0,0,w]		0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]		0,0,z+1/2 [0,0, $\bar{w}$ ]
8 j .2.		0,y,1/4 [0,v,0]		0, $\bar{y}$ ,1/4 [0, $\bar{v}$ ,0]		y,0,3/4 [ $\bar{v}$ ,0,0]		$\bar{y}$ ,0,3/4 [v,0,0]
8 i .2'.		x,1/2,1/4 [0,v,w]		$\bar{x}$ ,1/2,1/4 [0,v, $\bar{w}$ ]		1/2, $\bar{x}$ ,3/4 [ $\bar{v}$ ,0,w]		1/2,x,3/4 [ $\bar{v}$ ,0, $\bar{w}$ ]
8 h .2'.		1/2,y,1/4 [u,0,w]		1/2, $\bar{y}$ ,1/4 [u,0, $\bar{w}$ ]		y,1/2,3/4 [0, $\bar{u},\bar{w}$ ]		$\bar{y}$ ,1/2,3/4 [0, $\bar{u},w$ ]
8 g .2.		x,0,1/4 [u,0,0]		$\bar{x}$ ,0,1/4 [ $\bar{u}$ ,0,0]		0, $\bar{x}$ ,3/4 [0,u,0]		0,x,3/4 [0, $\bar{u}$ ,0]
4 f $\bar{4}$ '..		1/2,1/2,0 [0,0,0]		1/2,1/2,1/2 [0,0,0]				
4 e $\bar{4}$ ..		0,0,0 [0,0,w]		0,0,1/2 [0,0, $\bar{w}$ ]				
4 d 2'22'.		0,1/2,1/4 [0,v,0]		1/2,0,3/4 [ $\bar{v}$ ,0,0]				
4 c 22'2'.		1/2,1/2,1/4 [0,0,w]		1/2,1/2,3/4 [0,0, $\bar{w}$ ]				
4 b 2'22'.		1/2,0,1/4 [u,0,0]		0,1/2,3/4 [0, $\bar{u}$ ,0]				
4 a 222.		0,0,1/4 [0,0,0]		0,0,3/4 [0,0,0]				

**Symmetry of Special Projections**

Along [0,0,1]  $p_2-4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/2,1/2,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,1/4

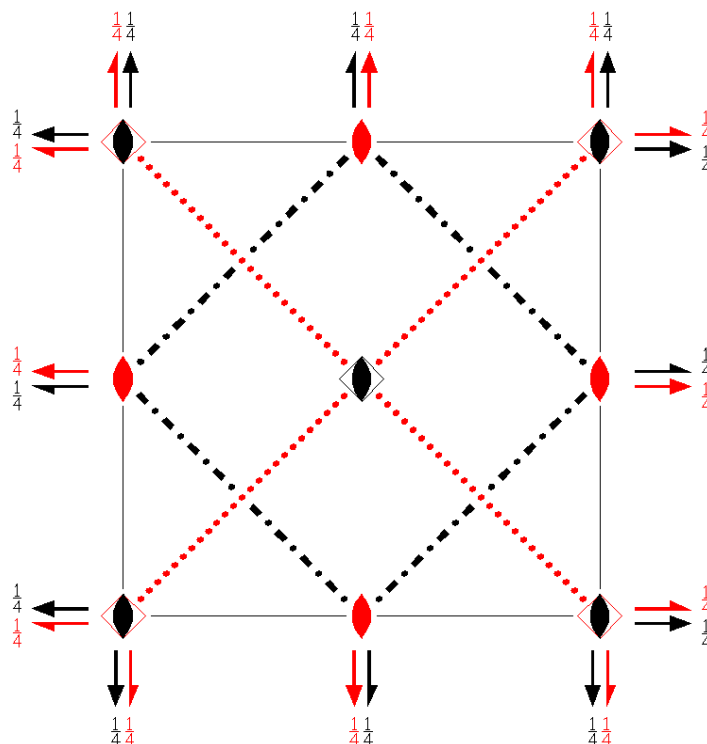
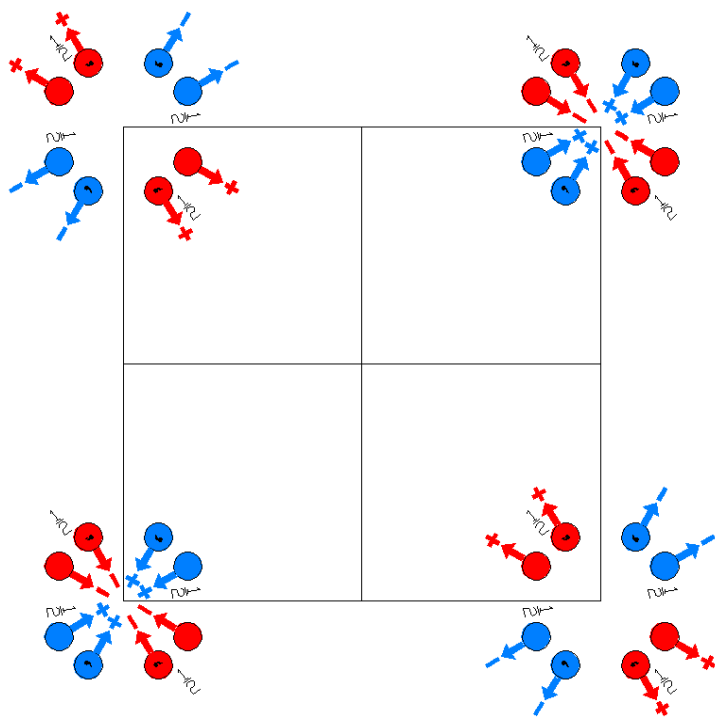
Along [1,1,0]  $p_{2a}-1m1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b} + \mathbf{c})/2$   
 Origin at x-1/4,x+1/4,0



$P\bar{4}'2c'$   
112.7.928

$\bar{4}2m1'$   
 $P\bar{4}'2c'$

Tetragonal



Origin on  $\bar{4}'1c'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)     | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)'          | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)' |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2) | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2) | (7) c' (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2)' | (8) c' (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)'       |

For (1,0,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1,0,0)<br>(1 1,0,0)'                   | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'           | (3) $\bar{4}^+$ 1/2,-1/2,z; 1/2,-1/2,0<br>( $\bar{4}_z$  1,0,0)    | (4) $\bar{4}^-$ 1/2,1/2,z; 1/2,1/2,0<br>( $\bar{4}_z^{-1}$  1,0,0) |
| (5) 2' 1/2,y,1/4<br>(2 <sub>y</sub>  1,0,1/2)' | (6) 2' (1,0,0) x,0,1/4<br>(2 <sub>x</sub>  1,0,1/2)' | (7) n (1/2,-1/2,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1,0,1/2) | (8) n (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1,0,1/2)            |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

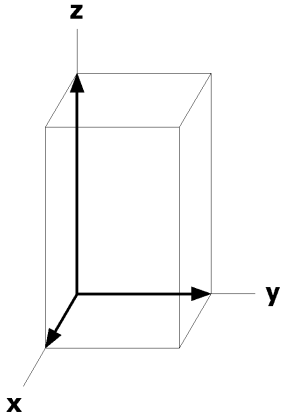
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(1,0,0)' +			
16 n 1	(1)	x,y,z [u,v,w]	(2)	$\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3)	y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(4)	$\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
	(5)	$\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6)	x, $\bar{y},\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ]	(7)	$\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(8)	y,x,z+1/2 [v,u,w]
8 m 2'..		0,1/2,z [u,v,0]		1/2,0, $\bar{z}$ [v, $\bar{u},0$ ]		0,1/2, $\bar{z}+1/2$ [ $\bar{u},v,0$ ]		1/2,0,z+1/2 [v,u,0]
8 l 2..		1/2,1/2,z [0,0,w]		1/2,1/2, $\bar{z}$ [0,0,w]		1/2,1/2, $\bar{z}+1/2$ [0,0,w]		1/2,1/2,z+1/2 [0,0,w]
8 k 2..		0,0,z [0,0,w]		0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]		0,0,z+1/2 [0,0,w]
8 j .2.		0,y,1/4 [0,v,0]		0, $\bar{y}$ ,1/4 [0, $\bar{v},0$ ]		y,0,3/4 [v,0,0]		$\bar{y},0,3/4$ [ $\bar{v},0,0$ ]
8 i .2'.		x,1/2,1/4 [0,v,w]		$\bar{x}$ ,1/2,1/4 [0,v, $\bar{w}$ ]		1/2, $\bar{x}$ ,3/4 [v,0, $\bar{w}$ ]		1/2,x,3/4 [v,0,w]
8 h .2'.		1/2,y,1/4 [u,0,w]		1/2, $\bar{y}$ ,1/4 [u,0, $\bar{w}$ ]		y,1/2,3/4 [0,u,w]		$\bar{y}$ ,1/2,3/4 [0,u, $\bar{w}$ ]
8 g .2.		x,0,1/4 [u,0,0]		$\bar{x}$ ,0,1/4 [ $\bar{u},0,0$ ]		0, $\bar{x}$ ,3/4 [0, $\bar{u},0$ ]		0,x,3/4 [0,u,0]
4 f $\bar{4}$ ..		1/2,1/2,0 [0,0,w]		1/2,1/2,1/2 [0,0,w]				
4 e $\bar{4}$ '..		0,0,0 [0,0,0]		0,0,1/2 [0,0,0]				
4 d 2'2'2.		0,1/2,1/4 [0,v,0]		1/2,0,3/4 [v,0,0]				
4 c 22'2'.		1/2,1/2,1/4 [0,0,w]		1/2,1/2,3/4 [0,0,w]				
4 b 2'22'.		1/2,0,1/4 [u,0,0]		0,1/2,3/4 [0,u,0]				
4 a 222.		0,0,1/4 [0,0,0]		0,0,3/4 [0,0,0]				

**Symmetry of Special Projections**

Along [0,0,1]  $p_4\bar{2}c'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,1/4

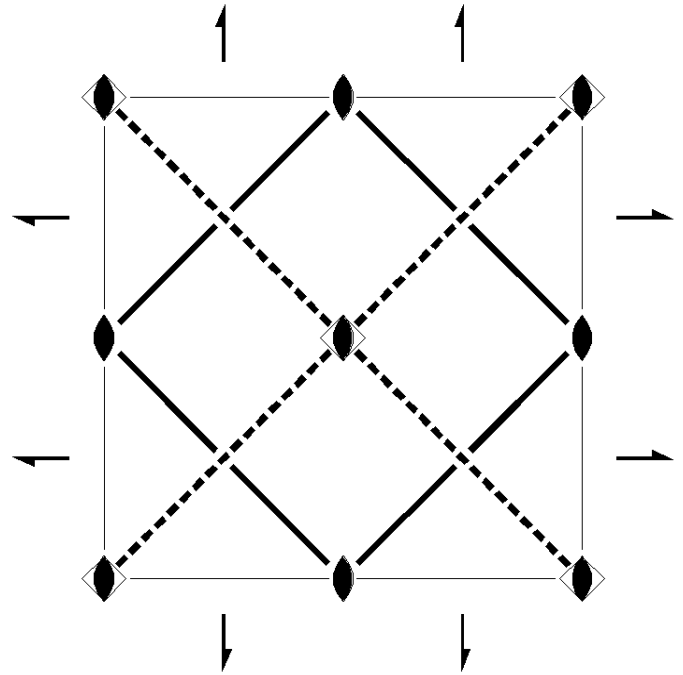
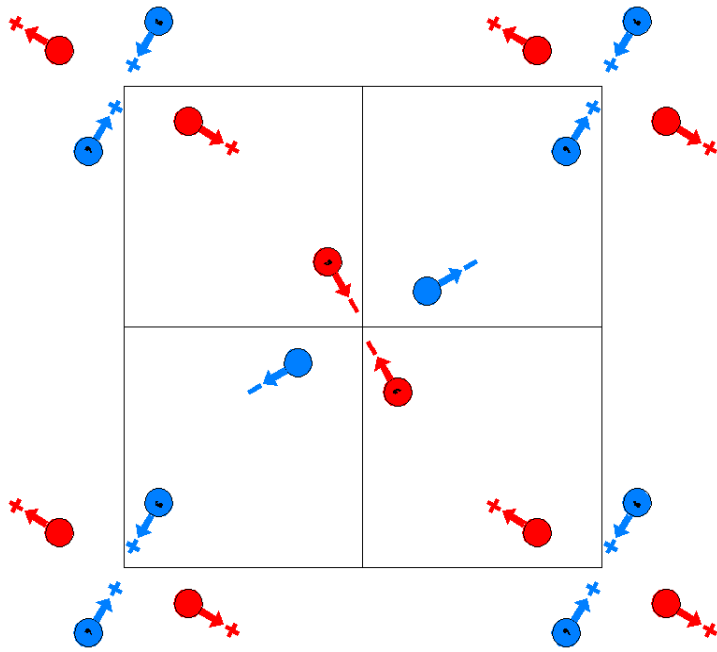
Along [1,1,0]  $p_{2a'}1m1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x-1/4,x+1/4,0



$P\bar{4}2_1m$   
113.1.929

$\bar{4}2m$   
 $P\bar{4}2_1m$

Tetragonal



Origin on  $\bar{4}1g$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$ ;  $y \leq 1/2 - x$

Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)   | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0) |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) | (7) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0) | (8) g (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0) |

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3); (5).

**Positions**

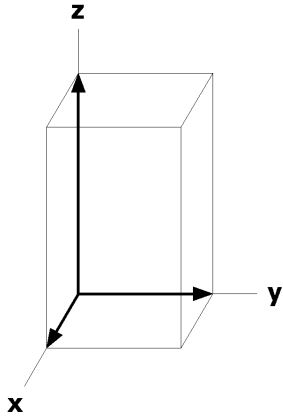
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	f	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $v,u,\bar{w}$ ]	(8) $y+1/2,x+1/2,z$ [ $\bar{v},\bar{u},\bar{w}$ ]		
4	e	$..m$	$x,x+1/2,z$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}+1/2,z$ [ $u,\bar{u},0$ ]	$x+1/2,\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,\bar{z}$ [ $u,u,0$ ]
4	d	$2..$	$0,0,z$ [ $0,0,w$ ]	$0,0,\bar{z}$ [ $0,0,w$ ]	$1/2,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,1/2,z$ [ $0,0,\bar{w}$ ]
2	c	$2.mm$	$0,1/2,z$ [ $0,0,0$ ]	$1/2,0,\bar{z}$ [ $0,0,0$ ]		
2	b	$\bar{4}..$	$0,0,1/2$ [ $0,0,w$ ]	$1/2,1/2,1/2$ [ $0,0,\bar{w}$ ]		
2	a	$\bar{4}..$	$0,0,0$ [ $0,0,w$ ]	$1/2,1/2,0$ [ $0,0,\bar{w}$ ]		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4'gm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,1/4,0$

Along  $[1,1,0]$   $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$

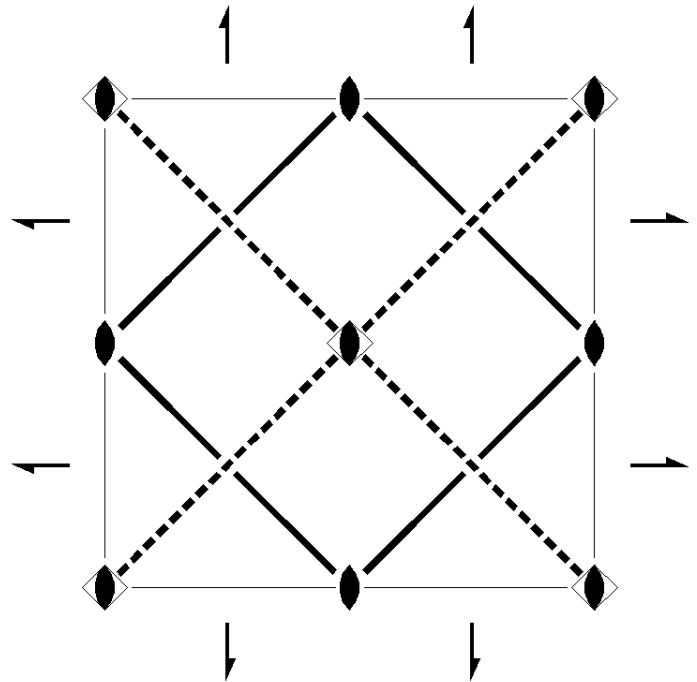
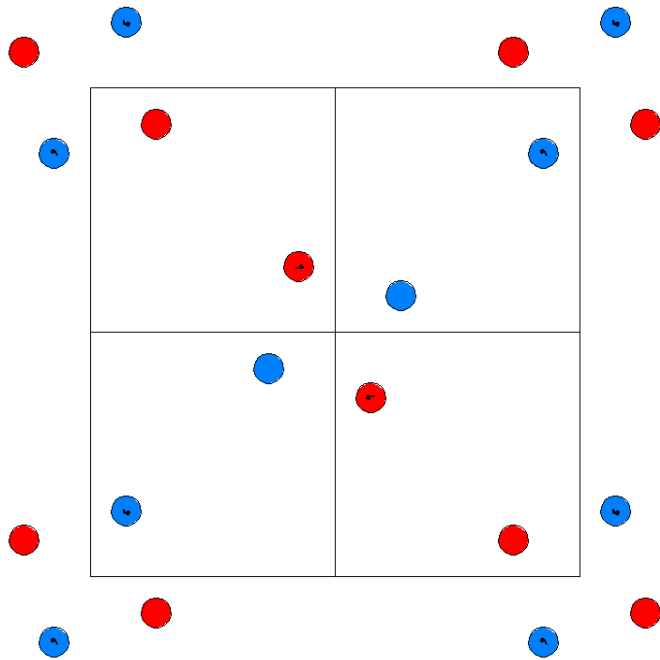


$P\bar{4}2_1m1'$   
113.2.930

$\bar{4}2m1'$   
 $P\bar{4}2_1m1'$

Tetragonal

1'



Origin on  $\bar{4}1g1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2-x$

**Symmetry Operations**

For 1 + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)     | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) | (7) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0) | (8) g (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)    |

For 1' + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1'<br>(1 0,0,0)'                                     | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                 | (3) $\bar{4}^+$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)'    | (4) $\bar{4}^-$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)' |
| (5) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (6) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' | (7) m' x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0)' | (8) g' (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)'     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +	1' +		
8 f 11'	(1) x,y,z [0,0,0]	(2) $\overline{x},\overline{y},z$ [0,0,0]		
	(3) $y,\overline{x},\overline{z}$ [0,0,0]	(4) $\overline{y},x,\overline{z}$ [0,0,0]		
	(5) $\overline{x}+1/2,y+1/2,\overline{z}$ [0,0,0]	(6) $x+1/2,\overline{y}+1/2,\overline{z}$ [0,0,0]		
	(7) $\overline{y}+1/2,\overline{x}+1/2,z$ [0,0,0]	(8) $y+1/2,x+1/2,z$ [0,0,0]		
4 e ..m1'	x,x+1/2,z [0,0,0]	$\overline{x},\overline{x}+1/2,z$ [0,0,0]	$x+1/2,\overline{x},\overline{z}$ [0,0,0]	$\overline{x}+1/2,x,\overline{z}$ [0,0,0]
4 d 2..1'	0,0,z [0,0,0]	$0,0,\overline{z}$ [0,0,0]	$1/2,1/2,\overline{z}$ [0,0,0]	$1/2,1/2,z$ [0,0,0]
2 c 2.mm1'	0,1/2,z [0,0,0]	$1/2,0,\overline{z}$ [0,0,0]		
2 b $\overline{4}..1'$	0,0,1/2 [0,0,0]	$1/2,1/2,1/2$ [0,0,0]		
2 a $\overline{4}..1'$	0,0,0 [0,0,0]	$1/2,1/2,0$ [0,0,0]		

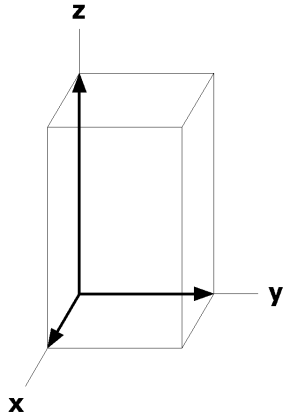
**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0

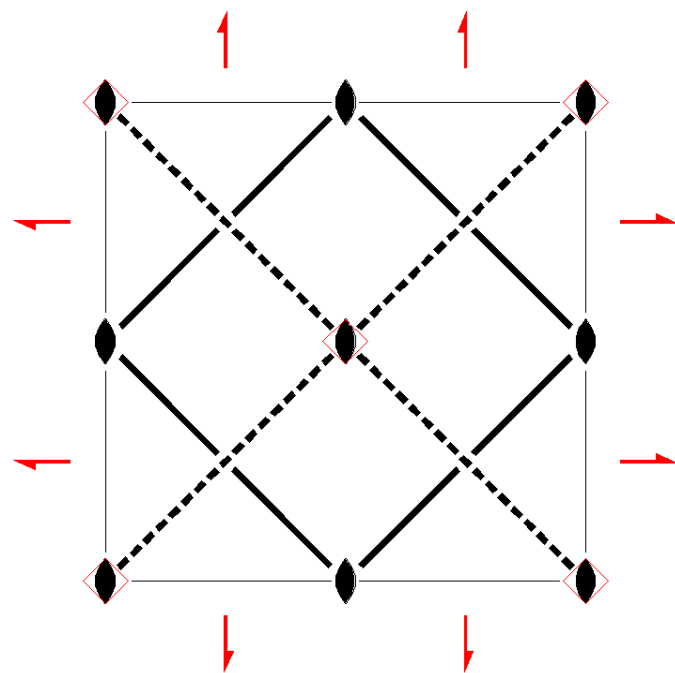
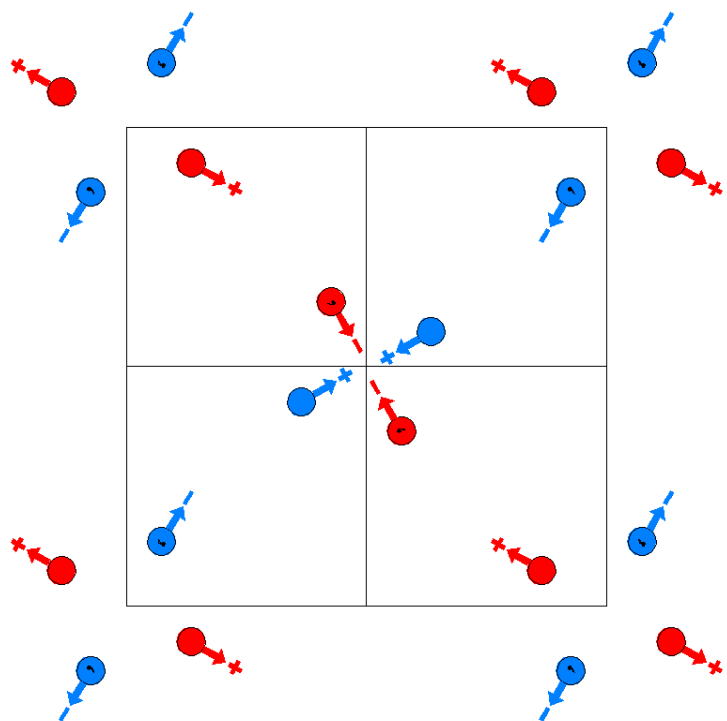




$P\bar{4}'2_1'm$   
113.3.931

$\bar{4}'2'm$   
 $P\bar{4}'2_1'm$

Tetragonal



Origin on  $\bar{4}'1g$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2 - x$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                           | (3) $\bar{4}'^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z$  0,0,0)' | (4) $\bar{4}'^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1}$  0,0,0)'    |
| (5) $2'$ $(0,1/2,0) \ 1/4,y,0$<br>( $2_y$   $1/2,1/2,0$ )' | (6) $2'$ $(1/2,0,0) \ x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )' | (7) $m \ x+1/2,\bar{x},z$<br>( $m_{xy}$   $1/2,1/2,0$ )   | (8) $g \ (1/2,1/2,0) \ x,x,z$<br>( $m_{\bar{xy}}$   $1/2,1/2,0$ ) |

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3); (5).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

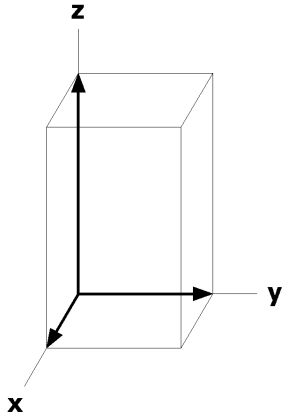
8	f	1	(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $y, \bar{x}, \bar{z}$ [ $v, \bar{u}, \bar{w}$ ]	(4) $\bar{y}, x, \bar{z}$ [ $\bar{v}, u, \bar{w}$ ]		
			(5) $\bar{x}+1/2, y+1/2, \bar{z}$ [ $u, \bar{v}, w$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $\bar{u}, v, w$ ]		
			(7) $\bar{y}+1/2, \bar{x}+1/2, z$ [ $v, u, \bar{w}$ ]	(8) $y+1/2, x+1/2, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
4	e	..m	$x, x+1/2, z$ [ $\bar{u}, u, 0$ ]	$\bar{x}, \bar{x}+1/2, z$ [ $u, \bar{u}, 0$ ]	$x+1/2, \bar{x}, \bar{z}$ [ $u, u, 0$ ]	$\bar{x}+1/2, x, \bar{z}$ [ $\bar{u}, \bar{u}, 0$ ]
4	d	2..	$0, 0, z$ [ $0, 0, w$ ]	$0, 0, \bar{z}$ [ $0, 0, \bar{w}$ ]	$1/2, 1/2, \bar{z}$ [ $0, 0, w$ ]	$1/2, 1/2, z$ [ $0, 0, \bar{w}$ ]
2	c	2.mm	$0, 1/2, z$ [ $0, 0, 0$ ]	$1/2, 0, \bar{z}$ [ $0, 0, 0$ ]		
2	b	$\bar{4}'..$	$0, 0, 1/2$ [ $0, 0, 0$ ]	$1/2, 1/2, 1/2$ [ $0, 0, 0$ ]		
2	a	$\bar{4}'..$	$0, 0, 0$ [ $0, 0, 0$ ]	$1/2, 1/2, 0$ [ $0, 0, 0$ ]		

**Symmetry of Special Projections**

Along  $[0, 0, 1]$   $p4g'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$   $p2'm'g$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 1/4, 0$

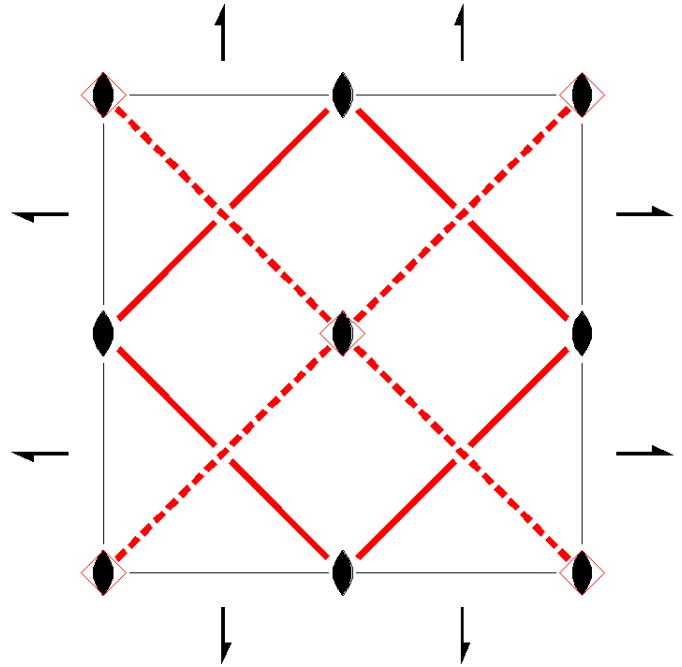
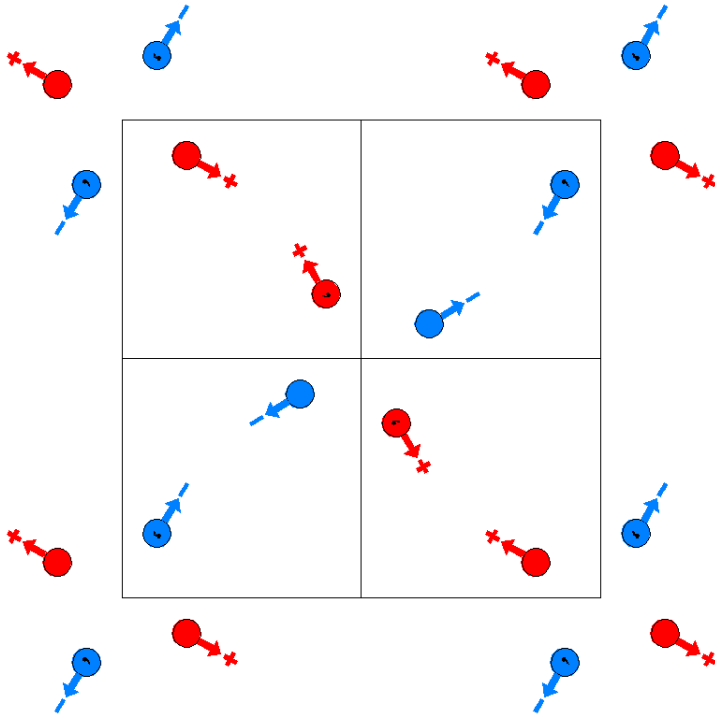
Along  $[1, 1, 0]$   $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 0$



$P\bar{4}'2_1m'$   
113.4.932

$\bar{4}'2m'$   
 $P\bar{4}'2_1m'$

Tetragonal



Origin on  $\bar{4}'1g'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2 - x$

Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) $\bar{4}'^+$ 0,0,z; 0,0,0<br>( $\bar{4}'_z$  0,0,0)'    | (4) $\bar{4}'^-$ 0,0,z; 0,0,0<br>( $\bar{4}'_z^{-1}$  0,0,0)' |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) | (7) m' x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0)' | (8) g' (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)'     |

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3); (5).

**Positions**

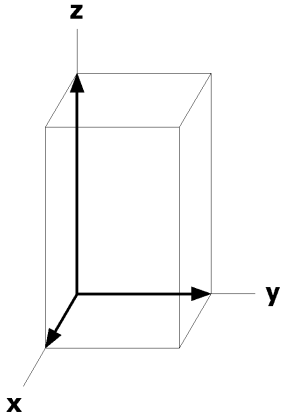
			Coordinates				
Multiplicity,	Wyckoff letter,	Site Symmetry.					
8	f	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]			
			(3) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]			
			(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]			
			(7) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $\bar{v},\bar{u},w$ ]	(8) $y+1/2,x+1/2,z$ [ $v,u,w$ ]			
4	e	..m'	$x,x+1/2,z$ [ $u,u,w$ ]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},w$ ]	$x+1/2,\bar{x},\bar{z}$ [ $u,\bar{u},\bar{w}$ ]	$\bar{x}+1/2,x,\bar{z}$ [ $\bar{u},u,\bar{w}$ ]	
4	d	2..	$0,0,z$ [ $0,0,w$ ]	$0,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,1/2,z$ [ $0,0,w$ ]	
2	c	2.m'm'	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,\bar{z}$ [ $0,0,\bar{w}$ ]			
2	b	$\bar{4}'..$	$0,0,1/2$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]			
2	a	$\bar{4}'..$	$0,0,0$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4gm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,1/4,0$

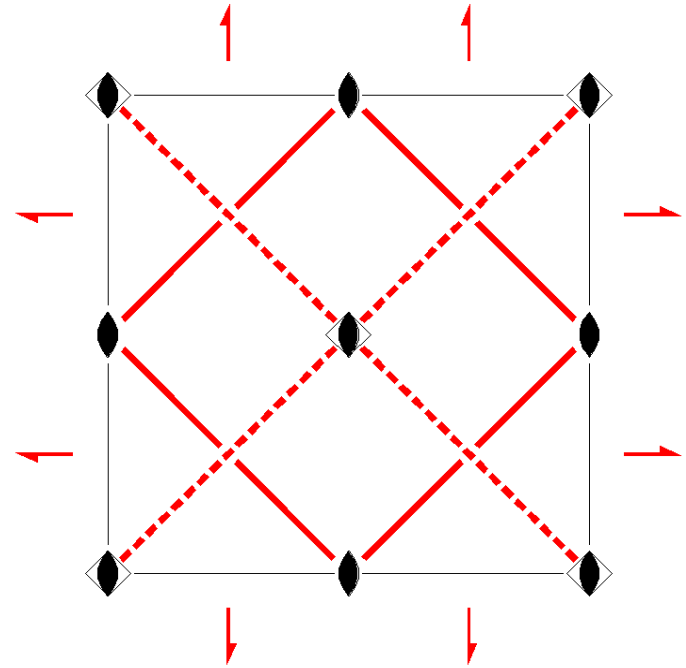
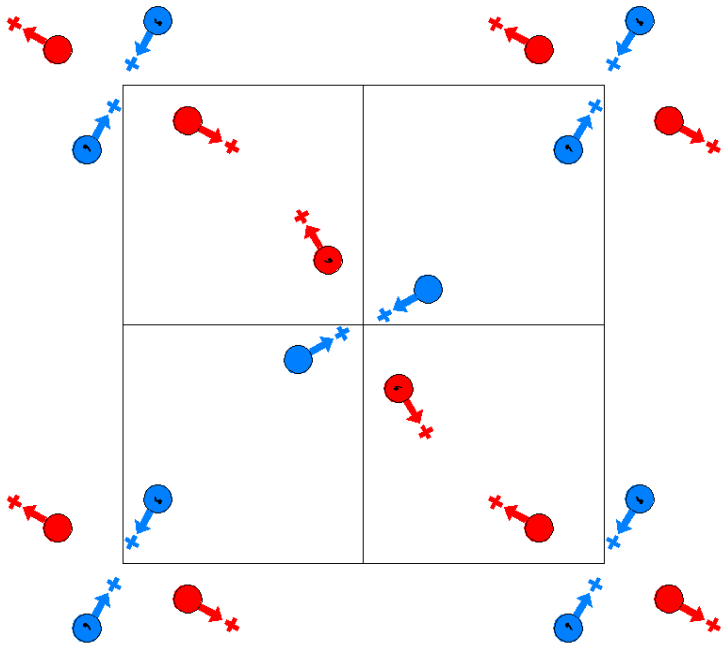
Along  $[1,1,0]$   $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$



$P\bar{4}2_1'm'$   
113.5.933

$\bar{4}2'm'$   
 $P\bar{4}2_1'm'$

Tetragonal



Origin on  $\bar{4}1g'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$ ;  $y \leq 1/2 - x$

### Symmetry Operations

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                           | (3) $\bar{4}^+$ $0,0,z$ ; $0,0,0$<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ $0,0,z$ ; $0,0,0$<br>( $\bar{4}_z^{-1}$  0,0,0)     |
| (5) $2'$ $(0,1/2,0)$ $1/4,y,0$<br>( $2_y$   $1/2,1/2,0$ )' | (6) $2'$ $(1/2,0,0)$ $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )' | (7) $m'$ $x+1/2,\bar{x},z$<br>( $m_{xy}$   $1/2,1/2,0$ )'  | (8) $g'$ $(1/2,1/2,0)$ $x,x,z$<br>( $m_{\bar{xy}}$   $1/2,1/2,0$ )' |

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

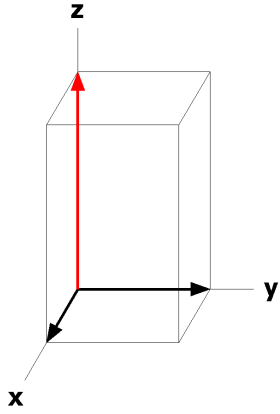
8	f	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]		
			(7) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $\bar{v},\bar{u},w$ ]	(8) $y+1/2,x+1/2,z$ [ $v,u,w$ ]		
4	e	$..m'$	$x,x+1/2,z$ [ $u,u,w$ ]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},w$ ]	$x+1/2,\bar{x},\bar{z}$ [ $\bar{u},u,w$ ]	$\bar{x}+1/2,x,\bar{z}$ [ $u,\bar{u},w$ ]
4	d	$2..$	$0,0,z$ [ $0,0,w$ ]	$0,0,\bar{z}$ [ $0,0,w$ ]	$1/2,1/2,\bar{z}$ [ $0,0,w$ ]	$1/2,1/2,z$ [ $0,0,w$ ]
2	c	$2.m'm'$	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,\bar{z}$ [ $0,0,w$ ]		
2	b	$\bar{4}..$	$0,0,1/2$ [ $0,0,w$ ]	$1/2,1/2,1/2$ [ $0,0,w$ ]		
2	a	$\bar{4}..$	$0,0,0$ [ $0,0,w$ ]	$1/2,1/2,0$ [ $0,0,w$ ]		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4'g'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2'm'g$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,1/4,0$

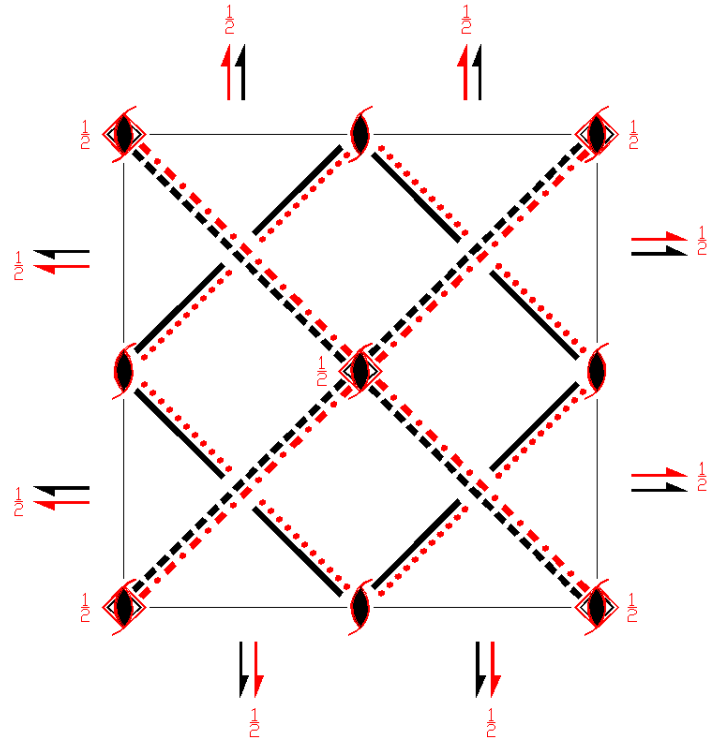
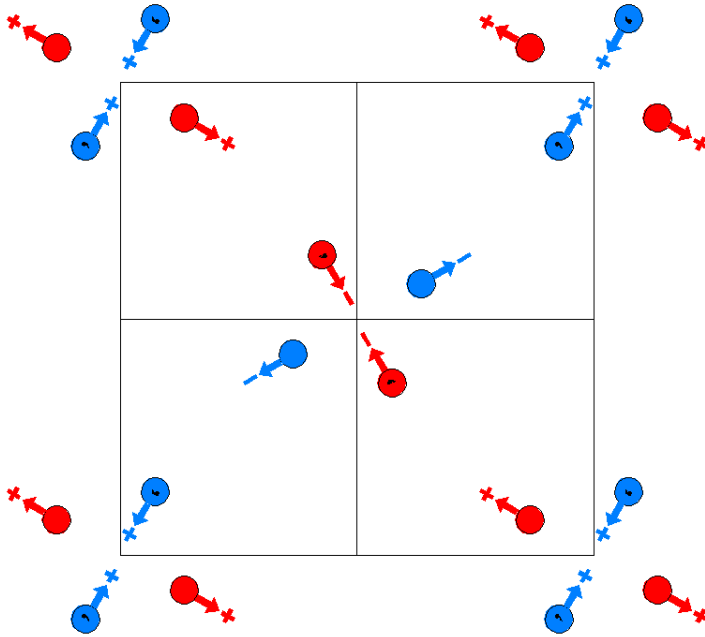
Along  $[1,1,0]$   $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$



$P_{2c} \bar{4}2_1m$   
113.6.934

$\bar{4}2m1'$   
 $P_{2c} \bar{4}2_1m$

Tetragonal



Origin on  $\bar{4}1g$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2 - x$

Symmetry Operations

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)   | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0) |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) | (7) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0) | (8) g (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0) |

For (0,0,1)' + set

- |  |  |   |  |
|--|--|---|--|
| (1) t' (0,0,1)<br>(1 0,0,1)'                               | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)'           | (3) $\bar{4}^+$ ' 0,0,z; 0,0,1/2<br>( $\bar{4}_z^+$  0,0,1)'        | (4) $\bar{4}^-$ ' 0,0,z; 0,0,1/2<br>( $\bar{4}_z^-$  0,0,1)' |
| (5) 2' (0,1/2,0) 1/4,y,1/2<br>(2 <sub>y</sub>  1/2,1/2,1)' | (6) 2' (1/2,0,0) x,1/4,1/2<br>(2 <sub>x</sub>  1/2,1/2,1)' | (7) c' (0,0,1) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1)' | (8) n' (1/2,1/2,1) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1)'    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +		(0,0,1)' +	
16	f	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $y, \bar{x}, \bar{z}$ [ $\bar{v}, u, w$ ]	(4) $\bar{y}, x, \bar{z}$ [ $v, \bar{u}, w$ ]
			(5) $\bar{x}+1/2, y+1/2, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]	(7) $\bar{y}+1/2, \bar{x}+1/2, z$ [ $v, u, \bar{w}$ ]	(8) $y+1/2, x+1/2, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]
8	e	..m	$x, x+1/2, z$ [ $\bar{u}, u, 0$ ]	$\bar{x}, \bar{x}+1/2, z$ [ $u, \bar{u}, 0$ ]	$x+1/2, \bar{x}, \bar{z}$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}+1/2, x, \bar{z}$ [ $u, u, 0$ ]
8	d	2..	$0, 0, z$ [0,0,w]	$0, 0, \bar{z}$ [0,0,w]	$1/2, 1/2, \bar{z}$ [0,0, $\bar{w}$ ]	$1/2, 1/2, z$ [0,0, $\bar{w}$ ]
4	c	2.mm	$0, 1/2, z$ [0,0,0]	$1/2, 0, \bar{z}$ [0,0,0]		
4	b	$\bar{4}'..$	$0, 0, 1/2$ [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]		
4	a	$\bar{4}'..$	$0, 0, 0$ [0,0,w]	$1/2, 1/2, 0$ [0,0, $\bar{w}$ ]		

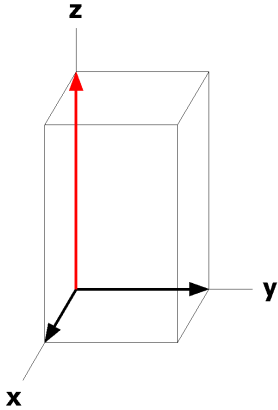
**Symmetry of Special Projections**

Along [0,0,1]  $p4gm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b} 2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 1/4, 0$

Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 0$





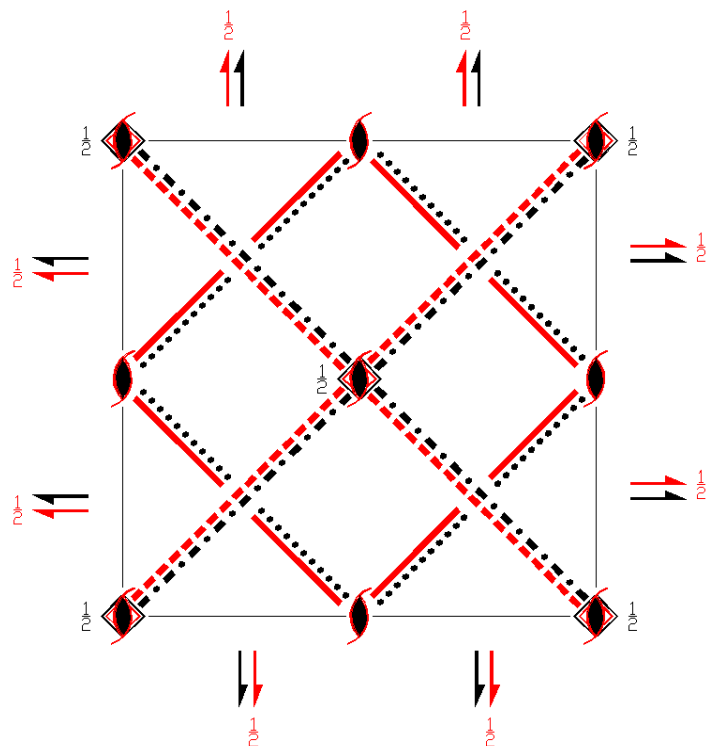
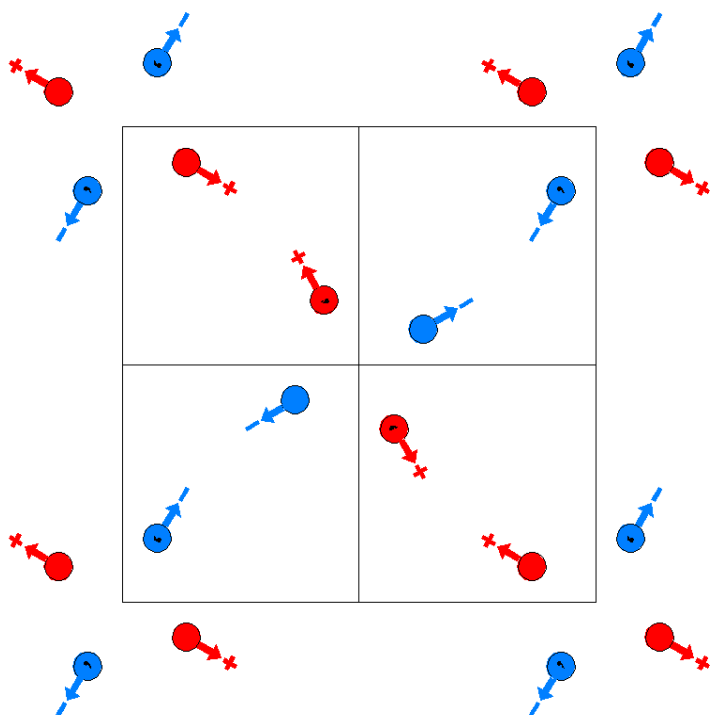
$P_{2c} \bar{4}' 2_1 m'$

113.7.935

$\bar{4} 2 m 1'$

$P_{2c} \bar{4}' 2_1 m'$

Tetragonal



Origin on  $\bar{4}' 1g'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2 - x$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) $\bar{4}^+ 0,0,z; 0,0,0$<br>( $\bar{4}_z^+ 0,0,0$ )'    | (4) $\bar{4}^- 0,0,z; 0,0,0$<br>( $\bar{4}_z^- 0,0,0$ )'  |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0) | (7) m' x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0)' | (8) g' (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)' |

For (0,0,1) + set

- |  |  |   |   |
|--|--|---|---|
| (1) t' (0,0,1)<br>(1 0,0,1)'                               | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)'           | (3) $\bar{4}^+ 0,0,z; 0,0,1/2$<br>( $\bar{4}_z^+ 0,0,1$ )         | (4) $\bar{4}^- 0,0,z; 0,0,1/2$<br>( $\bar{4}_z^- 0,0,1$ ) |
| (5) 2' (0,1/2,0) 1/4,y,1/2<br>(2 <sub>y</sub>  1/2,1/2,1)' | (6) 2' (1/2,0,0) x,1/4,1/2<br>(2 <sub>x</sub>  1/2,1/2,1)' | (7) c (0,0,1) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1) | (8) n (1/2,1/2,1) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

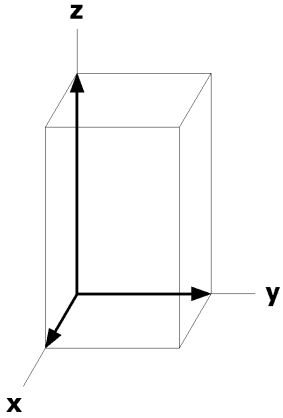
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(0,0,1)' +		
16	f	1	(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $y, \bar{x}, \bar{z}$ [ $v, \bar{u}, \bar{w}$ ]	(4) $\bar{y}, x, \bar{z}$ [ $\bar{v}, u, \bar{w}$ ]
			(5) $\bar{x}+1/2, y+1/2, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]	(7) $\bar{y}+1/2, \bar{x}+1/2, z$ [ $\bar{v}, \bar{u}, w$ ]	(8) $y+1/2, x+1/2, z$ [ $v, u, w$ ]
8	e	..m'	x,x+1/2,z [u,u,w]	$\bar{x}, \bar{x}+1/2, z$ [ $\bar{u}, \bar{u}, w$ ]	$x+1/2, \bar{x}, \bar{z}$ [ $u, \bar{u}, \bar{w}$ ]	$\bar{x}+1/2, x, \bar{z}$ [ $\bar{u}, u, \bar{w}$ ]
8	d	2..	0,0,z [0,0,w]	$0, 0, \bar{z}$ [ $0, 0, \bar{w}$ ]	$1/2, 1/2, \bar{z}$ [ $0, 0, \bar{w}$ ]	$1/2, 1/2, z$ [ $0, 0, w$ ]
4	c	2.m'm'	0,1/2,z [0,0,w]	$1/2, 0, \bar{z}$ [ $0, 0, \bar{w}$ ]		
4	b	$\bar{4}$ ..	0,0,1/2 [0,0,w]	$1/2, 1/2, 1/2$ [ $0, 0, w$ ]		
4	a	$\bar{4}$ '..	0,0,0 [0,0,0]	$1/2, 1/2, 0$ [ $0, 0, 0$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4gm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b} 2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

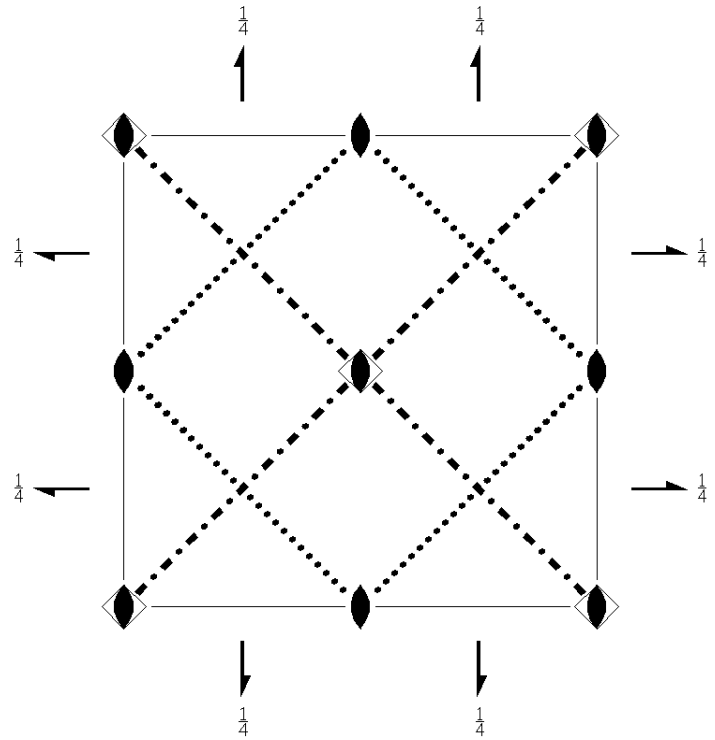
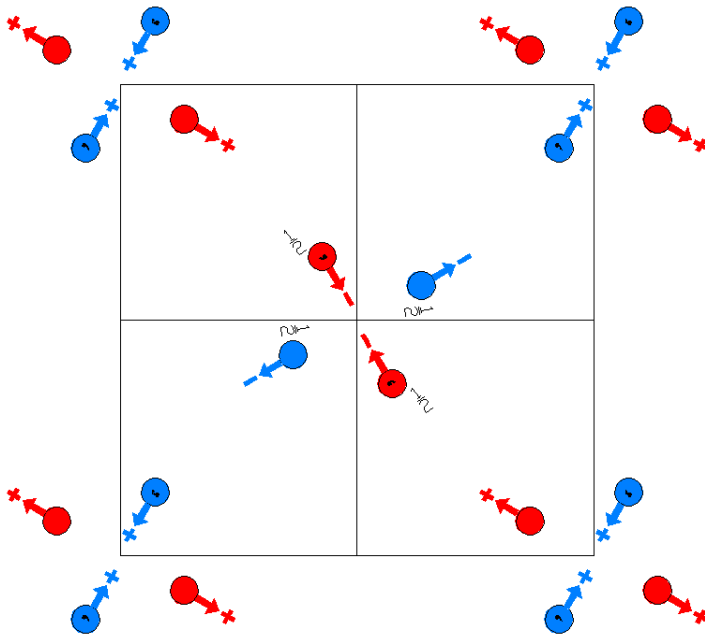
Along [1,1,0]  $p_{2b} 1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P\bar{4}2_1c$   
114.1.936

$\bar{4}2m$   
 $P\bar{4}2_1c$

Tetragonal



Origin on  $\bar{4}1n$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)               | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)     |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) | (7) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (8) n (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

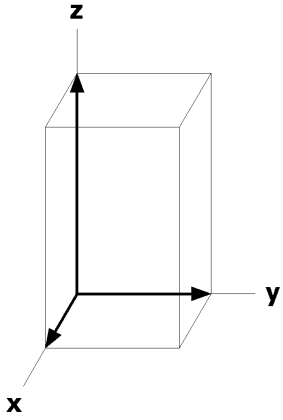
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	e	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $y, \bar{x}, \bar{z}$ [ $\bar{v}, u, w$ ]	(4) $\bar{y}, x, \bar{z}$ [ $v, \bar{u}, w$ ]		
			(5) $\bar{x}+1/2, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+1/2$ [ $u, \bar{v}, \bar{w}$ ]		
			(7) $\bar{y}+1/2, \bar{x}+1/2, z+1/2$ [ $v, u, \bar{w}$ ]	(8) $y+1/2, x+1/2, z+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
4	d	2..	$0, 1/2, z$ [0,0,w]	$1/2, 0, \bar{z}$ [0,0,w]	$1/2, 0, \bar{z}+1/2$ [0,0, $\bar{w}$ ]	$0, 1/2, z+1/2$ [0,0, $\bar{w}$ ]
4	c	2..	$0, 0, z$ [0,0,w]	$0, 0, \bar{z}$ [0,0,w]	$1/2, 1/2, \bar{z}+1/2$ [0,0, $\bar{w}$ ]	$1/2, 1/2, z+1/2$ [0,0, $\bar{w}$ ]
2	b	$\bar{4}..$	$0, 0, 1/2$ [0,0,w]	$1/2, 1/2, 0$ [0,0, $\bar{w}$ ]		
2	a	$\bar{4}..$	$0, 0, 0$ [0,0,w]	$1/2, 1/2, 1/2$ [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4'g'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [1,1,0]  $p_{2b}1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

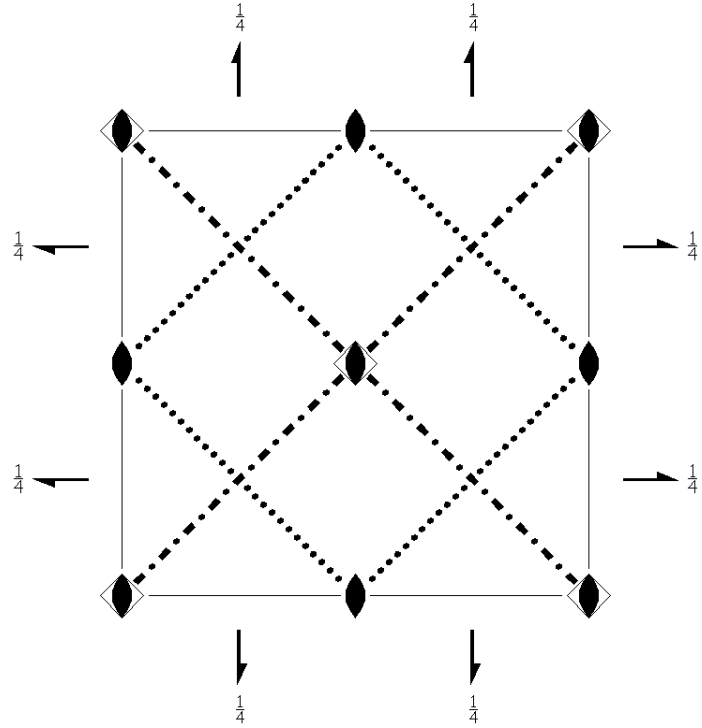
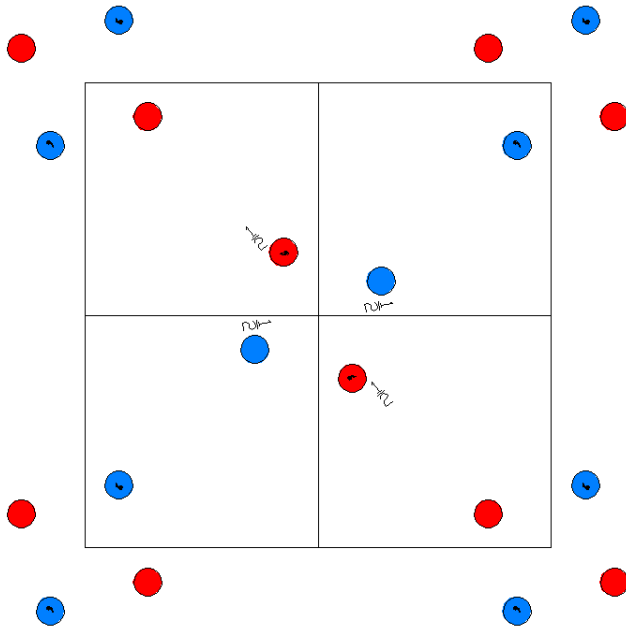


$P\bar{4}2_1c1'$   
114.2.937

$\bar{4}2m1'$   
 $P\bar{4}2_1c1'$

Tetragonal

1'



Origin on  $\bar{4}1n1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For 1 + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)               | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)     |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) | (7) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (8) n (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) |

For 1' + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1'<br>(1 0,0,0)'   | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                     | (3) $\bar{4}^+$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'              | (4) $\bar{4}^-$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'    |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' | (7) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)' | (8) n' (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

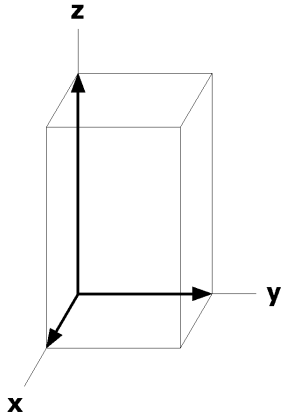
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +	1' +		
8 e 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]		
	(3) $y,\bar{x},\bar{z}$ [0,0,0]	(4) $\bar{y},x,\bar{z}$ [0,0,0]		
	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [0,0,0]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [0,0,0]		
	(7) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [0,0,0]	(8) $y+1/2,x+1/2,z+1/2$ [0,0,0]		
4 d 2..1'	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	0,1/2,z+1/2 [0,0,0]
4 c 2..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,1/2,z+1/2 [0,0,0]
2 b $\bar{4}..1'$	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2 a $\bar{4}..1'$	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

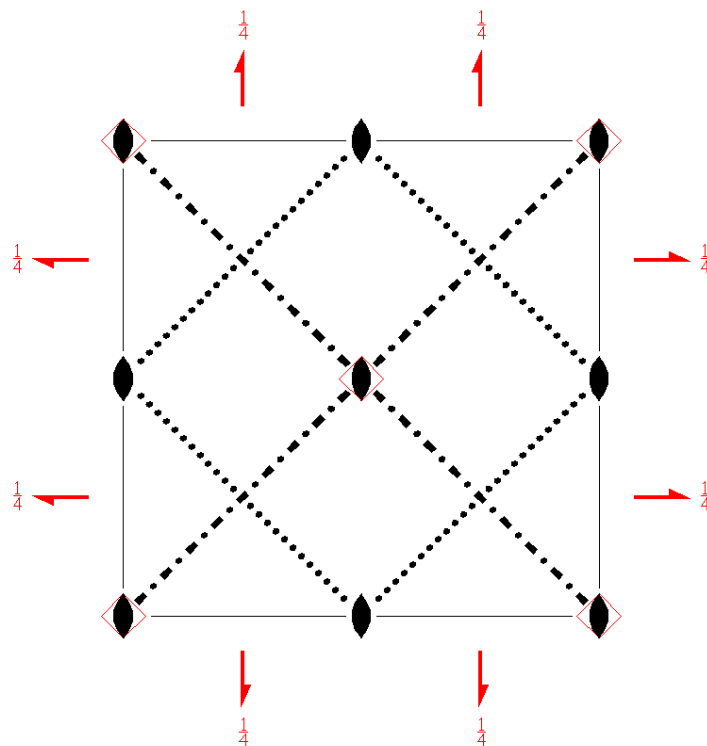
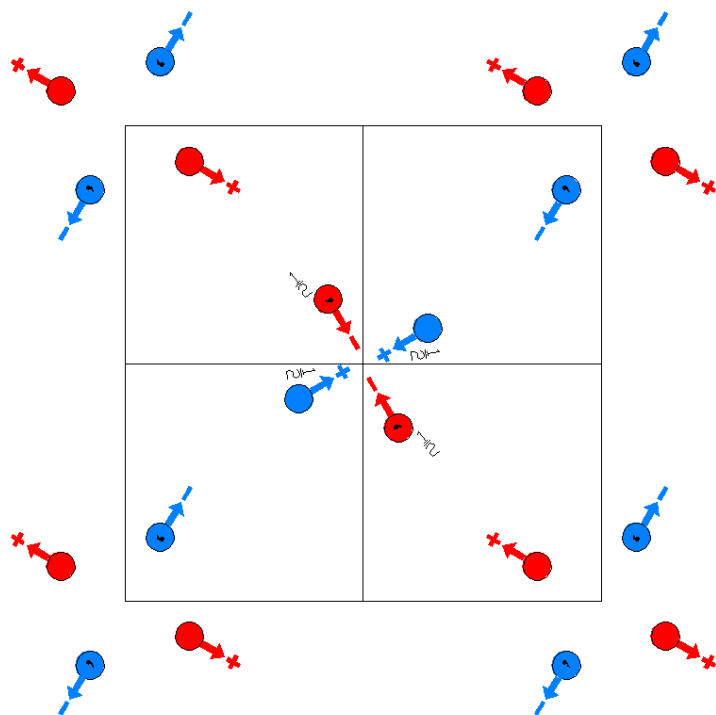
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P\bar{4}'2_1'c$   
114.3.938

$\bar{4}'2'm$   
 $P\bar{4}'2_1'c$

Tetragonal



Origin on  $\bar{4}'1n$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                               | (3) $\bar{4}'^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^+$  0,0,0)'         | (4) $\bar{4}'^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^-$  0,0,0)'         |
| (5) $2'$ $(0,1/2,0)$ $1/4,y,1/4$<br>( $2_y$   $1/2,1/2,1/2$ )' | (6) $2'$ $(1/2,0,0)$ $x,1/4,1/4$<br>( $2_x$   $1/2,1/2,1/2$ )' | (7) c $(0,0,1/2)$ $x+1/2,\bar{x},z$<br>( $m_{xy}$   $1/2,1/2,1/2$ ) | (8) n $(1/2,1/2,1/2)$ $x,x,z$<br>( $m_{\bar{xy}}$   $1/2,1/2,1/2$ ) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	e	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $y, \bar{x}, \bar{z}$ [v, $\bar{u}, \bar{w}$ ]	(4) $\bar{y}, x, \bar{z}$ [ $\bar{v}, u, \bar{w}$ ]		
			(5) $\bar{x}+1/2, y+1/2, \bar{z}+1/2$ [u, $\bar{v}, w$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]		
			(7) $\bar{y}+1/2, \bar{x}+1/2, z+1/2$ [v,u, $\bar{w}$ ]	(8) $y+1/2, x+1/2, z+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
4	d	2..	$0, 1/2, z$ [0,0,w]	$1/2, 0, \bar{z}$ [0,0, $\bar{w}$ ]	$1/2, 0, \bar{z}+1/2$ [0,0,w]	$0, 1/2, z+1/2$ [0,0, $\bar{w}$ ]
4	c	2..	$0, 0, z$ [0,0,w]	$0, 0, \bar{z}$ [0,0, $\bar{w}$ ]	$1/2, 1/2, \bar{z}+1/2$ [0,0,w]	$1/2, 1/2, z+1/2$ [0,0, $\bar{w}$ ]
2	b	$\bar{4}'..$	$0, 0, 1/2$ [0,0,0]	$1/2, 1/2, 0$ [0,0,0]		
2	a	$\bar{4}'..$	$0, 0, 0$ [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]		

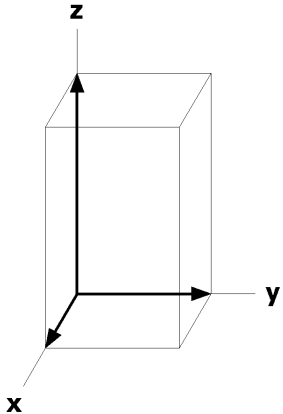
**Symmetry of Special Projections**

Along [0,0,1]  $p4g'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2'm'g$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [1,1,0]  $p_{2b}1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

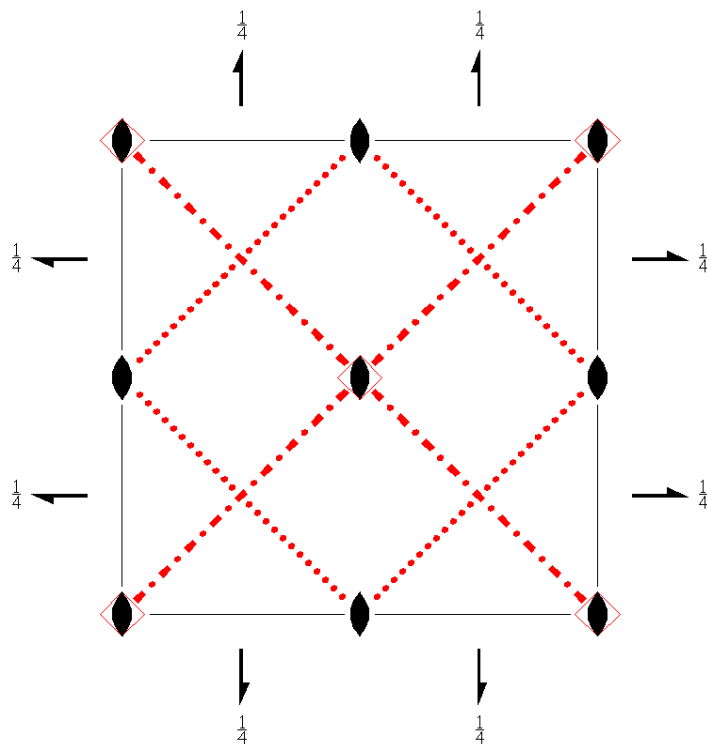
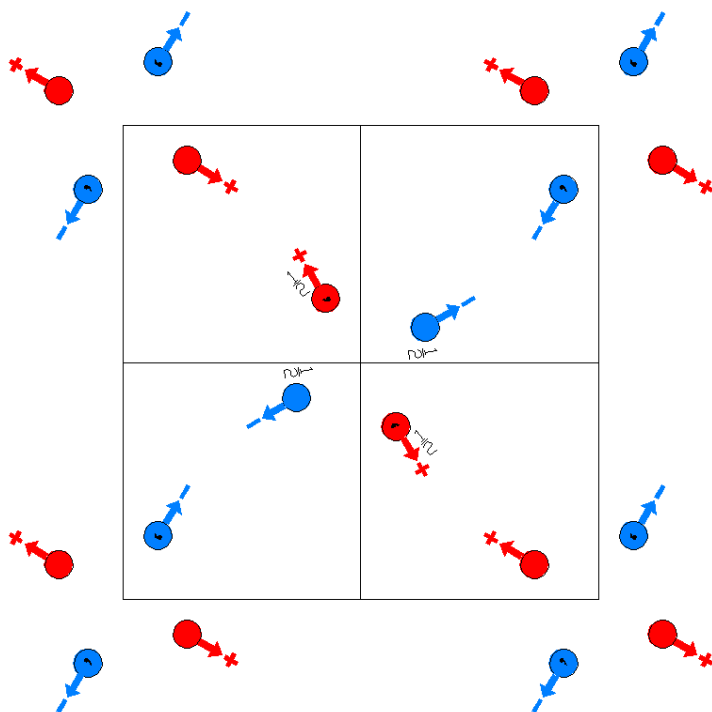




$P\bar{4}'2_1c'$   
114.4.939

$\bar{4}'2m'$   
 $P\bar{4}'2_1c'$

Tetragonal



Origin on  $\bar{4}'1n'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) $\bar{4}'^+$ 0,0,z; 0,0,0<br>( $\bar{4}'_z$  0,0,0)'                | (4) $\bar{4}'^-$ 0,0,z; 0,0,0<br>( $\bar{4}'_z^{-1}$  0,0,0)' |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) | (7) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)' | (8) n' (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

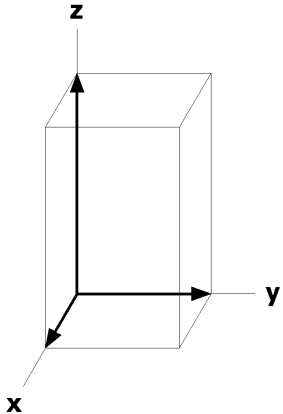
			Coordinates							
Multiplicity,	Wyckoff letter,	Site Symmetry.								
8	e	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $y, \bar{x}, \bar{z}$ [v, $\bar{u}, \bar{w}$ ]	(4) $\bar{y}, x, \bar{z}$ [ $\bar{v}, u, \bar{w}$ ]	(5) $\bar{x}+1/2, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+1/2$ [u, $\bar{v}, \bar{w}$ ]	(7) $\bar{y}+1/2, \bar{x}+1/2, z+1/2$ [ $\bar{v}, \bar{u}, w$ ]	(8) $y+1/2, x+1/2, z+1/2$ [v,u,w]
4	d	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0,w]				
4	c	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0,w]				
2	b	$\bar{4}'$ ..	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]						
2	a	$\bar{4}'$ ..	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]						

**Symmetry of Special Projections**

Along [0,0,1]  $p4gm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

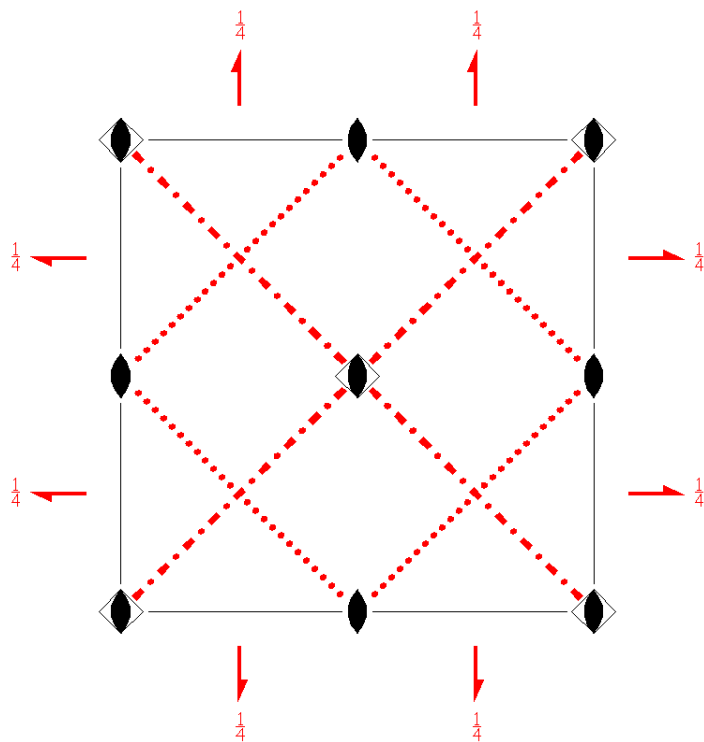
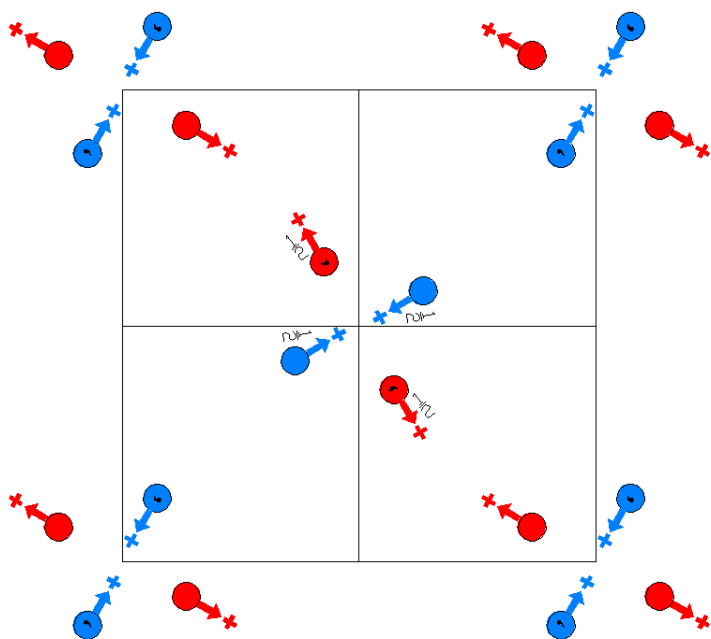
Along [1,1,0]  $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P\bar{4}2_1c'$   
114.5.940

$\bar{4}2'm'$   
 $P\bar{4}2_1c'$

Tetragonal



Origin on  $\bar{4}1n'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                       | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)                   | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)    |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' | (7) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)' | (8) n' (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

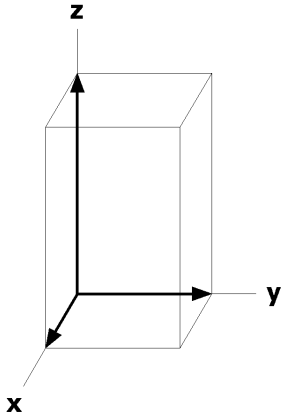
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	e	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $y, \bar{x}, \bar{z}$ [ $\bar{v}, u, w$ ]	(4) $\bar{y}, x, \bar{z}$ [ $v, \bar{u}, w$ ]		
			(5) $\bar{x}+1/2, y+1/2, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]		
			(7) $\bar{y}+1/2, \bar{x}+1/2, z+1/2$ [ $\bar{v}, \bar{u}, w$ ]	(8) $y+1/2, x+1/2, z+1/2$ [ $v, u, w$ ]		
4	d	2..	$0, 1/2, z$ [0,0,w]	$1/2, 0, \bar{z}$ [0,0,w]	$1/2, 0, \bar{z}+1/2$ [0,0,w]	$0, 1/2, z+1/2$ [0,0,w]
4	c	2..	$0, 0, z$ [0,0,w]	$0, 0, \bar{z}$ [0,0,w]	$1/2, 1/2, \bar{z}+1/2$ [0,0,w]	$1/2, 1/2, z+1/2$ [0,0,w]
2	b	$\bar{4}..$	$0, 0, 1/2$ [0,0,w]	$1/2, 1/2, 0$ [0,0,w]		
2	a	$\bar{4}..$	$0, 0, 0$ [0,0,w]	$1/2, 1/2, 1/2$ [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4'g'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2'm'g$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 1/4, 1/4$

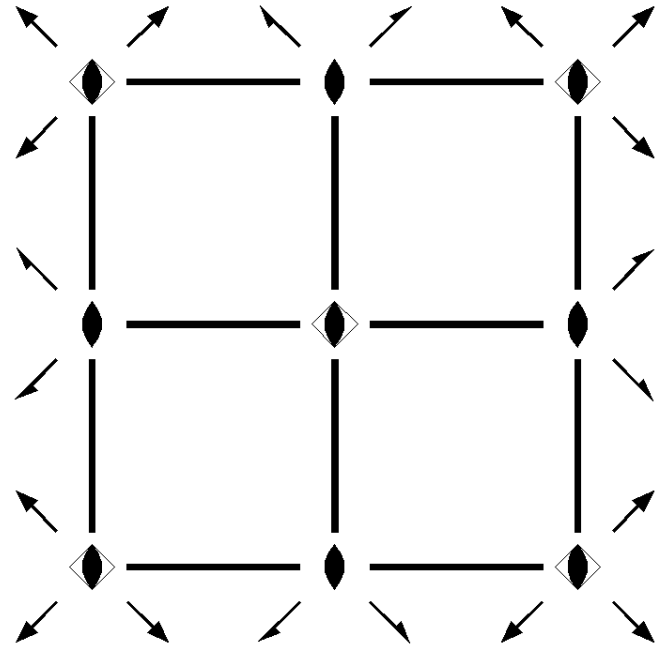
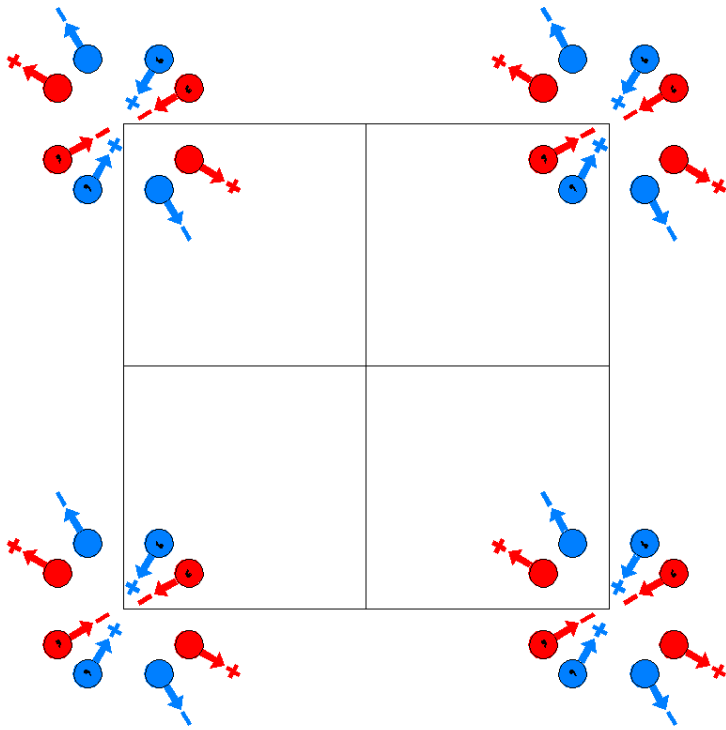
Along [1,1,0]  $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, x, 0$



$P\bar{4}m2$   
115.1.941

$\bar{4}m2$   
 $P\bar{4}m2$

Tetragonal



Origin on  $\bar{4}m2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (6) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)               | (8) 2 x, $\bar{x}$ ,0<br>(2 $\bar{xy}$  0,0,0)             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

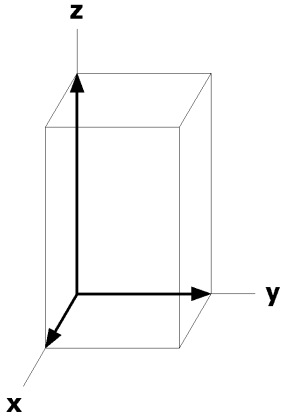
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	l	1	(1) x,y,z [u,v,w] (5) $\overline{x},\overline{y},z$ [ $\overline{u},v,\overline{w}$ ]	(2) $\overline{x},\overline{y},z$ [ $\overline{u},\overline{v},w$ ] (6) $\overline{x},y,z$ [ $u,\overline{v},\overline{w}$ ]	(3) y, $\overline{x},\overline{z}$ [ $\overline{v},u,w$ ] (7) y,x, $\overline{z}$ [v,u, $\overline{w}$ ]	(4) $\overline{y},x,\overline{z}$ [v, $\overline{u},w$ ] (8) $\overline{y},\overline{x},\overline{z}$ [ $\overline{v},\overline{u},\overline{w}$ ]
4	k	.m.	x,1/2,z [0,v,0]	$\overline{x},1/2,z$ [0, $\overline{v},0$ ]	1/2, $\overline{x},\overline{z}$ [ $\overline{v},0,0$ ]	1/2,x, $\overline{z}$ [v,0,0]
4	j	.m.	x,0,z [0,v,0]	$\overline{x},0,z$ [0, $\overline{v},0$ ]	0, $\overline{x},\overline{z}$ [ $\overline{v},0,0$ ]	0,x, $\overline{z}$ [v,0,0]
4	i	..2	x,x,1/2 [u,u,0]	$\overline{x},\overline{x},1/2$ [ $\overline{u},\overline{u},0$ ]	x, $\overline{x},1/2$ [ $\overline{u},u,0$ ]	$\overline{x},x,1/2$ [u, $\overline{u},0$ ]
4	h	..2	x,x,0 [u,u,0]	$\overline{x},\overline{x},0$ [ $\overline{u},\overline{u},0$ ]	x, $\overline{x},0$ [ $\overline{u},u,0$ ]	$\overline{x},x,0$ [u, $\overline{u},0$ ]
2	g	2mm.	0,1/2,z [0,0,0]	1/2,0, $\overline{z}$ [0,0,0]		
2	f	2mm.	1/2,1/2,z [0,0,0]	1/2,1/2, $\overline{z}$ [0,0,0]		
2	e	2mm.	0,0,z [0,0,0]	0,0, $\overline{z}$ [0,0,0]		
1	d	$\overline{4}m2$	0,0,1/2 [0,0,0]			
1	c	$\overline{4}m2$	1/2,1/2,1/2 [0,0,0]			
1	b	$\overline{4}m2$	1/2,1/2,0 [0,0,0]			
1	a	$\overline{4}m2$	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $p4'mm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0

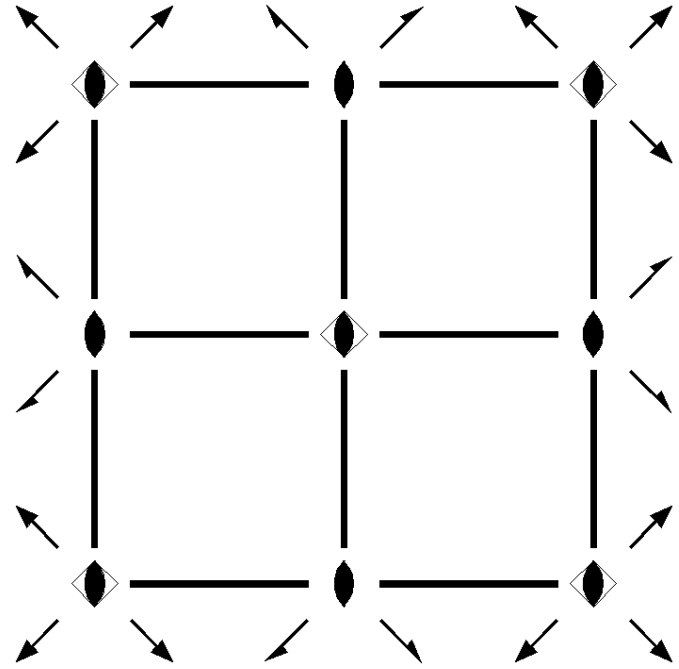
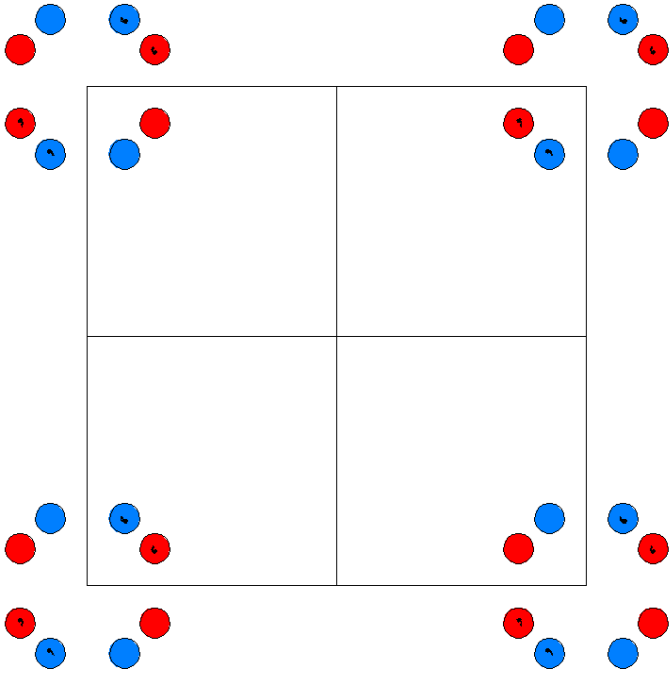


$P\bar{4}m21'$   
115.2.942

$\bar{4}m21'$   
 $P\bar{4}m21'$

Tetragonal

1'



Origin on  $\bar{4}m21'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For 1 + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)         |
| (5) m <sub>x</sub> x,0,z<br>(m <sub>y</sub>  0,0,0) | (6) m <sub>y</sub> 0,y,z<br>(m <sub>x</sub>  0,0,0) | (7) 2 <sub>xy</sub> x,x,0<br>(2 <sub>xy</sub>  0,0,0)   | (8) 2 <sub>xy</sub> x, $\bar{x}$ ,0<br>(2 <sub>xy</sub>  0,0,0) |

For 1' + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1'<br>(1 0,0,0)'                                   | (2) 2' <sub>z</sub> 0,0,z<br>(2' <sub>z</sub>  0,0,0)' | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'           |
| (5) m' <sub>x</sub> x,0,z<br>(m' <sub>y</sub>  0,0,0)' | (6) m' <sub>y</sub> 0,y,z<br>(m' <sub>x</sub>  0,0,0)' | (7) 2' <sub>xy</sub> x,x,0<br>(2' <sub>xy</sub>  0,0,0)' | (8) 2' <sub>xy</sub> x, $\bar{x}$ ,0<br>(2' <sub>xy</sub>  0,0,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
8 l 11'	(1) x,y,z [0,0,0]	(2) $\overline{x},\overline{y},z$ [0,0,0]	(3) $y,\overline{x},\overline{z}$ [0,0,0]	(4) $\overline{y},x,\overline{z}$ [0,0,0]
	(5) $x,\overline{y},z$ [0,0,0]	(6) $\overline{x},y,z$ [0,0,0]	(7) $y,x,\overline{z}$ [0,0,0]	(8) $\overline{y},\overline{x},\overline{z}$ [0,0,0]
4 k .m.1'	$x,1/2,z$ [0,0,0]	$\overline{x},1/2,z$ [0,0,0]	$1/2,\overline{x},\overline{z}$ [0,0,0]	$1/2,x,\overline{z}$ [0,0,0]
4 j .m.1'	$x,0,z$ [0,0,0]	$\overline{x},0,z$ [0,0,0]	$0,\overline{x},\overline{z}$ [0,0,0]	$0,x,\overline{z}$ [0,0,0]
4 i ..21'	$x,x,1/2$ [0,0,0]	$\overline{x},\overline{x},1/2$ [0,0,0]	$x,\overline{x},1/2$ [0,0,0]	$\overline{x},x,1/2$ [0,0,0]
4 h ..21'	$x,x,0$ [0,0,0]	$\overline{x},\overline{x},0$ [0,0,0]	$x,\overline{x},0$ [0,0,0]	$\overline{x},x,0$ [0,0,0]
2 g 2mm.1'	$0,1/2,z$ [0,0,0]	$1/2,0,\overline{z}$ [0,0,0]		
2 f 2mm.1'	$1/2,1/2,z$ [0,0,0]	$1/2,1/2,\overline{z}$ [0,0,0]		
2 e 2mm.1'	$0,0,z$ [0,0,0]	$0,0,\overline{z}$ [0,0,0]		
1 d $\overline{4}m21'$	$0,0,1/2$ [0,0,0]			
1 c $\overline{4}m21'$	$1/2,1/2,1/2$ [0,0,0]			
1 b $\overline{4}m21'$	$1/2,1/2,0$ [0,0,0]			
1 a $\overline{4}m21'$	$0,0,0$ [0,0,0]			

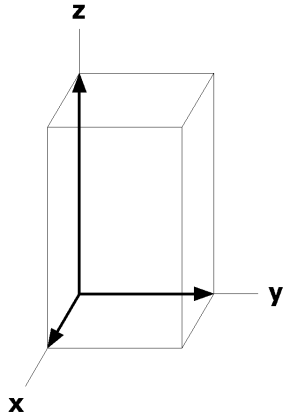
**Symmetry of Special Projections**

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0

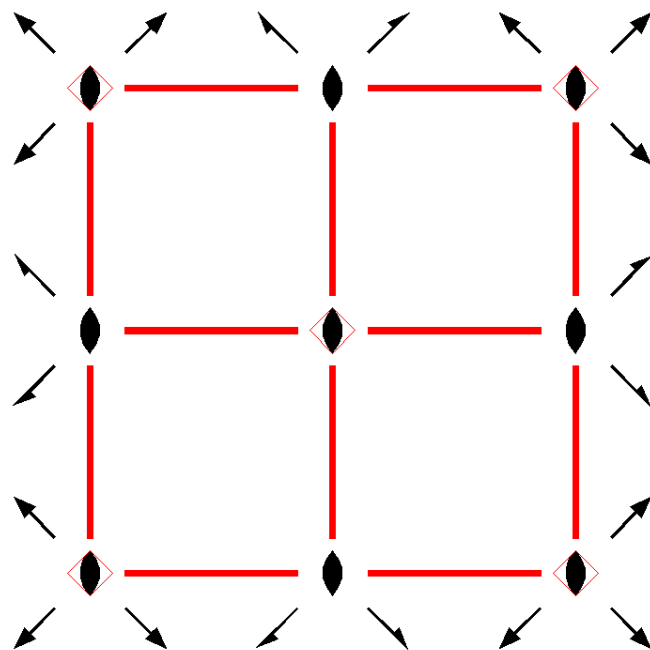
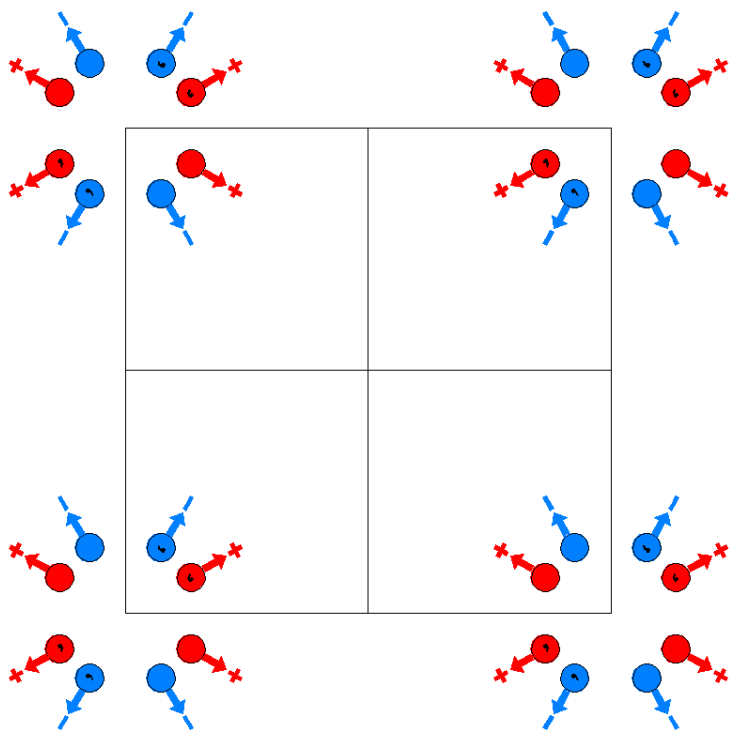




$P\bar{4}'m'2$   
115.3.943

$\bar{4}'m'2$   
 $P\bar{4}'m'2$

Tetragonal



Origin on  $\bar{4}'m'2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) $\bar{4}'^+$ 0,0,z; 0,0,0<br>( $\bar{4}'_z$  0,0,0)' | (4) $\bar{4}'^-$ 0,0,z; 0,0,0<br>( $\bar{4}'_z^{-1}$  0,0,0)'        |
| (5) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (6) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                  | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{x}y</math></sub>  0,0,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

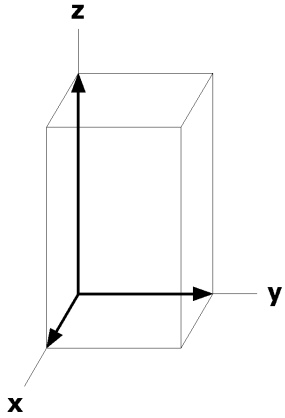
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	l	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(3) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ] (7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
4	k	.m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ]	1/2, $\bar{x},\bar{z}$ [0, $\bar{u},\bar{w}$ ]	1/2,x, $\bar{z}$ [0,u, $\bar{w}$ ]
4	j	.m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	0, $\bar{x},\bar{z}$ [0, $\bar{u},\bar{w}$ ]	0,x, $\bar{z}$ [0,u, $\bar{w}$ ]
4	i	..2	x,x,1/2 [u,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},1/2$ [u, $\bar{u},0$ ]	$\bar{x},x,1/2$ [ $\bar{u},u,0$ ]
4	h	..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},0$ [u, $\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]
2	g	2m'm'	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	f	2m'm'	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	e	2m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
1	d	$\bar{4}'m'2$	0,0,1/2 [0,0,0]			
1	c	$\bar{4}'m'2$	1/2,1/2,1/2 [0,0,0]			
1	b	$\bar{4}'m'2$	1/2,1/2,0 [0,0,0]			
1	a	$\bar{4}'m'2$	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

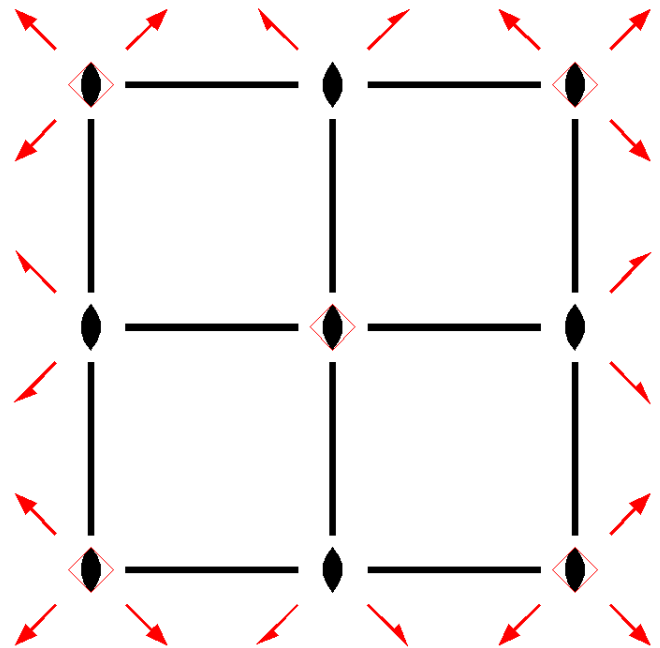
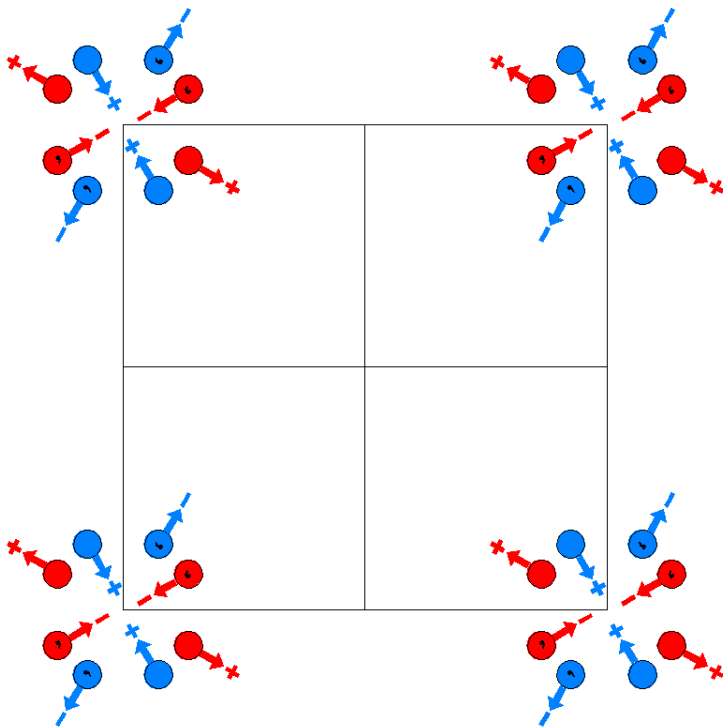
Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P\bar{4}'m2'$   
115.4.944

$\bar{4}'m2'$   
 $P\bar{4}'m2'$

Tetragonal



Origin on  $\bar{4}'m2'$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)' |
| (5) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (6) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'              | (8) 2' x, $\bar{x}$ ,0<br>(2 <sub>xy</sub>  0,0,0)'         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

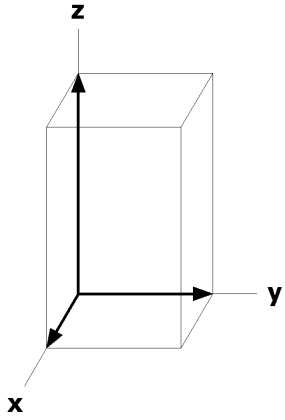
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	l	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ] (6) $\bar{x},y,z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) y, $\bar{x},z$ [v, $\bar{u},\bar{w}$ ] (7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ] (8) $\bar{y},\bar{x},z$ [v,u,w]
4	k	.m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v},0$ ]	1/2, $\bar{x},z$ [v,0,0]	1/2,x, $\bar{z}$ [ $\bar{v},0,0$ ]
4	j	.m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	0, $\bar{x},z$ [v,0,0]	0,x, $\bar{z}$ [ $\bar{v},0,0$ ]
4	i	..2'	x,x,1/2 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},1/2$ [u, $\bar{u},\bar{w}$ ]	$\bar{x},x,1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]
4	h	..2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},0$ [u, $\bar{u},\bar{w}$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},\bar{w}$ ]
2	g	2mm.	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
2	f	2mm.	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
2	e	2mm.	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
1	d	$\bar{4}'m2'$	0,0,1/2 [0,0,0]			
1	c	$\bar{4}'m2'$	1/2,1/2,1/2 [0,0,0]			
1	b	$\bar{4}'m2'$	1/2,1/2,0 [0,0,0]			
1	a	$\bar{4}'m2'$	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

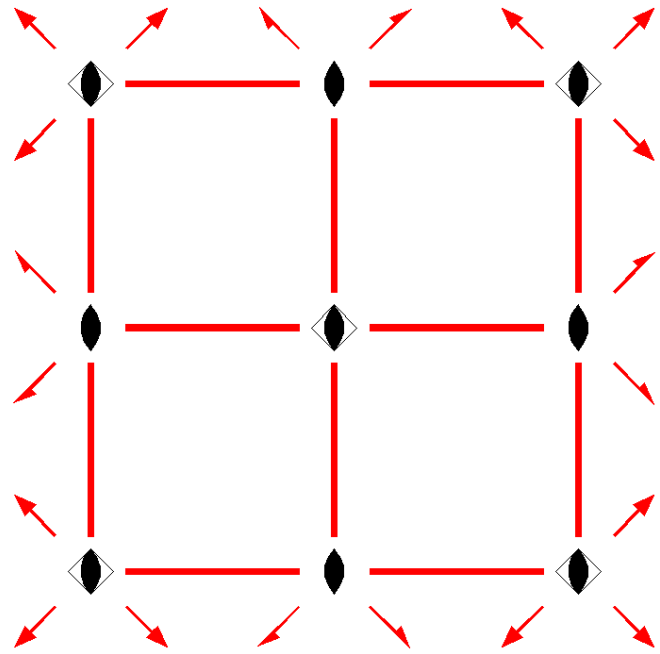
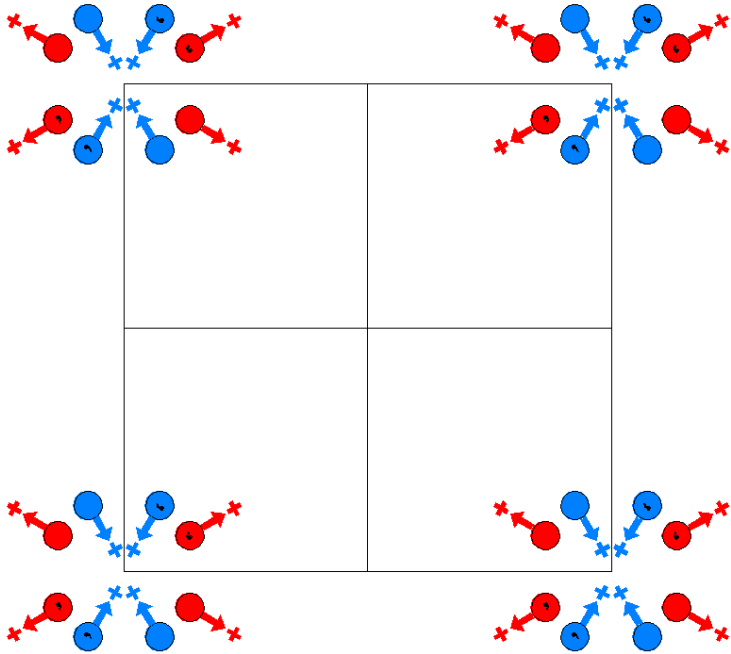
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$P\bar{4}m'2'$   
115.5.945

$\bar{4}m'2'$   
 $P\bar{4}m'2'$

Tetragonal



Origin on  $\bar{4}m'2'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 <sub>0,0,z</sub><br>(2 <sub>z</sub>  0,0,0)   | (3) $\bar{4}^+$ <sub>0,0,z</sub> ; 0,0,0<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ <sub>0,0,z</sub> ; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)                     |
| (5) m' <sub>x,0,z</sub><br>(m <sub>y</sub>  0,0,0)' | (6) m' <sub>0,y,z</sub><br>(m <sub>x</sub>  0,0,0)' | (7) 2' <sub>x,x,0</sub><br>(2 <sub>xy</sub>  0,0,0)'              | (8) 2' <sub>x,<math>\bar{x}</math>,0</sub><br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

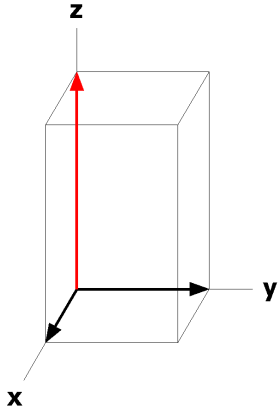
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	l	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(3) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ] (7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]
4	k	.m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ]	1/2, $\bar{x},\bar{z}$ [0,u,w]	1/2,x, $\bar{z}$ [0, $\bar{u},w$ ]
4	j	.m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	0, $\bar{x},\bar{z}$ [0,u,w]	0,x, $\bar{z}$ [0, $\bar{u},w$ ]
4	i	..2'	x,x,1/2 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},1/2$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,1/2$ [ $\bar{u},u,w$ ]
4	h	..2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,0$ [ $\bar{u},u,w$ ]
2	g	2m'm'	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]		
2	f	2m'm'	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
2	e	2m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
1	d	$\bar{4}m'2'$	0,0,1/2 [0,0,w]			
1	c	$\bar{4}m'2'$	1/2,1/2,1/2 [0,0,w]			
1	b	$\bar{4}m'2'$	1/2,1/2,0 [0,0,w]			
1	a	$\bar{4}m'2'$	0,0,0 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1]  $p4'm'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



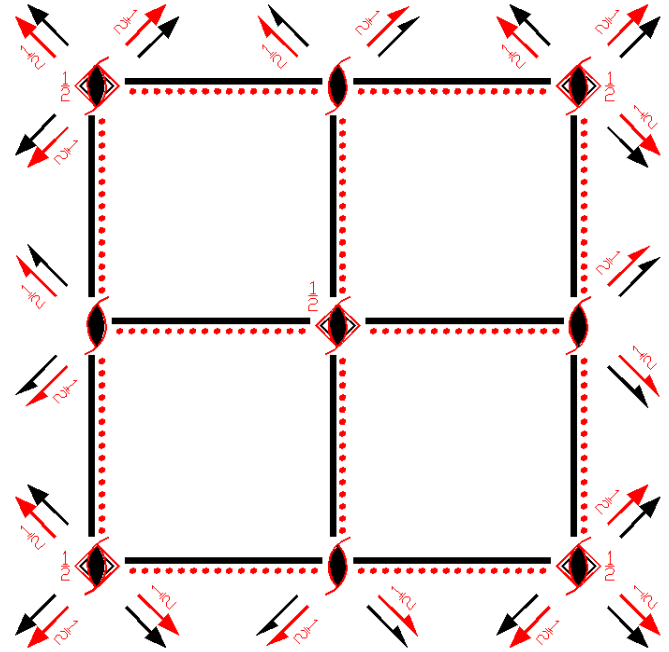
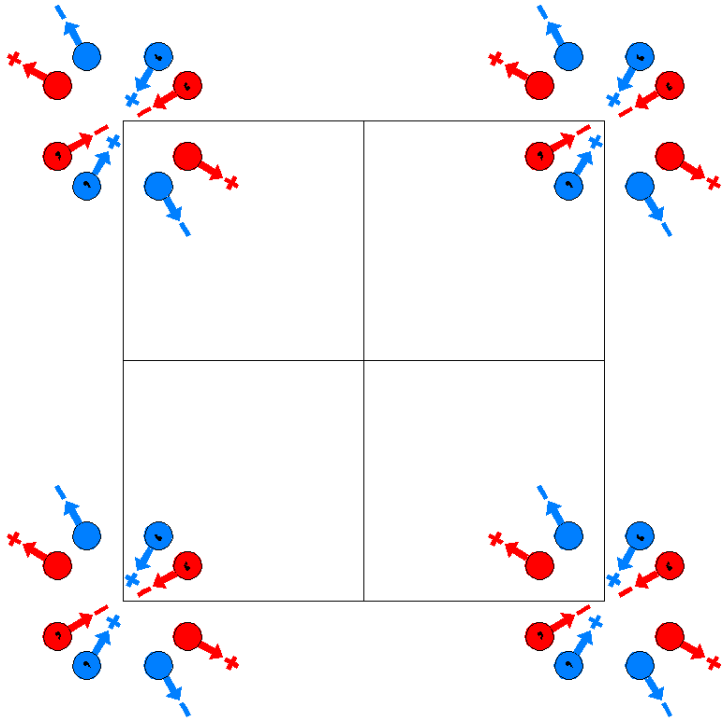
$P_{2c}\bar{4}m2$

115.6.946

$\bar{4}m21'$

$P_{2c}\bar{4}m2$

Tetragonal



Origin on  $\bar{4}m2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0) |
| (5) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (6) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                 | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub>-xy</sub>  0,0,0)      |

For (0,0,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (0,0,1)<br>(1 0,0,1)'                     | (2) 2' (0,01) 0,0,z<br>(2 <sub>z</sub>  0,0,1)'  | (3) $\bar{4}^+$ ' 0,0,z; 0,0,1/2<br>( $\bar{4}_z^+$  0,0,1)' | (4) $\bar{4}^-$ ' 0,0,z; 0,0,1/2<br>( $\bar{4}_z^-$  0,0,1)' |
| (5) c' (0,0,1) x,0,z<br>(m <sub>y</sub>  0,0,1)' | (6) c' (0,0,1) 0,y,z<br>(m <sub>x</sub>  0,0,1)' | (7) 2' x,x,1/2<br>(2 <sub>xy</sub>  0,0,1)'                  | (8) 2' x, $\bar{x}$ ,1/2<br>(2 <sub>-xy</sub>  0,0,1)'       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
		(0,0,0) +	(0,0,1)' +					
16 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(5) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
8 k .m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v},0$ ]	1/2, $\bar{x},\bar{z}$ [ $\bar{v},0,0$ ]	1/2,x, $\bar{z}$ [ $v,0,0$ ]				
8 j .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	0, $\bar{x},\bar{z}$ [ $\bar{v},0,0$ ]	0,x, $\bar{z}$ [ $v,0,0$ ]				
8 i ..2'	x,x,1/2 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/2$ [ $u,\bar{u},w$ ]	x, $\bar{x},1/2$ [ $u,u,\bar{w}$ ]	$\bar{x},x,1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]				
8 h ..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},0$ [ $\bar{u},u,0$ ]	$\bar{x},x,0$ [ $u,\bar{u},0$ ]				
4 g 2mm.	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]						
4 f 2mm.	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]						
4 e 2mm.	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]						
2 d $\bar{4}'m2'$	0,0,1/2 [0,0,0]							
2 c $\bar{4}'m2'$	1/2,1/2,1/2 [0,0,0]							
2 b $\bar{4}m2$	1/2,1/2,0 [0,0,0]							
2 a $\bar{4}m2$	0,0,0 [0,0,0]							

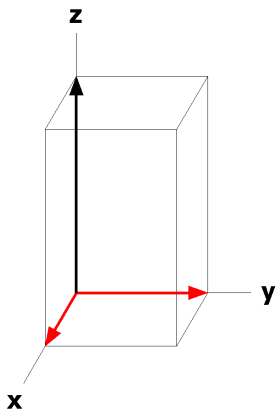
**Symmetry of Special Projections**

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p_{2a} 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0

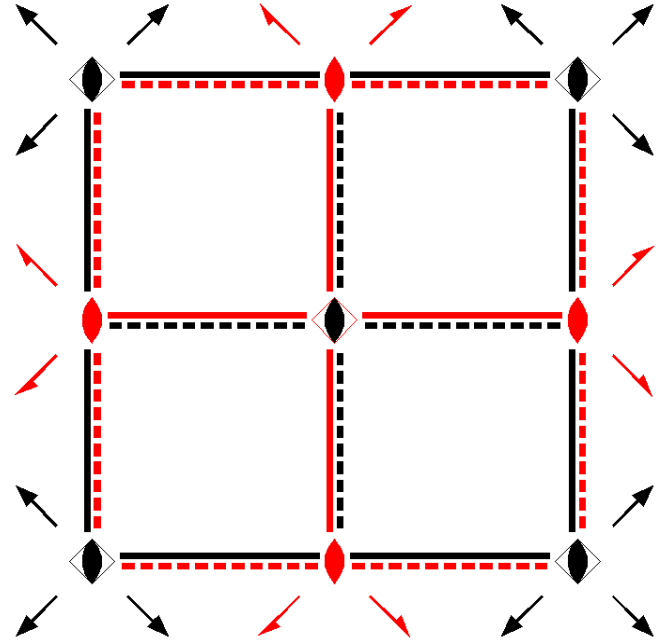
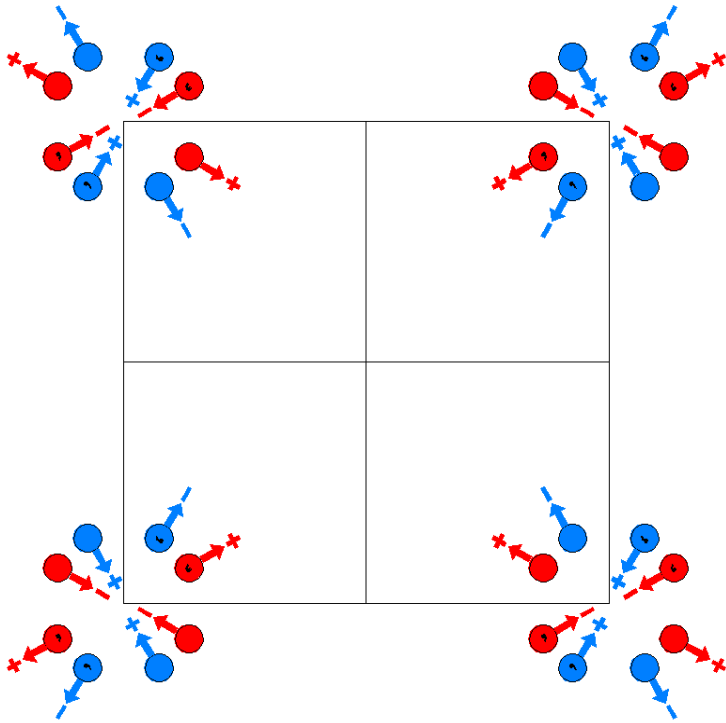




$P\bar{4}m2$   
115.7.947

$\bar{4}m21'$   
 $P\bar{4}m2$

Tetragonal



Origin on  $\bar{4}m2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0) |
| (5) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (6) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                 | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub>-xy</sub>  0,0,0)      |

For (1,0,0)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) t' (1,0,0)<br>(1 1,0,0)'                     | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)' | (3) $\bar{4}^+$ ' 1/2,-1/2,z; 1/2,-1/2,0<br>( $\bar{4}_z^+$  1,0,0)' | (4) $\bar{4}^-$ ' 1/2,1/2,z; 1/2,1/2,0<br>( $\bar{4}_z^-$  1,0,0)'    |
| (5) a' (1,0,0) x,0,z<br>(m <sub>y</sub>  1,0,0)' | (6) m' 1/2,y,z<br>(m <sub>x</sub>  1,0,0)' | (7) 2' (1/2,1/2,0) x+1/2,x,0<br>(2 <sub>xy</sub>  1,0,0)'            | (8) 2' (1/2,-1/2,0) x+1/2, $\bar{x}$ ,0<br>(2 <sub>-xy</sub>  1,0,0)' |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
		(0,0,0) +	(1,0,0)' +					
16 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(5) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
8 k .m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [u,0, $\bar{w}$ ]	1/2, $\bar{x},\bar{z}$ [0,u,w]	1/2,x, $\bar{z}$ [0, $\bar{u},\bar{w}$ ]				
8 j .m	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	0, $\bar{x},\bar{z}$ [ $\bar{v},0,0$ ]	0,x, $\bar{z}$ [v,0,0]				
8 i ..2	x,x,1/2 [u,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},1/2$ [ $\bar{u},u,0$ ]	$\bar{x},x,1/2$ [u, $\bar{u},0$ ]				
8 h ..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},0$ [ $\bar{u},u,0$ ]	$\bar{x},x,0$ [u, $\bar{u},0$ ]				
4 g 2'mm'	0,1/2,z [u,0,0]	1/2,0, $\bar{z}$ [0,u,0]						
4 f 2m'm'	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]						
4 e 2mm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]						
2 d $\bar{4}m2$	0,0,1/2 [0,0,0]							
2 c $\bar{4}'m'2$	1/2,1/2,1/2 [0,0,0]							
2 b $\bar{4}'m'2$	1/2,1/2,0 [0,0,0]							
2 a $\bar{4}m2$	0,0,0 [0,0,0]							

**Symmetry of Special Projections**

Along [0,0,1]  $p_p^*4m'm'$

$\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$

Origin at 0,0,z

Along [1,0,0]  $p1m11'$

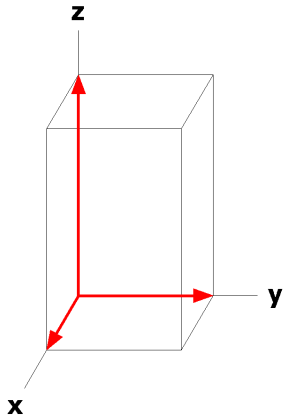
$\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$

Origin at x,0,0

Along [1,1,0]  $p_{2a}^*2m'm'$

$\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$

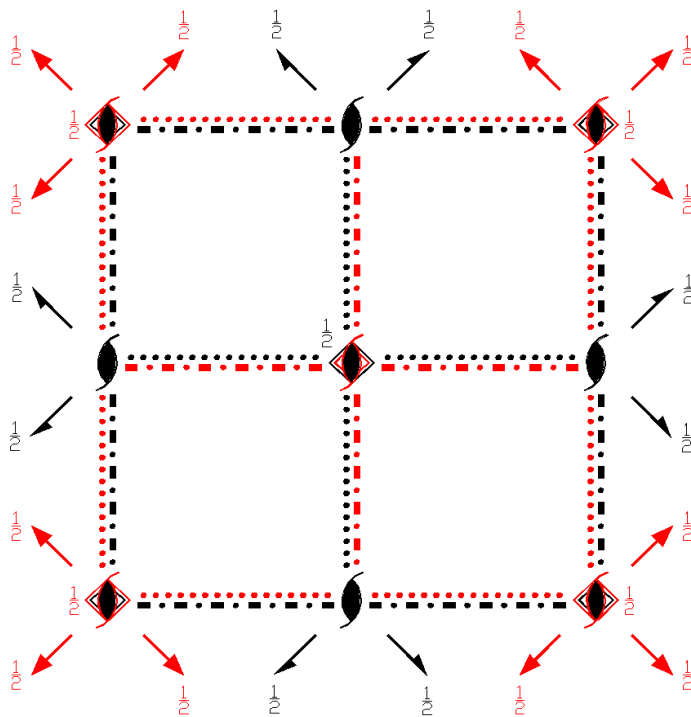
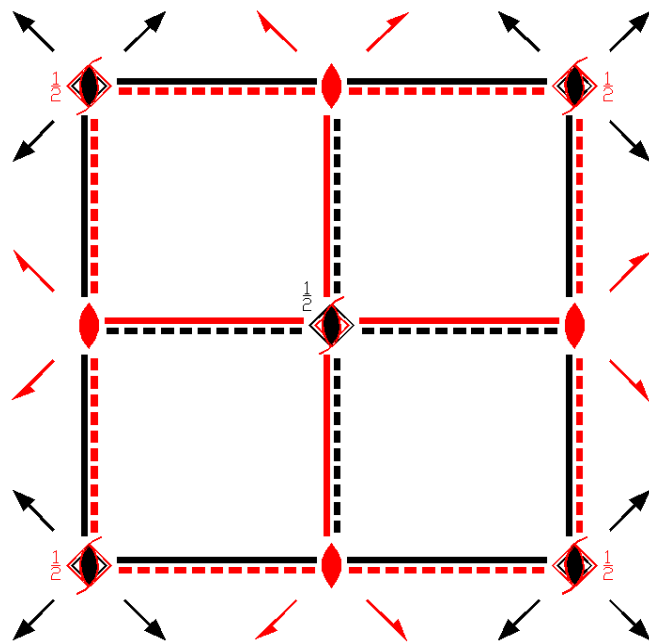
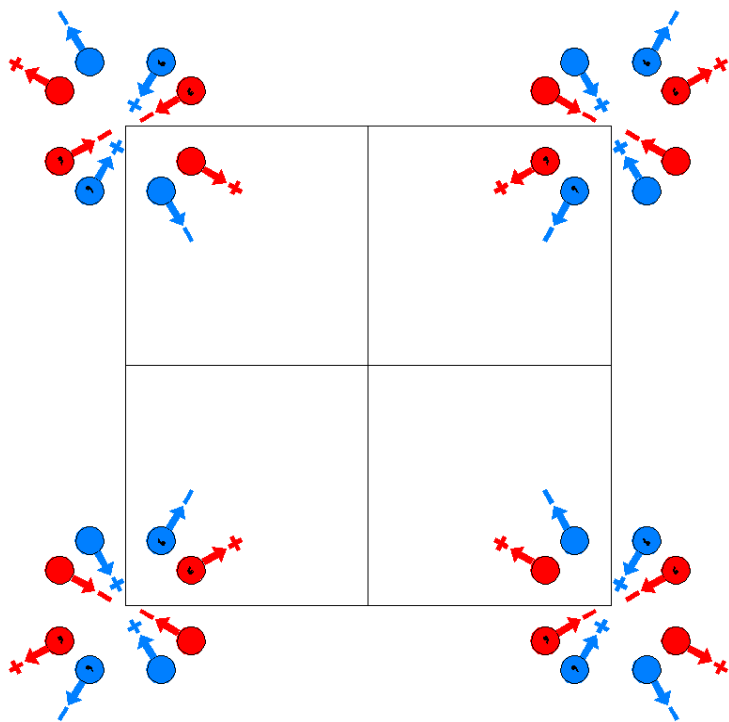
Origin at x,x,0



$P_1\bar{4}m2$   
115.8.948

$\bar{4}m21'$   
 $P_1\bar{4}m2$

Tetragonal



Origin on  $\bar{4}m2$ Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$ 

## Symmetry Operations

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)           |
| (5) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (6) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)               | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0) |

For (1,0,0)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) t' (1,0,0)<br>(1 1,0,0)'                     | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)' | (3) $\bar{4}^+$ ' 1/2,-1/2,z; 1/2,-1/2,0<br>( $\bar{4}_z$  1,0,0)' | (4) $\bar{4}^-$ ' 1/2,1/2,z; 1/2,1/2,0<br>( $\bar{4}_z^{-1}$  1,0,0)'                   |
| (5) a' (1,0,0) x,0,z<br>(m <sub>y</sub>  1,0,0)' | (6) m' 1/2,y,z<br>(m <sub>x</sub>  1,0,0)' | (7) 2' (1/2,1/2,0) x+1/2,x,0<br>(2 <sub>xy</sub>  1,0,0)'          | (8) 2' (1/2,-1/2,0) x+1/2, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  1,0,0)' |

Generators selected (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

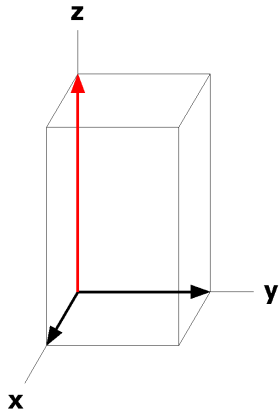
			(0,0,0) +	(1,0,0)' +		
16	l	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ] (6) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) y, $\bar{x},z$ [ $\bar{v},u,w$ ] (7) y,x, $\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ] (8) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	k	.m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [u,0, $\bar{w}$ ]	1/2, $\bar{x},z$ [0,u,w]	1/2,x, $\bar{z}$ [0,u, $\bar{w}$ ]
8	j	.m	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	0, $\bar{x},z$ [ $\bar{v},0,0$ ]	0,x, $\bar{z}$ [ $\bar{v},0,0$ ]
8	i	..2'	x,x,1/2 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]	x, $\bar{x},1/2$ [u,u, $\bar{w}$ ]	$\bar{x},x,1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	h	..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},0$ [ $\bar{u},u,0$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},0$ ]
4	g	2'mm'	0,1/2,z [u,0,0]	1/2,0, $\bar{z}$ [0,u,0]		
4	f	2m'm'	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
4	e	2mm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	d	$\bar{4}'m2'$	0,0,1/2 [0,0,0]			
2	c	$\bar{4}m2'$	1/2,1/2,1/2 [0,0,w]			
2	b	$\bar{4}'m2$	1/2,1/2,0 [0,0,0]			
2	a	$\bar{4}m2$	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,0,0$

Along  $[1,1,0]$   $p_c 2mm$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x-1/4, x+1/4, 1/2$



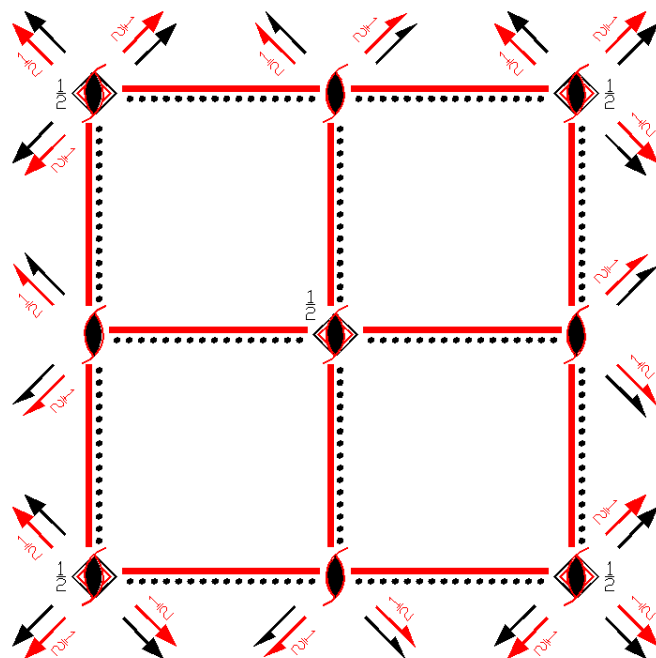
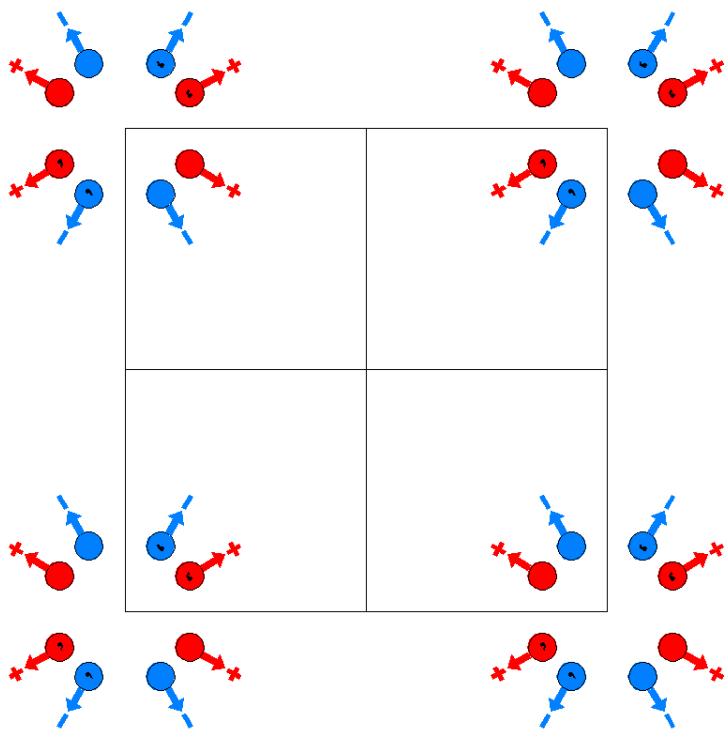
$P_{2c}\bar{4}m'2$

115.9.949

$\bar{4}m21'$

$P_{2c}\bar{4}m'2$

Tetragonal



Origin on  $\bar{4}m'2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)' |
| (5) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (6) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                  | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub>-xy</sub>  0,0,0)          |

For (0,0,1/2) + set

- |   |  |   |   |
|---|--|---|---|
| (1) t' (0,0,1)<br>(1 0,0,1)'                    | (2) 2' (0,01) 0,0,z<br>(2 <sub>z</sub> ' 0,0,1)' | (3) $\bar{4}^+$ 0,0,z; 0,0,1/2<br>( $\bar{4}_z^+$  0,0,1) | (4) $\bar{4}^-$ 0,0,z; 0,0,1/2<br>( $\bar{4}_z^{-1}$ ' 0,0,1) |
| (5) c (0,0,1) x,0,z<br>(m <sub>y</sub> ' 0,0,1) | (6) c (0,0,1) 0,y,z<br>(m <sub>x</sub> ' 0,0,1)  | (7) 2' x,x,1/2<br>(2 <sub>xy</sub> ' 0,0,1)'              | (8) 2' x, $\bar{x}$ ,1/2<br>(2 <sub>-xy</sub> ' 0,0,1)'       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

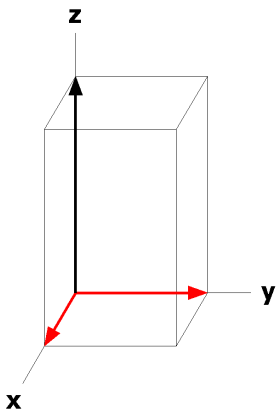
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(0,0,1)' +		
16	l	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(3) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ] (7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	k	.m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ]	1/2, $\bar{x},\bar{z}$ [0, $\bar{u},\bar{w}$ ]	1/2,x, $\bar{z}$ [0,u, $\bar{w}$ ]
8	j	.m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	0, $\bar{x},\bar{z}$ [0, $\bar{u},\bar{w}$ ]	0,x, $\bar{z}$ [0,u, $\bar{w}$ ]
8	i	..2'	x,x,1/2 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},1/2$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,1/2$ [u,u,w]
8	h	..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},0$ [u, $\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]
4	g	2m'm'	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4	f	2m'm'	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
4	e	2m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	d	$\bar{4}'m'2'$	0,0,1/2 [0,0,w]			
2	c	$\bar{4}'m'2'$	1/2,1/2,1/2 [0,0,w]			
2	b	$\bar{4}'m'2$	1/2,1/2,0 [0,0,0]			
2	a	$\bar{4}'m'2$	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b'}1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

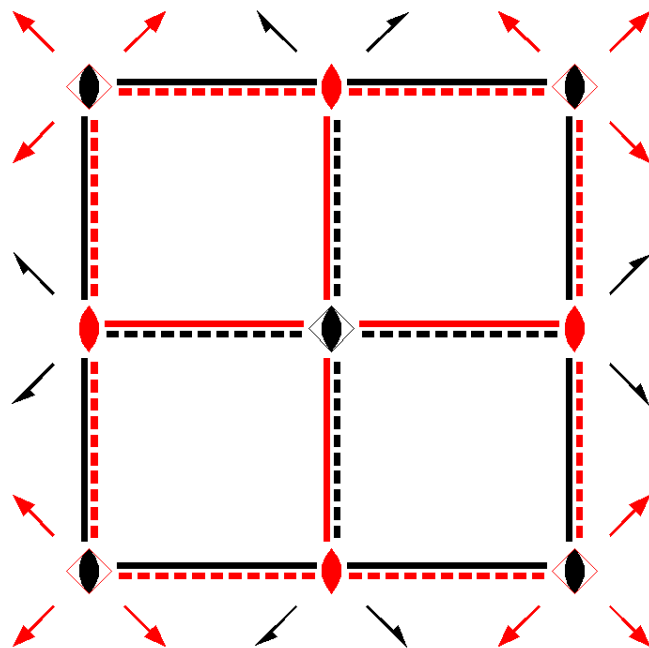
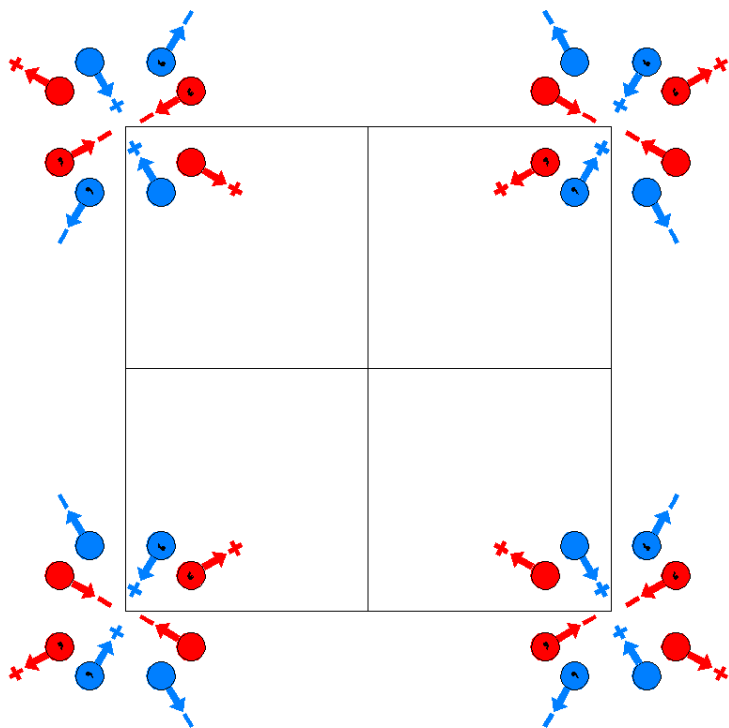
Along [1,1,0]  $p_{2a'}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/2



$P\bar{4}1m2'$   
115.10.950

$\bar{4}m21'$   
 $P\bar{4}1m2'$

Tetragonal



Origin on  $\bar{4}1m2'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'          |
| (5) m <sub>x</sub> x,0,z<br>(m <sub>y</sub>  0,0,0) | (6) m <sub>0</sub> 0,y,z<br>(m <sub>x</sub>  0,0,0) | (7) 2' <sub>x</sub> x,x,0<br>(2 <sub>xy</sub>  0,0,0)'   | (8) 2' <sub>x</sub> x, $\bar{x}$ ,0<br>(2 <sub>-xy</sub>  0,0,0)' |

For (1,0,0)' + set

- |  |   |  |   |
|--|---|--|---|
| (1) t' (1,0,0)<br>(1 1,0,0)'                     | (2) 2' <sub>z</sub> 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'   | (3) $\bar{4}^+$ 1/2,-1/2,z; 1/2,-1/2,0<br>( $\bar{4}_z^+$  1,0,0)          | (4) $\bar{4}^-$ 1/2,1/2,z; 1/2,1/2,0<br>( $\bar{4}_z^-$  1,0,0)     |
| (5) a' (1,0,0) x,0,z<br>(m <sub>y</sub>  1,0,0)' | (6) m' <sub>1/2</sub> 1/2,y,z<br>(m <sub>x</sub>  1,0,0)' | (7) 2' <sub>(1/2)</sub> (1/2,1/2,0) x+1/2,x,0<br>(2 <sub>xy</sub>  1,0,0)' | (8) 2 (1/2,-1/2,0) x+1/2, $\bar{x}$ ,0<br>(2 <sub>-xy</sub>  1,0,0) |



**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

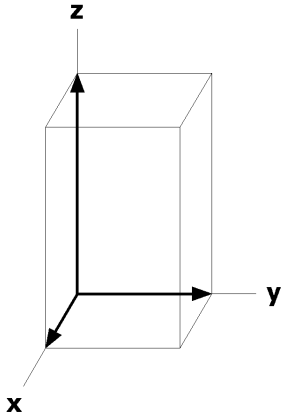
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1,0,0)' +		
16	l	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ] (6) $\bar{x},y,z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) y, $\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ] (7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	k	.m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [u,0, $\bar{w}$ ]	1/2, $\bar{x},\bar{z}$ [0, $\bar{u},\bar{w}$ ]	1/2,x, $\bar{z}$ [0, $\bar{u},\bar{w}$ ]
8	j	.m	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	0, $\bar{x},\bar{z}$ [ $\bar{v},0,0$ ]	0,x, $\bar{z}$ [ $\bar{v},0,0$ ]
8	i	..2	x,x,1/2 [u,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},1/2$ [u, $\bar{u},0$ ]	$\bar{x},x,1/2$ [ $\bar{u},\bar{u},0$ ]
8	h	..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},0$ [u, $\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},0$ ]
4	g	2'mm'	0,1/2,z [u,0,0]	1/2,0, $\bar{z}$ [0, $\bar{u},0$ ]		
4	f	2m'm'	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
4	e	2mm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	d	$\bar{4}'m2'$	0,0,1/2 [0,0,0]			
2	c	$\bar{4}m'2'$	1/2,1/2,1/2 [0,0,w]			
2	b	$\bar{4}m'2'$	1/2,1/2,0 [0,0,w]			
2	a	$\bar{4}'m2'$	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $p_p 4mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/2,1/2,z

Along [1,0,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

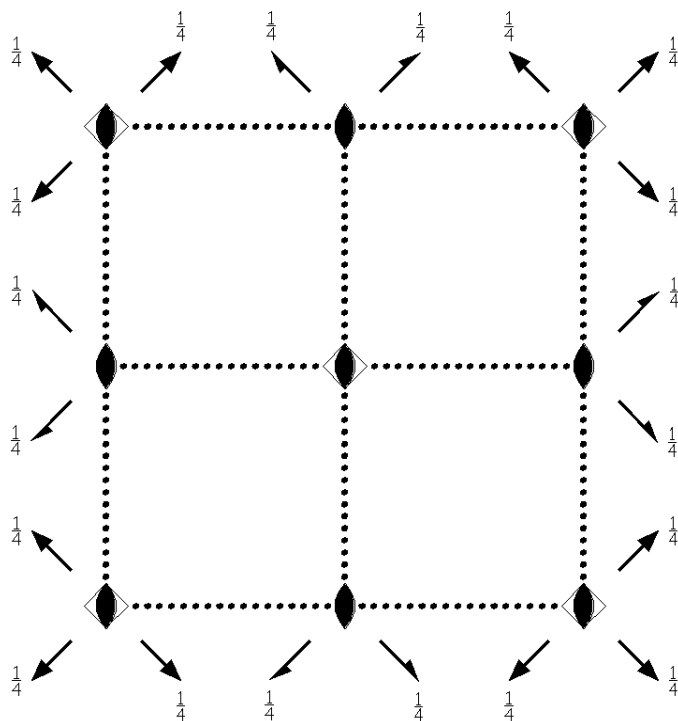
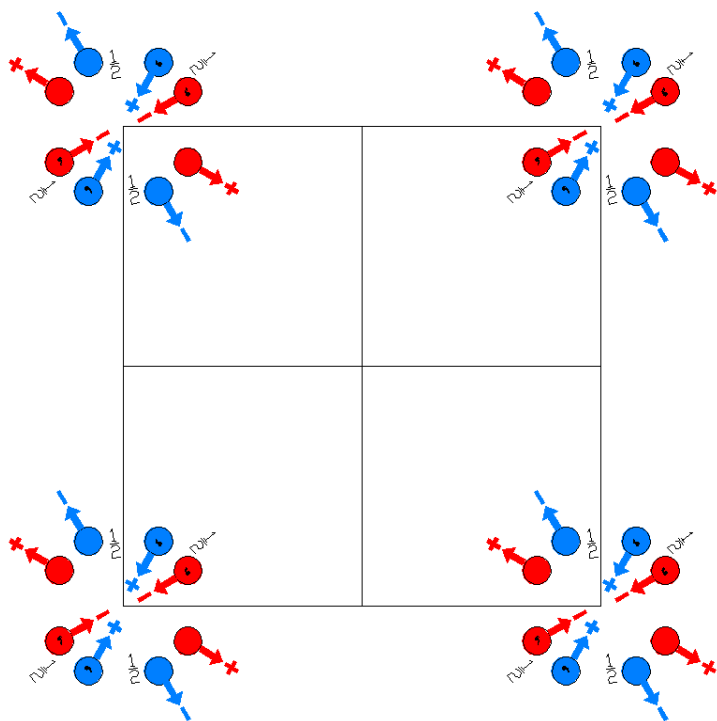
Along [1,1,0]  $p_{2a} 2mm$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x-1/4,x+1/4,0



$P\bar{4}c2$   
116.1.951

$\bar{4}m2$   
 $P\bar{4}c2$

Tetragonal



Origin on  $\bar{4}c1$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)             | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)               |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)           | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

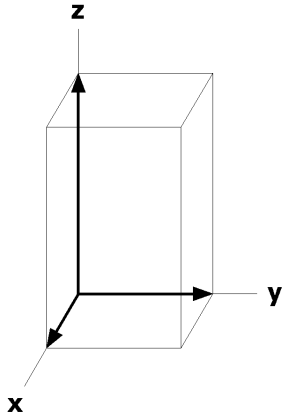
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	j	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},z+1/2 [\bar{u},v,\bar{w}]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$ (6) $\bar{x},y,z+1/2 [u,\bar{v},\bar{w}]$	(3) $y,\bar{x},\bar{z} [\bar{v},u,w]$ (7) $y,x,\bar{z}+1/2 [v,u,\bar{w}]$	(4) $\bar{y},x,\bar{z} [v,\bar{u},w]$ (8) $\bar{y},\bar{x},\bar{z}+1/2 [\bar{v},\bar{u},\bar{w}]$
4	i	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	h	2..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	g	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	f	..2	x,x,3/4 [u,u,0]	$\bar{x},\bar{x},3/4 [\bar{u},\bar{u},0]$	x, $\bar{x}$ ,1/4 [ $\bar{u}$ ,u,0]	$\bar{x},x,1/4 [u,\bar{u},0]$
4	e	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4 [\bar{u},\bar{u},0]$	x, $\bar{x}$ ,3/4 [ $\bar{u}$ ,u,0]	$\bar{x},x,3/4 [u,\bar{u},0]$
2	d	$\bar{4}$	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		
2	c	$\bar{4}$	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		
2	b	2.22	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	a	2.22	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>'1m'1  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4

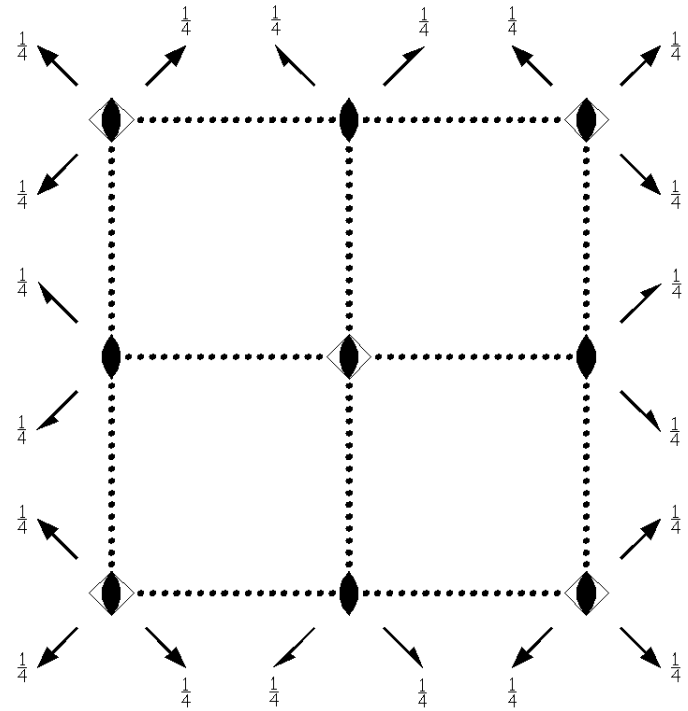
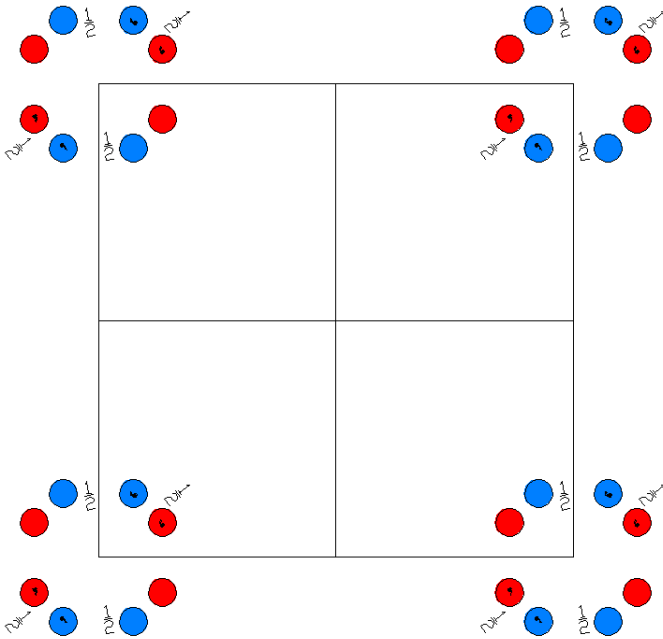


$P\bar{4}c21'$   
116.2.952

$\bar{4}m21'$   
 $P\bar{4}c21'$

Tetragonal

1'



Origin on  $\bar{4}c11'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

Symmetry Operations

For 1 + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)             | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)             | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub>-xy</sub>  0,0,1/2)     |

For 1' + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1'<br>(1 0,0,0)'                                 | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'             | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)' |
| (5) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'            | (8) 2' x, $\bar{x}$ ,1/4<br>(2 <sub>-xy</sub>  0,0,1/2)'    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

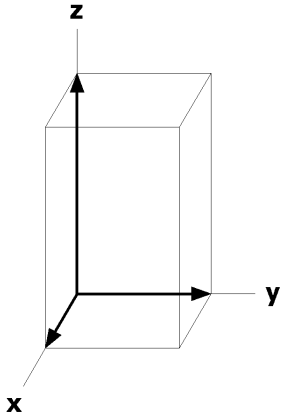
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +	1' +	
8 j 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) y, $\bar{x},\bar{z}$ [0,0,0]	(4) $\bar{y},x,\bar{z}$ [0,0,0]
	(5) x, $\bar{y},z+1/2$ [0,0,0]	(6) $\bar{x},y,z+1/2$ [0,0,0]	(7) y,x, $\bar{z}+1/2$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [0,0,0]
4 i 2..1'	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]
4 h 2..1'	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]
4 g 2..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]
4 f ..21'	x,x,3/4 [0,0,0]	$\bar{x},\bar{x},3/4$ [0,0,0]	x, $\bar{x},1/4$ [0,0,0]	$\bar{x},x,1/4$ [0,0,0]
4 e ..21'	x,x,1/4 [0,0,0]	$\bar{x},\bar{x},1/4$ [0,0,0]	x, $\bar{x},3/4$ [0,0,0]	$\bar{x},x,3/4$ [0,0,0]
2 d $\bar{4}1'$	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2 c $\bar{4}1'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
2 b 2.221'	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2 a 2.221'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

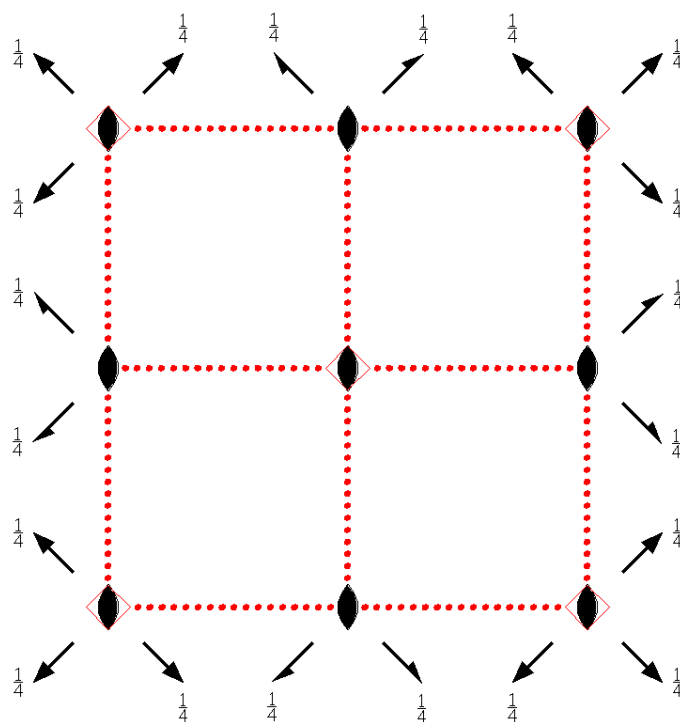
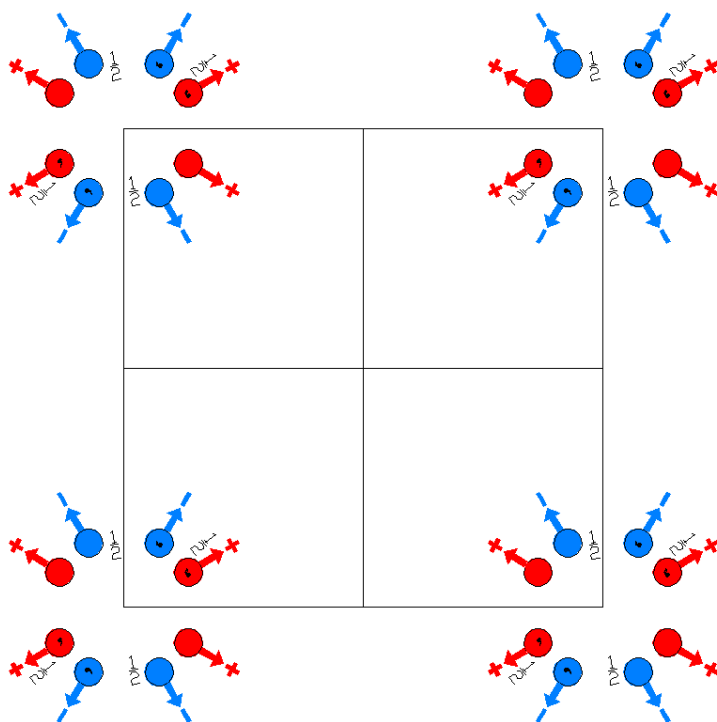
Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



$P\bar{4}'c'2$   
116.3.953

$\bar{4}'m'2$   
 $P\bar{4}'c'2$

Tetragonal



Origin on  $\bar{4}'c'1$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

Symmetry Operations

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                                   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)               | (3) $\bar{4}'^+$ 0,0,z; 0,0,0<br>( $\bar{4}'_z$  0,0,0)' | (4) $\bar{4}'^-$ 0,0,z; 0,0,0<br>( $\bar{4}'_z^{-1}$  0,0,0)' |
| (5) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)              | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub>xy</sub>  0,0,1/2)         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

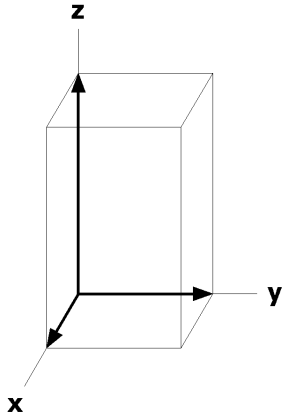
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	j	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
			(5) x, $\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(6) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]	(7) y,x, $\bar{z}+1/2$ [v,u, $\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
4	i	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	h	2..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	g	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	f	..2	x,x,3/4 [u,u,0]	$\bar{x},\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},1/4$ [u, $\bar{u},0$ ]	$\bar{x},x,1/4$ [ $\bar{u},u,0$ ]
4	e	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},3/4$ [u, $\bar{u},0$ ]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]
2	d	$\bar{4}'$	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	c	$\bar{4}'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
2	b	2.22	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	a	2.22	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

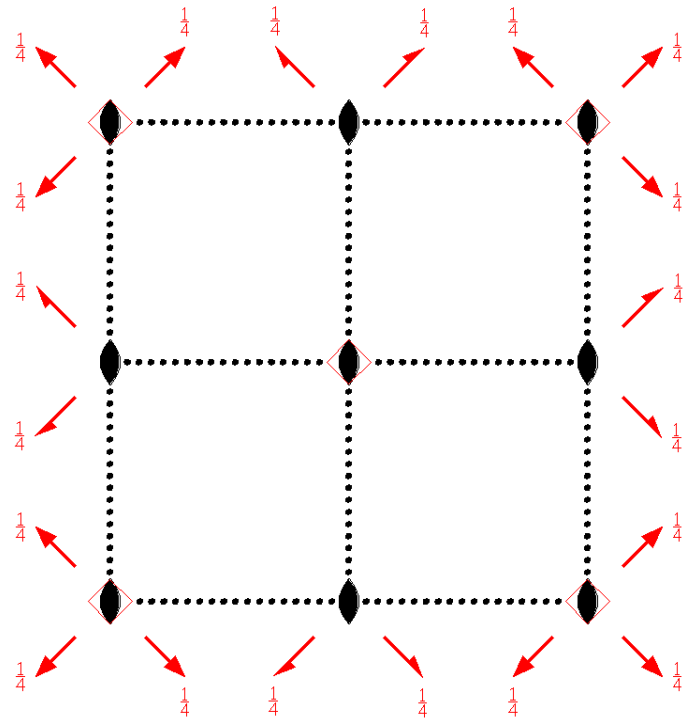
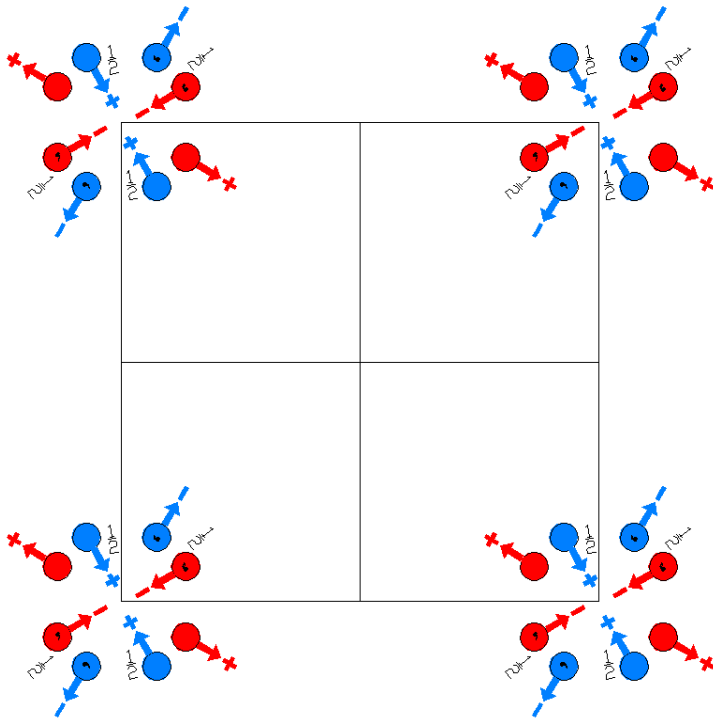
Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



$P\bar{4}'c2'$   
116.4.954

$\bar{4}'m2'$   
 $P\bar{4}'c2'$

Tetragonal



Origin on  $\bar{4}'c1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)             | (3) $\bar{4}'^+$ 0,0,z; 0,0,0<br>( $\bar{4}'_z$  0,0,0)' | (4) $\bar{4}'^-$ 0,0,z; 0,0,0<br>( $\bar{4}'_z^{-1}$  0,0,0)' |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'            | (8) 2' x, $\bar{x}$ ,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'       |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

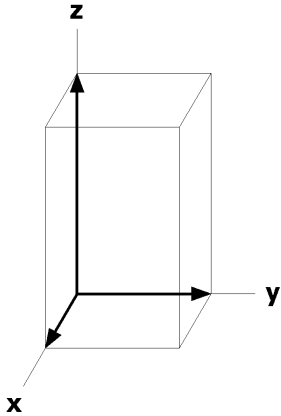
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	j	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
			(5) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x},y,z+1/2$ [u, $\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [v,u,w]
4	i	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0,w]
4	h	2..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]
4	g	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0,w]
4	f	..2'	x,x,3/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},3/4$ [u, $\bar{u},w$ ]	x, $\bar{x},1/4$ [u,u, $\bar{w}$ ]	$\bar{x},x,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
4	e	..2'	x,x,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [u, $\bar{u},w$ ]	x, $\bar{x},3/4$ [u,u, $\bar{w}$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
2	d	$\bar{4}'$	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	c	$\bar{4}'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
2	b	2.2'2'	1/2,1/2,1/4 [0,0,w]	1/2,1/2,3/4 [0,0, $\bar{w}$ ]		
2	a	2.2'2'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b}1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

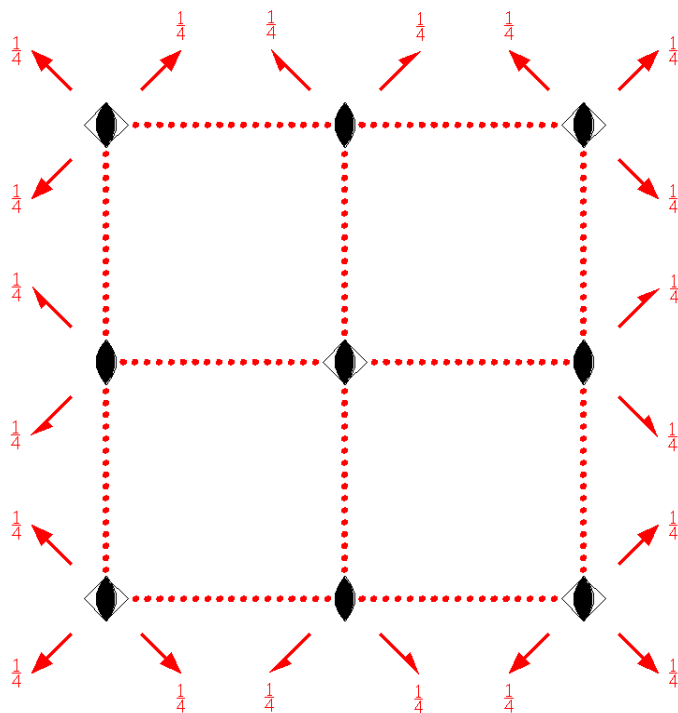
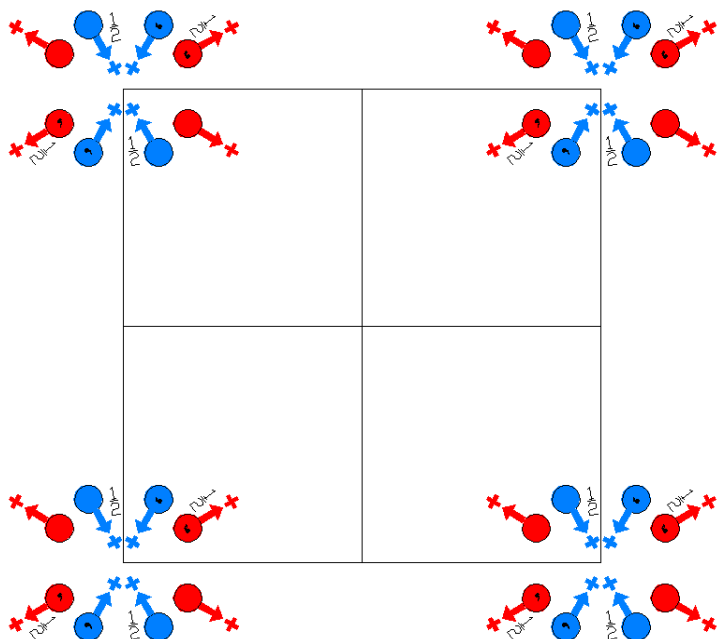
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



$P\bar{4}c'2'$   
116.5.955

$\bar{4}m'2'$   
 $P\bar{4}c'2'$

Tetragonal



Origin on  $\bar{4}c'1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 <sub>0,0,z</sub><br>(2 <sub>z</sub>  0,0,0)               | (3) $\bar{4}^+$ <sub>0,0,z</sub> ; 0,0,0<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ <sub>0,0,z</sub> ; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)                         |
| (5) c' <sub>(0,0,1/2)</sub> x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (6) c' <sub>(0,0,1/2)</sub> 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' | (7) 2' <sub>x,x,1/4</sub><br>(2 <sub>xy</sub>  0,0,1/2)'          | (8) 2' <sub>x,<math>\bar{x}</math>,1/4</sub><br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

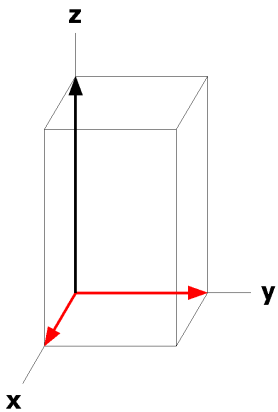
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
8	j	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
			(5) x, $\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(6) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]	(7) y,x, $\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $v,u,w$ ]
4	i	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]
4	h	2..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]
4	g	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]
4	f	..2'	x,x,3/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},3/4$ [ $u,\bar{u},w$ ]	x, $\bar{x},1/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,1/4$ [ $u,u,w$ ]
4	e	..2'	x,x,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [ $u,\bar{u},w$ ]	x, $\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,3/4$ [ $u,u,w$ ]
2	d	$\bar{4}$	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]		
2	c	$\bar{4}$	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]		
2	b	2.2'2'	1/2,1/2,1/4 [0,0,w]	1/2,1/2,3/4 [0,0,w]		
2	a	2.2'2'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4'm'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

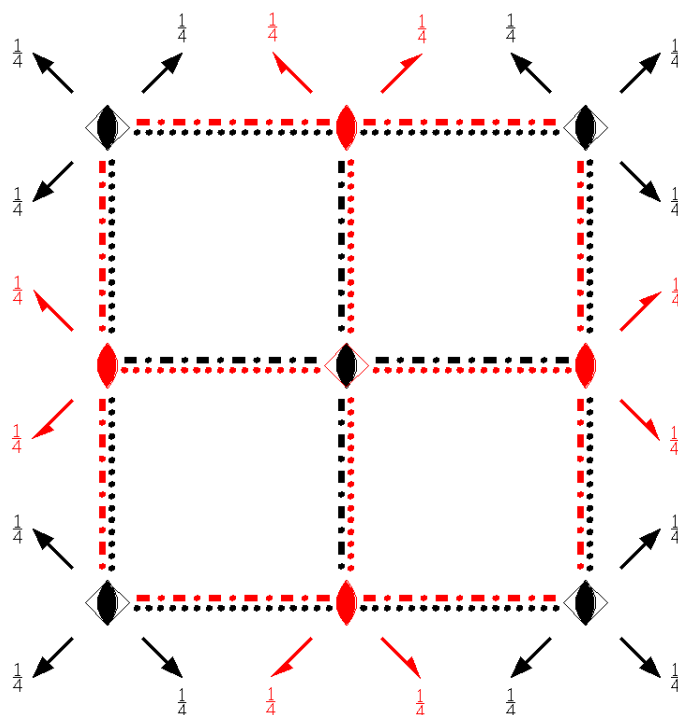
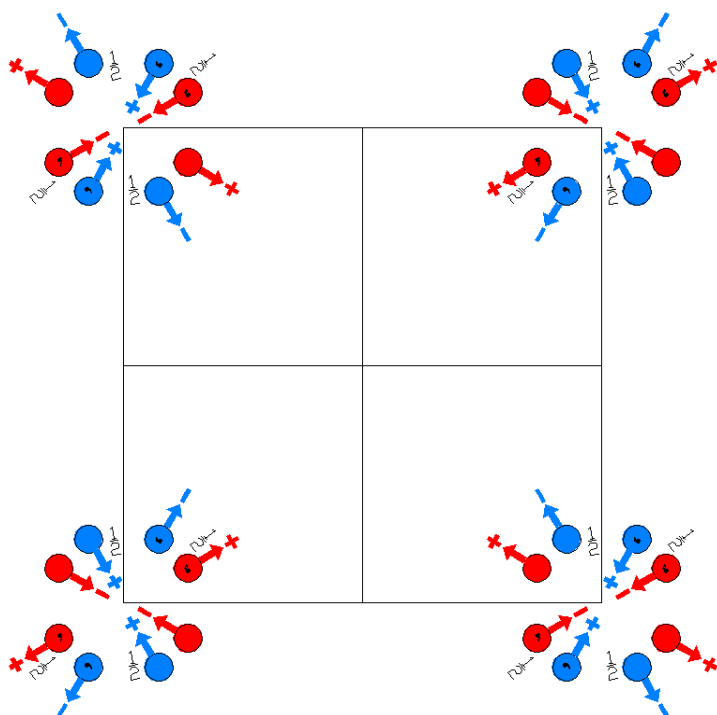
Along [1,1,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



$P_p\bar{4}c2$   
116.6.956

$\bar{4}m21'$   
 $P_p\bar{4}c2$

Tetragonal



Origin on  $\bar{4}c1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)             | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0) |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)             | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub>-xy</sub>  0,0,1/2)  |

For (1,0,0)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) t' (1,0,0)<br>(1 1,0,0)'                         | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'             | (3) $\bar{4}^+$ ' 1/2,-1/2,z; 1/2,-1/2,0<br>( $\bar{4}_z^+$  1,0,0)' | (4) $\bar{4}^-$ ' 1/2,1/2,z; 1/2,1/2,0<br>( $\bar{4}_z^-$  1,0,0)'        |
| (5) n' (1,0,1/2) x,0,z<br>(m <sub>y</sub>  1,0,1/2)' | (6) c' (0,0,1/2) 1/2,y,z<br>(m <sub>x</sub>  1,0,1/2)' | (7) 2' (1/2,1/2,0) x+1/2,x,1/4<br>(2 <sub>xy</sub>  1,0,1/2)'        | (8) 2' (1/2,-1/2,0) x+1/2, $\bar{x}$ ,1/4<br>(2 <sub>-xy</sub>  1,0,1/2)' |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

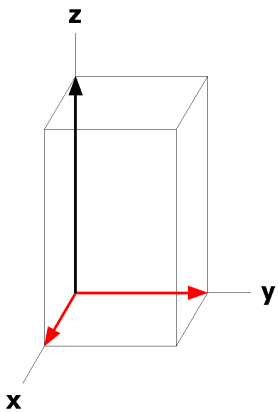
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1,0,0)' +		
16	j	1	(1) x,y,z [u,v,w] (5) x,y,z+1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $\bar{x},y,z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) y,x,z [ $\bar{v},u,w$ ] (7) y,x,z+1/2 [v,u, $\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [v, $\bar{u},w$ ] (8) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	i	2'..	0,1/2,z [u,v,0]	1/2,0, $\bar{z}$ [ $\bar{v},u,0$ ]	0,1/2,z+1/2 [u, $\bar{v},0$ ]	1/2,0, $\bar{z}+1/2$ [v,u,0]
8	h	2..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
8	g	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
8	f	..2	x,x,3/4 [u,u,0]	$\bar{x},\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},1/4$ [ $\bar{u},u,0$ ]	$\bar{x},x,1/4$ [u, $\bar{u},0$ ]
8	e	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},3/4$ [ $\bar{u},u,0$ ]	$\bar{x},x,3/4$ [u, $\bar{u},0$ ]
4	d	$\bar{4}'$	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4	c	$\bar{4}$	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		
4	b	2.22	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
4	a	2.22	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_4$ , 4m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/2,1/2,z

Along [1,0,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

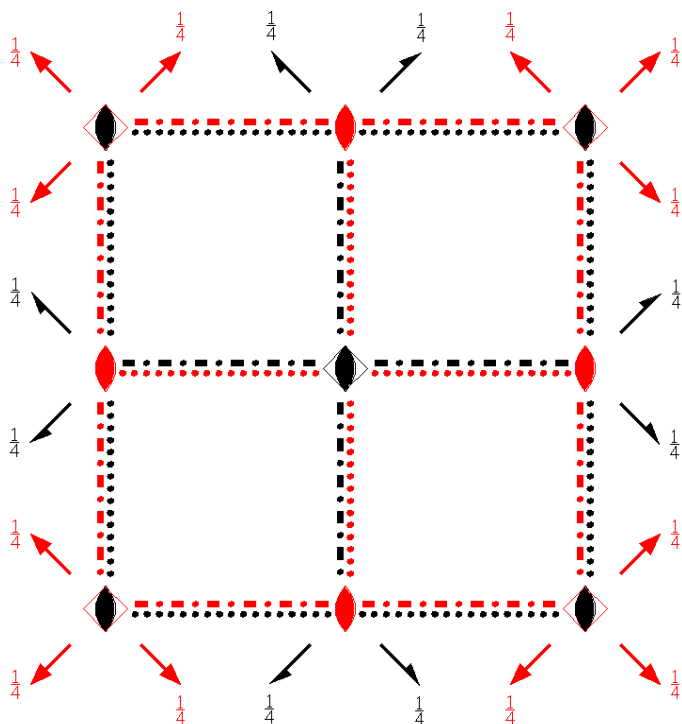
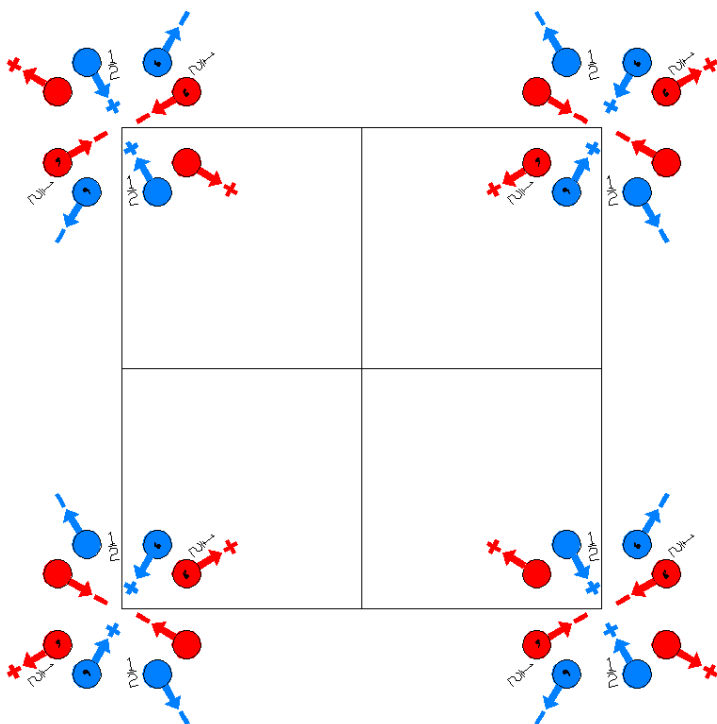
Along [1,1,0]  $p_{2a}$ , 2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



$P_p\bar{4}'c2'$   
116.7.957

$\bar{4}m21'$   
 $P_p\bar{4}'c2'$

Tetragonal



Origin on  $\bar{4}'c1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)             | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)' |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'            | (8) 2' x, $\bar{x}$ ,1/4<br>(2 <sub>-xy</sub>  0,0,1/2)' |

For (1,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) t' (1,0,0)<br>(1 1,0,0)'                         | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'             | (3) $\bar{4}^+$ 1/2,1/2,z; 1/2,1/2,0<br>( $\bar{4}_z^+$  1,0,0) | (4) $\bar{4}^-$ 1/2,-1/2,z; 1/2,-1/2,0<br>( $\bar{4}_z^-$  1,0,0)       |
| (5) n' (1,0,1/2) x,0,z<br>(m <sub>y</sub>  1,0,1/2)' | (6) c' (0,0,1/2) 1/2,y,z<br>(m <sub>x</sub>  1,0,1/2)' | (7) 2 (1/2,1/2,0) x+1/2,x,1/4<br>(2 <sub>xy</sub>  1,0,1/2)     | (8) 2 (1/2,-1/2,0) x+1/2, $\bar{x}$ ,1/4<br>(2 <sub>-xy</sub>  1,0,1/2) |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

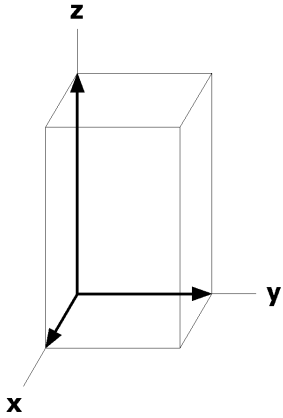
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(1,0,0)' +			
16 j 1	(1)	$x,y,z [u,v,w]$	(2)	$\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3)	$y,\bar{x},\bar{z} [v,\bar{u},\bar{w}]$	(4)	$\bar{y},x,\bar{z} [\bar{v},u,\bar{w}]$
	(5)	$x,\bar{y},z+1/2 [\bar{u},v,\bar{w}]$	(6)	$\bar{x},y,z+1/2 [u,\bar{v},\bar{w}]$	(7)	$y,x,\bar{z}+1/2 [\bar{v},\bar{u},w]$	(8)	$\bar{y},\bar{x},\bar{z}+1/2 [v,u,w]$
8 i 2'.		$0,1/2,z [u,v,0]$		$1/2,0,\bar{z} [v,\bar{u},0]$		$0,1/2,z+1/2 [u,\bar{v},0]$		$1/2,0,\bar{z}+1/2 [\bar{v},\bar{u},0]$
8 h 2..		$1/2,1/2,z [0,0,w]$		$1/2,1/2,\bar{z} [0,0,w]$		$1/2,1/2,z+1/2 [0,0,w]$		$1/2,1/2,\bar{z}+1/2 [0,0,w]$
8 g 2..		$0,0,z [0,0,w]$		$0,0,\bar{z} [0,0,\bar{w}]$		$0,0,z+1/2 [0,0,\bar{w}]$		$0,0,\bar{z}+1/2 [0,0,w]$
8 f ..2'		$x,x,3/4 [\bar{u},u,w]$		$\bar{x},\bar{x},3/4 [u,\bar{u},w]$		$x,\bar{x},1/4 [u,u,\bar{w}]$		$\bar{x},x,1/4 [\bar{u},\bar{u},\bar{w}]$
8 e ..2'		$x,x,1/4 [\bar{u},u,w]$		$\bar{x},\bar{x},1/4 [u,\bar{u},w]$		$x,\bar{x},3/4 [u,u,\bar{w}]$		$\bar{x},x,3/4 [\bar{u},\bar{u},\bar{w}]$
4 d $\bar{4}$		$1/2,1/2,0 [0,0,w]$		$1/2,1/2,1/2 [0,0,w]$				
4 c $\bar{4}'$		$0,0,0 [0,0,0]$		$0,0,1/2 [0,0,0]$				
4 b 2.2'2'		$1/2,1/2,1/4 [0,0,w]$		$1/2,1/2,3/4 [0,0,w]$				
4 a 2.2'2'		$0,0,1/4 [0,0,w]$		$0,0,3/4 [0,0,\bar{w}]$				

**Symmetry of Special Projections**

Along [0,0,1]  $p_4$ , 4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

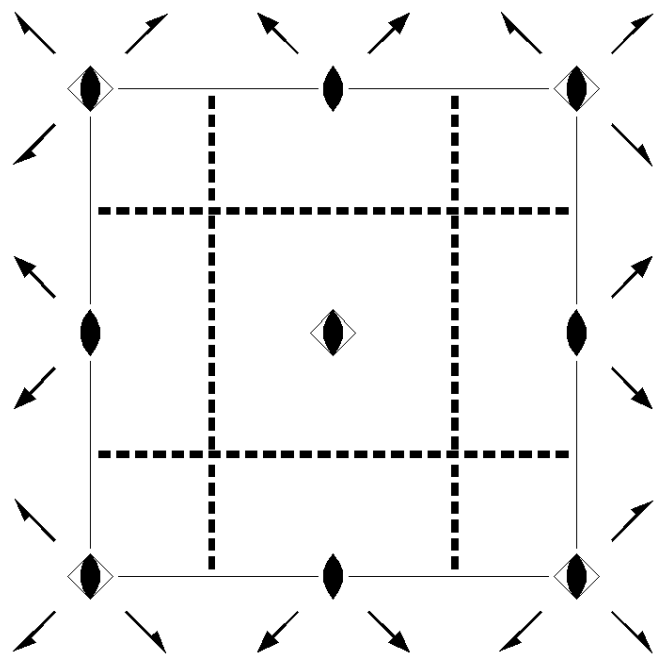
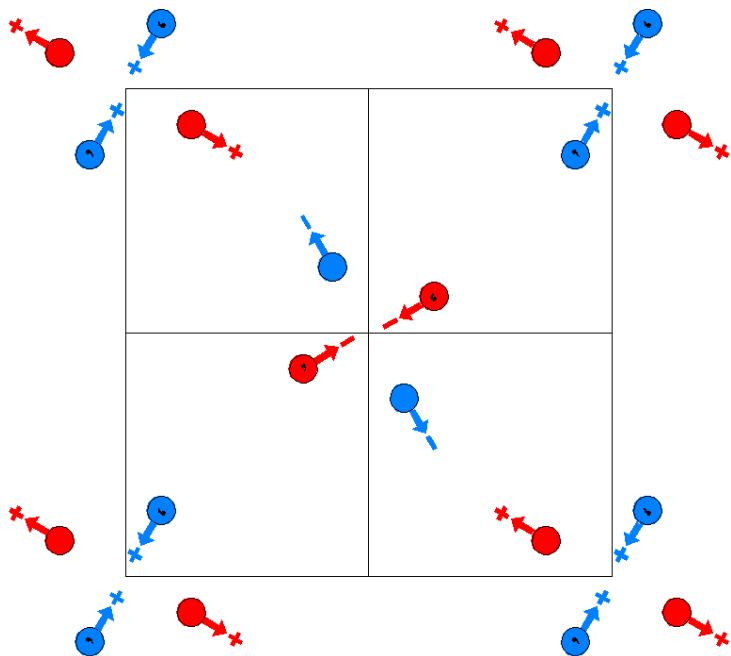
Along [1,1,0]  $p_{2a}$ , 2mm  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x-1/4, x+1/4, 1/4$



$P\bar{4}b2$   
117.1.958

$\bar{4}m2$   
 $P\bar{4}b2$

Tetragonal



Origin on  $\bar{4}12_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)   | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (6) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (7) 2 (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0) | (8) 2 x, $\bar{x}+1/2,0$<br>(2 <sub>xy</sub>  1/2,1/2,0)   |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

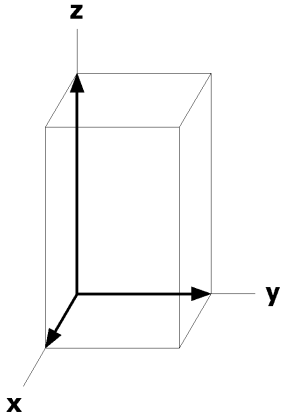
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]		
			(5) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x}+1/2,y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y+1/2,x+1/2,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
4	h	..2	$x,x+1/2,1/2$ [u,u,0]	$\bar{x},\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},1/2$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,x,1/2$ [ $u,\bar{u},0$ ]
4	g	..2	$x,x+1/2,0$ [u,u,0]	$\bar{x},\bar{x}+1/2,0$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},0$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,x,0$ [ $u,\bar{u},0$ ]
4	f	2..	$0,1/2,z$ [0,0,w]	$1/2,0,\bar{z}$ [0,0,w]	$1/2,0,z$ [0,0, $\bar{w}$ ]	$0,1/2,\bar{z}$ [0,0, $\bar{w}$ ]
4	e	2..	$0,0,z$ [0,0,w]	$0,0,\bar{z}$ [0,0,w]	$1/2,1/2,z$ [0,0, $\bar{w}$ ]	$1/2,1/2,\bar{z}$ [0,0, $\bar{w}$ ]
2	d	2.22	$0,1/2,1/2$ [0,0,0]	$1/2,0,1/2$ [0,0,0]		
2	c	2.22	$0,1/2,0$ [0,0,0]	$1/2,0,0$ [0,0,0]		
2	b	$\bar{4}..$	$0,0,1/2$ [0,0,w]	$1/2,1/2,1/2$ [0,0, $\bar{w}$ ]		
2	a	$\bar{4}..$	$0,0,0$ [0,0,w]	$1/2,1/2,0$ [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4'gm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,1/4,0$

Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$

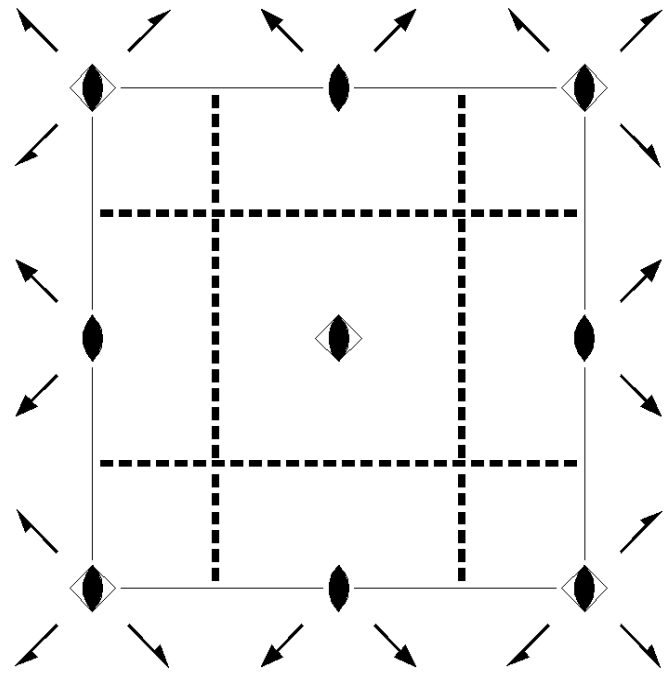
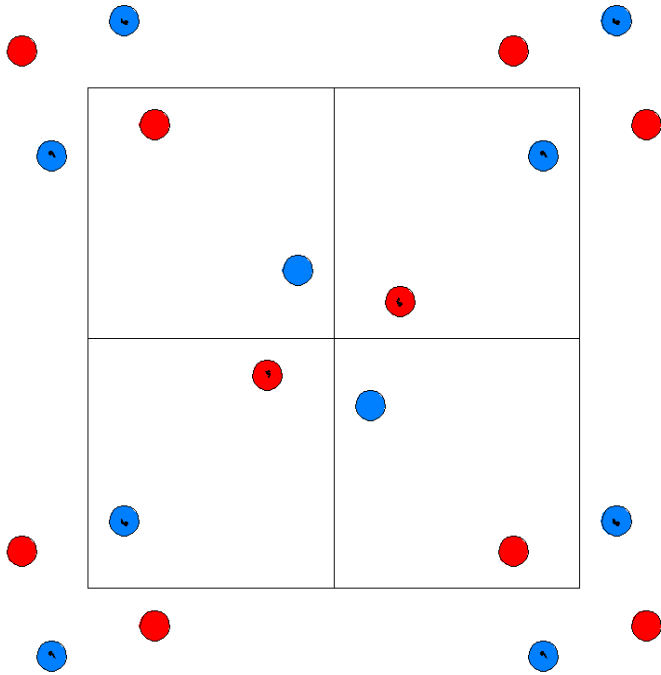


$P\bar{4}b21'$   
117.2.959

$\bar{4}m21'$   
 $P\bar{4}b21'$

Tetragonal

1'



Origin on  $\bar{4}12,1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

For 1 + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)   | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (6) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (7) 2 (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0) | (8) 2 x, $\bar{x}$ +1/2,0<br>(2 <sub>-xy</sub>  1/2,1/2,0) |

For 1' + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1'<br>(1 0,0,0)'                                     | (2) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                 | (3) $\bar{4}^+$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)'  | (4) $\bar{4}^-$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)' |
| (5) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (6) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' | (7) 2' (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)' | (8) 2' x, $\bar{x}$ +1/2,0<br>(2 <sub>-xy</sub>  1/2,1/2,0)'  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

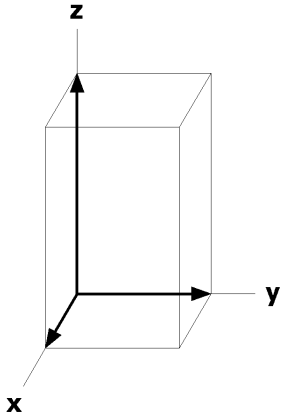
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +	1' +		
8 i 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]		
	(3) $y,\bar{x},\bar{z}$ [0,0,0]	(4) $\bar{y},x,\bar{z}$ [0,0,0]		
	(5) $x+1/2,\bar{y}+1/2,z$ [0,0,0]	(6) $\bar{x}+1/2,y+1/2,z$ [0,0,0]		
	(7) $y+1/2,x+1/2,\bar{z}$ [0,0,0]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}$ [0,0,0]		
4 h ..21'	$x,x+1/2,1/2$ [0,0,0]	$\bar{x},\bar{x}+1/2,1/2$ [0,0,0]	$x+1/2,\bar{x},1/2$ [0,0,0]	$\bar{x}+1/2,x,1/2$ [0,0,0]
4 g ..21'	$x,x+1/2,0$ [0,0,0]	$\bar{x},\bar{x}+1/2,0$ [0,0,0]	$x+1/2,\bar{x},0$ [0,0,0]	$\bar{x}+1/2,x,0$ [0,0,0]
4 f 2..1'	$0,1/2,z$ [0,0,0]	$1/2,0,\bar{z}$ [0,0,0]	$1/2,0,z$ [0,0,0]	$0,1/2,\bar{z}$ [0,0,0]
4 e 2..1'	$0,0,z$ [0,0,0]	$0,0,\bar{z}$ [0,0,0]	$1/2,1/2,z$ [0,0,0]	$1/2,1/2,\bar{z}$ [0,0,0]
2 d 2.221'	$0,1/2,1/2$ [0,0,0]	$1/2,0,1/2$ [0,0,0]		
2 c 2.221'	$0,1/2,0$ [0,0,0]	$1/2,0,0$ [0,0,0]		
2 b $\bar{4}..1'$	$0,0,1/2$ [0,0,0]	$1/2,1/2,1/2$ [0,0,0]		
2 a $\bar{4}..1'$	$0,0,0$ [0,0,0]	$1/2,1/2,0$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4gm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

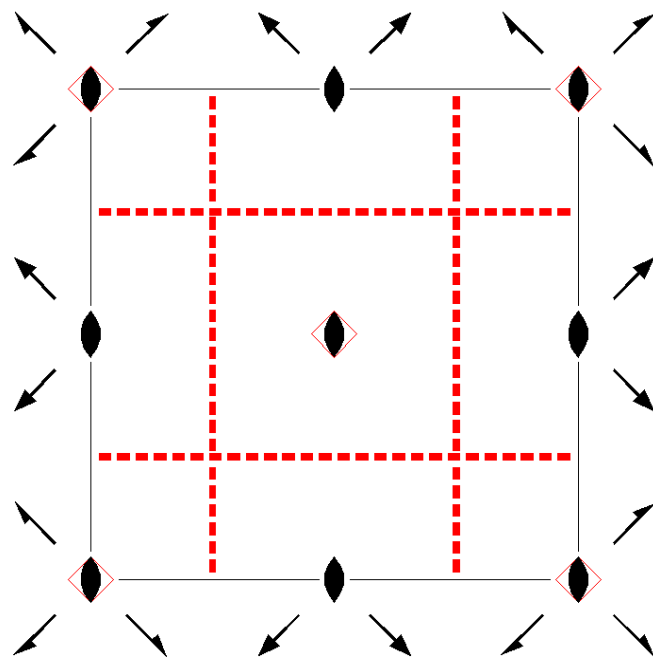
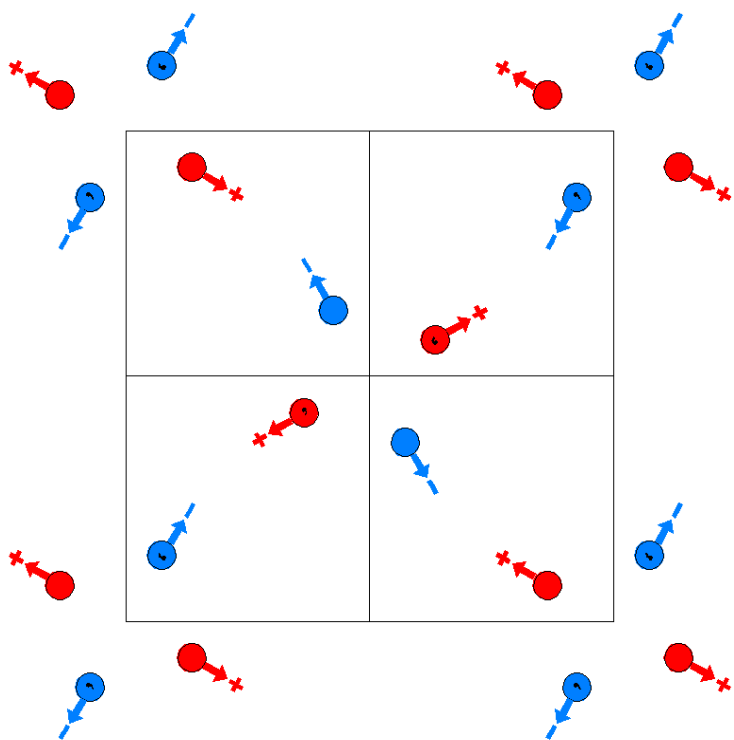
Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P\bar{4}'b'2$   
117.3.960

$\bar{4}'m'2$   
 $P\bar{4}'b'2$

Tetragonal



Origin on  $\bar{4}'12_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

**Symmetry Operations**

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                   | (3) $\bar{4}'^+$ 0,0,z; 0,0,0<br>( $\bar{4}'_z$  0,0,0)' | (4) $\bar{4}'^-$ 0,0,z; 0,0,0<br>( $\bar{4}'_z^{-1}$  0,0,0)' |
| (5) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (6) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' | (7) 2 (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)  | (8) 2 x, $\bar{x}$ +1/2,0<br>(2 <sub>xy</sub>  1/2,1/2,0)     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

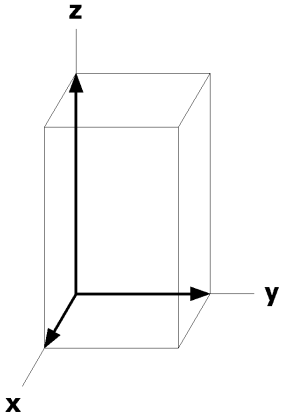
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	i	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $y,\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},\bar{v},w$ ]	(6) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]		
			(7) $y+1/2,x+1/2,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
4	h	..2	$x,x+1/2,1/2$ [u,u,0]	$\bar{x},\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,1/2$ [ $\bar{u},u,0$ ]
4	g	..2	$x,x+1/2,0$ [u,u,0]	$\bar{x},\bar{x}+1/2,0$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,0$ [ $\bar{u},u,0$ ]
4	f	2..	$0,1/2,z$ [0,0,w]	$1/2,0,\bar{z}$ [0,0, $\bar{w}$ ]	$1/2,0,z$ [0,0,w]	$0,1/2,\bar{z}$ [0,0, $\bar{w}$ ]
4	e	2..	$0,0,z$ [0,0,w]	$0,0,\bar{z}$ [0,0, $\bar{w}$ ]	$1/2,1/2,z$ [0,0,w]	$1/2,1/2,\bar{z}$ [0,0, $\bar{w}$ ]
2	d	2.22	$0,1/2,1/2$ [0,0,0]	$1/2,0,1/2$ [0,0,0]		
2	c	2.22	$0,1/2,0$ [0,0,0]	$1/2,0,0$ [0,0,0]		
2	b	$\bar{4}'..$	$0,0,1/2$ [0,0,0]	$1/2,1/2,1/2$ [0,0,0]		
2	a	$\bar{4}'..$	$0,0,0$ [0,0,0]	$1/2,1/2,0$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4g'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

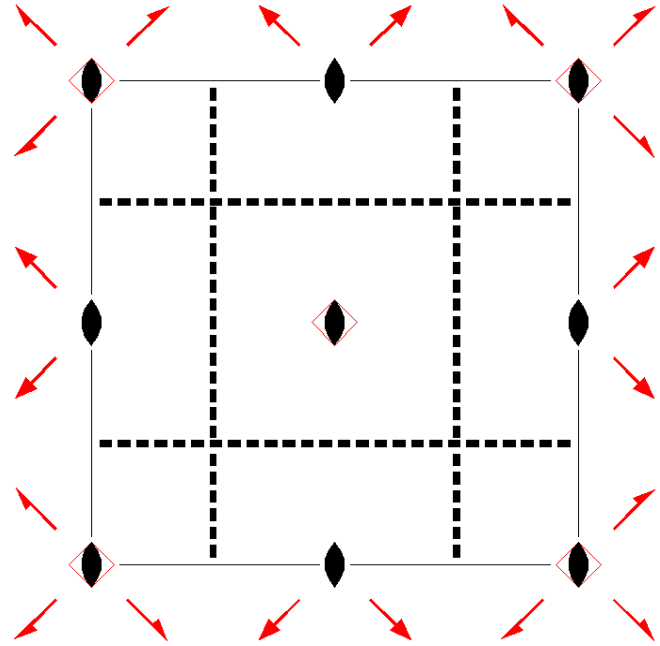
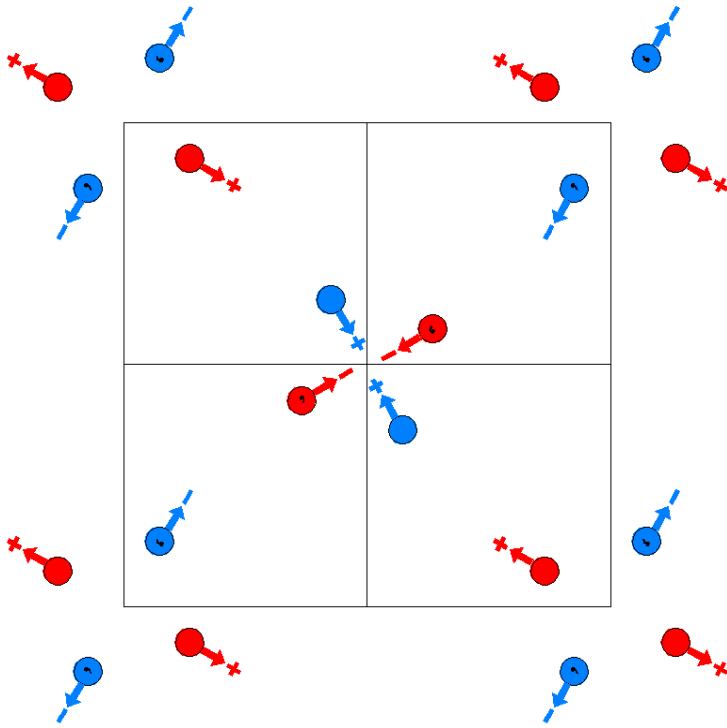
Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P\bar{4}'b2'$   
117.4.961

$\bar{4}'m2'$   
 $P\bar{4}'b2'$

Tetragonal



Origin on  $\bar{4}'12_1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2  $0,0,z$   
( $2_z$ |0,0,0)

(3)  $\bar{4}^+$   $0,0,z; 0,0,0$   
( $\bar{4}_z$ |0,0,0)'

(4)  $\bar{4}^-$   $0,0,z; 0,0,0$   
( $\bar{4}_z^{-1}$ |0,0,0)'

(5) a  $(1/2,0,0) \ x,1/4,z$   
( $m_y$ | $1/2,1/2,0$ )

(6) b  $(0,1/2,0) \ 1/4,y,z$   
( $m_x$ | $1/2,1/2,0$ )

(7)  $2'$   $(1/2,1/2,0) \ x,x,0$   
( $2_{xy}$ | $1/2,1/2,0$ )'

(8)  $2'$   $x,\bar{x}+1/2,0$   
( $2_{\bar{xy}}$ | $1/2,1/2,0$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

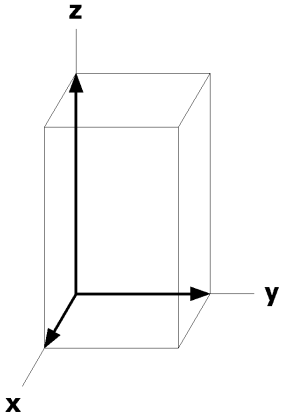
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x}+1/2,y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y+1/2,x+1/2,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}$ [ $v,u,w$ ]		
4	h	..2'	$x,x+1/2,1/2$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/2$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x},1/2$ [ $u,u,\bar{w}$ ]	$\bar{x}+1/2,x,1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]
4	g	..2'	$x,x+1/2,0$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,0$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x},0$ [ $u,u,\bar{w}$ ]	$\bar{x}+1/2,x,0$ [ $\bar{u},\bar{u},\bar{w}$ ]
4	f	2..	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,0,z$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}$ [ $0,0,w$ ]
4	e	2..	$0,0,z$ [ $0,0,w$ ]	$0,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,1/2,z$ [ $0,0,\bar{w}$ ]	$1/2,1/2,\bar{z}$ [ $0,0,w$ ]
2	d	2.2'2'	$0,1/2,1/2$ [ $0,0,w$ ]	$1/2,0,1/2$ [ $0,0,\bar{w}$ ]		
2	c	2.2'2'	$0,1/2,0$ [ $0,0,w$ ]	$1/2,0,0$ [ $0,0,\bar{w}$ ]		
2	b	$\bar{4}'..$	$0,0,1/2$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]		
2	a	$\bar{4}'..$	$0,0,0$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p4gm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [1,1,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



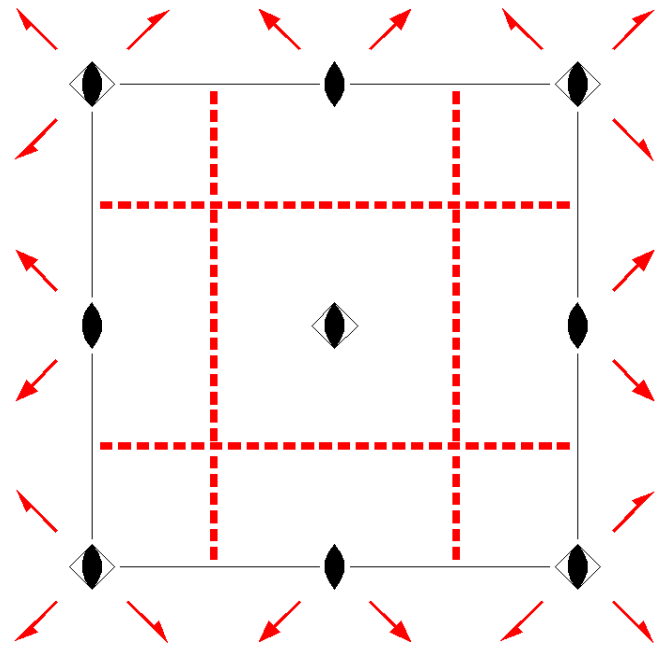
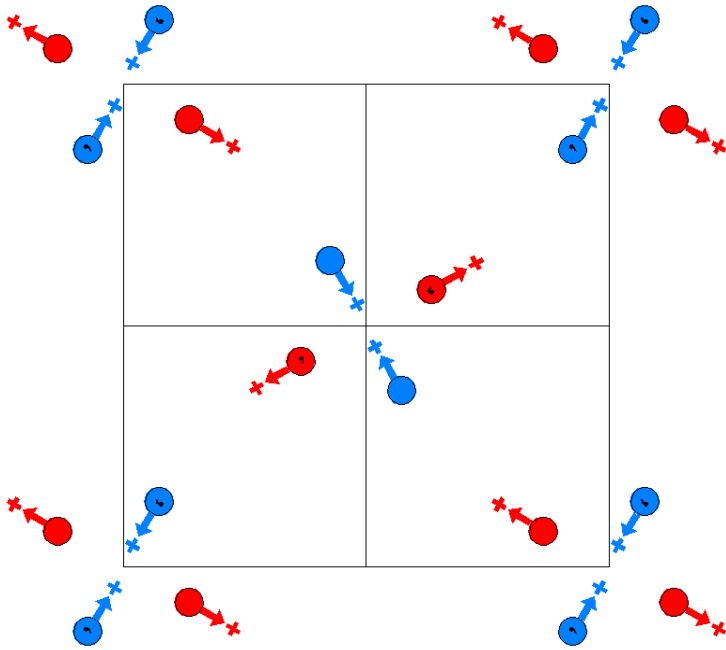
$P\bar{4}b'2'$

117.5.962

$\bar{4}m'2'$

$P\bar{4}b'2'$

Tetragonal



Origin on  $\bar{4}1'2_1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                           | (3) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z$  0,0,0)       | (4) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1}$  0,0,0)    |
| (5) $a'$ $(1/2,0,0) \ x,1/4,z$<br>( $m_y$   $1/2,1/2,0$ )' | (6) $b'$ $(0,1/2,0) \ 1/4,y,z$<br>( $m_x$   $1/2,1/2,0$ )' | (7) $2'$ $(1/2,1/2,0) \ x,x,0$<br>( $2_{xy}$   $1/2,1/2,0$ )' | (8) $2'$ $x,\bar{x}+1/2,0$<br>( $2_{\bar{xy}}$   $1/2,1/2,0$ )' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

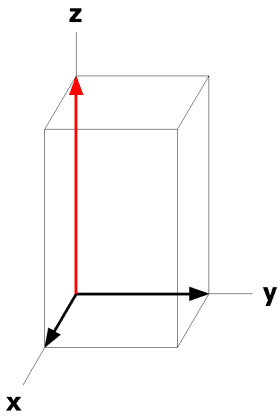
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]		
			(5) $x+1/2,\bar{y}+1/2,z$ [ $u,\bar{v},w$ ]	(6) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]		
			(7) $y+1/2,x+1/2,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}$ [ $v,u,w$ ]		
4	h	..2'	$x,x+1/2,1/2$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/2$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x},1/2$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,1/2$ [ $u,u,w$ ]
4	g	..2'	$x,x+1/2,0$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,0$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,0$ [ $u,u,w$ ]
4	f	2..	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,\bar{z}$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,w$ ]	$0,1/2,\bar{z}$ [ $0,0,w$ ]
4	e	2..	$0,0,z$ [ $0,0,w$ ]	$0,0,\bar{z}$ [ $0,0,w$ ]	$1/2,1/2,z$ [ $0,0,w$ ]	$1/2,1/2,\bar{z}$ [ $0,0,w$ ]
2	d	2.2'2'	$0,1/2,1/2$ [ $0,0,w$ ]	$1/2,0,1/2$ [ $0,0,w$ ]		
2	c	2.2'2'	$0,1/2,0$ [ $0,0,w$ ]	$1/2,0,0$ [ $0,0,w$ ]		
2	b	$\bar{4}..$	$0,0,1/2$ [ $0,0,w$ ]	$1/2,1/2,1/2$ [ $0,0,w$ ]		
2	a	$\bar{4}..$	$0,0,0$ [ $0,0,w$ ]	$1/2,1/2,0$ [ $0,0,w$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p4'g'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

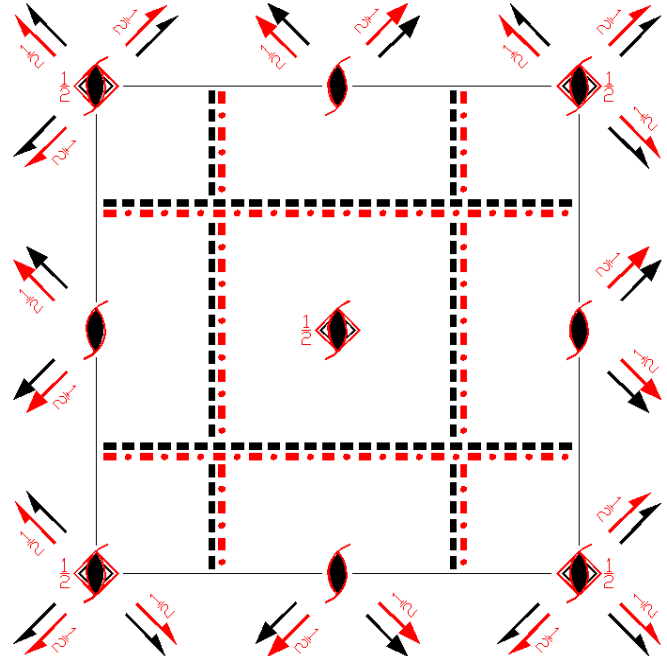
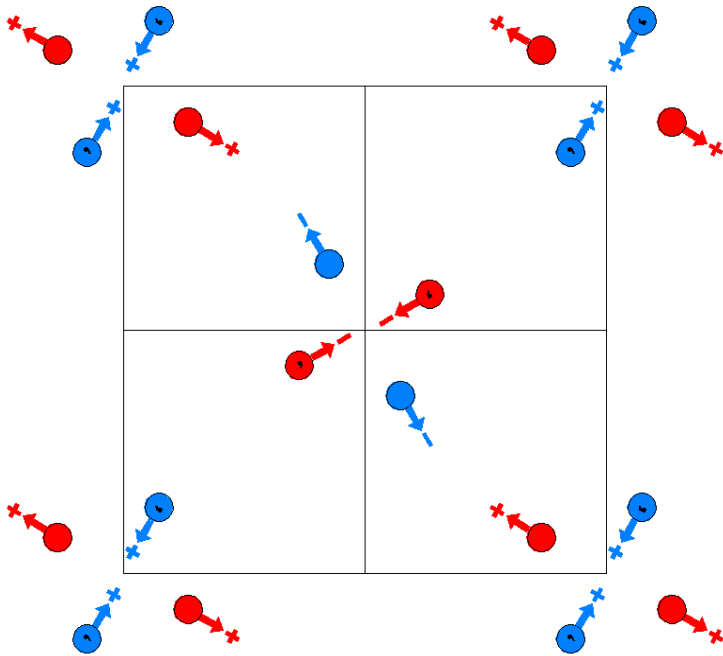
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$P_{2c}\bar{4}b2$   
117.6.963

$\bar{4}m21'$   
 $P_{2c}\bar{4}b2$

Tetragonal



Origin on  $\bar{4}12_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 <sub>0,0,z</sub><br>(2 <sub>z</sub>  0,0,0)                 | (3) $\bar{4}^+$ <sub>0,0,z</sub> ; 0,0,0<br>( $\bar{4}_z$  0,0,0)  | (4) $\bar{4}^-$ <sub>0,0,z</sub> ; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)                           |
| (5) a <sub>(1/2,0,0)</sub> x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (6) b <sub>(0,1/2,0)</sub> 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (7) 2 <sub>(1/2,1/2,0)</sub> x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0) | (8) 2 <sub>x,<math>\bar{x}+1/2,0</math></sub><br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,0) |

For (0,0,1)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (0,0,1)<br>(1 0,0,1)'                             | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)'         | (3) $\bar{4}^+$ ' <sub>0,0,z</sub> ; 0,0,1/2<br>( $\bar{4}_z$  0,0,1)' | (4) $\bar{4}^-$ ' <sub>0,0,z</sub> ; 0,0,1/2<br>( $\bar{4}_z^{-1}$  0,0,1)'                          |
| (5) n' (1/2,0,1) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1)' | (6) n' (0,1/2,1) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1)' | (7) 2' (1/2,1/2,0) x,x,1/2<br>(2 <sub>xy</sub>  1/2,1/2,1)'            | (8) 2' <sub>x,<math>\bar{x}+1/2,1/2</math></sub><br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (0,0,1)' +

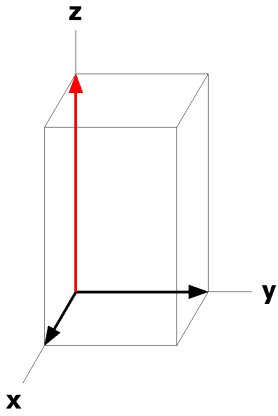
16	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]	(5) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $\bar{x}+1/2,y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]	(7) $y+1/2,x+1/2,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	h	..2'	$x,x+1/2,1/2$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/2$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x},1/2$ [ $u,u,\bar{w}$ ]	$\bar{x}+1/2,x,1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]				
8	g	..2	$x,x+1/2,0$ [ $u,u,0$ ]	$\bar{x},\bar{x}+1/2,0$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},0$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,x,0$ [ $u,\bar{u},0$ ]				
8	f	2..	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,\bar{z}$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]				
8	e	2..	$0,0,z$ [ $0,0,w$ ]	$0,0,\bar{z}$ [ $0,0,w$ ]	$1/2,1/2,z$ [ $0,0,\bar{w}$ ]	$1/2,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]				
4	d	2.2'2'	$0,1/2,1/2$ [ $0,0,w$ ]	$1/2,0,1/2$ [ $0,0,\bar{w}$ ]						
4	c	2.22	$0,1/2,0$ [ $0,0,0$ ]	$1/2,0,0$ [ $0,0,0$ ]						
4	b	$\bar{4}'..$	$0,0,1/2$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]						
4	a	$\bar{4}..$	$0,0,0$ [ $0,0,w$ ]	$1/2,1/2,0$ [ $0,0,\bar{w}$ ]						

**Symmetry of Special Projections**

Along [0,0,1]  $p4gm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0]  $p_c \cdot 1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,1/4,0$

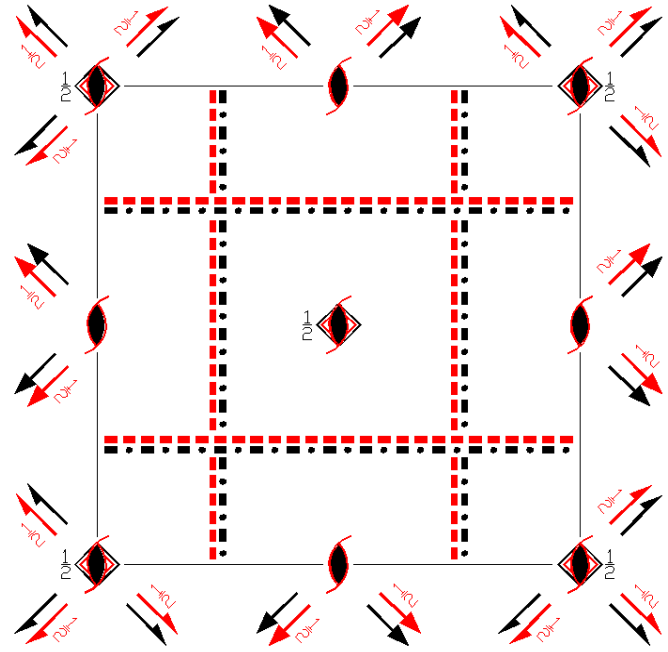
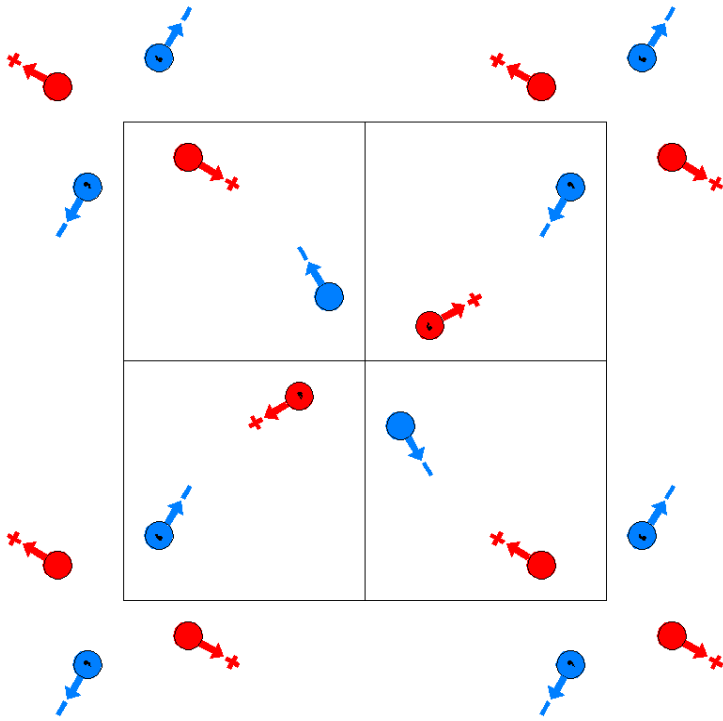
Along [1,1,0]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at  $x,x,0$



$P_{2c}\bar{4}'b'2$   
117.7.964

$\bar{4}m21'$   
 $P_{2c}\bar{4}'b'2$

Tetragonal



Origin on  $\bar{4}'12_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)      | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)' |
| (5) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (6) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' | (7) 2 (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)  | (8) 2 x, $\bar{x}$ +1/2,0<br>(2 <sub>xy</sub>  1/2,1/2,0)   |

For (0,0,1) + set

- |  |  |   |   |
|--|--|---|---|
| (1) t' (0,0,1)<br>(1 0,0,1)'                           | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)'       | (3) $\bar{4}^+$ 0,0,z; 0,0,1/2<br>( $\bar{4}_z^+$  0,0,1)   | (4) $\bar{4}^-$ 0,0,z; 0,0,1/2<br>( $\bar{4}_z^{-1}$  0,0,1)  |
| (5) n (1/2,0,1) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1) | (6) n (0,1/2,1) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1) | (7) 2' (1/2,1/2,0) x,x,1/2<br>(2 <sub>xy</sub>  1/2,1/2,1)' | (8) 2' x, $\bar{x}$ +1/2,1/2<br>(2 <sub>xy</sub>  1/2,1/2,1)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (0,0,1)' +

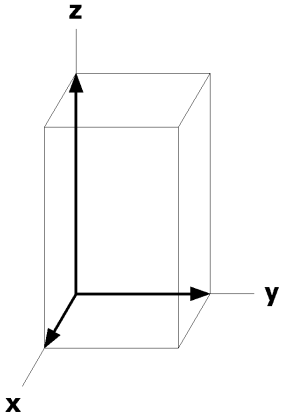
16	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(5) $x+1/2,\bar{y}+1/2,z$ [ $u,\bar{v},w$ ]	(6) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]	(7) $y+1/2,x+1/2,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	h	..2'	$x,x+1/2,1/2$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/2$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x},1/2$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,1/2$ [ $u,u,w$ ]				
8	g	..2	$x,x+1/2,0$ [ $u,u,0$ ]	$\bar{x},\bar{x}+1/2,0$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},0$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x,0$ [ $\bar{u},u,0$ ]				
8	f	2..	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,0,z$ [ $0,0,w$ ]	$0,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]				
8	e	2..	$0,0,z$ [ $0,0,w$ ]	$0,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,1/2,z$ [ $0,0,w$ ]	$1/2,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]				
4	d	2.2'2'	$0,1/2,1/2$ [ $0,0,w$ ]	$1/2,0,1/2$ [ $0,0,w$ ]						
4	c	2.22	$0,1/2,0$ [ $0,0,0$ ]	$1/2,0,0$ [ $0,0,0$ ]						
4	b	$\bar{4}$ ..	$0,0,1/2$ [ $0,0,w$ ]	$1/2,1/2,1/2$ [ $0,0,w$ ]						
4	a	$\bar{4}$ '..	$0,0,0$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]						

**Symmetry of Special Projections**

Along [0,0,1]  $p4gm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0]  $p_{2b}1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,0,0

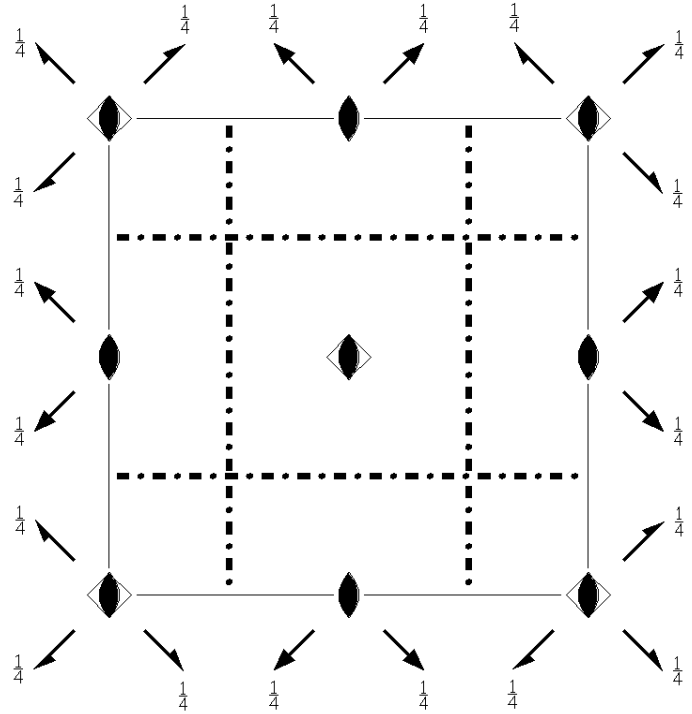
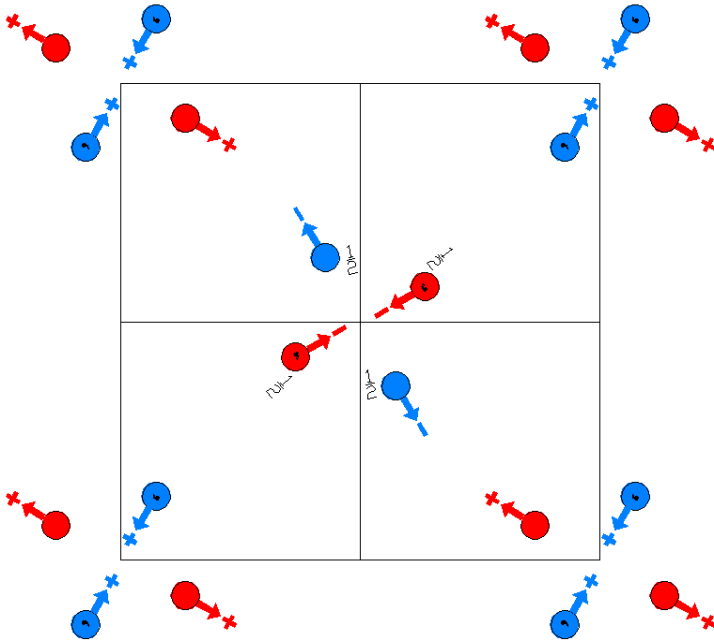
Along [1,1,0]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at x,x,0



$P\bar{4}n2$   
118.1.965

$\bar{4}m2$   
 $P\bar{4}n2$

Tetragonal



Origin on  $\bar{4}$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                           | (3) $\bar{4}^+$ $0,0,z$ ; $0,0,0$<br>( $\bar{4}_z$  0,0,0)    | (4) $\bar{4}^-$ $0,0,z$ ; $0,0,0$<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) n $(1/2,0,1/2)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,1/2$ ) | (6) n $(0,1/2,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,1/2$ ) | (7) 2 $(1/2,1/2,0)$ $x,x,1/4$<br>( $2_{xy}$   $1/2,1/2,1/2$ ) | (8) 2 $x,\bar{x}+1/2,1/4$<br>( $2_{\bar{xy}}$   $1/2,1/2,1/2$ ) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

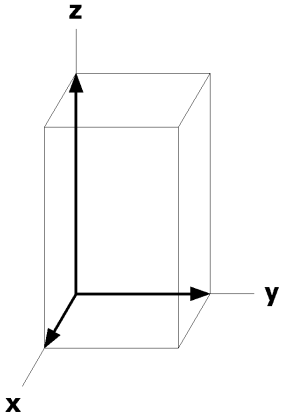
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	i	1	(1) x,y,z [u,v,w]		(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	
			(3) $y, \bar{x}, \bar{z}$ [ $\bar{v}, u, w$ ]		(4) $\bar{y}, x, \bar{z}$ [ $v, \bar{u}, w$ ]	
			(5) $x+1/2, \bar{y}+1/2, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]		(6) $\bar{x}+1/2, y+1/2, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]	
			(7) $y+1/2, x+1/2, \bar{z}+1/2$ [ $v, u, \bar{w}$ ]		(8) $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	
4	h	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	g	..2	x,x+1/2,1/4 [u,u,0]	$\bar{x}, \bar{x}+1/2, 1/4$ [ $\bar{u}, \bar{u}, 0$ ]	x+1/2, $\bar{x}, 3/4$ [ $\bar{u}, u, 0$ ]	$\bar{x}+1/2, x, 3/4$ [ $u, \bar{u}, 0$ ]
4	f	..2	x, $\bar{x}+1/2, 1/4$ [ $\bar{u}, u, 0$ ]	$\bar{x}, x+1/2, 1/4$ [ $u, \bar{u}, 0$ ]	$\bar{x}+1/2, \bar{x}, 3/4$ [ $\bar{u}, \bar{u}, 0$ ]	x+1/2,x,3/4 [u,u,0]
4	e	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
2	d	2.22	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]		
2	c	2.22	0,1/2,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]		
2	b	$\bar{4}$ ..	0,0,1/2 [0,0,w]	1/2,1/2,0 [0,0, $\bar{w}$ ]		
2	a	$\bar{4}$ ..	0,0,0 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p4'gm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4

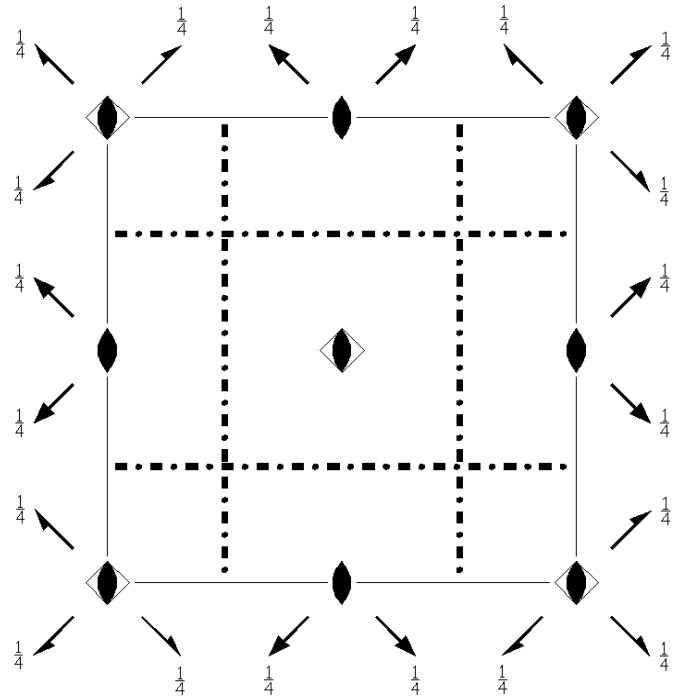
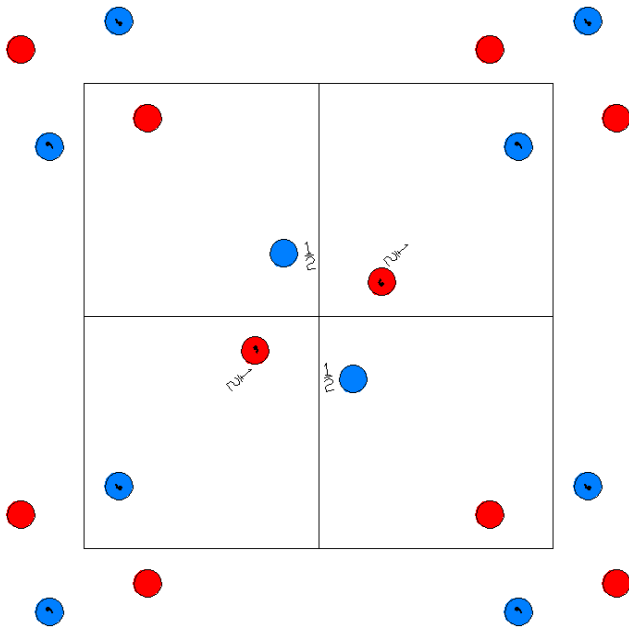


$P\bar{4}n21'$   
118.2.966

$\bar{4}m21'$   
 $P\bar{4}n21'$

Tetragonal

1'



Origin on  $\bar{4}1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

For 1 + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)        | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)     | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                          |
| (5) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (6) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2) | (8) 2 x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2) |

For 1' + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1'<br>(1 0,0,0)'   | (2) 2' <sub>z</sub> 0,0,z<br>(2' <sub>z</sub>  0,0,0)'       | (3) $\bar{4}^+$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'     | (4) $\bar{4}^-$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                          |
| (5) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (6) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2' <sub>xy</sub>  1/2,1/2,1/2)' | (8) 2' x, $\bar{x}$ +1/2,1/4<br>(2' <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

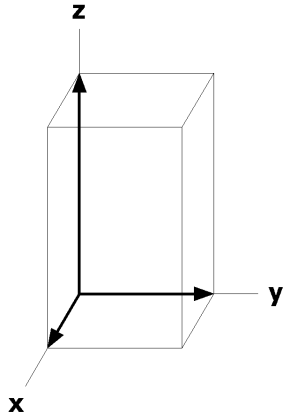
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		1 +		1' +
8 i 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $y,\bar{x},\bar{z}$ [0,0,0]	(4) $\bar{y},x,\bar{z}$ [0,0,0]
	(5) $x+1/2,\bar{y}+1/2,z+1/2$ [0,0,0]	(6) $\bar{x}+1/2,y+1/2,z+1/2$ [0,0,0]	(7) $y+1/2,x+1/2,\bar{z}+1/2$ [0,0,0]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [0,0,0]
4 h 2..1'	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	1/2,0,z+1/2 [0,0,0]	0,1/2, $\bar{z}+1/2$ [0,0,0]
4 g ..21'	x,x+1/2,1/4 [0,0,0]	$\bar{x},\bar{x}+1/2,1/4$ [0,0,0]	x+1/2, $\bar{x},3/4$ [0,0,0]	$\bar{x}+1/2,x,3/4$ [0,0,0]
4 f ..21'	x, $\bar{x}+1/2,1/4$ [0,0,0]	$\bar{x},x+1/2,1/4$ [0,0,0]	$\bar{x}+1/2,\bar{x},3/4$ [0,0,0]	x+1/2,x,3/4 [0,0,0]
4 e 2..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]
2 d 2.221'	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]		
2 c 2.221'	0,1/2,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]		
2 b $\bar{4}..1'$	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2 a $\bar{4}..1'$	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4gm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

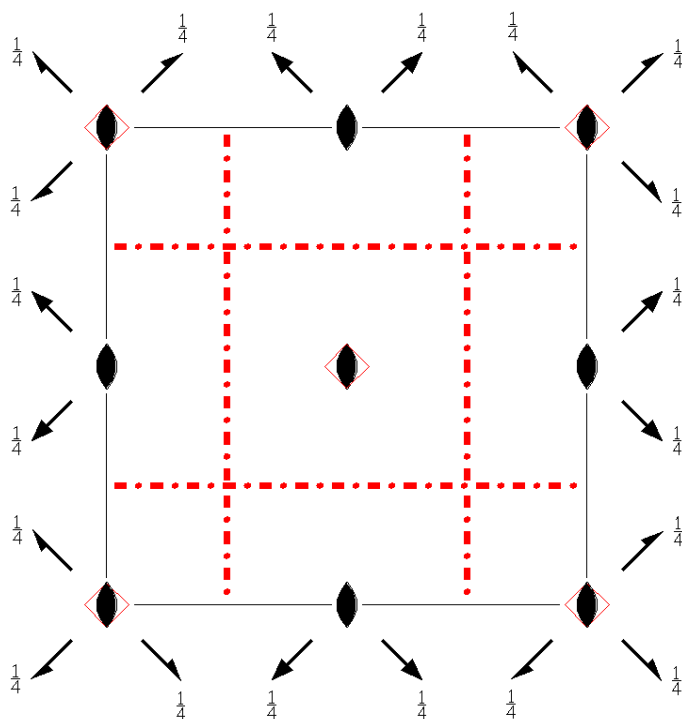
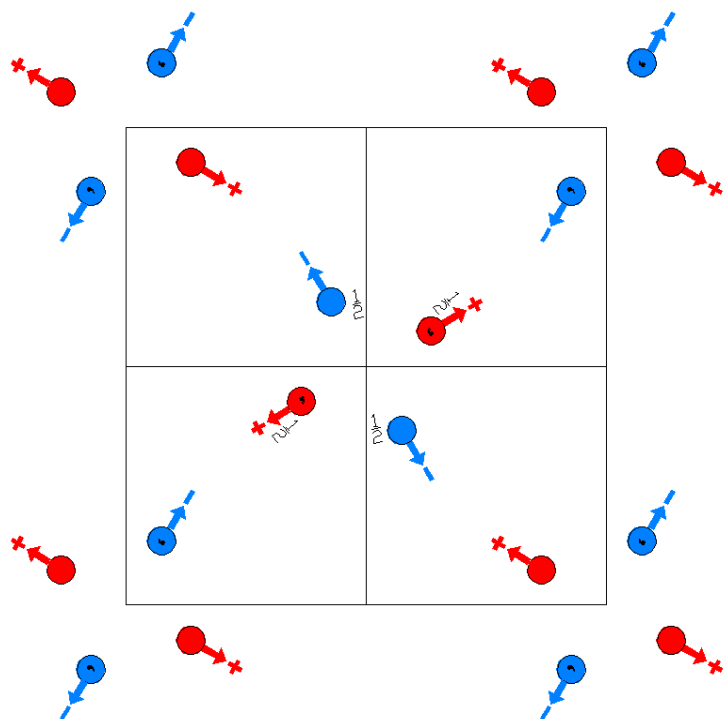
Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



$P\bar{4}'n'2$   
118.3.967

$\bar{4}'m'2$   
 $P\bar{4}'n'2$

Tetragonal



Origin on  $\bar{4}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                       | (3) $\bar{4}'^+$ 0,0,z; 0,0,0<br>( $\bar{4}'_z$  0,0,0)'    | (4) $\bar{4}'^-$ 0,0,z; 0,0,0<br>( $\bar{4}'_z^{-1}$  0,0,0)'   |
| (5) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (6) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2) | (8) 2 x, $\bar{x}$ +1/2,1/4<br>(2 <sub>xy</sub> ^- 1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

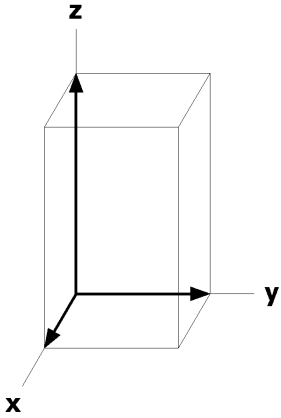
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	i	1	(1) x,y,z [u,v,w]		(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	
			(3) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]		(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	
			(5) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]		(6) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]	
			(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]		(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	
4	h	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	g	..2	x,x+1/2,1/4 [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	x+1/2, $\bar{x},3/4$ [u, $\bar{u},0$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},u,0$ ]
4	f	..2	x, $\bar{x}+1/2,1/4$ [ $\bar{u},u,0$ ]	$\bar{x},x+1/2,1/4$ [u, $\bar{u},0$ ]	$\bar{x}+1/2,\bar{x},3/4$ [u,u,0]	x+1/2,x,3/4 [ $\bar{u},\bar{u},0$ ]
4	e	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
2	d	2.22	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]		
2	c	2.22	0,1/2,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]		
2	b	$\bar{4}'..$	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a	$\bar{4}'..$	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4g'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

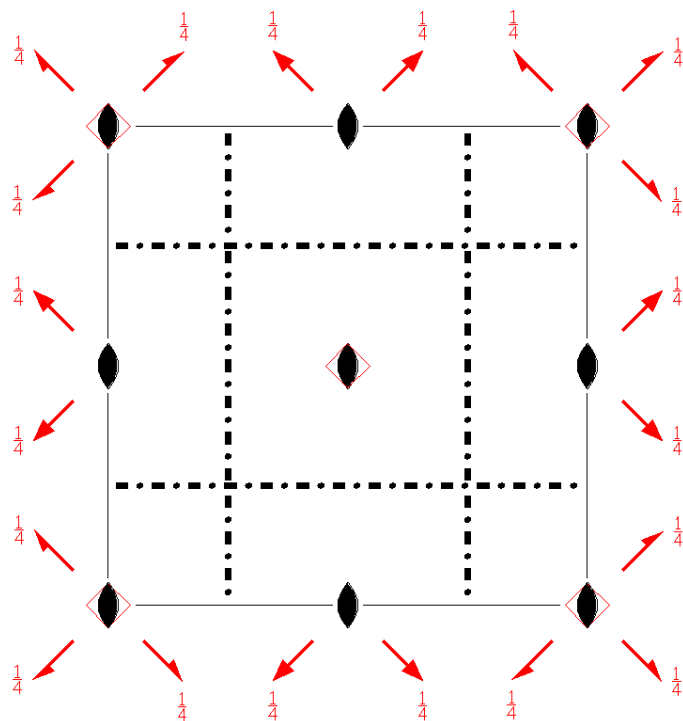
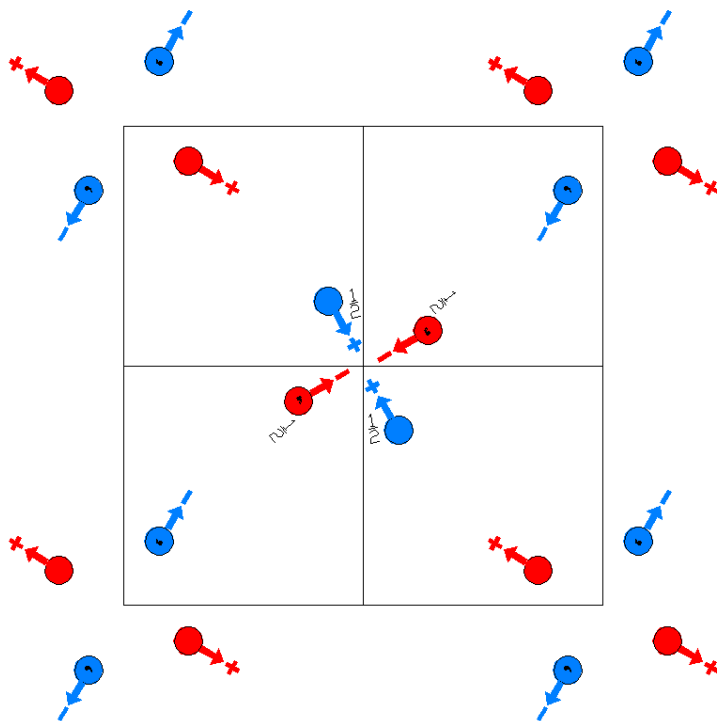
Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



$P\bar{4}'n2'$   
118.4.968

$\bar{4}'m2'$   
 $P\bar{4}'n2'$

Tetragonal



Origin on  $\bar{4}'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                           | (3) $\bar{4}'^+$ $0,0,z$ ; $0,0,0$<br>( $\bar{4}_z$  0,0,0)'      | (4) $\bar{4}'^-$ $0,0,z$ ; $0,0,0$<br>( $\bar{4}_z^{-1}$  0,0,0)'   |
| (5) n $(1/2,0,1/2)$ $x,1/4,z$<br>( $m_y$   $1/2,1/2,1/2$ ) | (6) n $(0,1/2,1/2)$ $1/4,y,z$<br>( $m_x$   $1/2,1/2,1/2$ ) | (7) $2'$ $(1/2,1/2,0)$ $x,x,1/4$<br>( $2_{xy}$   $1/2,1/2,1/2$ )' | (8) $2'$ $x,\bar{x}+1/2,1/4$<br>( $2_{\bar{xy}}$   $1/2,1/2,1/2$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

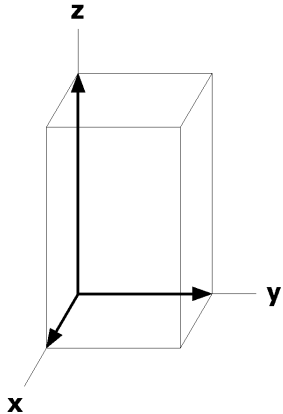
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	i	1	(1) x,y,z [u,v,w]		(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	
			(3) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]		(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	
			(5) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]		(6) $\bar{x}+1/2,y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]	
			(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]		(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $v,u,w$ ]	
4	h	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0,w]
4	g	..2'	x,x+1/2,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $u,\bar{u},w$ ]	x+1/2, $\bar{x},3/4$ [ $u,u,\bar{w}$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
4	f	..2'	x, $\bar{x}+1/2,1/4$ [ $u,u,w$ ]	$\bar{x},x+1/2,1/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,\bar{x},3/4$ [ $u,\bar{u},\bar{w}$ ]	x+1/2,x,3/4 [ $\bar{u},u,\bar{w}$ ]
4	e	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]
2	d	2.2'2'	0,1/2,3/4 [0,0,w]	1/2,0,1/4 [0,0, $\bar{w}$ ]		
2	c	2.2'2'	0,1/2,1/4 [0,0,w]	1/2,0,3/4 [0,0, $\bar{w}$ ]		
2	b	$\bar{4}'..$	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a	$\bar{4}'..$	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4gm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c_p-1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

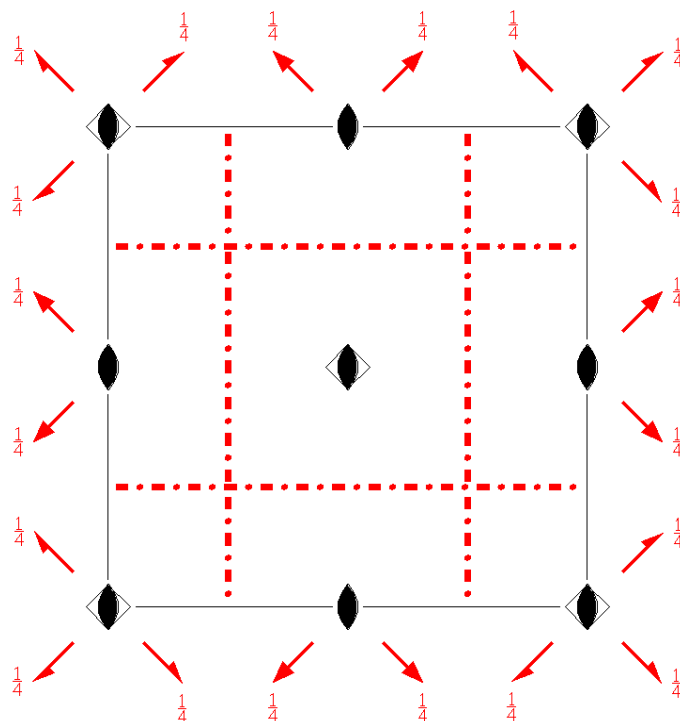
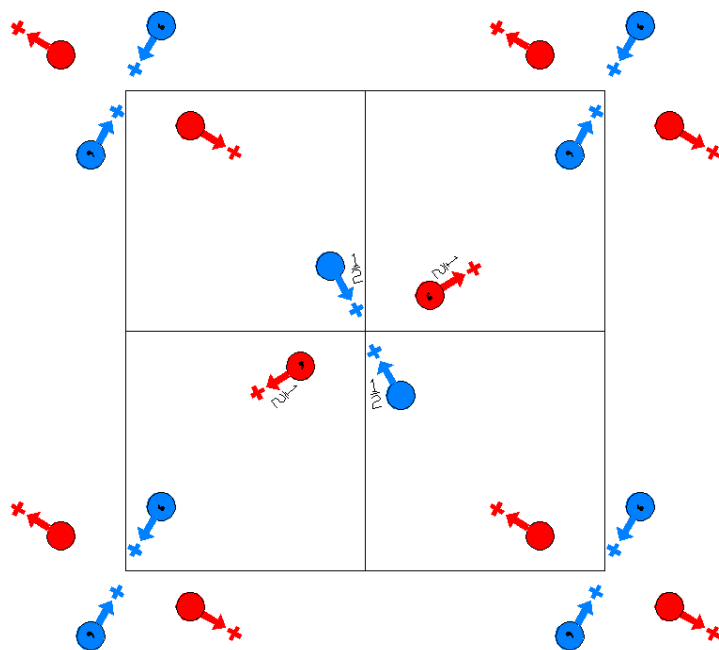
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



$P\bar{4}n'2'$   
118.5.969

$\bar{4}m'2'$   
 $P\bar{4}n'2'$

Tetragonal



Origin on  $\bar{4}$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                       | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)         | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)     |
| (5) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (6) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)' | (8) 2' x, $\bar{x}+1/2,1/4$<br>(2 <sub>xy</sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

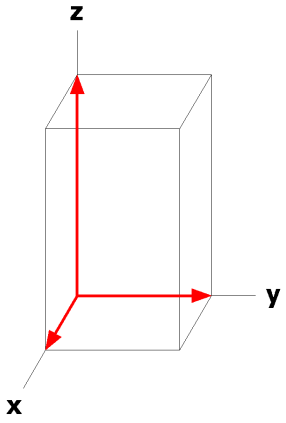
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
8	i	1	(1) x,y,z [u,v,w]		(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	
			(3) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]		(4) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]	
			(5) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]		(6) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]	
			(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]		(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $v,u,w$ ]	
4	h	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	1/2,0,z+1/2 [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]
4	g	..2'	x,x+1/2,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $u,\bar{u},w$ ]	x+1/2, $\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,3/4$ [ $u,u,w$ ]
4	f	..2'	x, $\bar{x}+1/2,1/4$ [ $u,u,w$ ]	$\bar{x},x+1/2,1/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,\bar{x},3/4$ [ $\bar{u},u,w$ ]	x+1/2,x,3/4 [ $u,\bar{u},w$ ]
4	e	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]
2	d	2.2'2'	0,1/2,3/4 [0,0,w]	1/2,0,1/4 [0,0,w]		
2	c	2.2'2'	0,1/2,1/4 [0,0,w]	1/2,0,3/4 [0,0,w]		
2	b	$\bar{4}..$	0,0,1/2 [0,0,w]	1/2,1/2,0 [0,0,w]		
2	a	$\bar{4}..$	0,0,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4'g'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

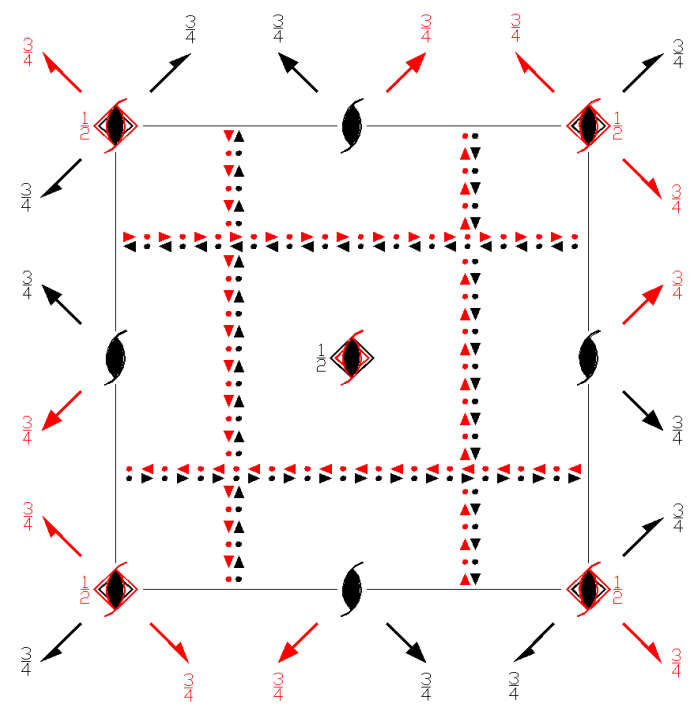
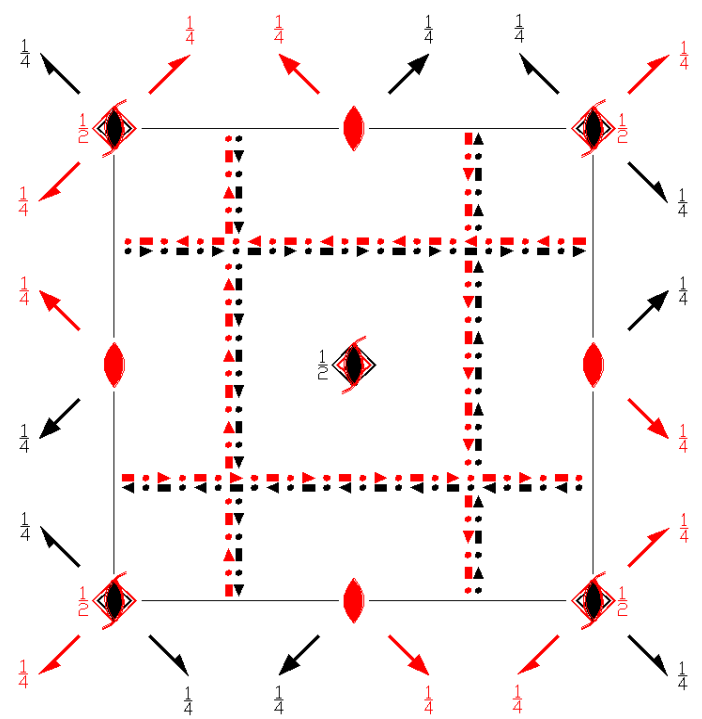
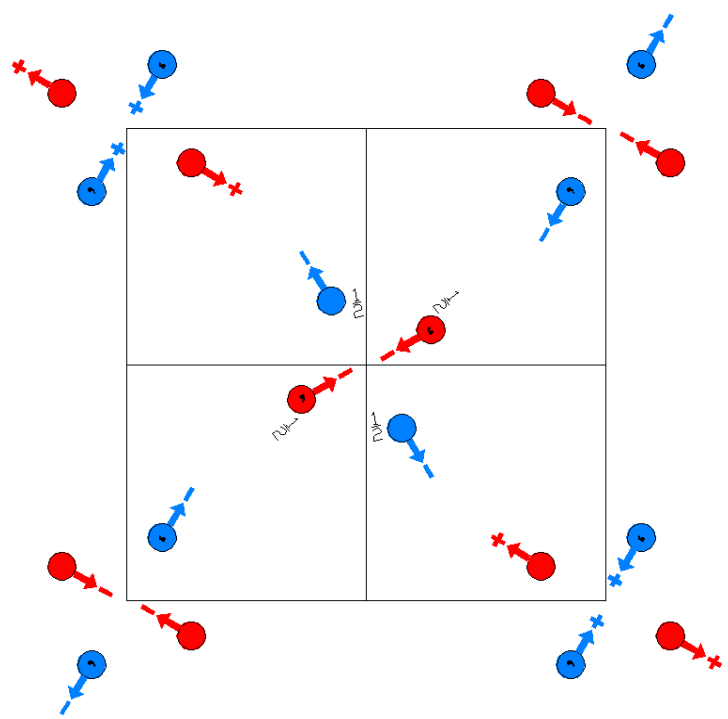
Along [1,1,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



$P_1\bar{4}n2$   
118.6.970

$\bar{4}m21'$   
 $P_1\bar{4}n2$

Tetragonal





Origin on  $\bar{4}$ Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$ 

## Symmetry Operations

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)       | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)    |
| (5) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (6) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2) | (8) 2 x, $\bar{x}$ +1/2,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2) |

For (1,0,0)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) t' (1,0,0)<br>(1 1,0,0)'                                 | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'                   | (3) $\bar{4}^+$ ' 1/2,1/2,z; 1/2,1/2,0<br>( $\bar{4}_z$  1,0,0)' | (4) $\bar{4}^-$ ' 1/2,-1/2,z; 1/2,-1/2,0<br>( $\bar{4}_z^{-1}$  1,0,0)'   |
| (5) n' (3/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  3/2,1/2,1/2)' | (6) n' (0,1/2,1/2) 3/4,y,z<br>(m <sub>x</sub>  3/2,1/2,1/2)' | (7) 2' x+1/2,x,1/4<br>(2 <sub>xy</sub>  3/2,1/2,1/2)'            | (8) 2' (1/2,1/2,0) x+1, $\bar{x}$ ,1/4<br>(2 <sub>xy</sub>  3/2,1/2,1/2)' |

Generators selected (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

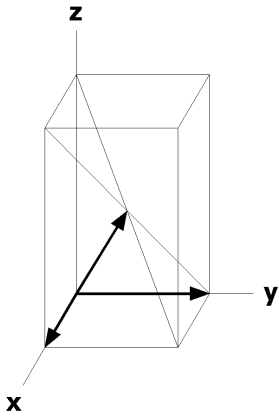
			(0,0,0) +	(1,0,0)' +			
16	i	1	(1) x,y,z [u,v,w] (3) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},u,w$ ] (5) x+1/2, $\bar{y}$ +1/2,z+1/2 [ $\bar{u},v,\bar{w}$ ] (7) y+1/2,x+1/2, $\bar{z}$ +1/2 [v,u, $\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (4) $\bar{y},x,\bar{z}$ [v, $\bar{u},w$ ] (6) $\bar{x}$ +1/2,y+1/2,z+1/2 [u, $\bar{v},\bar{w}$ ] (8) $\bar{y}$ +1/2, $\bar{x}$ +1/2, $\bar{z}$ +1/2 [ $\bar{v},\bar{u},\bar{w}$ ]			
8	h	2'..	0,1/2,z [u,v,0]      1/2,0, $\bar{z}$ [ $\bar{v},u,0$ ]	1/2,0,z+1/2 [ $\bar{u},v,0$ ]	0,1/2, $\bar{z}$ +1/2 [v,u,0]		
8	g	..2'	x,x+1/2,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}$ +1/2,1/4 [ $\bar{u},u,\bar{w}$ ]	x+1/2, $\bar{x}$ ,3/4 [u,u, $\bar{w}$ ]	$\bar{x}$ +1/2,x,3/4 [u,u,w]	
8	f	..2	x, $\bar{x}$ +1/2,1/4 [ $\bar{u},u,0$ ]	$\bar{x},x$ +1/2,1/4 [ $\bar{u},u,0$ ]	$\bar{x}$ +1/2, $\bar{x}$ ,3/4 [u,u,0]	x+1/2,x,3/4 [u,u,0]	
8	e	2..	0,0,z [0,0,w]      0,0, $\bar{z}$ [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ +1/2 [0,0, $\bar{w}$ ]		
4	d	2'.22'	0,1/2,3/4 [u,u,0]      1/2,0,1/4 [u, $\bar{u},0$ ]				
4	c	2'.2'2	0,1/2,1/4 [ $\bar{u},u,0$ ]	1/2,0,3/4 [u,u,0]			
4	b	$\bar{4}$ '..	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]			
4	a	$\bar{4}$ ..	0,0,0 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4gm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $c1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,0,0$

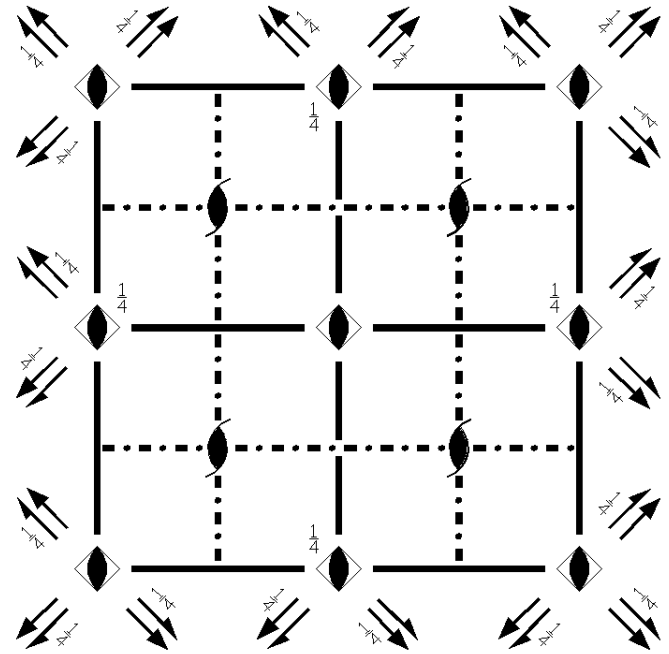
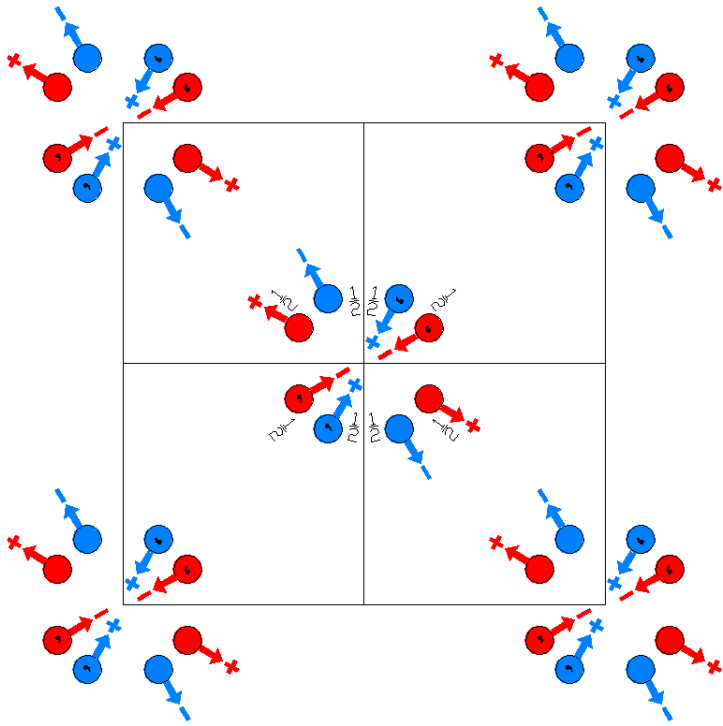
Along  $[1,1,0]$   $p_c 2mm$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x-1/4, x+1/4, -1/4$



$\bar{4}m2$   
119.1.971

$\bar{4}m2$   
 $\bar{4}m2$

Tetragonal



Origin on  $\bar{4}m2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)           |
| (5) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (6) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)               | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0) |

For (1/2,1/2,1/2) + set

- |  |  |   |  |
|--|--|---|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                     | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2) | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2)           |
| (5) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (6) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)       | (8) 2 x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

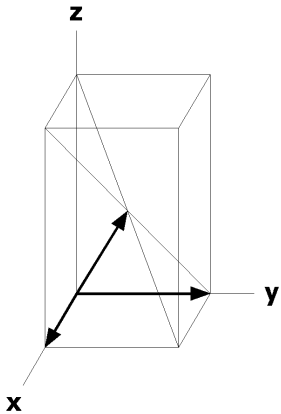
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates								
			(0,0,0) +	(1/2,1/2,1/2) +					
16 j 1	(1)	$x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $y,\bar{x},\bar{z} [\bar{v},u,w]$	(4) $\bar{y},x,\bar{z} [v,\bar{u},w]$	(5) $x,\bar{y},z [\bar{u},v,\bar{w}]$	(6) $\bar{x},y,z [u,\bar{v},\bar{w}]$	(7) $y,x,\bar{z} [v,u,\bar{w}]$	(8) $\bar{y},\bar{x},\bar{z} [\bar{v},\bar{u},\bar{w}]$
8 i .m.		$x,0,z [0,v,0]$	$\bar{x},0,z [0,\bar{v},0]$	$0,\bar{x},\bar{z} [\bar{v},0,0]$	$0,x,\bar{z} [v,0,0]$				
8 h ..2		$x,x+1/2,1/4 [u,u,0]$	$\bar{x},\bar{x}+1/2,1/4 [\bar{u},\bar{u},0]$	$x+1/2,\bar{x},3/4 [\bar{u},u,0]$	$\bar{x}+1/2,x,3/4 [u,\bar{u},0]$				
8 g ..2		$x,x,0 [u,u,0]$	$\bar{x},\bar{x},0 [\bar{u},\bar{u},0]$	$x,\bar{x},0 [\bar{u},u,0]$	$\bar{x},x,0 [u,\bar{u},0]$				
4 f 2mm.		$0,1/2,z [0,0,0]$	$1/2,0,\bar{z} [0,0,0]$						
4 e 2mm.		$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$						
2 d $\bar{4}m2$		$0,1/2,3/4 [0,0,0]$							
2 c $\bar{4}m2$		$0,1/2,1/4 [0,0,0]$							
2 b $\bar{4}m2$		$0,0,1/2 [0,0,0]$							
2 a $\bar{4}m2$		$0,0,0 [0,0,0]$							

**Symmetry of Special Projections**

Along [0,0,1]  $p4'm'm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$\bar{4}m21'$

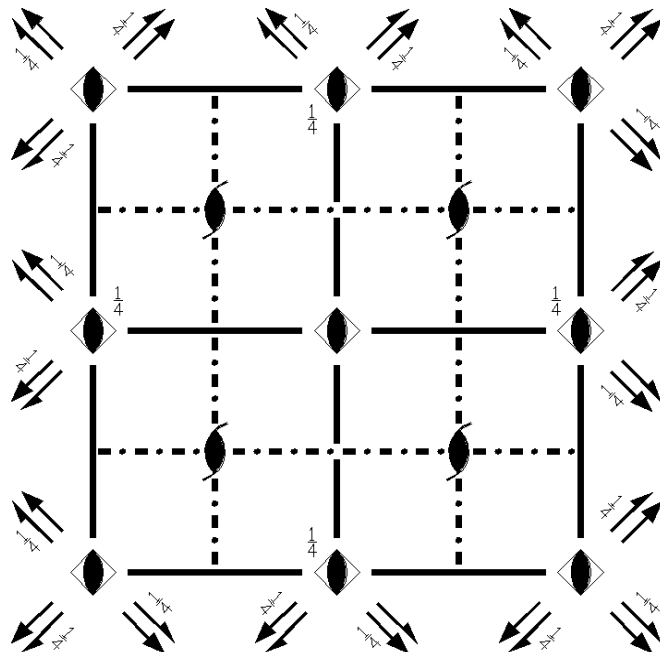
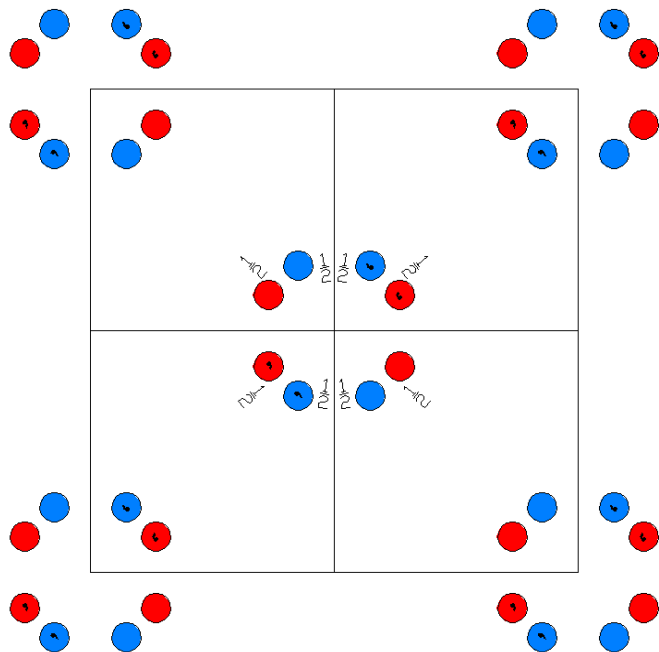
119.2.972

$\bar{4}m21'$

$\bar{4}m21'$

Tetragonal

1'



Origin on  $\bar{4}m21'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1   0,0,0)                    | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$   0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$   0,0,0) |
| (5) m x,0,z<br>(m <sub>y</sub>   0,0,0) | (6) m 0,y,z<br>(m <sub>x</sub>   0,0,0) | (7) 2 x,x,0<br>(2 <sub>xy</sub>   0,0,0)               | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub>xy</sub>   0,0,0)          |

For (1/2,1/2,1/2) + set

- |   |   |  |   |
|---|---|--|---|
| (1) t (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)                    | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2) | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$   1/2,1/2,1/2) | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$   1/2,1/2,1/2) |
| (5) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,1/2) | (6) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,1/2) | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>   1/2,1/2,1/2)       | (8) 2 x, $\bar{x}$ +1/2,1/4<br>(2 <sub>xy</sub>   1/2,1/2,1/2)          |

## For (0,0,0)' + set

(1) $1'$ (1 0,0,0)'	(2) $2'$ 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'	(4) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z^{-1}$  0,0,0)'
(5) $m'$ x,0,z (m <sub>y</sub>  0,0,0)'	(6) $m'$ 0,y,z (m <sub>x</sub>  0,0,0)'	(7) $2'$ x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) $2'$ x, $\bar{x}$ ,0 (2 <sub>xy</sub>  0,0,0)'

## For (1/2,1/2,1/2)' + set

(1) $t'$ (1/2,1/2,1/2) (1 1/2,1/2,1/2)'	(2) $2'$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>  1/2,1/2,1/2)'	(3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$  1/2,1/2,1/2)'	(4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$  1/2,1/2,1/2)'
(5) $n'$ (1/2,0,1/2) x,1/4,z (m <sub>y</sub>  1/2,1/2,1/2)'	(6) $n'$ (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1/2)'	(7) $2'$ (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(8) $2'$ x, $\bar{x}+1/2$ ,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

**Positions**

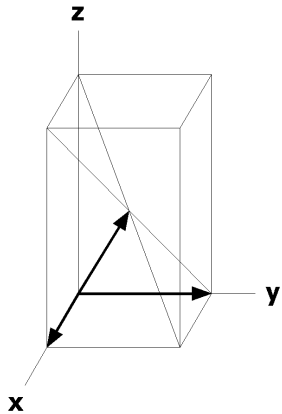
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'		
16	j	11'	(1) x,y,z [0,0,0] (5) x, $\bar{y}$ ,z [0,0,0]	(2) $\bar{x}$ , $\bar{y}$ ,z [0,0,0] (6) $\bar{x}$ ,y,z [0,0,0]	(3) y, $\bar{x}$ , $\bar{z}$ [0,0,0] (7) y,x, $\bar{z}$ [0,0,0]	(4) $\bar{y}$ ,x, $\bar{z}$ [0,0,0] (8) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [0,0,0]
8	i	.m.1'	x,0,z [0,0,0]	$\bar{x}$ ,0,z [0,0,0]	0, $\bar{x}$ , $\bar{z}$ [0,0,0]	0,x, $\bar{z}$ [0,0,0]
8	h	..21'	x,x+1/2,1/4 0,0,0]	$\bar{x}$ , $\bar{x}+1/2$ ,1/4 [0,0,0]	x+1/2, $\bar{x}$ ,3/4 [0,0,0]	$\bar{x}+1/2$ ,x,3/4 [0,0,0]
8	g	..21'	x,x,0 [0,0,0]	$\bar{x}$ , $\bar{x}$ ,0 [0,0,0]	x, $\bar{x}$ ,0 [0,0,0]	$\bar{x}$ ,x,0 [0,0,0]
4	f	2mm.1'	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
4	e	2mm.1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	d	$\bar{4}m21'$	0,1/2,3/4 [0,0,0]			
2	c	$\bar{4}m21'$	0,1/2,1/4 [0,0,0]			
2	b	$\bar{4}m21'$	0,0,1/2 [0,0,0]			
2	a	$\bar{4}m21'$	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



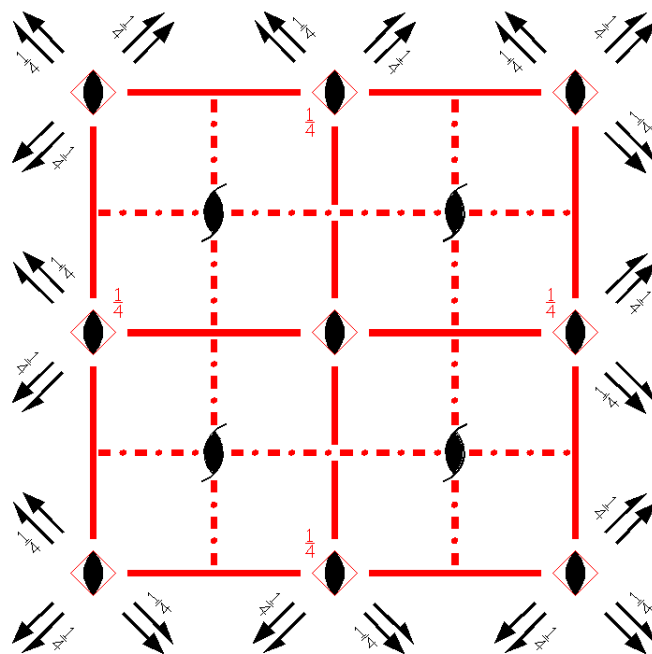
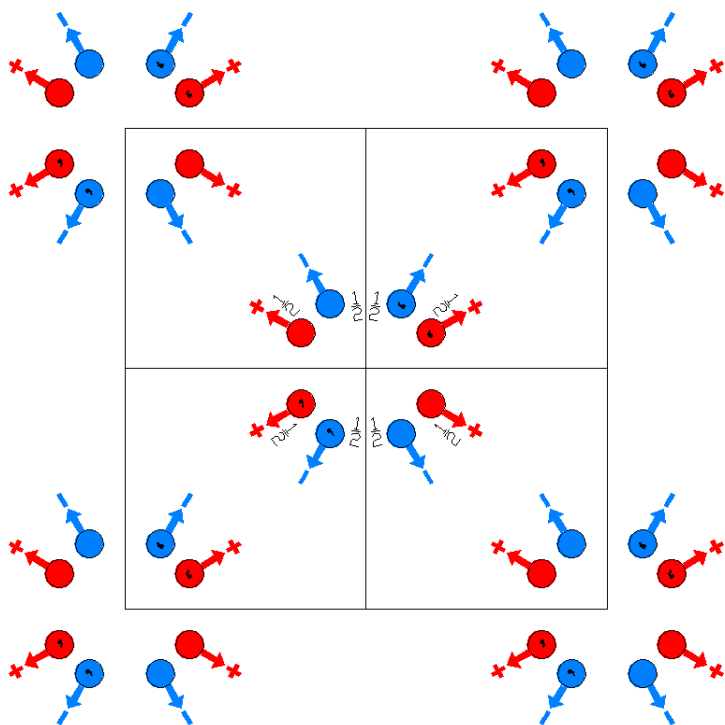
$\bar{4}m'2$

119.3.973

$\bar{4}m'2$

$\bar{4}m'2$

Tetragonal



Origin on  $\bar{4}m'2$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)' |
| (5) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (6) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub>-xy</sub>  0,0,0)          |

For (1/2,1/2,1/2) + set

- |  |  |  |   |
|--|--|--|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                       | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)   | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2)' | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2)' |
| (5) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (6) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)        | (8) 2 x, $\bar{x}$ +1/2,1/4<br>(2 <sub>-xy</sub>  1/2,1/2,1/2)          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates									
			(0,0,0) +		(1/2,1/2,1/2) +					
16	j	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(5) x, $\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(6) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	i	.m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	0, $\bar{x},\bar{z}$ [0, $\bar{u},\bar{w}$ ]	0,x, $\bar{z}$ [0,u, $\bar{w}$ ]				
8	h	..2	x,x+1/2,1/4 [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	x+1/2, $\bar{x},3/4$ [u, $\bar{u},0$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},u,0$ ]				
8	g	..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},0$ [u, $\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]				
4	f	2m'm'	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]						
4	e	2m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]						
2	d	$\bar{4}'m'2$	0,1/2,3/4 [0,0,0]							
2	c	$\bar{4}'m'2$	0,1/2,1/4 [0,0,0]							
2	b	$\bar{4}'m'2$	0,0,1/2 [0,0,0]							
2	a	$\bar{4}'m'2$	0,0,0 [0,0,0]							

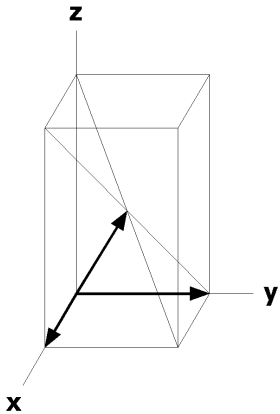
**Symmetry of Special Projections**

Along [0,0,1]  $p4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

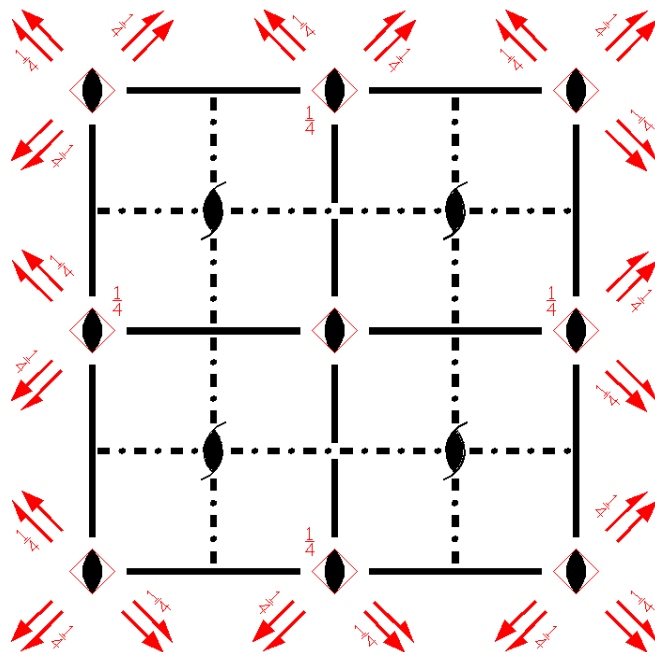
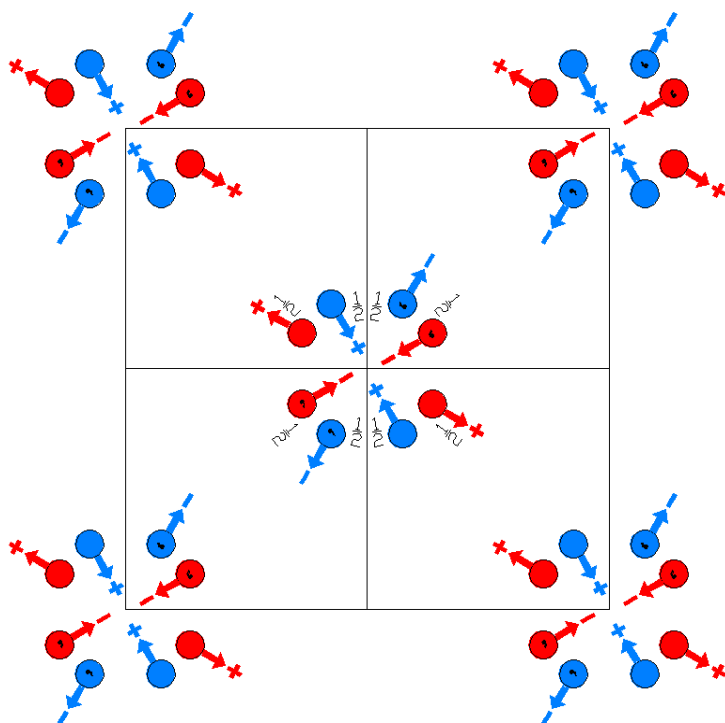




$\bar{4}'m2'$   
119.4.974

$\bar{4}'m2'$   
 $\bar{4}'m2'$

Tetragonal



Origin on  $\bar{4}'m2'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'               |
| (5) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (6) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                | (8) 2' x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)' |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                     | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2)' | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2)'               |
| (5) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (6) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'        | (8) 2' x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

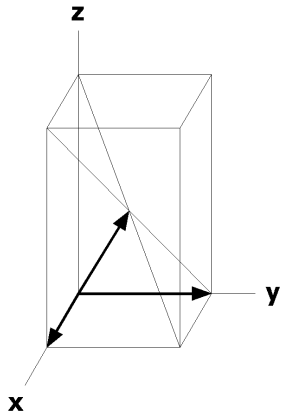
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
		(0,0,0) +	(1/2,1/2,1/2) +					
16 j 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(5) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [v,u,w]
8 i .m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	0, $\bar{x},\bar{z}$ [v,0,0]	0,x, $\bar{z}$ [ $\bar{v},0,0$ ]				
8 h ..2'	x,x+1/2,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [u, $\bar{u},w$ ]	x+1/2, $\bar{x},3/4$ [u,u, $\bar{w}$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]				
8 g ..2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [u, $\bar{u},w$ ]	x, $\bar{x},0$ [u,u, $\bar{w}$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},\bar{w}$ ]				
4 f 2mm.	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]						
4 e 2mm.	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]						
2 d $\bar{4}'m2'$	0,1/2,3/4 [0,0,0]							
2 c $\bar{4}'m2'$	0,1/2,1/4 [0,0,0]							
2 b $\bar{4}'m2'$	0,0,1/2 [0,0,0]							
2 a $\bar{4}'m2'$	0,0,0 [0,0,0]							

**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c1m11'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



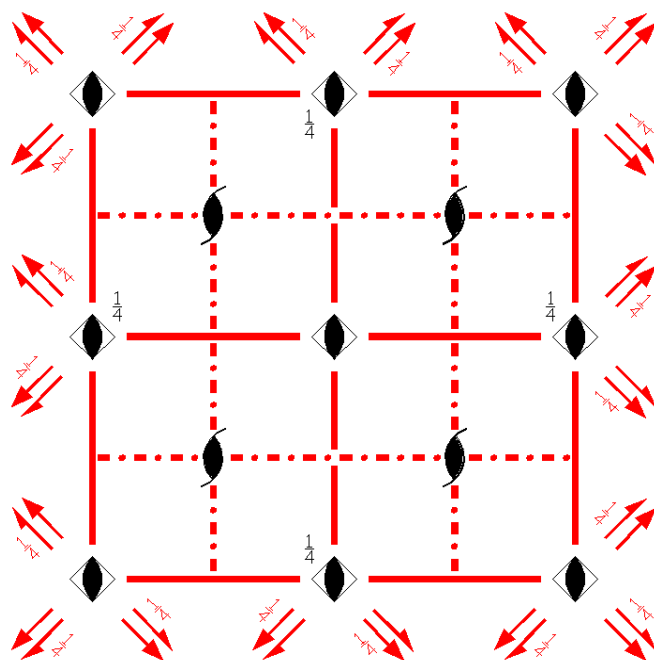
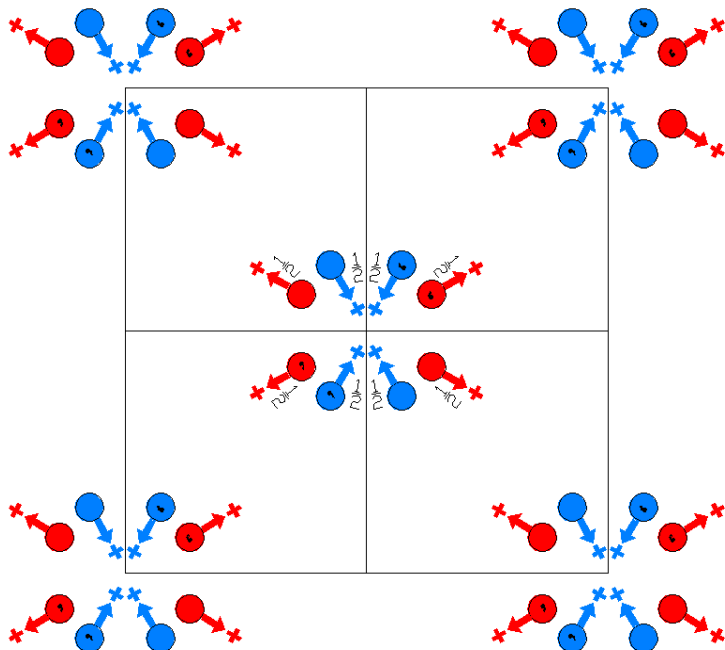
$\bar{4}m'2'$

119.5.975

$\bar{4}m'2'$

$\bar{4}m'2'$

Tetragonal



Origin on  $\bar{4}m'2'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (6) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'             | (8) 2' x, $\bar{x}$ ,0<br>(2 <sub>xy</sub>  0,0,0)'        |

For (1/2,1/2,1/2) + set

- |  |  |   |  |
|--|--|---|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                       | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)   | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2) | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2) |
| (5) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (6) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'     | (8) 2' x, $\bar{x}$ +1/2,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

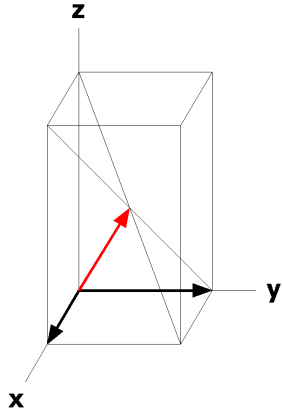
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates									
			(0,0,0) +		(1/2,1/2,1/2) +					
16	j	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(5) x, $\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(6) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]
8	i	.m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	0, $\bar{x},\bar{z}$ [0,u,w]	0,x, $\bar{z}$ [0, $\bar{u},w$ ]				
8	h	..2'	x,x+1/2,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},w$ ]	x+1/2, $\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},u,w$ ]				
8	g	..2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,0$ [ $\bar{u},u,w$ ]				
4	f	2m'm'	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]						
4	e	2m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]						
2	d	$\bar{4}m'2'$	0,1/2,3/4 [0,0,w]							
2	c	$\bar{4}m'2'$	0,1/2,1/4 [0,0,w]							
2	b	$\bar{4}m'2'$	0,0,1/2 [0,0,w]							
2	a	$\bar{4}m'2'$	0,0,0 [0,0,w]							

**Symmetry of Special Projections**

Along [0,0,1]  $p4'mm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

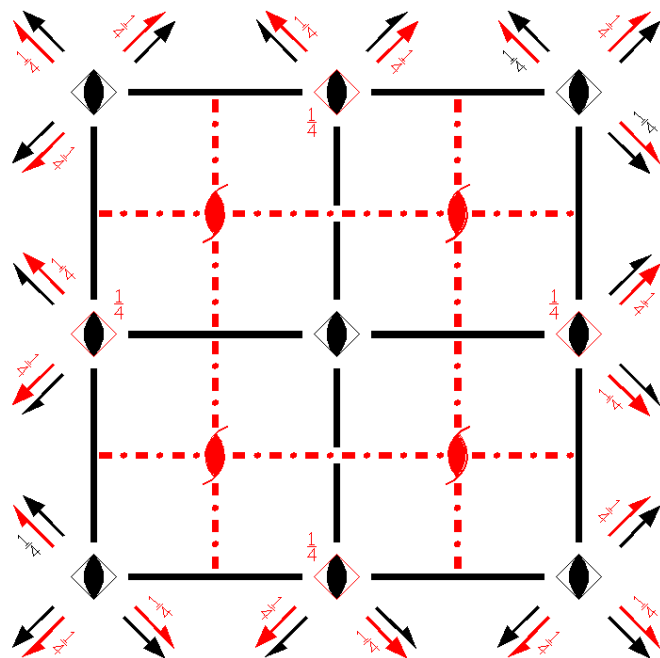
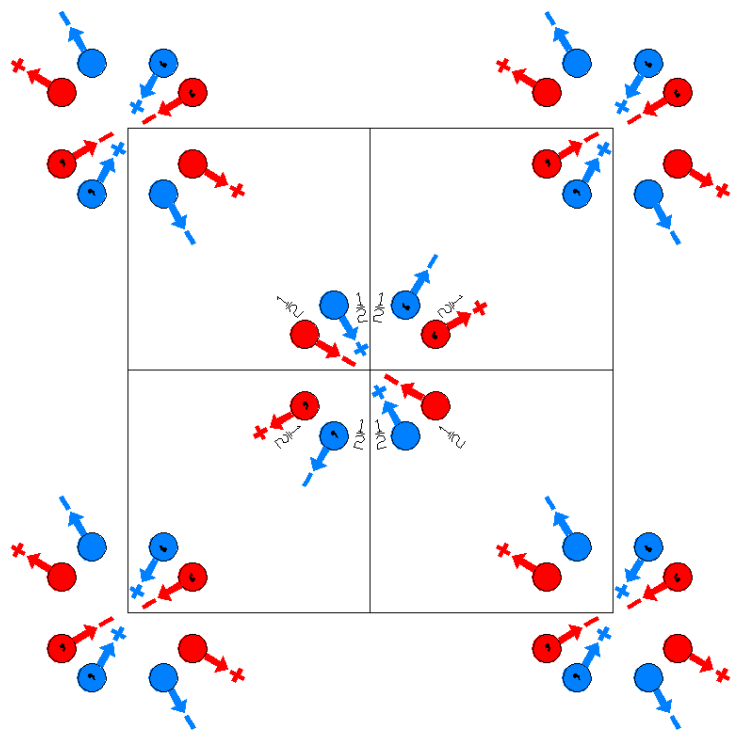
Along [1,1,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$I_p\bar{4}m2$   
119.6.976

$\bar{4}m21'$   
 $I_p\bar{4}m2$

Tetragonal



Origin on  $\bar{4}m2$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)           |
| (5) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (6) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)               | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0) |

For (1/2,1/2,1/2)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'                     | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2)' | (4) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2)'          |
| (5) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (6) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'        | (8) 2' x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

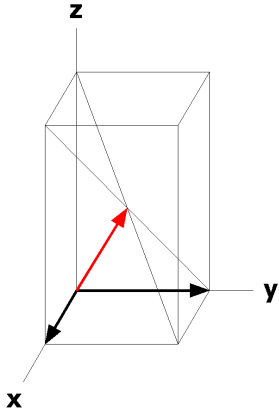
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1/2,1/2,1/2)' +		
16	j	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(3) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ] (7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	i	.m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0]	0, $\bar{x},\bar{z}$ [ $\bar{v},0,0$ ]	0,x, $\bar{z}$ [v,0,0]
8	h	..2'	x,x+1/2,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $u,\bar{u},w$ ]	x+1/2, $\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,3/4$ [u,u,w]
8	g	..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},0$ [ $\bar{u},u,0$ ]	$\bar{x},x,0$ [u, $\bar{u},0$ ]
4	f	2mm.	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
4	e	2mm.	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	d	$\bar{4}'m2'$	0,1/2,3/4 [0,0,0]			
2	c	$\bar{4}'m2'$	0,1/2,1/4 [0,0,0]			
2	b	$\bar{4}m2$	0,0,1/2 [0,0,0]			
2	a	$\bar{4}m2$	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $p_p\bar{4}m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,1/2,z

Along [1,0,0]  $c1m11'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

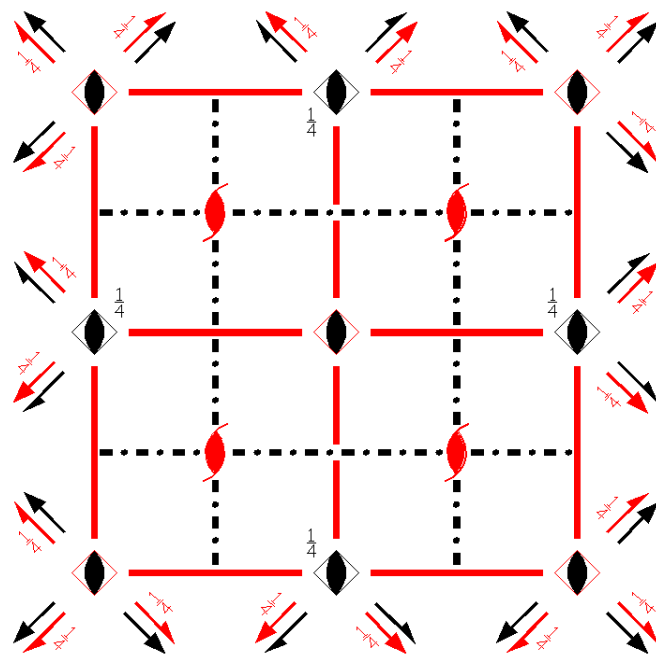
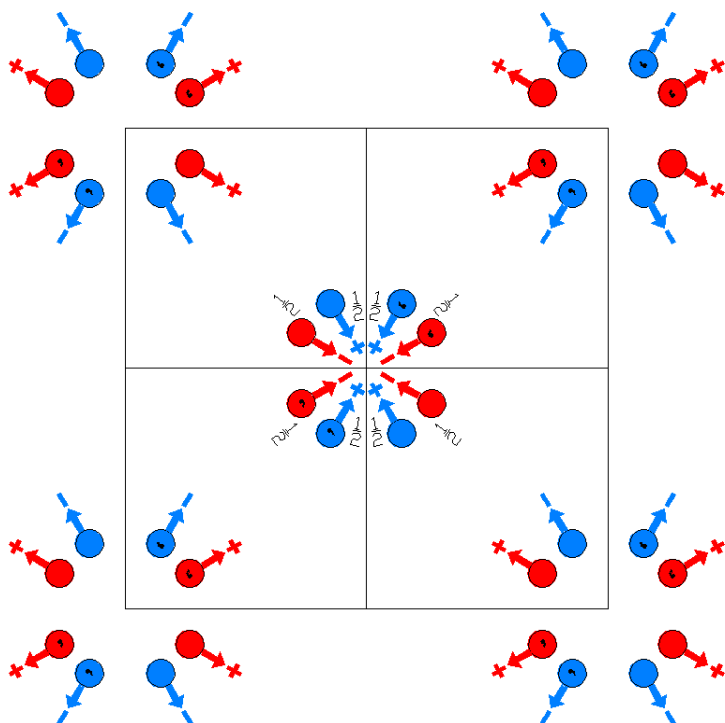
Along [1,1,0]  $p_{2a}\bar{2}m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$I_p\bar{4}'m'2$   
119.7.977

$\bar{4}m21'$   
 $I_p\bar{4}'m'2$

Tetragonal



Origin on  $\bar{4}'m'2$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'             |
| (5) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (6) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                  | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0) |

For (1/2,1/2,1/2)' + set

- |  |  |   |  |
|--|--|---|--|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'                   | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2) | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2)                |
| (5) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (6) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)   | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'       | (8) 2' x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates									
			(0,0,0) +	(1/2,1/2,1/2)' +						
16	j	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(5) x, $\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(6) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	i	.m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	0, $\bar{x},\bar{z}$ [0, $\bar{u},\bar{w}$ ]	0,x, $\bar{z}$ [0,u, $\bar{w}$ ]				
8	h	..2'	x,x+1/2,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},w$ ]	x+1/2, $\bar{x},3/4$ [u,u, $\bar{w}$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]				
8	g	..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},0$ [u, $\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]				
4	f	2m'm'	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]						
4	e	2m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]						
2	d	$\bar{4}m'2'$	0,1/2,3/4 [0,0,w]							
2	c	$\bar{4}m'2'$	0,1/2,1/4 [0,0,w]							
2	b	$\bar{4}'m'2$	0,0,1/2 [0,0,0]							
2	a	$\bar{4}'m'2$	0,0,0 [0,0,0]							

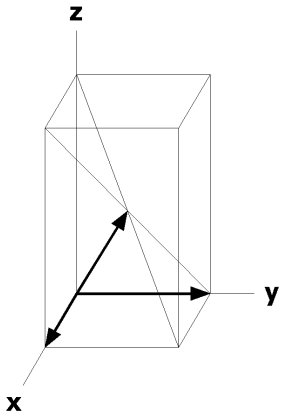
**Symmetry of Special Projections**

Along [0,0,1]  $p_p \cdot 4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 1m'1$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0

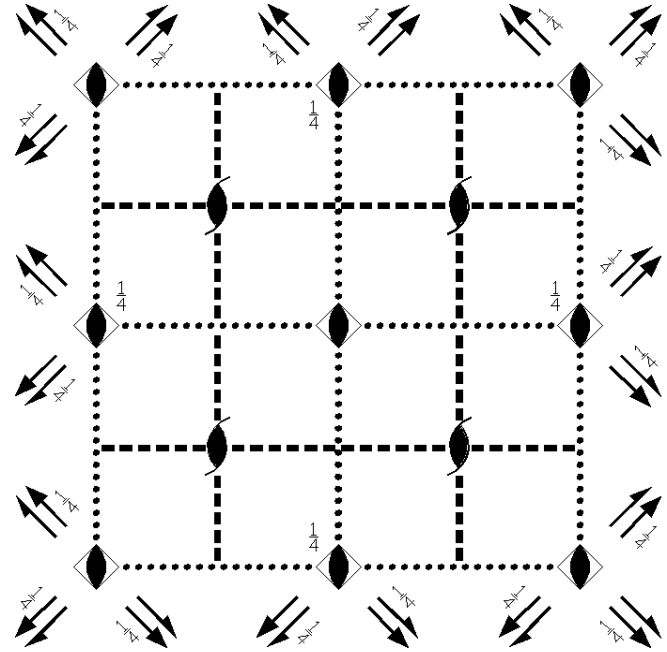
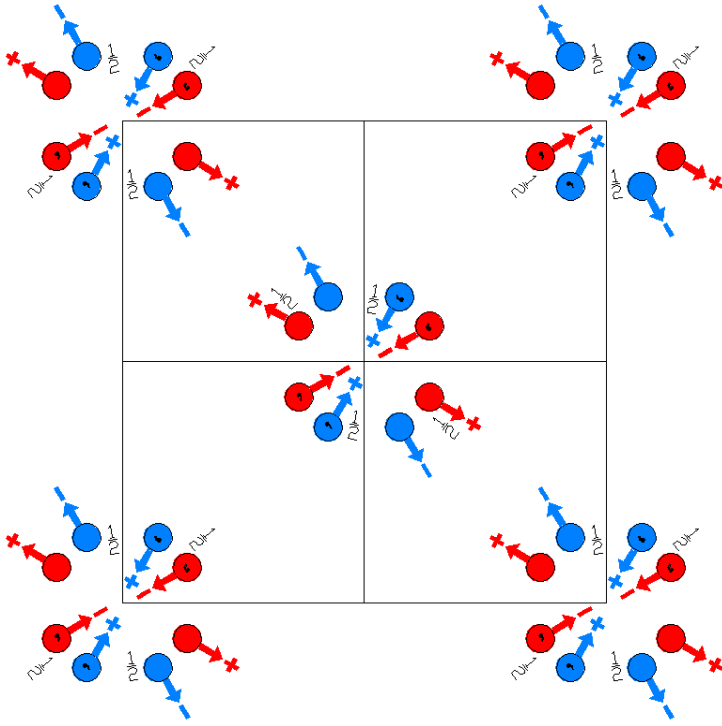




$\bar{4}c2$   
120.1.978

$\bar{4}m2$   
 $\bar{4}c2$

Tetragonal



Origin on  $\bar{4}c2_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)             | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)           | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub>-xy</sub>  0,0,1/2)     |

For (1/2,1/2,1/2) + set

- |  |  |   |  |
|--|--|---|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                 | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2) | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2) |
| (5) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (6) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)     | (7) 2 (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)           | (8) 2 x, $\bar{x}$ +1/2,0<br>(2 <sub>-xy</sub>  1/2,1/2,0)             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

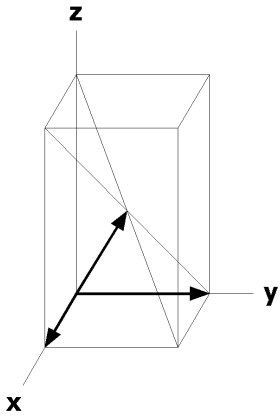
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
16	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]
			(5) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	h	..2	x,x+1/2,0 [u,u,0]	$\bar{x},\bar{x}+1/2,0$ [ $\bar{u},\bar{u},0$ ]	x+1/2, $\bar{x},0$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,x,0$ [ $u,\bar{u},0$ ]
8	g	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
8	f	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
8	e	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},3/4$ [ $\bar{u},u,0$ ]	$\bar{x},x,3/4$ [ $u,\bar{u},0$ ]
4	d	2.22	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
4	c	$\bar{4}..$	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0, $\bar{w}$ ]		
4	b	$\bar{4}..$	0,1/2,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		
4	a	2.22	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4'm'm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b}1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$\bar{4}c21'$

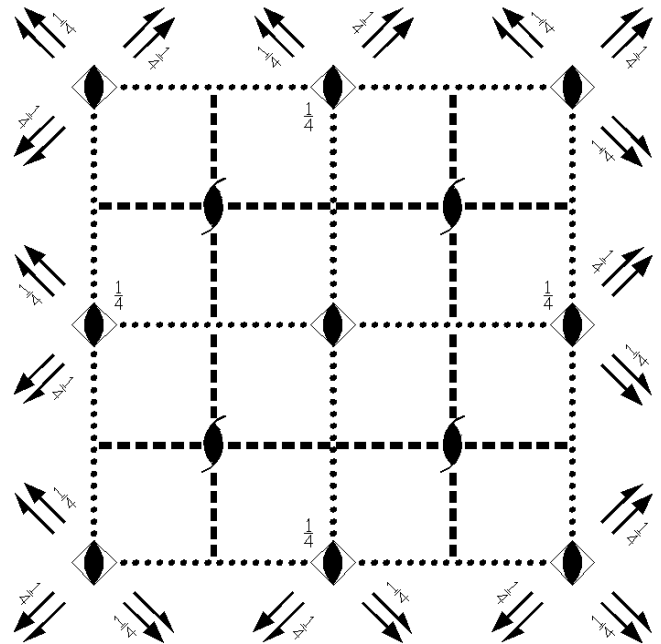
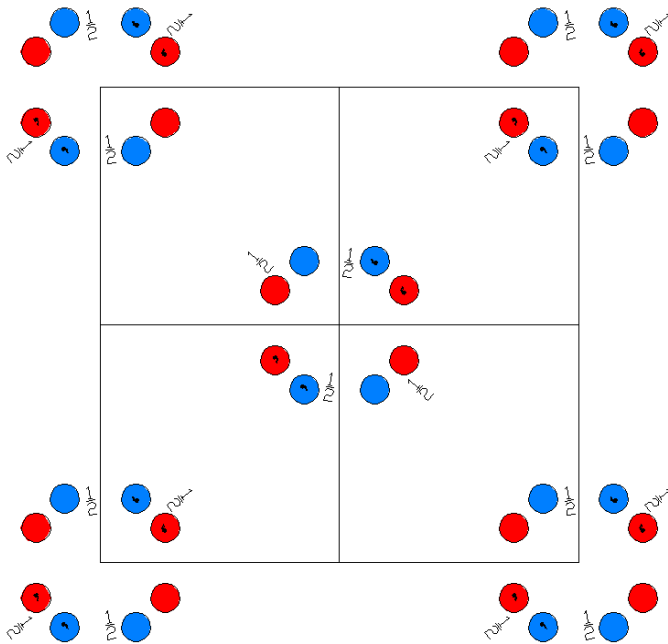
120.2.979

$\bar{4}m21'$

$\bar{4}c21'$

Tetragonal

1'



Origin on  $\bar{4}c2,1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)             | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)               |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)           | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2) |

For (1/2,1/2,1/2) + set

- |  |  |   |  |
|--|--|---|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                 | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2) | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2)       |
| (5) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (6) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)     | (7) 2 (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)           | (8) 2 x, $\bar{x}$ +1/2,0<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,0) |

## For (0,0,0)' + set

(1) $1'$ (1 0,0,0)'	(2) $2'$ 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'	(4) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z^{-1}$  0,0,0)'
(5) $c'$ (0,0,1/2) x,0,z (m <sub>y</sub>  0,0,1/2)'	(6) $c'$ (0,0,1/2) 0,y,z (m <sub>x</sub>  0,0,1/2)'	(7) $2'$ x,x,1/4 (2 <sub>xy</sub>  0,0,1/2)'	(8) $2'$ x, $\bar{x}$ ,1/4 (2 <sub>xy</sub>  0,0,1/2)'

## For (1/2,1/2,1/2)' + set

(1) $t'$ (1/2,1/2,1/2) (1 1/2,1/2,1/2)'	(2) $2'$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>  1/2,1/2,1/2)'	(3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$  1/2,1/2,1/2)'	(4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$  1/2,1/2,1/2)'
(5) $a'$ (1/2,0,0) x,1/4,z (m <sub>y</sub>  1/2,1/2,0)'	(6) $b'$ (0,1/2,0) 1/4,y,z (m <sub>x</sub>  1/2,1/2,0)'	(7) $2'$ (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>  1/2,1/2,0)'	(8) $2'$ x, $\bar{x}$ +1/2,0 (2 <sub>xy</sub>  1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

**Positions**

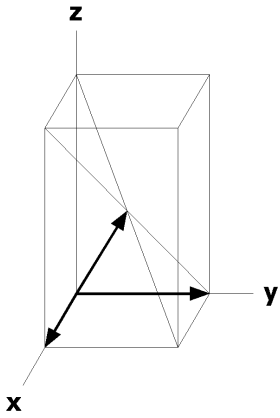
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
		(0,0,0) + (0,0,0)' +	(1/2,1/2,1/2) + (1/2,1/2,1/2)' +					
16 i 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) y, $\bar{x},\bar{z}$ [0,0,0]	(4) $\bar{y},x,\bar{z}$ [0,0,0]	(5) x, $\bar{y},z+1/2$ [0,0,0]	(6) $\bar{x},y,z+1/2$ [0,0,0]	(7) y,x, $\bar{z}+1/2$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [0,0,0]
8 h ..21'	x,x+1/2,0 [0,0,0]	$\bar{x},\bar{x}+1/2,0$ [0,0,0]	x+1/2, $\bar{x},0$ [0,0,0]	$\bar{x}+1/2,x,0$ [0,0,0]				
8 g 2..1'	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]				
8 f 2..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]				
8 e ..21'	x,x,1/4 [0,0,0]	$\bar{x},\bar{x},1/4$ [0,0,0]	x, $\bar{x},3/4$ [0,0,0]	$\bar{x},x,3/4$ [0,0,0]				
4 d 2.221'	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]						
4 c $\bar{4}..1'$	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]						
4 b $\bar{4}..1'$	0,1/2,0 [0,0,0]	0,0,1/2 [0,0,0]						
4 a 2.221'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]						

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

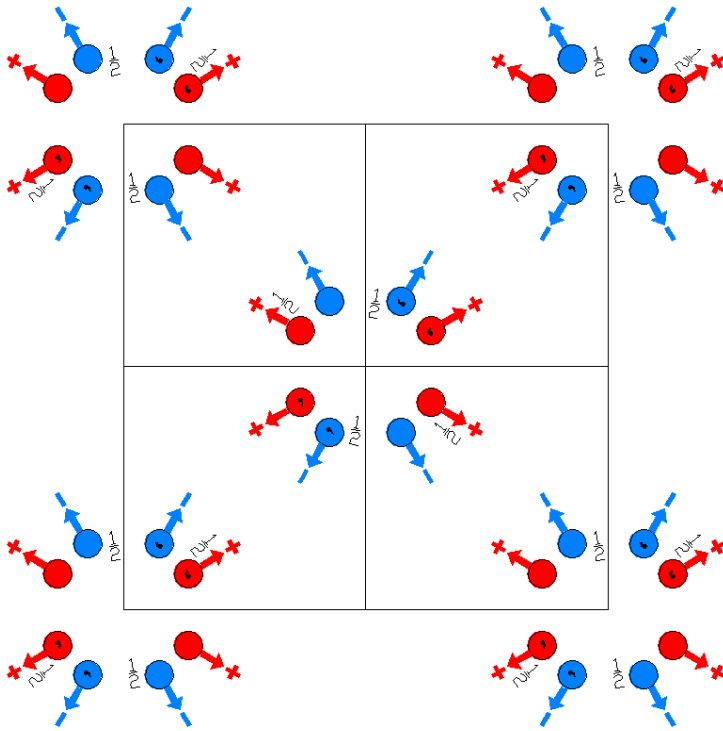
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$\bar{4}^+c'2$   
120.3.980

$\bar{4}^+m'2$   
 $\bar{4}^+c'2$

Tetragonal



Origin on  $\bar{4}^+c'2_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

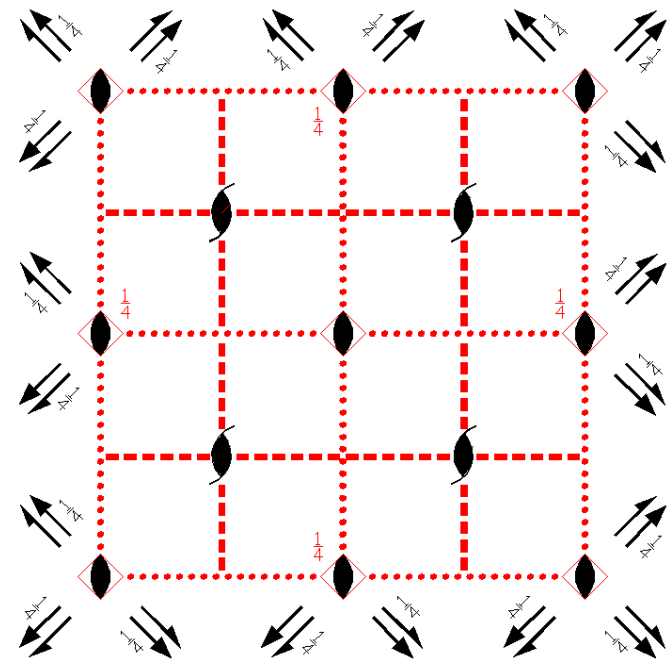
### Symmetry Operations

For (0,0,0) + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                                   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)               | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)' |
| (5) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)            | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub>xy</sub>  0,0,1/2)       |

For (1/2,1/2,1/2) + set

- |  |  |  |   |
|--|--|--|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                   | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2)' | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2)' |
| (5) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (6) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)'   | (7) 2 (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)            | (8) 2 x, $\bar{x}$ +1/2,0<br>(2 <sub>xy</sub>  1/2,1/2,0)               |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

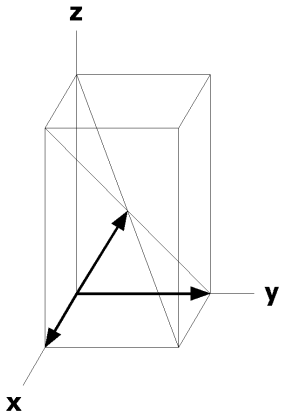
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
16	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
			(5) x, $\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(6) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]	(7) y,x, $\bar{z}+1/2$ [v,u, $\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	h	..2	x,x+1/2,0 [u,u,0]	$\bar{x},\bar{x}+1/2,0$ [ $\bar{u},\bar{u},0$ ]	x+1/2, $\bar{x},0$ [u, $\bar{u},0$ ]	$\bar{x}+1/2,x,0$ [ $\bar{u},u,0$ ]
8	g	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
8	f	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
8	e	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},3/4$ [u, $\bar{u},0$ ]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]
4	d	2.22	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
4	c	$\bar{4}'..$	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]		
4	b	$\bar{4}'..$	0,1/2,0 [0,0,0]	0,0,1/2 [0,0,0]		
4	a	2.22	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

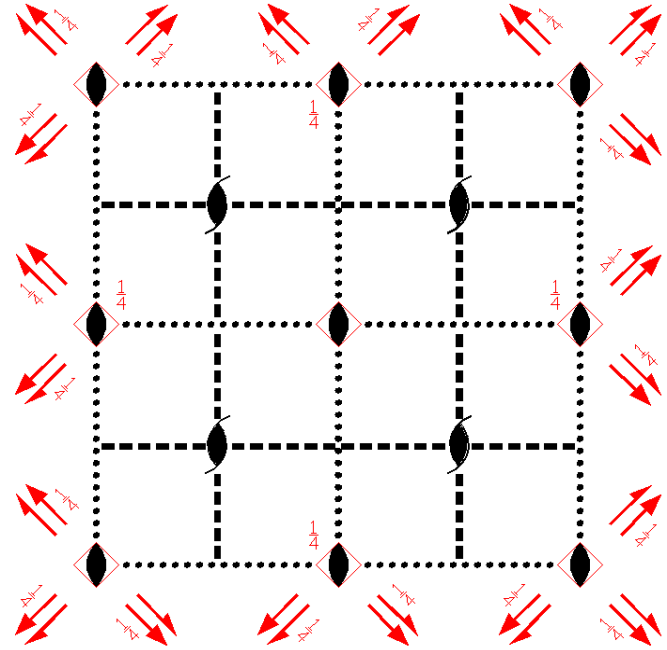
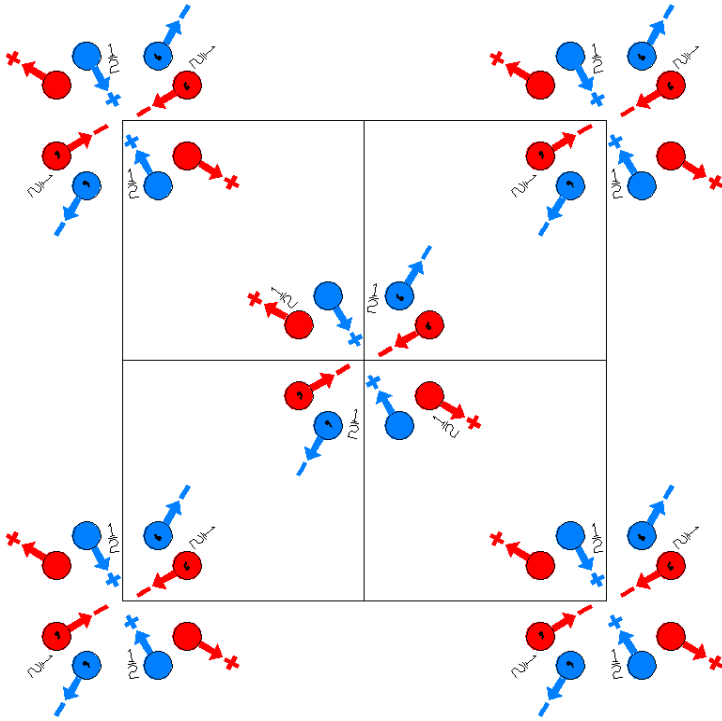
Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$\bar{4}'c_2'$   
120.4.981

$\bar{4}'m_2'$   
 $\bar{4}'c_2'$

Tetragonal



Origin on  $\bar{4}'c_2'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)             | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)' |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'          | (8) 2' x, $\bar{x}$ ,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'     |

For (1/2,1/2,1/2) + set

- |  |  |  |   |
|--|--|--|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                 | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2)' | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2)' |
| (5) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (6) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)     | (7) 2' (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)'          | (8) 2' x, $\bar{x}$ +1/2,0<br>(2 <sub>xy</sub>  1/2,1/2,0)'             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
16	i	1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $y,\bar{x},\bar{z} [v,\bar{u},\bar{w}]$	(4) $\bar{y},x,\bar{z} [\bar{v},u,\bar{w}]$
			(5) $x,\bar{y},z+1/2 [\bar{u},v,\bar{w}]$	(6) $\bar{x},y,z+1/2 [u,\bar{v},\bar{w}]$	(7) $y,x,\bar{z}+1/2 [\bar{v},\bar{u},w]$	(8) $\bar{y},\bar{x},\bar{z}+1/2 [v,u,w]$
8	h	..2'	$x,x+1/2,0 [\bar{u},u,w]$	$\bar{x},\bar{x}+1/2,0 [u,\bar{u},w]$	$x+1/2,\bar{x},0 [u,u,\bar{w}]$	$\bar{x}+1/2,x,0 [\bar{u},\bar{u},\bar{w}]$
8	g	2..	$0,1/2,z [0,0,w]$	$1/2,0,\bar{z} [0,0,\bar{w}]$	$0,1/2,z+1/2 [0,0,\bar{w}]$	$1/2,0,\bar{z}+1/2 [0,0,w]$
8	f	2..	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,\bar{w}]$	$0,0,z+1/2 [0,0,\bar{w}]$	$0,0,\bar{z}+1/2 [0,0,w]$
8	e	..2'	$x,x,1/4 [\bar{u},u,w]$	$\bar{x},\bar{x},1/4 [u,\bar{u},w]$	$x,\bar{x},3/4 [u,u,\bar{w}]$	$\bar{x},x,3/4 [\bar{u},\bar{u},\bar{w}]$
4	d	2.2'2'	$0,1/2,0 [0,0,w]$	$1/2,0,0 [0,0,\bar{w}]$		
4	c	$\bar{4}'..$	$0,1/2,1/4 [0,0,0]$	$0,1/2,3/4 [0,0,0]$		
4	b	$\bar{4}'..$	$0,1/2,0 [0,0,0]$	$0,0,1/2 [0,0,0]$		
4	a	2.2'2'	$0,0,1/4 [0,0,w]$	$0,0,3/4 [0,0,\bar{w}]$		

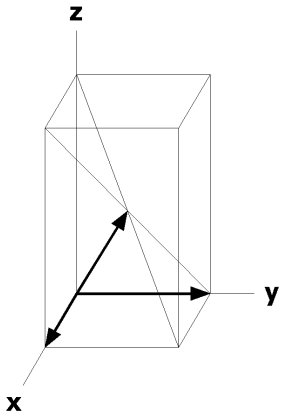
**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2b}1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$

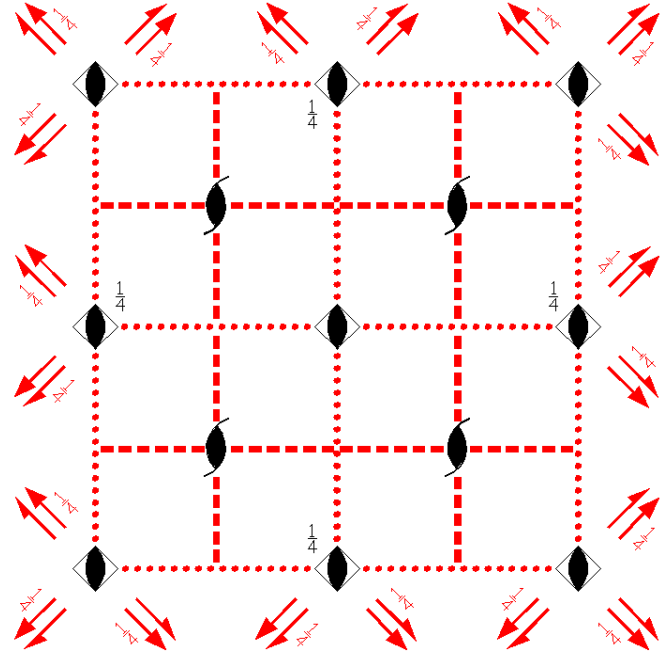
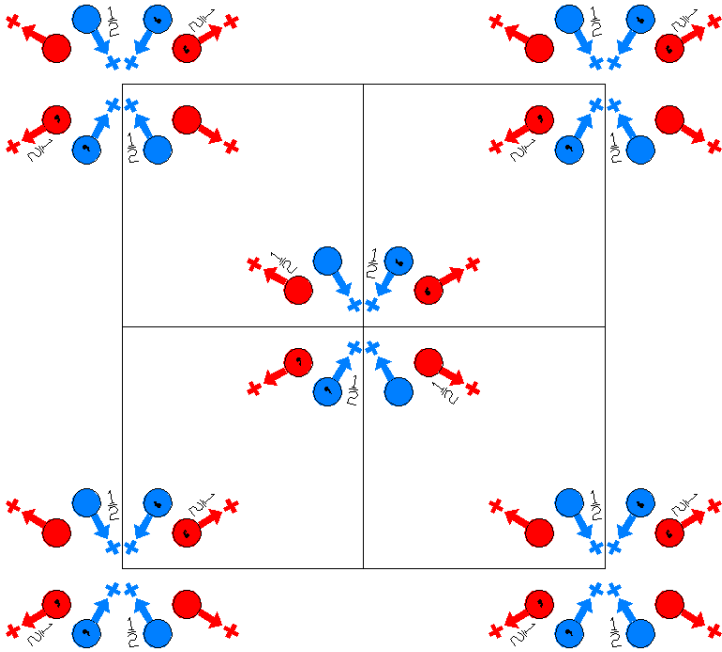




$\bar{4}c'2'$   
120.5.982

$\bar{4}m'2'$   
 $\bar{4}c'2'$

Tetragonal



Origin on  $\bar{4}c'2'_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1   0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0)               | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$   0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$   0,0,0) |
| (5) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>   0,0,1/2)' | (6) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>   0,0,1/2)' | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>   0,0,1/2)'         | (8) 2' x, $\bar{x}$ ,1/4<br>(2 <sub>-xy</sub>   0,0,1/2)'   |

For (1/2,1/2,1/2) + set

- |   |   |  |   |
|---|---|--|---|
| (1) t (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)                  | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2) | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$   1/2,1/2,1/2) | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$   1/2,1/2,1/2) |
| (5) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0)' | (6) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)'   | (7) 2' (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>   1/2,1/2,0)'         | (8) 2' x, $\bar{x}$ +1/2,0<br>(2 <sub>-xy</sub>   1/2,1/2,0)'           |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

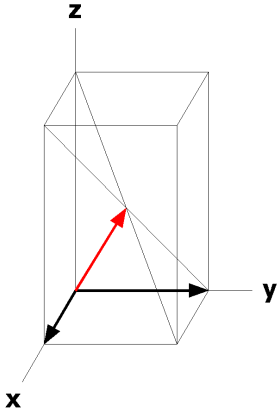
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(1/2,1/2,1/2) +			
16	i	1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $y,\bar{x},\bar{z} [\bar{v},u,w]$	(4) $\bar{y},x,\bar{z} [v,\bar{u},w]$		
			(5) $x,\bar{y},z+1/2 [u,\bar{v},w]$	(6) $\bar{x},y,z+1/2 [\bar{u},v,w]$	(7) $y,x,\bar{z}+1/2 [\bar{v},\bar{u},w]$	(8) $\bar{y},\bar{x},\bar{z}+1/2 [v,u,w]$		
8	h	..2'	$x,x+1/2,0 [\bar{u},u,w]$	$\bar{x},\bar{x}+1/2,0 [u,\bar{u},w]$	$x+1/2,\bar{x},0 [\bar{u},\bar{u},w]$	$\bar{x}+1/2,x,0 [u,u,w]$		
8	g	2..	$0,1/2,z [0,0,w]$	$1/2,0,\bar{z} [0,0,w]$	$0,1/2,z+1/2 [0,0,w]$	$1/2,0,\bar{z}+1/2 [0,0,w]$		
8	f	2..	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,w]$	$0,0,z+1/2 [0,0,w]$	$0,0,\bar{z}+1/2 [0,0,w]$		
8	e	..2'	$x,x,1/4 [\bar{u},u,w]$	$\bar{x},\bar{x},1/4 [u,\bar{u},w]$	$x,\bar{x},3/4 [\bar{u},\bar{u},w]$	$\bar{x},x,3/4 [u,u,w]$		
4	d	2.2'2'	$0,1/2,0 [0,0,w]$	$1/2,0,0 [0,0,w]$				
4	c	$\bar{4}..$	$0,1/2,1/4 [0,0,w]$	$0,1/2,3/4 [0,0,w]$				
4	b	$\bar{4}..$	$0,1/2,0 [0,0,w]$	$0,0,1/2 [0,0,w]$				
4	a	2.2'2'	$0,0,1/4 [0,0,w]$	$0,0,3/4 [0,0,w]$				

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4'mm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,0,0$

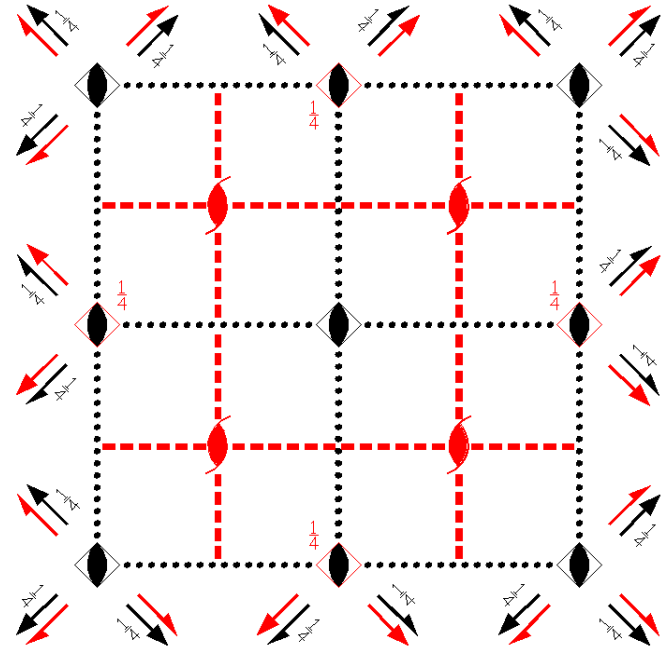
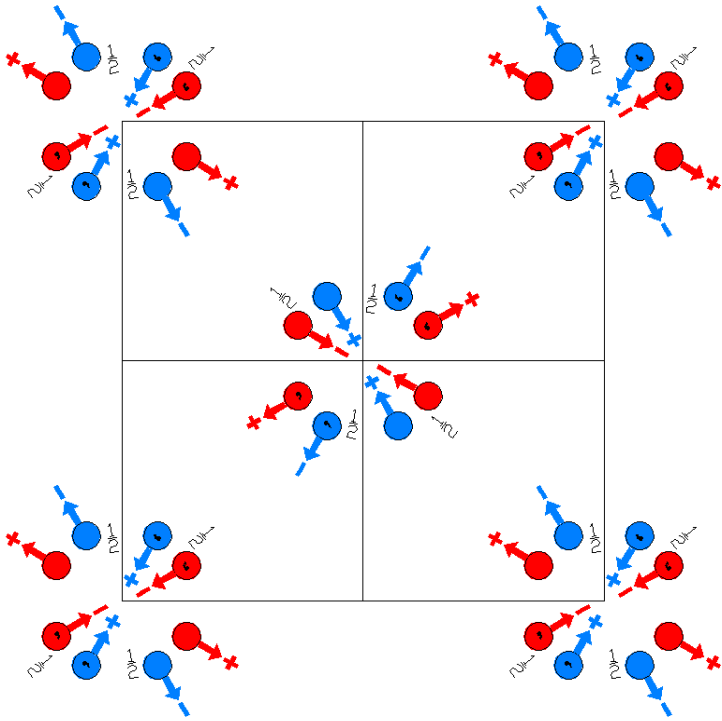
Along  $[1,1,0]$   $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,0$



$I_p \bar{4}c2$   
120.6.983

$\bar{4}m21'$   
 $I_p \bar{4}c2$

Tetragonal



Origin on  $\bar{4}c2_1$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)             | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)           | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub>-xy</sub>  0,0,1/2)     |

For (1/2,1/2,1/2)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'                 | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2)' | (4) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2)' |
| (5) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (6) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)'     | (7) 2' (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)'            | (8) 2' x, $\bar{x}$ +1/2,0<br>(2 <sub>-xy</sub>  1/2,1/2,0)'              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

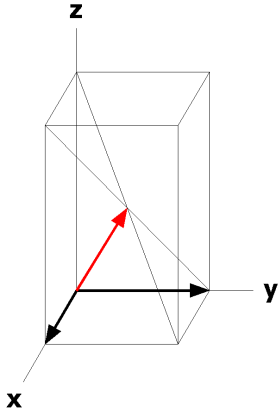
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2)' +		
16	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]
			(5) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	h	..2'	x,x+1/2,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,0$ [ $u,\bar{u},w$ ]	x+1/2, $\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,0$ [ $u,u,w$ ]
8	g	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
8	f	2..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
8	e	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},3/4$ [ $\bar{u},u,0$ ]	$\bar{x},x,3/4$ [ $u,\bar{u},0$ ]
4	d	2.2'2'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]		
4	c	$\bar{4}'..$	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]		
4	b	$\bar{4}..$	0,1/2,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		
4	a	2.22	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_p\bar{4}mm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,1/2,z

Along [1,0,0]  $p_{2b}\bar{1}m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0]  $p_{2a}\bar{2}m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



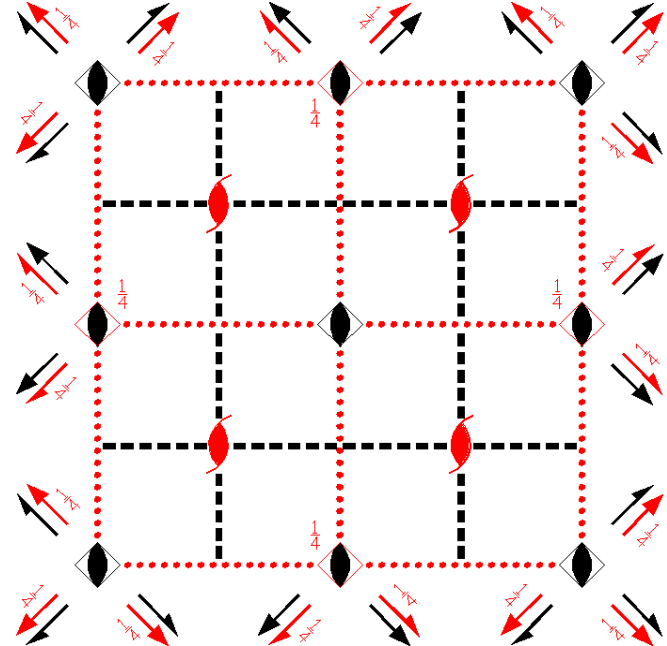
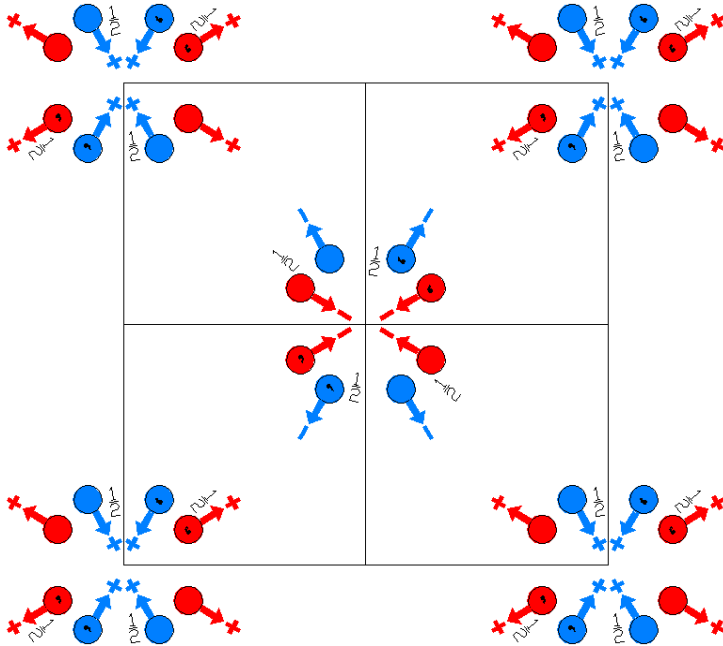
$I_p \bar{4}c'2'$

120.7.984

$\bar{4}m21'$

$I_p \bar{4}c'2'$

Tetragonal



Origin on  $\bar{4}c'2_1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                                   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)               | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'         | (8) 2' x, $\bar{x}$ ,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'    |

For (1/2,1/2,1/2)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'               | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2)' | (4) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2)' |
| (5) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (6) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)       | (7) 2 (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)              | (8) 2 x, $\bar{x}$ +1/2,0<br>(2 <sub>xy</sub>  1/2,1/2,0)                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

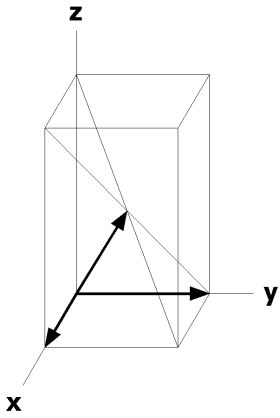
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2)' +		
16	i	1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $y,\bar{x},\bar{z} [\bar{v},u,w]$	(4) $\bar{y},x,\bar{z} [v,\bar{u},w]$
			(5) $x,\bar{y},z+1/2 [u,\bar{v},w]$	(6) $\bar{x},y,z+1/2 [\bar{u},v,w]$	(7) $y,x,\bar{z}+1/2 [\bar{v},\bar{u},w]$	(8) $\bar{y},\bar{x},\bar{z}+1/2 [v,u,w]$
8	h	..2	$x,x+1/2,0 [u,u,0]$	$\bar{x},\bar{x}+1/2,0 [\bar{u},\bar{u},0]$	$x+1/2,\bar{x},0 [\bar{u},u,0]$	$\bar{x}+1/2,x,0 [u,\bar{u},0]$
8	g	2..	$0,1/2,z [0,0,w]$	$1/2,0,\bar{z} [0,0,w]$	$0,1/2,z+1/2 [0,0,w]$	$1/2,0,\bar{z}+1/2 [0,0,w]$
8	f	2..	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,w]$	$0,0,z+1/2 [0,0,w]$	$0,0,\bar{z}+1/2 [0,0,w]$
8	e	..2'	$x,x,1/4 [\bar{u},u,w]$	$\bar{x},\bar{x},1/4 [u,\bar{u},w]$	$x,\bar{x},3/4 [\bar{u},\bar{u},w]$	$\bar{x},x,3/4 [u,u,w]$
4	d	2.22	$0,1/2,0 [0,0,0]$	$1/2,0,0 [0,0,0]$		
4	c	$\bar{4}'..$	$0,1/2,1/4 [0,0,0]$	$0,1/2,3/4 [0,0,0]$		
4	b	$\bar{4}..$	$0,1/2,0 [0,0,w]$	$0,0,1/2 [0,0,w]$		
4	a	2.2'2'	$0,0,1/4 [0,0,w]$	$0,0,3/4 [0,0,w]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_p\bar{4}m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,1/2,z$

Along  $[1,0,0]$   $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,0,0$

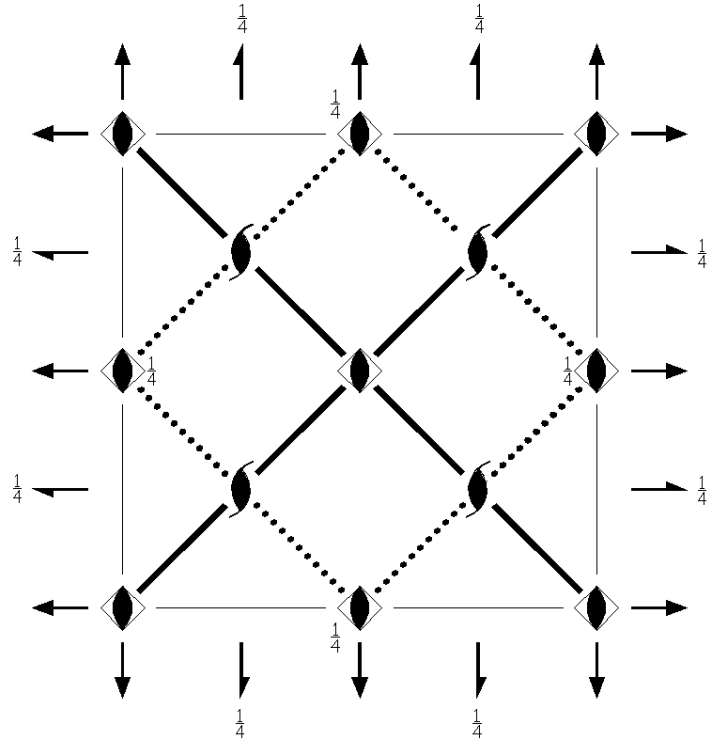
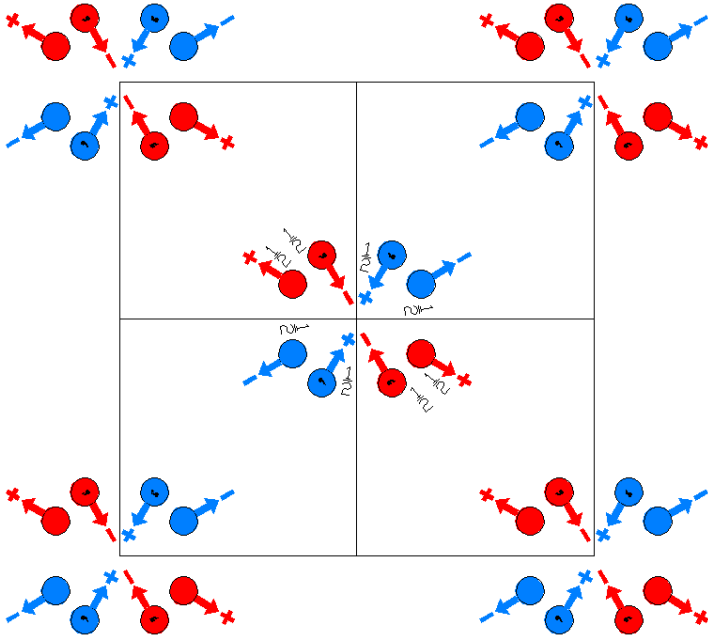
Along  $[1,1,0]$   $p_{2a}\bar{2}m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,0$



$\bar{4}2m$   
121.1.985

$\bar{4}2m$   
 $\bar{4}2m$

Tetragonal



Origin on  $\bar{4}2m$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$ ;  $x \leq y$

### Symmetry Operations

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) m x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)     | (8) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                    |

For (1/2,1/2,1/2) + set

- |  |  |   |  |
|--|--|---|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                     | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2)     | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2) |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) | (7) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (8) n (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)            |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
16	j	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(3) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ] (7) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [v, $\bar{u},w$ ] (8) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
8	i	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [u, $\bar{u},0$ ]	x, $\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,\bar{z}$ [u,u,0]
8	h	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0,z [0,0, $\bar{w}$ ]
8	g	.2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0, $\bar{x},1/2$ [0,u,0]	0,x,1/2 [0, $\bar{u},0$ ]
8	f	.2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0, $\bar{x},0$ [0,u,0]	0,x,0 [0, $\bar{u},0$ ]
4	e	2.mm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4	d	$\bar{4}..$	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0, $\bar{w}$ ]		
4	c	222.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
2	b	$\bar{4}2m$	0,0,1/2 [0,0,0]			
2	a	$\bar{4}2m$	0,0,0 [0,0,0]			

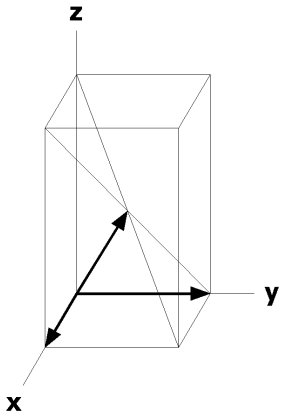
**Symmetry of Special Projections**

Along [0,0,1]  $p4'm'm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0





$\bar{4}2m1'$

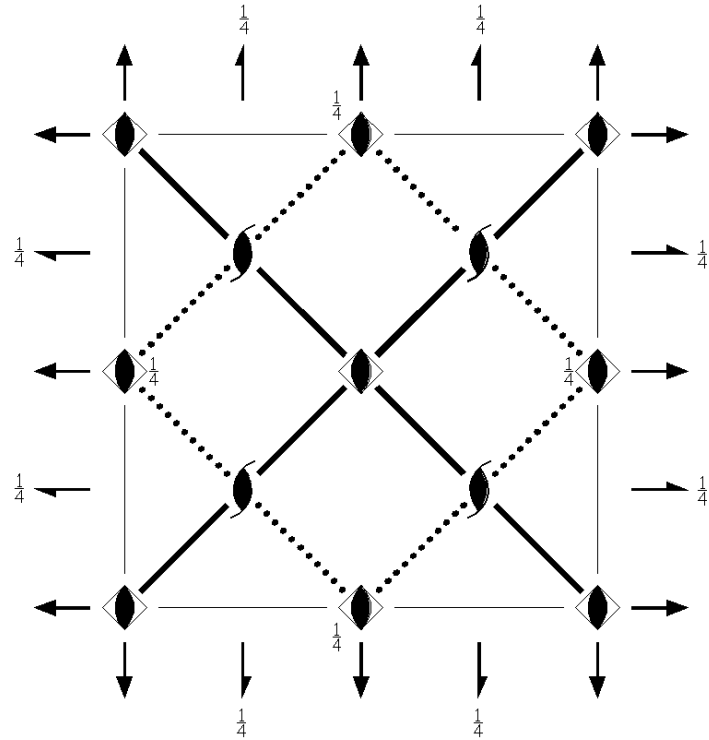
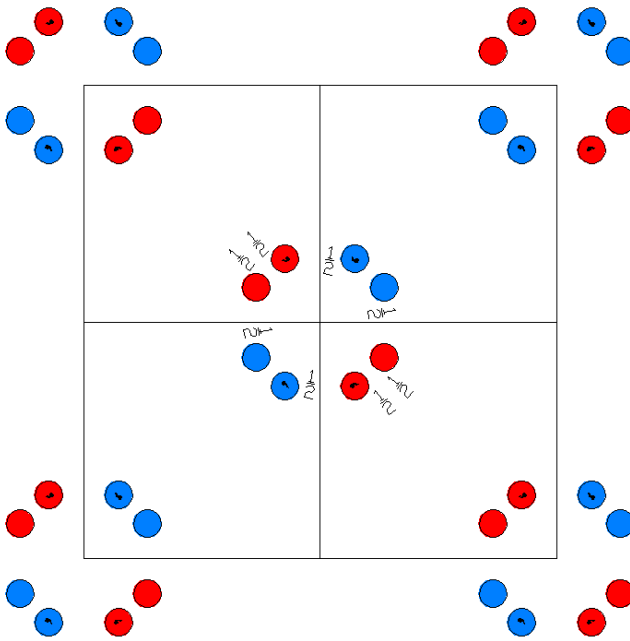
121.2.986

$\bar{4}2m1'$

$\bar{4}2m1'$

Tetragonal

1'



Origin on  $\bar{4}2m1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

Symmetry Operations

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) m x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)     | (8) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                    |

For (1/2,1/2,1/2) + set

- |  |  |   |  |
|--|--|---|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                     | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2)     | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2) |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) | (7) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (8) n (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)            |

## For (0,0,0)' + set

(1) $1'$ (1 0,0,0)'	(2) $2'$ 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'	(4) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z^{-1}$  0,0,0)'
(5) $2'$ 0,y,0 (2 <sub>y</sub>  0,0,0)'	(6) $2'$ x,0,0 (2 <sub>x</sub>  0,0,0)'	(7) $m'$ x, $\bar{x}$ ,z ( $m_{xy}$  0,0,0)'	(8) $m'$ x,x,z ( $m_{\bar{xy}}$  0,0,0)'

## For (1/2,1/2,1/2)' + set

(1) $t'$ (1/2,1/2,1/2) (1 1/2,1/2,1/2)'	(2) $2'$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>  1/2,1/2,1/2)'	(3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$  1/2,1/2,1/2)'	(4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$  1/2,1/2,1/2)'
(5) $2'$ (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>  1/2,1/2,1/2)'	(6) $2'$ (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>  1/2,1/2,1/2)'	(7) $c'$ (0,0,1/2) x+1/2, $\bar{x}$ ,z ( $m_{xy}$  1/2,1/2,1/2)'	(8) $n'$ (1/2,1/2,1/2) x,x,z ( $m_{\bar{xy}}$  1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

**Positions**

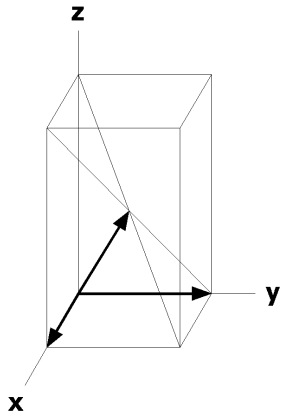
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) + (0,0,0)'			(1/2,1/2,1/2) + (1/2,1/2,1/2)'		
16 j 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) y, $\bar{x},\bar{z}$ [0,0,0]	(4) $\bar{y},x,\bar{z}$ [0,0,0]	(5) $\bar{x},y,\bar{z}$ [0,0,0]	(6) x, $\bar{y},\bar{z}$ [0,0,0]	(7) $\bar{y},\bar{x},z$ [0,0,0]	(8) y,x,z [0,0,0]
8 i ..m1'	x,x,z [0,0,0]	$\bar{x},\bar{x},z$ [0,0,0]	x, $\bar{x},\bar{z}$ [0,0,0]	$\bar{x},x,\bar{z}$ [0,0,0]				
8 h 2..1'	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0,z [0,0,0]				
8 g .2.1'	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]	0, $\bar{x},1/2$ [0,0,0]	0,x,1/2 [0,0,0]				
8 f .2.1'	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0, $\bar{x},0$ [0,0,0]	0,x,0 [0,0,0]				
4 e 2.mm1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]						
4 d $\bar{4}..1'$	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]						
4 c 222.1'	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]						
2 b $\bar{4}2m1'$	0,0,1/2 [0,0,0]							
2 a $\bar{4}2m1'$	0,0,0 [0,0,0]							

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

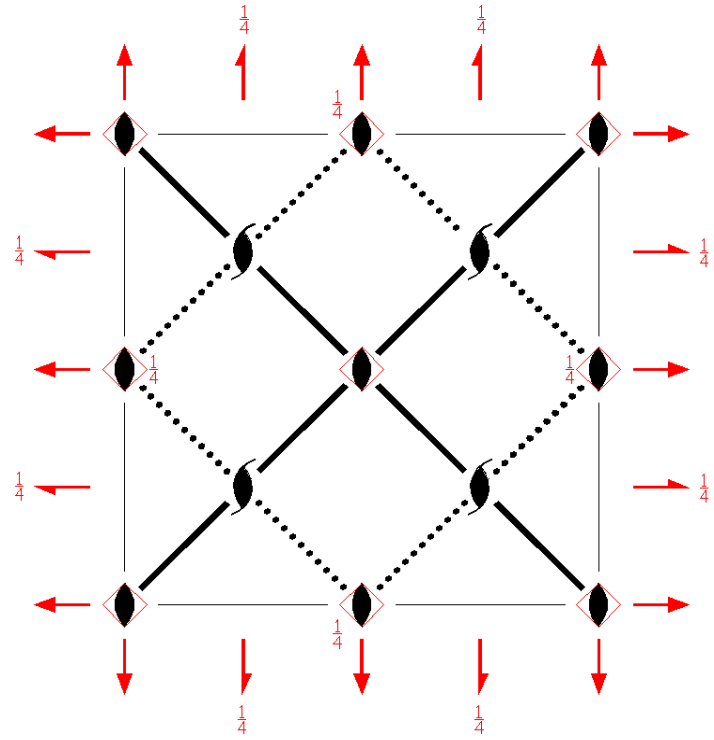
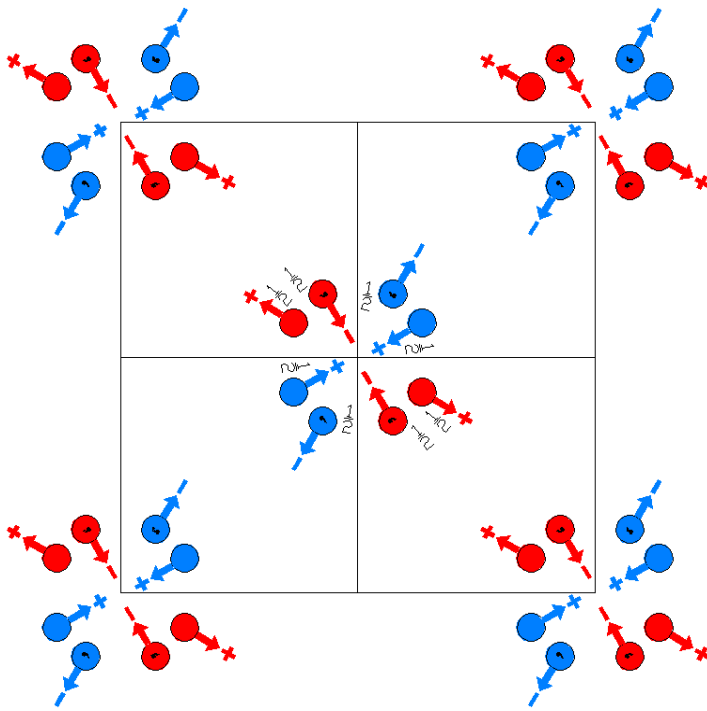
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$\bar{4}'2'm$   
121.3.987

$\bar{4}'2'm$   
 $\bar{4}'2'm$

Tetragonal



Origin on  $\bar{4}'2'm$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$ ;  $x \leq y$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)' |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' | (7) m x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)        | (8) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                  |

For (1/2,1/2,1/2) + set

- |  |  |   |  |
|--|--|---|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                       | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)   | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2)'  | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2)' |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' | (7) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (8) n (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

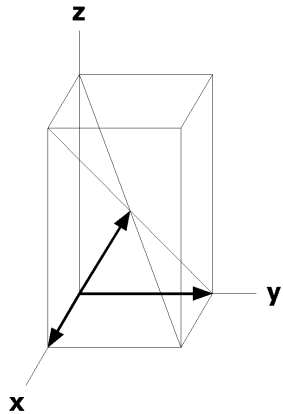
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
16	j	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x,y,z [ $\bar{u},\bar{v},w$ ]	(3) y,x,z [v,u,w] (7) $\bar{y},\bar{x},z$ [v,u,w]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ] (8) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
8	i	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [u,u,0]	x,x,z [u,u,0]	$\bar{x},x,\bar{z}$ [ $\bar{u},\bar{u},0$ ]
8	h	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]
8	g	.2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0,v,w]	0,x,1/2 [v,0,w]	0,x,1/2 [ $\bar{v},0,\bar{w}$ ]
8	f	.2'	x,0,0 [0,v,w]	$\bar{x},0,0$ [0,v,w]	0,x,0 [v,0,w]	0,x,0 [ $\bar{v},0,\bar{w}$ ]
4	e	2.mm	0,0,z [0,0,0]	0,0,z [0,0,0]		
4	d	$\bar{4}'..$	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]		
4	c	22'2'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]		
2	b	$\bar{4}'2'm$	0,0,1/2 [0,0,0]			
2	a	$\bar{4}'2'm$	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $p4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

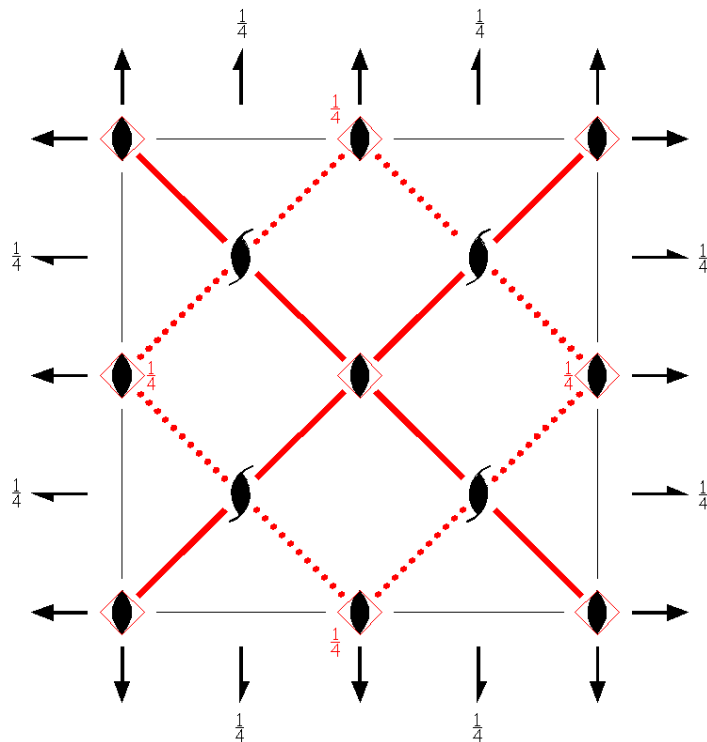
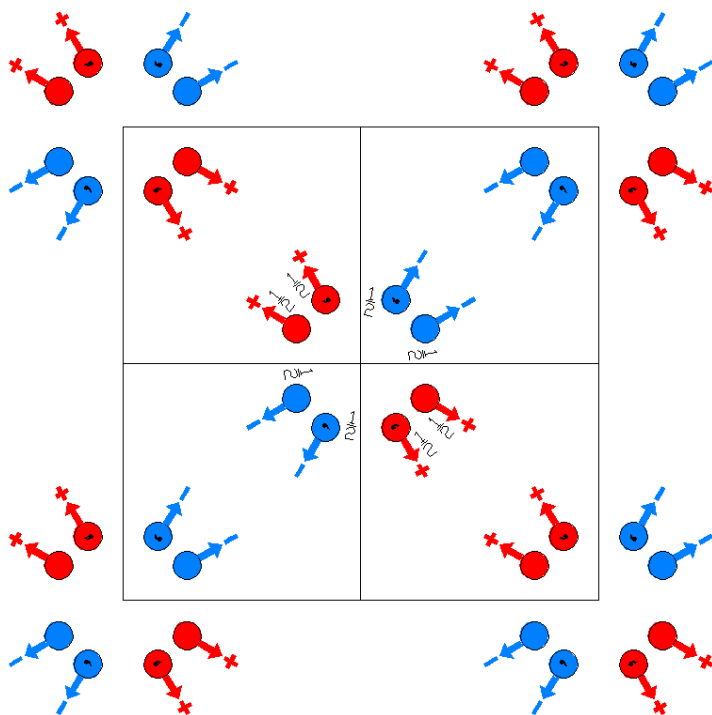
Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$\bar{4}'2m'$   
121.4.988

$\bar{4}'2m'$   
 $\bar{4}'2m'$

Tetragonal



Origin on  $\bar{4}'2m'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)' |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) m' x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)'      | (8) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                |

For (1/2,1/2,1/2) + set

- |  |  |   |  |
|--|--|---|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                     | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2)'    | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2)' |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) | (7) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)' | (8) n' (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)'        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

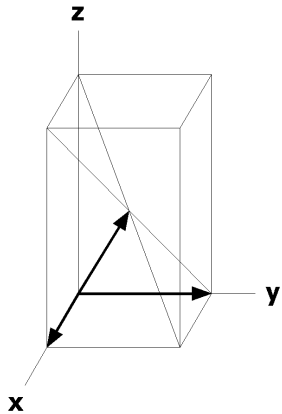
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates									
			(0,0,0) +		(1/2,1/2,1/2) +					
16	j	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(8) $y,x,z$ [ $v,u,w$ ]
8	i	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x},\bar{z}$ [ $u,\bar{u},\bar{w}$ ]	$\bar{x},x,\bar{z}$ [ $\bar{u},u,\bar{w}$ ]				
8	h	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0,z [0,0,w]				
8	g	.2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0, $\bar{x},1/2$ [0, $\bar{u},0$ ]	0,x,1/2 [0,u,0]				
8	f	.2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0, $\bar{x},0$ [0, $\bar{u},0$ ]	0,x,0 [0,u,0]				
4	e	2.m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]						
4	d	$\bar{4}'..$	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]						
4	c	222.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]						
2	b	$\bar{4}'2m'$	0,0,1/2 [0,0,0]							
2	a	$\bar{4}'2m'$	0,0,0 [0,0,0]							

**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



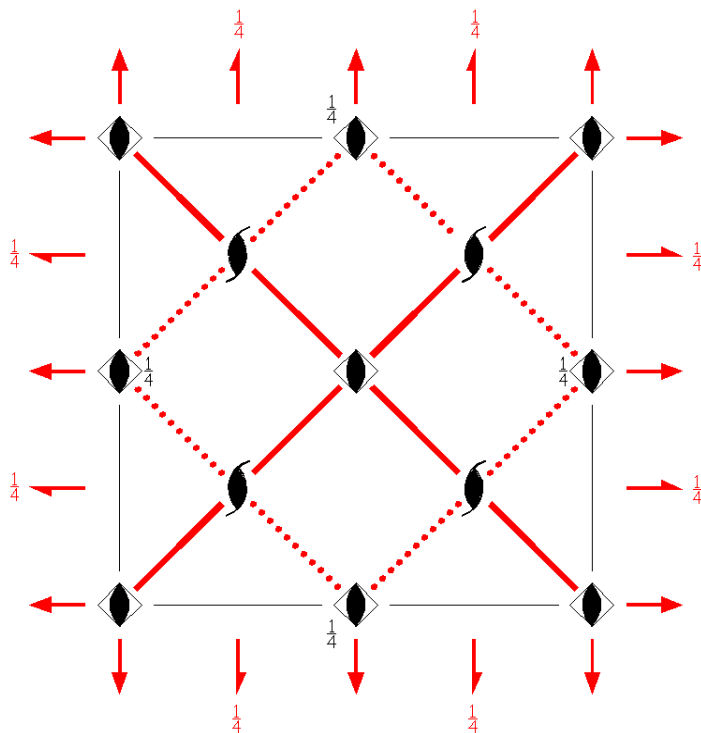
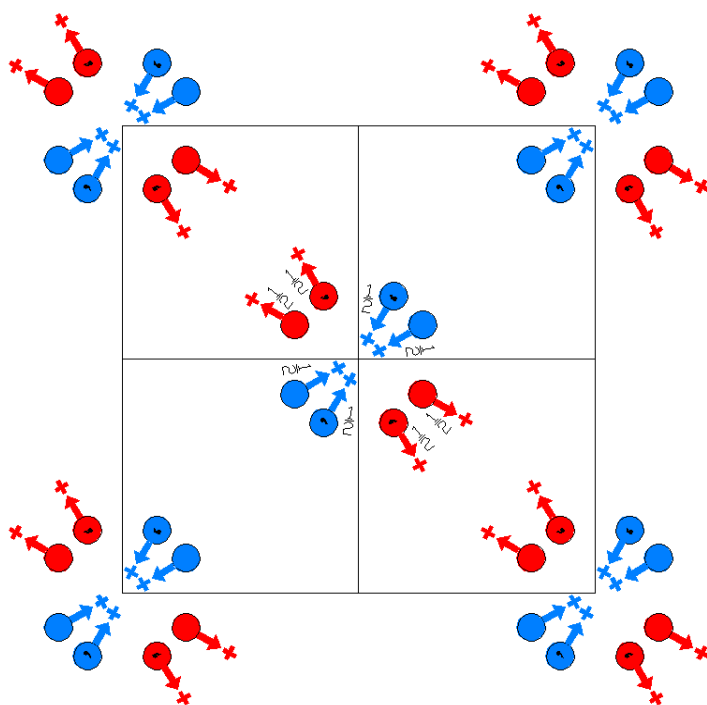
$\bar{1}42'm'$

121.5.989

$\bar{4}2'm'$

$\bar{1}42'm'$

Tetragonal



Origin on  $\bar{4}2'm'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0) |
| (5) 2' 0,y,0<br>(2 <sub>y</sub> ' 0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub> ' 0,0,0)' | (7) m' x, $\bar{x}$ ,z<br>(m <sub>xy</sub> ' 0,0,0)'    | (8) m' x,x,z<br>(m <sub>xy</sub> ' 0,0,0)'              |

For (1/2,1/2,1/2) + set

- |   |   |  |   |
|---|---|--|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                        | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)    | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2)      | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2) |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub> ' 1/2,1/2,1/2)' | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub> ' 1/2,1/2,1/2)' | (7) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub> ' 1/2,1/2,1/2)' | (8) n' (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub> ' 1/2,1/2,1/2)'      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
			(0,0,0) +		(1/2,1/2,1/2) +			
16	j	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u, $\bar{v}$ ,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v}$ ,w] (6) x, $\bar{y},\bar{z}$ [ $\bar{u},v$ ,w]	(3) y, $\bar{x},\bar{z}$ [ $\bar{v},u$ ,w] (7) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u}$ ,w]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u}$ ,w] (8) y,x,z [v,u,w]		
8	i	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u}$ ,w]	x, $\bar{x},\bar{z}$ [ $\bar{u},u$ ,w]	$\bar{x},x,\bar{z}$ [u, $\bar{u}$ ,w]		
8	h	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0,z [0,0,w]		
8	g	.2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v}$ ,w]	0, $\bar{x},1/2$ [ $\bar{v},0$ ,w]	0,x,1/2 [v,0,w]		
8	f	.2'	x,0,0 [0,v,w]	$\bar{x},0,0$ [0, $\bar{v}$ ,w]	0, $\bar{x},0$ [ $\bar{v},0$ ,w]	0,x,0 [v,0,w]		
4	e	2.m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]				
4	d	$\bar{4}..$	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0,w]				
4	c	22'2'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]				
2	b	$\bar{4}2'm'$	0,0,1/2 [0,0,w]					
2	a	$\bar{4}2'm'$	0,0,0 [0,0,w]					

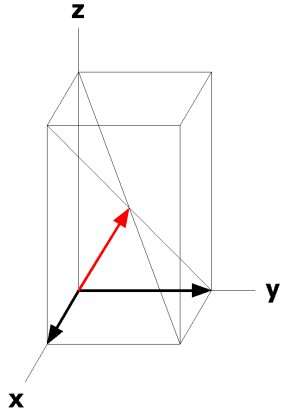
**Symmetry of Special Projections**

Along [0,0,1]  $p4'mm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0]  $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0





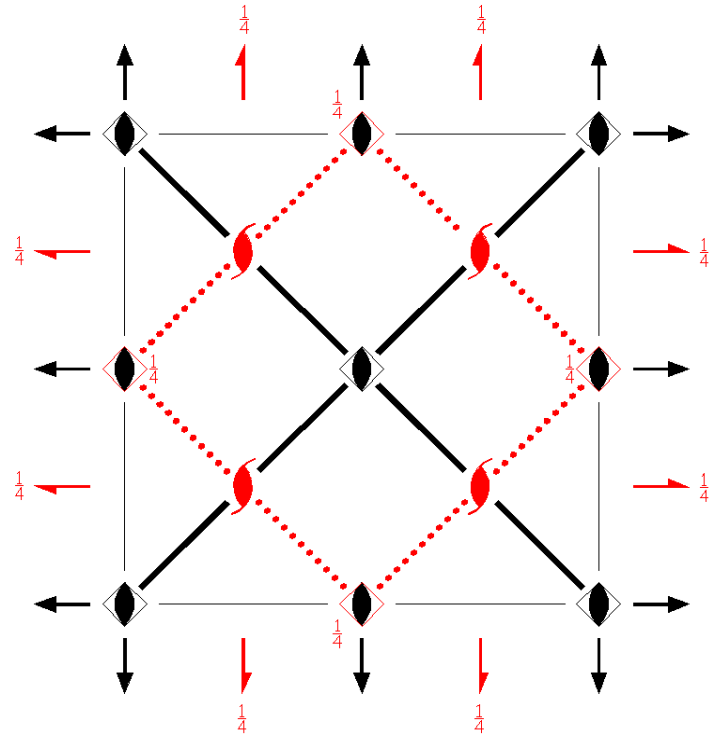
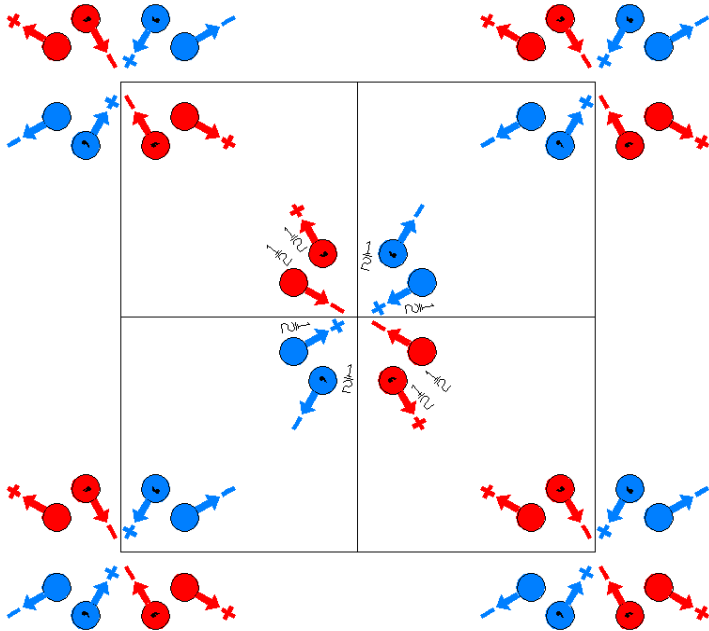
$I_p \bar{4}2m$

121.6.990

$\bar{4}2m1'$

$I_p \bar{4}2m$

Tetragonal



Origin on  $\bar{4}2m$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

Symmetry Operations

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) m x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)       | (8) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                 |

For (1/2,1/2,1/2)' + set

- |  |  |   |  |
|--|--|---|--|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'                     | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2)'  | (4) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2)' |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' | (7) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)' | (8) n' (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)'          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

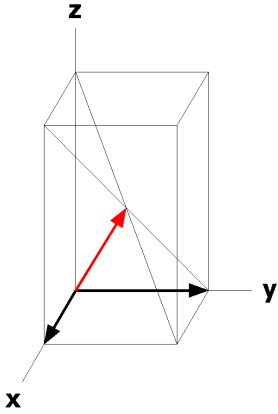
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates							
		(0,0,0) +	(1/2,1/2,1/2)' +					
16 j 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]	(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(8) $y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]
8 i ..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]	x, $\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,\bar{z}$ [ $u,u,0$ ]				
8 h 2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0,z [0,0, $\bar{w}$ ]				
8 g .2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0, $\bar{x},1/2$ [0,u,0]	0,x,1/2 [0, $\bar{u},0$ ]				
8 f .2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0, $\bar{x},0$ [0,u,0]	0,x,0 [0, $\bar{u},0$ ]				
4 e 2.mm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]						
4 d $\bar{4}'..$	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]						
4 c 222.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]						
2 b $\bar{4}2m$	0,0,1/2 [0,0,0]							
2 a $\bar{4}2m$	0,0,0 [0,0,0]							

**Symmetry of Special Projections**

Along [0,0,1]  $p_2-4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/2,0,z

Along [1,0,0]  $c2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



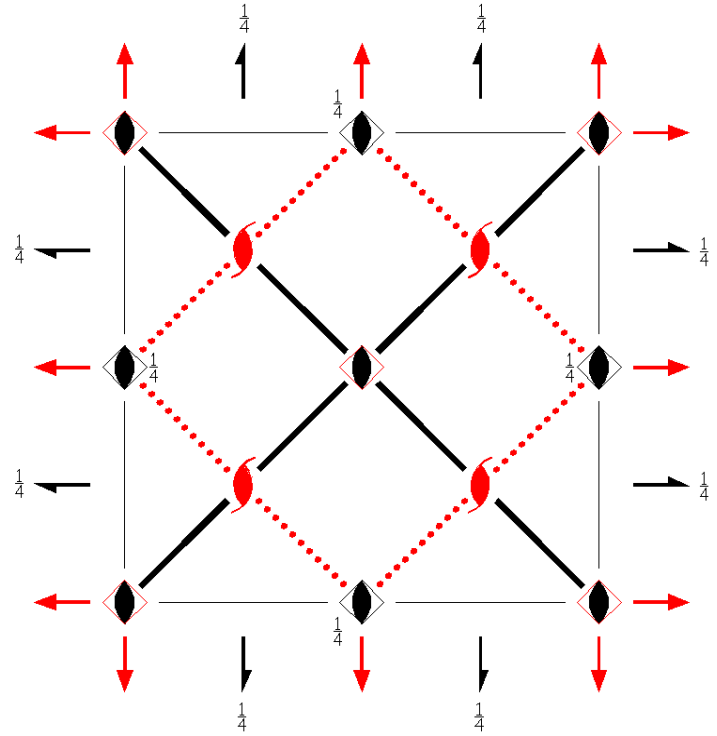
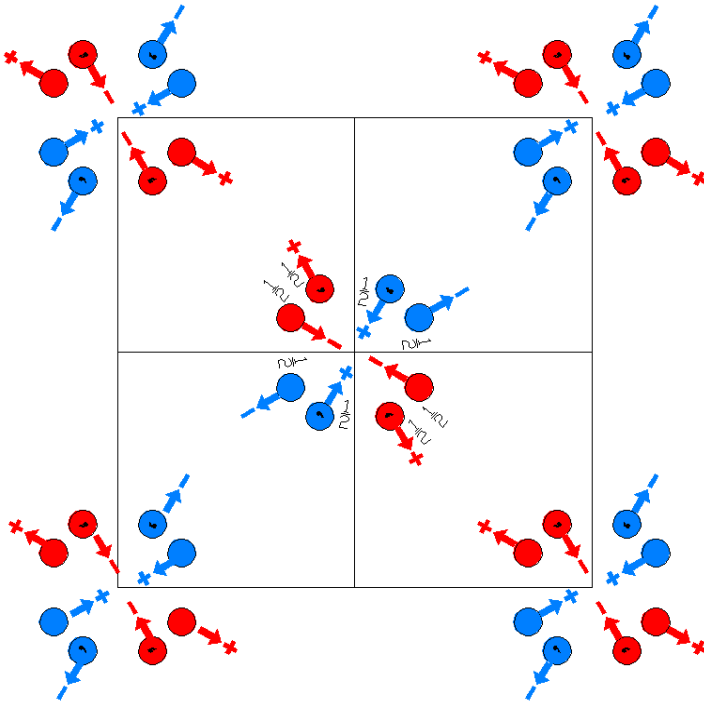
$I_p \bar{4}'2'm$

121.7.991

$\bar{4}2m1'$

$I_p \bar{4}'2'm$

Tetragonal



Origin on  $\bar{4}'2'm$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)' |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' | (7) m x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)        | (8) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                  |

For (1/2,1/2,1/2) + set

- |  |  |   |   |
|--|--|---|---|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'                   | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2)     | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2) |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)   | (7) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)' | (8) n' (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)'       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

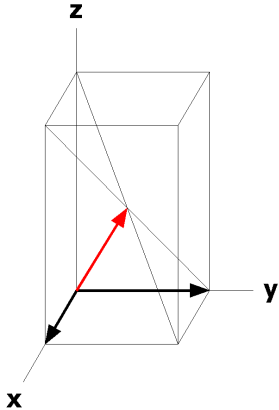
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2)' +		
16	j	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(3) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ] (7) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ] (8) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
8	i	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [u, $\bar{u},0$ ]	x, $\bar{x},\bar{z}$ [u,u,0]	$\bar{x},x,\bar{z}$ [ $\bar{u},\bar{u},0$ ]
8	h	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]
8	g	.2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	0, $\bar{x},1/2$ [v,0, $\bar{w}$ ]	0,x,1/2 [ $\bar{v},0,\bar{w}$ ]
8	f	.2'	x,0,0 [0,v,w]	$\bar{x},0,0$ [0, $\bar{v},w$ ]	0, $\bar{x},0$ [v,0, $\bar{w}$ ]	0,x,0 [ $\bar{v},0,\bar{w}$ ]
4	e	2.mm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4	d	$\bar{4}..$	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0,w]		
4	c	22'2'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]		
2	b	$\bar{4}'2'm$	0,0,1/2 [0,0,0]			
2	a	$\bar{4}'2'm$	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $p_p\bar{4}m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c_p\bar{2}'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



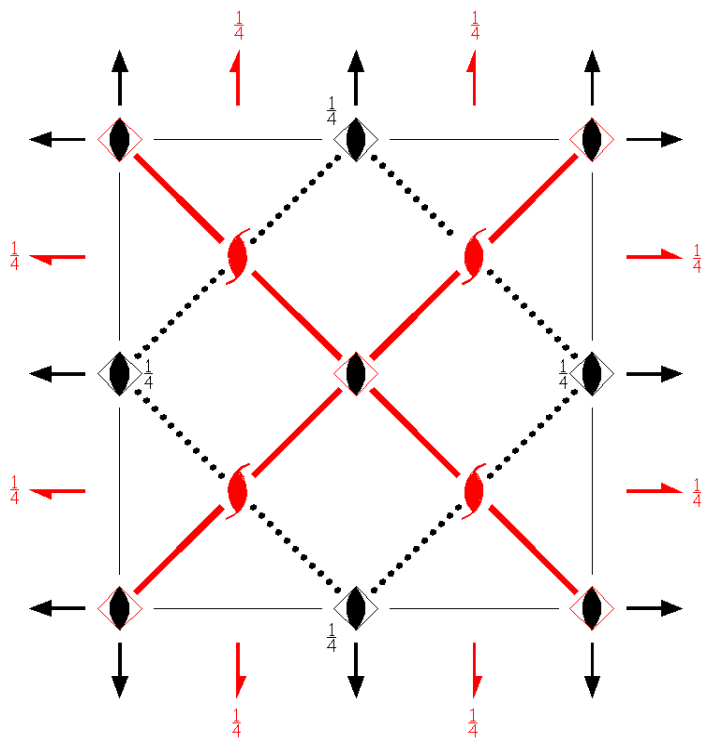
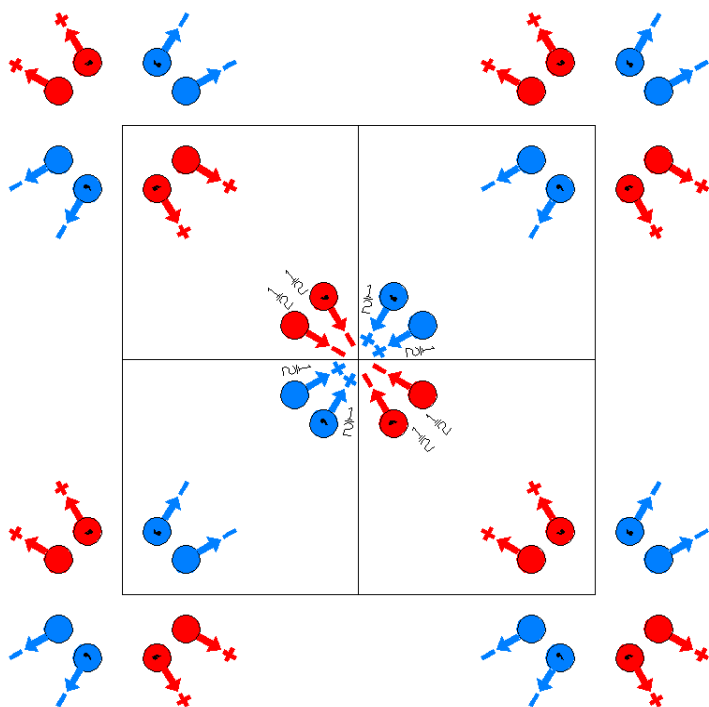
$I_p\bar{4}'2m'$

121.8.992

$\bar{4}2m1'$

$I_p\bar{4}'2m'$

Tetragonal



Origin on  $\bar{4}'2m'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)' | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)' |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0) | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0) | (7) m' x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)'      | (8) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                |

For (1/2,1/2,1/2) + set

- |  |  |   |   |
|--|--|---|---|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'                     | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2)   | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2) |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' | (7) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (8) n (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

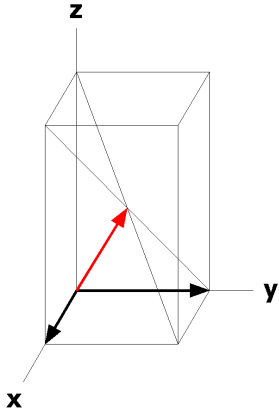
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2)' +		
16	j	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(3) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ] (7) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ] (8) y,x,z [v,u,w]
8	i	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},\bar{z}$ [u, $\bar{u},\bar{w}$ ]	$\bar{x},x,\bar{z}$ [ $\bar{u},u,\bar{w}$ ]
8	h	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0,z [0,0,w]
8	g	.2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0, $\bar{x},1/2$ [0, $\bar{u},0$ ]	0,x,1/2 [0,u,0]
8	f	.2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0, $\bar{x},0$ [0, $\bar{u},0$ ]	0,x,0 [0,u,0]
4	e	2.m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4	d	$\bar{4}$ ..	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0, $\bar{w}$ ]		
4	c	222.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
2	b	$\bar{4}'2m'$	0,0,1/2 [0,0,0]			
2	a	$\bar{4}'2m'$	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $p_p$ -4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c_p$ -2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

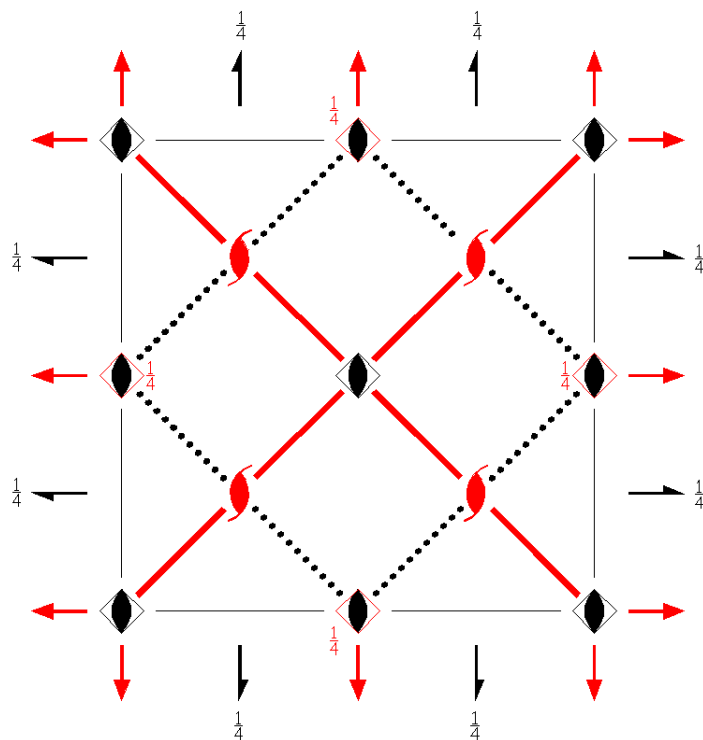
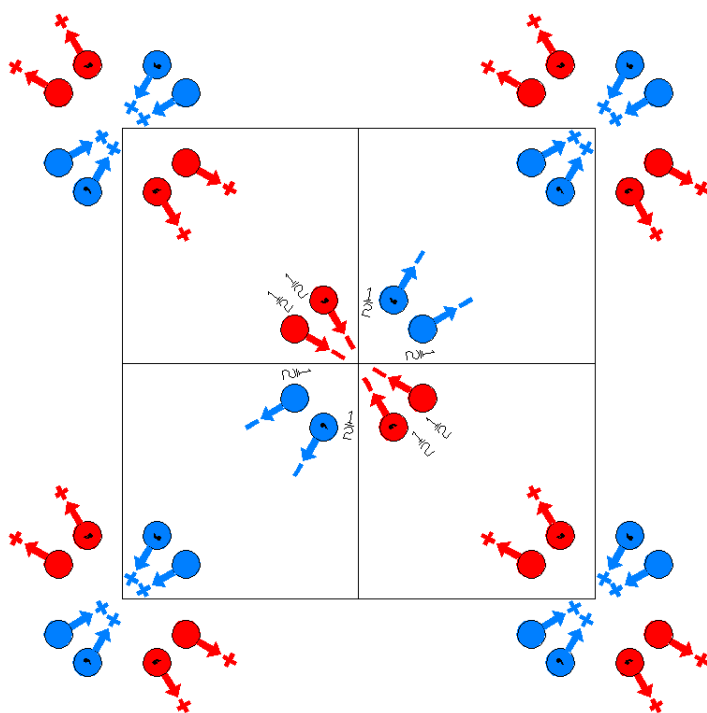
Along [1,1,0]  $p_{2b}$ -1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I_p \bar{4}2m'$   
121.9.993

$\bar{4}2m1'$   
 $I_p \bar{4}2m'$

Tetragonal



Origin on  $\bar{4}2m'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

Symmetry Operations

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0) | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0) |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)' | (7) m' x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)'     | (8) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'               |

For (1/2,1/2,1/2) + set

- |  |  |   |  |
|--|--|---|--|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'                   | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2)' | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2)'  | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2)' |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)   | (7) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (8) n (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2)' +		
16	j	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(7) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(8) $y,x,z$ [ $v,u,w$ ]
8	i	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x},\bar{z}$ [ $\bar{u},u,w$ ]	$\bar{x},x,\bar{z}$ [ $u,\bar{u},w$ ]
8	h	2..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0,z [0,0,w]
8	g	.2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	0, $\bar{x},1/2$ [ $\bar{v},0,w$ ]	0,x,1/2 [ $v,0,w$ ]
8	f	.2'	x,0,0 [0,v,w]	$\bar{x},0,0$ [0, $\bar{v},w$ ]	0, $\bar{x},0$ [ $\bar{v},0,w$ ]	0,x,0 [ $v,0,w$ ]
4	e	2.m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
4	d	$\bar{4}'..$	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]		
4	c	22'2'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]		
2	b	$\bar{4}2'm'$	0,0,1/2 [0,0,w]			
2	a	$\bar{4}2'm'$	0,0,0 [0,0,w]			

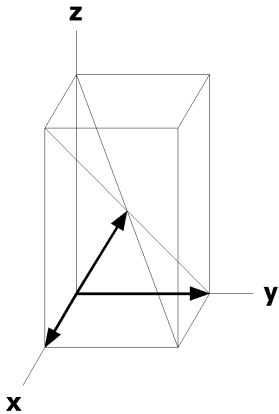
**Symmetry of Special Projections**

Along [0,0,1]  $p_p\bar{4}m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/2,0,z

Along [1,0,0]  $c_p\bar{2}'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0]  $p_{2b}\bar{1}m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0





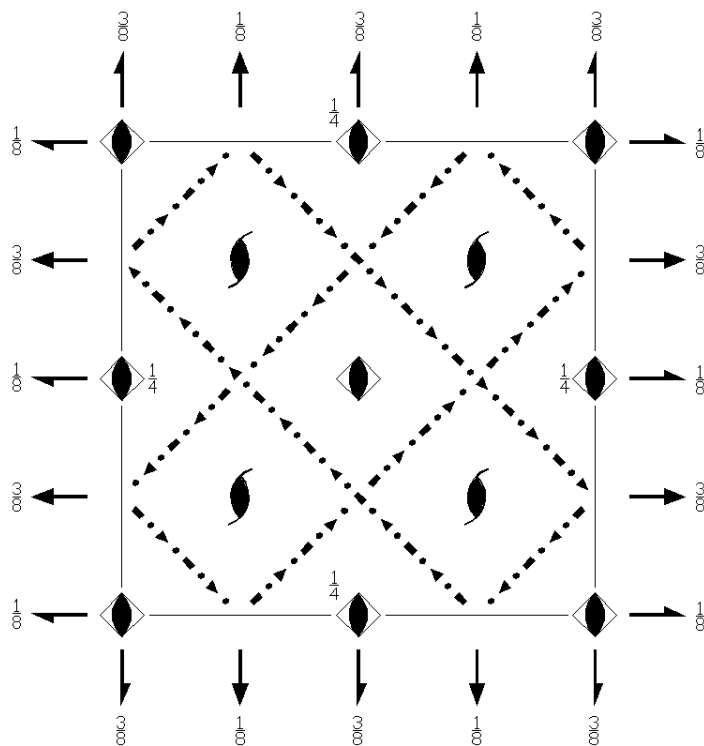
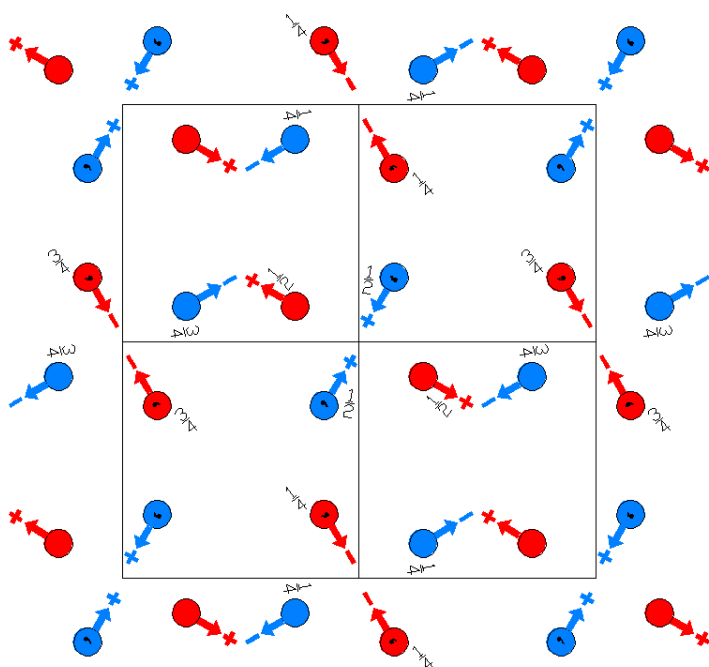
$\bar{4}2d$

122.1.994

$\bar{4}2m$

$\bar{4}2d$

Tetragonal



Origin on  $\bar{4}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/8$

Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)         | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)                    | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)                       |
| (5) 2 (0,1/2,0) 0,y,1/8<br>(2 <sub>y</sub>  0,1/2,1/4) | (6) 2 x,1/4,1/8<br>(2 <sub>x</sub>  0,1/2,1/4) | (7) d (-1/4,1/4,1/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,1/2,1/4) | (8) d (1/4,1/4,1/4) x-1/4,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,1/2,1/4) |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)         | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2)        | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2)           |
| (5) 2 1/4,y,3/8<br>(2 <sub>y</sub>  1/2,0,3/4) | (6) 2 (1/2,0,0) x,0,3/8<br>(2 <sub>x</sub>  1/2,0,3/4)     | (7) d (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,0,3/4) | (8) d (1/4,1/4,3/4) x+1/4,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,0,3/4) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

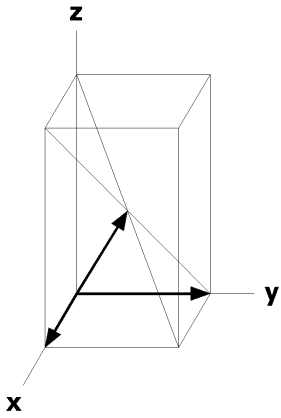
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
16	e	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $\bar{y},\bar{x}+1/2,z+1/4$ [ $v,u,\bar{w}$ ]	(8) $y,x+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	d	.2.	$x,1/4,1/8$ [u,0,0]	$\bar{x},3/4,1/8$ [ $\bar{u},0,0$ ]	$1/4,\bar{x},7/8$ [0,u,0]	$3/4,x,7/8$ [0, $\bar{u}$ ,0]
8	c	2..	0,0,z [0,0,w]	$0,0,\bar{z}$ [0,0,w]	$0,1/2,z+1/4$ [0,0, $\bar{w}$ ]	$0,1/2,\bar{z}+1/4$ [0,0, $\bar{w}$ ]
4	b	$\bar{4}..$	$0,0,1/2$ [0,0,w]	$0,1/2,3/4$ [0,0, $\bar{w}$ ]		
4	a	$\bar{4}..$	0,0,0 [0,0,w]	$0,1/2,1/4$ [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4'g'm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

Along [1,1,0]  $c1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$\bar{1}42d1'$

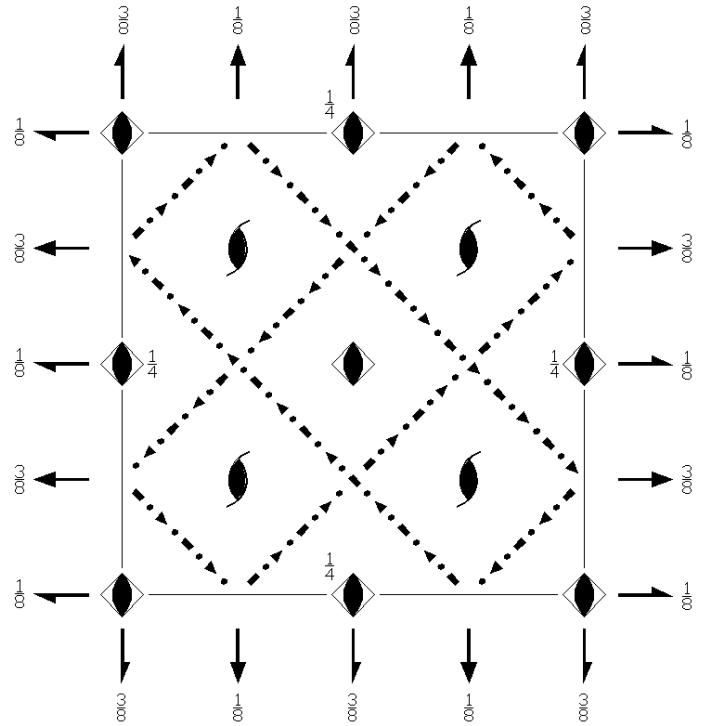
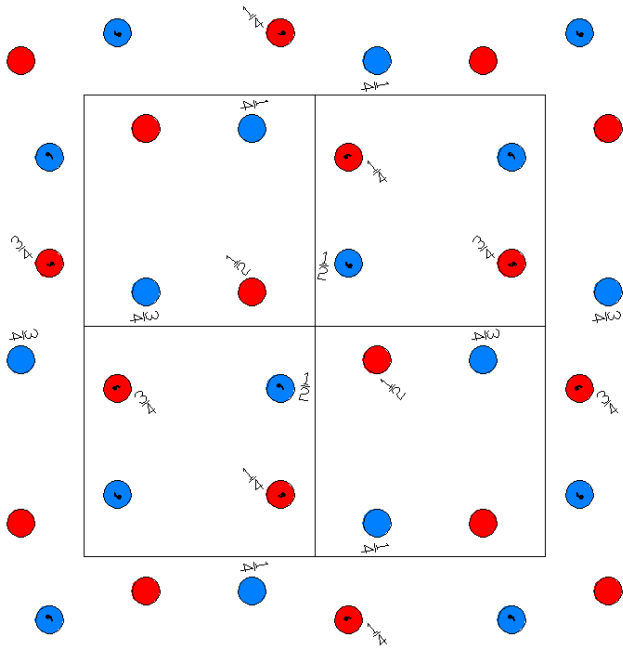
122.2.995

$\bar{4}2m1'$

$\bar{1}42d1'$

Tetragonal

1'



Origin on  $\bar{4}1'$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)         | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)                  | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)       |
| (5) 2 (0,1/2,0) 0,y,1/8<br>(2 <sub>y</sub>  0,1/2,1/4) | (6) 2 x,1/4,1/8<br>(2 <sub>x</sub>  0,1/2,1/4) | (7) d (-1/4,1/4,1/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,1/2,1/4) | (8) d (1/4,1/4,1/4) x-1/4,x,z<br>(m <sub>xy</sub>  0,1/2,1/4) |

For (1/2,1/2,1/2) + set

- |  |  |  |   |
|--|--|--|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)         | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2)      | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2) |
| (5) 2 1/4,y,3/8<br>(2 <sub>y</sub>  1/2,0,3/4) | (6) 2 (1/2,0,0) x,0,3/8<br>(2 <sub>x</sub>  1/2,0,3/4)     | (7) d (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,0,3/4) | (8) d (1/4,1/4,3/4) x+1/4,x,z<br>(m <sub>xy</sub>  1/2,0,3/4)       |

## For (0,0,0)' + set

(1) $1'$ (1 0,0,0)'	(2) $2'$ 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) $\bar{4}^+$ ' 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'	(4) $\bar{4}^-$ ' 0,0,z; 0,0,0 ( $\bar{4}_z^{-1}$  0,0,0)'
(5) $2'$ (0,1/2,0) 0,y,1/8 (2 <sub>y</sub>  0,1/2,1/4)'	(6) $2'$ x,1/4,1/8 (2 <sub>x</sub>  0,1/2,1/4)'	(7) $d'$ (-1/4,1/4,1/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>  0,1/2,1/4)'	(8) $d'$ (1/4,1/4,1/4) x-1/4,x,z (m <sub><math>\bar{xy}</math></sub>  0,1/2,1/4)'

## For (1/2,1/2,1/2)' + set

(1) $t'$ (1/2,1/2,1/2) (1 1/2,1/2,1/2)'	(2) $2'$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>  1/2,1/2,1/2)'	(3) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$  1/2,1/2,1/2)'	(4) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$  1/2,1/2,1/2)'
(5) $2'$ 1/4,y,3/8 (2 <sub>y</sub>  1/2,0,3/4)'	(6) $2'$ (1/2,0,0) x,0,3/8 (2 <sub>x</sub>  1/2,0,3/4)'	(7) $d'$ (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,0,3/4)'	(8) $d'$ (1/4,1/4,3/4) x+1/4,x,z (m <sub><math>\bar{xy}</math></sub>  1/2,0,3/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

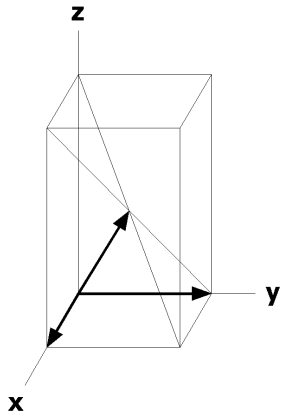
			(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'		
16	e	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]		
			(3) y, $\bar{x},\bar{z}$ [0,0,0]	(4) $\bar{y},x,\bar{z}$ [0,0,0]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [0,0,0]	(6) x, $\bar{y}+1/2,\bar{z}+1/4$ [0,0,0]		
			(7) $\bar{y},\bar{x}+1/2,z+1/4$ [0,0,0]	(8) y,x+1/2,z+1/4 [0,0,0]		
8	d	.2.1'	x,1/4,1/8 [0,0,0]	$\bar{x},3/4,1/8$ [0,0,0]	1/4, $\bar{x},7/8$ [0,0,0]	3/4,x,7/8 [0,0,0]
8	c	2..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,1/2,z+1/4 [0,0,0]	0,1/2, $\bar{z}+1/4$ [0,0,0]
4	b	$\bar{4}..1'$	0,0,1/2 [0,0,0]	0,1/2,3/4 [0,0,0]		
4	a	$\bar{4}..1'$	0,0,0 [0,0,0]	0,1/2,1/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

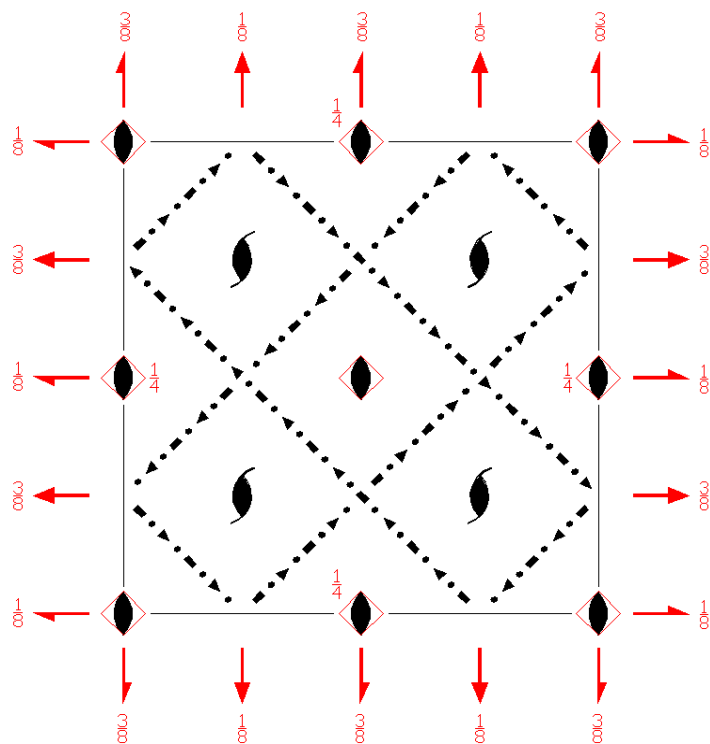
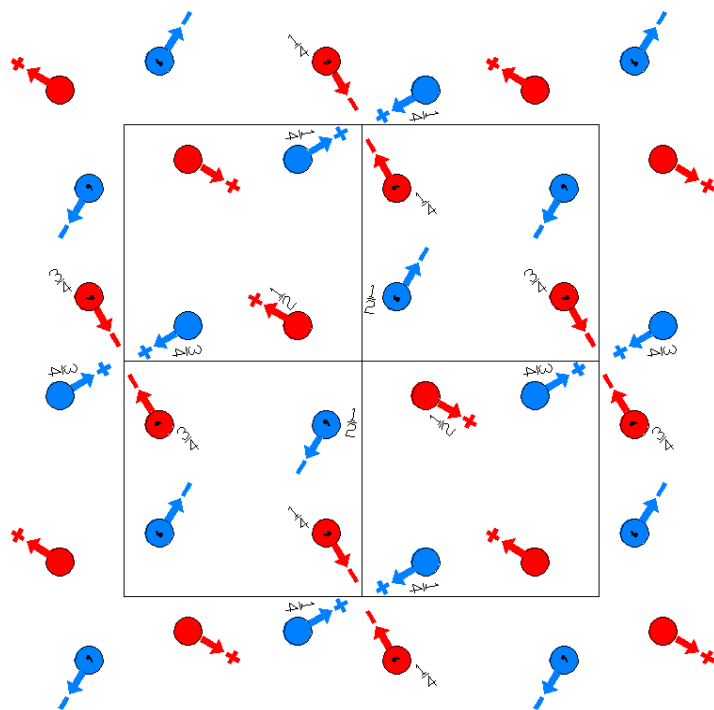
Along [1,1,0] c1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$\bar{4}'2'd$   
122.3.996

$\bar{4}'2'm$   
 $\bar{4}'2'd$

Tetragonal



Origin on  $\bar{4}'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)           | (3) $\bar{4}'^+$ 0,0,z; 0,0,0<br>( $\bar{4}'_z$  0,0,0)'                 | (4) $\bar{4}'^-$ 0,0,z; 0,0,0<br>( $\bar{4}'_z^{-1}$  0,0,0)' |
| (5) 2' (0,1/2,0) 0,y,1/8<br>(2 <sub>y</sub>  0,1/2,1/4)' | (6) 2' x,1/4,1/8<br>(2 <sub>x</sub>  0,1/2,1/4)' | (7) d (-1/4,1/4,1/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,1/2,1/4) | (8) d (1/4,1/4,1/4) x-1/4,x,z<br>(m <sub>xy</sub>  0,1/2,1/4) |

For (1/2,1/2,1/2) + set

- |  |  |  |   |
|--|--|--|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)           | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) $\bar{4}'^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}'_z$  1/2,1/2,1/2)'     | (4) $\bar{4}'^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}'_z^{-1}$  1/2,1/2,1/2)' |
| (5) 2' 1/4,y,3/8<br>(2 <sub>y</sub>  1/2,0,3/4)' | (6) 2' (1/2,0,0) x,0,3/8<br>(2 <sub>x</sub>  1/2,0,3/4)'   | (7) d (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,0,3/4) | (8) d (1/4,1/4,3/4) x+1/4,x,z<br>(m <sub>xy</sub>  1/2,0,3/4)             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

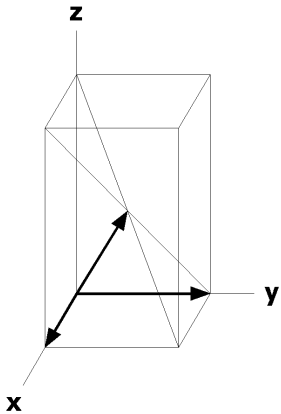
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
16	e	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},w$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},v,w$ ]		
			(7) $\bar{y},\bar{x}+1/2,z+1/4$ [ $v,u,\bar{w}$ ]	(8) $y,x+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	d	.2'	$x,1/4,1/8$ [0,v,w]	$\bar{x},3/4,1/8$ [0, $\bar{v}$ ,w]	$1/4,\bar{x},7/8$ [v,0, $\bar{w}$ ]	$3/4,x,7/8$ [ $\bar{v},0,\bar{w}$ ]
8	c	2..	0,0,z [0,0,w]	$0,0,\bar{z}$ [0,0, $\bar{w}$ ]	$0,1/2,z+1/4$ [0,0, $\bar{w}$ ]	$0,1/2,\bar{z}+1/4$ [0,0,w]
4	b	$\bar{4}'..$	0,0,1/2 [0,0,0]	0,1/2,3/4 [0,0,0]		
4	a	$\bar{4}'..$	0,0,0 [0,0,0]	0,1/2,1/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4g'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

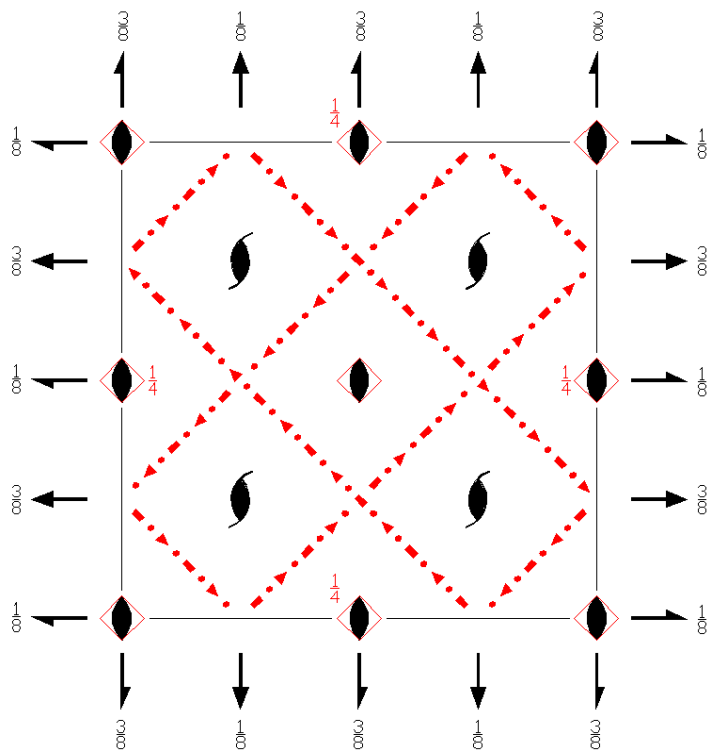
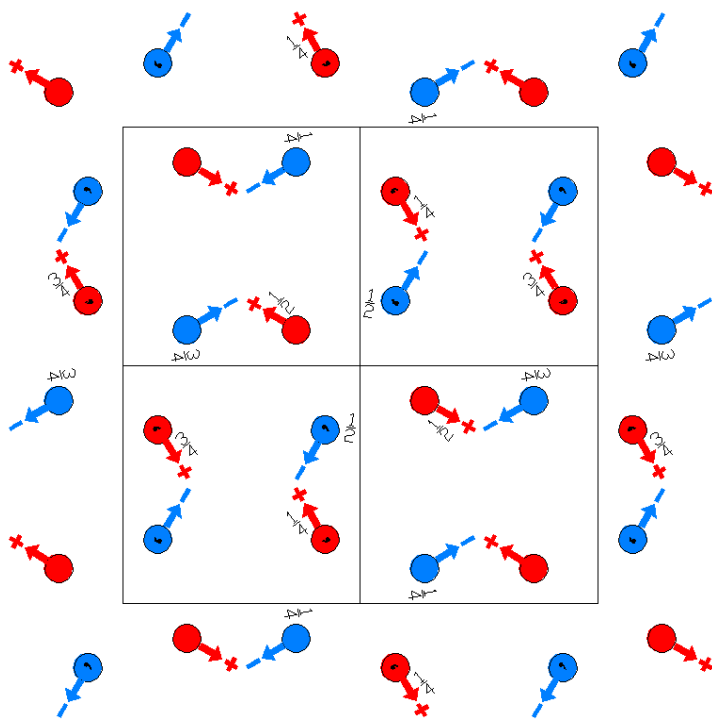
Along [1,1,0]  $c_2^*1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$\bar{4}'2d'$   
122.4.997

$\bar{4}'2m'$   
 $\bar{4}'2d'$

Tetragonal



Origin on  $\bar{4}'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)         | (3) $\bar{4}^+$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)'                   | (4) $\bar{4}^-$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)'                      |
| (5) 2 (0,1/2,0) 0,y,1/8<br>(2 <sub>y</sub>  0,1/2,1/4) | (6) 2 x,1/4,1/8<br>(2 <sub>x</sub>  0,1/2,1/4) | (7) d' (-1/4,1/4,1/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,1/2,1/4)' | (8) d' (1/4,1/4,1/4) x-1/4,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,1/2,1/4)' |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)         | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2)'       | (4) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2)'          |
| (5) 2 1/4,y,3/8<br>(2 <sub>y</sub>  1/2,0,3/4) | (6) 2 (1/2,0,0) x,0,3/8<br>(2 <sub>x</sub>  1/2,0,3/4)     | (7) d' (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,0,3/4)' | (8) d' (1/4,1/4,3/4) x+1/4,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,0,3/4)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
16	e	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $y,\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(4) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [u, $\bar{v},\bar{w}$ ]		
			(7) $\bar{y},\bar{x}+1/2,z+1/4$ [ $\bar{v},\bar{u},w$ ]	(8) $y,x+1/2,z+1/4$ [v,u,w]		
8	d	.2.	$x,1/4,1/8$ [u,0,0]	$\bar{x},3/4,1/8$ [ $\bar{u},0,0$ ]	$1/4,\bar{x},7/8$ [0, $\bar{u},0$ ]	$3/4,x,7/8$ [0,u,0]
8	c	2..	0,0,z [0,0,w]	$0,0,\bar{z}$ [0,0, $\bar{w}$ ]	$0,1/2,z+1/4$ [0,0,w]	$0,1/2,\bar{z}+1/4$ [0,0, $\bar{w}$ ]
4	b	$\bar{4}'..$	$0,0,1/2$ [0,0,0]	$0,1/2,3/4$ [0,0,0]		
4	a	$\bar{4}'..$	0,0,0 [0,0,0]	$0,1/2,1/4$ [0,0,0]		

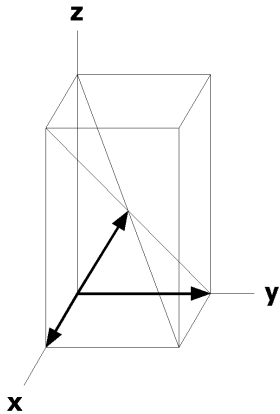
**Symmetry of Special Projections**

Along [0,0,1] p4gm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

Along [1,1,0] c1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

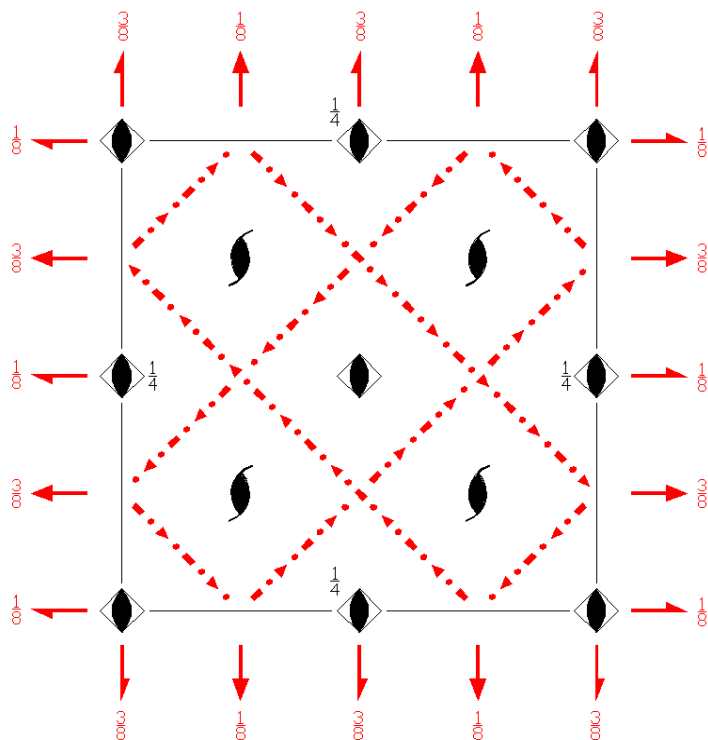
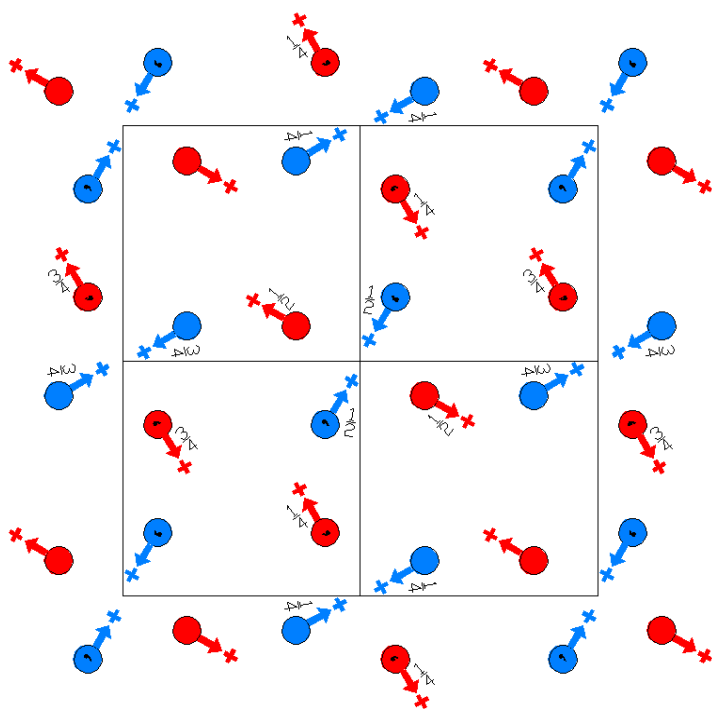




$\bar{1}42'd'$   
122.5.998

$\bar{4}2'm'$   
 $\bar{1}42'd'$

Tetragonal



Origin on  $\bar{4}$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/8$

### Symmetry Operations

For (0,0,0) + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)           | (3) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)                      | (4) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)      |
| (5) 2' (0,1/2,0) 0,y,1/8<br>(2 <sub>y</sub>  0,1/2,1/4)' | (6) 2' x,1/4,1/8<br>(2 <sub>x</sub>  0,1/2,1/4)' | (7) d' (-1/4,1/4,1/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,1/2,1/4)' | (8) d' (1/4,1/4,1/4) x-1/4,x,z<br>(m <sub>xy</sub>  0,1/2,1/4)' |

For (1/2,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)           | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,1/2) | (3) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,1/2)          | (4) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,1/2) |
| (5) 2' 1/4,y,3/8<br>(2 <sub>y</sub>  1/2,0,3/4)' | (6) 2' (1/2,0,0) x,0,3/8<br>(2 <sub>x</sub>  1/2,0,3/4)'   | (7) d' (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,0,3/4)' | (8) d' (1/4,1/4,3/4) x+1/4,x,z<br>(m <sub>xy</sub>  1/2,0,3/4)'        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

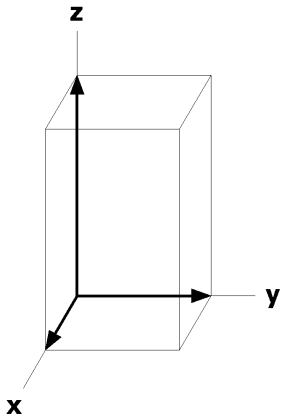
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
16	e	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(4) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},w$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},v,w$ ]		
			(7) $\bar{y},\bar{x}+1/2,z+1/4$ [ $\bar{v},\bar{u},w$ ]	(8) $y,x+1/2,z+1/4$ [ $v,u,w$ ]		
8	d	.2'	$x,1/4,1/8$ [0,v,w]	$\bar{x},3/4,1/8$ [0, $\bar{v}$ ,w]	$1/4,\bar{x},7/8$ [ $\bar{v},0,w$ ]	$3/4,x,7/8$ [v,0,w]
8	c	2..	0,0,z [0,0,w]	$0,0,\bar{z}$ [0,0,w]	$0,1/2,z+1/4$ [0,0,w]	$0,1/2,\bar{z}+1/4$ [0,0,w]
4	b	$\bar{4}..$	$0,0,1/2$ [0,0,w]	$0,1/2,3/4$ [0,0,w]		
4	a	$\bar{4}..$	0,0,0 [0,0,w]	$0,1/2,1/4$ [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4'gm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,3/8

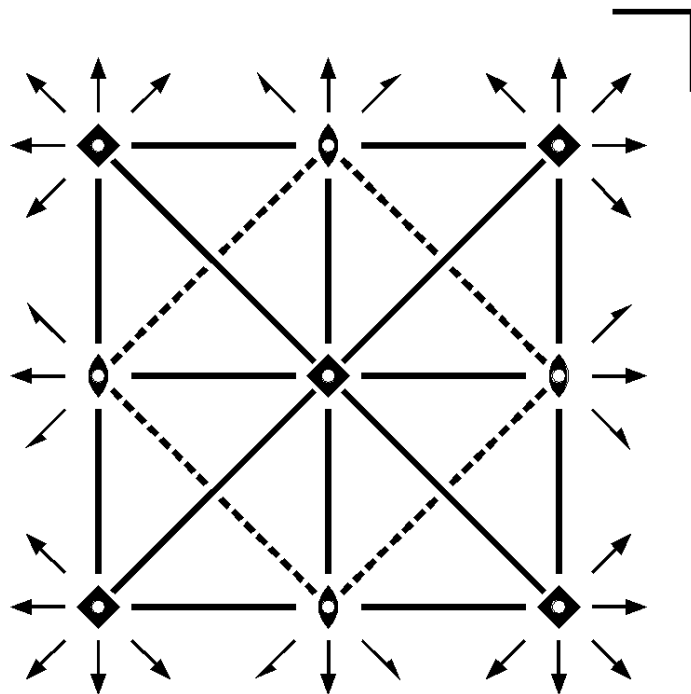
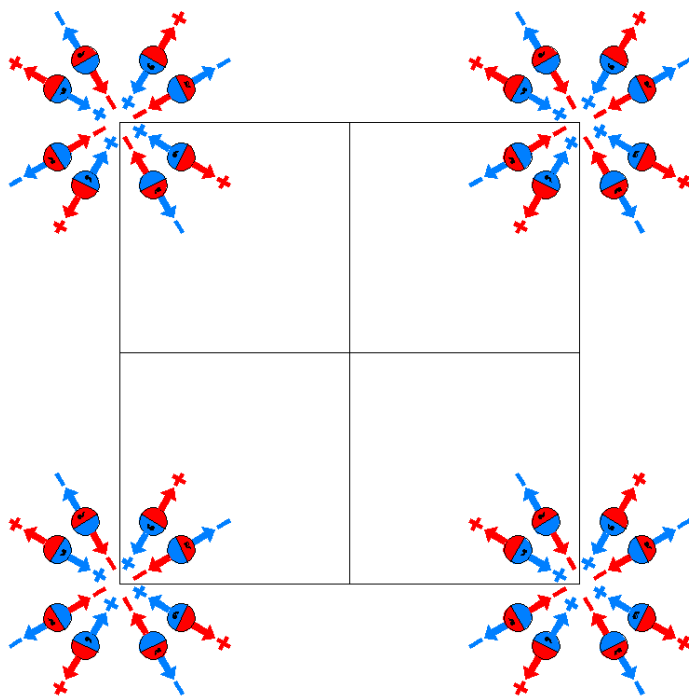
Along [1,1,0]  $c1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



P4/mmm  
123.1.999

4/mmm  
P4/m2/m2/m

Tetragonal



Origin at center ( 4/mmm )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y$

### Symmetry Operations

- |  |   |  |  |
|--|---|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)      | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)    |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)     | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                  | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0) |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0) | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)             |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)    | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (15) m x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)       | (16) m x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,0)          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	u	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (9) $\bar{x},\bar{y},\bar{z}$ [u,v,w] (13) x, $\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ] (14) $\bar{x},\bar{y},z$ [u, $\bar{v},\bar{w}$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ] (7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ] (11) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ] (15) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ] (12) $\bar{y},x,\bar{z}$ [v, $\bar{u},w$ ] (16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
8	t	.m.	x,1/2,z [0,v,0] $\bar{x},1/2,\bar{z}$ [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v},0$ ] x,1/2, $\bar{z}$ [0, $\bar{v},0$ ]	1/2,x,z [ $\bar{v},0,0$ ] 1/2,x, $\bar{z}$ [ $\bar{v},0,0$ ]	1/2, $\bar{x},z$ [v,0,0] 1/2, $\bar{x},\bar{z}$ [v,0,0]
8	s	.m.	x,0,z [0,v,0] $\bar{x},0,\bar{z}$ [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ] x,0, $\bar{z}$ [0, $\bar{v},0$ ]	0,x,z [ $\bar{v},0,0$ ] 0,x, $\bar{z}$ [ $\bar{v},0,0$ ]	0, $\bar{x},z$ [v,0,0] 0, $\bar{x},\bar{z}$ [v,0,0]
8	r	..m	x,x,z [ $\bar{u},u,0$ ] $\bar{x},x,\bar{z}$ [u,u,0]	$\bar{x},\bar{x},z$ [u, $\bar{u},0$ ] x, $\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,z$ [ $\bar{u},\bar{u},0$ ] x,x, $\bar{z}$ [u, $\bar{u},0$ ]	x, $\bar{x},z$ [u,u,0] $\bar{x},\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]
8	q	m..	x,y,1/2 [0,0,w] $\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	$\bar{x},\bar{y},1/2$ [0,0,w] x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]	$\bar{y},x,1/2$ [0,0,w] y,x,1/2 [0,0, $\bar{w}$ ]	y, $\bar{x},1/2$ [0,0,w] $\bar{y},\bar{x},1/2$ [0,0, $\bar{w}$ ]
8	p	m..	x,y,0 [0,0,w] $\bar{x},y,0$ [0,0, $\bar{w}$ ]	$\bar{x},\bar{y},0$ [0,0,w] x, $\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{y},x,0$ [0,0,w] y,x,0 [0,0, $\bar{w}$ ]	y, $\bar{x},0$ [0,0,w] $\bar{y},\bar{x},0$ [0,0, $\bar{w}$ ]
4	o	m2m.	x,1/2,1/2 [0,0,0]	$\bar{x},1/2,1/2$ [0,0,0]	1/2,x,1/2 [0,0,0]	1/2, $\bar{x},1/2$ [0,0,0]
4	n	m2m.	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]	1/2,x,0 [0,0,0]	1/2, $\bar{x},0$ [0,0,0]
4	m	m2m.	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]	0,x,1/2 [0,0,0]	0, $\bar{x},1/2$ [0,0,0]
4	l	m2m.	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x},0$ [0,0,0]
4	k	m.2m	x,x,1/2 [0,0,0]	$\bar{x},\bar{x},1/2$ [0,0,0]	$\bar{x},x,1/2$ [0,0,0]	x, $\bar{x},1/2$ [0,0,0]
4	j	m.2m	x,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x},x,0$ [0,0,0]	x, $\bar{x},0$ [0,0,0]
4	i	2mm.	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]
2	h	4mm	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
2	g	4mm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	f	mmm.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		

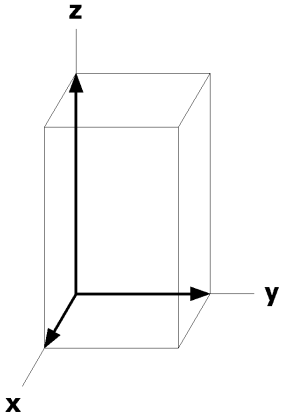
2	e	mmm.	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]
1	d	4/mmm	1/2,1/2,1/2 [0,0,0]	
1	c	4/mmm	1/2,1/2,0 [0,0,0]	
1	b	4/mmm	0,0,1/2 [0,0,0]	
1	a	4/mmm	0,0,0 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4/mmm1'

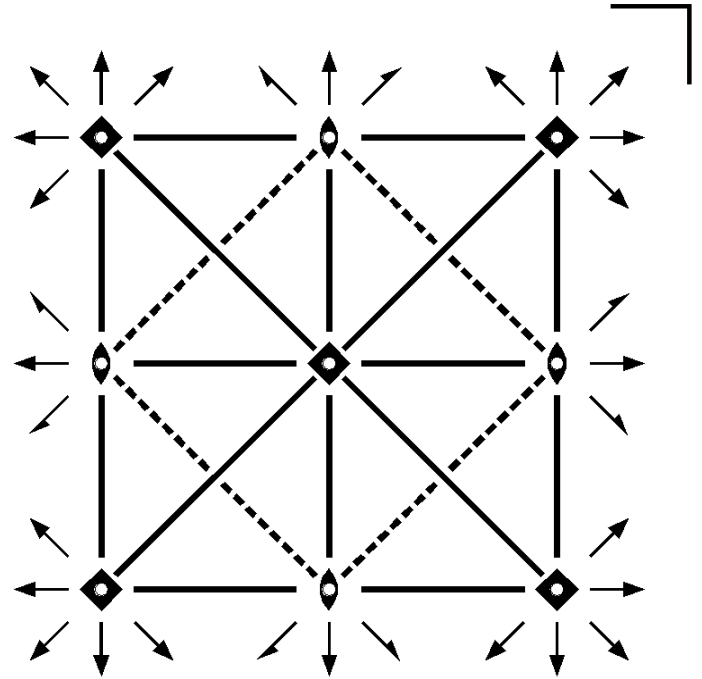
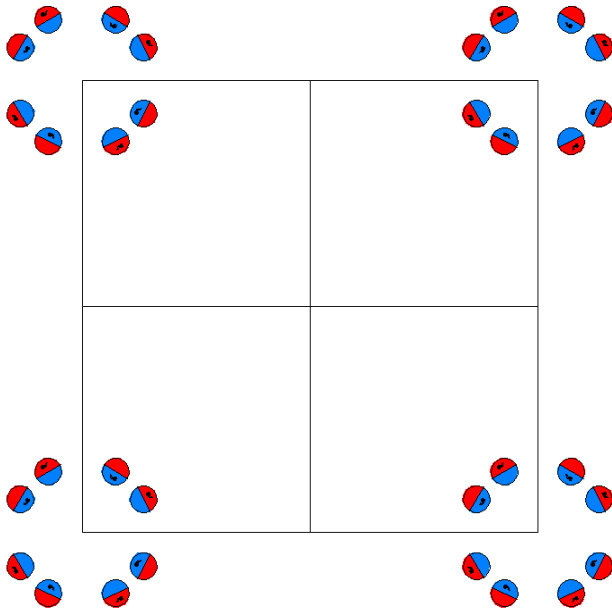
123.2.1000

4/mmm1'

P4/m2/m2/m1'

Tetragonal

1'



Origin at center ( 4/mmm1' )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

Symmetry Operations

For 1 + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                      | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)         |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                  | (8) 2 x,x̄,0<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,0)                    |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)              | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (15) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                                | (16) m x,x,z<br>(m <sub>xy</sub> <sup>-1</sup>  0,0,0)                    |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)'	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(5) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(6) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'	(7) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) 2' x, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  0,0,0)'
(9) $\bar{1}$ ' 0,0,0 ( $\bar{1}$  0,0,0)'	(10) m' x,y,0 (m <sub>z</sub>  0,0,0)'	(11) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z^+$  0,0,0)'	(12) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z^-$  0,0,0)'
(13) m' x,0,z (m <sub>y</sub>  0,0,0)'	(14) m' 0,y,z (m <sub>x</sub>  0,0,0)'	(15) m' x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)'	(16) m' x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

**Positions**

			Coordinates			
			1 +		1' +	
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	u	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z$ [0,0,0]	(4) y, $\bar{x},z$ [0,0,0]
			(5) $\bar{x},y,\bar{z}$ [0,0,0]	(6) x, $\bar{y},\bar{z}$ [0,0,0]	(7) y,x, $\bar{z}$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}$ [0,0,0]
			(9) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(10) x,y, $\bar{z}$ [0,0,0]	(11) y, $\bar{x},\bar{z}$ [0,0,0]	(12) $\bar{y},x,\bar{z}$ [0,0,0]
			(13) x, $\bar{y},z$ [0,0,0]	(14) $\bar{x},y,z$ [0,0,0]	(15) $\bar{y},\bar{x},z$ [0,0,0]	(16) y,x,z [0,0,0]
8	t	.m.1'	x,1/2,z [0,0,0]	$\bar{x},1/2,z$ [0,0,0]	1/2,x,z [0,0,0]	1/2, $\bar{x},z$ [0,0,0]
			$\bar{x},1/2,\bar{z}$ [0,0,0]	x,1/2, $\bar{z}$ [0,0,0]	1/2,x, $\bar{z}$ [0,0,0]	1/2, $\bar{x},\bar{z}$ [0,0,0]
8	s	.m.1'	x,0,z [0,0,0]	$\bar{x},0,z$ [0,0,0]	0,x,z [0,0,0]	0, $\bar{x},z$ [0,0,0]
			$\bar{x},0,\bar{z}$ [0,0,0]	x,0, $\bar{z}$ [0,0,0]	0,x, $\bar{z}$ [0,0,0]	0, $\bar{x},\bar{z}$ [0,0,0]
8	r	..m1'	x,x,z [0,0,0]	$\bar{x},\bar{x},z$ [0,0,0]	$\bar{x},x,z$ [0,0,0]	x, $\bar{x},z$ [0,0,0]
			$\bar{x},x,\bar{z}$ [0,0,0]	x, $\bar{x},\bar{z}$ [0,0,0]	x,x, $\bar{z}$ [0,0,0]	$\bar{x},\bar{x},\bar{z}$ [0,0,0]
8	q	m..1'	x,y,1/2 [0,0,0]	$\bar{x},\bar{y},1/2$ [0,0,0]	$\bar{y},x,1/2$ [0,0,0]	y, $\bar{x},1/2$ [0,0,0]
			$\bar{x},y,1/2$ [0,0,0]	x, $\bar{y},1/2$ [0,0,0]	y,x,1/2 [0,0,0]	$\bar{y},\bar{x},1/2$ [0,0,0]
8	p	m..1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{y},x,0$ [0,0,0]	y, $\bar{x},0$ [0,0,0]
			$\bar{x},y,0$ [0,0,0]	x, $\bar{y},0$ [0,0,0]	y,x,0 [0,0,0]	$\bar{y},\bar{x},0$ [0,0,0]
4	o	m2m.1'	x,1/2,1/2 [0,0,0]	$\bar{x},1/2,1/2$ [0,0,0]	1/2,x,1/2 [0,0,0]	1/2, $\bar{x},1/2$ [0,0,0]
4	n	m2m.1'	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]	1/2,x,0 [0,0,0]	1/2, $\bar{x},0$ [0,0,0]

4	m	m2m.1'	$x, 0, 1/2 [0, 0, 0]$	$\bar{x}, 0, 1/2 [0, 0, 0]$	$0, x, 1/2 [0, 0, 0]$	$0, \bar{x}, 1/2 [0, 0, 0]$
4	l	m2m.1'	$x, 0, 0 [0, 0, 0]$	$\bar{x}, 0, 0 [0, 0, 0]$	$0, x, 0 [0, 0, 0]$	$0, \bar{x}, 0 [0, 0, 0]$
4	k	m.2m1'	$x, x, 1/2 [0, 0, 0]$	$\bar{x}, \bar{x}, 1/2 [0, 0, 0]$	$\bar{x}, x, 1/2 [0, 0, 0]$	$x, \bar{x}, 1/2 [0, 0, 0]$
4	j	m.2m1'	$x, x, 0 [0, 0, 0]$	$\bar{x}, \bar{x}, 0 [0, 0, 0]$	$\bar{x}, x, 0 [0, 0, 0]$	$x, \bar{x}, 0 [0, 0, 0]$
4	i	2mm.1'	$0, 1/2, z [0, 0, 0]$	$1/2, 0, z [0, 0, 0]$	$0, 1/2, \bar{z} [0, 0, 0]$	$1/2, 0, \bar{z} [0, 0, 0]$
2	h	4mm1'	$1/2, 1/2, z [0, 0, 0]$	$1/2, 1/2, \bar{z} [0, 0, 0]$		
2	g	4mm1'	$0, 0, z [0, 0, 0]$	$0, 0, \bar{z} [0, 0, 0]$		
2	f	mmm.1'	$0, 1/2, 0 [0, 0, 0]$	$1/2, 0, 0 [0, 0, 0]$		
2	e	mmm.1'	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$		
1	d	4/mmm1'	$1/2, 1/2, 1/2 [0, 0, 0]$			
1	c	4/mmm1'	$1/2, 1/2, 0 [0, 0, 0]$			
1	b	4/mmm1'	$0, 0, 1/2 [0, 0, 0]$			
1	a	4/mmm1'	$0, 0, 0 [0, 0, 0]$			

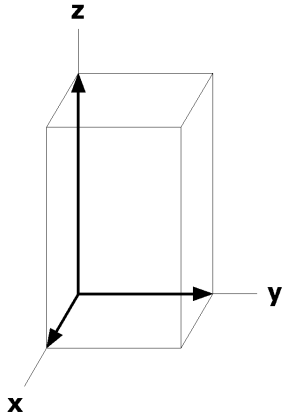
### Symmetry of Special Projections

Along  $[0, 0, 1]$  p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$  p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 0, 0$

Along  $[1, 1, 0]$  p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 0$

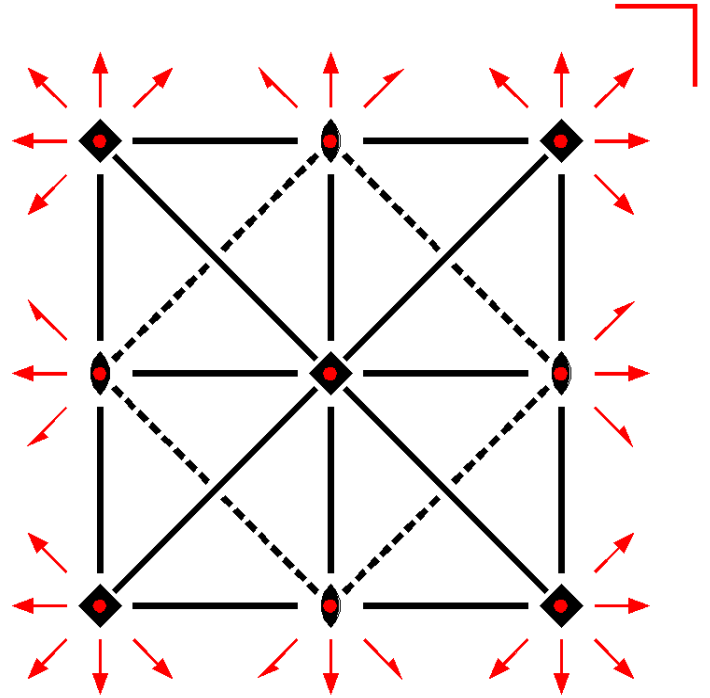
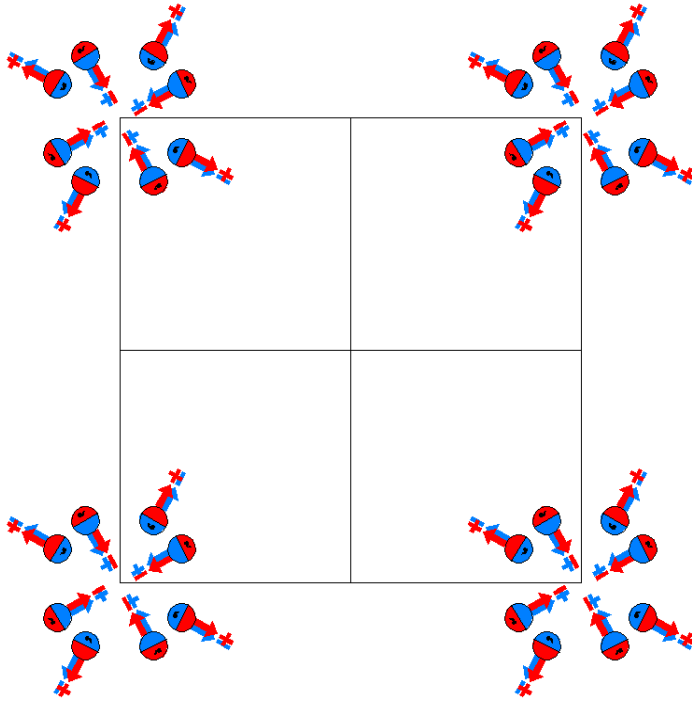




P4/m'mm  
123.3.1001

4/m'mm  
P4/m'2'/m2'/m

Tetragonal



Origin at center ( 4/m'mm )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $x \leq y$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                             | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)     | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)          | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)      |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'       | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'   | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                    | (8) 2' x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)' |
| (9) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$ ' 0,0,0)' | (10) m' x,y,0<br>(m <sub>z</sub> ' 0,0,0)' | (11) $\bar{4}^+$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^+$ ' 0,0,0)' | (12) $\bar{4}^-$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^-$ ' 0,0,0)'           |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)        | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)    | (15) m x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)           | (16) m x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,0)            |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	u	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ]
			(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [v,u,w]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(11) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
			(13) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ]	(16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
8	t	.m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v},0$ ]	1/2,x,z [ $\bar{v},0,0$ ]	1/2, $\bar{x},z$ [v,0,0]
			$\bar{x},1/2,\bar{z}$ [0, $\bar{v},0$ ]	x,1/2, $\bar{z}$ [0,v,0]	1/2,x, $\bar{z}$ [ $\bar{v},0,0$ ]	1/2, $\bar{x},\bar{z}$ [v,0,0]
8	s	.m.	x,0,z [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ]	0,x,z [ $\bar{v},0,0$ ]	0, $\bar{x},z$ [v,0,0]
			$\bar{x},0,\bar{z}$ [0, $\bar{v},0$ ]	x,0, $\bar{z}$ [0,v,0]	0,x, $\bar{z}$ [ $\bar{v},0,0$ ]	0, $\bar{x},\bar{z}$ [v,0,0]
8	r	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [u, $\bar{u},0$ ]	$\bar{x},x,z$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},z$ [u,u,0]
			$\bar{x},x,\bar{z}$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},\bar{z}$ [u,u,0]	x,x, $\bar{z}$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},\bar{z}$ [u, $\bar{u},0$ ]
8	q	m'..	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},u,0$ ]	y, $\bar{x},1/2$ [v, $\bar{u},0$ ]
			$\bar{x},y,1/2$ [u, $\bar{v},0$ ]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]	y,x,1/2 [ $\bar{v},\bar{u},0$ ]	$\bar{y},\bar{x},1/2$ [v,u,0]
8	p	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},u,0$ ]	y, $\bar{x},0$ [v, $\bar{u},0$ ]
			$\bar{x},y,0$ [u, $\bar{v},0$ ]	x, $\bar{y},0$ [ $\bar{u},v,0$ ]	y,x,0 [ $\bar{v},\bar{u},0$ ]	$\bar{y},\bar{x},0$ [v,u,0]
4	o	m'2'm.	x,1/2,1/2 [0,v,0]	$\bar{x},1/2,1/2$ [0, $\bar{v},0$ ]	1/2,x,1/2 [ $\bar{v},0,0$ ]	1/2, $\bar{x},1/2$ [v,0,0]
4	n	m'2'm.	x,1/2,0 [0,v,0]	$\bar{x},1/2,0$ [0, $\bar{v},0$ ]	1/2,x,0 [ $\bar{v},0,0$ ]	1/2, $\bar{x},0$ [v,0,0]
4	m	m'2'm.	x,0,1/2 [0,v,0]	$\bar{x},0,1/2$ [0, $\bar{v},0$ ]	0,x,1/2 [ $\bar{v},0,0$ ]	0, $\bar{x},1/2$ [v,0,0]
4	l	m'2'm.	x,0,0 [0,v,0]	$\bar{x},0,0$ [0, $\bar{v},0$ ]	0,x,0 [ $\bar{v},0,0$ ]	0, $\bar{x},0$ [v,0,0]
4	k	m'.2'm	x,x,1/2 [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},1/2$ [u, $\bar{u},0$ ]	$\bar{x},x,1/2$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},1/2$ [u,u,0]
4	j	m'.2'm	x,x,0 [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},0$ [u, $\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},0$ [u,u,0]
4	i	2mm.	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]
2	h	4mm	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
2	g	4mm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	f	m'mm.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		

Continued

123.3.1001

P4/m'mm

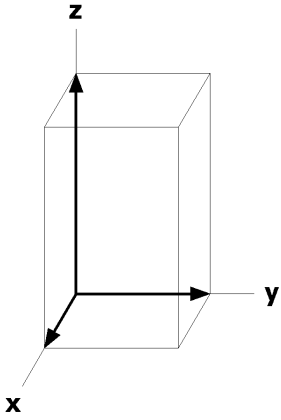
2	e	mmm.	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]
1	d	4/m'mm	1/2,1/2,1/2 [0,0,0]	
1	c	4/m'mm	1/2,1/2,0 [0,0,0]	
1	b	4/m'mm	0,0,1/2 [0,0,0]	
1	a	4/m'mm	0,0,0 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] p4mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

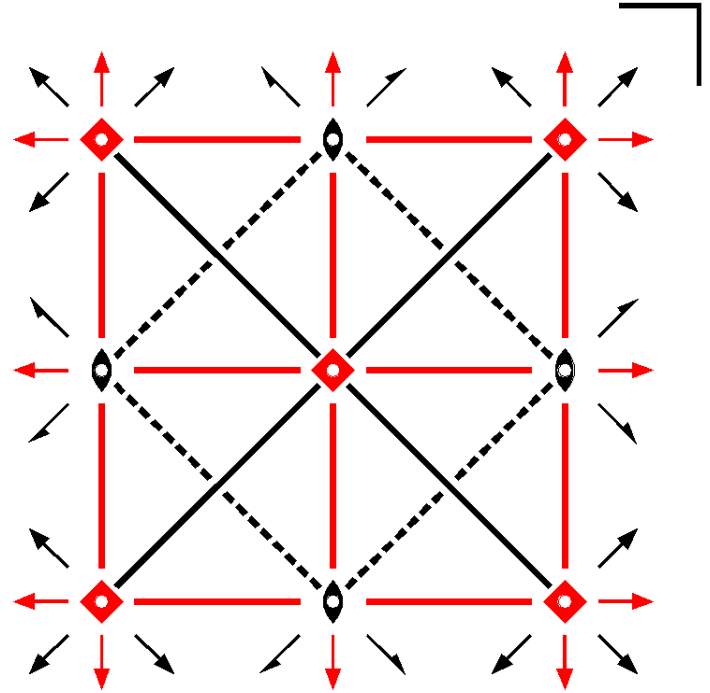
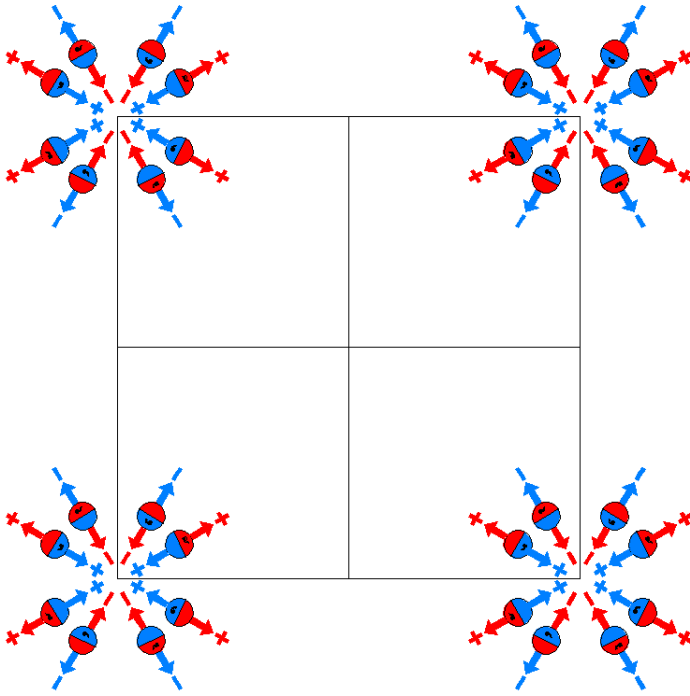
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4'/mm'm  
123.4.1002

4'/mm'm  
P4'/m2'/m'2'/m

Tetragonal



Origin at center ( 4'/mm'm )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

### Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)     | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)'         | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'         |
| (5) 2' 0,y,0<br>(2 <sub>y</sub> ' 0,0,0)'  | (6) 2' x,0,0<br>(2 <sub>x</sub> ' 0,0,0)'  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                   | (8) 2 x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)                                 |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)                 | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)    | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)' | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)' |
| (13) m' x,0,z<br>(m <sub>y</sub> ' 0,0,0)' | (14) m' 0,y,z<br>(m <sub>x</sub> ' 0,0,0)' | (15) m x,x̄,z<br>(m <sub>xȳ</sub>  0,0,0)                                | (16) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                                  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
16	u	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w] (9) $\bar{x},\bar{y},\bar{z}$ [u,v,w] (13) x, $\bar{y}$ ,z [u, $\bar{v}$ ,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ] (14) $\bar{x},\bar{y},z$ [ $\bar{u},v,w$ ]	(3) $\bar{y},x,z$ [v, $\bar{u},\bar{w}$ ] (7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ] (11) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ] (15) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ] (12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ] (16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
8	t	.m'	x,1/2,z [u,0,w] $\bar{x},1/2,\bar{z}$ [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ] x,1/2, $\bar{z}$ [ $\bar{u},0,w$ ]	1/2,x,z [0, $\bar{u},\bar{w}$ ] 1/2,x, $\bar{z}$ [0,u, $\bar{w}$ ]	1/2, $\bar{x},z$ [0,u, $\bar{w}$ ] 1/2, $\bar{x},\bar{z}$ [0, $\bar{u},\bar{w}$ ]
8	s	.m'	x,0,z [u,0,w] $\bar{x},0,\bar{z}$ [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ] x,0, $\bar{z}$ [ $\bar{u},0,w$ ]	0,x,z [0, $\bar{u},\bar{w}$ ] 0,x, $\bar{z}$ [0,u, $\bar{w}$ ]	0, $\bar{x},z$ [0,u, $\bar{w}$ ] 0, $\bar{x},\bar{z}$ [0, $\bar{u},\bar{w}$ ]
8	r	..m	x,x,z [ $\bar{u},u,0$ ] $\bar{x},x,\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},\bar{x},z$ [u, $\bar{u},0$ ] x, $\bar{x},\bar{z}$ [u,u,0]	$\bar{x},x,z$ [u,u,0] x,x, $\bar{z}$ [u, $\bar{u},0$ ]	x, $\bar{x},z$ [ $\bar{u},\bar{u},0$ ] $\bar{x},\bar{x},\bar{z}$ [ $\bar{u},u,0$ ]
8	q	m..	x,y,1/2 [0,0,w] $\bar{x},y,1/2$ [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0,w] x, $\bar{y},1/2$ [0,0,w]	$\bar{y},x,1/2$ [0,0, $\bar{w}$ ] y,x,1/2 [0,0, $\bar{w}$ ]	y, $\bar{x},1/2$ [0,0, $\bar{w}$ ] $\bar{y},\bar{x},1/2$ [0,0, $\bar{w}$ ]
8	p	m..	x,y,0 [0,0,w] $\bar{x},y,0$ [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w] x, $\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0, $\bar{w}$ ] y,x,0 [0,0, $\bar{w}$ ]	y, $\bar{x},0$ [0,0, $\bar{w}$ ] $\bar{y},\bar{x},0$ [0,0, $\bar{w}$ ]
4	o	m2'm'	x,1/2,1/2 [0,0,w]	$\bar{x},1/2,1/2$ [0,0,w]	1/2,x,1/2 [0,0, $\bar{w}$ ]	1/2, $\bar{x},1/2$ [0,0, $\bar{w}$ ]
4	n	m2'm'	x,1/2,0 [0,0,w]	$\bar{x},1/2,0$ [0,0,w]	1/2,x,0 [0,0, $\bar{w}$ ]	1/2, $\bar{x},0$ [0,0, $\bar{w}$ ]
4	m	m2'm'	x,0,1/2 [0,0,w]	$\bar{x},0,1/2$ [0,0,w]	0,x,1/2 [0,0, $\bar{w}$ ]	0, $\bar{x},1/2$ [0,0, $\bar{w}$ ]
4	l	m2'm'	x,0,0 [0,0,w]	$\bar{x},0,0$ [0,0,w]	0,x,0 [0,0, $\bar{w}$ ]	0, $\bar{x},0$ [0,0, $\bar{w}$ ]
4	k	m.2m	x,x,1/2 [0,0,0]	$\bar{x},\bar{x},1/2$ [0,0,0]	$\bar{x},x,1/2$ [0,0,0]	x, $\bar{x},1/2$ [0,0,0]
4	j	m.2m	x,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x},x,0$ [0,0,0]	x, $\bar{x},0$ [0,0,0]
4	i	2m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
2	h	4'm'm	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
2	g	4'm'm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	f	mm'm'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]		

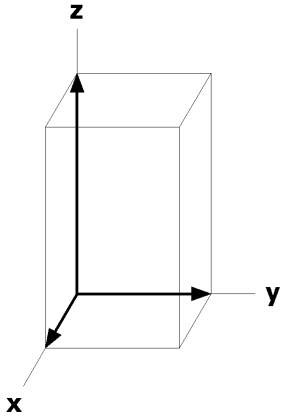
2	e	mm'm'	0,1/2,1/2 [0,0,w]	1/2,0,1/2 [0,0, $\bar{w}$ ]
1	d	4'/mm'm	1/2,1/2,1/2 [0,0,0]	
1	c	4'/mm'm	1/2,1/2,0 [0,0,0]	
1	b	4'/mm'm	0,0,1/2 [0,0,0]	
1	a	4'/mm'm	0,0,0 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



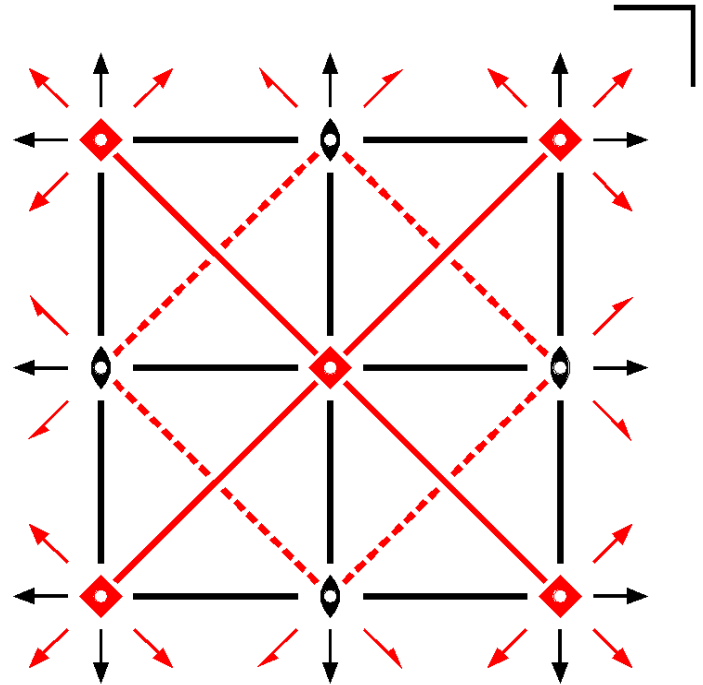
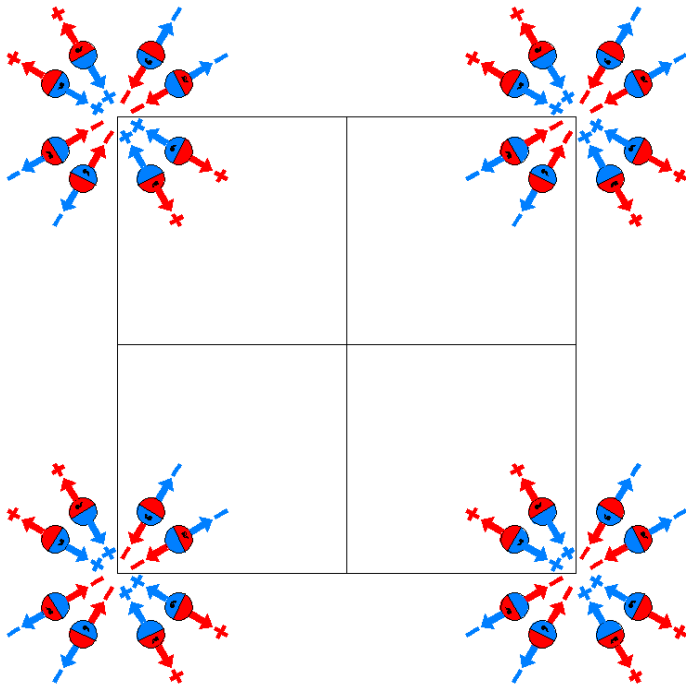
P4'/mmm'

123.5.1003

4'/mmm'

P4'/m2/m2'/m'

Tetragonal



Origin at center ( 4'/mmm' )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $x \leq y$

**Symmetry Operations**

- |  |   |   |  |
|--|---|---|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'      | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'     |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)     | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                 | (8) 2' x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)' |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)' | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'              |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)    | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (15) m' x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)'      | (16) m' x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,0)'          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	u	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (9) $\bar{x},\bar{y},\bar{z}$ [u,v,w] (13) x, $\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ] (14) $\bar{x},\bar{y},z$ [u, $\bar{v},\bar{w}$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ] (7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ] (11) y, $\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ] (15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ] (8) $\bar{y},\bar{x},\bar{z}$ [v,u,w] (12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ] (16) y,x,z [v,u,w]
8	t	.m.	x,1/2,z [0,v,0] $\bar{x},1/2,\bar{z}$ [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v},0$ ] x,1/2, $\bar{z}$ [0, $\bar{v},0$ ]	1/2,x,z [v,0,0] 1/2,x, $\bar{z}$ [ $\bar{v},0,0$ ]	1/2, $\bar{x},z$ [ $\bar{v},0,0$ ] 1/2, $\bar{x},\bar{z}$ [v,0,0]
8	s	.m.	x,0,z [0,v,0] $\bar{x},0,\bar{z}$ [0,v,0]	$\bar{x},0,z$ [0, $\bar{v},0$ ] x,0, $\bar{z}$ [0, $\bar{v},0$ ]	0,x,z [v,0,0] 0,x, $\bar{z}$ [ $\bar{v},0,0$ ]	0, $\bar{x},z$ [ $\bar{v},0,0$ ] 0, $\bar{x},\bar{z}$ [v,0,0]
8	r	..m'	x,x,z [u,u,w] $\bar{x},x,\bar{z}$ [ $\bar{u},\bar{u},\bar{w}$ ]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ] x, $\bar{x},\bar{z}$ [u, $\bar{u},\bar{w}$ ]	$\bar{x},x,z$ [u, $\bar{u},\bar{w}$ ] x,x, $\bar{z}$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},z$ [ $\bar{u},\bar{u},\bar{w}$ ] $\bar{x},\bar{x},\bar{z}$ [u,u,w]
8	q	m..	x,y,1/2 [0,0,w] $\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	$\bar{x},\bar{y},1/2$ [0,0,w] x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]	$\bar{y},x,1/2$ [0,0, $\bar{w}$ ] y,x,1/2 [0,0,w]	y, $\bar{x},1/2$ [0,0, $\bar{w}$ ] $\bar{y},\bar{x},1/2$ [0,0,w]
8	p	m..	x,y,0 [0,0,w] $\bar{x},y,0$ [0,0, $\bar{w}$ ]	$\bar{x},\bar{y},0$ [0,0,w] x, $\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{y},x,0$ [0,0, $\bar{w}$ ] y,x,0 [0,0,w]	y, $\bar{x},0$ [0,0, $\bar{w}$ ] $\bar{y},\bar{x},0$ [0,0,w]
4	o	m2m.	x,1/2,1/2 [0,0,0]	$\bar{x},1/2,1/2$ [0,0,0]	1/2,x,1/2 [0,0,0]	1/2, $\bar{x},1/2$ [0,0,0]
4	n	m2m.	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]	1/2,x,0 [0,0,0]	1/2, $\bar{x},0$ [0,0,0]
4	m	m2m.	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]	0,x,1/2 [0,0,0]	0, $\bar{x},1/2$ [0,0,0]
4	l	m2m.	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x},0$ [0,0,0]
4	k	m.2'm'	x,x,1/2 [0,0,w]	$\bar{x},\bar{x},1/2$ [0,0,w]	$\bar{x},x,1/2$ [0,0, $\bar{w}$ ]	x, $\bar{x},1/2$ [0,0, $\bar{w}$ ]
4	j	m.2'm'	x,x,0 [0,0,w]	$\bar{x},\bar{x},0$ [0,0,w]	$\bar{x},x,0$ [0,0, $\bar{w}$ ]	x, $\bar{x},0$ [0,0, $\bar{w}$ ]
4	i	2mm.	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]
2	h	4'mm'	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
2	g	4'mm'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	f	mmm.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		



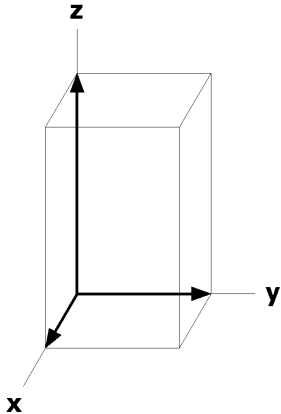
2	e	mmm.	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]
1	d	4'/mmm'	1/2,1/2,1/2 [0,0,0]	
1	c	4'/mmm'	1/2,1/2,0 [0,0,0]	
1	b	4'/mmm'	0,0,1/2 [0,0,0]	
1	a	4'/mmm'	0,0,0 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



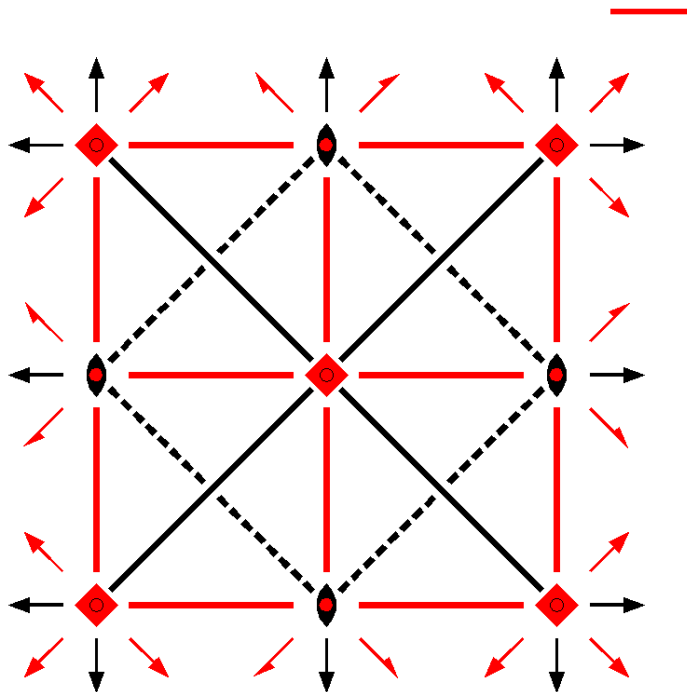
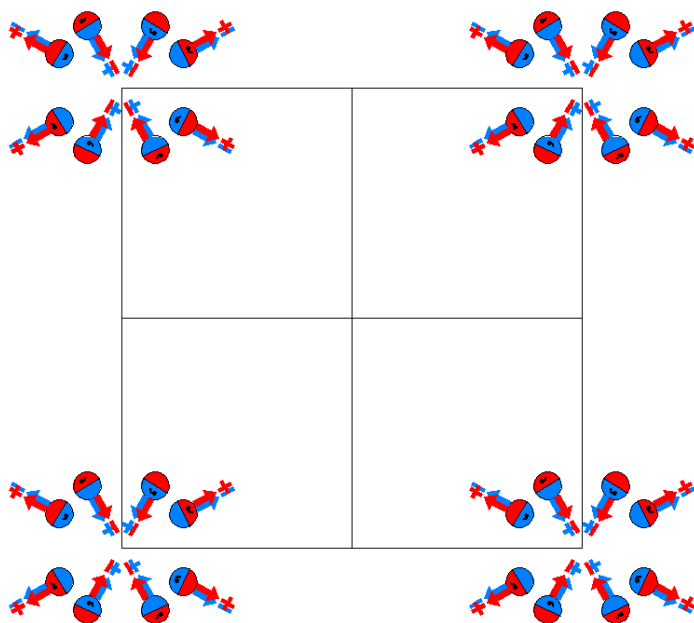
P4'/m'm'm

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4'/m'm'm

P4'/m'2/m'2'/m

Tetragonal



Origin at center ( 4'/m'm'm )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'        | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'        |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)    | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)    | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                   | (8) 2' x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)'                               |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'               | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub>  0,0,0) | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (15) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                   | (16) m x,x,z<br>(m <sub>xȳ</sub>  0,0,0)                                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	u	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
			(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(13) x, $\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},\bar{v},w$ ]	(15) $\bar{y},\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]	(16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
8	t	.m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ]	1/2,x,z [0, $\bar{u},\bar{w}$ ]	1/2, $\bar{x},z$ [0,u, $\bar{w}$ ]
			$\bar{x},1/2,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	x,1/2, $\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	1/2,x, $\bar{z}$ [0, $\bar{u},w$ ]	1/2, $\bar{x},\bar{z}$ [0,u,w]
8	s	.m'	x,0,z [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ]	0,x,z [0, $\bar{u},\bar{w}$ ]	0, $\bar{x},z$ [0,u, $\bar{w}$ ]
			$\bar{x},0,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	x,0, $\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	0,x, $\bar{z}$ [0, $\bar{u},w$ ]	0, $\bar{x},\bar{z}$ [0,u,w]
8	r	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,z$ [u,u,0]	x, $\bar{x},z$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},x,\bar{z}$ [u,u,0]	x, $\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]	x,x, $\bar{z}$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]
8	q	m'..	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},\bar{u},0$ ]	y, $\bar{x},1/2$ [ $\bar{v},u,0$ ]
			$\bar{x},y,1/2$ [ $\bar{u},\bar{v},0$ ]	x, $\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	y,x,1/2 [ $\bar{v},\bar{u},0$ ]	$\bar{y},\bar{x},1/2$ [ $\bar{v},u,0$ ]
8	p	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},\bar{u},0$ ]	y, $\bar{x},0$ [ $\bar{v},u,0$ ]
			$\bar{x},y,0$ [ $\bar{u},\bar{v},0$ ]	x, $\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	y,x,0 [ $\bar{v},\bar{u},0$ ]	$\bar{y},\bar{x},0$ [ $\bar{v},u,0$ ]
4	o	m'2m'	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	1/2,x,1/2 [0, $\bar{u},0$ ]	1/2, $\bar{x},1/2$ [0,u,0]
4	n	m'2m'	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	1/2,x,0 [0, $\bar{u},0$ ]	1/2, $\bar{x},0$ [0,u,0]
4	m	m'2m'	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,1/2 [0, $\bar{u},0$ ]	0, $\bar{x},1/2$ [0,u,0]
4	l	m'2m'	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0, $\bar{u},0$ ]	0, $\bar{x},0$ [0,u,0]
4	k	m'.2'm	x,x,1/2 [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/2$ [u,u,0]	x, $\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]
4	j	m'.2'm	x,x,0 [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [u,u,0]	x, $\bar{x},0$ [ $\bar{u},\bar{u},0$ ]
4	i	2m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]
2	h	4'm'm	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
2	g	4'm'm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	f	m'm'm'	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		

Continued

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P4'/m'm'm

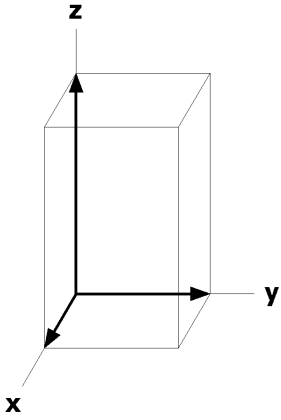
2	e	m'm'm'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]
1	d	4'/m'm'm	1/2,1/2,1/2 [0,0,0]	
1	c	4'/m'm'm	1/2,1/2,0 [0,0,0]	
1	b	4'/m'm'm	0,0,1/2 [0,0,0]	
1	a	4'/m'm'm	0,0,0 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] p4'm'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

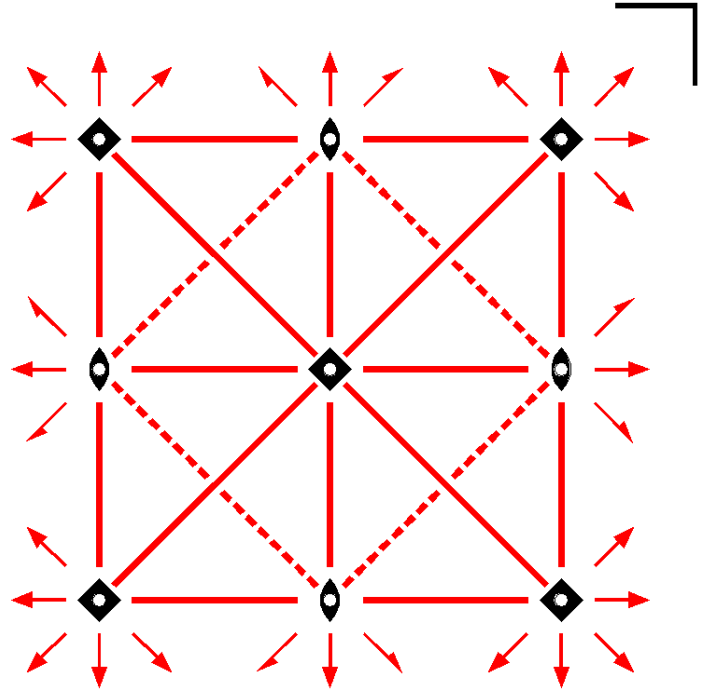
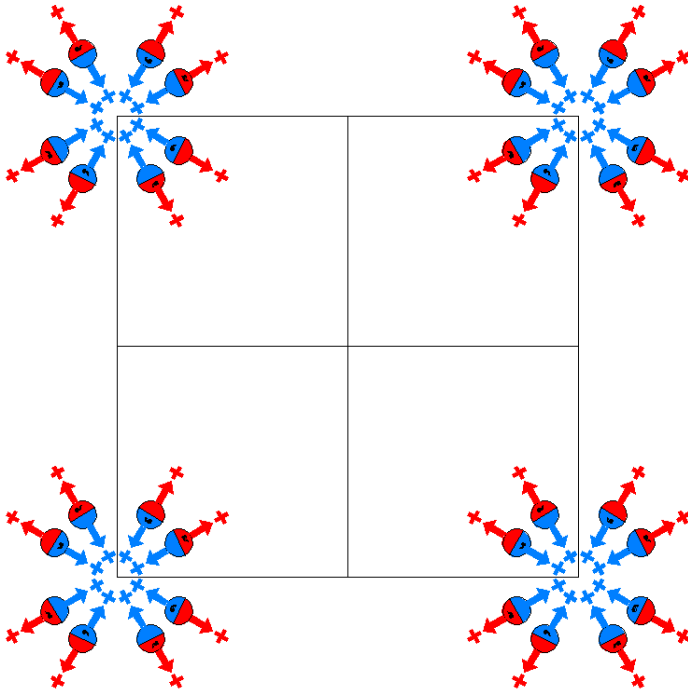
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4/mm'm'  
123.7.1005

4/mm'm'  
P4/m2'/m'2'/m'

Tetragonal



Origin at center ( 4/mm'm' )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $x \leq y$

### Symmetry Operations

- |  |   |  |   |
|--|---|--|---|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)      | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'   | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'  | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                | (8) 2' x,x̄,0<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,0)'          |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)   | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0) | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)          |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)'  | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (15) m' x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'              | (16) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
16	u	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u,v,w] (9) $\bar{x},\bar{y},\bar{z}$ [u,v,w] (13) x, $\bar{y}$ ,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ] (10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ] (14) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ] (7) y,x, $\bar{z}$ [ $\bar{v},u,w$ ] (11) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ] (15) $\bar{y},\bar{x},z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ] (8) $\bar{y},\bar{x},\bar{z}$ [v,u,w] (12) $\bar{y},x,\bar{z}$ [v, $\bar{u},w$ ] (16) y,x,z [v,u,w]
8	t	.m'	x,1/2,z [u,0,w] $\bar{x},1/2,\bar{z}$ [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ] x,1/2, $\bar{z}$ [ $\bar{u},0,w$ ]	1/2,x,z [0,u,w] 1/2,x, $\bar{z}$ [0, $\bar{u},w$ ]	1/2, $\bar{x},z$ [0, $\bar{u},w$ ] 1/2, $\bar{x},\bar{z}$ [0,u,w]
8	s	.m'	x,0,z [u,0,w] $\bar{x},0,\bar{z}$ [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ] x,0, $\bar{z}$ [ $\bar{u},0,w$ ]	0,x,z [0,u,w] 0,x, $\bar{z}$ [0, $\bar{u},w$ ]	0, $\bar{x},z$ [0, $\bar{u},w$ ] 0, $\bar{x},\bar{z}$ [0,u,w]
8	r	..m'	x,x,z [u,u,w] $\bar{x},x,\bar{z}$ [u, $\bar{u},w$ ]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ] x, $\bar{x},\bar{z}$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,z$ [ $\bar{u},u,w$ ] x,x, $\bar{z}$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},z$ [u, $\bar{u},w$ ] $\bar{x},\bar{x},\bar{z}$ [u,u,w]
8	q	m..	x,y,1/2 [0,0,w] $\bar{x},y,1/2$ [0,0,w]	$\bar{x},\bar{y},1/2$ [0,0,w] x, $\bar{y},1/2$ [0,0,w]	$\bar{y},x,1/2$ [0,0,w] y,x,1/2 [0,0,w]	y, $\bar{x},1/2$ [0,0,w] $\bar{y},\bar{x},1/2$ [0,0,w]
8	p	m..	x,y,0 [0,0,w] $\bar{x},y,0$ [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w] x, $\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0,w] y,x,0 [0,0,w]	y, $\bar{x},0$ [0,0,w] $\bar{y},\bar{x},0$ [0,0,w]
4	o	m2'm'	x,1/2,1/2 [0,0,w]	$\bar{x},1/2,1/2$ [0,0,w]	1/2,x,1/2 [0,0,w]	1/2, $\bar{x},1/2$ [0,0,w]
4	n	m2'm'	x,1/2,0 [0,0,w]	$\bar{x},1/2,0$ [0,0,w]	1/2,x,0 [0,0,w]	1/2, $\bar{x},0$ [0,0,w]
4	m	m2'm'	x,0,1/2 [0,0,w]	$\bar{x},0,1/2$ [0,0,w]	0,x,1/2 [0,0,w]	0, $\bar{x},1/2$ [0,0,w]
4	l	m2'm'	x,0,0 [0,0,w]	$\bar{x},0,0$ [0,0,w]	0,x,0 [0,0,w]	0, $\bar{x},0$ [0,0,w]
4	k	m.2'm'	x,x,1/2 [0,0,w]	$\bar{x},\bar{x},1/2$ [0,0,w]	$\bar{x},x,1/2$ [0,0,w]	x, $\bar{x},1/2$ [0,0,w]
4	j	m.2'm'	x,x,0 [0,0,w]	$\bar{x},\bar{x},0$ [0,0,w]	$\bar{x},x,0$ [0,0,w]	x, $\bar{x},0$ [0,0,w]
4	i	2m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]
2	h	4m'm'	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]		
2	g	4m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
2	f	mm'm'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]		

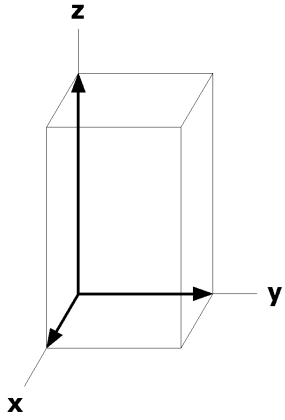
2	e	mm'm'	0,1/2,1/2 [0,0,w]	1/2,0,1/2 [0,0,w]
1	d	4/mm'm'	1/2,1/2,1/2 [0,0,w]	
1	c	4/mm'm'	1/2,1/2,0 [0,0,w]	
1	b	4/mm'm'	0,0,1/2 [0,0,w]	
1	a	4/mm'm'	0,0,0 [0,0,w]	

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



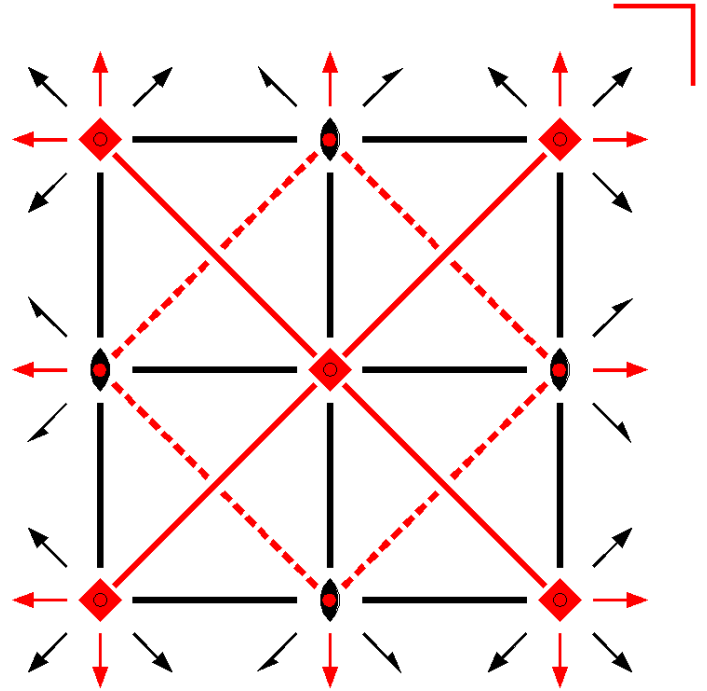
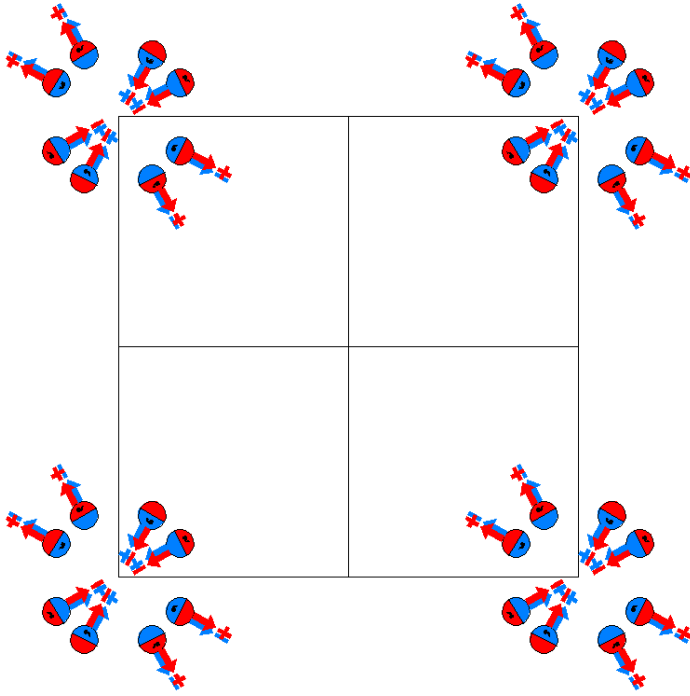
P4'/m'mm'

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4'/m'mm'

P4'/m'2'/m2/m'

Tetragonal



Origin at center ( 4'/m'mm' )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $x \leq y$

**Symmetry Operations**

- |  |   |  |   |
|--|---|--|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'                     | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'        |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                  | (8) 2 x,x̄,0<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,0)                     |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'              | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)  | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   | (15) m' x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'                              | (16) m' x,x,z<br>(m <sub>xy</sub> <sup>-</sup>  0,0,0)'                   |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	u	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u, $\bar{v}$ ,w] (9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (13) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (10) x,y, $\bar{z}$ [u,v, $\bar{w}$ ] (14) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(3) $\bar{y},x,z$ [v, $\bar{u},\bar{w}$ ] (7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ] (11) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ] (15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ] (12) $\bar{y},x,\bar{z}$ [v, $\bar{u},w$ ] (16) y,x,z [v,u,w]
8	t	.m.	x,1/2,z [0,v,0] $\bar{x},1/2,\bar{z}$ [0, $\bar{v}$ ,0]	$\bar{x},1/2,z$ [0, $\bar{v}$ ,0] x,1/2, $\bar{z}$ [0,v,0]	1/2,x,z [v,0,0] 1/2,x, $\bar{z}$ [v,0,0]	1/2, $\bar{x},z$ [ $\bar{v}$ ,0,0] 1/2, $\bar{x},\bar{z}$ [ $\bar{v}$ ,0,0]
8	s	.m.	x,0,z [0,v,0] $\bar{x},0,\bar{z}$ [0, $\bar{v}$ ,0]	$\bar{x},0,z$ [0, $\bar{v}$ ,0] x,0, $\bar{z}$ [0,v,0]	0,x,z [v,0,0] 0,x, $\bar{z}$ [v,0,0]	0, $\bar{x},z$ [ $\bar{v}$ ,0,0] 0, $\bar{x},\bar{z}$ [ $\bar{v}$ ,0,0]
8	r	..m'	x,x,z [u,u,w] $\bar{x},x,\bar{z}$ [u, $\bar{u},w$ ]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ] x, $\bar{x},\bar{z}$ [ $\bar{u},u,w$ ]	$\bar{x},x,z$ [u, $\bar{u},\bar{w}$ ] x,x, $\bar{z}$ [u,u, $\bar{w}$ ]	x, $\bar{x},z$ [ $\bar{u},u,\bar{w}$ ] $\bar{x},\bar{x},\bar{z}$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	q	m'..	x,y,1/2 [u,v,0] $\bar{x},y,1/2$ [u, $\bar{v}$ ,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ] x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]	$\bar{y},x,1/2$ [v, $\bar{u},0$ ] y,x,1/2 [v,u,0]	y, $\bar{x},1/2$ [ $\bar{v},u,0$ ] $\bar{y},\bar{x},1/2$ [ $\bar{v},\bar{u},0$ ]
8	p	m'..	x,y,0 [u,v,0] $\bar{x},y,0$ [u, $\bar{v}$ ,0]	$\bar{x},y,0$ [ $\bar{u},\bar{v},0$ ] x, $\bar{y},0$ [ $\bar{u},v,0$ ]	$\bar{y},x,0$ [v, $\bar{u},0$ ] y,x,0 [v,u,0]	y, $\bar{x},0$ [ $\bar{v},u,0$ ] $\bar{y},\bar{x},0$ [ $\bar{v},\bar{u},0$ ]
4	o	m'2'm.	x,1/2,1/2 [0,v,0]	$\bar{x},1/2,1/2$ [0, $\bar{v}$ ,0]	1/2,x,1/2 [v,0,0]	1/2, $\bar{x},1/2$ [ $\bar{v}$ ,0,0]
4	n	m'2'm.	x,1/2,0 [0,v,0]	$\bar{x},1/2,0$ [0, $\bar{v}$ ,0]	1/2,x,0 [v,0,0]	1/2, $\bar{x},0$ [ $\bar{v}$ ,0,0]
4	m	m'2'm.	x,0,1/2 [0,v,0]	$\bar{x},0,1/2$ [0, $\bar{v}$ ,0]	0,x,1/2 [v,0,0]	0, $\bar{x},1/2$ [ $\bar{v}$ ,0,0]
4	l	m'2'm.	x,0,0 [0,v,0]	$\bar{x},0,0$ [0, $\bar{v}$ ,0]	0,x,0 [v,0,0]	0, $\bar{x},0$ [ $\bar{v}$ ,0,0]
4	k	m'.2m'	x,x,1/2 [u,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/2$ [u, $\bar{u},0$ ]	x, $\bar{x},1/2$ [ $\bar{u},u,0$ ]
4	j	m'.2m'	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [u, $\bar{u},0$ ]	x, $\bar{x},0$ [ $\bar{u},u,0$ ]
4	i	2mm.	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]
2	h	4'mm'	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
2	g	4'mm'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	f	m'mm.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		

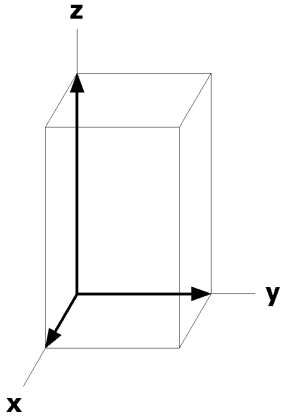
2	e	m'mm.	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]
1	d	4'/m'mm'	1/2,1/2,1/2 [0,0,0]	
1	c	4'/m'mm'	1/2,1/2,0 [0,0,0]	
1	b	4'/m'mm'	0,0,1/2 [0,0,0]	
1	a	4'/m'mm'	0,0,0 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



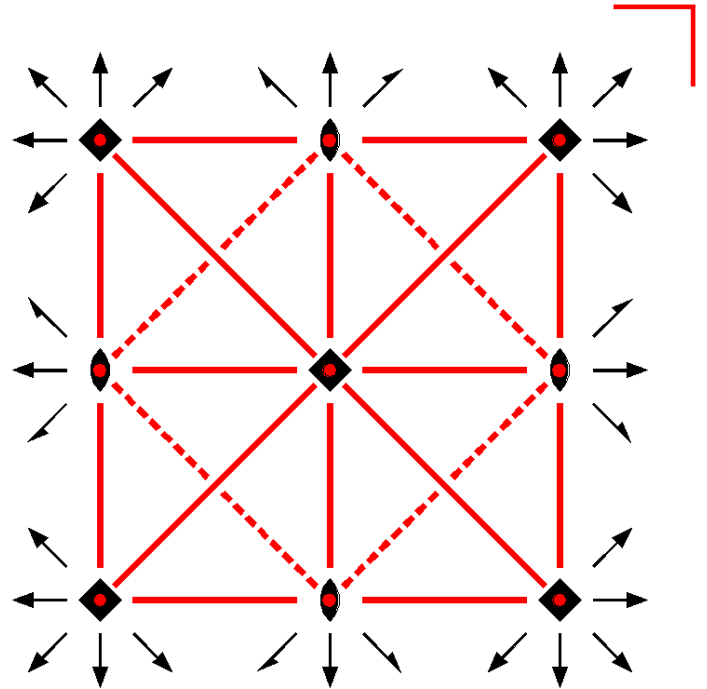
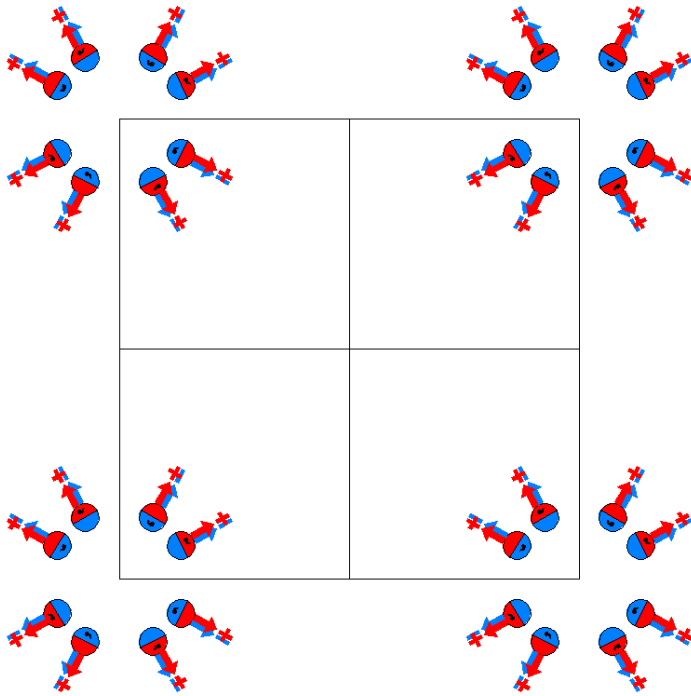
P4/m'm'm'

123.9.1007

4/m'm'm'

P4/m'2/m'2/m'

Tetragonal



Origin at center ( 4/m'm'm' )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y$

**Symmetry Operations**

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                       | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)          |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)    | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)    | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                   | (8) 2 x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)                                  |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'               | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)' | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (15) m' x,x̄,z<br>(m <sub>xȳ</sub>  0,0,0)'                              | (16) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	u	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (13) x, $\bar{y}$ ,z [u, $\bar{v}$ ,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (10) x,y, $\bar{z}$ [u,v, $\bar{w}$ ] (14) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ] (7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ] (11) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ] (15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ] (12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ] (16) y,x,z [v,u,w]
8	t	.m'	x,1/2,z [u,0,w] $\bar{x},1/2,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ] x,1/2, $\bar{z}$ [u,0, $\bar{w}$ ]	1/2,x,z [0,u,w] 1/2,x, $\bar{z}$ [0,u, $\bar{w}$ ]	1/2, $\bar{x},z$ [0, $\bar{u},w$ ] 1/2, $\bar{x},\bar{z}$ [0, $\bar{u},\bar{w}$ ]
8	s	.m'	x,0,z [u,0,w] $\bar{x},0,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	$\bar{x},0,z$ [ $\bar{u},0,w$ ] x,0, $\bar{z}$ [u,0, $\bar{w}$ ]	0,x,z [0,u,w] 0,x, $\bar{z}$ [0,u, $\bar{w}$ ]	0, $\bar{x},z$ [0, $\bar{u},w$ ] 0, $\bar{x},\bar{z}$ [0, $\bar{u},\bar{w}$ ]
8	r	..m'	x,x,z [u,u,w] $\bar{x},x,\bar{z}$ [ $\bar{u},u,\bar{w}$ ]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ] x, $\bar{x},\bar{z}$ [u, $\bar{u},\bar{w}$ ]	$\bar{x},x,z$ [ $\bar{u},u,w$ ] x,x, $\bar{z}$ [u,u, $\bar{w}$ ]	x, $\bar{x},z$ [u, $\bar{u},w$ ] $\bar{x},\bar{x},\bar{z}$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	q	m'..	x,y,1/2 [u,v,0] $\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ] x, $\bar{y},1/2$ [u, $\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},u,0$ ] y,x,1/2 [v,u,0]	y, $\bar{x},1/2$ [v, $\bar{u},0$ ] $\bar{y},\bar{x},1/2$ [ $\bar{v},\bar{u},0$ ]
8	p	m'..	x,y,0 [u,v,0] $\bar{x},y,0$ [ $\bar{u},v,0$ ]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ] x, $\bar{y},0$ [u, $\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},u,0$ ] y,x,0 [v,u,0]	y, $\bar{x},0$ [v, $\bar{u},0$ ] $\bar{y},\bar{x},0$ [ $\bar{v},\bar{u},0$ ]
4	o	m'2m'	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	1/2,x,1/2 [0,u,0]	1/2, $\bar{x},1/2$ [0, $\bar{u},0$ ]
4	n	m'2m'	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	1/2,x,0 [0,u,0]	1/2, $\bar{x},0$ [0, $\bar{u},0$ ]
4	m	m'2m'	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,1/2 [0,u,0]	0, $\bar{x},1/2$ [0, $\bar{u},0$ ]
4	l	m'2m'	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0,u,0]	0, $\bar{x},0$ [0, $\bar{u},0$ ]
4	k	m'.2m'	x,x,1/2 [u,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/2$ [ $\bar{u},u,0$ ]	x, $\bar{x},1/2$ [u, $\bar{u},0$ ]
4	j	m'.2m'	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]	x, $\bar{x},0$ [u, $\bar{u},0$ ]
4	i	2m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
2	h	4m'm'	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	g	4m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	f	m'm'm'	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		

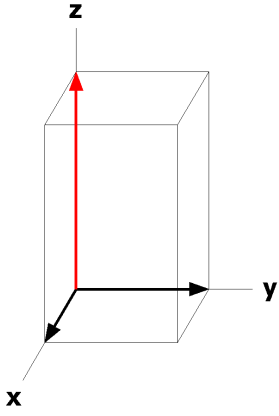
2	e	m'm'm'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]
1	d	4/m'm'm'	1/2,1/2,1/2 [0,0,0]	
1	c	4/m'm'm'	1/2,1/2,0 [0,0,0]	
1	b	4/m'm'm'	0,0,1/2 [0,0,0]	
1	a	4/m'm'm'	0,0,0 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1]  $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



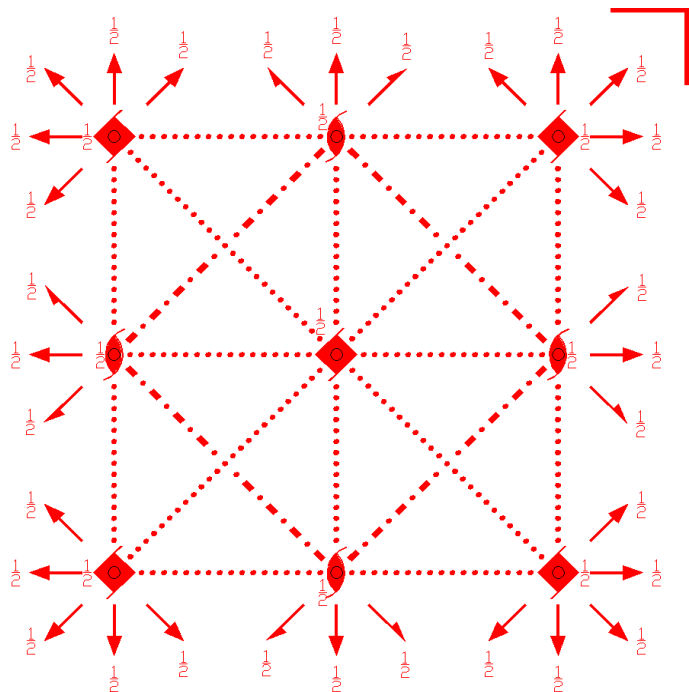
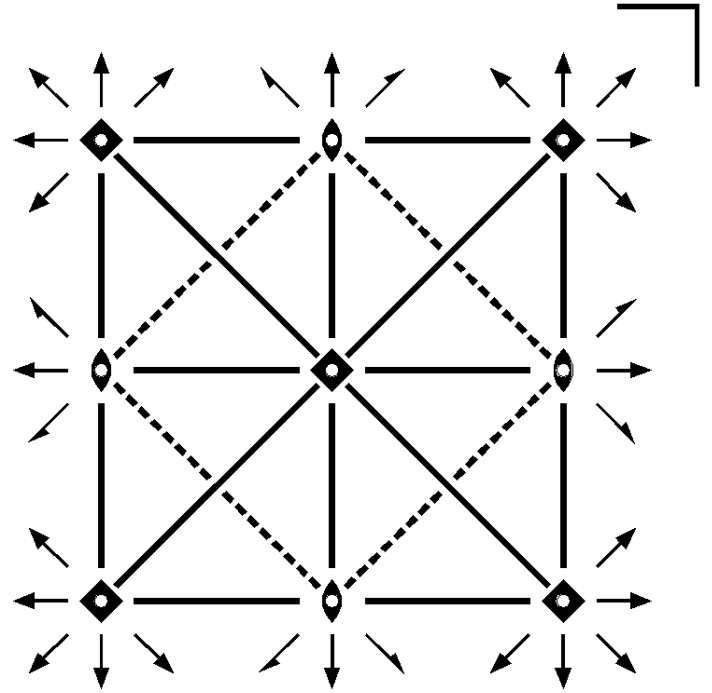
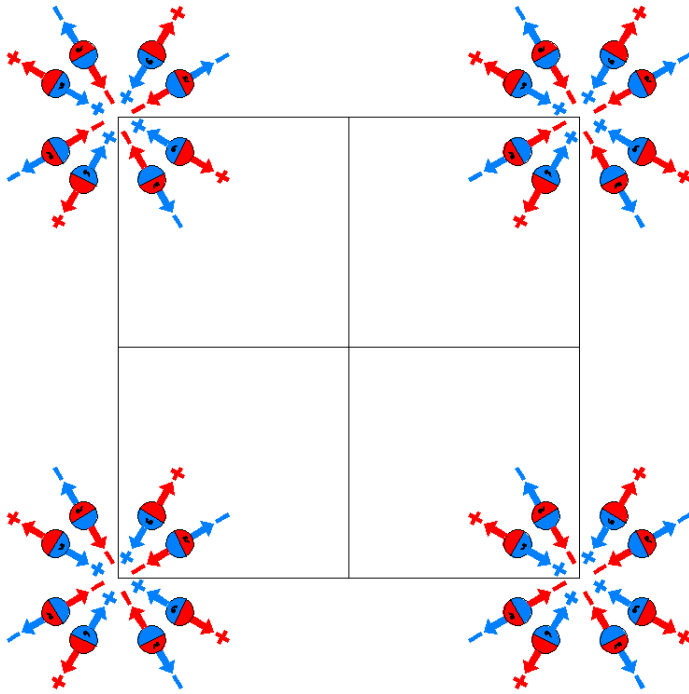
$P_{2c} 4/mmm$

123.10.1008

$4/mmm1'$

$P_{2c} 4/m2/m2/m$

Tetragonal



Origin at center ( 4/mmm )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $x \leq y$ 

## Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)
(5) 2 0,y,0 (2 <sub>y</sub>  0,0,0)	(6) 2 x,0,0 (2 <sub>x</sub>  0,0,0)	(7) 2 x,x,0 (2 <sub>xy</sub>  0,0,0)	(8) 2 x, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  0,0,0)
(9) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(10) m x,y,0 (m <sub>z</sub>  0,0,0)	(11) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z^+$  0,0,0)	(12) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z^-$  0,0,0)
(13) m x,0,z (m <sub>y</sub>  0,0,0)	(14) m 0,y,z (m <sub>x</sub>  0,0,0)	(15) m x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)	(16) m x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,0)

For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 2' (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)'	(3) 4 <sup>+</sup> ' (0,0,1) 0,0,z (4 <sub>z</sub>  0,0,1)'	(4) 4 <sup>-</sup> ' (0,0,1) 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,1)'
(5) 2' 0,y,1/2 (2 <sub>y</sub>  0,0,1)'	(6) 2' x,0,1/2 (2 <sub>x</sub>  0,0,1)'	(7) 2' x,x,1/2 (2 <sub>xy</sub>  0,0,1)'	(8) 2' x, $\bar{x}$ ,1/2 (2 <sub><math>\bar{xy}</math></sub>  0,0,1)'
(9) $\bar{1}$ ' 0,0,1/2 ( $\bar{1}$  0,0,1)'	(10) m' x,y,1/2 (m <sub>z</sub>  0,0,1)'	(11) $\bar{4}^+$ ' 0,0,z; 0,0,1/2 ( $\bar{4}_z^+$  0,0,1)'	(12) $\bar{4}^-$ ' 0,0,z; 0,0,1/2 ( $\bar{4}_z^-$  0,0,1)'
(13) c' (0,0,1) x,0,z (m <sub>y</sub>  0,0,1)'	(14) c' (0,0,1) 0,y,z (m <sub>x</sub>  0,0,1)'	(15) c' (0,0,1) x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,1)'	(16) c' (0,0,1) x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,1)'

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

## Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
32 u 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [ $v,\bar{u},w$ ]
	(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) x, $\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
	(9) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
	(13) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
16 t .m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v}$ ,0]	1/2,x,z [ $\bar{v}$ ,0,0]	1/2, $\bar{x},z$ [v,0,0]
	$\bar{x},1/2,\bar{z}$ [0,v,0]	x,1/2, $\bar{z}$ [0, $\bar{v}$ ,0]	1/2,x, $\bar{z}$ [ $\bar{v}$ ,0,0]	1/2, $\bar{x},\bar{z}$ [v,0,0]

16	s	.m.	$x,0,z [0,v,0]$	$\bar{x},0,z [0,\bar{v},0]$	$0,x,z [\bar{v},0,0]$	$0,\bar{x},z [v,0,0]$
			$\bar{x},0,\bar{z} [0,v,0]$	$x,0,\bar{z} [0,\bar{v},0]$	$0,x,\bar{z} [\bar{v},0,0]$	$0,\bar{x},\bar{z} [v,0,0]$
16	r	..m	$x,x,z [\bar{u},u,0]$	$\bar{x},\bar{x},z [u,\bar{u},0]$	$\bar{x},x,z [\bar{u},\bar{u},0]$	$x,\bar{x},z [u,u,0]$
			$\bar{x},x,\bar{z} [u,u,0]$	$x,\bar{x},\bar{z} [\bar{u},\bar{u},0]$	$x,x,\bar{z} [u,\bar{u},0]$	$\bar{x},\bar{x},\bar{z} [\bar{u},\bar{u},0]$
16	q	m..	$x,y,1/2 [u,v,0]$	$\bar{x},\bar{y},1/2 [\bar{u},\bar{v},0]$	$\bar{y},x,1/2 [\bar{v},u,0]$	$y,\bar{x},1/2 [v,\bar{u},0]$
			$\bar{x},y,1/2 [u,\bar{v},0]$	$x,\bar{y},1/2 [\bar{u},v,0]$	$y,x,1/2 [\bar{v},\bar{u},0]$	$\bar{y},\bar{x},1/2 [v,u,0]$
16	p	m..	$x,y,0 [0,0,w]$	$\bar{x},\bar{y},0 [0,0,w]$	$\bar{y},x,0 [0,0,w]$	$y,\bar{x},0 [0,0,w]$
			$\bar{x},y,0 [0,0,\bar{w}]$	$x,\bar{y},0 [0,0,\bar{w}]$	$y,x,0 [0,0,\bar{w}]$	$\bar{y},\bar{x},0 [0,0,\bar{w}]$
8	o	m'2'm.	$x,1/2,1/2 [0,v,0]$	$\bar{x},1/2,1/2 [0,\bar{v},0]$	$1/2,x,1/2 [\bar{v},0,0]$	$1/2,\bar{x},1/2 [v,0,0]$
8	n	m2m.	$x,1/2,0 [0,0,0]$	$\bar{x},1/2,0 [0,0,0]$	$1/2,x,0 [0,0,0]$	$1/2,\bar{x},0 [0,0,0]$
8	m	m'2m'.	$x,0,1/2 [0,v,0]$	$\bar{x},0,1/2 [0,\bar{v},0]$	$0,x,1/2 [\bar{v},0,0]$	$0,\bar{x},1/2 [v,0,0]$
8	l	m2m.	$x,0,0 [0,0,0]$	$\bar{x},0,0 [0,0,0]$	$0,x,0 [0,0,0]$	$0,\bar{x},0 [0,0,0]$
8	k	m'.2'm	$x,x,1/2 [\bar{u},u,0]$	$\bar{x},\bar{x},1/2 [u,\bar{u},0]$	$\bar{x},x,1/2 [\bar{u},\bar{u},0]$	$x,\bar{x},1/2 [u,u,0]$
8	j	m.2m	$x,x,0 [0,0,0]$	$\bar{x},\bar{x},0 [0,0,0]$	$\bar{x},x,0 [0,0,0]$	$x,\bar{x},0 [0,0,0]$
8	i	2mm.	$0,1/2,z [0,0,0]$	$1/2,0,z [0,0,0]$	$0,1/2,\bar{z} [0,0,0]$	$1/2,0,\bar{z} [0,0,0]$
4	h	4mm	$1/2,1/2,z [0,0,0]$	$1/2,1/2,\bar{z} [0,0,0]$		
4	g	4mm	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$		
4	f	mmm.	$0,1/2,0 [0,0,0]$	$1/2,0,0 [0,0,0]$		
4	e	m'mm.	$0,1/2,1/2 [0,0,0]$	$1/2,0,1/2 [0,0,0]$		
2	d	4/m'mm	$1/2,1/2,1/2 [0,0,0]$			
2	c	4/mmm	$1/2,1/2,0 [0,0,0]$			
2	b	4/m'mm	$0,0,1/2 [0,0,0]$			
2	a	4/mmm	$0,0,0 [0,0,0]$			

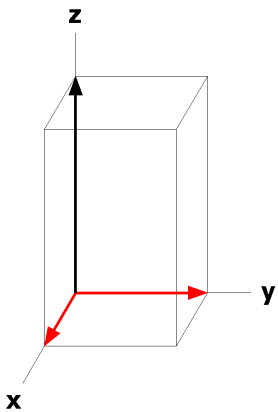
### Symmetry of Special Projections

Along  $[0,0,1]$  p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$  p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$

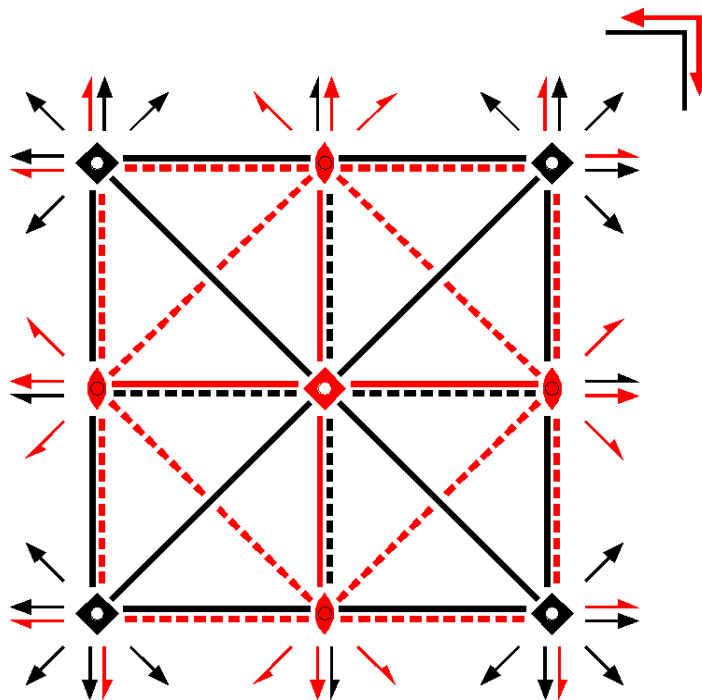
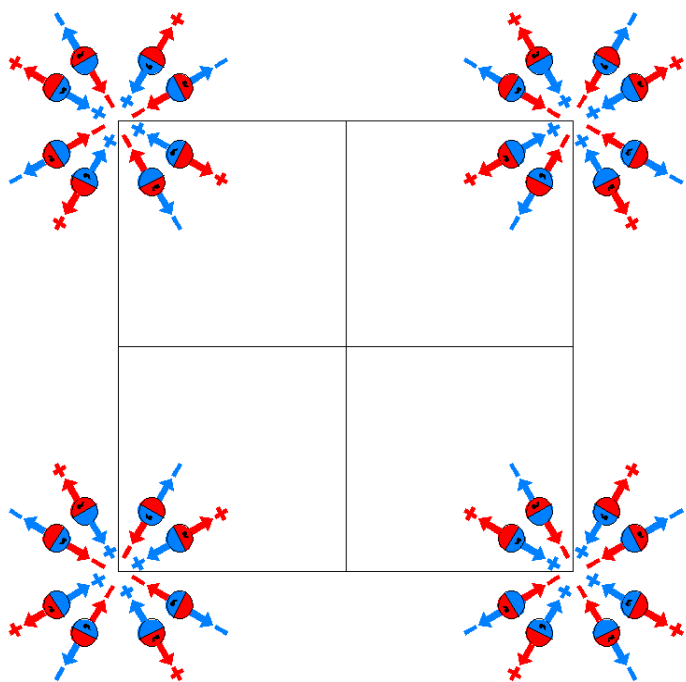




$P_4/mmm$   
123.11.1009

$4/mmm1'$   
 $P_4/m2/m2/m$

Tetragonal



Origin at center ( $4/mmm$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                      | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)         |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                  | (8) 2 x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)                                 |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)              | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (15) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                                | (16) m x,x,z<br>(m <sub>xȳ</sub>  0,0,0)                                 |

For (1,0,0)<sup>+</sup> + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> -1/2,1/2,z (4 <sub>z</sub>  1,0,0)'	(4) 4' 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,0)'
(5) 2' 1/2,y,0 (2 <sub>y</sub>  1,0,0)'	(6) 2' (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)'	(7) 2' (1/2,1/2,0) x+1/2,x,0 (2 <sub>xy</sub>  1,0,0)'	(8) 2' (1/2,-1/2,0) x+1/2,x̄,0 (2 <sub>xy</sub> <sup>-</sup>  1,0,0)'
(9) 1̄' 1/2,0,0 (1̄ 1,0,0)'	(10) a' (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)'	(11) 4 <sup>+</sup> 1/2,-1/2,z; 1/2,-1/2,0 (4 <sub>z</sub>  1,0,0)'	(12) 4' 1/2,1/2,z; 1/2,1/2,0 (4 <sub>z</sub> <sup>-1</sup>  1,0,0)'
(13) a' (1,0,0) x,0,z (m <sub>y</sub>  1,0,0)'	(14) m' 1/2,y,z (m <sub>x</sub>  1,0,0)'	(15) g' (1/2,-1/2,0) x+1/2,x̄,z (m <sub>xy</sub>  1,0,0)'	(16) g' (1/2,1/2,0) x+1/2,x,z (m <sub>xy</sub> <sup>-</sup>  1,0,0)'

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1,0,0) <sup>+</sup> +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	u	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w]	(3) ȳ,x,z [v̄,u,w]	(4) y,x,z [v,ū,w]
			(5) x̄,y,z [ū,v,w]	(6) x,y,z [u,v̄,w]	(7) y,x,z [v,u,w]	(8) ȳ,x,z [v̄,ū,w]
			(9) x̄,ȳ,z [u,v,w]	(10) x,y,z [ū,v̄,w]	(11) y,x,z [v̄,u,w]	(12) ȳ,x,z [v,ū,w]
			(13) x,y,z [ū,v,w]	(14) x̄,y,z [u,v̄,w]	(15) ȳ,x,z [v,u,w]	(16) y,x,z [v̄,ū,w]
16	t	.m'	x,1/2,z [u,0,w]	x̄,1/2,z [u,0,w̄]	1/2,x,z [0,ū,w]	1/2,x̄,z [0,ū,w]
			x̄,1/2,z [ū,0,w̄]	x,1/2,z [u,0,w]	1/2,x,z [0,u,w̄]	1/2,x̄,z [0,u,w]
16	s	.m.	x,0,z [0,v,0]	x̄,0,z [0,v̄,0]	0,x,z [v̄,0,0]	0,x̄,z [v,0,0]
			x̄,0,z [0,v,0]	x,0,z [0,v̄,0]	0,x,z [v,0,0]	0,x̄,z [v̄,0,0]
16	r	..m	x,x,z [ū,u,0]	x̄,x,z [u,ū,0]	x̄,x,z [ū,ū,0]	x,x,z [u,u,0]
			x̄,x,z [u,u,0]	x,x,z [ū,ū,0]	x,x,z [u,ū,0]	x̄,x,z [ū,ū,0]
16	q	m..	x,y,1/2 [0,0,w]	x̄,ȳ,1/2 [0,0,w]	ȳ,x,1/2 [0,0,w]	y,x̄,1/2 [0,0,w]
			x̄,y,1/2 [0,0,w̄]	x,ȳ,1/2 [0,0,w̄]	y,x,1/2 [0,0,w̄]	ȳ,x̄,1/2 [0,0,w̄]
16	p	m..	x,y,0 [0,0,w]	x̄,ȳ,0 [0,0,w]	ȳ,x,0 [0,0,w]	y,x̄,0 [0,0,w]
			x̄,y,0 [0,0,w̄]	x,ȳ,0 [0,0,w̄]	y,x,0 [0,0,w̄]	ȳ,x̄,0 [0,0,w̄]
8	o	m2'm'	x,1/2,1/2 [0,0,w]	x̄,1/2,1/2 [0,0,w̄]	1/2,x,1/2 [0,0,w̄]	1/2,x̄,1/2 [0,0,w]
8	n	m2'm'	x,1/2,0 [0,0,w]	x̄,1/2,0 [0,0,w̄]	1/2,x,0 [0,0,w̄]	1/2,x̄,0 [0,0,w]
8	m	m2m.	x,0,1/2 [0,0,0]	x̄,0,1/2 [0,0,0]	0,x,1/2 [0,0,0]	0,x̄,1/2 [0,0,0]

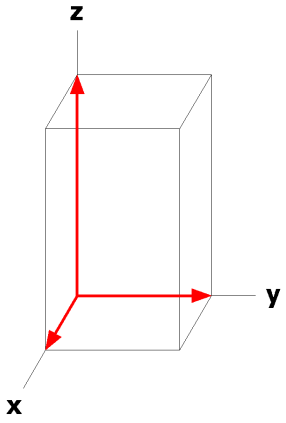
8	l	m2m.	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,0 [0,0,0]	$0,\bar{x},0$ [0,0,0]
8	k	m.2m	x,x,1/2 [0,0,0]	$\bar{x},\bar{x},1/2$ [0,0,0]	$\bar{x},x,1/2$ [0,0,0]	$x,\bar{x},1/2$ [0,0,0]
8	j	m.2m	x,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x},x,0$ [0,0,0]	$x,\bar{x},0$ [0,0,0]
8	i	2'mm'.	0,1/2,z [u,0,0]	1/2,0,z [0, $\bar{u}$ ,0]	0,1/2, $\bar{z}$ [ $\bar{u}$ ,0,0]	1/2,0, $\bar{z}$ [0,u,0]
4	h	4'm'm	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
4	g	4mm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4	f	mmm'.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
4	e	mmm'.	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	d	4'/mm'm	1/2,1/2,1/2 [0,0,0]			
2	c	4'/mm'm	1/2,1/2,0 [0,0,0]			
2	b	4/mmm	0,0,1/2 [0,0,0]			
2	a	4/mmm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

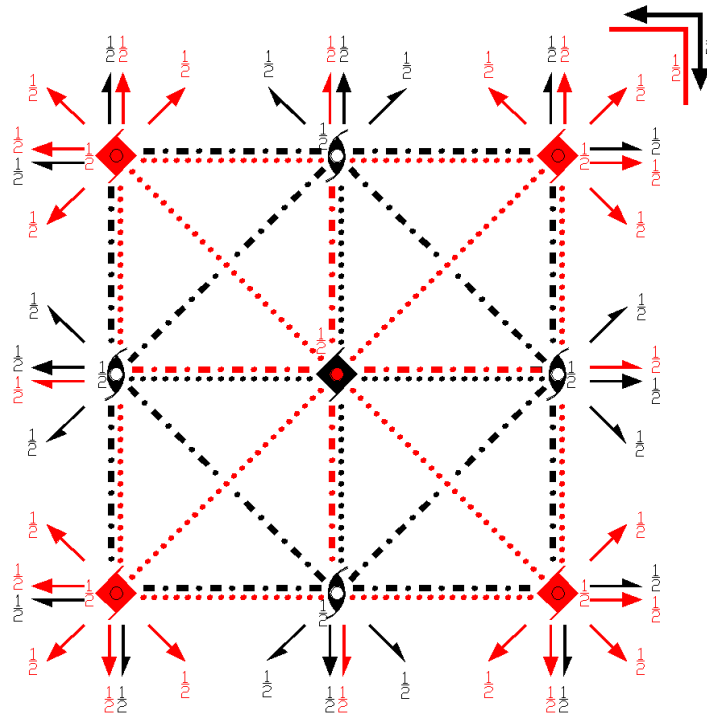
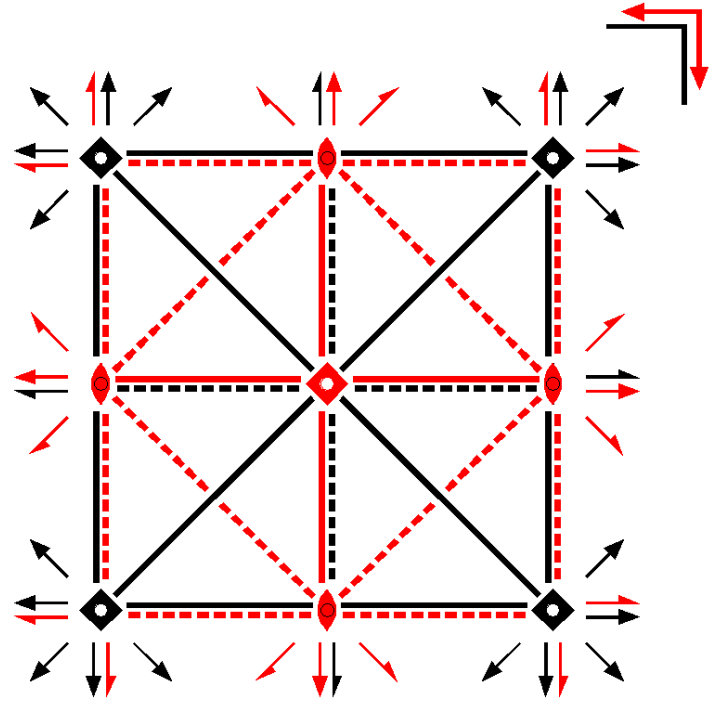
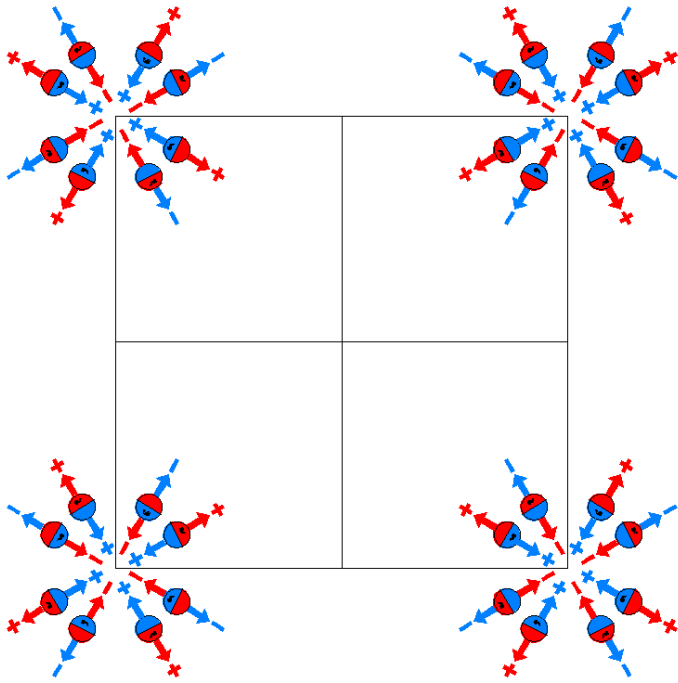
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_14/mmm$   
123.12.1010

$4/mmm1'$   
 $P_14/m2/m2/m$

Tetragonal



Origin at center ( 4/mmm )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y$ 

## Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)
(5) 2 0,y,0 (2 <sub>y</sub>  0,0,0)	(6) 2 x,0,0 (2 <sub>x</sub>  0,0,0)	(7) 2 x,x,0 (2 <sub>xy</sub>  0,0,0)	(8) 2 x, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  0,0,0)
(9) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(10) m x,y,0 (m <sub>z</sub>  0,0,0)	(11) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z^+$  0,0,0)	(12) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z^-$  0,0,0)
(13) m x,0,z (m <sub>y</sub>  0,0,0)	(14) m 0,y,z (m <sub>x</sub>  0,0,0)	(15) m x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)	(16) m x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,0)

For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> ' -1/2,1/2,z (4 <sub>z</sub>  1,0,0)'	(4) 4 <sup>-</sup> ' 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,0)'
(5) 2' 1/2,y,0 (2 <sub>y</sub>  1,0,0)'	(6) 2' (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)'	(7) 2' (1/2,1/2,0) x+1/2,x,0 (2 <sub>xy</sub>  1,0,0)'	(8) 2' (1/2,-1/2,0) x+1/2, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  1,0,0)'
(9) $\bar{1}$ ' 1/2,0,0 ( $\bar{1}$  1,0,0)'	(10) a' (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)'	(11) $\bar{4}^+$ ' 1/2,-1/2,z; 1/2,-1/2,0 ( $\bar{4}_z^+$  1,0,0)'	(12) $\bar{4}^-$ ' 1/2,1/2,z; 1/2,1/2,0 ( $\bar{4}_z^-$  1,0,0)'
(13) a' (1,0,0) x,0,z (m <sub>y</sub>  1,0,0)'	(14) m' 1/2,y,z (m <sub>x</sub>  1,0,0)'	(15) g' (1/2,-1/2,0) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1,0,0)'	(16) g' (1/2,1/2,0) x+1/2,x,z (m <sub><math>\bar{xy}</math></sub>  1,0,0)'

Generators selected (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5); (9).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

		(0,0,0) +	(1,0,0)' +		
32	u 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ]
		(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
		(9) $\bar{x},\bar{y},z$ [u,v,w]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [v, $\bar{u},w$ ]
		(13) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ]	(16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
16	t .m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [u,0, $\bar{w}$ ]	1/2,x,z [0, $\bar{u},\bar{w}$ ]	1/2, $\bar{x},z$ [0, $\bar{u},w$ ]
		$\bar{x},1/2,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	x,1/2, $\bar{z}$ [ $\bar{u},0,w$ ]	1/2,x, $\bar{z}$ [0,u, $\bar{w}$ ]	1/2, $\bar{x},\bar{z}$ [0,u,w]

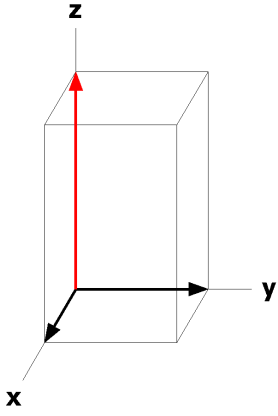
16	s	.m.	$x,0,z [0,v,0]$	$\bar{x},0,z [0,\bar{v},0]$	$0,x,z [\bar{v},0,0]$	$0,\bar{x},z [v,0,0]$
			$\bar{x},0,\bar{z} [0,v,0]$	$x,0,\bar{z} [0,\bar{v},0]$	$0,x,\bar{z} [\bar{v},0,0]$	$0,\bar{x},\bar{z} [v,0,0]$
16	r	..m	$x,x,z [\bar{u},u,0]$	$\bar{x},\bar{x},z [u,\bar{u},0]$	$\bar{x},x,z [\bar{u},\bar{u},0]$	$x,\bar{x},z [u,u,0]$
			$\bar{x},x,\bar{z} [u,u,0]$	$x,\bar{x},\bar{z} [\bar{u},\bar{u},0]$	$x,x,\bar{z} [u,\bar{u},0]$	$\bar{x},\bar{x},\bar{z} [\bar{u},u,0]$
16	q	m'..	$x,y,1/2 [u,v,0]$	$\bar{x},\bar{y},1/2 [\bar{u},\bar{v},0]$	$\bar{y},x,1/2 [\bar{v},u,0]$	$y,\bar{x},1/2 [v,\bar{u},0]$
			$\bar{x},y,1/2 [u,\bar{v},0]$	$x,\bar{y},1/2 [\bar{u},v,0]$	$y,x,1/2 [\bar{v},\bar{u},0]$	$\bar{y},\bar{x},1/2 [v,u,0]$
16	p	m..	$x,y,0 [0,0,w]$	$\bar{x},\bar{y},0 [0,0,w]$	$\bar{y},x,0 [0,0,w]$	$y,\bar{x},0 [0,0,w]$
			$\bar{x},y,0 [0,0,\bar{w}]$	$x,\bar{y},0 [0,0,\bar{w}]$	$y,x,0 [0,0,\bar{w}]$	$\bar{y},\bar{x},0 [0,0,\bar{w}]$
8	o	m'2m'.	$x,1/2,1/2 [u,0,0]$	$\bar{x},1/2,1/2 [u,0,0]$	$1/2,x,1/2 [0,\bar{u},0]$	$1/2,\bar{x},1/2 [0,\bar{u},0]$
8	n	m2'm'.	$x,1/2,0 [0,0,w]$	$\bar{x},1/2,0 [0,0,\bar{w}]$	$1/2,x,0 [0,0,\bar{w}]$	$1/2,\bar{x},0 [0,0,w]$
8	m	m'2'm.	$x,0,1/2 [0,v,0]$	$\bar{x},0,1/2 [0,\bar{v},0]$	$0,x,1/2 [\bar{v},0,0]$	$0,\bar{x},1/2 [v,0,0]$
8	l	m2m.	$x,0,0 [0,0,0]$	$\bar{x},0,0 [0,0,0]$	$0,x,0 [0,0,0]$	$0,\bar{x},0 [0,0,0]$
8	k	m'.2'm	$x,x,1/2 [\bar{u},u,0]$	$\bar{x},\bar{x},1/2 [u,\bar{u},0]$	$\bar{x},x,1/2 [\bar{u},\bar{u},0]$	$x,\bar{x},1/2 [u,u,0]$
8	j	m.2m	$x,x,0 [0,0,0]$	$\bar{x},\bar{x},0 [0,0,0]$	$\bar{x},x,0 [0,0,0]$	$x,\bar{x},0 [0,0,0]$
8	i	2'mm'.	$0,1/2,z [u,0,0]$	$1/2,0,z [0,\bar{u},0]$	$0,1/2,\bar{z} [\bar{u},0,0]$	$1/2,0,\bar{z} [0,u,0]$
4	h	4'm'm	$1/2,1/2,z [0,0,0]$	$1/2,1/2,\bar{z} [0,0,0]$		
4	g	4mm	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$		
4	f	mm'm.	$0,1/2,0 [0,0,0]$	$1/2,0,0 [0,0,0]$		
4	e	m'mm'.	$0,1/2,1/2 [u,0,0]$	$1/2,0,1/2 [0,\bar{u},0]$		
2	d	4'/m'm'm	$1/2,1/2,1/2 [0,0,0]$			
2	c	4'/mm'm	$1/2,1/2,0 [0,0,0]$			
2	b	4/m'mm	$0,0,1/2 [0,0,0]$			
2	a	4/mmm	$0,0,0 [0,0,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$  p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

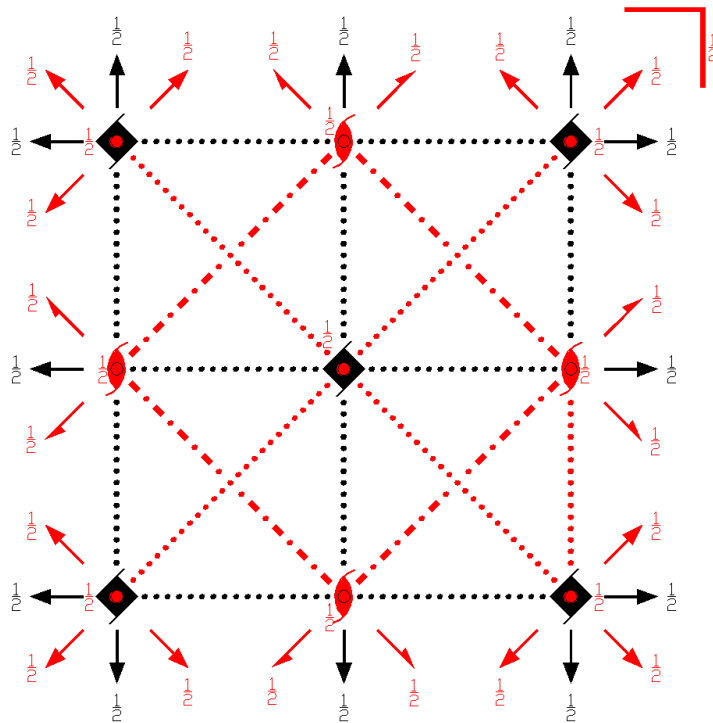
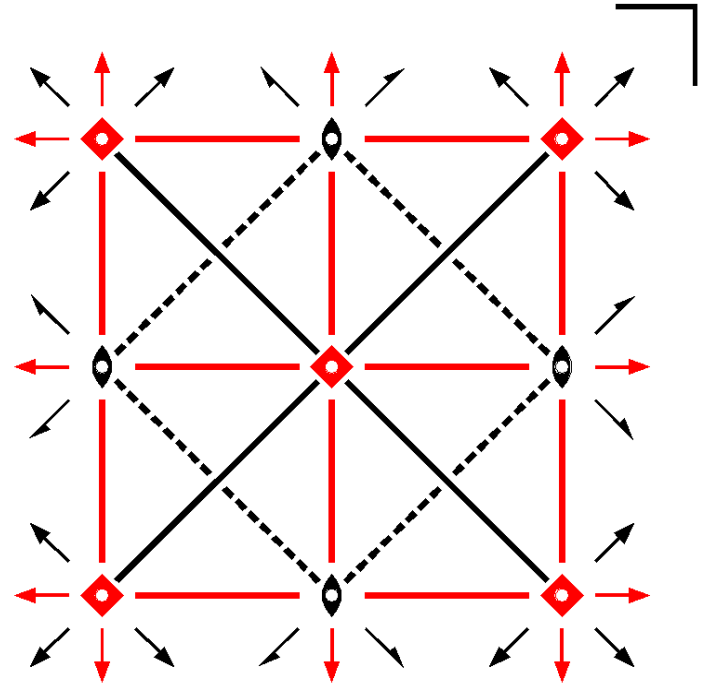
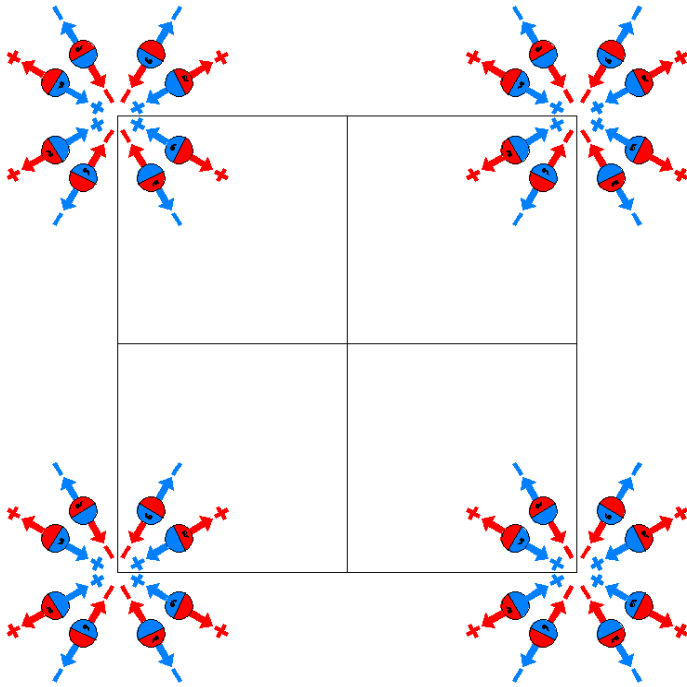
Along  $[1,1,0]$  p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$



$P_{2c} 4'/mm'm$   
123.13.1011

$4/mmm1'$   
 $P_{2c} 4'/m2'/m'2'/m$

Tetragonal



Origin at center ( 4'/mm'm )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $x \leq y$ 

## Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)'	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(5) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(6) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'	(7) 2 x,x,0 (2 <sub>xy</sub>  0,0,0)	(8) 2 x, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  0,0,0)
(9) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(10) m x,y,0 (m <sub>z</sub>  0,0,0)	(11) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z^+$  0,0,0)'	(12) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z^-$  0,0,0)'
(13) m' x,0,z (m <sub>y</sub>  0,0,0)'	(14) m' 0,y,z (m <sub>x</sub>  0,0,0)'	(15) m x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)	(16) m x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,0)

For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 2' (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)'	(3) 4 <sup>+</sup> (0,0,1) 0,0,z (4 <sub>z</sub>  0,0,1)	(4) 4 <sup>-</sup> (0,0,1) 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,1)
(5) 2 0,y,1/2 (2 <sub>y</sub>  0,0,1)	(6) 2 x,0,1/2 (2 <sub>x</sub>  0,0,1)	(7) 2' x,x,1/2 (2 <sub>xy</sub>  0,0,1)'	(8) 2' x, $\bar{x}$ ,1/2 (2 <sub><math>\bar{xy}</math></sub>  0,0,1)'
(9) $\bar{1}$ ' 0,0,1/2 ( $\bar{1}$ ' 0,0,1)'	(10) m' x,y,1/2 (m <sub>z</sub> ' 0,0,1)'	(11) $\bar{4}^+$ 0,0,z; 0,0,1/2 ( $\bar{4}_z^+$  0,0,1)	(12) $\bar{4}^-$ 0,0,z; 0,0,1/2 ( $\bar{4}_z^-$ ' 0,0,1)
(13) c (0,0,1) x,0,z (m <sub>y</sub>  0,0,1)	(14) c (0,0,1) 0,y,z (m <sub>x</sub>  0,0,1)	(15) c' (0,0,1) x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,1)'	(16) c' (0,0,1) x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,1)'

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

## Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
32 u 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $v,\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
	(5) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(6) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(7) y,x, $\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
	(9) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
	(13) x, $\bar{y},z$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(15) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
16 t .m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ]	1/2,x,z [0, $\bar{u},\bar{w}$ ]	1/2, $\bar{x},z$ [0,u, $\bar{w}$ ]
	$\bar{x},1/2,\bar{z}$ [ $u,0,w$ ]	x,1/2, $\bar{z}$ [ $\bar{u},0,w$ ]	1/2,x, $\bar{z}$ [0,u, $\bar{w}$ ]	1/2, $\bar{x},\bar{z}$ [0, $\bar{u},\bar{w}$ ]



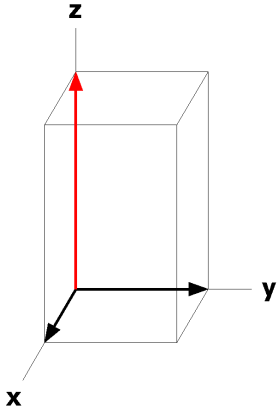
16	s	.m'	x,0,z [u,0,w]	$\bar{x},0,z [\bar{u},0,w]$	0,x,z [0, $\bar{u},\bar{w}$ ]	0, $\bar{x},z [0,u,\bar{w}]$
			$\bar{x},0,\bar{z} [u,0,w]$	x,0, $\bar{z} [\bar{u},0,w]$	0,x, $\bar{z} [0,u,\bar{w}]$	0, $\bar{x},\bar{z} [0,\bar{u},\bar{w}]$
16	r	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z [u,\bar{u},0]$	$\bar{x},x,z [u,u,0]$	x, $\bar{x},z [\bar{u},\bar{u},0]$
			$\bar{x},x,\bar{z} [\bar{u},\bar{u},0]$	x, $\bar{x},\bar{z} [u,u,0]$	x,x, $\bar{z} [u,\bar{u},0]$	$\bar{x},\bar{x},\bar{z} [\bar{u},u,0]$
16	q	m'..	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2 [\bar{u},\bar{v},0]$	$\bar{y},x,1/2 [v,\bar{u},0]$	y, $\bar{x},1/2 [\bar{v},u,0]$
			$\bar{x},y,1/2 [\bar{u},v,0]$	x, $\bar{y},1/2 [u,\bar{v},0]$	y,x,1/2 [ $\bar{v},\bar{u},0$ ]	$\bar{y},\bar{x},1/2 [v,u,0]$
16	p	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0 [0,0,w]$	$\bar{y},x,0 [0,0,\bar{w}]$	y, $\bar{x},0 [0,0,\bar{w}]$
			$\bar{x},y,0 [0,0,w]$	x, $\bar{y},0 [0,0,w]$	y,x,0 [0,0, $\bar{w}$ ]	$\bar{y},\bar{x},0 [0,0,\bar{w}]$
8	o	m'2m'	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2 [\bar{u},0,0]$	1/2,x,1/2 [0, $\bar{u},0$ ]	1/2, $\bar{x},1/2 [0,u,0]$
8	n	m2'm'	x,1/2,0 [0,0,w]	$\bar{x},1/2,0 [0,0,w]$	1/2,x,0 [0,0, $\bar{w}$ ]	1/2, $\bar{x},0 [0,0,\bar{w}]$
8	m	m'2m'	x,0,1/2 [u,0,0]	$\bar{x},0,1/2 [\bar{u},0,0]$	0,x,1/2 [0, $\bar{u},0$ ]	0, $\bar{x},1/2 [0,u,0]$
8	l	m2'm'	x,0,0 [0,0,w]	$\bar{x},0,0 [0,0,w]$	0,x,0 [0,0, $\bar{w}$ ]	0, $\bar{x},0 [0,0,\bar{w}]$
8	k	m'.2'm	x,x,1/2 [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},1/2 [u,\bar{u},0]$	$\bar{x},x,1/2 [u,u,0]$	x, $\bar{x},1/2 [\bar{u},\bar{u},0]$
8	j	m.2m	x,x,0 [0,0,w]	$\bar{x},\bar{x},0 [0,0,\bar{w}]$	$\bar{x},x,0 [0,0,w]$	x, $\bar{x},0 [0,0,\bar{w}]$
8	i	2m'm'	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z} [0,0,0]$	1/2,0, $\bar{z} [0,0,0]$
4	h	4'm'm	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z} [0,0,0]$		
4	g	4'm'm	0,0,z [0,0,0]	0,0, $\bar{z} [0,0,0]$		
4	f	mm'm'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]		
4	e	m'mm.	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	d	4'/m'm'm	1/2,1/2,1/2 [0,0,0]			
2	c	4'/mm'm	1/2,1/2,0 [0,0,0]			
2	b	4'/m'm'm	0,0,1/2 [0,0,0]			
2	a	4'/mm'm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'2'mm1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

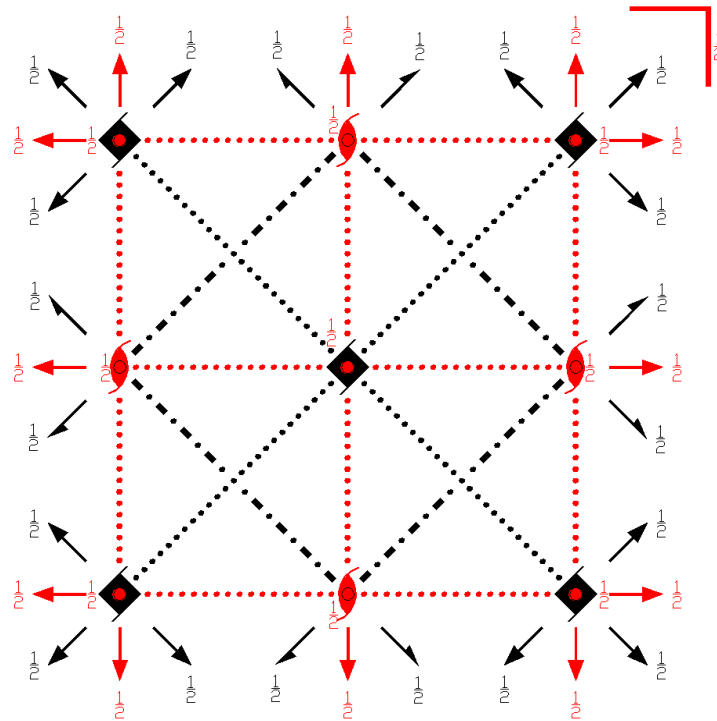
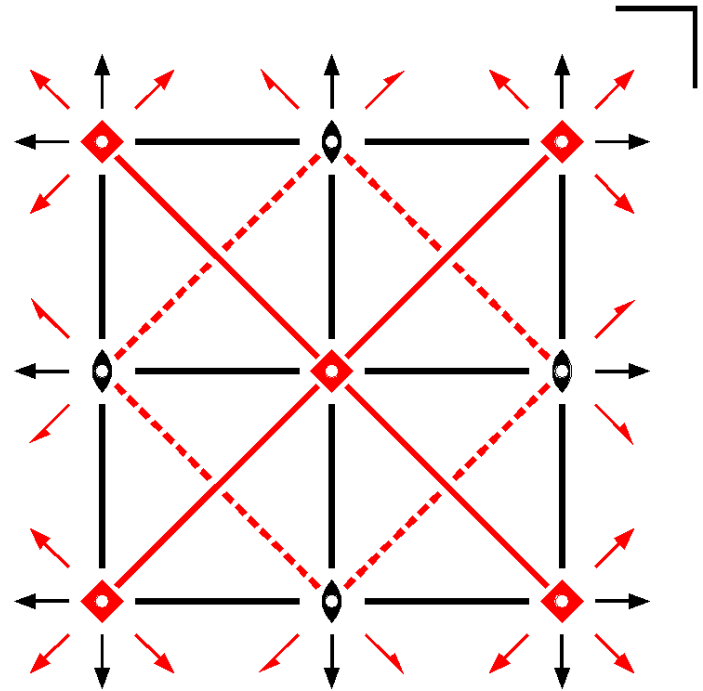
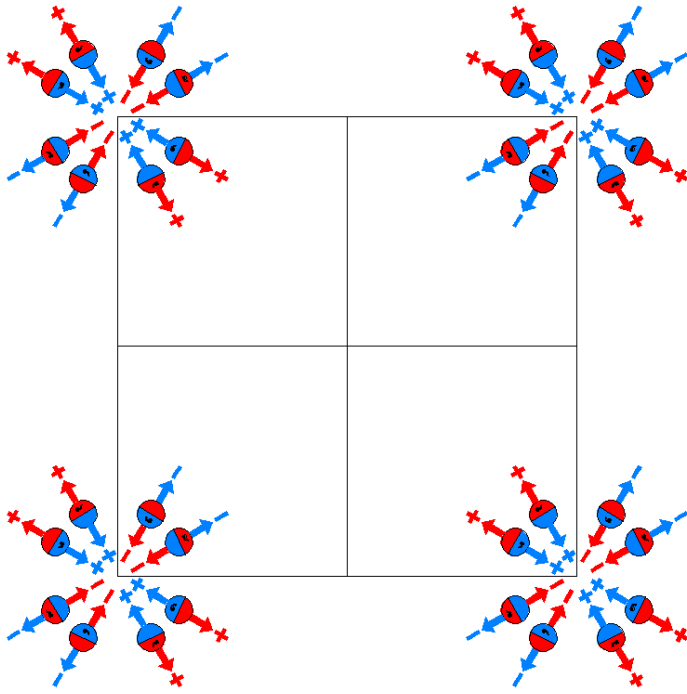
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_{2c} 4'/mmm'$   
123.14.1012

$4/mmm1'$   
 $P_{2c} 4'/m2/m2'/m'$

Tetragonal



Origin at center ( 4'/mmm' )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y$ 

## Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)'	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(5) 2 0,y,0 (2 <sub>y</sub>  0,0,0)	(6) 2 x,0,0 (2 <sub>x</sub>  0,0,0)	(7) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) 2' x, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  0,0,0)'
(9) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(10) m x,y,0 (m <sub>z</sub>  0,0,0)	(11) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z^+$  0,0,0)'	(12) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z^-$  0,0,0)'
(13) m x,0,z (m <sub>y</sub>  0,0,0)	(14) m 0,y,z (m <sub>x</sub>  0,0,0)	(15) m' x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)'	(16) m' x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,0)'

For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 2' (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)'	(3) 4 <sup>+</sup> (0,0,1) 0,0,z (4 <sub>z</sub>  0,0,1)	(4) 4 <sup>-</sup> (0,0,1) 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,1)
(5) 2' 0,y,1/2 (2 <sub>y</sub>  0,0,1)'	(6) 2' x,0,1/2 (2 <sub>x</sub>  0,0,1)'	(7) 2 x,x,1/2 (2 <sub>xy</sub>  0,0,1)	(8) 2 x, $\bar{x}$ ,1/2 (2 <sub><math>\bar{xy}</math></sub>  0,0,1)
(9) $\bar{1}$ ' 0,0,1/2 ( $\bar{1}$  0,0,1)'	(10) m' x,y,1/2 (m <sub>z</sub>  0,0,1)'	(11) $\bar{4}^+$ 0,0,z; 0,0,1/2 ( $\bar{4}_z^+$  0,0,1)	(12) $\bar{4}^-$ 0,0,z; 0,0,1/2 ( $\bar{4}_z^-$  0,0,1)
(13) c' (0,0,1) x,0,z (m <sub>y</sub>  0,0,1)'	(14) c' (0,0,1) 0,y,z (m <sub>x</sub>  0,0,1)'	(15) c (0,0,1) x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,1)	(16) c (0,0,1) x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,1)

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

## Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
32 u 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},w$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,w$ ]
	(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) x, $\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},u,w$ ]	(8) $\bar{y},x,\bar{z}$ [ $\bar{v},u,w$ ]
	(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
	(13) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(16) y,x,z [ $\bar{v},u,w$ ]
16 t .m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0, $\bar{v}$ ,0]	1/2,x,z [v,0,0]	1/2, $\bar{x},z$ [ $\bar{v}$ ,0,0]
	$\bar{x},1/2,\bar{z}$ [0,v,0]	x,1/2, $\bar{z}$ [0, $\bar{v}$ ,0]	1/2,x, $\bar{z}$ [ $\bar{v}$ ,0,0]	1/2, $\bar{x},\bar{z}$ [ $\bar{v},0,0$ ]

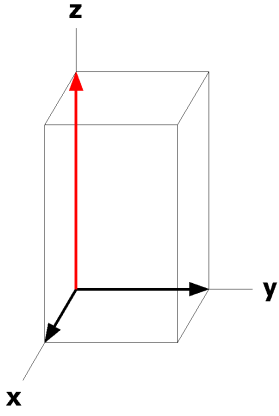
16	s	.m.	x,0,z [0,v,0]	$\bar{x},0,z [0,\bar{v},0]$	0,x,z [v,0,0]	0, $\bar{x}$ ,z [ $\bar{v}$ ,0,0]
			$\bar{x},0,\bar{z} [0,v,0]$	x,0, $\bar{z} [0,\bar{v},0]$	0,x, $\bar{z} [\bar{v},0,0]$	0, $\bar{x}$ , $\bar{z} [v,0,0]$
16	r	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z [\bar{u},\bar{u},w]$	$\bar{x},x,z [u,\bar{u},\bar{w}]$	x, $\bar{x}$ ,z [ $\bar{u},u,\bar{w}]$
			$\bar{x},x,\bar{z} [\bar{u},u,\bar{w}]$	x, $\bar{x},\bar{z} [u,\bar{u},\bar{w}]$	x,x, $\bar{z} [\bar{u},\bar{u},w]$	$\bar{x},\bar{x},\bar{z} [u,u,w]$
16	q	m'..	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2 [\bar{u},\bar{v},0]$	$\bar{y},x,1/2 [v,\bar{u},0]$	y, $\bar{x}$ ,1/2 [ $\bar{v},u,0]$
			$\bar{x},y,1/2 [u,\bar{v},0]$	x, $\bar{y},1/2 [\bar{u},v,0]$	y,x,1/2 [v,u,0]	$\bar{y},\bar{x},1/2 [\bar{v},\bar{u},0]$
16	p	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0 [0,0,w]$	$\bar{y},x,0 [0,0,\bar{w}]$	y, $\bar{x}$ ,0 [0,0, $\bar{w}]$
			$\bar{x},y,0 [0,0,\bar{w}]$	x, $\bar{y},0 [0,0,\bar{w}]$	y,x,0 [0,0,w]	$\bar{y},\bar{x},0 [0,0,w]$
8	o	m'2'm.	x,1/2,1/2 [0,v,0]	$\bar{x},1/2,1/2 [0,\bar{v},0]$	1/2,x,1/2 [v,0,0]	1/2, $\bar{x}$ ,1/2 [ $\bar{v},0,0]$
8	n	m2m.	x,1/2,0 [0,0,0]	$\bar{x},1/2,0 [0,0,0]$	1/2,x,0 [0,0,0]	1/2, $\bar{x}$ ,0 [0,0,0]
8	m	m'2'm.	x,0,1/2 [0,v,0]	$\bar{x},0,1/2 [0,\bar{v},0]$	0,x,1/2 [v,0,0]	0, $\bar{x}$ ,1/2 [ $\bar{v},0,0]$
8	l	m2m.	x,0,0 [0,0,0]	$\bar{x},0,0 [0,0,0]$	0,x,0 [0,0,0]	0, $\bar{x}$ ,0 [0,0,0]
8	k	m'.2'm	x,x,1/2 [ $\bar{u},u,0]$	$\bar{x},\bar{x},1/2 [u,\bar{u},0]$	$\bar{x},x,1/2 [u,u,0]$	x, $\bar{x}$ ,1/2 [ $\bar{u},\bar{u},0]$
8	j	m.2'm'	x,x,0 [0,0,w]	$\bar{x},\bar{x},0 [0,0,w]$	$\bar{x},x,0 [0,0,\bar{w}]$	x, $\bar{x}$ ,0 [0,0, $\bar{w}]$
8	i	2mm.	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z} [0,0,0]$	1/2,0, $\bar{z} [0,0,0]$
4	h	4'mm'	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z} [0,0,0]$		
4	g	4'mm'	0,0,z [0,0,0]	0,0, $\bar{z} [0,0,0]$		
4	f	mmm.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
4	e	m'mm.	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	d	4'/m'mm'	1/2,1/2,1/2 [0,0,0]			
2	c	4'/mmm'	1/2,1/2,0 [0,0,0]			
2	b	4'/m'mm'	0,0,1/2 [0,0,0]			
2	a	4'/mmm'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

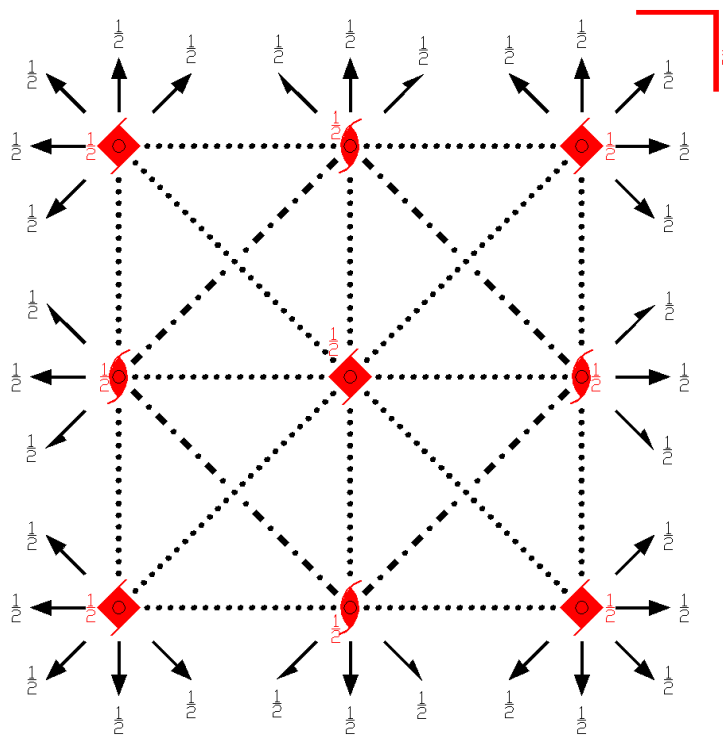
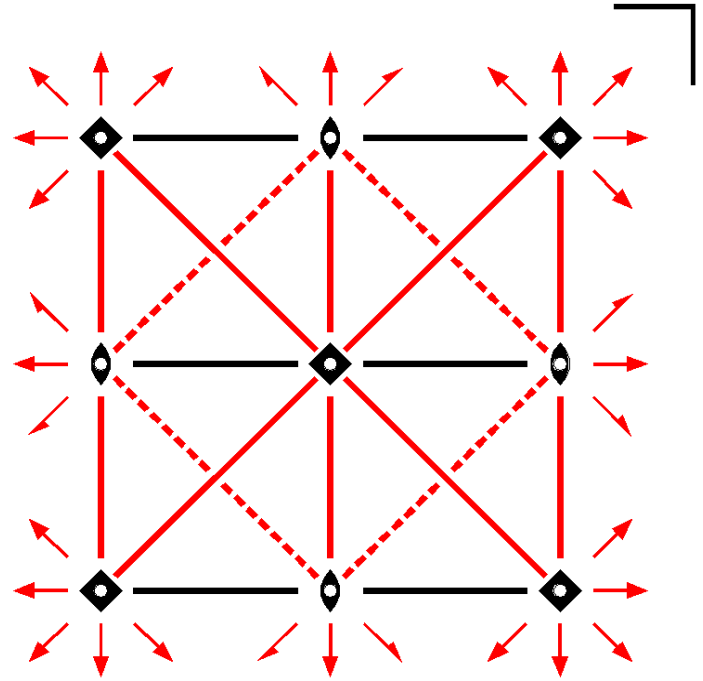
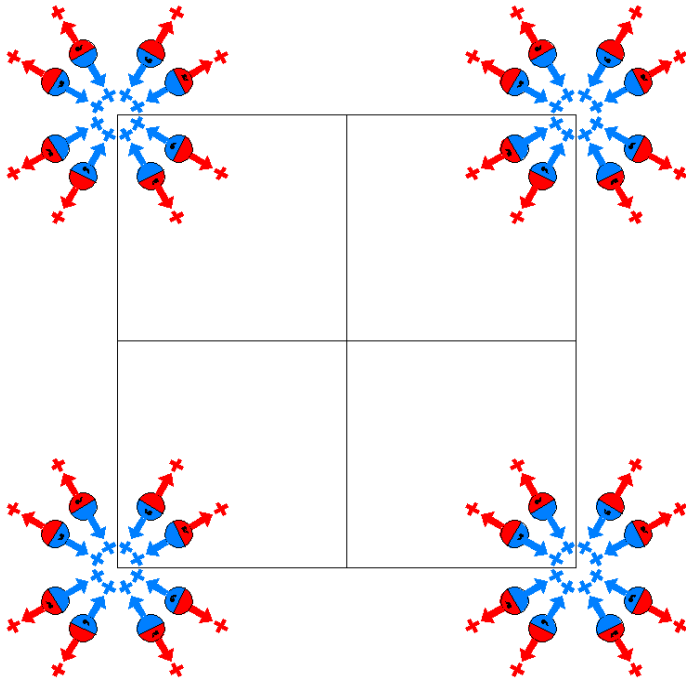
Along [1,1,0] p<sub>2a</sub>2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$P_{2c} 4/m\bar{m}'m'$   
123.15.1013

$4/m\bar{m}m1'$   
 $P_{2c} 4/m2'/m'2'/m'$

Tetragonal



Origin at center ( 4/mm'm' )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $x \leq y$ 

## Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)
(5) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(6) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'	(7) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) 2' x, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  0,0,0)'
(9) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(10) m x,y,0 (m <sub>z</sub>  0,0,0)	(11) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z^+$  0,0,0)	(12) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z^-$  0,0,0)
(13) m' x,0,z (m <sub>y</sub>  0,0,0)'	(14) m' 0,y,z (m <sub>x</sub>  0,0,0)'	(15) m' x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)'	(16) m' x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,0)'

For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 2' (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)'	(3) 4 <sup>+</sup> ' (0,0,1) 0,0,z (4 <sub>z</sub>  0,0,1)'	(4) 4 <sup>-</sup> ' (0,0,1) 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,1)'
(5) 2 0,y,1/2 (2 <sub>y</sub>  0,0,1)	(6) 2 x,0,1/2 (2 <sub>x</sub>  0,0,1)	(7) 2 x,x,1/2 (2 <sub>xy</sub>  0,0,1)	(8) 2 x, $\bar{x}$ ,1/2 (2 <sub><math>\bar{xy}</math></sub>  0,0,1)
(9) $\bar{1}$ ' 0,0,1/2 ( $\bar{1}$  0,0,1)'	(10) m' x,y,1/2 (m <sub>z</sub>  0,0,1)'	(11) $\bar{4}^+$ ' 0,0,z; 0,0,1/2 ( $\bar{4}_z^+$  0,0,1)'	(12) $\bar{4}^-$ ' 0,0,z; 0,0,1/2 ( $\bar{4}_z^-$  0,0,1)'
(13) c (0,0,1) x,0,z (m <sub>y</sub>  0,0,1)	(14) c (0,0,1) 0,y,z (m <sub>x</sub>  0,0,1)	(15) c (0,0,1) x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,1)	(16) c (0,0,1) x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,1)

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

## Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
		(0,0,0) +	(0,0,1)' +	
32 u 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [ $v,\bar{u},w$ ]
	(5) $\bar{x},y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]
	(9) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
	(13) x, $\bar{y},z$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(16) y,x,z [ $v,u,w$ ]
16 t .m'	x,1/2,z [u,0,w]	$\bar{x},1/2,z$ [ $\bar{u},0,w$ ]	1/2,x,z [0,u,w]	1/2, $\bar{x},z$ [0, $\bar{u},w$ ]
	$\bar{x},1/2,\bar{z}$ [ $u,0,w$ ]	x,1/2, $\bar{z}$ [ $\bar{u},0,w$ ]	1/2,x, $\bar{z}$ [0, $\bar{u},w$ ]	1/2, $\bar{x},\bar{z}$ [0,u,w]

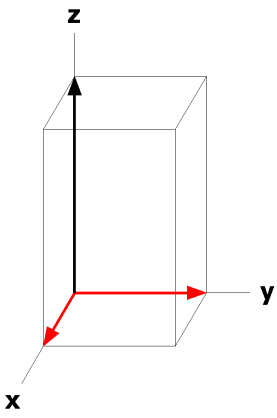
16	s	.m'	x,0,z [u,0,w]	$\bar{x},0,z [\bar{u},0,w]$	0,x,z [0,u,w]	0, $\bar{x},z [0,\bar{u},w]$
			$\bar{x},0,\bar{z} [u,0,w]$	x,0, $\bar{z} [\bar{u},0,w]$	0,x, $\bar{z} [0,\bar{u},w]$	0, $\bar{x},\bar{z} [0,u,w]$
16	r	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z [\bar{u},\bar{u},w]$	$\bar{x},x,z [\bar{u},u,w]$	x, $\bar{x},z [u,\bar{u},w]$
			$\bar{x},x,\bar{z} [u,\bar{u},w]$	x, $\bar{x},\bar{z} [\bar{u},u,w]$	x,x, $\bar{z} [\bar{u},\bar{u},w]$	$\bar{x},\bar{x},\bar{z} [u,u,w]$
16	q	m'..	x,y,1/2 [u,v,0]	$\bar{x},\bar{y},1/2 [\bar{u},\bar{v},0]$	$\bar{y},x,1/2 [\bar{v},u,0]$	y, $\bar{x},1/2 [v,\bar{u},0]$
			$\bar{x},y,1/2 [\bar{u},v,0]$	x, $\bar{y},1/2 [u,\bar{v},0]$	y,x,1/2 [v,u,0]	$\bar{y},\bar{x},1/2 [\bar{v},\bar{u},0]$
16	p	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0 [0,0,w]$	$\bar{y},x,0 [0,0,w]$	y, $\bar{x},0 [0,0,w]$
			$\bar{x},y,0 [0,0,w]$	x, $\bar{y},0 [0,0,w]$	y,x,0 [0,0,w]	$\bar{y},\bar{x},0 [0,0,w]$
8	o	m'2m'	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2 [\bar{u},0,0]$	1/2,x,1/2 [0,u,0]	1/2, $\bar{x},1/2 [0,\bar{u},0]$
8	n	m2'm'	x,1/2,0 [0,0,w]	$\bar{x},1/2,0 [0,0,w]$	1/2,x,0 [0,0,w]	1/2, $\bar{x},0 [0,0,w]$
8	m	m'2m'	x,0,1/2 [u,0,0]	$\bar{x},0,1/2 [\bar{u},0,0]$	0,x,1/2 [0,u,0]	0, $\bar{x},1/2 [0,\bar{u},0]$
8	l	m2'm'	x,0,0 [0,0,w]	$\bar{x},0,0 [0,0,w]$	0,x,0 [0,0,w]	0, $\bar{x},0 [0,0,w]$
8	k	m'.2m'	x,x,1/2 [u,u,0]	$\bar{x},\bar{x},1/2 [\bar{u},\bar{u},0]$	$\bar{x},x,1/2 [\bar{u},u,0]$	x, $\bar{x},1/2 [u,\bar{u},0]$
8	j	m.2'm'	x,x,0 [0,0,w]	$\bar{x},\bar{x},0 [0,0,w]$	$\bar{x},x,0 [0,0,w]$	x, $\bar{x},0 [0,0,w]$
8	i	2m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z} [0,0,w]$	1/2,0, $\bar{z} [0,0,w]$
4	h	4m'm'	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z} [0,0,w]$		
4	g	4m'm'	0,0,z [0,0,w]	0,0, $\bar{z} [0,0,w]$		
4	f	mm'm'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]		
4	e	m'mm.	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	d	4/m'm'm'	1/2,1/2,1/2 [0,0,0]			
2	c	4/mm'm'	1/2,1/2,0 [0,0,w]			
2	b	4/m'm'm'	0,0,1/2 [0,0,0]			
2	a	4/mm'm'	0,0,0 [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'-2'mm1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

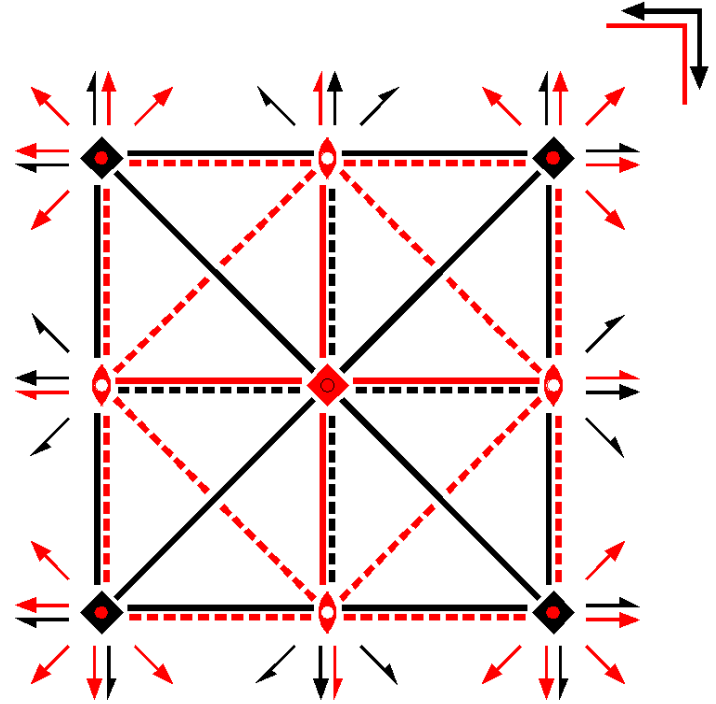
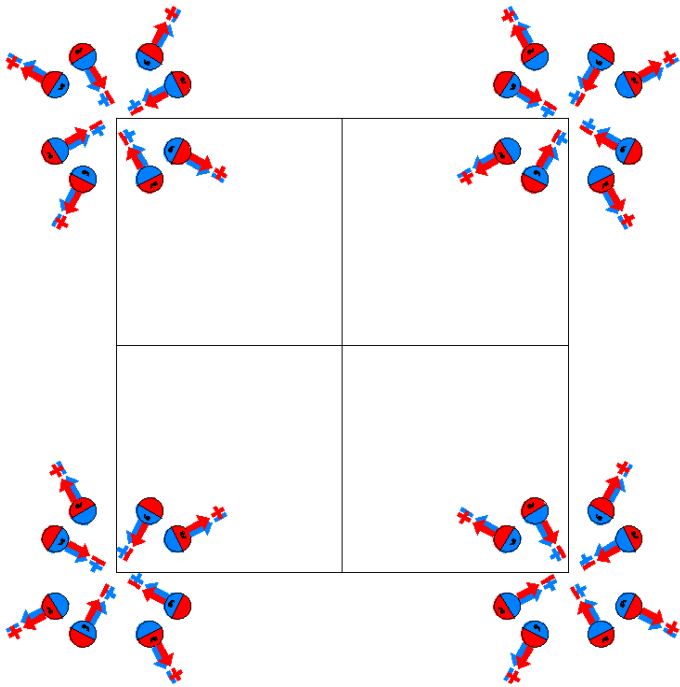
Along [1,1,0] p<sub>2a</sub>'-2'mm1'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$P_4/m'mm$   
123.16.1014

$4/mmm1'$   
 $P_4/m'2'/m2'/m$

Tetragonal



Origin at center ( $4/m'mm$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

Symmetry Operations

For (0,0,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                         | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)           |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'  | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                                   | (8) 2' x,x̄,0<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,0)'                    |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'              | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) 4̄ <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (12) 4̄ <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)  | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   | (15) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                                   | (16) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                                    |



For (1,0,0)<sup>+</sup> + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> -1/2,1/2,z (4 <sub>z</sub>  1,0,0)'	(4) 4 <sup>-</sup> 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,0)'
(5) 2 1/2,y,0 (2 <sub>y</sub>  1,0,0)	(6) 2 (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)	(7) 2 (1/2,1/2,0) x+1/2,x,0 (2 <sub>xy</sub>  1,0,0)	(8) 2 (1/2,-1/2,0) x+1/2,x̄,0 (2 <sub>xy</sub> <sup>-</sup>  1,0,0)
(9) 1̄ 1/2,0,0 (1̄ 1,0,0)	(10) a (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)	(11) 4 <sup>+</sup> 1/2,-1/2,z; 1/2,-1/2,0 (4 <sub>z</sub>  1,0,0)	(12) 4 <sup>-</sup> 1/2,1/2,z; 1/2,1/2,0 (4 <sub>z</sub> <sup>-1</sup>  1,0,0)
(13) a' (1,0,0) x,0,z (m <sub>y</sub>  1,0,0)'	(14) m' 1/2,y,z (m <sub>x</sub>  1,0,0)'	(15) g' (1/2,-1/2,0) x+1/2,x̄,z (m <sub>xy</sub>  1,0,0)'	(16) g' (1/2,1/2,0) x+1/2,x,z (m <sub>xy</sub> <sup>-</sup>  1,0,0)'

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1,0,0) <sup>+</sup> +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	u	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w]	(3) ȳ,x,z [v̄,u,w]	(4) y,x,z [v,ū,w]
			(5) x̄,y,z [ū,v̄,w]	(6) x,y,z [u,v,w]	(7) y,x,z [v̄,ū,w]	(8) ȳ,x̄,z [v,u,w]
			(9) x̄,ȳ,z [ū,v̄,w̄]	(10) x,y,z [u,v,w̄]	(11) y,x,z [v,ū,w̄]	(12) ȳ,x̄,z [v̄,ū,w̄]
			(13) x,y,z [ū,v,w̄]	(14) x̄,y,z [u,v̄,w̄]	(15) ȳ,x,z [v,ū,w̄]	(16) y,x,z [v̄,ū,w̄]
16	t	.m'	x,1/2,z [u,0,w]	x̄,1/2,z [u,0,w̄]	1/2,x,z [0,ū,w̄]	1/2,x̄,z [0,ū,w]
			x̄,1/2,z [u,0,w]	x,1/2,z [u,0,w̄]	1/2,x,z [0,ū,w]	1/2,x̄,z [0,ū,w̄]
16	s	.m.	x,0,z [0,v,0]	x̄,0,z [0,v̄,0]	0,x,z [v̄,0,0]	0,x̄,z [v,0,0]
			x̄,0,z [0,v̄,0]	x,0,z [0,v,0]	0,x,z [v̄,0,0]	0,x̄,z [v,0,0]
16	r	.m	x,x,z [ū,u,0]	x̄,x̄,z [ū,ū,0]	x̄,x,z [ū,ū,0]	x,x̄,z [u,ū,0]
			x̄,x,z [ū,ū,0]	x,x̄,z [ū,ū,0]	x,x,z [ū,ū,0]	x̄,x̄,z [u,ū,0]
16	q	m'..	x,y,1/2 [u,v,0]	x̄,ȳ,1/2 [ū,v̄,0]	ȳ,x,1/2 [v̄,u,0]	y,x̄,1/2 [v,ū,0]
			x̄,y,1/2 [u,v̄,0]	x,ȳ,1/2 [ū,v,0]	y,x,1/2 [v̄,ū,0]	ȳ,x̄,1/2 [v,u,0]
16	p	m'..	x,y,0 [u,v,0]	x̄,ȳ,0 [ū,v̄,0]	ȳ,x,0 [v̄,u,0]	y,x̄,0 [v,ū,0]
			x̄,y,0 [u,v̄,0]	x,ȳ,0 [ū,v,0]	y,x,0 [v̄,ū,0]	ȳ,x̄,0 [v,u,0]
8	o	m'2m'	x,1/2,1/2 [u,0,0]	x̄,1/2,1/2 [u,0,0]	1/2,x,1/2 [0,ū,0]	1/2,x̄,1/2 [0,ū,0]
8	n	m'2m'	x,1/2,0 [u,0,0]	x̄,1/2,0 [u,0,0]	1/2,x,0 [0,ū,0]	1/2,x̄,0 [0,ū,0]
8	m	m'2'm.	x,0,1/2 [0,v,0]	x̄,0,1/2 [0,v̄,0]	0,x,1/2 [v̄,0,0]	0,x̄,1/2 [v,0,0]

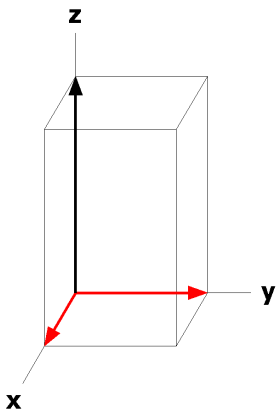
8	l	$m'2'm.$	$x,0,0 [0,v,0]$	$\bar{x},0,0 [0,\bar{v},0]$	$0,x,0 [\bar{v},0,0]$	$0,\bar{x},0 [v,0,0]$
8	k	$m'.2'm$	$x,x,1/2 [\bar{u},u,0]$	$\bar{x},\bar{x},1/2 [u,\bar{u},0]$	$\bar{x},x,1/2 [\bar{u},\bar{u},0]$	$x,\bar{x},1/2 [u,u,0]$
8	j	$m'.2'm$	$x,x,0 [\bar{u},u,0]$	$\bar{x},\bar{x},0 [u,\bar{u},0]$	$\bar{x},x,0 [\bar{u},\bar{u},0]$	$x,\bar{x},0 [u,u,0]$
8	i	$2'mm'.$	$0,1/2,z [u,0,0]$	$1/2,0,z [0,\bar{u},0]$	$0,1/2,\bar{z} [u,0,0]$	$1/2,0,\bar{z} [0,\bar{u},0]$
4	h	$4'm'm$	$1/2,1/2,z [0,0,0]$	$1/2,1/2,\bar{z} [0,0,0]$		
4	g	$4mm$	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$		
4	f	$mm'm.$	$0,1/2,0 [0,0,0]$	$1/2,0,0 [0,0,0]$		
4	e	$mm'm.$	$0,1/2,1/2 [0,0,0]$	$1/2,0,1/2 [0,0,0]$		
2	d	$4'/mm'm$	$1/2,1/2,1/2 [0,0,0]$			
2	c	$4'/mm'm$	$1/2,1/2,0 [0,0,0]$			
2	b	$4/m'mm$	$0,0,1/2 [0,0,0]$			
2	a	$4/m'mm$	$0,0,0 [0,0,0]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_4, 4mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

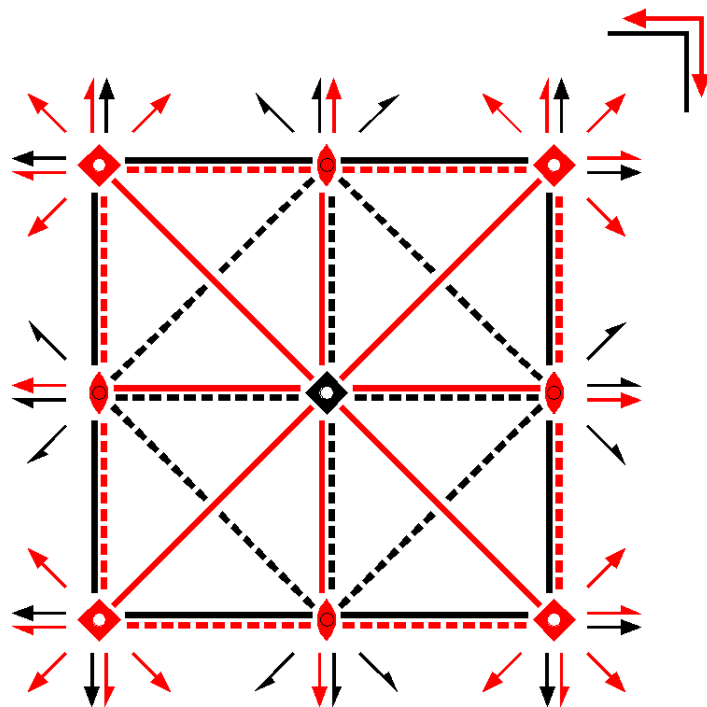
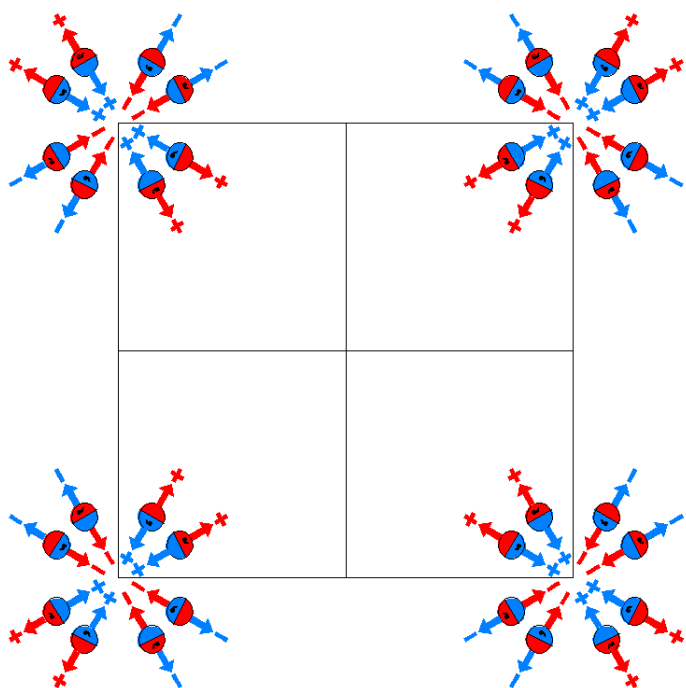
Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$



$P_4 4'/mmm'$   
123.17.1015

$4/mmm1'$   
 $P_4 4'/m2/m2'/m'$

Tetragonal



Origin at center ( $4'/mmm'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'         | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'         |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                    | (8) 2' x,x̄,0<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,0)'                    |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)              | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub>  0,0,0)' | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (15) m' x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'                  | (16) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                                 |

## For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> -1/2,1/2,z (4 <sub>z</sub>  1,0,0)	(4) 4 <sup>-</sup> 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,0)
(5) 2' 1/2,y,0 (2 <sub>y</sub>  1,0,0)'	(6) 2' (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)'	(7) 2 (1/2,1/2,0) x+1/2,x,0 (2 <sub>xy</sub>  1,0,0)	(8) 2 (1/2,-1/2,0) x+1/2,x̄,0 (2 <sub>xy</sub> <sup>-</sup>  1,0,0)
(9) 1̄' 1/2,0,0 (1̄ 1,0,0)'	(10) a' (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)'	(11) 4 <sup>+</sup> 1/2,-1/2,z; 1/2,-1/2,0 (4 <sub>z</sub>  1,0,0)	(12) 4 <sup>-</sup> 1/2,1/2,z; 1/2,1/2,0 (4 <sub>z</sub> <sup>-1</sup>  1,0,0)
(13) a' (1,0,0) x,0,z (m <sub>y</sub>  1,0,0)'	(14) m' 1/2,y,z (m <sub>x</sub>  1,0,0)'	(15) g (1/2,-1/2,0) x+1/2,x̄,z (m <sub>xy</sub>  1,0,0)	(16) g (1/2,1/2,0) x+1/2,x,z (m <sub>xy</sub> <sup>-</sup>  1,0,0)

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1,0,0)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	u	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w]	(3) ȳ,x,z [v̄,ū,w̄]	(4) y,x,z [v̄,ū,w̄]
			(5) x̄,y,z [ū,v,w]	(6) x,y,z̄ [u,v̄,w̄]	(7) y,x,z̄ [v̄,ū,w̄]	(8) ȳ,x̄,z̄ [v̄,ū,w̄]
			(9) x̄,ȳ,z̄ [u,v,w]	(10) x,y,z̄ [ū,v̄,w̄]	(11) y,x̄,z̄ [v̄,ū,w̄]	(12) ȳ,x̄,z̄ [v̄,ū,w̄]
			(13) x,ȳ,z [ū,v,w̄]	(14) x̄,y,z [u,v̄,w̄]	(15) ȳ,x̄,z [v̄,ū,w̄]	(16) y,x,z [v̄,ū,w̄]
16	t	.m'	x,1/2,z [u,0,w]	x̄,1/2,z [ū,0,w̄]	1/2,x,z [0,u,w]	1/2,x̄,z [0,ū,w̄]
			x̄,1/2,z̄ [ū,0,w̄]	x,1/2,z̄ [u,0,w]	1/2,x,z̄ [0,ū,w̄]	1/2,x̄,z̄ [0,ū,w̄]
16	s	.m.	x,0,z [0,v,0]	x̄,0,z [0,v̄,0]	0,x,z [v,0,0]	0,x̄,z [v̄,0,0]
			x̄,0,z̄ [0,v,0]	x,0,z̄ [0,v̄,0]	0,x,z̄ [v̄,0,0]	0,x̄,z̄ [v̄,0,0]
16	r	..m'	x,x,z [u,u,w]	x̄,x̄,z [ū,ū,w̄]	x̄,x,z [u,ū,w̄]	x,x̄,z [ū,ū,w̄]
			x̄,x,z̄ [ū,ū,w̄]	x,x̄,z̄ [u,ū,w̄]	x,x,z̄ [ū,ū,w̄]	x̄,x̄,z̄ [u,ū,w̄]
16	q	m..	x,y,1/2 [0,0,w]	x̄,ȳ,1/2 [0,0,w̄]	ȳ,x,1/2 [0,0,w̄]	y,x̄,1/2 [0,0,w̄]
			x̄,y,1/2 [0,0,w̄]	x,ȳ,1/2 [0,0,w̄]	y,x,1/2 [0,0,w]	ȳ,x̄,1/2 [0,0,w]
16	p	m..	x,y,0 [0,0,w]	x̄,ȳ,0 [0,0,w̄]	ȳ,x,0 [0,0,w̄]	y,x̄,0 [0,0,w̄]
			x̄,y,0 [0,0,w̄]	x,ȳ,0 [0,0,w̄]	y,x,0 [0,0,w]	ȳ,x̄,0 [0,0,w]
8	o	m2'm'	x,1/2,1/2 [0,0,w]	x̄,1/2,1/2 [0,0,w̄]	1/2,x,1/2 [0,0,w]	1/2,x̄,1/2 [0,0,w̄]
8	n	m2'm'	x,1/2,0 [0,0,w]	x̄,1/2,0 [0,0,w̄]	1/2,x,0 [0,0,w]	1/2,x̄,0 [0,0,w̄]
8	m	m2m.	x,0,1/2 [0,0,0]	x̄,0,1/2 [0,0,0]	0,x,1/2 [0,0,0]	0,x̄,1/2 [0,0,0]

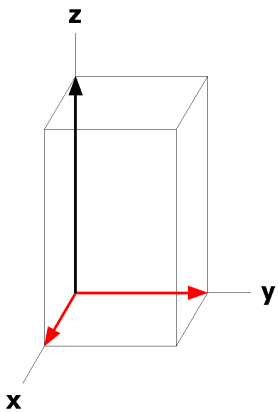
8	l	$m2m'$	$x,0,0 [0,0,0]$	$\bar{x},0,0 [0,0,0]$	$0,x,0 [0,0,0]$	$0,\bar{x},0 [0,0,0]$
8	k	$m.2'm'$	$x,x,1/2 [0,0,w]$	$\bar{x},\bar{x},1/2 [0,0,w]$	$\bar{x},x,1/2 [0,0,\bar{w}]$	$x,\bar{x},1/2 [0,0,\bar{w}]$
8	j	$m.2'm'$	$x,x,0 [0,0,w]$	$\bar{x},\bar{x},0 [0,0,w]$	$\bar{x},x,0 [0,0,\bar{w}]$	$x,\bar{x},0 [0,0,\bar{w}]$
8	i	$2'mm'$	$0,1/2,z [u,0,0]$	$1/2,0,z [0,u,0]$	$0,1/2,\bar{z} [\bar{u},0,0]$	$1/2,0,\bar{z} [0,\bar{u},0]$
4	h	$4m'm'$	$1/2,1/2,z [0,0,w]$	$1/2,1/2,\bar{z} [0,0,w]$		
4	g	$4'mm'$	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$		
4	f	$mmm'$	$0,1/2,0 [0,0,0]$	$1/2,0,0 [0,0,0]$		
4	e	$mmm'$	$0,1/2,1/2 [0,0,0]$	$1/2,0,1/2 [0,0,0]$		
2	d	$4/mm'm'$	$1/2,1/2,1/2 [0,0,w]$			
2	c	$4/mm'm'$	$1/2,1/2,0 [0,0,w]$			
2	b	$4'/mmm'$	$0,0,1/2 [0,0,0]$			
2	a	$4'/mmm'$	$0,0,0 [0,0,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p_{2a}2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x-1/4, x+1/4, 0$



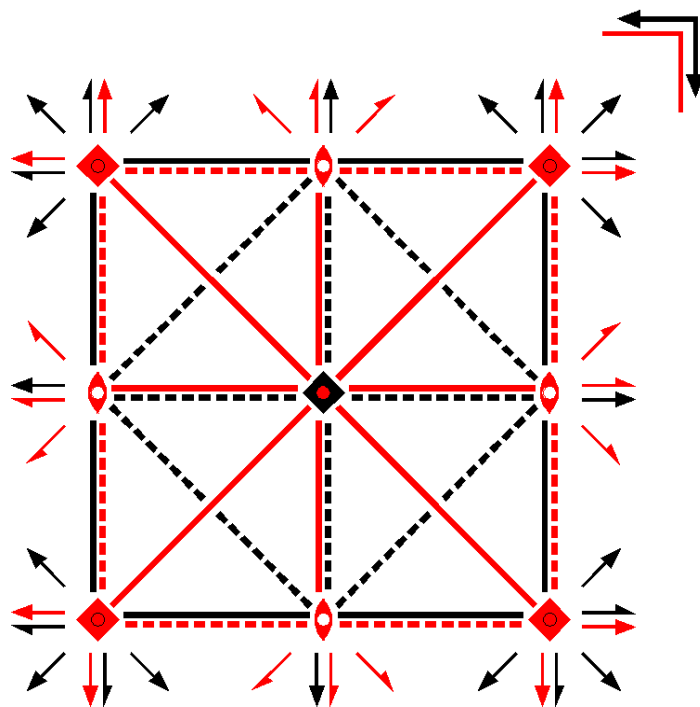
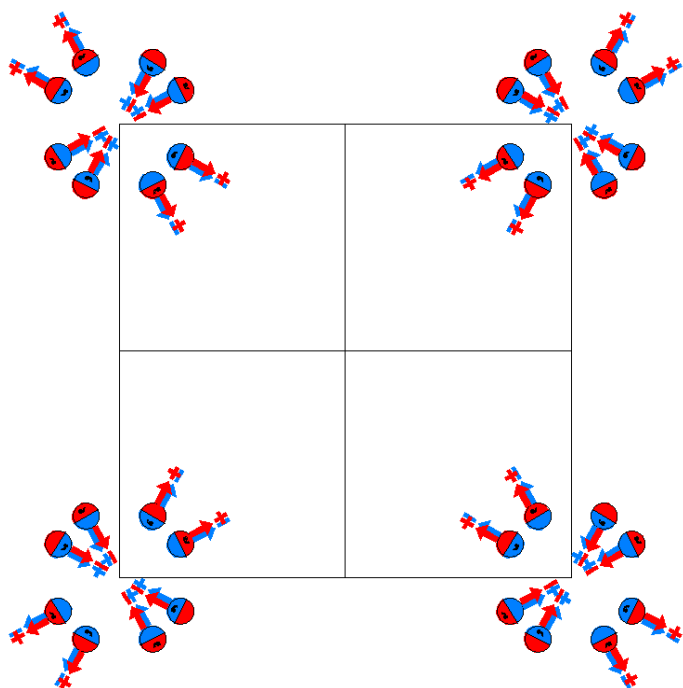
$P_4 4'/m'mm'$

123.18.1016

$4/mmm1'$

$P_4 4'/m'2'/m2/m'$

Tetragonal



Origin at center ( $4'/m'mm'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |  |  |
|--|---|--|--|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)'        | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'        |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                  | (8) 2 x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)                                |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'              | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0) |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)  | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   | (15) m' x,x̄,z<br>(m <sub>xȳ</sub>  0,0,0)'                             | (16) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                               |

## For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> -1/2,1/2,z (4 <sub>z</sub>  1,0,0)	(4) 4 <sup>-</sup> 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,0)
(5) 2 1/2,y,0 (2 <sub>y</sub>  1,0,0)	(6) 2 (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)	(7) 2' (1/2,1/2,0) x+1/2,x,0 (2 <sub>xy</sub>  1,0,0)'	(8) 2' (1/2,-1/2,0) x+1/2,x̄,0 (2 <sub>xy</sub> <sup>-</sup>  1,0,0)'
(9) 1̄ 1/2,0,0 (1̄ 1,0,0)	(10) a (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)	(11) 4 <sup>+</sup> 1/2,-1/2,z; 1/2,-1/2,0 (4 <sub>z</sub>  1,0,0)'	(12) 4 <sup>-</sup> 1/2,1/2,z; 1/2,1/2,0 (4 <sub>z</sub> <sup>-1</sup>  1,0,0)'
(13) a' (1,0,0) x,0,z (m <sub>y</sub>  1,0,0)'	(14) m' 1/2,y,z (m <sub>x</sub>  1,0,0)'	(15) g (1/2,-1/2,0) x+1/2,x̄,z (m <sub>xy</sub>  1,0,0)	(16) g (1/2,1/2,0) x+1/2,x,z (m <sub>xy</sub> <sup>-</sup>  1,0,0)

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1,0,0)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	u	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w]	(3) ȳ,x,z [v̄,ū,w̄]	(4) y,x,z [v̄,ū,w̄]
			(5) x̄,y,z [ū,v̄,w]	(6) x,y,z̄ [ū,v̄,w]	(7) y,x,z̄ [v̄,ū,w̄]	(8) ȳ,x̄,z̄ [v̄,ū,w̄]
			(9) x̄,ȳ,z̄ [ū,v̄,w̄]	(10) x,y,z̄ [ū,v̄,w̄]	(11) y,x̄,z̄ [v̄,ū,w̄]	(12) ȳ,x̄,z̄ [v̄,ū,w̄]
			(13) x,y,z̄ [ū,v̄,w̄]	(14) x̄,y,z [ū,v̄,w̄]	(15) ȳ,x̄,z [v̄,ū,w̄]	(16) y,x,z [v̄,ū,w̄]
16	t	.m'	x,1/2,z [u,0,w]	x̄,1/2,z [ū,0,w̄]	1/2,x,z [0,u,w]	1/2,x̄,z [0,ū,w̄]
			x̄,1/2,z̄ [ū,0,w̄]	x,1/2,z̄ [u,0,w]	1/2,x,z̄ [0,ū,w̄]	1/2,x̄,z̄ [0,ū,w̄]
16	s	.m.	x,0,z [0,v,0]	x̄,0,z [0,v̄,0]	0,x,z [v,0,0]	0,x̄,z [v̄,0,0]
			x̄,0,z̄ [0,v̄,0]	x,0,z̄ [0,v,0]	0,x,z̄ [v,0,0]	0,x̄,z̄ [v̄,0,0]
16	r	..m'	x,x,z [u,u,w]	x̄,x̄,z [ū,ū,w̄]	x̄,x,z [u,ū,w̄]	x,x̄,z [ū,ū,w̄]
			x̄,x,z̄ [ū,ū,w̄]	x,x̄,z̄ [u,ū,w̄]	x,x,z̄ [u,ū,w̄]	x̄,x̄,z̄ [ū,ū,w̄]
16	q	m'..	x,y,1/2 [u,v,0]	x̄,ȳ,1/2 [ū,v̄,0]	ȳ,x,1/2 [v̄,ū,0]	y,x̄,1/2 [v̄,ū,0]
			x̄,y,1/2 [ū,v̄,0]	x,ȳ,1/2 [u,v,0]	y,x,1/2 [v,ū,0]	ȳ,x̄,1/2 [v̄,ū,0]
16	p	m'..	x,y,0 [u,v,0]	x̄,ȳ,0 [ū,v̄,0]	ȳ,x,0 [v̄,ū,0]	y,x̄,0 [v̄,ū,0]
			x̄,y,0 [ū,v̄,0]	x,ȳ,0 [u,v,0]	y,x,0 [v,ū,0]	ȳ,x̄,0 [v̄,ū,0]
8	o	m'2m'	x,1/2,1/2 [u,0,0]	x̄,1/2,1/2 [ū,0,0]	1/2,x,1/2 [0,ū,0]	1/2,x̄,1/2 [0,ū,0]
8	n	m'2m'	x,1/2,0 [u,0,0]	x̄,1/2,0 [ū,0,0]	1/2,x,0 [0,ū,0]	1/2,x̄,0 [0,ū,0]
8	m	m'2'm.	x,0,1/2 [0,v,0]	x̄,0,1/2 [0,v̄,0]	0,x,1/2 [v,0,0]	0,x̄,1/2 [v̄,0,0]

8	l	$m'2'm'$	$x,0,0 [0,v,0]$	$\bar{x},0,0 [0,\bar{v},0]$	$0,x,0 [v,0,0]$	$0,\bar{x},0 [\bar{v},0,0]$
8	k	$m'.2m'$	$x,x,1/2 [u,u,0]$	$\bar{x},\bar{x},1/2 [\bar{u},\bar{u},0]$	$\bar{x},x,1/2 [u,\bar{u},0]$	$x,\bar{x},1/2 [\bar{u},u,0]$
8	j	$m'.2m'$	$x,x,0 [u,u,0]$	$\bar{x},\bar{x},0 [\bar{u},\bar{u},0]$	$\bar{x},x,0 [u,\bar{u},0]$	$x,\bar{x},0 [\bar{u},u,0]$
8	i	$2'mm'$	$0,1/2,z [u,0,0]$	$1/2,0,z [0,u,0]$	$0,1/2,\bar{z} [u,0,0]$	$1/2,0,\bar{z} [0,u,0]$
4	h	$4m'm'$	$1/2,1/2,z [0,0,w]$	$1/2,1/2,\bar{z} [0,0,\bar{w}]$		
4	g	$4'mm'$	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$		
4	f	$m'mm'$	$0,1/2,0 [u,0,0]$	$1/2,0,0 [0,u,0]$		
4	e	$m'mm'$	$0,1/2,1/2 [u,0,0]$	$1/2,0,1/2 [0,u,0]$		
2	d	$4/m'm'm'$	$1/2,1/2,1/2 [0,0,0]$			
2	c	$4/m'm'm'$	$1/2,1/2,0 [0,0,0]$			
2	b	$4'/m'mm'$	$0,0,1/2 [0,0,0]$			
2	a	$4'/m'mm'$	$0,0,0 [0,0,0]$			

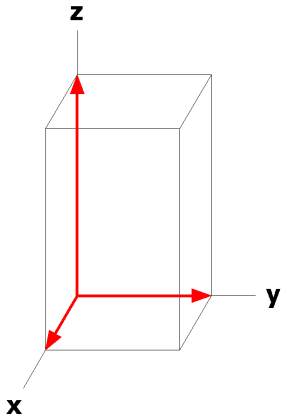
### Symmetry of Special Projections

Along  $[0,0,1]$   $p_4 4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $1/2,1/2,z$

Along  $[1,0,0]$   $p_2 2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p_{2a} 2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$





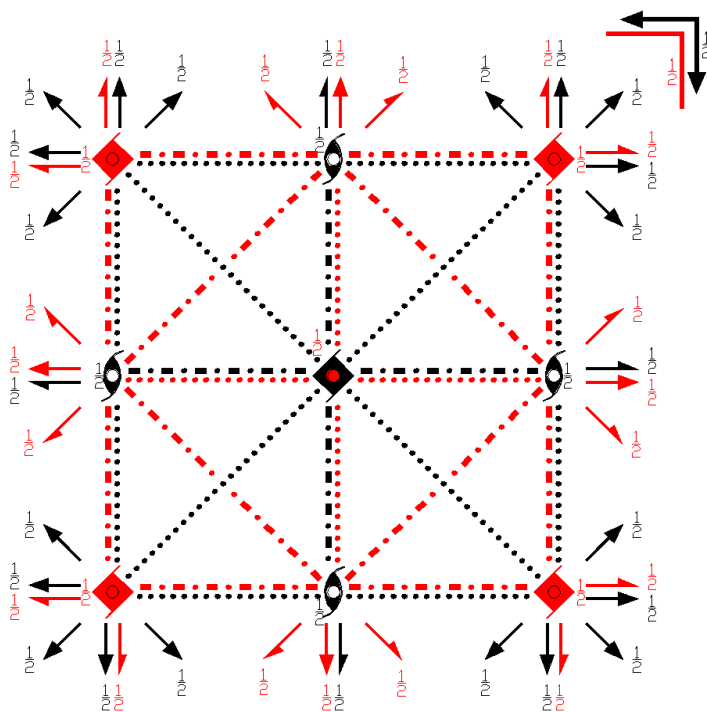
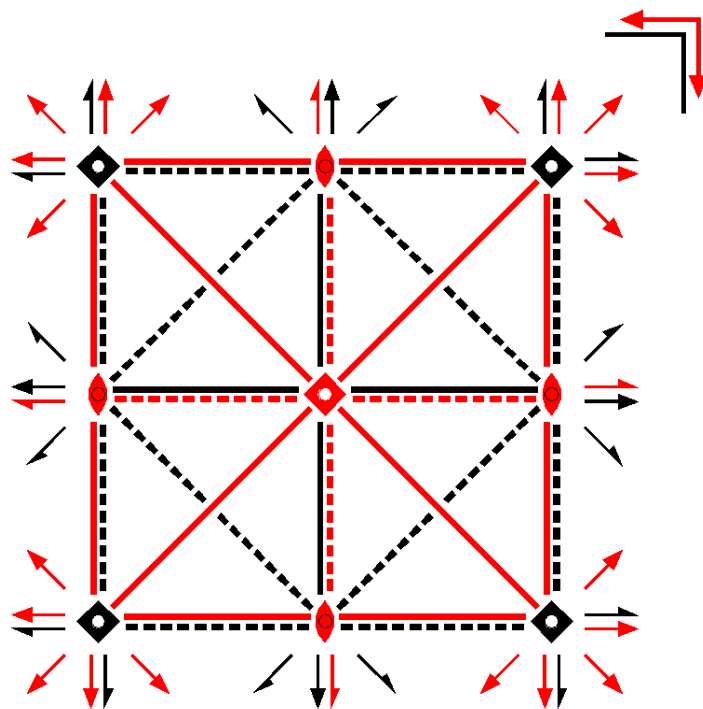
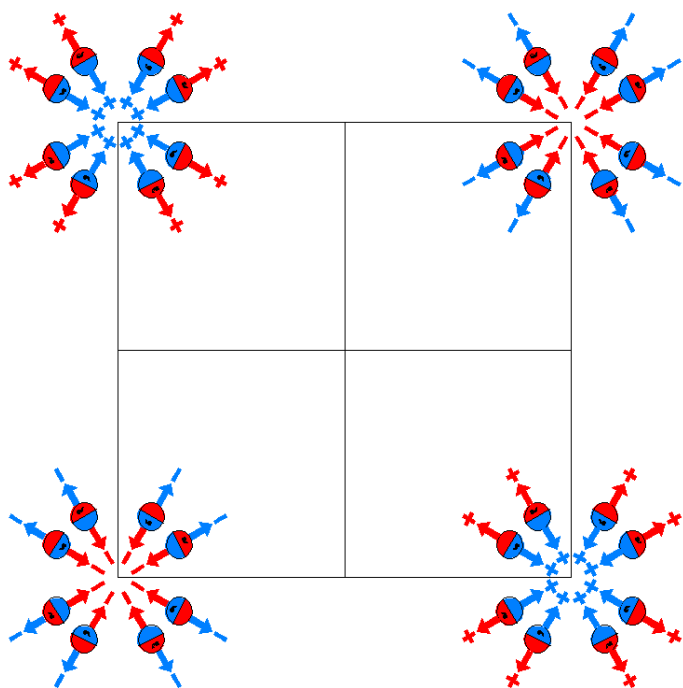
$P_14/m\bar{m}'m'$

123.19.1017

$4/m\bar{m}m1'$

$P_14/m2'/m'2'/m'$

Tetragonal



Origin at center ( 4/mmm'm' )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $x \leq y$ 

## Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)
(5) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(6) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'	(7) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) 2' x, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  0,0,0)'
(9) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(10) m x,y,0 (m <sub>z</sub>  0,0,0)	(11) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z^+$  0,0,0)	(12) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z^-$  0,0,0)
(13) m' x,0,z (m <sub>y</sub>  0,0,0)'	(14) m' 0,y,z (m <sub>x</sub>  0,0,0)'	(15) m' x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)'	(16) m' x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,0)'

For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> ' -1/2,1/2,z (4 <sub>z</sub>  1,0,0)'	(4) 4 <sup>-</sup> ' 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,0)'
(5) 2 1/2,y,0 (2 <sub>y</sub>  1,0,0)	(6) 2 (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)	(7) 2 (1/2,1/2,0) x+1/2,x,0 (2 <sub>xy</sub>  1,0,0)	(8) 2 (1/2,-1/2,0) x+1/2, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  1,0,0)
(9) $\bar{1}$ ' 1/2,0,0 ( $\bar{1}$  1,0,0)'	(10) a' (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)'	(11) $\bar{4}^+$ ' 1/2,-1/2,z; 1/2,-1/2,0 ( $\bar{4}_z^+$  1,0,0)'	(12) $\bar{4}^-$ ' 1/2,1/2,z; 1/2,1/2,0 ( $\bar{4}_z^-$  1,0,0)'
(13) a (1,0,0) x,0,z (m <sub>y</sub>  1,0,0)	(14) m 1/2,y,z (m <sub>x</sub>  1,0,0)	(15) g (1/2,-1/2,0) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1,0,0)	(16) g (1/2,1/2,0) x+1/2,x,z (m <sub><math>\bar{xy}</math></sub>  1,0,0)

Generators selected (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5); (9).

## Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1,0,0)' +		
32 u 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ]
	(5) $\bar{x},y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [v,u,w]
	(9) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [v, $\bar{u},w$ ]
	(13) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(16) y,x,z [v,u,w]
16 t .m.	x,1/2,z [0,v,0]	$\bar{x},1/2,z$ [0,v,0]	1/2,x,z [v,0,0]	1/2, $\bar{x},z$ [v,0,0]
	$\bar{x},1/2,\bar{z}$ [0, $\bar{v},0$ ]	x,1/2, $\bar{z}$ [0, $\bar{v},0$ ]	1/2,x, $\bar{z}$ [ $\bar{v},0,0$ ]	1/2, $\bar{x},\bar{z}$ [ $\bar{v},0,0$ ]

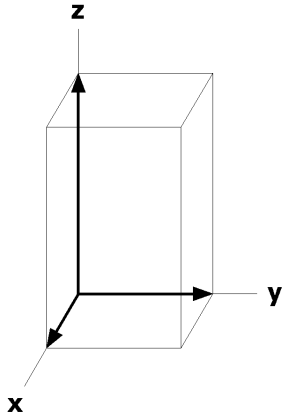
16	s	.m'	x,0,z [u,0,w] $\bar{x},0,\bar{z}$ [u,0,w]	$\bar{x},0,z$ [ $\bar{u},0,w$ ] x,0, $\bar{z}$ [ $\bar{u},0,w$ ]	0,x,z [0,u,w] 0,x, $\bar{z}$ [0, $\bar{u},w$ ]	0, $\bar{x},z$ [0, $\bar{u},w$ ] 0, $\bar{x},\bar{z}$ [0,u,w]
16	r	..m'	x,x,z [u,u,w] $\bar{x},x,\bar{z}$ [u, $\bar{u},w$ ]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ] x, $\bar{x},\bar{z}$ [ $\bar{u},u,w$ ]	$\bar{x},x,z$ [ $\bar{u},u,w$ ] x,x, $\bar{z}$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},z$ [u, $\bar{u},w$ ] $\bar{x},\bar{x},\bar{z}$ [u,u,w]
16	q	m'..	x,y,1/2 [u,v,0] $\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ] x, $\bar{y},1/2$ [u, $\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},u,0$ ] y,x,1/2 [v,u,0]	y, $\bar{x},1/2$ [v, $\bar{u},0$ ] $\bar{y},\bar{x},1/2$ [ $\bar{v},\bar{u},0$ ]
16	p	m..	x,y,0 [0,0,w] $\bar{x},y,0$ [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w] x, $\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0,w] y,x,0 [0,0,w]	y, $\bar{x},0$ [0,0,w] $\bar{y},\bar{x},0$ [0,0,w]
8	o	m'2'm.	x,1/2,1/2 [0,v,0]	$\bar{x},1/2,1/2$ [0,v,0]	1/2,x,1/2 [v,0,0]	1/2, $\bar{x},1/2$ [v,0,0]
8	n	m2m.	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]	1/2,x,0 [0,0,0]	1/2, $\bar{x},0$ [0,0,0]
8	m	m'2m'.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,1/2 [0,u,0]	0, $\bar{x},1/2$ [0, $\bar{u},0$ ]
8	l	m2'm'.	x,0,0 [0,0,w]	$\bar{x},0,0$ [0,0,w]	0,x,0 [0,0,w]	0, $\bar{x},0$ [0,0,w]
8	k	m'.2m'	x,x,1/2 [u,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/2$ [ $\bar{u},u,0$ ]	x, $\bar{x},1/2$ [u, $\bar{u},0$ ]
8	j	m.2'm'	x,x,0 [0,0,w]	$\bar{x},\bar{x},0$ [0,0,w]	$\bar{x},x,0$ [0,0,w]	x, $\bar{x},0$ [0,0,w]
8	i	2'm'm.	0,1/2,z [0,v,0]	1/2,0,z [v,0,0]	0,1/2, $\bar{z}$ [0, $\bar{v},0$ ]	1/2,0, $\bar{z}$ [ $\bar{v},0,0$ ]
4	h	4'mm'	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]		
4	g	4m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
4	f	mm'm.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
4	e	m'm'm.	0,1/2,1/2 [0,v,0]	1/2,0,1/2 [v,0,0]		
2	d	4'/m'mm'	1/2,1/2,1/2 [0,0,0]			
2	c	4'/mmm'	1/2,1/2,0 [0,0,0]			
2	b	4/m'm'm'	0,0,1/2 [0,0,0]			
2	a	4/mm'm'	0,0,0 [0,0,w]			

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

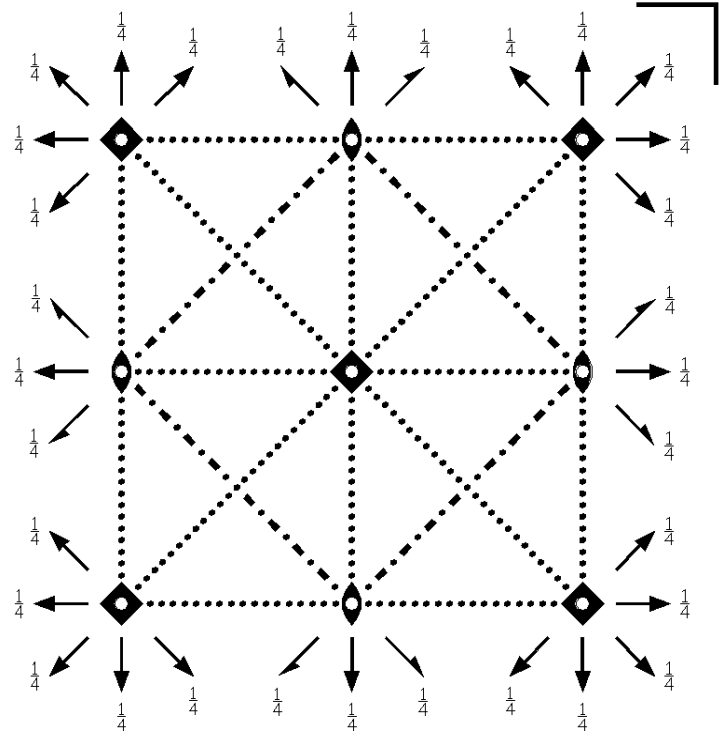
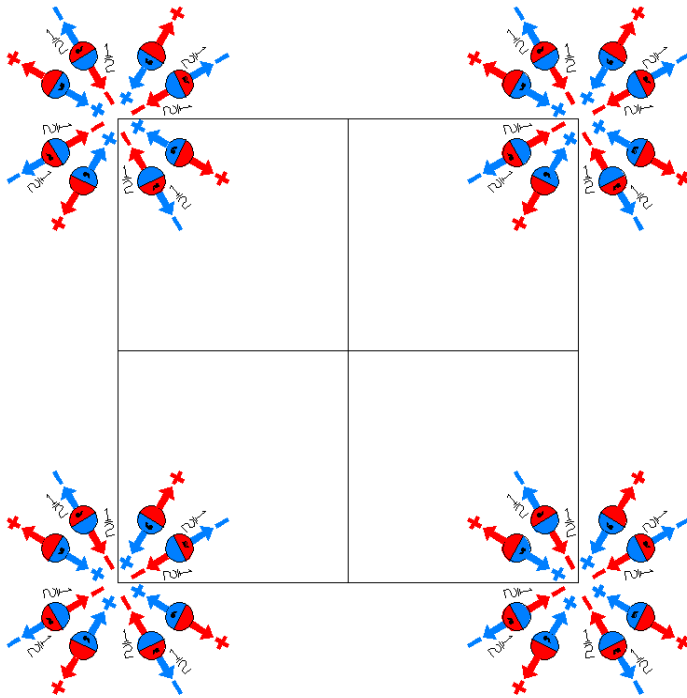
Along [1,1,0] p<sub>c</sub>2mm  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x-1/4,x+1/4,0



P4/mcc  
124.1.1018

4/mmm  
P4/m2/c2/c

Tetragonal



Origin at center ( 4/m ) at 4/mcc

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)              | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)            | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)        |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)          | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)          | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                    | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2) |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)          | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)             | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)       | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                 |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (15) c (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2) | (16) c (0,0,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,1/2)  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

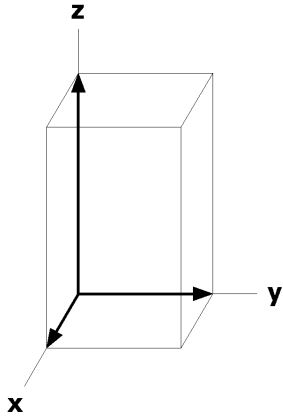
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
16	n	1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $\bar{y},x,z [\bar{v},u,w]$	(4) $y,\bar{x},z [v,\bar{u},w]$
			(5) $\bar{x},y,\bar{z}+1/2 [\bar{u},v,\bar{w}]$	(6) $x,\bar{y},\bar{z}+1/2 [u,\bar{v},\bar{w}]$	(7) $y,x,\bar{z}+1/2 [v,u,\bar{w}]$	(8) $\bar{y},\bar{x},\bar{z}+1/2 [\bar{v},\bar{u},\bar{w}]$
			(9) $\bar{x},\bar{y},\bar{z} [u,v,w]$	(10) $x,y,\bar{z} [\bar{u},\bar{v},w]$	(11) $y,\bar{x},\bar{z} [\bar{v},u,w]$	(12) $\bar{y},x,\bar{z} [v,\bar{u},w]$
			(13) $x,\bar{y},z+1/2 [\bar{u},v,\bar{w}]$	(14) $\bar{x},y,z+1/2 [u,\bar{v},\bar{w}]$	(15) $\bar{y},\bar{x},z+1/2 [v,u,\bar{w}]$	(16) $y,x,z+1/2 [\bar{v},\bar{u},\bar{w}]$
8	m	m..	$x,y,0 [0,0,w]$	$\bar{x},\bar{y},0 [0,0,w]$	$\bar{y},x,0 [0,0,w]$	$y,\bar{x},0 [0,0,w]$
			$\bar{x},y,1/2 [0,0,\bar{w}]$	$x,\bar{y},1/2 [0,0,\bar{w}]$	$y,x,1/2 [0,0,\bar{w}]$	$\bar{y},\bar{x},1/2 [0,0,\bar{w}]$
8	l	.2.	$x,1/2,1/4 [u,0,0]$	$\bar{x},1/2,1/4 [\bar{u},0,0]$	$1/2,x,1/4 [0,u,0]$	$1/2,\bar{x},1/4 [0,\bar{u},0]$
			$\bar{x},1/2,3/4 [u,0,0]$	$x,1/2,3/4 [\bar{u},0,0]$	$1/2,\bar{x},3/4 [0,u,0]$	$1/2,x,3/4 [0,\bar{u},0]$
8	k	.2.	$x,0,1/4 [u,0,0]$	$\bar{x},0,1/4 [\bar{u},0,0]$	$0,x,1/4 [0,u,0]$	$0,\bar{x},1/4 [0,\bar{u},0]$
			$\bar{x},0,3/4 [u,0,0]$	$x,0,3/4 [\bar{u},0,0]$	$0,\bar{x},3/4 [0,u,0]$	$0,x,3/4 [0,\bar{u},0]$
8	j	..2	$x,x,1/4 [u,u,0]$	$\bar{x},\bar{x},1/4 [\bar{u},\bar{u},0]$	$\bar{x},x,1/4 [\bar{u},u,0]$	$x,\bar{x},1/4 [u,\bar{u},0]$
			$\bar{x},\bar{x},3/4 [u,u,0]$	$x,x,3/4 [\bar{u},\bar{u},0]$	$x,\bar{x},3/4 [\bar{u},u,0]$	$\bar{x},x,3/4 [u,\bar{u},0]$
8	i	2..	$0,1/2,z [0,0,w]$	$1/2,0,z [0,0,w]$	$0,1/2,\bar{z}+1/2 [0,0,\bar{w}]$	$1/2,0,\bar{z}+1/2 [0,0,\bar{w}]$
			$0,1/2,\bar{z} [0,0,w]$	$1/2,0,\bar{z} [0,0,w]$	$0,1/2,z+1/2 [0,0,\bar{w}]$	$1/2,0,z+1/2 [0,0,\bar{w}]$
4	h	4..	$1/2,1/2,z [0,0,w]$	$1/2,1/2,\bar{z}+1/2 [0,0,\bar{w}]$	$1/2,1/2,\bar{z} [0,0,w]$	$1/2,1/2,z+1/2 [0,0,\bar{w}]$
4	g	4..	$0,0,z [0,0,w]$	$0,0,\bar{z}+1/2 [0,0,\bar{w}]$	$0,0,\bar{z} [0,0,w]$	$0,0,z+1/2 [0,0,\bar{w}]$
4	f	222.	$0,1/2,1/4 [0,0,0]$	$1/2,0,1/4 [0,0,0]$	$0,1/2,3/4 [0,0,0]$	$1/2,0,3/4 [0,0,0]$
4	e	2/m..	$0,1/2,0 [0,0,w]$	$1/2,0,0 [0,0,w]$	$0,1/2,1/2 [0,0,\bar{w}]$	$1/2,0,1/2 [0,0,\bar{w}]$
2	d	4/m..	$1/2,1/2,0 [0,0,w]$	$1/2,1/2,1/2 [0,0,\bar{w}]$		
2	c	422	$1/2,1/2,1/4 [0,0,0]$	$1/2,1/2,3/4 [0,0,0]$		
2	b	4/m..	$0,0,0 [0,0,w]$	$0,0,1/2 [0,0,\bar{w}]$		
2	a	422	$0,0,1/4 [0,0,0]$	$0,0,3/4 [0,0,0]$		

## Symmetry of Special Projections

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2a^*2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $x,0,1/4$

Along  $[1,1,0]$   $p2a^*2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at  $x,x,1/4$

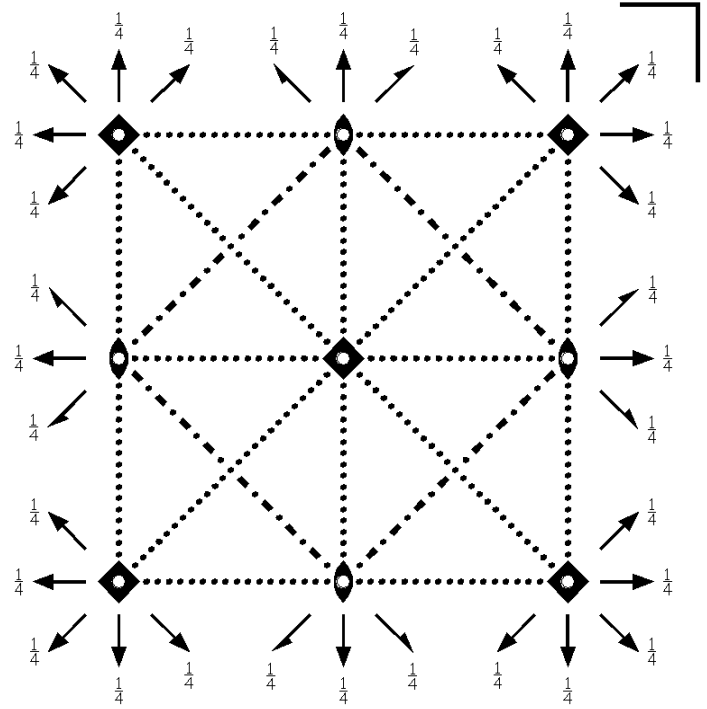
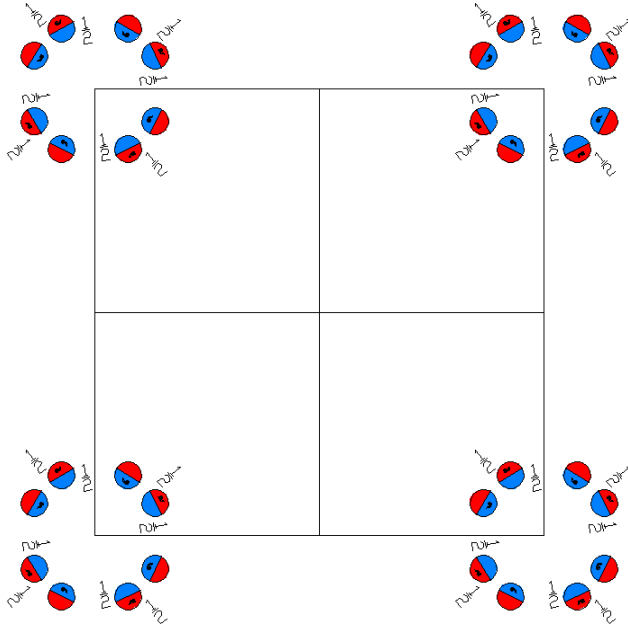


P4/mcc1'  
124.2.1019

4/mmm1'  
P4/m2/c2/c1'

Tetragonal

1'



Origin at center ( 4/m1' ) at 4/mcc1'

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For 1 + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)              | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)         |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)          | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)          | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                      | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2) |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)          | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)             | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)         | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                 |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (15) c (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2)   | (16) c (0,0,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,1/2)  |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)'	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(5) 2' 0,y,1/4 (2 <sub>y</sub>  0,0,1/2)'	(6) 2' x,0,1/4 (2 <sub>x</sub>  0,0,1/2)'	(7) 2' x,x,1/4 (2 <sub>xy</sub>  0,0,1/2)'	(8) 2' x, $\bar{x}$ ,1/4 (2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)'
(9) $\bar{1}$ ' 0,0,0 ( $\bar{1}$  0,0,0)'	(10) m' x,y,0 (m <sub>z</sub>  0,0,0)'	(11) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'	(12) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z^{-1}$  0,0,0)'
(13) c' (0,0,1/2) x,0,z (m <sub>y</sub>  0,0,1/2)'	(14) c' (0,0,1/2) 0,y,z (m <sub>x</sub>  0,0,1/2)'	(15) c' (0,0,1/2) x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,1/2)'	(16) c' (0,0,1/2) x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			1 +		1' +	
			16	n	11'	(1) x,y,z [0,0,0]
			(5) $\bar{x},y,\bar{z}+1/2$ [0,0,0]	(6) x, $\bar{y},\bar{z}+1/2$ [0,0,0]	(7) y,x, $\bar{z}+1/2$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [0,0,0]
			(9) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(10) x,y, $\bar{z}$ [0,0,0]	(11) y, $\bar{x},\bar{z}$ [0,0,0]	(12) $\bar{y},x,\bar{z}$ [0,0,0]
			(13) x, $\bar{y},z+1/2$ [0,0,0]	(14) $\bar{x},y,z+1/2$ [0,0,0]	(15) $\bar{y},\bar{x},z+1/2$ [0,0,0]	(16) y,x,z+1/2 [0,0,0]
8	m	m..1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{y},x,0$ [0,0,0]	y, $\bar{x},0$ [0,0,0]
			$\bar{x},y,1/2$ [0,0,0]	x, $\bar{y},1/2$ [0,0,0]	y,x,1/2 [0,0,0]	$\bar{y},\bar{x},1/2$ [0,0,0]
8	l	.2.1'	x,1/2,1/4 [0,0,0]	$\bar{x},1/2,1/4$ [0,0,0]	1/2,x,1/4 [0,0,0]	1/2, $\bar{x},1/4$ [0,0,0]
			$\bar{x},1/2,3/4$ [0,0,0]	x,1/2,3/4 [0,0,0]	1/2, $\bar{x},3/4$ [0,0,0]	1/2,x,3/4 [0,0,0]
8	k	.2.1'	x,0,1/4 [0,0,0]	$\bar{x},0,1/4$ [0,0,0]	0,x,1/4 [0,0,0]	0, $\bar{x},1/4$ [0,0,0]
			$\bar{x},0,3/4$ [0,0,0]	x,0,3/4 [0,0,0]	0, $\bar{x},3/4$ [0,0,0]	0,x,3/4 [0,0,0]
8	j	..21'	x,x,1/4 [0,0,0]	$\bar{x},\bar{x},1/4$ [0,0,0]	$\bar{x},x,1/4$ [0,0,0]	x, $\bar{x},1/4$ [0,0,0]
			$\bar{x},\bar{x},3/4$ [0,0,0]	x,x,3/4 [0,0,0]	x, $\bar{x},3/4$ [0,0,0]	$\bar{x},x,3/4$ [0,0,0]
8	i	2..1'	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]
			0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0,z+1/2 [0,0,0]
4	h	4..1'	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	1/2,1/2,z+1/2 [0,0,0]
4	g	4..1'	0,0,z [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0,z+1/2 [0,0,0]
4	f	222.1'	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,3/4 [0,0,0]



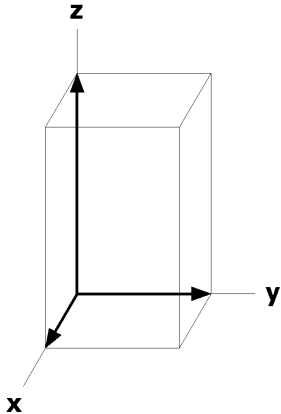
4	e	2/m..1'	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0]
2	d	4/m..1'	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
2	c	4221'	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]	
2	b	4/m..1'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]	
2	a	4221'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

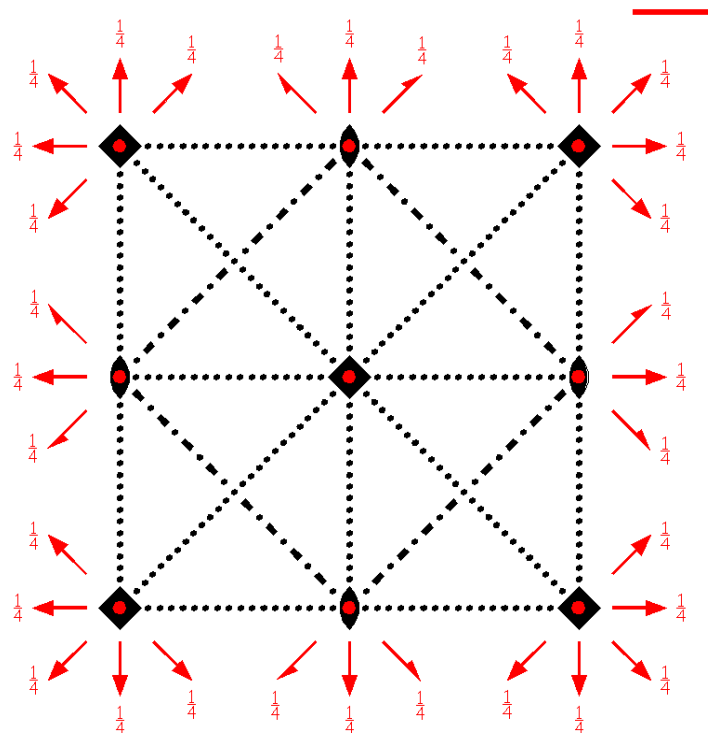
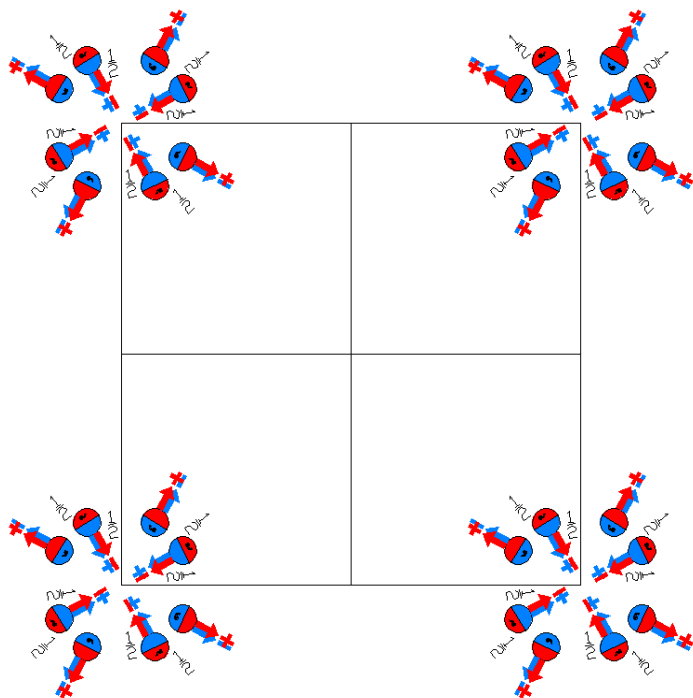
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



P4/m'cc  
124.3.1020

4/m'mm  
P4/m'2'/c2'/c

Tetragonal



Origin at center ( $4/m'$ ) at  $4/m'cc$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)              | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)            | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)          |
| (5) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'        | (6) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'        | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                  | (8) 2' x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)' |
| (9) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$ ' 0,0,0)'      | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'           | (11) $\bar{4}^+$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^+$ ' 0,0,0)'   | (12) $\bar{4}^-$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^-$ ' 0,0,0)'               |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (15) c (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2) | (16) c (0,0,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,1/2)    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

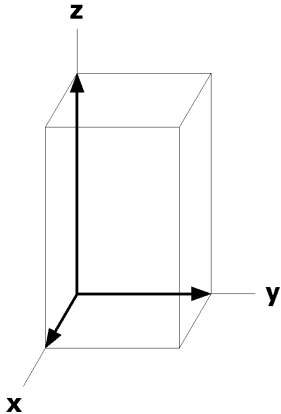
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	n	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [v, $\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [v,u,w]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [u,v, $\bar{w}$ ]	(11) $y,\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
			(13) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [u, $\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z+1/2$ [v,u, $\bar{w}$ ]	(16) $y,x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	m	m'..	$x,y,0$ [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},u,0$ ]	$y,\bar{x},0$ [v, $\bar{u},0$ ]
			$\bar{x},y,1/2$ [u, $\bar{v},0$ ]	$x,\bar{y},1/2$ [ $\bar{u},v,0$ ]	$y,x,1/2$ [ $\bar{v},\bar{u},0$ ]	$\bar{y},\bar{x},1/2$ [v,u,0]
8	l	.2'	$x,1/2,1/4$ [0,v,w]	$\bar{x},1/2,1/4$ [0, $\bar{v},w$ ]	$1/2,x,1/4$ [ $\bar{v},0,w$ ]	$1/2,\bar{x},1/4$ [v,0,w]
			$\bar{x},1/2,3/4$ [0, $\bar{v},\bar{w}$ ]	$x,1/2,3/4$ [0,v, $\bar{w}$ ]	$1/2,\bar{x},3/4$ [v,0, $\bar{w}$ ]	$1/2,x,3/4$ [ $\bar{v},0,\bar{w}$ ]
8	k	.2'	$x,0,1/4$ [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	$0,x,1/4$ [ $\bar{v},0,w$ ]	$0,\bar{x},1/4$ [v,0,w]
			$\bar{x},0,3/4$ [0, $\bar{v},\bar{w}$ ]	$x,0,3/4$ [0,v, $\bar{w}$ ]	$0,\bar{x},3/4$ [v,0, $\bar{w}$ ]	$0,x,3/4$ [ $\bar{v},0,\bar{w}$ ]
8	j	..2'	$x,x,1/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [u, $\bar{u},w$ ]	$\bar{x},x,1/4$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x},1/4$ [u,u,w]
			$\bar{x},\bar{x},3/4$ [u, $\bar{u},\bar{w}$ ]	$x,x,3/4$ [ $\bar{u},u,\bar{w}$ ]	$x,\bar{x},3/4$ [u,u, $\bar{w}$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	i	2..	$0,1/2,z$ [0,0,w]	$1/2,0,z$ [0,0,w]	$0,1/2,\bar{z}+1/2$ [0,0,w]	$1/2,0,\bar{z}+1/2$ [0,0,w]
			$0,1/2,\bar{z}$ [0,0, $\bar{w}$ ]	$1/2,0,\bar{z}$ [0,0, $\bar{w}$ ]	$0,1/2,z+1/2$ [0,0, $\bar{w}$ ]	$1/2,0,z+1/2$ [0,0, $\bar{w}$ ]
4	h	4..	$1/2,1/2,z$ [0,0,w]	$1/2,1/2,\bar{z}+1/2$ [0,0,w]	$1/2,1/2,\bar{z}$ [0,0, $\bar{w}$ ]	$1/2,1/2,z+1/2$ [0,0, $\bar{w}$ ]
4	g	4..	$0,0,z$ [0,0,w]	$0,0,\bar{z}+1/2$ [0,0,w]	$0,0,\bar{z}$ [0,0, $\bar{w}$ ]	$0,0,z+1/2$ [0,0, $\bar{w}$ ]
4	f	22'2'	$0,1/2,1/4$ [0,0,w]	$1/2,0,1/4$ [0,0,w]	$0,1/2,3/4$ [0,0, $\bar{w}$ ]	$1/2,0,3/4$ [0,0, $\bar{w}$ ]
4	e	2/m'..	$0,1/2,0$ [0,0,0]	$1/2,0,0$ [0,0,0]	$0,1/2,1/2$ [0,0,0]	$1/2,0,1/2$ [0,0,0]
2	d	4/m'..	$1/2,1/2,0$ [0,0,0]	$1/2,1/2,1/2$ [0,0,0]		
2	c	42'2'	$1/2,1/2,1/4$ [0,0,w]	$1/2,1/2,3/4$ [0,0, $\bar{w}$ ]		
2	b	4/m'..	$0,0,0$ [0,0,0]	$0,0,1/2$ [0,0,0]		
2	a	42'2'	$0,0,1/4$ [0,0,w]	$0,0,3/4$ [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $x,0,0$

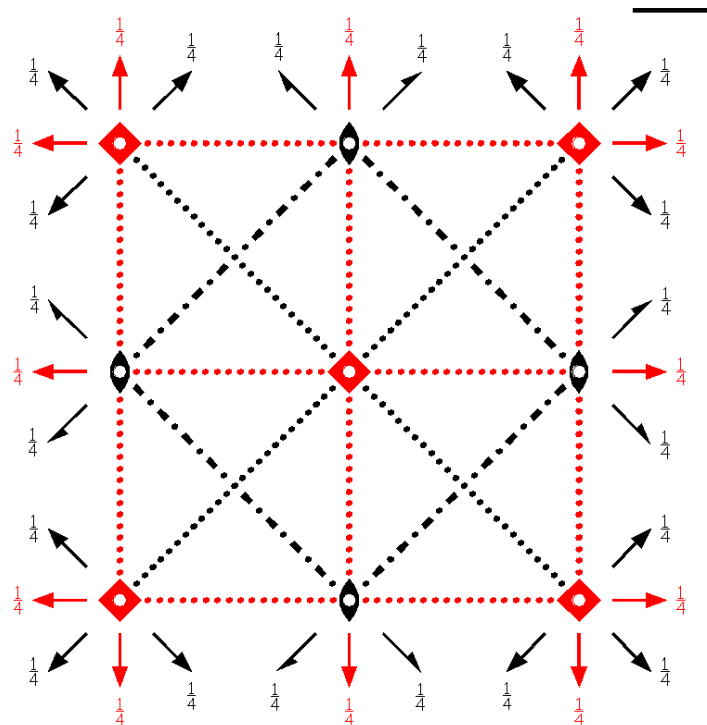
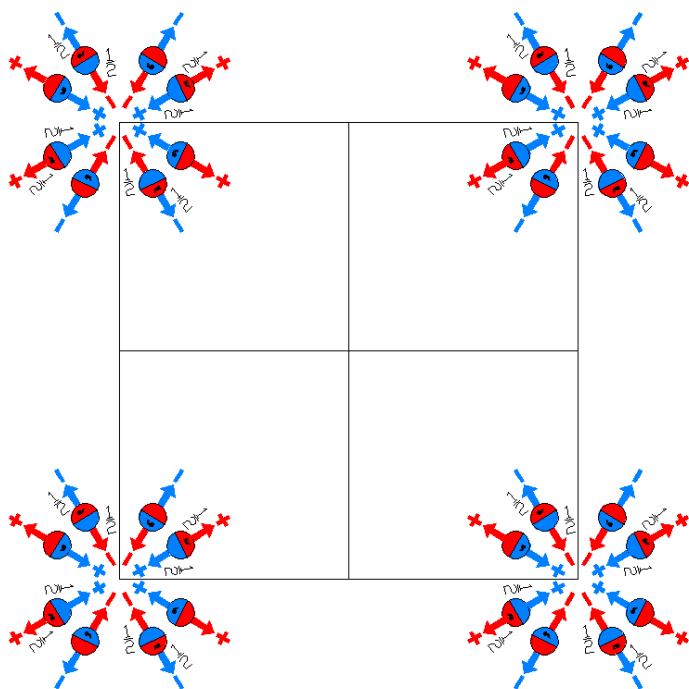
Along  $[1,1,0]$   $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at  $x,x,0$



P4'/mc'c  
124.4.1021

4'/mm'm  
P4'/m2'/c'2/c

Tetragonal



Origin at center ( $4'/m$ ) at  $4'/mc'c$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                                    | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'        |
| (5) 2' 0,y,1/4<br>(2 <sub>y</sub> ' 0,0,1/2)'         | (6) 2' x,0,1/4<br>(2 <sub>x</sub> ' 0,0,1/2)'         | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                       | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2) |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)            | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)               | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'         | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                |
| (13) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (14) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' | (15) c (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2)    | (16) c (0,0,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,1/2)  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

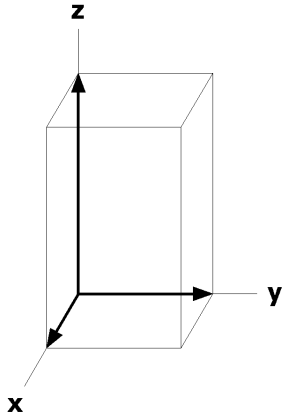
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	n	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [v, $\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}+1/2$ [v,u, $\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(10) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
			(13) $x,\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]	(15) $\bar{y},\bar{x},z+1/2$ [v,u, $\bar{w}$ ]	(16) $y,x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	m	m..	$x,y,0$ [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0, $\bar{w}$ ]	$y,\bar{x},0$ [0,0, $\bar{w}$ ]
			$\bar{x},y,1/2$ [0,0,w]	$x,\bar{y},1/2$ [0,0,w]	$y,x,1/2$ [0,0, $\bar{w}$ ]	$\bar{y},\bar{x},1/2$ [0,0, $\bar{w}$ ]
8	l	.2'	$x,1/2,1/4$ [0,v,w]	$\bar{x},1/2,1/4$ [0, $\bar{v},w$ ]	$1/2,x,1/4$ [v,0, $\bar{w}$ ]	$1/2,\bar{x},1/4$ [ $\bar{v},0,\bar{w}$ ]
			$\bar{x},1/2,3/4$ [0,v,w]	$x,1/2,3/4$ [0, $\bar{v},w$ ]	$1/2,\bar{x},3/4$ [v,0, $\bar{w}$ ]	$1/2,x,3/4$ [ $\bar{v},0,\bar{w}$ ]
8	k	.2'	$x,0,1/4$ [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	$0,x,1/4$ [v,0, $\bar{w}$ ]	$0,\bar{x},1/4$ [ $\bar{v},0,\bar{w}$ ]
			$\bar{x},0,3/4$ [0,v,w]	$x,0,3/4$ [0, $\bar{v},w$ ]	$0,\bar{x},3/4$ [v,0, $\bar{w}$ ]	$0,x,3/4$ [ $\bar{v},0,\bar{w}$ ]
8	j	..2	$x,x,1/4$ [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/4$ [u, $\bar{u},0$ ]	$x,\bar{x},1/4$ [ $\bar{u},u,0$ ]
			$\bar{x},\bar{x},3/4$ [u,u,0]	$x,x,3/4$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},3/4$ [u, $\bar{u},0$ ]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]
8	i	2..	$0,1/2,z$ [0,0,w]	$1/2,0,z$ [0,0, $\bar{w}$ ]	$0,1/2,\bar{z}+1/2$ [0,0,w]	$1/2,0,\bar{z}+1/2$ [0,0, $\bar{w}$ ]
			$0,1/2,\bar{z}$ [0,0,w]	$1/2,0,\bar{z}$ [0,0, $\bar{w}$ ]	$0,1/2,z+1/2$ [0,0,w]	$1/2,0,z+1/2$ [0,0, $\bar{w}$ ]
4	h	4'..	$1/2,1/2,z$ [0,0,0]	$1/2,1/2,\bar{z}+1/2$ [0,0,0]	$1/2,1/2,\bar{z}$ [0,0,0]	$1/2,1/2,z+1/2$ [0,0,0]
4	g	4'..	$0,0,z$ [0,0,0]	$0,0,\bar{z}+1/2$ [0,0,0]	$0,0,\bar{z}$ [0,0,0]	$0,0,z+1/2$ [0,0,0]
4	f	22'2'	$0,1/2,1/4$ [0,0,w]	$1/2,0,1/4$ [0,0, $\bar{w}$ ]	$0,1/2,3/4$ [0,0,w]	$1/2,0,3/4$ [0,0, $\bar{w}$ ]
4	e	2/m..	$0,1/2,0$ [0,0,w]	$1/2,0,0$ [0,0, $\bar{w}$ ]	$0,1/2,1/2$ [0,0,w]	$1/2,0,1/2$ [0,0, $\bar{w}$ ]
2	d	4'/m..	$1/2,1/2,0$ [0,0,0]	$1/2,1/2,1/2$ [0,0,0]		
2	c	4'2'2	$1/2,1/2,1/4$ [0,0,0]	$1/2,1/2,3/4$ [0,0,0]		
2	b	4'/m..	$0,0,0$ [0,0,0]	$0,0,1/2$ [0,0,0]		
2	a	4'2'2	$0,0,1/4$ [0,0,0]	$0,0,3/4$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
Origin at x,0,0

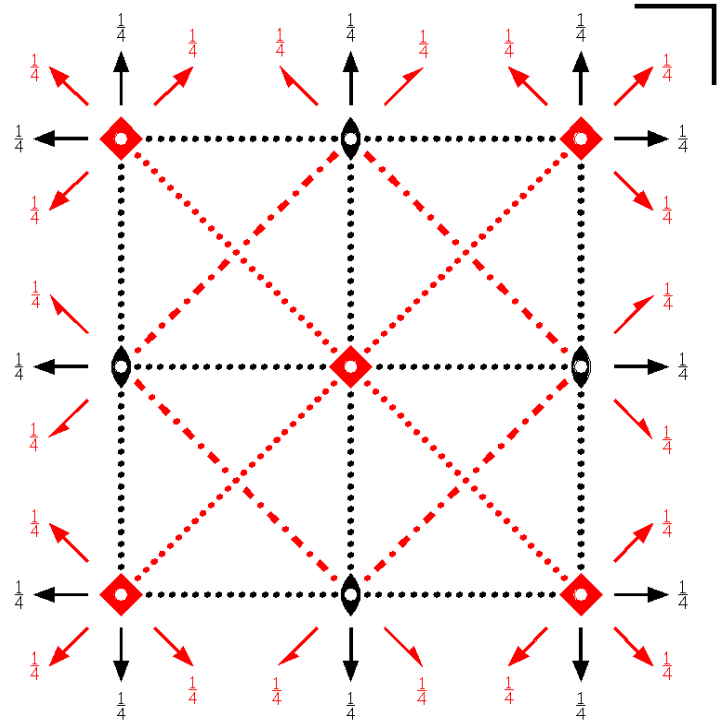
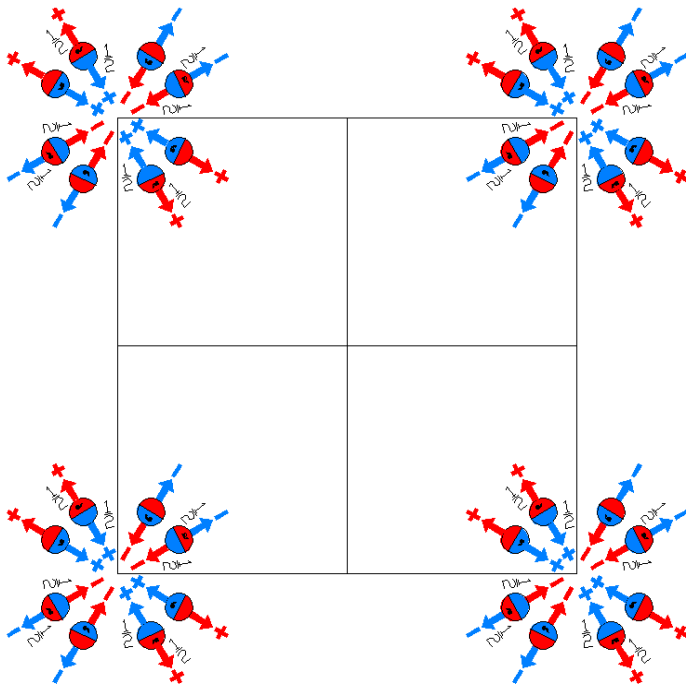
Along [1,1,0]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at x,x,1/4



P4'/mcc'  
124.5.1022

4'/mmm'  
P4'/m2/c2'/c'

Tetragonal



Origin at center ( $4'/m$ ) at  $4'/mcc'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                              | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                | (3) $4^+$ $0,0,z$<br>( $4_z$  0,0,0)'                      | (4) $4^-$ $0,0,z$<br>( $4_z^{-1}$  0,0,0)'                     |
| (5) 2 $0,y,1/4$<br>( $2_y$  0,0,1/2)            | (6) 2 $x,0,1/4$<br>( $2_x$  0,0,1/2)            | (7) $2'$ $x,x,1/4$<br>( $2_{xy}$  0,0,1/2)'                | (8) $2'$ $x,\bar{x},1/4$<br>( $2_{\bar{xy}}$  0,0,1/2)'        |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)    | (10) m $x,y,0$<br>( $m_z$  0,0,0)               | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z$  0,0,0)'  | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1}$  0,0,0)' |
| (13) c $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2) | (14) c $(0,0,1/2)$ $0,y,z$<br>( $m_x$  0,0,1/2) | (15) c' $(0,0,1/2)$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2)' | (16) c' $(0,0,1/2)$ $x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2)'     |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

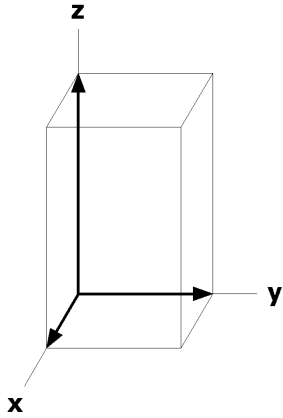
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	n	1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $\bar{y},x,z [v,\bar{u},\bar{w}]$	(4) $y,\bar{x},z [\bar{v},u,\bar{w}]$
			(5) $\bar{x},y,\bar{z}+1/2 [\bar{u},v,\bar{w}]$	(6) $x,\bar{y},\bar{z}+1/2 [u,\bar{v},\bar{w}]$	(7) $y,x,\bar{z}+1/2 [\bar{v},\bar{u},w]$	(8) $\bar{y},\bar{x},\bar{z}+1/2 [v,u,w]$
			(9) $\bar{x},\bar{y},\bar{z} [u,v,w]$	(10) $x,y,\bar{z} [\bar{u},\bar{v},w]$	(11) $y,\bar{x},\bar{z} [v,\bar{u},\bar{w}]$	(12) $\bar{y},x,\bar{z} [\bar{v},u,\bar{w}]$
			(13) $x,\bar{y},z+1/2 [\bar{u},v,\bar{w}]$	(14) $\bar{x},y,z+1/2 [u,\bar{v},\bar{w}]$	(15) $\bar{y},\bar{x},z+1/2 [\bar{v},\bar{u},w]$	(16) $y,x,z+1/2 [v,u,w]$
8	m	m..	$x,y,0 [0,0,w]$	$\bar{x},\bar{y},0 [0,0,w]$	$\bar{y},x,0 [0,0,\bar{w}]$	$y,\bar{x},0 [0,0,\bar{w}]$
			$\bar{x},y,1/2 [0,0,\bar{w}]$	$x,\bar{y},1/2 [0,0,\bar{w}]$	$y,x,1/2 [0,0,w]$	$\bar{y},\bar{x},1/2 [0,0,w]$
8	l	.2.	$x,1/2,1/4 [u,0,0]$	$\bar{x},1/2,1/4 [\bar{u},0,0]$	$1/2,x,1/4 [0,\bar{u},0]$	$1/2,\bar{x},1/4 [0,u,0]$
			$\bar{x},1/2,3/4 [u,0,0]$	$x,1/2,3/4 [\bar{u},0,0]$	$1/2,\bar{x},3/4 [0,\bar{u},0]$	$1/2,x,3/4 [0,u,0]$
8	k	.2.	$x,0,1/4 [u,0,0]$	$\bar{x},0,1/4 [\bar{u},0,0]$	$0,x,1/4 [0,\bar{u},0]$	$0,\bar{x},1/4 [0,u,0]$
			$\bar{x},0,3/4 [u,0,0]$	$x,0,3/4 [\bar{u},0,0]$	$0,\bar{x},3/4 [0,\bar{u},0]$	$0,x,3/4 [0,u,0]$
8	j	..2'	$x,x,1/4 [\bar{u},u,w]$	$\bar{x},\bar{x},1/4 [u,\bar{u},w]$	$\bar{x},x,1/4 [u,u,\bar{w}]$	$x,\bar{x},1/4 [\bar{u},\bar{u},\bar{w}]$
			$\bar{x},\bar{x},3/4 [\bar{u},u,w]$	$x,x,3/4 [u,\bar{u},w]$	$x,\bar{x},3/4 [u,u,\bar{w}]$	$\bar{x},x,3/4 [\bar{u},\bar{u},\bar{w}]$
8	i	2..	$0,1/2,z [0,0,w]$	$1/2,0,z [0,0,\bar{w}]$	$0,1/2,\bar{z}+1/2 [0,0,\bar{w}]$	$1/2,0,\bar{z}+1/2 [0,0,w]$
			$0,1/2,\bar{z} [0,0,w]$	$1/2,0,\bar{z} [0,0,\bar{w}]$	$0,1/2,z+1/2 [0,0,\bar{w}]$	$1/2,0,z+1/2 [0,0,w]$
4	h	4'..	$1/2,1/2,z [0,0,0]$	$1/2,1/2,\bar{z}+1/2 [0,0,0]$	$1/2,1/2,\bar{z} [0,0,0]$	$1/2,1/2,z+1/2 [0,0,0]$
4	g	4'..	$0,0,z [0,0,0]$	$0,0,\bar{z}+1/2 [0,0,0]$	$0,0,\bar{z} [0,0,0]$	$0,0,z+1/2 [0,0,0]$
4	f	222.	$0,1/2,1/4 [0,0,0]$	$1/2,0,1/4 [0,0,0]$	$0,1/2,3/4 [0,0,0]$	$1/2,0,3/4 [0,0,0]$
4	e	2/m..	$0,1/2,0 [0,0,w]$	$1/2,0,0 [0,0,\bar{w}]$	$0,1/2,1/2 [0,0,\bar{w}]$	$1/2,0,1/2 [0,0,w]$
2	d	4'/m..	$1/2,1/2,0 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$		
2	c	4'22'	$1/2,1/2,1/4 [0,0,0]$	$1/2,1/2,3/4 [0,0,0]$		
2	b	4'/m..	$0,0,0 [0,0,0]$	$0,0,1/2 [0,0,0]$		
2	a	4'22'	$0,0,1/4 [0,0,0]$	$0,0,3/4 [0,0,0]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $x,0,1/4$

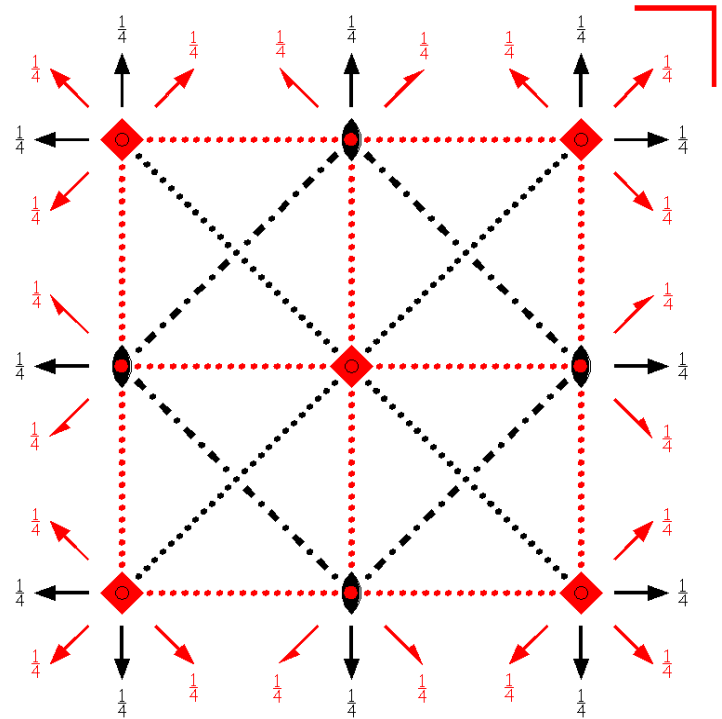
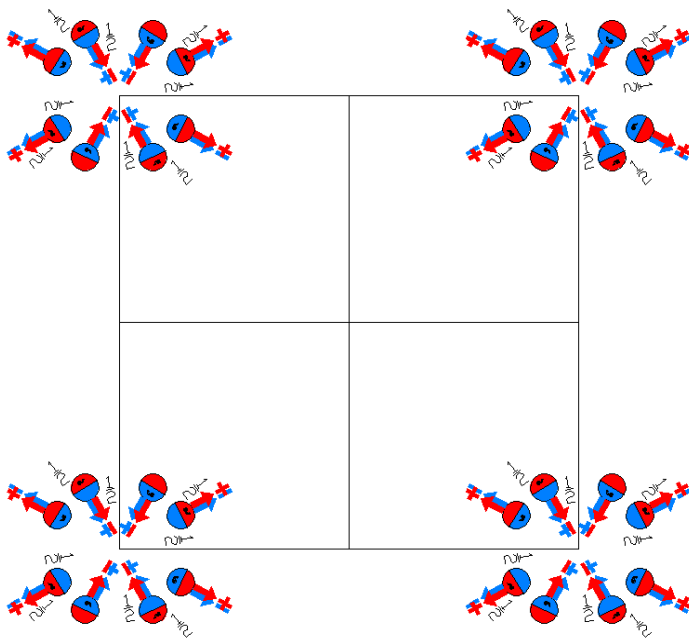
Along  $[1,1,0]$   $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at  $x,x,0$



P4'/m'c'c  
124.6.1023

4'/m'm'm  
P4'/m'2/c'2'/c

Tetragonal



Origin at center ( $4'/m'$ ) at  $4'/m'c'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

**Symmetry Operations**

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                    | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)'        | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'        |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)            | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)            | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                            | (8) 2' x,x̄,1/4<br>(2 <sub>xȳ</sub>  0,0,1/2)'                          |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'                           | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'             | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0) |
| (13) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (14) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' | (15) c (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)                    | (16) c (0,0,1/2) x,x,z<br>(m <sub>xȳ</sub>  0,0,1/2)                    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

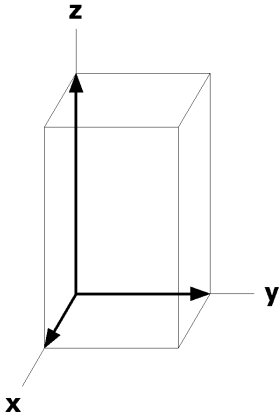
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	n	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $v,\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $v,u,w$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
			(13) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y,x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	m	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $v,\bar{u},0$ ]	$y,\bar{x},0$ [ $\bar{v},u,0$ ]
			$\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	$x,\bar{y},1/2$ [ $u,\bar{v},0$ ]	$y,x,1/2$ [ $\bar{v},\bar{u},0$ ]	$\bar{y},\bar{x},1/2$ [ $v,u,0$ ]
8	l	.2.	x,1/2,1/4 [u,0,0]	$\bar{x},1/2,1/4$ [ $\bar{u},0,0$ ]	1/2,x,1/4 [0, $\bar{u},0$ ]	1/2, $\bar{x},1/4$ [0,u,0]
			$\bar{x},1/2,3/4$ [ $\bar{u},0,0$ ]	x,1/2,3/4 [u,0,0]	1/2, $\bar{x},3/4$ [0,u,0]	1/2,x,3/4 [0, $\bar{u},0$ ]
8	k	.2.	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	0,x,1/4 [0, $\bar{u},0$ ]	0, $\bar{x},1/4$ [0,u,0]
			$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [u,0,0]	0, $\bar{x},3/4$ [0,u,0]	0,x,3/4 [0, $\bar{u},0$ ]
8	j	..2'	x,x,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [ $u,\bar{u},w$ ]	$\bar{x},x,1/4$ [ $u,u,\bar{w}$ ]	$x,\bar{x},1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x},\bar{x},3/4$ [ $u,\bar{u},\bar{w}$ ]	x,x,3/4 [ $\bar{u},u,\bar{w}$ ]	$x,\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,3/4$ [ $u,u,w$ ]
8	i	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0,w]
			0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]
4	h	4'..	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	1/2,1/2,z+1/2 [0,0,0]
4	g	4'..	0,0,z [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0,z+1/2 [0,0,0]
4	f	222.	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,3/4 [0,0,0]
4	e	2/m'..	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]
2	d	4'/m'..	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	c	4'22'	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	b	4'/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
2	a	4'22'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4'm'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,0,0

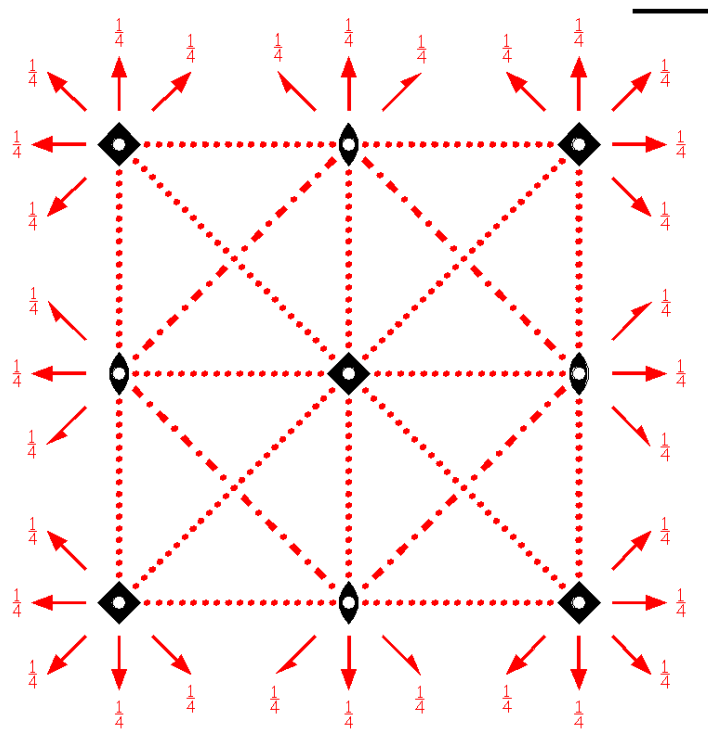
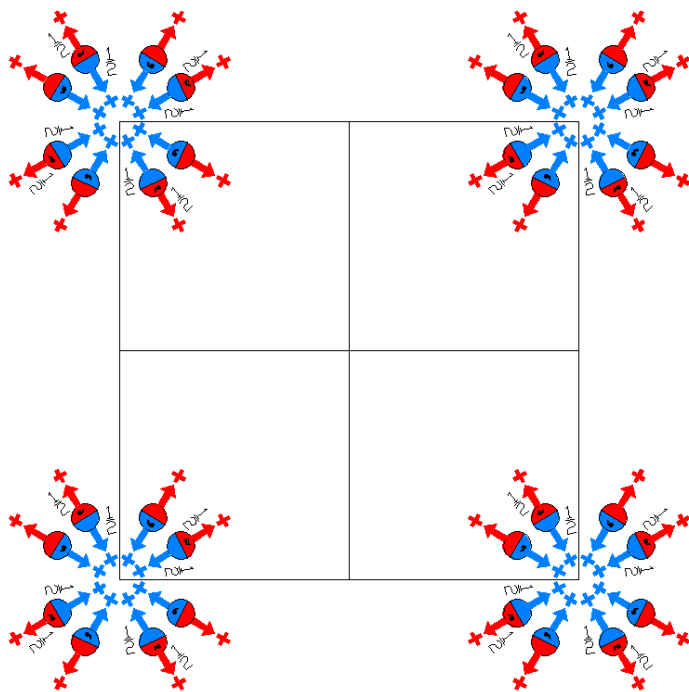
Along [1,1,0]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at x,x,0



P4/mc'c'  
124.7.1024

4/mm'm'  
P4/m2'/c'2'/c'

Tetragonal



Origin at center ( $4/m$ ) at  $4/mc'c'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                    | (3) $4^+$ $0,0,z$<br>( $4_z$  0,0,0)                         | (4) $4^-$ $0,0,z$<br>( $4_z^{-1}$  0,0,0)                     |
| (5) $2'$ $0,y,1/4$<br>( $2_y$  0,0,1/2)'            | (6) $2'$ $x,0,1/4$<br>( $2_x$  0,0,1/2)'            | (7) $2'$ $x,x,1/4$<br>( $2_{xy}$  0,0,1/2)'                  | (8) $2'$ $x,\bar{x},1/4$<br>( $2_{\bar{xy}}$  0,0,1/2)'       |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)        | (10) m $x,y,0$<br>( $m_z$  0,0,0)                   | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z$  0,0,0)     | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (13) $c'$ $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2)' | (14) $c'$ $(0,0,1/2)$ $0,y,z$<br>( $m_x$  0,0,1/2)' | (15) $c'$ $(0,0,1/2)$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2)' | (16) $c'$ $(0,0,1/2)$ $x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2)'  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	n	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $v,u,w$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(10) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
			(13) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x,z+1/2$ [ $v,u,w$ ]
8	m	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0,w]	$y,\bar{x},0$ [0,0,w]
			$\bar{x},y,1/2$ [0,0,w]	$x,\bar{y},1/2$ [0,0,w]	$y,x,1/2$ [0,0,w]	$\bar{y},\bar{x},1/2$ [0,0,w]
8	l	.2'	x,1/2,1/4 [0,v,w]	$\bar{x},1/2,1/4$ [0, $\bar{v},w$ ]	1/2,x,1/4 [ $\bar{v},0,w$ ]	1/2, $\bar{x},1/4$ [ $v,0,w$ ]
			$\bar{x},1/2,3/4$ [0,v,w]	$x,1/2,3/4$ [0, $\bar{v},w$ ]	1/2, $\bar{x},3/4$ [ $\bar{v},0,w$ ]	1/2,x,3/4 [ $v,0,w$ ]
8	k	.2'	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	0,x,1/4 [ $\bar{v},0,w$ ]	0, $\bar{x},1/4$ [ $v,0,w$ ]
			$\bar{x},0,3/4$ [0,v,w]	$x,0,3/4$ [0, $\bar{v},w$ ]	0, $\bar{x},3/4$ [ $\bar{v},0,w$ ]	0,x,3/4 [ $v,0,w$ ]
8	j	..2'	x,x,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [ $u,\bar{u},w$ ]	$\bar{x},x,1/4$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x},1/4$ [ $u,u,w$ ]
			$\bar{x},\bar{x},3/4$ [ $\bar{u},u,w$ ]	$x,x,3/4$ [ $u,\bar{u},w$ ]	$x,\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,3/4$ [ $u,u,w$ ]
8	i	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]
			0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0,z+1/2 [0,0,w]
4	h	4..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2,z+1/2 [0,0,w]
4	g	4..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0,w]
4	f	22'2'	0,1/2,1/4 [0,0,w]	1/2,0,1/4 [0,0,w]	0,1/2,3/4 [0,0,w]	1/2,0,3/4 [0,0,w]
4	e	2/m..	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]	0,1/2,1/2 [0,0,w]	1/2,0,1/2 [0,0,w]
2	d	4/m..	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]		
2	c	42'2'	1/2,1/2,1/4 [0,0,w]	1/2,1/2,3/4 [0,0,w]		
2	b	4/m..	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]		
2	a	42'2'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		

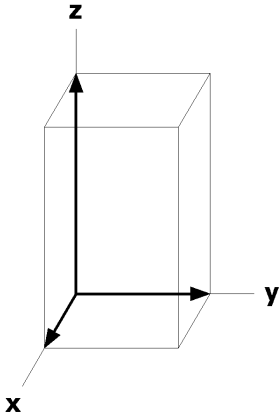
## Symmetry of Special Projections

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $x,0,0$

Along  $[1,1,0]$   $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at  $x,x,0$

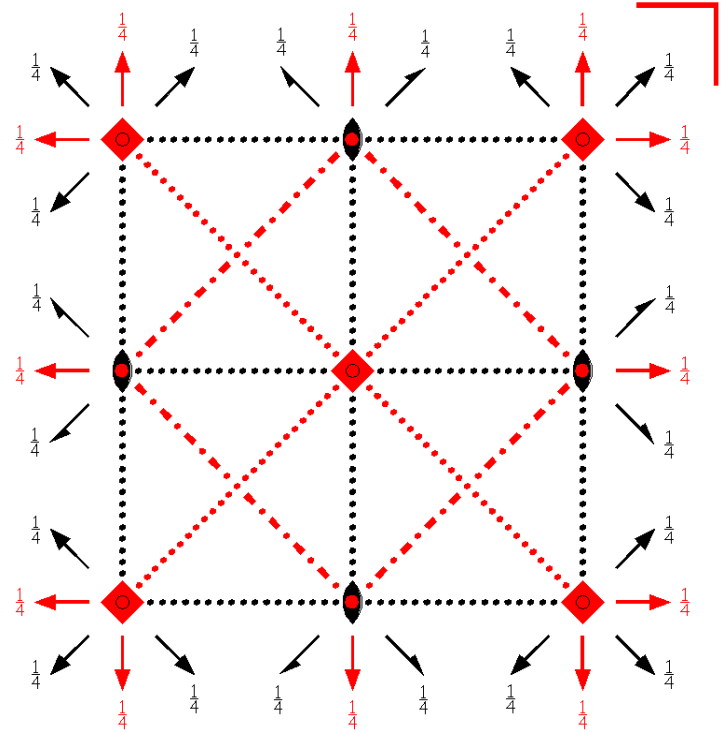
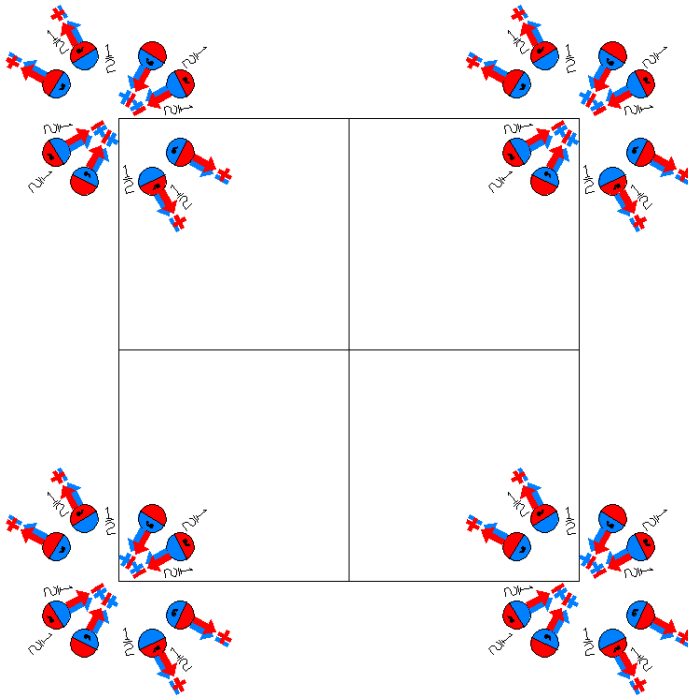




P4'/m'cc'  
124.8.1025

4'/m'mm'  
P4'/m'2'/c2'/c'

Tetragonal



Origin at center ( $4'/m'$ ) at  $4'/m'cc'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)              | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'                                      | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'                         |
| (5) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'        | (6) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'        | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)   | (8) 2 x,x̄,1/4<br>(2 <sub>xȳ</sub>  0,0,1/2)  |
| (9) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$ ' 0,0,0)'      | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'           | (11) $\bar{4}$ <sup>+</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>+</sup>  0,0,0) | (12) $\bar{4}$ <sup>-</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (15) c' (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)'                                   | (16) c' (0,0,1/2) x,x,z<br>(m <sub>xȳ</sub>  0,0,1/2)'                                    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

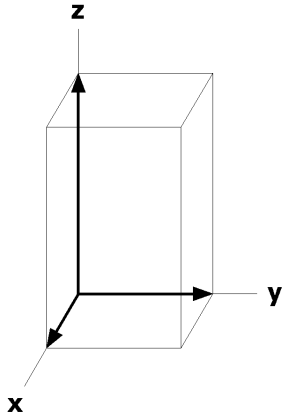
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	n	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]
			(13) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x,z+1/2$ [ $\bar{v},u,w$ ]
8	m	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},\bar{u},0$ ]	$y,\bar{x},0$ [ $\bar{v},u,0$ ]
			$\bar{x},y,1/2$ [ $\bar{u},\bar{v},0$ ]	$x,\bar{y},1/2$ [ $\bar{u},v,0$ ]	$y,x,1/2$ [ $\bar{v},u,0$ ]	$\bar{y},\bar{x},1/2$ [ $\bar{v},\bar{u},0$ ]
8	l	.2'	x,1/2,1/4 [0,v,w]	$\bar{x},1/2,1/4$ [0, $\bar{v},w$ ]	1/2,x,1/4 [v,0, $\bar{w}$ ]	1/2, $\bar{x},1/4$ [ $\bar{v},0,\bar{w}$ ]
			$\bar{x},1/2,3/4$ [0, $\bar{v},\bar{w}$ ]	$x,1/2,3/4$ [0,v, $\bar{w}$ ]	1/2, $\bar{x},3/4$ [ $\bar{v},0,w$ ]	1/2,x,3/4 [v,0,w]
8	k	.2'	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	0,x,1/4 [v,0, $\bar{w}$ ]	0, $\bar{x},1/4$ [ $\bar{v},0,\bar{w}$ ]
			$\bar{x},0,3/4$ [0, $\bar{v},\bar{w}$ ]	$x,0,3/4$ [0,v, $\bar{w}$ ]	0, $\bar{x},3/4$ [ $\bar{v},0,w$ ]	0,x,3/4 [v,0,w]
8	j	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/4$ [u, $\bar{u},0$ ]	$x,\bar{x},1/4$ [ $\bar{u},u,0$ ]
			$\bar{x},\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	$x,x,3/4$ [u,u,0]	$x,\bar{x},3/4$ [u, $\bar{u},0$ ]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]
8	i	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
			0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0,w]
4	h	4'..	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	1/2,1/2,z+1/2 [0,0,0]
4	g	4'..	0,0,z [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0,z+1/2 [0,0,0]
4	f	22'2'	0,1/2,1/4 [0,0,w]	1/2,0,1/4 [0,0, $\bar{w}$ ]	0,1/2,3/4 [0,0, $\bar{w}$ ]	1/2,0,3/4 [0,0,w]
4	e	2/m'..	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]
2	d	4'/m'..	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	c	4'2'2	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	b	4'/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
2	a	4'2'2	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4'mm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
Origin at x,0,0

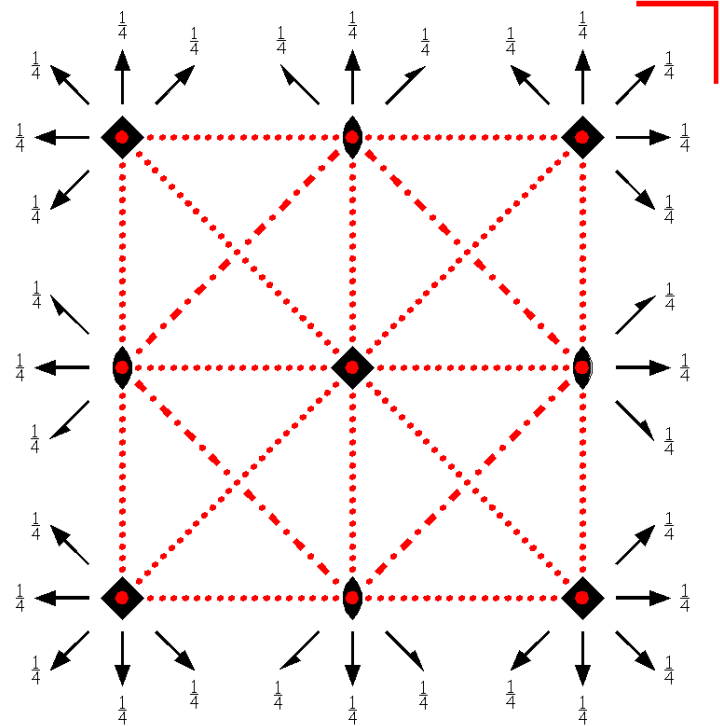
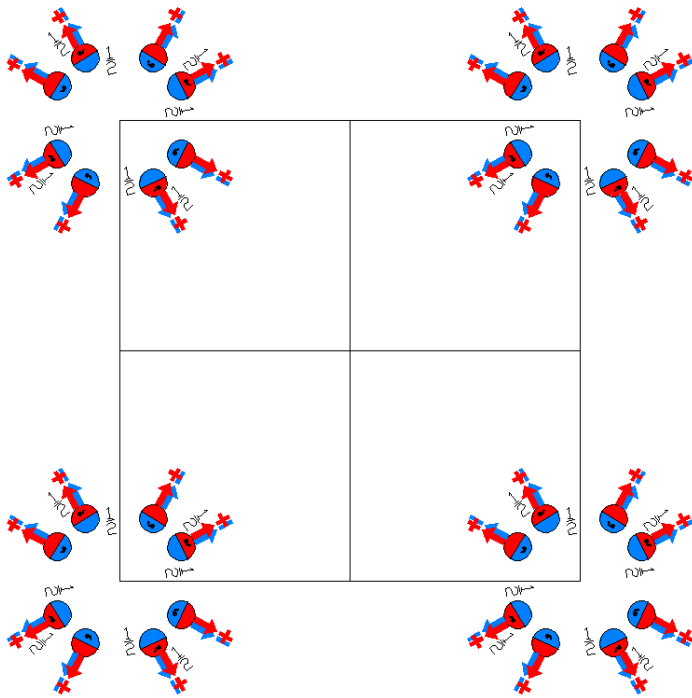
Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,x,0



P4/m'c'c'  
124.9.1026

4/m'm'm'  
P4/m'2/c'2/c'

Tetragonal



Origin at center ( 4/m' ) at 4/m'c'c'

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

**Symmetry Operations**

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                                    | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                       | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)          |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)            | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)            | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                               | (8) 2 x,x̄,1/4<br>(2 <sub>xȳ</sub>  0,0,1/2)                              |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'                           | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'             | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)' | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (13) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (14) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' | (15) c' (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)'                   | (16) c' (0,0,1/2) x,x,z<br>(m <sub>xȳ</sub>  0,0,1/2)'                    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

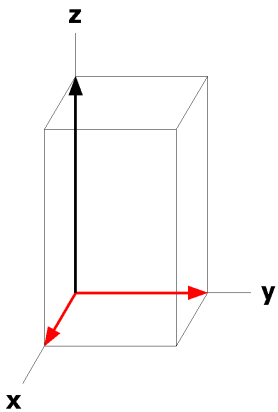
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	n	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
			(13) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x,z+1/2$ [ $v,u,w$ ]
8	m	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},u,0$ ]	$y,\bar{x},0$ [ $v,\bar{u},0$ ]
			$\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	$x,\bar{y},1/2$ [ $u,\bar{v},0$ ]	$y,x,1/2$ [ $v,u,0$ ]	$\bar{y},\bar{x},1/2$ [ $\bar{v},\bar{u},0$ ]
8	l	.2.	x,1/2,1/4 [u,0,0]	$\bar{x},1/2,1/4$ [ $\bar{u},0,0$ ]	1/2,x,1/4 [0,u,0]	1/2, $\bar{x},1/4$ [0, $\bar{u},0$ ]
			$\bar{x},1/2,3/4$ [ $\bar{u},0,0$ ]	x,1/2,3/4 [u,0,0]	1/2, $\bar{x},3/4$ [0, $\bar{u},0$ ]	1/2,x,3/4 [0,u,0]
8	k	.2.	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	0,x,1/4 [0,u,0]	0, $\bar{x},1/4$ [0, $\bar{u},0$ ]
			$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [u,0,0]	0, $\bar{x},3/4$ [0, $\bar{u},0$ ]	0,x,3/4 [0,u,0]
8	j	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/4$ [ $\bar{u},u,0$ ]	x, $\bar{x},1/4$ [ $u,\bar{u},0$ ]
			$\bar{x},\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	x,x,3/4 [u,u,0]	x, $\bar{x},3/4$ [ $u,\bar{u},0$ ]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]
8	i	2..	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
			0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0,w]	1/2,0,z+1/2 [0,0,w]
4	h	4..	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0,w]
4	g	4..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]
4	f	222.	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,3/4 [0,0,0]
4	e	2/m'..	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]
2	d	4/m'..	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	c	422	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	b	4/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
2	a	422	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,0,0

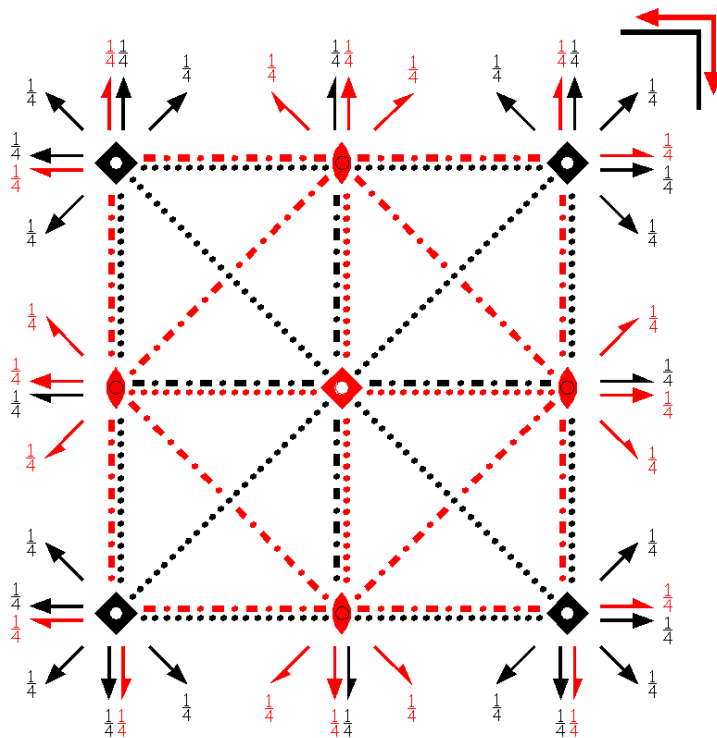
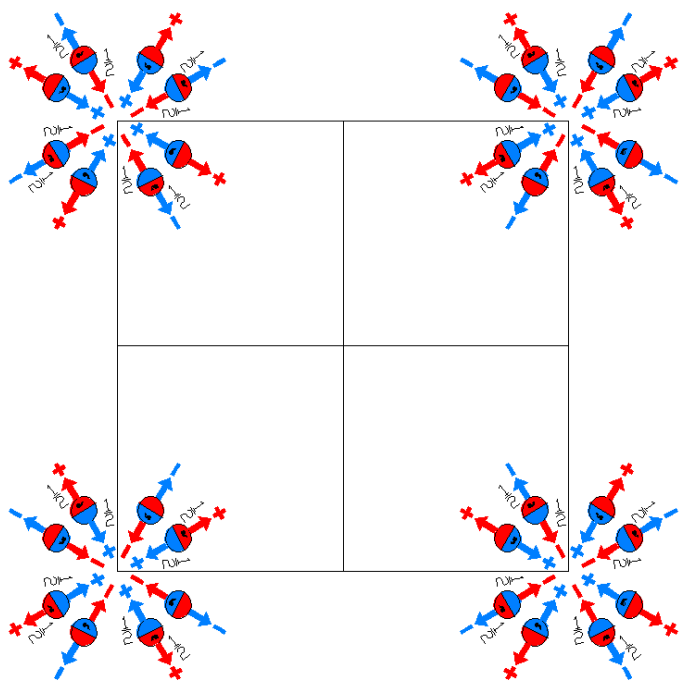
Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,x,0



$P_4/mcc$   
124.10.1027

$4/mmm1'$   
 $P_4/m2/c2/c$

Tetragonal



Origin at center ( $4/m$ ) at  $4/mcc$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                                | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                  | (3) $4^+$ $0,0,z$<br>( $4_z$  0,0,0)                       | (4) $4^-$ $0,0,z$<br>( $4_z^{-1}$  0,0,0)                     |
| (5) 2 $0,y,1/4$<br>( $2_y$  0,0,1/2)              | (6) 2 $x,0,1/4$<br>( $2_x$  0,0,1/2)              | (7) 2 $x,x,1/4$<br>( $2_{xy}$  0,0,1/2)                    | (8) 2 $x,\bar{x},1/4$<br>( $2_{\bar{xy}}$  0,0,1/2)           |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)      | (10) $m$ $x,y,0$<br>( $m_z$  0,0,0)               | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z$  0,0,0)   | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (13) $c$ $(0,0,1/2) \ x,0,z$<br>( $m_y$  0,0,1/2) | (14) $c$ $(0,0,1/2) \ 0,y,z$<br>( $m_x$  0,0,1/2) | (15) $c$ $(0,0,1/2) \ x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2) | (16) $c$ $(0,0,1/2) \ x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2)    |

For (1,0,0)<sup>'</sup> + set

(1) t <sup>'</sup> (1,0,0) (1 1,0,0) <sup>'</sup>	(2) 2 <sup>'</sup> 1/2,0,z (2 <sub>z</sub>  1,0,0) <sup>'</sup>	(3) 4 <sup>+</sup> -1/2,1/2,z (4 <sub>z</sub>  1,0,0) <sup>'</sup>	(4) 4 <sup>'</sup> 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,0) <sup>'</sup>
(5) 2 <sup>'</sup> 1/2,y,1/4 (2 <sub>y</sub>  1,0,1/2) <sup>'</sup>	(6) 2 <sup>'</sup> (1,0,0) x,0,1/4 (2 <sub>x</sub>  1,0,1/2) <sup>'</sup>	(7) 2 <sup>'</sup> (1/2,1/2,0) x+1/2,x,1/4 (2 <sub>xy</sub>  1,0,1/2) <sup>'</sup>	(8) 2 <sup>'</sup> (1/2,-1/2,0) x+1/2,x̄,1/4 (2 <sub>xy</sub> <sup>-</sup>  1,0,1/2) <sup>'</sup>
(9) 1̄ <sup>'</sup> 1/2,0,0 (1̄ 1,0,0) <sup>'</sup>	(10) a <sup>'</sup> (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0) <sup>'</sup>	(11) 4 <sup>+</sup> 1/2,-1/2,z; 1/2,-1/2,0 (4 <sub>z</sub>  1,0,0) <sup>'</sup>	(12) 4 <sup>'</sup> 1/2,1/2,z; 1/2,1/2,0 (4 <sub>z</sub> <sup>-1</sup>  1,0,0) <sup>'</sup>
(13) n <sup>'</sup> (1,0,1/2) x,0,z (m <sub>y</sub>  1,0,1/2) <sup>'</sup>	(14) c <sup>'</sup> (0,0,1/2) 1/2,y,z (m <sub>x</sub>  1,0,1/2) <sup>'</sup>	(15) n <sup>'</sup> (1/2,-1/2,1/2) x+1/2,x̄,z (m <sub>xy</sub>  1,0,1/2) <sup>'</sup>	(16) n <sup>'</sup> (1/2,1/2,1/2)x+1/2,x,z (m <sub>xy</sub> <sup>-</sup>  1,0,1/2) <sup>'</sup>

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1,0,0) <sup>'</sup> +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	n	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w]	(3) ȳ,x,z [v̄,u,w]	(4) y,x,z [v,u,w]
			(5) x̄,y,z+1/2 [ū,v̄,w̄]	(6) x,y,z+1/2 [u,v̄,w̄]	(7) y,x,z+1/2 [v,u,w̄]	(8) ȳ,x̄,z+1/2 [v̄,ū,w̄]
			(9) x̄,ȳ,z̄ [u,v,w]	(10) x,y,z̄ [ū,v̄,w]	(11) y,x,z̄ [v̄,u,w]	(12) ȳ,x,z̄ [v,u,w]
			(13) x̄,y,z+1/2 [ū,v̄,w̄]	(14) x̄,y,z+1/2 [u,v̄,w̄]	(15) ȳ,x,z+1/2 [v,u,w̄]	(16) y,x,z+1/2 [v̄,ū,w̄]
16	m	m..	x,y,0 [0,0,w]	x̄,y,0 [0,0,w]	ȳ,x,0 [0,0,w]	y,x,0 [0,0,w]
			x̄,y,1/2 [0,0,w̄]	x,y,1/2 [0,0,w̄]	y,x,1/2 [0,0,w̄]	ȳ,x̄,1/2 [0,0,w̄]
16	l	.2'	x,1/2,1/4 [0,v,w]	x̄,1/2,1/4 [0,v,w̄]	1/2,x,1/4 [v,0,w̄]	1/2,x̄,1/4 [v,0,w]
			x̄,1/2,3/4 [0,v̄,w̄]	x,1/2,3/4 [0,v̄,w]	1/2,x̄,3/4 [v̄,0,w]	1/2,x,3/4 [v̄,0,w̄]
16	k	.2.	x,0,1/4 [u,0,0]	x̄,0,1/4 [ū,0,0]	0,x,1/4 [0,u,0]	0,x̄,1/4 [0,ū,0]
			x̄,0,3/4 [u,0,0]	x,0,3/4 [ū,0,0]	0,x̄,3/4 [0,u,0]	0,x,3/4 [0,ū,0]
16	j	..2	x,x,1/4 [u,u,0]	x̄,x̄,1/4 [ū,ū,0]	x̄,x,1/4 [ū,u,0]	x,x̄,1/4 [u,ū,0]
			x̄,x̄,3/4 [u,u,0]	x,x,3/4 [ū,ū,0]	x,x̄,3/4 [ū,u,0]	x̄,x,3/4 [u,ū,0]
16	i	2'..	0,1/2,z [u,v,0]	1/2,0,z [v,ū,0]	0,1/2,z̄+1/2 [ū,v,0]	1/2,0,z̄+1/2 [v,u,0]
			0,1/2,z̄ [ū,v̄,0]	1/2,0,z̄ [v̄,u,0]	0,1/2,z+1/2 [u,v̄,0]	1/2,0,z+1/2 [v̄,ū,0]
8	h	4'..	1/2,1/2,z [0,0,0]	1/2,1/2,z̄+1/2 [0,0,0]	1/2,1/2,z̄ [0,0,0]	1/2,1/2,z+1/2 [0,0,0]
8	g	4..	0,0,z [0,0,w]	0,0,z̄+1/2 [0,0,w̄]	0,0,z̄ [0,0,w]	0,0,z+1/2 [0,0,w̄]
8	f	2'2'2.	0,1/2,1/4 [0,v,0]	1/2,0,1/4 [v,0,0]	0,1/2,3/4 [0,v̄,0]	1/2,0,3/4 [v̄,0,0]



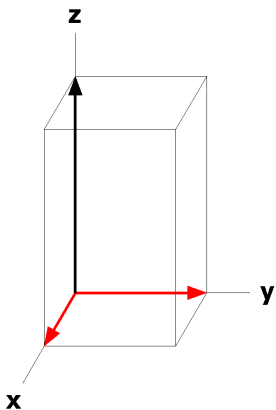
8	e	2'/m..	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0]
4	d	4'/m..	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
4	c	4'2'2	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]	
4	b	4/m..	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]	
4	a	422	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

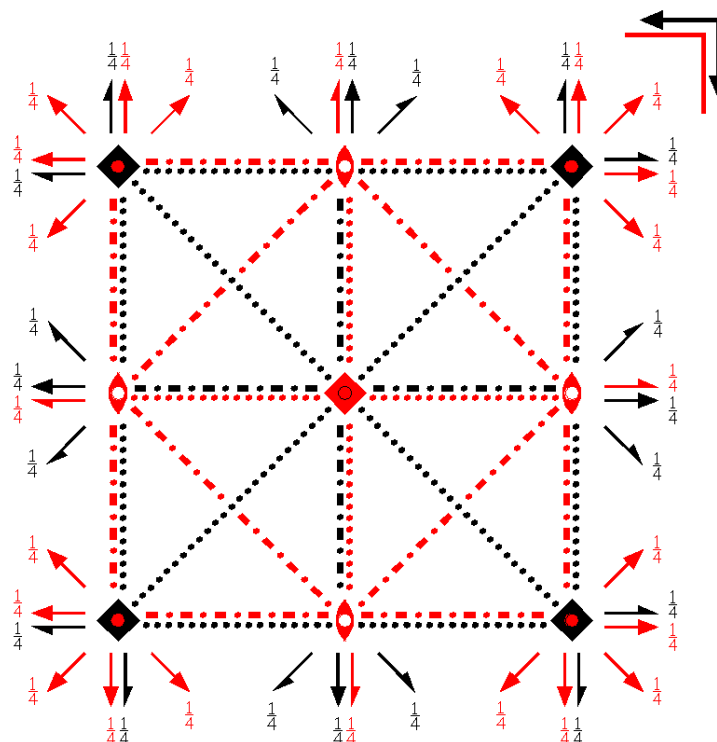
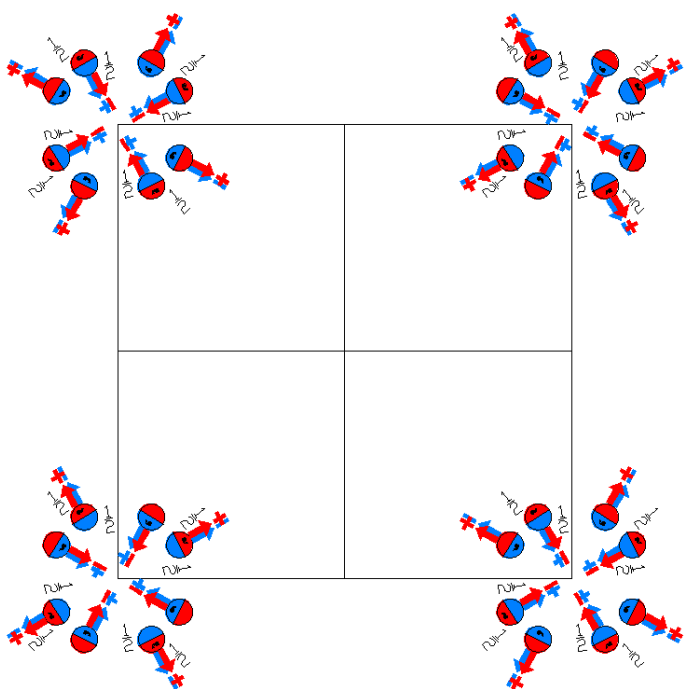
Along [1,1,0] p<sub>c</sub>2mm  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x-1/4,x+1/4,0



$P_P 4/m'cc$   
124.11.1028

$4/mmm1'$   
 $P_P 4/m'2'/c2'/c$

Tetragonal



Origin at center ( $4/m'$ ) at  $4/m'cc$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)              | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)            | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)            |
| (5) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'        | (6) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'        | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                  | (8) 2' x,x̄,1/4<br>(2 <sub>xȳ</sub>  0,0,1/2)'                              |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'                         | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'           | (11) 4̄ <sup>+</sup> 0,0,z; 0,0,0<br>(4̄ <sub>z</sub>  0,0,0)' | (12) 4̄ <sup>-</sup> 0,0,z; 0,0,0<br>(4̄ <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (15) c (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)          | (16) c (0,0,1/2) x,x,z<br>(m <sub>xȳ</sub>  0,0,1/2)                        |

## For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> ' -1/2,1/2,z (4 <sub>z</sub>  1,0,0)'	(4) 4 <sup>-</sup> ' 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,0)'
(5) 2 1/2,y,1/4 (2 <sub>y</sub>  1,0,1/2)	(6) 2 (1,0,0) x,0,1/4 (2 <sub>x</sub>  1,0,1/2)	(7) 2 (1/2,1/2,0) x+1/2,x,1/4 (2 <sub>xy</sub>  1,0,1/2)	(8) 2 (1/2,-1/2,0) x+1/2,x̄,1/4 (2 <sub>xy</sub> <sup>-</sup>  1,0,1/2)
(9) 1̄ 1/2,0,0 (1̄ 1,0,0)	(10) a (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)	(11) 4 <sup>+</sup> 1/2,-1/2,z; 1/2,-1/2,0 (4 <sub>z</sub>  1,0,0)	(12) 4 <sup>-</sup> 1/2,1/2,z; 1/2,1/2,0 (4 <sub>z</sub> <sup>-1</sup>  1,0,0)'
(13) n' (1,0,1/2) x,0,z (m <sub>y</sub>  1,0,1/2)'	(14) c' (0,0,1/2) 1/2,y,z (m <sub>x</sub>  1,0,1/2)'	(15) n' (1/2,-1/2,1/2) x+1/2,x̄,z (m <sub>xy</sub>  1,0,1/2)'	(16) n' (1/2,1/2,1/2)x+1/2,x,z (m <sub>xy</sub> <sup>-</sup>  1,0,1/2)'

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

			(0,0,0) +	(1,0,0)' +		
32	n	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w]	(3) ȳ,x,z [v̄,u,w]	(4) y,x,z [v,u,w]
			(5) x̄,y,z+1/2 [ū,v̄,w]	(6) x,y,z+1/2 [u,v,w]	(7) y,x,z+1/2 [v̄,u,w]	(8) ȳ,x̄,z+1/2 [v,u,w]
			(9) x̄,y,z [ū,v̄,w̄]	(10) x,y,z [u,v,w̄]	(11) y,x,z [v̄,u,w̄]	(12) ȳ,x,z [v,u,w̄]
			(13) x,y,z+1/2 [ū,v̄,w̄]	(14) x̄,y,z+1/2 [u,v̄,w̄]	(15) ȳ,x,z+1/2 [v̄,u,w̄]	(16) y,x,z+1/2 [v,u,w̄]
16	m	m'..	x,y,0 [u,v,0]	x̄,y,0 [ū,v̄,0]	ȳ,x,0 [v̄,u,0]	y,x,0 [v,u,0]
			x̄,y,1/2 [ū,v̄,0]	x,y,1/2 [u,v,0]	y,x,1/2 [v̄,u,0]	ȳ,x̄,1/2 [v,u,0]
16	l	.2.	x,1/2,1/4 [u,0,0]	x̄,1/2,1/4 [ū,0,0]	1/2,x,1/4 [0,ū,0]	1/2,x̄,1/4 [0,ū,0]
			x̄,1/2,3/4 [ū,0,0]	x,1/2,3/4 [u,0,0]	1/2,x̄,3/4 [0,ū,0]	1/2,x,3/4 [0,ū,0]
16	k	.2'.	x,0,1/4 [0,v,w]	x̄,0,1/4 [0,v̄,w]	0,x,1/4 [v̄,0,w]	0,x̄,1/4 [v,0,w]
			x̄,0,3/4 [0,v̄,w̄]	x,0,3/4 [0,v,w̄]	0,x̄,3/4 [v̄,0,w̄]	0,x,3/4 [v,0,w̄]
16	j	..2'	x,x,1/4 [ū,u,w]	x̄,x̄,1/4 [ū,ū,w]	x̄,x,1/4 [ū,ū,w]	x,x̄,1/4 [u,u,w]
			x̄,x̄,3/4 [ū,ū,w̄]	x,x,3/4 [ū,u,w̄]	x,x̄,3/4 [u,u,w̄]	x̄,x,3/4 [ū,ū,w̄]
16	i	2'..	0,1/2,z [u,v,0]	1/2,0,z [v̄,ū,0]	0,1/2,z+1/2 [u,v̄,0]	1/2,0,z+1/2 [v̄,ū,0]
			0,1/2,z̄ [u,v,0]	1/2,0,z̄ [v̄,ū,0]	0,1/2,z+1/2 [u,v̄,0]	1/2,0,z+1/2 [v̄,ū,0]
8	h	4'..	1/2,1/2,z [0,0,0]	1/2,1/2,z̄+1/2 [0,0,0]	1/2,1/2,z̄ [0,0,0]	1/2,1/2,z+1/2 [0,0,0]
8	g	4..	0,0,z [0,0,w]	0,0,z̄+1/2 [0,0,w]	0,0,z̄ [0,0,w̄]	0,0,z+1/2 [0,0,w̄]
8	f	2'22'.	0,1/2,1/4 [u,0,0]	1/2,0,1/4 [0,ū,0]	0,1/2,3/4 [u,0,0]	1/2,0,3/4 [0,ū,0]

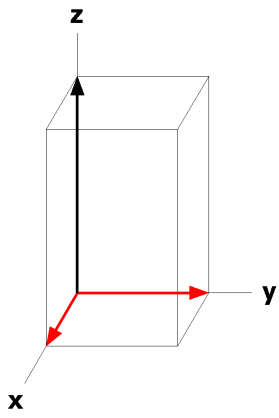
8	e	$2'/m'..$	$0,1/2,0 [u,v,0]$	$1/2,0,0 [v,\bar{u},0]$	$0,1/2,1/2 [u,\bar{v},0]$	$1/2,0,1/2 [\bar{v},\bar{u},0]$
4	d	$4'/m'..$	$1/2,1/2,0 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$		
4	c	$4'22'$	$1/2,1/2,1/4 [0,0,0]$	$1/2,1/2,3/4 [0,0,0]$		
4	b	$4/m'..$	$0,0,0 [0,0,0]$	$0,0,1/2 [0,0,0]$		
4	a	$42'2'$	$0,0,1/4 [0,0,w]$	$0,0,3/4 [0,0,\bar{w}]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_4 \cdot 4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,0,0$

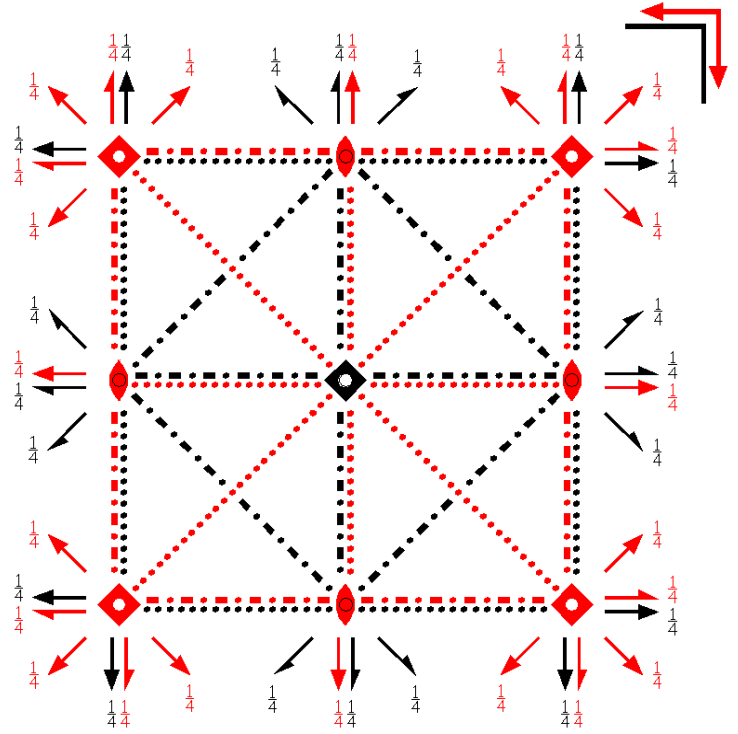
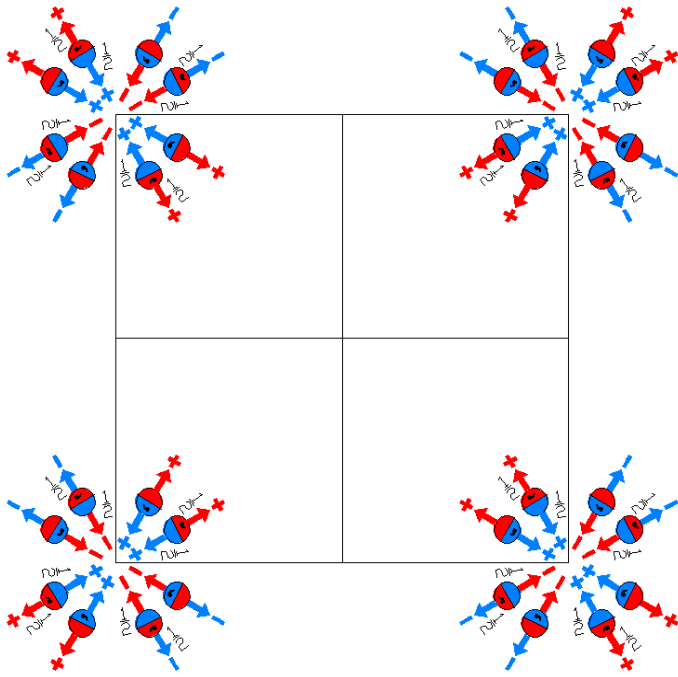
Along  $[1,1,0]$   $p_2 \cdot 2mm$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x-1/4, x+1/4, 1/4$



$P_P 4'/mcc'$   
124.12.1029

$4/mmm1'$   
 $P_P 4'/m2/c2'/c'$

Tetragonal



Origin at center ( $4'/m$ ) at  $4'/mcc'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)              | (3) $4^+ 0,0,z$<br>( $4_z^+$  0,0,0)'                     | (4) $4^- 0,0,z$<br>( $4_z^-$  0,0,0)'                     |
| (5) 2 $0,y,1/4$<br>( $2_y$  0,0,1/2)          | (6) 2 $x,0,1/4$<br>( $2_x$  0,0,1/2)          | (7) $2' x,x,1/4$<br>( $2_{xy}$  0,0,1/2)'                 | (8) $2' x,\bar{x},1/4$<br>( $2_{\bar{xy}}$  0,0,1/2)'     |
| (9) $\bar{1} 0,0,0$<br>( $\bar{1}$  0,0,0)    | (10) m $x,y,0$<br>( $m_z$  0,0,0)             | (11) $\bar{4}^+ 0,0,z; 0,0,0$<br>( $\bar{4}_z^+$  0,0,0)' | (12) $\bar{4}^- 0,0,z; 0,0,0$<br>( $\bar{4}_z^-$  0,0,0)' |
| (13) c (0,0,1/2) $x,0,z$<br>( $m_y$  0,0,1/2) | (14) c (0,0,1/2) $0,y,z$<br>( $m_x$  0,0,1/2) | (15) $c' (0,0,1/2) x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2)'  | (16) $c' (0,0,1/2) x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2)'  |

## For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> -1/2,1/2,z (4 <sub>z</sub>  1,0,0)	(4) 4 <sup>-</sup> 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,0)
(5) 2' 1/2,y,1/4 (2 <sub>y</sub>  1,0,1/2)'	(6) 2' (1,0,0) x,0,1/4 (2 <sub>x</sub>  1,0,1/2)'	(7) 2 (1/2,1/2,0) x+1/2,x,1/4 (2 <sub>xy</sub>  1,0,1/2)	(8) 2 (1/2,-1/2,0) x+1/2,x̄,1/4 (2 <sub>xy</sub> <sup>-</sup>  1,0,1/2)
(9) 1̄' 1/2,0,0 (1̄ 1,0,0)'	(10) a' (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)'	(11) 4 <sup>+</sup> 1/2,-1/2,z; 1/2,-1/2,0 (4 <sub>z</sub>  1,0,0)	(12) 4 <sup>-</sup> 1/2,1/2,z; 1/2,1/2,0 (4 <sub>z</sub> <sup>-1</sup>  1,0,0)
(13) n' (1,0,1/2) x,0,z (m <sub>y</sub>  1,0,1/2)'	(14) c' (0,0,1/2) 1/2,y,z (m <sub>x</sub>  1,0,1/2)'	(15) n (1/2,-1/2,1/2) x+1/2,x̄,z (m <sub>xy</sub>  1,0,1/2)	(16) n (1/2,1/2,1/2)x+1/2,x,z (m <sub>xy</sub> <sup>-</sup>  1,0,1/2)

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1,0,0)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	n	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w]	(3) ȳ,x,z [v̄,ū,w̄]	(4) y,x,z [v̄,u,w̄]
			(5) x̄,y,z+1/2 [ū,v̄,w̄]	(6) x,y,z+1/2 [u,v̄,w̄]	(7) y,x,z+1/2 [v̄,ū,w]	(8) ȳ,x̄,z+1/2 [v,u,w]
			(9) x̄,ȳ,z [u,v,w]	(10) x,y,z [ū,v̄,w]	(11) y,x,z [v̄,ū,w̄]	(12) ȳ,x,z [v̄,u,w̄]
			(13) x,y,z+1/2 [ū,v̄,w̄]	(14) x̄,y,z+1/2 [u,v̄,w̄]	(15) ȳ,x,z+1/2 [v̄,ū,w]	(16) y,x,z+1/2 [v,u,w]
16	m	m..	x,y,0 [0,0,w]	x̄,y,0 [0,0,w]	ȳ,x,0 [0,0,w̄]	y,x,0 [0,0,w̄]
			x̄,y,1/2 [0,0,w̄]	x,y,1/2 [0,0,w̄]	y,x,1/2 [0,0,w]	ȳ,x̄,1/2 [0,0,w]
16	l	.2'	x,1/2,1/4 [0,v,w]	x̄,1/2,1/4 [0,v̄,w̄]	1/2,x,1/4 [v̄,0,w]	1/2,x̄,1/4 [v̄,0,w̄]
			x̄,1/2,3/4 [0,v̄,w̄]	x,1/2,3/4 [0,v̄,w]	1/2,x̄,3/4 [v,0,w̄]	1/2,x,3/4 [v,0,w]
16	k	.2.	x,0,1/4 [u,0,0]	x̄,0,1/4 [ū,0,0]	0,x,1/4 [0,ū,0]	0,x̄,1/4 [0,u,0]
			x̄,0,3/4 [u,0,0]	x,0,3/4 [ū,0,0]	0,x̄,3/4 [0,ū,0]	0,x,3/4 [0,u,0]
16	j	..2'	x,x,1/4 [ū,u,w]	x̄,x̄,1/4 [u,ū,w]	x̄,x,1/4 [u,u,w̄]	x,x̄,1/4 [ū,ū,w̄]
			x̄,x̄,3/4 [ū,u,w]	x,x,3/4 [u,ū,w]	x,x̄,3/4 [u,u,w̄]	x̄,x,3/4 [ū,ū,w̄]
16	i	2'..	0,1/2,z [u,v,0]	1/2,0,z [v̄,u,0]	0,1/2,z+1/2 [ū,v,0]	1/2,0,z+1/2 [v̄,ū,0]
			0,1/2,z̄ [ū,v̄,0]	1/2,0,z̄ [v,ū,0]	0,1/2,z+1/2 [u,v̄,0]	1/2,0,z+1/2 [v,u,0]
8	h	4..	1/2,1/2,z [0,0,w]	1/2,1/2,z̄+1/2 [0,0,w]	1/2,1/2,z̄ [0,0,w]	1/2,1/2,z+1/2 [0,0,w]
8	g	4'..	0,0,z [0,0,0]	0,0,z̄+1/2 [0,0,0]	0,0,z̄ [0,0,0]	0,0,z+1/2 [0,0,0]
8	f	2'2'.2.	0,1/2,1/4 [0,v,0]	1/2,0,1/4 [v̄,0,0]	0,1/2,3/4 [0,v̄,0]	1/2,0,3/4 [v,0,0]

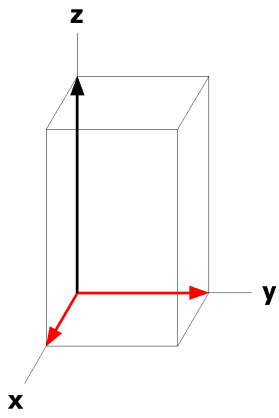
8	e	2'/m..	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0]
4	d	4'/m..	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
4	c	4'2'2	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]	
4	b	4'/m..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]	
4	a	4'22'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

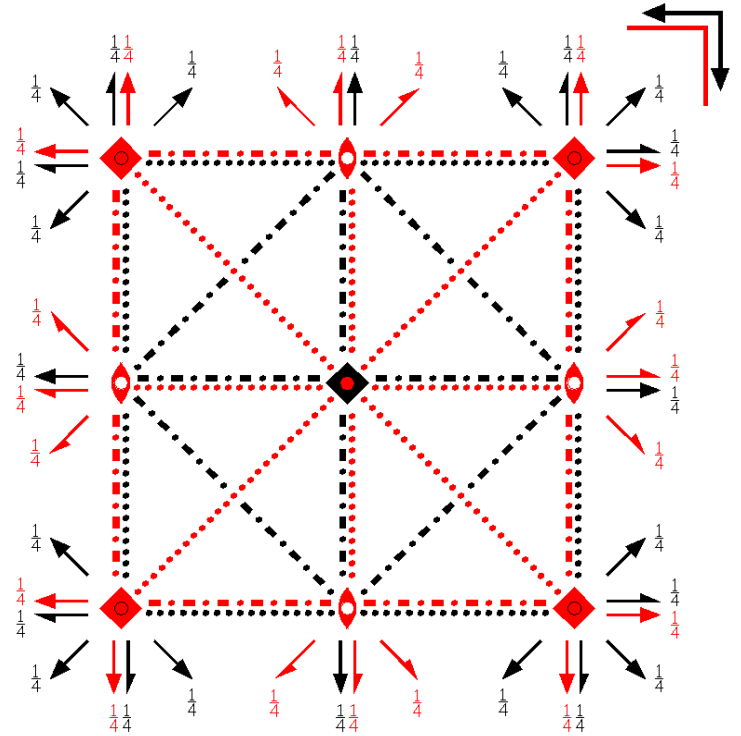
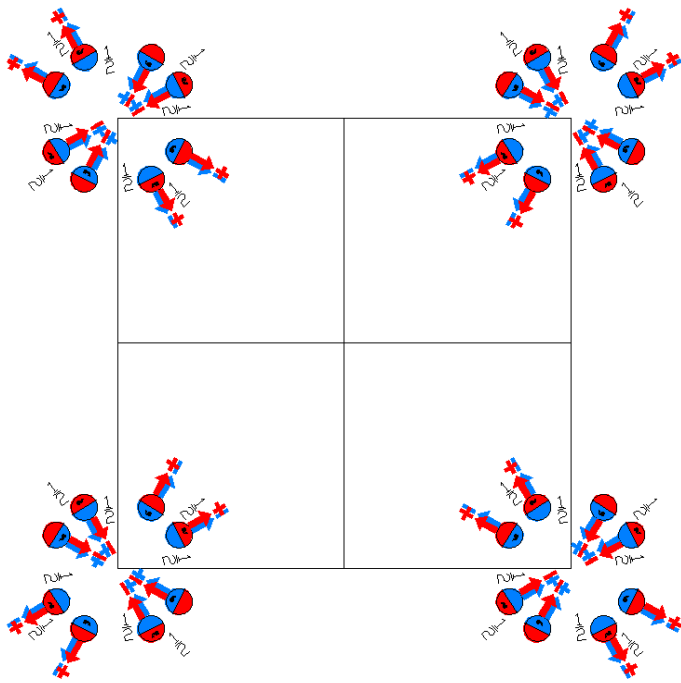
Along [1,1,0]  $p_{2a}2mm$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x-1/4, x+1/4, 0$



$P_P 4'/m'cc'$   
124.13.1030

$4/mmm1'$   
 $P_P 4'/m'2'/c2'/c'$

Tetragonal



Origin at center ( $4'/m'$ ) at  $4'/m'cc'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)              | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)'                         | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'                         |
| (5) 2' 0,y,1/4<br>(2 <sub>y</sub> ' 0,0,1/2)'       | (6) 2' x,0,1/4<br>(2 <sub>x</sub> ' 0,0,1/2)'       | (7) 2 x,x,1/4<br>(2 <sub>xy</sub> ' 0,0,1/2)  | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub> ' 0,0,1/2)                 |
| (9) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$ ' 0,0,0)'      | (10) m' x,y,0<br>(m <sub>z</sub> ' 0,0,0)'          | (11) $\bar{4}$ <sup>+</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>+</sup>  0,0,0) | (12) $\bar{4}$ <sup>-</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>-</sup>  0,0,0) |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (15) c' (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub> ' 0,0,1/2)'                         | (16) c' (0,0,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub> ' 0,0,1/2)'                |



## For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> -1/2,1/2,z (4 <sub>z</sub>  1,0,0)	(4) 4 <sup>-</sup> 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,0)
(5) 2 1/2,y,1/4 (2 <sub>y</sub>  1,0,1/2)	(6) 2 (1,0,0) x,0,1/4 (2 <sub>x</sub>  1,0,1/2)	(7) 2' (1/2,1/2,0) x+1/2,x,1/4 (2 <sub>xy</sub>  1,0,1/2)'	(8) 2' (1/2,-1/2,0) x+1/2,x̄,1/4 (2 <sub>xy</sub> <sup>-</sup>  1,0,1/2)'
(9) 1̄ 1/2,0,0 (1̄ 1,0,0)	(10) a (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)	(11) 4 <sup>+</sup> 1/2,-1/2,z; 1/2,-1/2,0 (4 <sub>z</sub>  1,0,0)'	(12) 4 <sup>-</sup> 1/2,1/2,z; 1/2,1/2,0 (4 <sub>z</sub> <sup>-1</sup>  1,0,0)'
(13) n' (1,0,1/2) x,0,z (m <sub>y</sub>  1,0,1/2)'	(14) c' (0,0,1/2) 1/2,y,z (m <sub>x</sub>  1,0,1/2)'	(15) n (1/2,-1/2,1/2) x+1/2,x̄,z (m <sub>xy</sub>  1,0,1/2)	(16) n (1/2,1/2,1/2)x+1/2,x,z (m <sub>xy</sub> <sup>-</sup>  1,0,1/2)

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1,0,0)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	n	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w]	(3) ȳ,x,z [v̄,ū,w̄]	(4) y,x,z [v̄,ū,w̄]
			(5) x̄,y,z+1/2 [ū,v̄,w]	(6) x,y,z+1/2 [ū,v̄,w]	(7) y,x,z+1/2 [v̄,ū,w̄]	(8) ȳ,x̄,z+1/2 [v̄,ū,w̄]
			(9) x̄,ȳ,z [ū,v̄,w̄]	(10) x,y,z [ū,v̄,w̄]	(11) y,x,z [v̄,ū,w]	(12) ȳ,x,z [v̄,ū,w]
			(13) x,y,z+1/2 [ū,v̄,w̄]	(14) x̄,y,z+1/2 [ū,v̄,w̄]	(15) ȳ,x,z+1/2 [v̄,ū,w]	(16) y,x,z+1/2 [v̄,ū,w]
16	m	m'..	x,y,0 [u,v,0]	x̄,y,0 [ū,v̄,0]	ȳ,x,0 [v̄,ū,0]	y,x,0 [v̄,ū,0]
			x̄,y,1/2 [ū,v̄,0]	x,y,1/2 [ū,v̄,0]	y,x,1/2 [v̄,ū,0]	ȳ,x̄,1/2 [v̄,ū,0]
16	l	.2.	x,1/2,1/4 [u,0,0]	x̄,1/2,1/4 [ū,0,0]	1/2,x,1/4 [0,ū,0]	1/2,x̄,1/4 [0,ū,0]
			x̄,1/2,3/4 [ū,0,0]	x,1/2,3/4 [ū,0,0]	1/2,x̄,3/4 [0,ū,0]	1/2,x,3/4 [0,ū,0]
16	k	.2'.	x,0,1/4 [0,v,w]	x̄,0,1/4 [0,v̄,w]	0,x,1/4 [v,0,w̄]	0,x̄,1/4 [v̄,0,w̄]
			x̄,0,3/4 [0,v̄,w̄]	x,0,3/4 [0,v̄,w̄]	0,x̄,3/4 [v̄,0,w]	0,x,3/4 [v,0,w]
16	j	..2	x,x,1/4 [u,u,0]	x̄,x̄,1/4 [ū,ū,0]	x̄,x,1/4 [ū,ū,0]	x,x̄,1/4 [ū,ū,0]
			x̄,x̄,3/4 [ū,ū,0]	x,x,3/4 [ū,ū,0]	x,x̄,3/4 [ū,ū,0]	x̄,x,3/4 [ū,ū,0]
16	i	2'..	0,1/2,z [u,v,0]	1/2,0,z [v̄,ū,0]	0,1/2,z+1/2 [ū,v̄,0]	1/2,0,z+1/2 [v̄,ū,0]
			0,1/2,z̄ [ū,v̄,0]	1/2,0,z̄ [v̄,ū,0]	0,1/2,z+1/2 [ū,v̄,0]	1/2,0,z+1/2 [v̄,ū,0]
8	h	4..	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w̄]	1/2,1/2,z̄ [0,0,w̄]	1/2,1/2,z+1/2 [0,0,w]
8	g	4'..	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	0,0,z̄ [0,0,0]	0,0,z+1/2 [0,0,0]
8	f	2'22'.	0,1/2,1/4 [u,0,0]	1/2,0,1/4 [0,ū,0]	0,1/2,3/4 [u,0,0]	1/2,0,3/4 [0,ū,0]

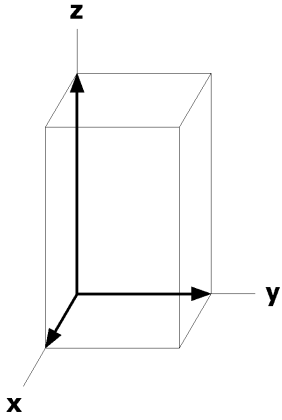
8	e	$2'/m'..$	$0,1/2,0 [u,v,0]$	$1/2,0,0 [\bar{v},u,0]$	$0,1/2,1/2 [u,\bar{v},0]$	$1/2,0,1/2 [v,u,0]$
4	d	$4/m'..$	$1/2,1/2,0 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$		
4	c	422	$1/2,1/2,1/4 [0,0,0]$	$1/2,1/2,3/4 [0,0,0]$		
4	b	$4'/m'..$	$0,0,0 [0,0,0]$	$0,0,1/2 [0,0,0]$		
4	a	$4'2'2$	$0,0,1/4 [0,0,0]$	$0,0,3/4 [0,0,0]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_4 \cdot 4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $1/2,1/2,z$

Along  $[1,0,0]$   $p_2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,0,0$

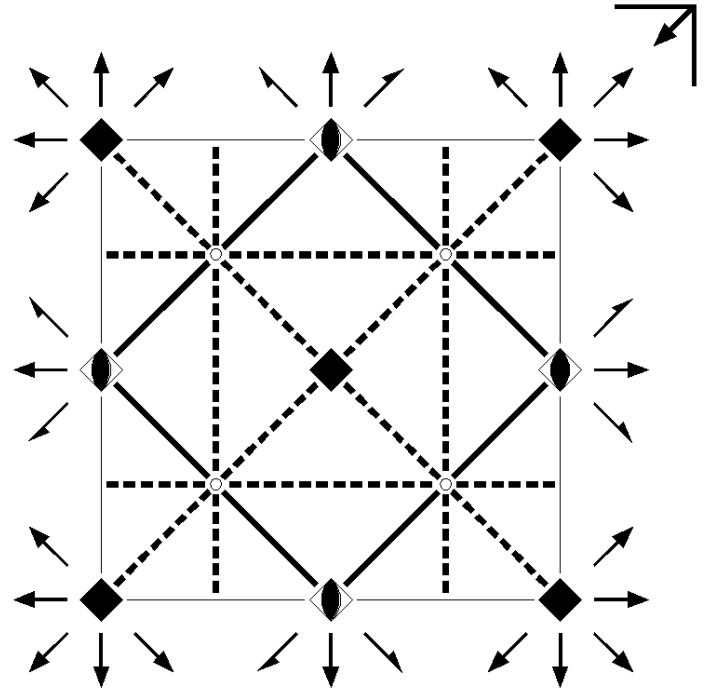
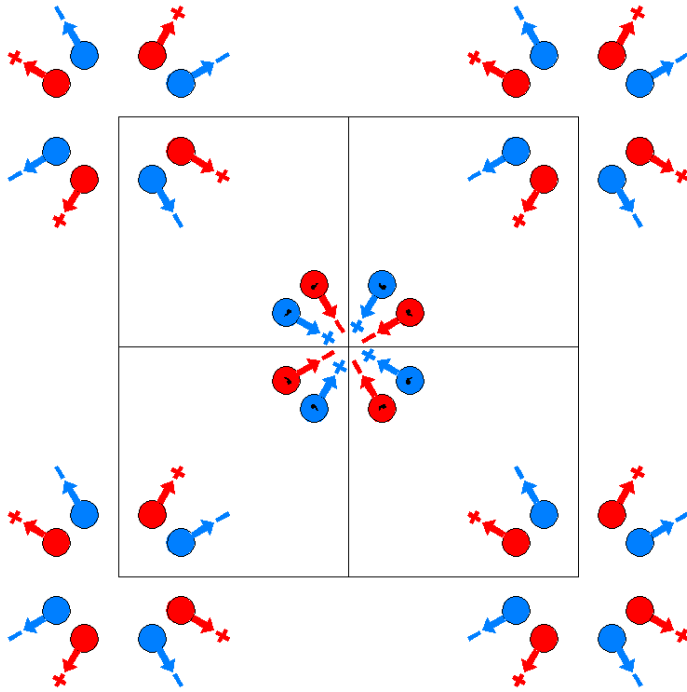
Along  $[1,1,0]$   $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



P4/nbm  
125.1.1031

4/mmm  
P4/n2/b2/m

Tetragonal



Origin at 422 at 4/n22/g, at  $-1/4, -1/4, 0$  from center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)              | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)    |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                  | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                          | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0) |
| (9) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)      | (10) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (11) $\bar{4}^+$ 1/2,0,z; 1/2,0,0<br>( $\bar{4}_z^+$  1/2,1/2,0) | (12) $\bar{4}^-$ 0,1/2,z; 0,1/2,0<br>( $\bar{4}_z^-$  1/2,1/2,0)     |
| (13) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (14) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (15) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0)       | (16) g (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

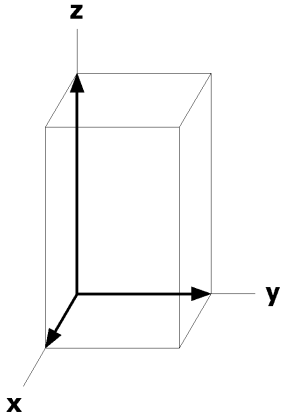
			Coordinates									
Multiplicity, Wyckoff letter, Site Symmetry.												
16	n	1										
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y},x,z$	$[\bar{v},u,w]$	(4)	$y,\bar{x},z$	$[v,\bar{u},w]$	
(5)	$\bar{x},y,\bar{z}$	$[\bar{u},v,\bar{w}]$	(6)	$x,\bar{y},\bar{z}$	$[u,\bar{v},\bar{w}]$	(7)	$y,x,\bar{z}$	$[v,u,\bar{w}]$	(8)	$\bar{y},\bar{x},\bar{z}$	$[\bar{v},\bar{u},\bar{w}]$	
(9)	$\bar{x}+1/2,\bar{y}+1/2,\bar{z}$	$[\bar{u},v,w]$	(10)	$x+1/2,y+1/2,\bar{z}$	$[\bar{u},\bar{v},w]$	(11)	$y+1/2,\bar{x}+1/2,\bar{z}$	$[\bar{v},u,w]$	(12)	$\bar{y}+1/2,x+1/2,\bar{z}$	$[v,\bar{u},w]$	
(13)	$x+1/2,\bar{y}+1/2,z$	$[\bar{u},v,\bar{w}]$	(14)	$\bar{x}+1/2,y+1/2,z$	$[u,\bar{v},\bar{w}]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[v,u,\bar{w}]$	(16)	$y+1/2,x+1/2,z$	$[\bar{v},\bar{u},\bar{w}]$	
8	m	..m	$x,x+1/2,z$	$[\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,z$	$[u,\bar{u},0]$	$\bar{x}+1/2,x,z$	$[\bar{u},\bar{u},0]$	$x+1/2,\bar{x},z$	$[u,u,0]$	$\bar{x}+1/2,\bar{x},z$	$[\bar{u},\bar{u},0]$
8	l	..2	$x,0,1/2$	$[u,0,0]$	$\bar{x},0,1/2$	$[\bar{u},0,0]$	$0,x,1/2$	$[0,u,0]$	$0,\bar{x},1/2$	$[0,\bar{u},0]$	$1/2,x+1/2,1/2$	$[0,\bar{u},0]$
8	k	..2	$x,0,0$	$[u,0,0]$	$\bar{x},0,0$	$[\bar{u},0,0]$	$0,x,0$	$[0,u,0]$	$0,\bar{x},0$	$[0,\bar{u},0]$	$1/2,x+1/2,0$	$[0,\bar{u},0]$
8	j	..2	$x,x,1/2$	$[u,u,0]$	$\bar{x},\bar{x},1/2$	$[\bar{u},\bar{u},0]$	$\bar{x},x,1/2$	$[\bar{u},u,0]$	$x,\bar{x},1/2$	$[u,\bar{u},0]$	$\bar{x}+1/2,\bar{x}+1/2,1/2$	$[u,\bar{u},0]$
8	i	..2	$x,x,0$	$[u,u,0]$	$\bar{x},\bar{x},0$	$[\bar{u},\bar{u},0]$	$\bar{x},x,0$	$[\bar{u},u,0]$	$x,\bar{x},0$	$[u,\bar{u},0]$	$\bar{x}+1/2,\bar{x}+1/2,0$	$[u,\bar{u},0]$
4	h	2.mm	$0,1/2,z$	$[0,0,0]$	$1/2,0,z$	$[0,0,0]$	$0,1/2,\bar{z}$	$[0,0,0]$	$1/2,0,\bar{z}$	$[0,0,0]$		
4	g	4..	$0,0,z$	$[0,0,w]$	$0,0,\bar{z}$	$[0,0,\bar{w}]$	$1/2,1/2,\bar{z}$	$[0,0,w]$	$1/2,1/2,z$	$[0,0,\bar{w}]$		
4	f	..2/m	$1/4,1/4,1/2$	$[u,u,0]$	$3/4,3/4,1/2$	$[\bar{u},\bar{u},0]$	$3/4,1/4,1/2$	$[\bar{u},u,0]$	$1/4,3/4,1/2$	$[u,\bar{u},0]$		
4	e	..2/m	$1/4,1/4,0$	$[u,u,0]$	$3/4,3/4,0$	$[\bar{u},\bar{u},0]$	$3/4,1/4,0$	$[\bar{u},u,0]$	$1/4,3/4,0$	$[u,\bar{u},0]$		
2	d	$\bar{4}2m$	$0,1/2,1/2$	$[0,0,0]$	$1/2,0,1/2$	$[0,0,0]$						
2	c	$\bar{4}2m$	$0,1/2,0$	$[0,0,0]$	$1/2,0,0$	$[0,0,0]$						
2	b	422	$0,0,1/2$	$[0,0,0]$	$1/2,1/2,1/2$	$[0,0,0]$						
2	a	422	$0,0,0$	$[0,0,0]$	$1/2,1/2,0$	$[0,0,0]$						

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_4$  4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a}$  2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,0,0$

Along  $[1,1,0]$   $p_{2mm1'}$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,x,0$

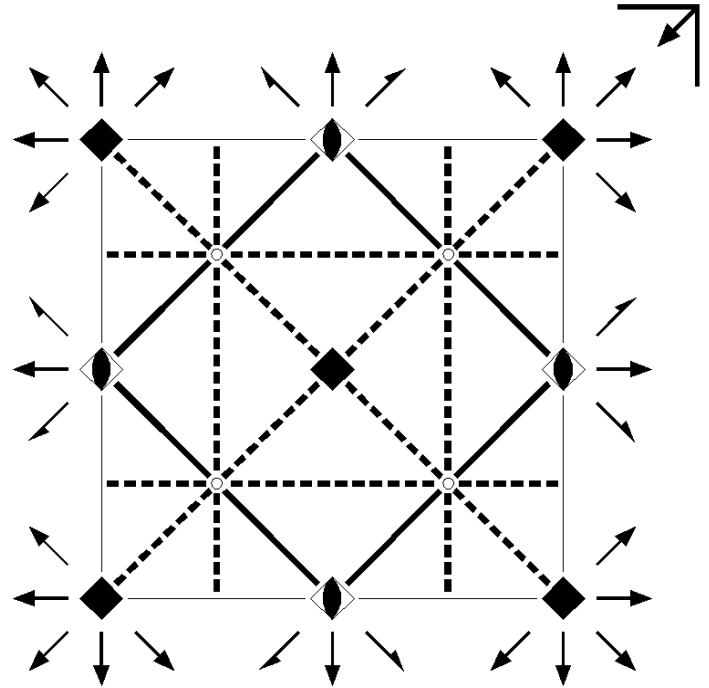
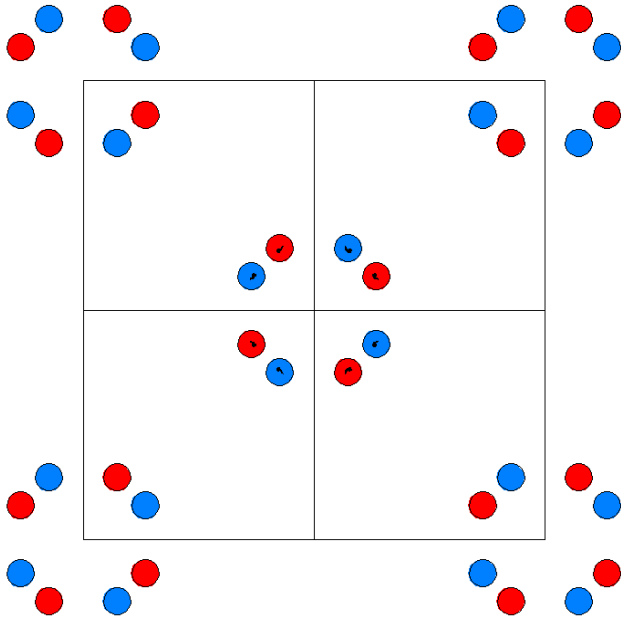


P4/nbm1'  
125.2.1032

4/mmm1'  
P4/n2/b2/m1'

Tetragonal

1'



Origin at 4221' at 4/n22/g1', at -1/4,-1/4,0 from center ( 2/m1' )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

For 1 + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)              | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                  | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                          | (8) 2 x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)                         |
| (9) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)      | (10) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (11) $\bar{4}^+$ 1/2,0,z; 1/2,0,0<br>( $\bar{4}_z^+$  1/2,1/2,0) | (12) $\bar{4}^-$ 0,1/2,z; 0,1/2,0<br>( $\bar{4}_z^-$  1/2,1/2,0)  |
| (13) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (14) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (15) m x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)                | (16) g (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)          |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)'	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(5) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(6) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'	(7) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) 2' x, $\bar{x}$ ,0 (2 <sub>xy</sub> <sup>-</sup>  0,0,0)'
(9) $\bar{1}$ ' 1/4,1/4,0 ( $\bar{1}$  1/2,1/2,0)'	(10) n' (1/2,1/2,0) x,y,0 (m <sub>z</sub>  1/2,1/2,0)'	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,0 ( $\bar{4}_z$  1/2,1/2,0)'	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,0 ( $\bar{4}_z^{-1}$  1/2,1/2,0)'
(13) a' (1/2,0,0) x,1/4,z (m <sub>y</sub>  1/2,1/2,0)'	(14) b' (0,1/2,0) 1/4,y,z ( (m <sub>x</sub>  1/2,1/2,0)'	(15) m' x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,0)'	(16) g' (1/2,1/2,0) x,x,z (m <sub>xy</sub> <sup>-</sup>  1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +	1 +	1 +	1 +
16 n 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z$ [0,0,0]	(4) y, $\bar{x},z$ [0,0,0]
	(5) $\bar{x},y,\bar{z}$ [0,0,0]	(6) x, $\bar{y},\bar{z}$ [0,0,0]	(7) y,x, $\bar{z}$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}$ [0,0,0]
	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [0,0,0]	(10) x+1/2,y+1/2, $\bar{z}$ [0,0,0]	(11) y+1/2, $\bar{x}+1/2,\bar{z}$ [0,0,0]	(12) $\bar{y}+1/2,x+1/2,\bar{z}$ [0,0,0]
	(13) x+1/2, $\bar{y}+1/2,z$ [0,0,0]	(14) $\bar{x}+1/2,y+1/2,z$ [0,0,0]	(15) $\bar{y}+1/2,\bar{x}+1/2,z$ [0,0,0]	(16) y+1/2,x+1/2,z [0,0,0]
8 m ..m1'	x,x+1/2,z [0,0,0]	$\bar{x},\bar{x}+1/2,z$ [0,0,0]	$\bar{x}+1/2,x,z$ [0,0,0]	x+1/2, $\bar{x},z$ [0,0,0]
	$\bar{x},x+1/2,\bar{z}$ [0,0,0]	x, $\bar{x}+1/2,\bar{z}$ [0,0,0]	x+1/2,x, $\bar{z}$ [0,0,0]	$\bar{x}+1/2,\bar{x},\bar{z}$ [0,0,0]
8 l .2.1'	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]	0,x,1/2 [0,0,0]	0, $\bar{x},1/2$ [0,0,0]
	$\bar{x}+1/2,1/2,1/2$ [0,0,0]	x+1/2,1/2,1/2 [0,0,0]	1/2, $\bar{x}+1/2,1/2$ [0,0,0]	1/2,x+1/2,1/2 [0,0,0]
8 k .2.1'	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x},0$ [0,0,0]
	$\bar{x}+1/2,1/2,0$ [0,0,0]	x+1/2,1/2,0 [0,0,0]	1/2, $\bar{x}+1/2,0$ [0,0,0]	1/2,x+1/2,0 [0,0,0]
8 j ..21'	x,x,1/2 [0,0,0]	$\bar{x},\bar{x},1/2$ [0,0,0]	$\bar{x},x,1/2$ [0,0,0]	x, $\bar{x},1/2$ [0,0,0]
	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [0,0,0]	x+1/2,x+1/2,1/2 [0,0,0]	x+1/2, $\bar{x}+1/2,1/2$ [0,0,0]	$\bar{x}+1/2,x+1/2,1/2$ [0,0,0]
8 i ..21'	x,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x},x,0$ [0,0,0]	x, $\bar{x},0$ [0,0,0]
	$\bar{x}+1/2,\bar{x}+1/2,0$ [0,0,0]	x+1/2,x+1/2,0 [0,0,0]	x+1/2, $\bar{x}+1/2,0$ [0,0,0]	$\bar{x}+1/2,x+1/2,0$ [0,0,0]
4 h 2.mm1'	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]

4	g	4..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	1/2,1/2,z [0,0,0]
4	f	..2/m1'	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]
4	e	..2/m1'	1/4,1/4,0 [0,0,0]	3/4,3/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]	1/4,3/4,0 [0,0,0]
2	d	$\bar{4}2m1'$	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	c	$\bar{4}2m1'$	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
2	b	4221'	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	a	4221'	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

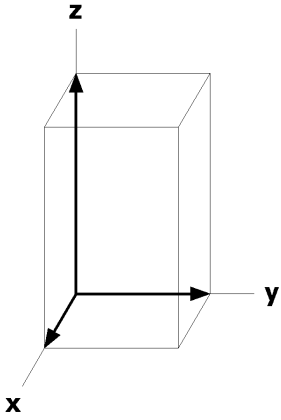
### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0

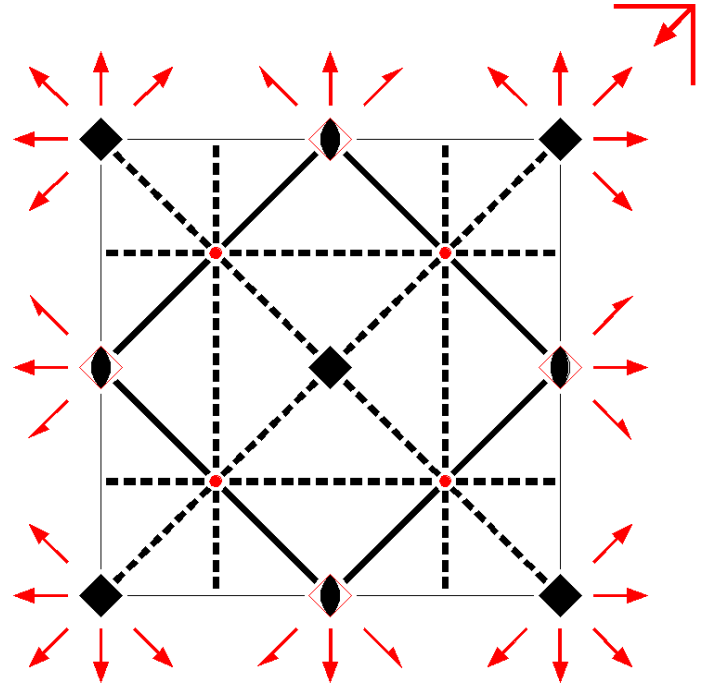
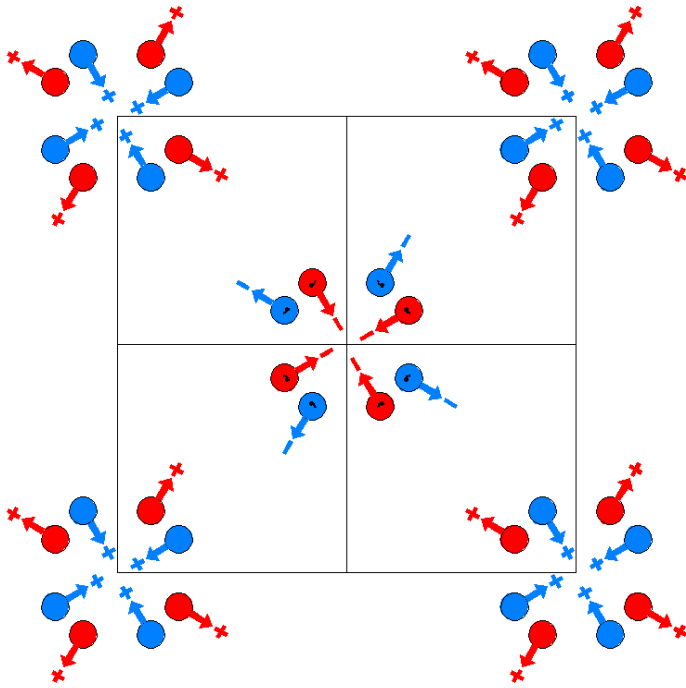




P4/n'bm  
125.3.1033

4/m'mm  
P4/n'2'/b2'/m

Tetragonal



Origin at  $4_2 2'$  at  $4/n'2'2'/g$ , at  $-1/4, -1/4, 0$  from center ( $2'/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

**Symmetry Operations**

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)               | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                  | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                         | (8) 2' x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)'                       |
| (9) $\bar{1}'$ 1/4,1/4,0<br>( $\bar{1}'$  1/2,1/2,0)'   | (10) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (11) $\bar{4}^+$ 1/2,0,z; 1/2,0,0<br>( $\bar{4}_z^+$  1/2,1/2,0)' | (12) $\bar{4}^-$ 0,1/2,z; 0,1/2,0<br>( $\bar{4}_z^-$  1/2,1/2,0)' |
| (13) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (14) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)   | (15) m x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)                 | (16) g (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

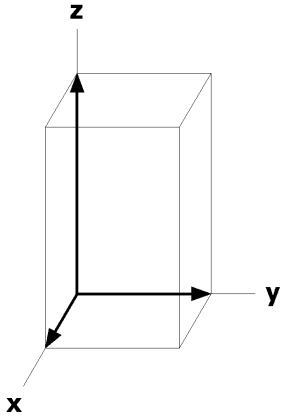
			Coordinates								
Multiplicity, Wyckoff letter, Site Symmetry.											
16	n	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y},x,z$	$[\bar{v},u,w]$	(4)	$y,\bar{x},z$	$[v,\bar{u},w]$
(5)	$\bar{x},y,\bar{z}$	$[u,\bar{v},w]$	(6)	$x,\bar{y},\bar{z}$	$[\bar{u},v,w]$	(7)	$y,x,\bar{z}$	$[\bar{v},\bar{u},w]$	(8)	$\bar{y},\bar{x},\bar{z}$	$[v,u,w]$
(9)	$\bar{x}+1/2,\bar{y}+1/2,\bar{z}$	$[\bar{u},\bar{v},\bar{w}]$	(10)	$x+1/2,y+1/2,\bar{z}$	$[u,v,\bar{w}]$	(11)	$y+1/2,\bar{x}+1/2,\bar{z}$	$[v,\bar{u},\bar{w}]$	(12)	$\bar{y}+1/2,x+1/2,\bar{z}$	$[\bar{v},u,\bar{w}]$
(13)	$x+1/2,\bar{y}+1/2,z$	$[\bar{u},v,\bar{w}]$	(14)	$\bar{x}+1/2,y+1/2,z$	$[u,\bar{v},\bar{w}]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[v,u,\bar{w}]$	(16)	$y+1/2,x+1/2,z$	$[\bar{v},\bar{u},\bar{w}]$
8	m	..m	$x,x+1/2,z$	$[\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,z$	$[u,\bar{u},0]$	$\bar{x}+1/2,x,z$	$[\bar{u},\bar{u},0]$	$x+1/2,\bar{x},z$	$[u,u,0]$	
			$\bar{x},x+1/2,\bar{z}$	$[\bar{u},\bar{u},0]$	$x,\bar{x}+1/2,\bar{z}$	$[u,u,0]$	$x+1/2,x,\bar{z}$	$[\bar{u},u,0]$	$\bar{x}+1/2,\bar{x},\bar{z}$	$[u,\bar{u},0]$	
8	l	.2'	$x,0,1/2$	$[0,v,w]$	$\bar{x},0,1/2$	$[0,\bar{v},w]$	$0,x,1/2$	$[\bar{v},0,w]$	$0,\bar{x},1/2$	$[v,0,w]$	
			$\bar{x}+1/2,1/2,1/2$	$[0,\bar{v},\bar{w}]$	$x+1/2,1/2,1/2$	$[0,v,\bar{w}]$	$1/2,\bar{x}+1/2,1/2$	$[v,0,\bar{w}]$	$1/2,x+1/2,1/2$	$[\bar{v},0,\bar{w}]$	
8	k	.2'	$x,0,0$	$[0,v,w]$	$\bar{x},0,0$	$[0,\bar{v},w]$	$0,x,0$	$[\bar{v},0,w]$	$0,\bar{x},0$	$[v,0,w]$	
			$\bar{x}+1/2,1/2,0$	$[0,\bar{v},\bar{w}]$	$x+1/2,1/2,0$	$[0,v,\bar{w}]$	$1/2,\bar{x}+1/2,0$	$[v,0,\bar{w}]$	$1/2,x+1/2,0$	$[\bar{v},0,\bar{w}]$	
8	j	..2'	$x,x,1/2$	$[\bar{u},u,w]$	$\bar{x},\bar{x},1/2$	$[u,\bar{u},w]$	$\bar{x},x,1/2$	$[\bar{u},\bar{u},w]$	$x,\bar{x},1/2$	$[u,u,w]$	
			$\bar{x}+1/2,\bar{x}+1/2,1/2$	$[u,\bar{u},\bar{w}]$	$x+1/2,x+1/2,1/2$	$[\bar{u},u,\bar{w}]$	$x+1/2,\bar{x}+1/2,1/2$	$[u,u,\bar{w}]$	$\bar{x}+1/2,x+1/2,1/2$	$[\bar{u},\bar{u},\bar{w}]$	
8	i	..2'	$x,x,0$	$[\bar{u},u,w]$	$\bar{x},\bar{x},0$	$[u,\bar{u},w]$	$\bar{x},x,0$	$[\bar{u},\bar{u},w]$	$x,\bar{x},0$	$[u,u,w]$	
			$\bar{x}+1/2,\bar{x}+1/2,0$	$[u,\bar{u},\bar{w}]$	$x+1/2,x+1/2,0$	$[\bar{u},u,\bar{w}]$	$x+1/2,\bar{x}+1/2,0$	$[u,u,\bar{w}]$	$\bar{x}+1/2,x+1/2,0$	$[\bar{u},\bar{u},\bar{w}]$	
4	h	2.mm	$0,1/2,z$	$[0,0,0]$	$1/2,0,z$	$[0,0,0]$	$0,1/2,\bar{z}$	$[0,0,0]$	$1/2,0,\bar{z}$	$[0,0,0]$	
4	g	4..	$0,0,z$	$[0,0,w]$	$0,0,\bar{z}$	$[0,0,w]$	$1/2,1/2,\bar{z}$	$[0,0,\bar{w}]$	$1/2,1/2,z$	$[0,0,\bar{w}]$	
4	f	..2'/m	$1/4,1/4,1/2$	$[0,0,0]$	$3/4,3/4,1/2$	$[0,0,0]$	$3/4,1/4,1/2$	$[0,0,0]$	$1/4,3/4,1/2$	$[0,0,0]$	
4	e	..2'/m	$1/4,1/4,0$	$[0,0,0]$	$3/4,3/4,0$	$[0,0,0]$	$3/4,1/4,0$	$[0,0,0]$	$1/4,3/4,0$	$[0,0,0]$	
2	d	$\bar{4}'2'm$	$0,1/2,1/2$	$[0,0,0]$	$1/2,0,1/2$	$[0,0,0]$					
2	c	$\bar{4}'2'm$	$0,1/2,0$	$[0,0,0]$	$1/2,0,0$	$[0,0,0]$					
2	b	$4'2'2'$	$0,0,1/2$	$[0,0,w]$	$1/2,1/2,1/2$	$[0,0,\bar{w}]$					
2	a	$4'2'2'$	$0,0,0$	$[0,0,w]$	$1/2,1/2,0$	$[0,0,\bar{w}]$					

**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,0,0

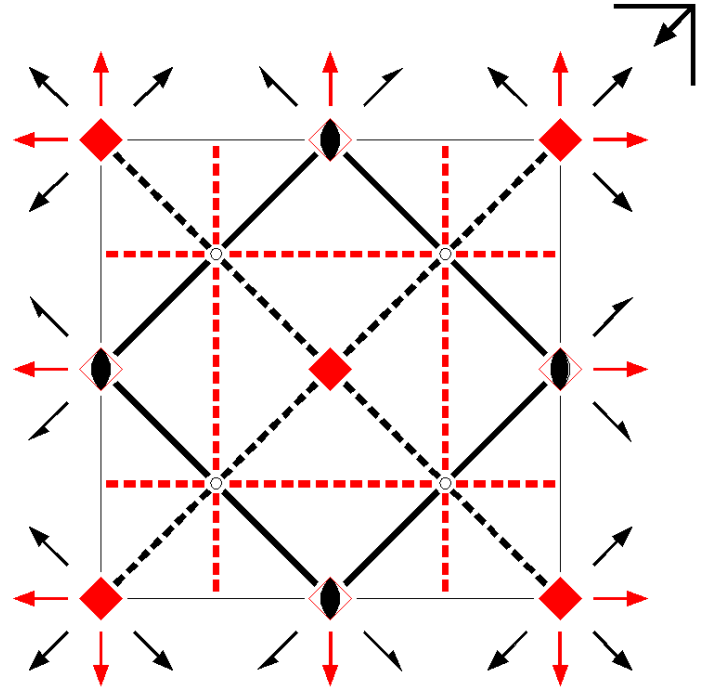
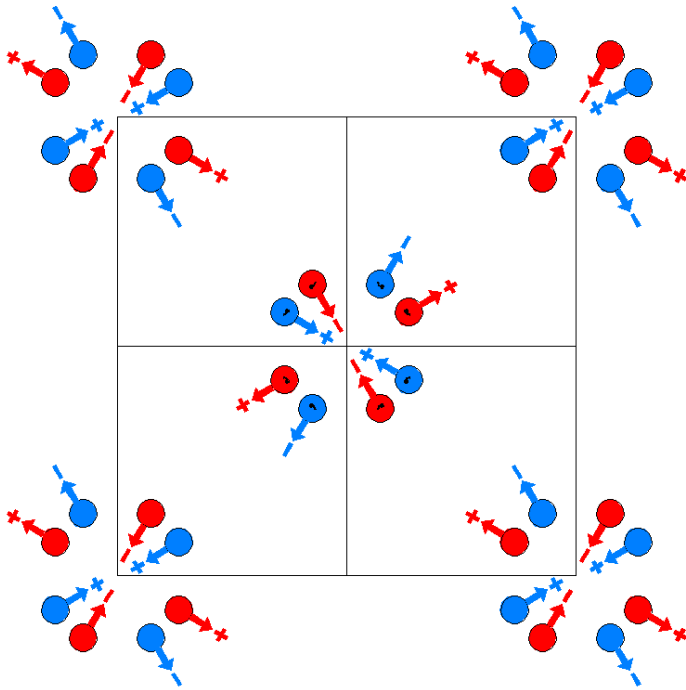
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,x,0



P4'/nb'm  
125.4.1034

4'/mm'm  
P4'/n2'/b'2/m

Tetragonal



Origin at 4'2'2 at 4'/n2'2/g, at  $-1/4, -1/4, 0$  from center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)' |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                  | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                           | (8) 2 x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)                         |
| (9) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)        | (10) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)   | (11) $\bar{4}^+$ 1/2,0,z; 1/2,0,0<br>( $\bar{4}_z^+$  1/2,1/2,0)' | (12) $\bar{4}^-$ 0,1/2,z; 0,1/2,0<br>( $\bar{4}_z^-$  1/2,1/2,0)' |
| (13) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (14) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' | (15) m x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)                 | (16) g (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

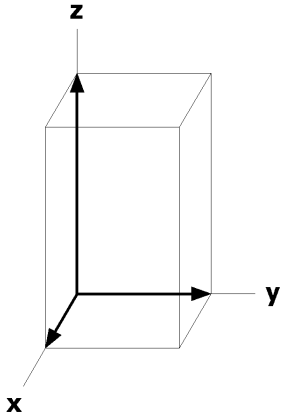
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
16	n	1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $\bar{y},x,z [v,\bar{u},\bar{w}]$	(4) $y,\bar{x},z [\bar{v},u,\bar{w}]$
			(5) $\bar{x},y,\bar{z} [u,\bar{v},w]$	(6) $x,\bar{y},\bar{z} [\bar{u},v,w]$	(7) $y,x,\bar{z} [v,u,\bar{w}]$	(8) $\bar{y},\bar{x},\bar{z} [\bar{v},\bar{u},\bar{w}]$
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z} [u,v,w]$	(10) $x+1/2,y+1/2,\bar{z} [\bar{u},\bar{v},w]$	(11) $y+1/2,\bar{x}+1/2,\bar{z} [v,\bar{u},\bar{w}]$	(12) $\bar{y}+1/2,x+1/2,\bar{z} [\bar{v},u,\bar{w}]$
			(13) $x+1/2,\bar{y}+1/2,z [u,\bar{v},w]$	(14) $\bar{x}+1/2,y+1/2,z [\bar{u},v,w]$	(15) $\bar{y}+1/2,\bar{x}+1/2,z [v,u,\bar{w}]$	(16) $y+1/2,x+1/2,z [\bar{v},\bar{u},\bar{w}]$
8	m	..m	$x,x+1/2,z [\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,z [u,\bar{u},0]$	$\bar{x}+1/2,x,z [u,u,0]$	$x+1/2,\bar{x},z [\bar{u},\bar{u},0]$
			$\bar{x},x+1/2,\bar{z} [\bar{u},\bar{u},0]$	$x,\bar{x}+1/2,\bar{z} [u,u,0]$	$x+1/2,x,\bar{z} [u,\bar{u},0]$	$\bar{x}+1/2,\bar{x},\bar{z} [\bar{u},u,0]$
8	l	.2'	$x,0,1/2 [0,v,w]$	$\bar{x},0,1/2 [0,\bar{v},w]$	$0,x,1/2 [v,0,\bar{w}]$	$0,\bar{x},1/2 [\bar{v},0,\bar{w}]$
			$\bar{x}+1/2,1/2,1/2 [0,v,w]$	$x+1/2,1/2,1/2 [0,\bar{v},w]$	$1/2,\bar{x}+1/2,1/2 [v,0,\bar{w}]$	$1/2,x+1/2,1/2 [\bar{v},0,\bar{w}]$
8	k	.2'	$x,0,0 [0,v,w]$	$\bar{x},0,0 [0,\bar{v},w]$	$0,x,0 [v,0,\bar{w}]$	$0,\bar{x},0 [\bar{v},0,\bar{w}]$
			$\bar{x}+1/2,1/2,0 [0,v,w]$	$x+1/2,1/2,0 [0,\bar{v},w]$	$1/2,\bar{x}+1/2,0 [v,0,\bar{w}]$	$1/2,x+1/2,0 [\bar{v},0,\bar{w}]$
8	j	..2	$x,x,1/2 [u,u,0]$	$\bar{x},\bar{x},1/2 [\bar{u},\bar{u},0]$	$\bar{x},x,1/2 [u,\bar{u},0]$	$x,\bar{x},1/2 [\bar{u},u,0]$
			$\bar{x}+1/2,\bar{x}+1/2,1/2 [u,u,0]$	$x+1/2,x+1/2,1/2 [\bar{u},\bar{u},0]$	$x+1/2,\bar{x}+1/2,1/2 [u,\bar{u},0]$	$\bar{x}+1/2,x+1/2,1/2 [\bar{u},u,0]$
8	i	..2	$x,x,0 [u,u,0]$	$\bar{x},\bar{x},0 [\bar{u},\bar{u},0]$	$\bar{x},x,0 [u,\bar{u},0]$	$x,\bar{x},0 [\bar{u},u,0]$
			$\bar{x}+1/2,\bar{x}+1/2,0 [u,u,0]$	$x+1/2,x+1/2,0 [\bar{u},\bar{u},0]$	$x+1/2,\bar{x}+1/2,0 [u,\bar{u},0]$	$\bar{x}+1/2,x+1/2,0 [\bar{u},u,0]$
4	h	2.mm	$0,1/2,z [0,0,0]$	$1/2,0,z [0,0,0]$	$0,1/2,\bar{z} [0,0,0]$	$1/2,0,\bar{z} [0,0,0]$
4	g	4'..	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$	$1/2,1/2,\bar{z} [0,0,0]$	$1/2,1/2,z [0,0,0]$
4	f	..2/m	$1/4,1/4,1/2 [u,u,0]$	$3/4,3/4,1/2 [\bar{u},\bar{u},0]$	$3/4,1/4,1/2 [u,\bar{u},0]$	$1/4,3/4,1/2 [\bar{u},u,0]$
4	e	..2/m	$1/4,1/4,0 [u,u,0]$	$3/4,3/4,0 [\bar{u},\bar{u},0]$	$3/4,1/4,0 [u,\bar{u},0]$	$1/4,3/4,0 [\bar{u},u,0]$
2	d	$\bar{4}'2'm$	$0,1/2,1/2 [0,0,0]$	$1/2,0,1/2 [0,0,0]$		
2	c	$\bar{4}'2'm$	$0,1/2,0 [0,0,0]$	$1/2,0,0 [0,0,0]$		
2	b	4'2'2	$0,0,1/2 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$		
2	a	4'2'2	$0,0,0 [0,0,0]$	$1/2,1/2,0 [0,0,0]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_4$  4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $1/2, 0, z$

Along  $[1,0,0]$   $p_{2a}$  2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $x, 0, 0$

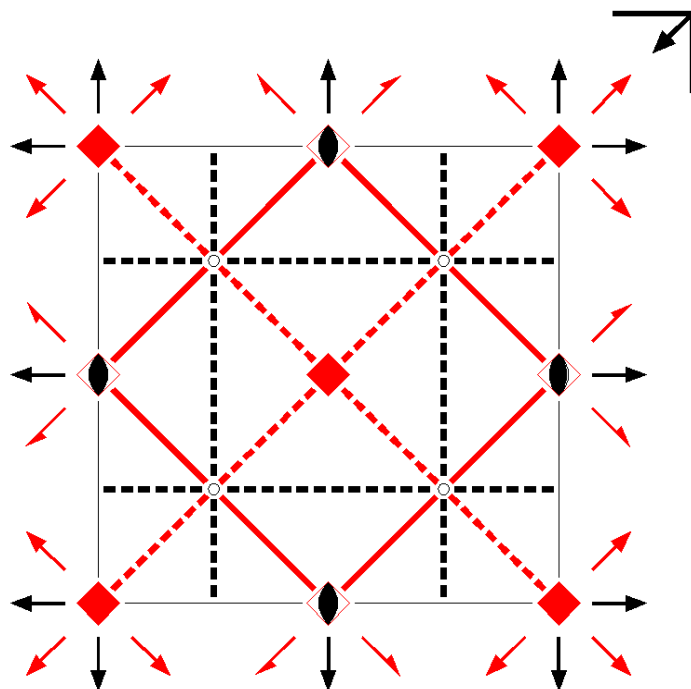
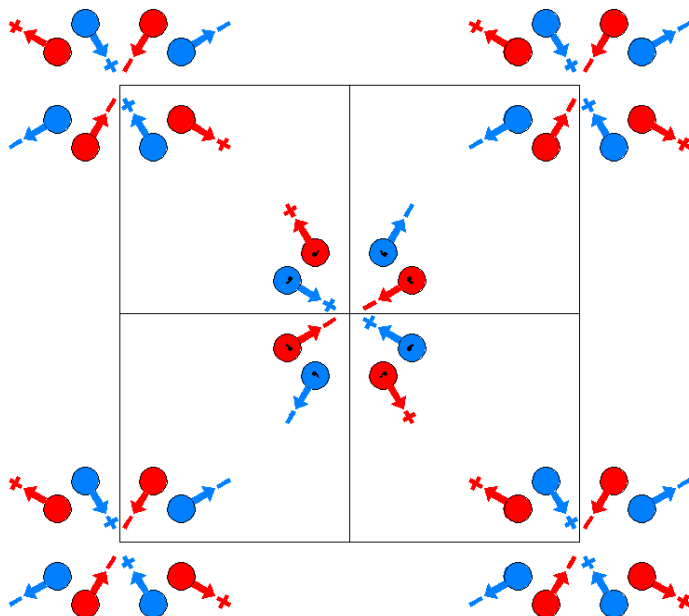
Along  $[1,1,0]$   $p_2$  2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at  $x, x, 0$



P4'/n**bm**'  
125.5.1035

4'/**mmm**'  
P4'/n2/b2'/**m**'

Tetragonal



Origin at 4'**22**' at 4'/n**22**'/g', at -1/4, -1/4, 0 from center ( 2'/**m**' )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'              |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                  | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                  | (7) 2' x,x,0<br>(2 <sub>xy</sub> ' 0,0,0)'                        | (8) 2' x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub> ' 0,0,0)'        |
| (9) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)      | (10) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (11) $\bar{4}^+$ 1/2,0,z; 1/2,0,0<br>( $\bar{4}_z^+$  1/2,1/2,0)' | (12) $\bar{4}^-$ 0,1/2,z; 0,1/2,0<br>( $\bar{4}_z^-$  1/2,1/2,0)'              |
| (13) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (14) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (15) m' x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub> ' 1/2,1/2,0)'     | (16) g' (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub> ' 1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates								
Multiplicity, Wyckoff letter, Site Symmetry.											
16	n	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y},x,z$	$[v,\bar{u},\bar{w}]$	(4)	$y,\bar{x},z$	$[\bar{v},u,\bar{w}]$
(5)	$\bar{x},y,\bar{z}$	$[\bar{u},v,\bar{w}]$	(6)	$x,\bar{y},\bar{z}$	$[u,\bar{v},\bar{w}]$	(7)	$y,x,\bar{z}$	$[\bar{v},\bar{u},w]$	(8)	$\bar{y},\bar{x},\bar{z}$	$[v,u,w]$
(9)	$\bar{x}+1/2,\bar{y}+1/2,\bar{z}$	$[\bar{u},v,w]$	(10)	$x+1/2,y+1/2,\bar{z}$	$[\bar{u},\bar{v},w]$	(11)	$y+1/2,\bar{x}+1/2,\bar{z}$	$[v,\bar{u},\bar{w}]$	(12)	$\bar{y}+1/2,x+1/2,\bar{z}$	$[\bar{v},u,\bar{w}]$
(13)	$x+1/2,\bar{y}+1/2,z$	$[\bar{u},v,\bar{w}]$	(14)	$\bar{x}+1/2,y+1/2,z$	$[u,\bar{v},\bar{w}]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[\bar{v},\bar{u},w]$	(16)	$y+1/2,x+1/2,z$	$[v,u,w]$
8	m	..m'	$x,x+1/2,z$	$[\bar{x},\bar{x}+1/2,z$	$[\bar{u},\bar{u},w]$	$\bar{x}+1/2,x,z$	$[u,\bar{u},\bar{w}]$	$x+1/2,\bar{x},z$	$[\bar{u},u,\bar{w}]$	$\bar{x}+1/2,\bar{x},z$	$[u,u,w]$
8	l	.2.	$x,0,1/2$	$[\bar{x},0,1/2$	$[\bar{u},0,0]$	$0,x,1/2$	$[0,\bar{u},0]$	$0,\bar{x},1/2$	$[0,u,0]$	$1/2,\bar{x}+1/2,1/2$	$[0,\bar{u},0]$
8	k	.2.	$x,0,0$	$[\bar{x},0,0$	$[\bar{u},0,0]$	$0,x,0$	$[0,\bar{u},0]$	$0,\bar{x},0$	$[0,u,0]$	$1/2,x+1/2,0$	$[0,\bar{u},0]$
8	j	..2'	$x,x,1/2$	$[\bar{x},\bar{x},1/2$	$[u,\bar{u},w]$	$\bar{x},x,1/2$	$[u,\bar{u},\bar{w}]$	$x,\bar{x},1/2$	$[\bar{u},\bar{u},\bar{w}]$	$\bar{x}+1/2,\bar{x}+1/2,1/2$	$[\bar{u},u,w]$
8	i	..2'	$x,x,0$	$[\bar{x},\bar{x},0$	$[u,\bar{u},w]$	$\bar{x},x,0$	$[u,\bar{u},\bar{w}]$	$x,\bar{x},0$	$[\bar{u},\bar{u},\bar{w}]$	$x+1/2,\bar{x}+1/2,0$	$[u,\bar{u},w]$
4	h	2.m'm'	$0,1/2,z$	$[0,0,w]$	$1/2,0,z$	$[0,0,\bar{w}]$	$0,1/2,\bar{z}$	$[0,0,\bar{w}]$	$1/2,0,\bar{z}$	$[0,0,w]$	
4	g	4'..	$0,0,z$	$[0,0,0]$	$0,0,\bar{z}$	$[0,0,0]$	$1/2,1/2,\bar{z}$	$[0,0,0]$	$1/2,1/2,z$	$[0,0,0]$	
4	f	..2'/m'	$1/4,1/4,1/2$	$[u,\bar{u},w]$	$3/4,3/4,1/2$	$[\bar{u},u,w]$	$3/4,1/4,1/2$	$[\bar{u},\bar{u},\bar{w}]$	$1/4,3/4,1/2$	$[u,u,\bar{w}]$	
4	e	..2'/m'	$1/4,1/4,0$	$[u,\bar{u},w]$	$3/4,3/4,0$	$[\bar{u},u,w]$	$3/4,1/4,0$	$[\bar{u},\bar{u},\bar{w}]$	$1/4,3/4,0$	$[u,u,\bar{w}]$	
2	d	$\bar{4}'2m'$	$0,1/2,1/2$	$[0,0,0]$	$1/2,0,1/2$	$[0,0,0]$					
2	c	$\bar{4}'2m'$	$0,1/2,0$	$[0,0,0]$	$1/2,0,0$	$[0,0,0]$					
2	b	4'22'	$0,0,1/2$	$[0,0,0]$	$1/2,1/2,1/2$	$[0,0,0]$					
2	a	4'22'	$0,0,0$	$[0,0,0]$	$1/2,1/2,0$	$[0,0,0]$					

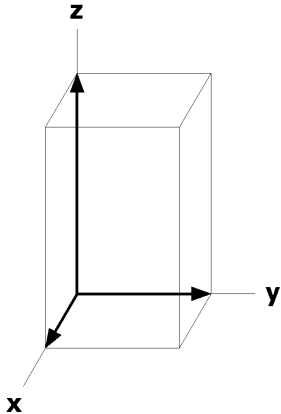


**Symmetry of Special Projections**

Along [0,0,1]  $p_4$  4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 1/2,0,z

Along [1,0,0]  $p_{2a}$  2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,0,0

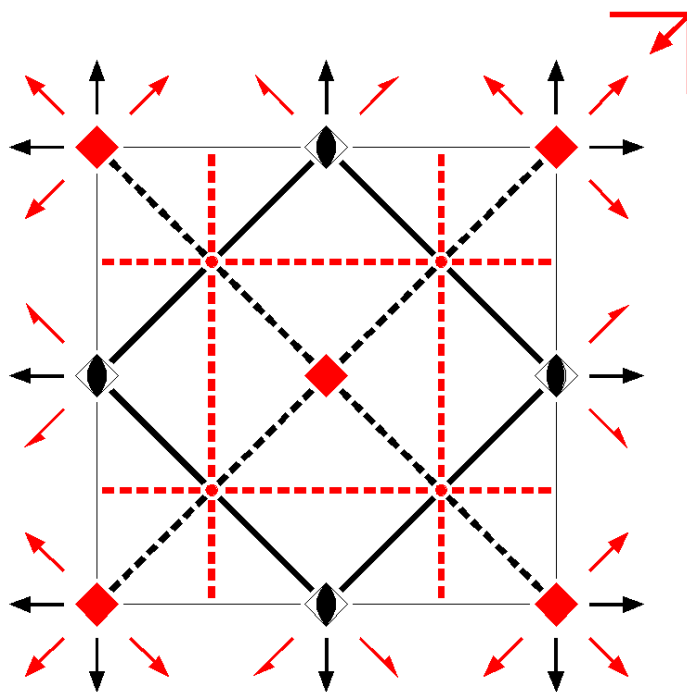
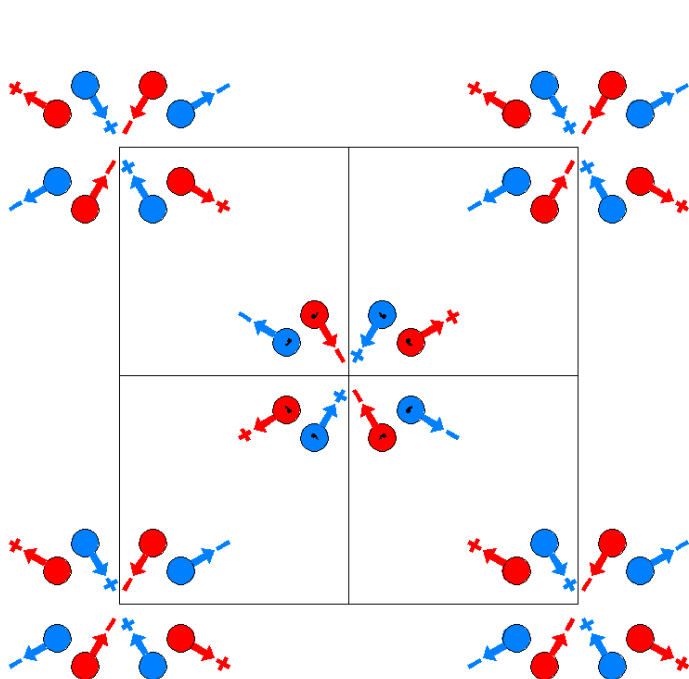
Along [1,1,0]  $p_{2b}$  2mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at x,x,0



P4'/n'b'm  
125.6.1036

4'/m'm'm  
P4'/n'2/b'2'/m

Tetragonal



Origin at 4'22' at 4'/n'22'/g, at  $-1/4, -1/4, 0$  from center ( $2'/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) 4 <sup>+</sup> <sub>z</sub> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)'                | (4) 4 <sup>-</sup> <sub>z</sub> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'                |
| (5) 2 <sub>y</sub> 0,y,0<br>(2 <sub>y</sub>  0,0,0)                     | (6) 2 <sub>x</sub> x,0,0<br>(2 <sub>x</sub>  0,0,0)                     | (7) 2' <sub>xy</sub> x,x,0<br>(2' <sub>xy</sub>  0,0,0)'                                      | (8) 2' <sub>xy</sub> x,x̄,0<br>(2' <sub>xy</sub>  0,0,0)'                                     |
| (9) 1̄ <sub>1</sub> 1/4,1/4,0<br>(1̄ <sub>1</sub>  1/2,1/2,0)'          | (10) n' <sub>z</sub> (1/2,1/2,0) x,y,0<br>(n' <sub>z</sub>  1/2,1/2,0)' | (11) 4 <sup>+</sup> <sub>z</sub> 1/2,0,z; 1/2,0,0<br>(4 <sub>z</sub> <sup>+</sup>  1/2,1/2,0) | (12) 4 <sup>-</sup> <sub>z</sub> 0,1/2,z; 0,1/2,0<br>(4 <sub>z</sub> <sup>-</sup>  1/2,1/2,0) |
| (13) a' <sub>y</sub> (1/2,0,0) x,1/4,z<br>(a' <sub>y</sub>  1/2,1/2,0)' | (14) b' <sub>x</sub> (0,1/2,0) 1/4,y,z<br>(b' <sub>x</sub>  1/2,1/2,0)' | (15) m <sub>xy</sub> x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)                               | (16) g <sub>xy</sub> (1/2,1/2,0) x,x,z<br>(g <sub>xy</sub>  1/2,1/2,0)                        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

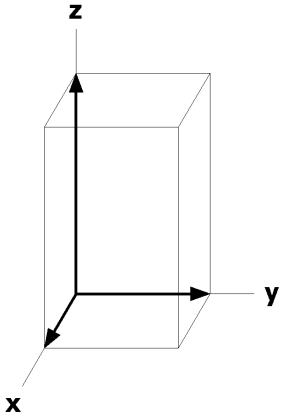
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	n	1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $\bar{y},x,z [v,\bar{u},\bar{w}]$	(4) $y,\bar{x},z [\bar{v},u,\bar{w}]$
			(5) $\bar{x},y,\bar{z} [\bar{u},v,\bar{w}]$	(6) $x,\bar{y},\bar{z} [u,\bar{v},\bar{w}]$	(7) $y,x,\bar{z} [v,\bar{u},w]$	(8) $\bar{y},\bar{x},\bar{z} [v,u,w]$
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z} [\bar{u},\bar{v},\bar{w}]$	(10) $x+1/2,y+1/2,\bar{z} [u,v,\bar{w}]$	(11) $y+1/2,\bar{x}+1/2,\bar{z} [v,\bar{u},w]$	(12) $\bar{y}+1/2,x+1/2,\bar{z} [v,\bar{u},w]$
			(13) $x+1/2,\bar{y}+1/2,z [u,\bar{v},w]$	(14) $\bar{x}+1/2,y+1/2,z [\bar{u},v,w]$	(15) $\bar{y}+1/2,\bar{x}+1/2,z [v,u,\bar{w}]$	(16) $y+1/2,x+1/2,z [\bar{v},\bar{u},\bar{w}]$
8	m	..m	$x,x+1/2,z [\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,z [u,\bar{u},0]$	$\bar{x}+1/2,x,z [u,u,0]$	$x+1/2,\bar{x},z [\bar{u},\bar{u},0]$
			$\bar{x},x+1/2,\bar{z} [u,u,0]$	$x,\bar{x}+1/2,\bar{z} [\bar{u},\bar{u},0]$	$x+1/2,x,\bar{z} [\bar{u},u,0]$	$\bar{x}+1/2,\bar{x},\bar{z} [u,\bar{u},0]$
8	l	.2.	$x,0,1/2 [u,0,0]$	$\bar{x},0,1/2 [\bar{u},0,0]$	$0,x,1/2 [0,\bar{u},0]$	$0,\bar{x},1/2 [0,u,0]$
			$\bar{x}+1/2,1/2,1/2 [\bar{u},0,0]$	$x+1/2,1/2,1/2 [u,0,0]$	$1/2,\bar{x}+1/2,1/2 [0,u,0]$	$1/2,x+1/2,1/2 [0,\bar{u},0]$
8	k	.2.	$x,0,0 [u,0,0]$	$\bar{x},0,0 [\bar{u},0,0]$	$0,x,0 [0,\bar{u},0]$	$0,\bar{x},0 [0,u,0]$
			$\bar{x}+1/2,1/2,0 [\bar{u},0,0]$	$x+1/2,1/2,0 [u,0,0]$	$1/2,\bar{x}+1/2,0 [0,u,0]$	$1/2,x+1/2,0 [0,\bar{u},0]$
8	j	..2'	$x,x,1/2 [\bar{u},u,w]$	$\bar{x},\bar{x},1/2 [u,\bar{u},w]$	$\bar{x},x,1/2 [u,u,\bar{w}]$	$x,\bar{x},1/2 [\bar{u},\bar{u},\bar{w}]$
			$\bar{x}+1/2,\bar{x}+1/2,1/2 [u,\bar{u},\bar{w}]$	$x+1/2,x+1/2,1/2 [\bar{u},u,\bar{w}]$	$x+1/2,\bar{x}+1/2,1/2 [\bar{u},\bar{u},w]$	$\bar{x}+1/2,x+1/2,1/2 [u,u,w]$
8	i	..2'	$x,x,0 [\bar{u},u,w]$	$\bar{x},\bar{x},0 [u,\bar{u},w]$	$\bar{x},x,0 [u,u,\bar{w}]$	$x,\bar{x},0 [\bar{u},\bar{u},\bar{w}]$
			$\bar{x}+1/2,\bar{x}+1/2,0 [u,\bar{u},\bar{w}]$	$x+1/2,x+1/2,0 [\bar{u},u,\bar{w}]$	$x+1/2,\bar{x}+1/2,0 [\bar{u},\bar{u},w]$	$\bar{x}+1/2,x+1/2,0 [u,u,w]$
4	h	2.mm	$0,1/2,z [0,0,0]$	$1/2,0,z [0,0,0]$	$0,1/2,\bar{z} [0,0,0]$	$1/2,0,\bar{z} [0,0,0]$
4	g	4'..	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$	$1/2,1/2,\bar{z} [0,0,0]$	$1/2,1/2,z [0,0,0]$
4	f	..2'/m	$1/4,1/4,1/2 [0,0,0]$	$3/4,3/4,1/2 [0,0,0]$	$3/4,1/4,1/2 [0,0,0]$	$1/4,3/4,1/2 [0,0,0]$
4	e	..2'/m	$1/4,1/4,0 [0,0,0]$	$3/4,3/4,0 [0,0,0]$	$3/4,1/4,0 [0,0,0]$	$1/4,3/4,0 [0,0,0]$
2	d	$\bar{4}2m$	$0,1/2,1/2 [0,0,0]$	$1/2,0,1/2 [0,0,0]$		
2	c	$\bar{4}2m$	$0,1/2,0 [0,0,0]$	$1/2,0,0 [0,0,0]$		
2	b	4'22'	$0,0,1/2 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$		
2	a	4'22'	$0,0,0 [0,0,0]$	$1/2,1/2,0 [0,0,0]$		

**Symmetry of Special Projections**

Along [0,0,1]  $p4'mm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 0,0,z

Along [1,0,0]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,0,0

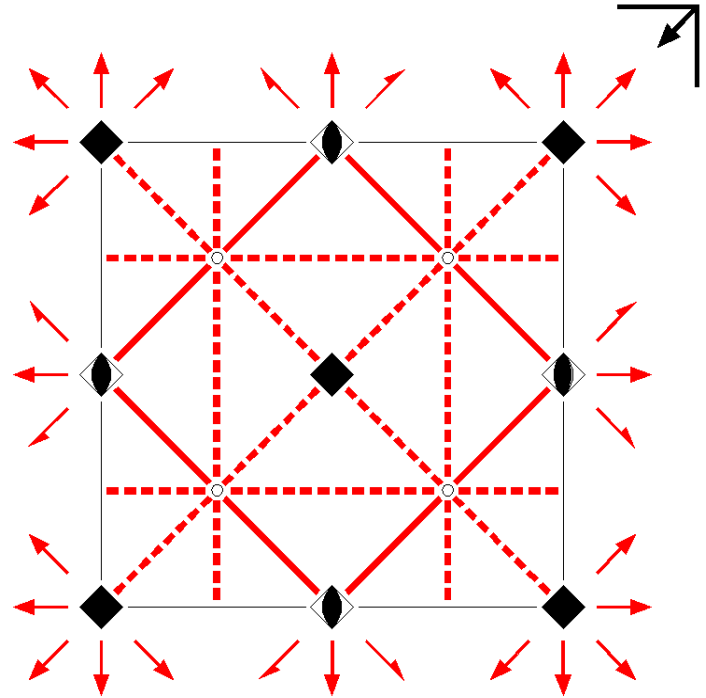
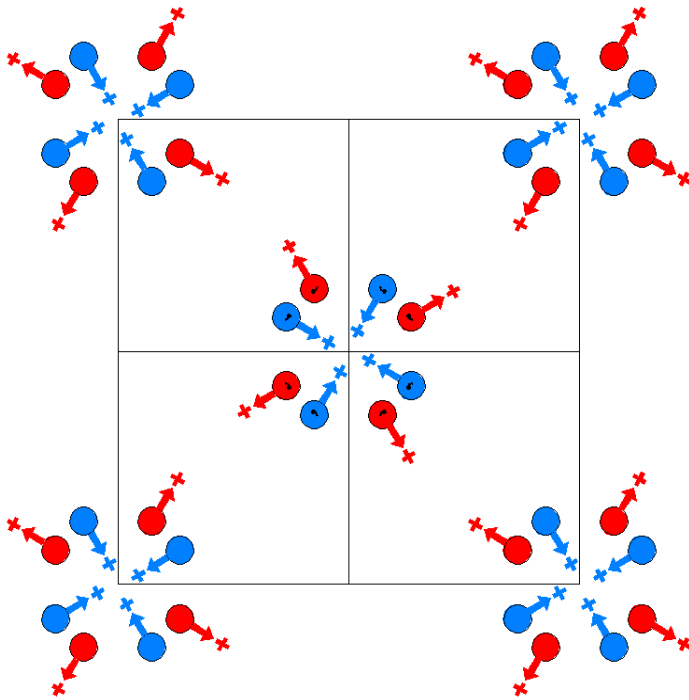
Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,x,0



P4/nb'm'  
125.7.1037

4/mm'm'  
P4/n2'/b2'/m'

Tetragonal



Origin at  $42'2'$  at  $4/n2'2'/g'$ , at  $-1/4, -1/4, 0$  from center ( $2'/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)       | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)              | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)        |
| (5) 2' <sub>y</sub> 0,y,0<br>(2 <sub>y</sub>  0,0,0)'     | (6) 2' <sub>x</sub> x,0,0<br>(2 <sub>x</sub>  0,0,0)'     | (7) 2' <sub>xy</sub> x,x,0<br>(2 <sub>xy</sub>  0,0,0)'          | (8) 2' <sub>xy</sub> x,x̄,0<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,0)'   |
| (9) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)        | (10) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)   | (11) $\bar{4}^+$ 1/2,0,z; 1/2,0,0<br>( $\bar{4}_z^+$  1/2,1/2,0) | (12) $\bar{4}^-$ 0,1/2,z; 0,1/2,0<br>( $\bar{4}_z^-$  1/2,1/2,0)         |
| (13) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (14) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' | (15) m' x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)'              | (16) g' (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub> <sup>-1</sup>  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

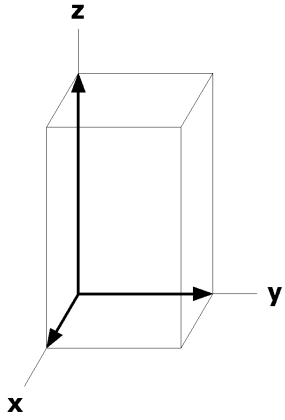
			Coordinates								
Multiplicity, Wyckoff letter, Site Symmetry.											
16	n	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y},x,z$	$[\bar{v},u,w]$	(4)	y, $\bar{x},z$	$[v,\bar{u},w]$
(5)	$\bar{x},y,\bar{z}$	$[u,\bar{v},w]$	(6)	x, $\bar{y},\bar{z}$	$[\bar{u},v,w]$	(7)	y,x, $\bar{z}$	$[\bar{v},\bar{u},w]$	(8)	$\bar{y},\bar{x},\bar{z}$	$[\bar{v},\bar{u},\bar{w}]$
(9)	$\bar{x}+1/2,\bar{y}+1/2,\bar{z}$	$[u,v,w]$	(10)	x+1/2,y+1/2, $\bar{z}$	$[\bar{u},\bar{v},w]$	(11)	y+1/2, $\bar{x}+1/2,\bar{z}$	$[\bar{v},u,w]$	(12)	$\bar{y}+1/2,x+1/2,\bar{z}$	$[v,\bar{u},w]$
(13)	x+1/2, $\bar{y}+1/2,z$	$[u,\bar{v},w]$	(14)	$\bar{x}+1/2,y+1/2,z$	$[\bar{u},v,w]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[\bar{v},\bar{u},w]$	(16)	y+1/2,x+1/2,z	$[\bar{v},\bar{u},\bar{w}]$
8	m	..m'	x,x+1/2,z	$[\bar{x},\bar{x}+1/2,z$	$[\bar{u},\bar{u},w]$	$\bar{x}+1/2,x,z$	$[\bar{u},u,w]$	x+1/2, $\bar{x},z$	$[u,\bar{u},w]$		
			$\bar{x},x+1/2,\bar{z}$	$[\bar{u},\bar{u},w]$	x, $\bar{x}+1/2,\bar{z}$	$[\bar{u},u,w]$	x+1/2,x, $\bar{z}$	$[\bar{u},\bar{u},w]$	$\bar{x}+1/2,\bar{x},\bar{z}$	$[u,u,w]$	
8	l	.2'	x,0,1/2	$[0,v,w]$	$\bar{x},0,1/2$	$[0,\bar{v},w]$	0,x,1/2	$[\bar{v},0,w]$	0, $\bar{x},1/2$	$[v,0,w]$	
			$\bar{x}+1/2,1/2,1/2$	$[0,v,w]$	x+1/2,1/2,1/2	$[0,\bar{v},w]$	1/2, $\bar{x}+1/2,1/2$	$[\bar{v},0,w]$	1/2,x+1/2,1/2	$[v,0,w]$	
8	k	.2'	x,0,0	$[0,v,w]$	$\bar{x},0,0$	$[0,\bar{v},w]$	0,x,0	$[\bar{v},0,w]$	0, $\bar{x},0$	$[v,0,w]$	
			$\bar{x}+1/2,1/2,0$	$[0,v,w]$	x+1/2,1/2,0	$[0,\bar{v},w]$	1/2, $\bar{x}+1/2,0$	$[\bar{v},0,w]$	1/2,x+1/2,0	$[v,0,w]$	
8	j	..2'	x,x,1/2	$[\bar{u},u,w]$	$\bar{x},\bar{x},1/2$	$[u,\bar{u},w]$	$\bar{x},x,1/2$	$[\bar{u},\bar{u},w]$	x, $\bar{x},1/2$	$[u,u,w]$	
			$\bar{x}+1/2,\bar{x}+1/2,1/2$	$[\bar{u},u,w]$	x+1/2,x+1/2,1/2	$[u,\bar{u},w]$	x+1/2, $\bar{x}+1/2,1/2$	$[\bar{u},\bar{u},w]$	$\bar{x}+1/2,x+1/2,1/2$	$[u,u,w]$	
8	i	..2'	x,x,0	$[\bar{u},u,w]$	$\bar{x},\bar{x},0$	$[u,\bar{u},w]$	$\bar{x},x,0$	$[\bar{u},\bar{u},w]$	x, $\bar{x},0$	$[u,u,w]$	
			$\bar{x}+1/2,\bar{x}+1/2,0$	$[\bar{u},u,w]$	x+1/2,x+1/2,0	$[u,\bar{u},w]$	x+1/2, $\bar{x}+1/2,0$	$[\bar{u},\bar{u},w]$	$\bar{x}+1/2,x+1/2,0$	$[u,u,w]$	
4	h	2.m'm'	0,1/2,z	$[0,0,w]$	1/2,0,z	$[0,0,w]$	0,1/2, $\bar{z}$	$[0,0,w]$	1/2,0, $\bar{z}$	$[0,0,w]$	
4	g	4..	0,0,z	$[0,0,w]$	0,0, $\bar{z}$	$[0,0,w]$	1/2,1/2, $\bar{z}$	$[0,0,w]$	1/2,1/2,z	$[0,0,w]$	
4	f	..2'/m'	1/4,1/4,1/2	$[\bar{u},u,w]$	3/4,3/4,1/2	$[u,\bar{u},w]$	3/4,1/4,1/2	$[\bar{u},\bar{u},w]$	1/4,3/4,1/2	$[u,u,w]$	
4	e	..2'/m'	1/4,1/4,0	$[\bar{u},u,w]$	3/4,3/4,0	$[u,\bar{u},w]$	3/4,1/4,0	$[\bar{u},\bar{u},w]$	1/4,3/4,0	$[u,u,w]$	
2	d	$\bar{4}2'm'$	0,1/2,1/2	$[0,0,w]$	1/2,0,1/2	$[0,0,w]$					
2	c	$\bar{4}2'm'$	0,1/2,0	$[0,0,w]$	1/2,0,0	$[0,0,w]$					
2	b	42'2'	0,0,1/2	$[0,0,w]$	1/2,1/2,1/2	$[0,0,w]$					
2	a	42'2'	0,0,0	$[0,0,w]$	1/2,1/2,0	$[0,0,w]$					

**Symmetry of Special Projections**

Along [0,0,1]  $p_4$  4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 0,0,z

Along [1,0,0]  $p_2$  m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,0,0

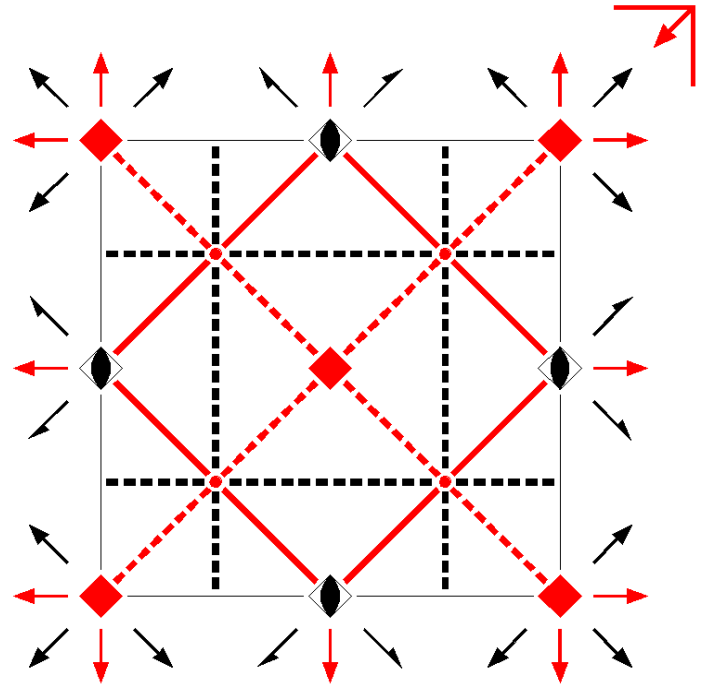
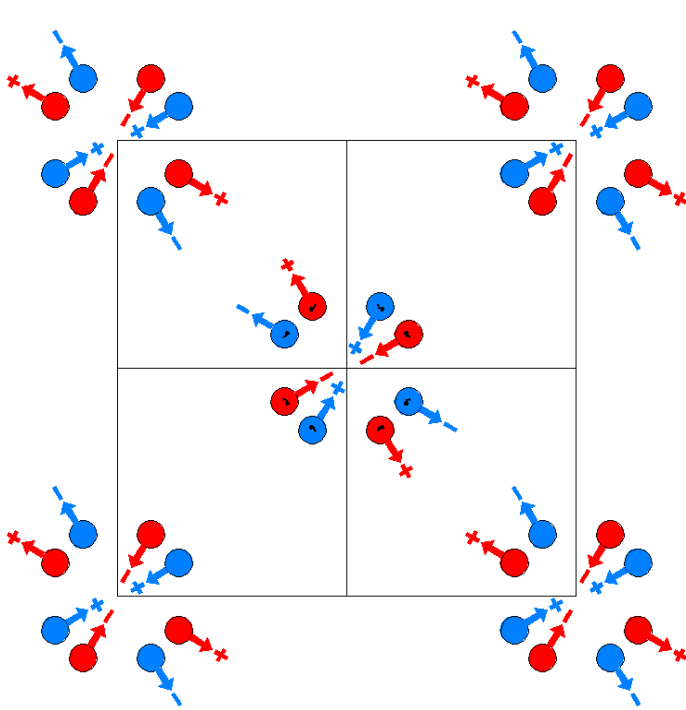
Along [1,1,0]  $p_2$  mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at x,x,0



P4'/n'bm'  
125.8.1038

4'/m'mm'  
P4'/n'2'/b2/m'

Tetragonal



Origin at 4'2'2 at 4'/n'2'2/g', at -1/4,-1/4,0 from center ( 2/m' )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)                                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)'                | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'                |
| (5) 2' 0,y,0<br>(2 <sub>y</sub> ' 0,0,0)'               | (6) 2' x,0,0<br>(2 <sub>x</sub> ' 0,0,0)'                  | (7) 2 x,x,0<br>(2 <sub>xy</sub> ' 0,0,0)   | (8) 2 x,x̄,0<br>(2 <sub>xȳ</sub> ' 0,0,0)                                       |
| (9) 1̄ 1/4,1/4,0<br>(1̄ 1/2,1/2,0)'                     | (10) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub> ' 1/2,1/2,0)' | (11) 4 <sup>+</sup> 1/2,0,z; 1/2,0,0<br>(4 <sub>z</sub> <sup>+</sup>  1/2,1/2,0) | (12) 4 <sup>-</sup> 0,1/2,z; 0,1/2,0<br>(4 <sub>z</sub> <sup>-</sup>  1/2,1/2,0) |
| (13) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (14) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)    | (15) m' x+1/2,x̄,z<br>(m <sub>xy</sub> ' 1/2,1/2,0)'                             | (16) g' (1/2,1/2,0) x,x,z<br>(m <sub>xȳ</sub> ' 1/2,1/2,0)'                     |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

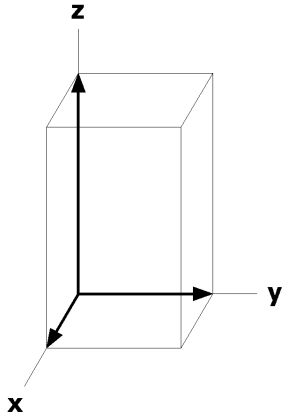
			Coordinates								
Multiplicity, Wyckoff letter, Site Symmetry.											
16	n	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y},x,z$	$[v,\bar{u},\bar{w}]$	(4)	$y,\bar{x},z$	$[\bar{v},u,\bar{w}]$
(5)	$\bar{x},y,\bar{z}$	$[u,\bar{v},w]$	(6)	$x,\bar{y},\bar{z}$	$[\bar{u},v,w]$	(7)	$y,x,\bar{z}$	$[v,u,\bar{w}]$	(8)	$\bar{y},\bar{x},\bar{z}$	$[\bar{v},\bar{u},\bar{w}]$
(9)	$\bar{x}+1/2,\bar{y}+1/2,\bar{z}$	$[\bar{u},\bar{v},\bar{w}]$	(10)	$x+1/2,y+1/2,\bar{z}$	$[u,v,\bar{w}]$	(11)	$y+1/2,\bar{x}+1/2,\bar{z}$	$[\bar{v},u,w]$	(12)	$\bar{y}+1/2,x+1/2,\bar{z}$	$[v,\bar{u},w]$
(13)	$x+1/2,\bar{y}+1/2,z$	$[\bar{u},v,\bar{w}]$	(14)	$\bar{x}+1/2,y+1/2,z$	$[u,\bar{v},\bar{w}]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[\bar{v},\bar{u},w]$	(16)	$y+1/2,x+1/2,z$	$[v,u,w]$
8	m	..m'	$x,x+1/2,z$	$[\bar{x},\bar{x}+1/2,z$	$[\bar{u},\bar{u},w]$	$\bar{x}+1/2,x,z$	$[u,\bar{u},\bar{w}]$	$x+1/2,\bar{x},z$	$[u,\bar{u},w]$	$\bar{x}+1/2,\bar{x},z$	$[\bar{u},\bar{u},\bar{w}]$
8	l	.2'	$x,0,1/2$	$[0,\bar{x},1/2$	$[0,\bar{v},w]$	$0,x,1/2$	$[v,0,\bar{w}]$	$0,\bar{x},1/2$	$[\bar{v},0,\bar{w}]$	$1/2,x+1/2,1/2$	$[v,0,w]$
8	k	.2'	$x,0,0$	$[0,\bar{x},0,0$	$[0,\bar{v},w]$	$0,x,0$	$[v,0,\bar{w}]$	$0,\bar{x},0$	$[\bar{v},0,\bar{w}]$	$1/2,x+1/2,0$	$[v,0,w]$
8	j	..2	$x,x,1/2$	$[u,\bar{x},1/2$	$[\bar{u},\bar{u},0]$	$\bar{x},x,1/2$	$[u,\bar{u},0]$	$x,\bar{x},1/2$	$[\bar{u},u,0]$	$\bar{x}+1/2,\bar{x}+1/2,1/2$	$[\bar{u},\bar{u},0]$
8	i	..2	$x,x,0$	$[u,\bar{x},x,0$	$[\bar{u},\bar{u},0]$	$\bar{x},x,0$	$[u,\bar{u},0]$	$x,\bar{x},0$	$[\bar{u},u,0]$	$\bar{x}+1/2,\bar{x}+1/2,0$	$[\bar{u},\bar{u},0]$
4	h	2.m'm'	$0,1/2,z$	$[0,0,\bar{x},1/2,z$	$[0,0,\bar{w}]$	$0,1/2,\bar{z}$	$[0,0,w]$	$1/2,0,\bar{z}$	$[0,0,\bar{w}]$		
4	g	4'..	$0,0,z$	$[0,0,0,\bar{x},0,z$	$[0,0,0]$	$1/2,1/2,\bar{z}$	$[0,0,0]$	$1/2,1/2,z$	$[0,0,0]$		
4	f	..2/m'	$1/4,1/4,1/2$	$[0,0,0,\bar{x},3/4,3/4,1/2$	$[0,0,0]$	$3/4,1/4,1/2$	$[0,0,0]$	$1/4,3/4,1/2$	$[0,0,0]$		
4	e	..2/m'	$1/4,1/4,0$	$[0,0,0,\bar{x},3/4,3/4,0$	$[0,0,0]$	$3/4,1/4,0$	$[0,0,0]$	$1/4,3/4,0$	$[0,0,0]$		
2	d	$\bar{4}2'm'$	$0,1/2,1/2$	$[0,0,\bar{x},1/2,0,1/2$	$[0,0,\bar{w}]$						
2	c	$\bar{4}2'm'$	$0,1/2,0$	$[0,0,\bar{x},1/2,0,0$	$[0,0,\bar{w}]$						
2	b	4'2'2	$0,0,1/2$	$[0,0,0,\bar{x},1/2,1/2,1/2$	$[0,0,0]$						
2	a	4'2'2	$0,0,0$	$[0,0,0,\bar{x},1/2,1/2,0$	$[0,0,0]$						

**Symmetry of Special Projections**

Along [0,0,1]  $p4'm'm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 0,0,z

Along [1,0,0]  $p_{2a}2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,1/4,0

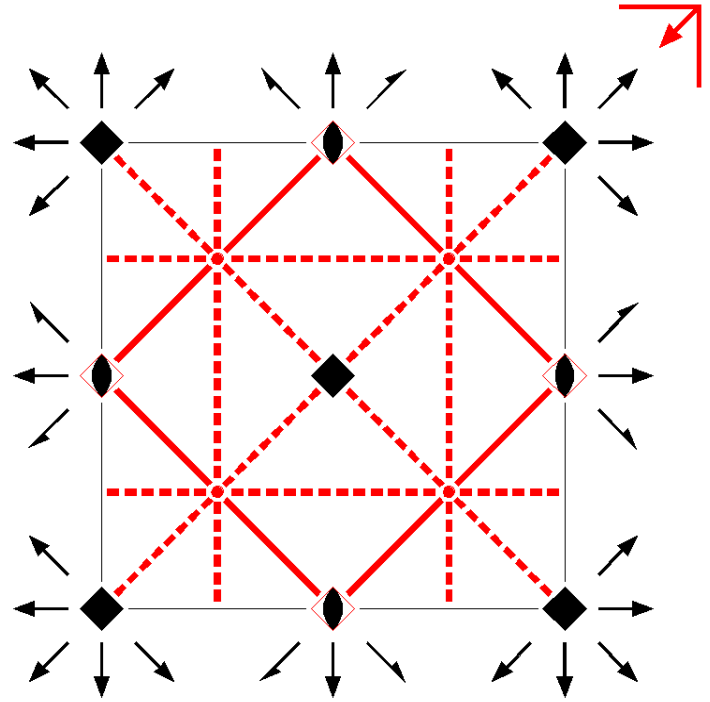
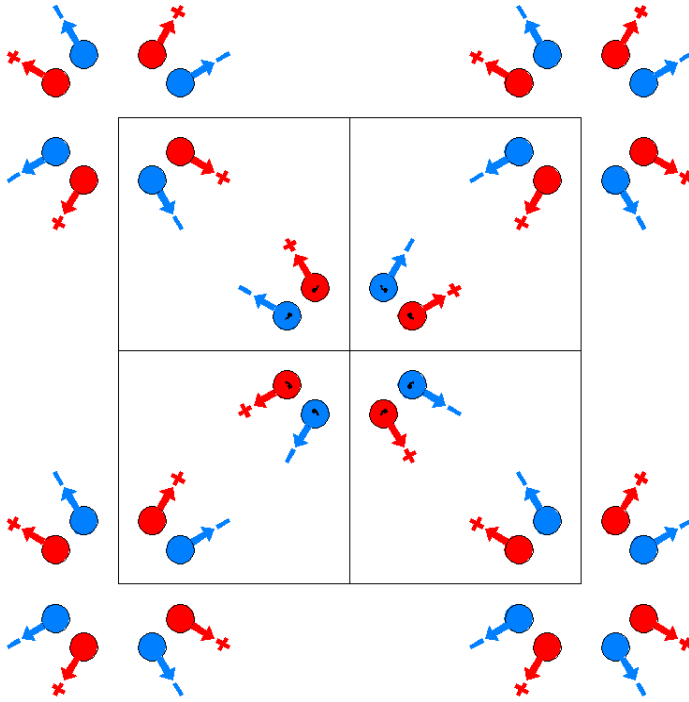
Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,x,0



P4/n'b'm'  
125.9.1039

4/m'm'm'  
P4/n'2/b'2/m'

Tetragonal



Origin at 422 at 4/n'22/g', at  $-1/4, -1/4, 0$  from center ( $2/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                                      | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)                                      |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                     | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                     | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)  | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)                                   |
| (9) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$ ' 1/2,1/2,0)'     | (10) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub> ' 1/2,1/2,0)' | (11) $\bar{4}$ <sup>+</sup> ' 1/2,0,z; 1/2,0,0<br>( $\bar{4}$ <sub>z</sub> ' 1/2,1/2,0)' | (12) $\bar{4}$ <sup>-</sup> ' 0,1/2,z; 0,1/2,0<br>( $\bar{4}$ <sub>z</sub> <sup>-1</sup> ' 1/2,1/2,0)' |
| (13) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub> ' 1/2,1/2,0)' | (14) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub> ' 1/2,1/2,0)' | (15) m' x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub> ' 1/2,1/2,0)'                            | (16) g' (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub> ' 1/2,1/2,0)'                         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

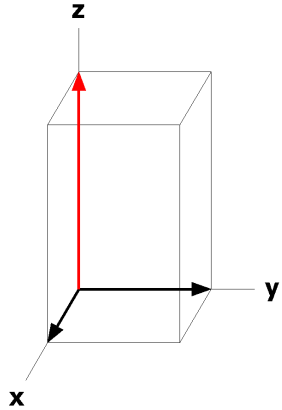
			Coordinates								
Multiplicity, Wyckoff letter, Site Symmetry.											
16	n	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y},x,z$	$[\bar{v},u,w]$	(4)	$y,\bar{x},z$	$[v,\bar{u},w]$
(5)	$\bar{x},y,\bar{z}$	$[\bar{u},v,\bar{w}]$	(6)	$x,\bar{y},\bar{z}$	$[u,\bar{v},\bar{w}]$	(7)	$y,x,\bar{z}$	$[v,u,\bar{w}]$	(8)	$\bar{y},\bar{x},\bar{z}$	$[\bar{v},\bar{u},\bar{w}]$
(9)	$\bar{x}+1/2,\bar{y}+1/2,\bar{z}$	$[\bar{u},\bar{v},\bar{w}]$	(10)	$x+1/2,y+1/2,\bar{z}$	$[u,v,\bar{w}]$	(11)	$y+1/2,\bar{x}+1/2,\bar{z}$	$[v,\bar{u},\bar{w}]$	(12)	$\bar{y}+1/2,x+1/2,\bar{z}$	$[\bar{v},u,\bar{w}]$
(13)	$x+1/2,\bar{y}+1/2,z$	$[u,\bar{v},w]$	(14)	$\bar{x}+1/2,y+1/2,z$	$[\bar{u},\bar{v},w]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[\bar{v},\bar{u},w]$	(16)	$y+1/2,x+1/2,z$	$[v,u,w]$
8	m	..m'	$x,x+1/2,z$	$[\bar{x},\bar{x}+1/2,z$	$[\bar{u},\bar{u},w]$	$\bar{x}+1/2,x,z$	$[\bar{u},u,w]$	$x+1/2,\bar{x},z$	$[u,\bar{u},w]$	$\bar{x}+1/2,\bar{x},z$	$[\bar{u},\bar{u},\bar{w}]$
8	l	..2.	$x,0,1/2$	$[\bar{x},0,1/2$	$[\bar{u},0,0]$	$0,x,1/2$	$[0,u,0]$	$0,\bar{x},1/2$	$[0,\bar{u},0]$	$1/2,x+1/2,1/2$	$[0,u,0]$
8	k	..2.	$x,0,0$	$[\bar{x},0,0$	$[\bar{u},0,0]$	$0,x,0$	$[0,u,0]$	$0,\bar{x},0$	$[0,\bar{u},0]$	$1/2,x+1/2,0$	$[0,u,0]$
8	j	..2	$x,x,1/2$	$[\bar{x},\bar{x},1/2$	$[\bar{u},\bar{u},0]$	$\bar{x},x,1/2$	$[\bar{u},u,0]$	$x,\bar{x},1/2$	$[u,\bar{u},0]$	$\bar{x}+1/2,\bar{x}+1/2,1/2$	$[u,u,0]$
8	i	..2	$x,x,0$	$[\bar{x},\bar{x},0$	$[\bar{u},\bar{u},0]$	$\bar{x},x,0$	$[\bar{u},u,0]$	$x,\bar{x},0$	$[u,\bar{u},0]$	$\bar{x}+1/2,\bar{x}+1/2,0$	$[u,u,0]$
4	h	2.m'm'	$0,1/2,z$	$[0,0,w]$	$1/2,0,z$	$[0,0,w]$	$0,1/2,\bar{z}$	$[0,0,\bar{w}]$	$1/2,0,\bar{z}$	$[0,0,\bar{w}]$	
4	g	4..	$0,0,z$	$[0,0,w]$	$0,0,\bar{z}$	$[0,0,w]$	$1/2,1/2,\bar{z}$	$[0,0,\bar{w}]$	$1/2,1/2,z$	$[0,0,\bar{w}]$	
4	f	..2/m'	$1/4,1/4,1/2$	$[0,0,0]$	$3/4,3/4,1/2$	$[0,0,0]$	$3/4,1/4,1/2$	$[0,0,0]$	$1/4,3/4,1/2$	$[0,0,0]$	
4	e	..2/m'	$1/4,1/4,0$	$[0,0,0]$	$3/4,3/4,0$	$[0,0,0]$	$3/4,1/4,0$	$[0,0,0]$	$1/4,3/4,0$	$[0,0,0]$	
2	d	$\bar{4}'2m'$	$0,1/2,1/2$	$[0,0,0]$	$1/2,0,1/2$	$[0,0,0]$					
2	c	$\bar{4}'2m'$	$0,1/2,0$	$[0,0,0]$	$1/2,0,0$	$[0,0,0]$					
2	b	422	$0,0,1/2$	$[0,0,0]$	$1/2,1/2,1/2$	$[0,0,0]$					
2	a	422	$0,0,0$	$[0,0,0]$	$1/2,1/2,0$	$[0,0,0]$					

**Symmetry of Special Projections**

Along [0,0,1]  $p4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 0,0,z

Along [1,0,0]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,0,0

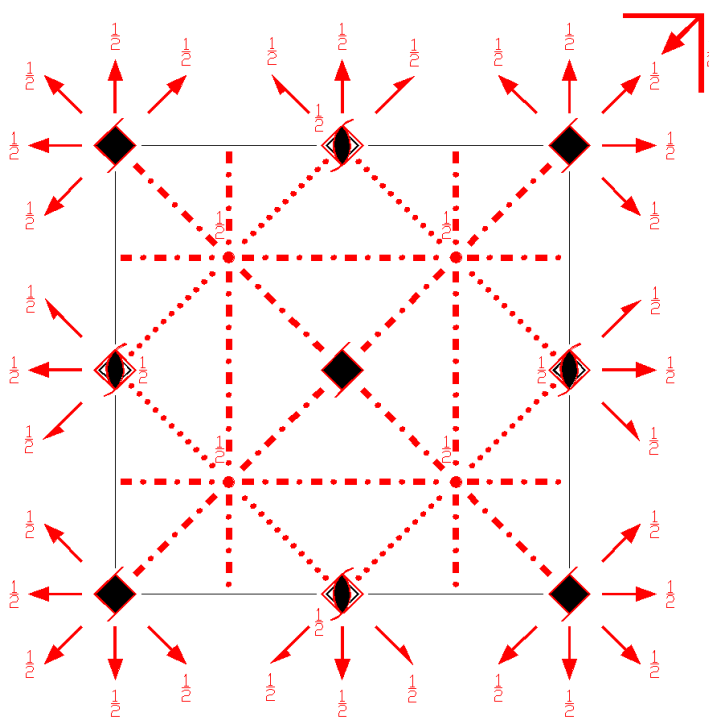
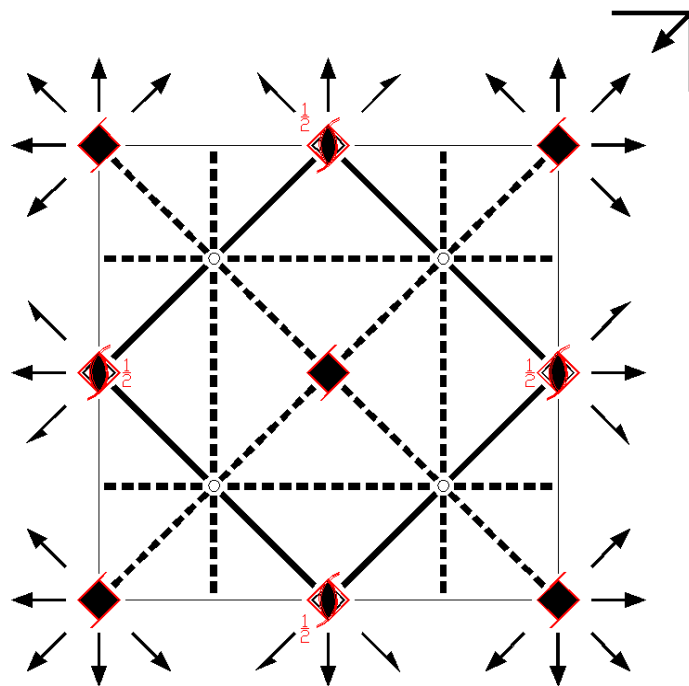
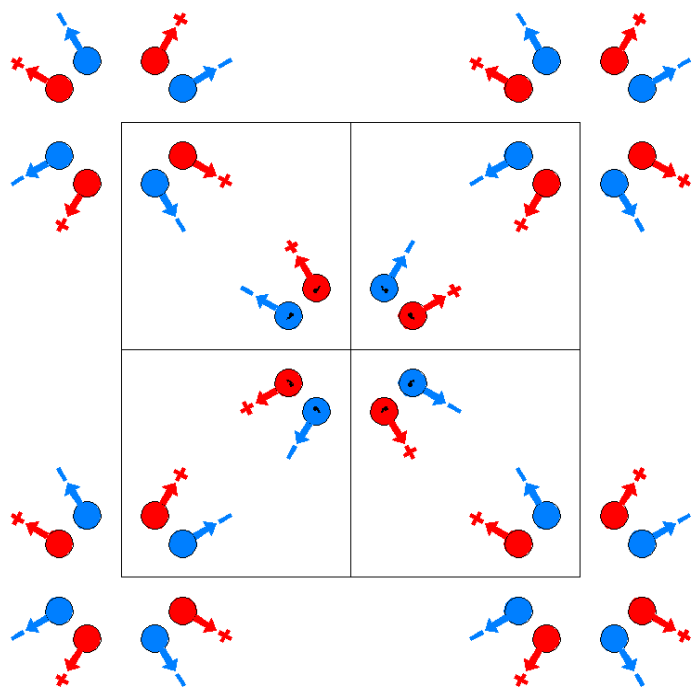
Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,x,0



$P_{2c} 4/nbm$   
125.10.1040

$4/mmm1'$   
 $P_{2c} 4/n2/b2/m$

Tetragonal



**Origin** at 422 at 4/n22/g, at -1/4,-1/4,0 from center ( 2/m )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)
(5) 2 0,y,0 (2 <sub>y</sub>  0,0,0)	(6) 2 x,0,0 (2 <sub>x</sub>  0,0,0)	(7) 2 x,x,0 (2 <sub>xy</sub>  0,0,0)	(8) 2 x, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  0,0,0)
(9) $\bar{1}$ 1/4,1/4,0 ( $\bar{1}$  1/2,1/2,0)	(10) n (1/2,1/2,0) x,y,0 (m <sub>z</sub>  1/2,1/2,0)	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,0 ( $\bar{4}_z^+$  1/2,1/2,0)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,0 ( $\bar{4}_z^-$  1/2,1/2,0)
(13) a (1/2,0,0) x,1/4,z (m <sub>y</sub>  1/2,1/2,0)	(14) b (0,1/2,0) 1/4,y,z (m <sub>x</sub>  1/2,1/2,0)	(15) m x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,0)	(16) g (1/2,1/2,0) x,x,z (m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)

For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 2' (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)'	(3) 4 <sup>+</sup> ' (0,0,1) 0,0,z (4 <sub>z</sub>  0,0,1)'	(4) 4 <sup>-</sup> ' (0,0,1) 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,1)'
(5) 2' 0,y,1/2 (2 <sub>y</sub>  0,0,1)'	(6) 2' x,0,1/2 (2 <sub>x</sub>  0,0,1)'	(7) 2' x,x,1/2 (2 <sub>xy</sub>  0,0,1)'	(8) 2' x, $\bar{x}$ ,1/2 (2 <sub><math>\bar{xy}</math></sub>  0,0,1)'
(9) $\bar{1}$ ' 1/4,1/4,1/2 ( $\bar{1}$  1/2,1/2,1)'	(10) n' (1/2,1/2,0) x,y,1/2 (m <sub>z</sub>  1/2,1/2,1)'	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/2 ( $\bar{4}_z^+$  1/2,1/2,1)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/2 ( $\bar{4}_z^-$  1/2,1/2,1)'
(13) n' (1/2,0,1) x,1/4,z (m <sub>y</sub>  1/2,1/2,1)'	(14) n' (0,1/2,1) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1)'	(15) c' (0,0,1) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,1)'	(16) n' (1/2,1/2,1) x,x,z (m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
32 n 1				
(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ]	
(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	
(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [u,v,w]	(10) x+1/2,y+1/2, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y+1/2, $\bar{x}+1/2,\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}$ [v, $\bar{u},w$ ]	
(13) x+1/2, $\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z$ [u, $\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z$ [v,u, $\bar{w}$ ]	(16) y+1/2,x+1/2,z [ $\bar{v},\bar{u},\bar{w}$ ]	
16 m ..m	x,x+1/2,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}+1/2,z$ [u, $\bar{u},0$ ]	$\bar{x}+1/2,x,z$ [ $\bar{u},\bar{u},0$ ]	x+1/2, $\bar{x},z$ [u,u,0]
	$\bar{x},x+1/2,\bar{z}$ [u,u,0]	x, $\bar{x}+1/2,\bar{z}$ [ $\bar{u},\bar{u},0$ ]	x+1/2,x, $\bar{z}$ [u, $\bar{u},0$ ]	$\bar{x}+1/2,\bar{x},\bar{z}$ [ $\bar{u},u,0$ ]

16	l	.2'	$x,0,1/2 [0,v,w]$	$\bar{x},0,1/2 [0,\bar{v},w]$	$0,x,1/2 [\bar{v},0,w]$	$0,\bar{x},1/2 [v,0,w]$
			$\bar{x}+1/2,1/2,1/2 [0,\bar{v},\bar{w}]$	$x+1/2,1/2,1/2 [0,v,\bar{w}]$	$1/2,\bar{x}+1/2,1/2 [v,0,\bar{w}]$	$1/2,x+1/2,1/2 [\bar{v},0,\bar{w}]$
16	k	.2.	$x,0,0 [u,0,0]$	$\bar{x},0,0 [\bar{u},0,0]$	$0,x,0 [0,u,0]$	$0,\bar{x},0 [0,\bar{u},0]$
			$\bar{x}+1/2,1/2,0 [u,0,0]$	$x+1/2,1/2,0 [\bar{u},0,0]$	$1/2,\bar{x}+1/2,0 [0,u,0]$	$1/2,x+1/2,0 [0,\bar{u},0]$
16	j	..2'	$x,x,1/2 [\bar{u},u,w]$	$\bar{x},\bar{x},1/2 [u,\bar{u},w]$	$\bar{x},x,1/2 [\bar{u},\bar{u},w]$	$x,\bar{x},1/2 [u,u,w]$
			$\bar{x}+1/2,\bar{x}+1/2,1/2 [u,\bar{u},\bar{w}]$	$x+1/2,x+1/2,1/2 [\bar{u},u,\bar{w}]$	$x+1/2,\bar{x}+1/2,1/2 [u,u,\bar{w}]$	$\bar{x}+1/2,x+1/2,1/2 [\bar{u},\bar{u},\bar{w}]$
16	i	..2	$x,x,0 [u,u,0]$	$\bar{x},\bar{x},0 [\bar{u},\bar{u},0]$	$\bar{x},x,0 [\bar{u},u,0]$	$x,\bar{x},0 [u,\bar{u},0]$
			$\bar{x}+1/2,\bar{x}+1/2,0 [u,u,0]$	$x+1/2,x+1/2,0 [\bar{u},\bar{u},0]$	$x+1/2,\bar{x}+1/2,0 [\bar{u},u,0]$	$\bar{x}+1/2,x+1/2,0 [u,\bar{u},0]$
8	h	2.mm	$0,1/2,z [0,0,0]$	$1/2,0,z [0,0,0]$	$0,1/2,\bar{z} [0,0,0]$	$1/2,0,\bar{z} [0,0,0]$
8	g	4..	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,\bar{w}]$	$1/2,1/2,\bar{z} [0,0,w]$	$1/2,1/2,z [0,0,\bar{w}]$
8	f	..2/m'	$1/4,1/4,1/2 [0,0,0]$	$3/4,3/4,1/2 [0,0,0]$	$3/4,1/4,1/2 [0,0,0]$	$1/4,3/4,1/2 [0,0,0]$
8	e	..2/m	$1/4,1/4,0 [u,u,0]$	$3/4,3/4,0 [\bar{u},\bar{u},0]$	$3/4,1/4,0 [\bar{u},u,0]$	$1/4,3/4,0 [u,\bar{u},0]$
4	d	$\bar{4}'2'm$	$0,1/2,1/2 [0,0,0]$	$1/2,0,1/2 [0,0,0]$		
4	c	$\bar{4}2m$	$0,1/2,0 [0,0,0]$	$1/2,0,0 [0,0,0]$		
4	b	42'2'	$0,0,1/2 [0,0,w]$	$1/2,1/2,1/2 [0,0,\bar{w}]$		
4	a	422	$0,0,0 [0,0,0]$	$1/2,1/2,0 [0,0,0]$		

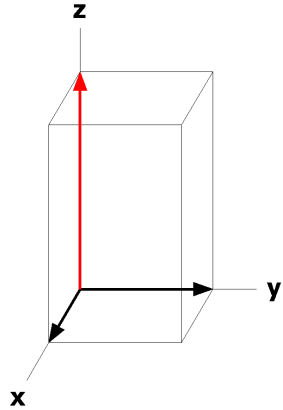
### Symmetry of Special Projections

Along  $[0,0,1]$  p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p<sub>c</sub>2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,1/4,1/2$

Along  $[1,1,0]$  p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$

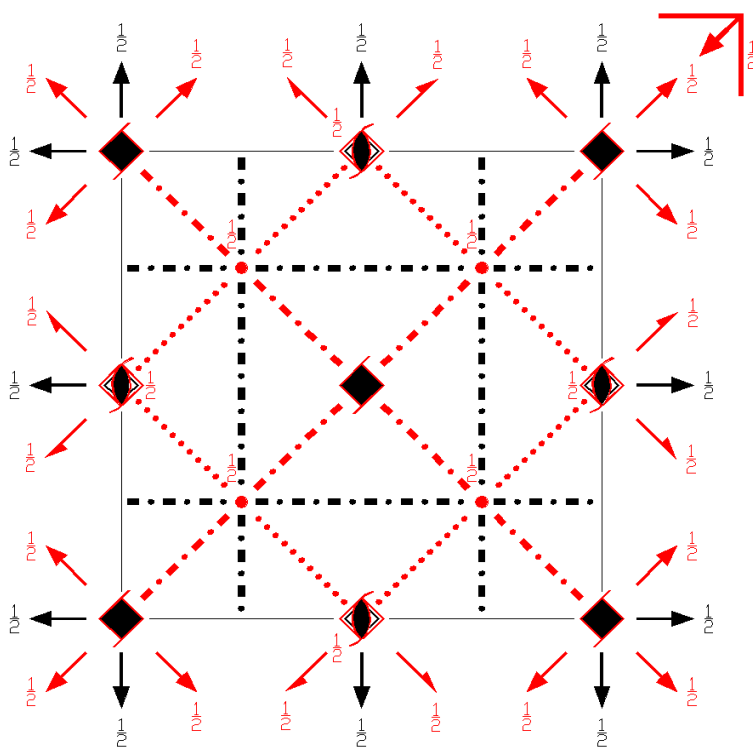
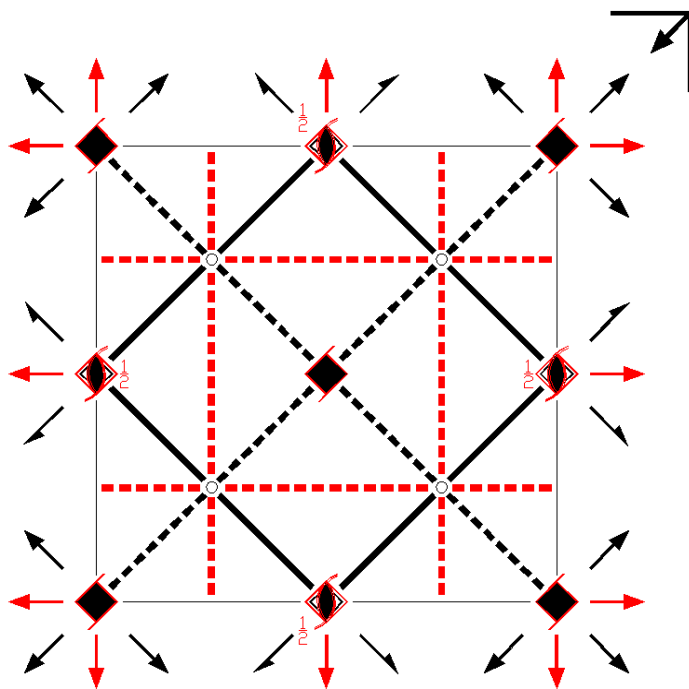
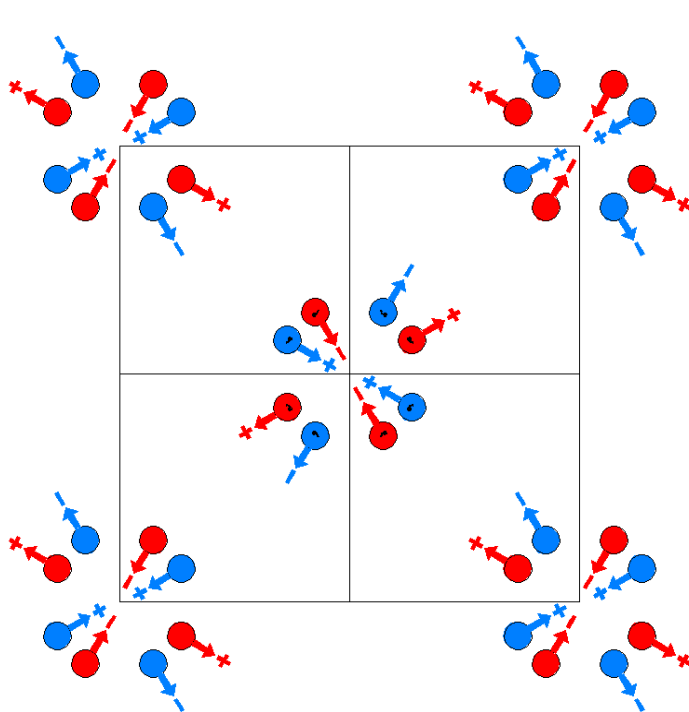




$P_{2c} 4/nb'm$   
125.11.1041

$4/mmm1'$   
 $P_{2c} 4/n2'/b'2/m$

Tetragonal



**Origin** at 4'2'2 at 4'/n2'2/g, at -1/4,-1/4,0 from center ( 2/m )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)'	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(5) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(6) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'	(7) 2 x,x,0 (2 <sub>xy</sub>  0,0,0)	(8) 2 x,x̄,0 (2 <sub>xy</sub> <sup>-</sup>  0,0,0)
(9) $\bar{1}$ 1/4,1/4,0 ( $\bar{1}$  1/2,1/2,0)	(10) n (1/2,1/2,0) x,y,0 (m <sub>z</sub>  1/2,1/2,0)	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,0 ( $\bar{4}_z^+$  1/2,1/2,0)'	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,0 ( $\bar{4}_z^-$  1/2,1/2,0)'
(13) a' (1/2,0,0) x,1/4,z (m <sub>y</sub>  1/2,1/2,0)'	(14) b' (0,1/2,0) 1/4,y,z (m <sub>x</sub>  1/2,1/2,0)'	(15) m x+1/2,x̄,z (m <sub>xy</sub>  1/2,1/2,0)	(16) g (1/2,1/2,0) x,x,z (m <sub>xy</sub> <sup>-</sup>  1/2,1/2,0)

For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 2' (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)'	(3) 4 <sup>+</sup> (0,0,1) 0,0,z (4 <sub>z</sub>  0,0,1)	(4) 4 <sup>-</sup> (0,0,1) 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,1)
(5) 2 0,y,1/2 (2 <sub>y</sub>  0,0,1)	(6) 2 x,0,1/2 (2 <sub>x</sub>  0,0,1)	(7) 2' x,x,1/2 (2 <sub>xy</sub>  0,0,1)'	(8) 2' x,x̄,1/2 (2 <sub>xy</sub> <sup>-</sup>  0,0,1)'
(9) $\bar{1}$ ' 1/4,1/4,1/2 ( $\bar{1}$ ' 1/2,1/2,1)'	(10) n' (1/2,1/2,0) x,y,1/2 (m <sub>z</sub> ' 1/2,1/2,1)'	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/2 ( $\bar{4}_z^+$  1/2,1/2,1)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/2 ( $\bar{4}_z^-$ ' 1/2,1/2,1)
(13) n (1/2,0,1) x,1/4,z (m <sub>y</sub>  1/2,1/2,1)	(14) n (0,1/2,1) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1)	(15) c' (0,0,1) x+1/2,x̄,z (m <sub>xy</sub>  1/2,1/2,1)'	(16) n' (1/2,1/2,1) x,x,z (m <sub>xy</sub> <sup>-</sup> ' 1/2,1/2,1)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
32 n 1				
(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]	
(5) $\bar{x},y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	
(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [u,v,w]	(10) $x+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y+1/2,\bar{x}+1/2,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	
(13) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},\bar{v},w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $\bar{v},u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	
16 m ..m	$x,x+1/2,z$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}+1/2,z$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x,z$ [ $u,u,0$ ]	$x+1/2,\bar{x},z$ [ $\bar{u},\bar{u},0$ ]
	$\bar{x},x+1/2,\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x}+1/2,\bar{z}$ [ $u,u,0$ ]	$x+1/2,x,\bar{z}$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,\bar{x},\bar{z}$ [ $\bar{u},u,0$ ]

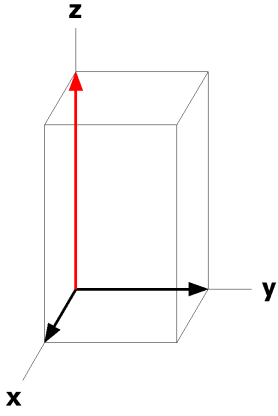
16	l	.2.	x,0,1/2 [u,0,0] $\bar{x}+1/2,1/2,1/2 [\bar{u},0,0]$	$\bar{x},0,1/2 [\bar{u},0,0]$ x+1/2,1/2,1/2 [u,0,0]	0,x,1/2 [0, $\bar{u}$ ,0] 1/2, $\bar{x}+1/2,1/2 [0,u,0]$	0, $\bar{x},1/2 [0,u,0]$ 1/2,x+1/2,1/2 [0, $\bar{u}$ ,0]
16	k	.2'	x,0,0 [0,v,w] $\bar{x}+1/2,1/2,0 [0,v,w]$	$\bar{x},0,0 [0,\bar{v},w]$ x+1/2,1/2,0 [0, $\bar{v},w]$	0,x,0 [v,0, $\bar{w}$ ] 1/2, $\bar{x}+1/2,0 [v,0,\bar{w}]$	0, $\bar{x},0 [\bar{v},0,\bar{w}]$ 1/2,x+1/2,0 [ $\bar{v},0,\bar{w}]$
16	j	..2'	x,x,1/2 [ $\bar{u}$ ,u,w] $\bar{x}+1/2,\bar{x}+1/2,1/2 [u,\bar{u},\bar{w}]$	$\bar{x},\bar{x},1/2 [u,\bar{u},w]$ x+1/2,x+1/2,1/2 [ $\bar{u},u,\bar{w}]$	$\bar{x},x,1/2 [u,u,\bar{w}]$ x+1/2, $\bar{x}+1/2,1/2 [u,\bar{u},\bar{w}]$	x, $\bar{x},1/2 [\bar{u},\bar{u},\bar{w}]$ $\bar{x}+1/2,x+1/2,1/2 [u,u,w]$
16	i	..2	x,x,0 [u,u,0] $\bar{x}+1/2,\bar{x}+1/2,0 [u,u,0]$	$\bar{x},\bar{x},0 [u,\bar{u},0]$ x+1/2,x+1/2,0 [ $\bar{u},\bar{u},0]$	$\bar{x},x,0 [u,\bar{u},0]$ x+1/2, $\bar{x}+1/2,0 [u,\bar{u},0]$	x, $\bar{x},0 [u,\bar{u},0]$ $\bar{x}+1/2,x+1/2,0 [\bar{u},u,0]$
8	h	2.mm	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z} [0,0,0]$	1/2,0, $\bar{z} [0,0,0]$
8	g	4'..	0,0,z [0,0,0]	0,0, $\bar{z} [0,0,0]$	1/2,1/2, $\bar{z} [0,0,0]$	1/2,1/2,z [0,0,0]
8	f	..2'/m'	1/4,1/4,1/2 [u,v,0]	3/4,3/4,1/2 [ $\bar{u},\bar{v},0]$	3/4,1/4,1/2 [v, $\bar{u}$ ,0]	1/4,3/4,1/2 [ $\bar{v},u,0]$
8	e	..2/m	1/4,1/4,0 [u,u,0]	3/4,3/4,0 [ $\bar{u},\bar{u},0]$	3/4,1/4,0 [u, $\bar{u}$ ,0]	1/4,3/4,0 [ $\bar{u},u,0]$
4	d	$\bar{4}2m$	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
4	c	$\bar{4}'2'm$	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
4	b	4'22'	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4	a	4'2'2	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,1/2

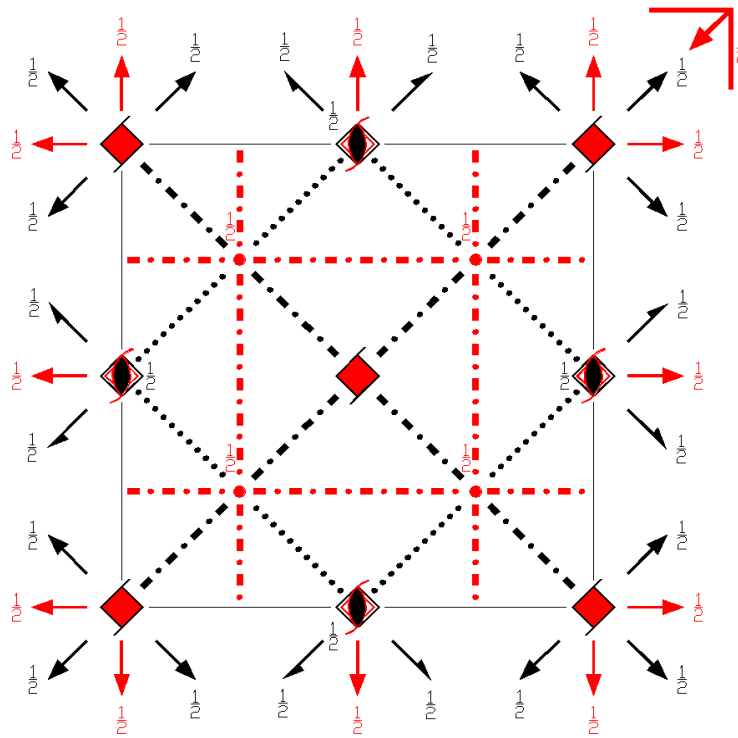
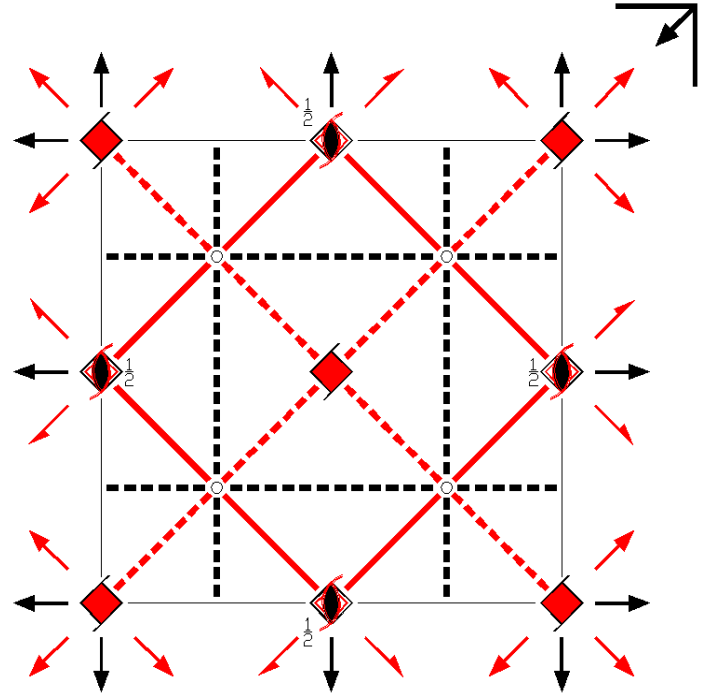
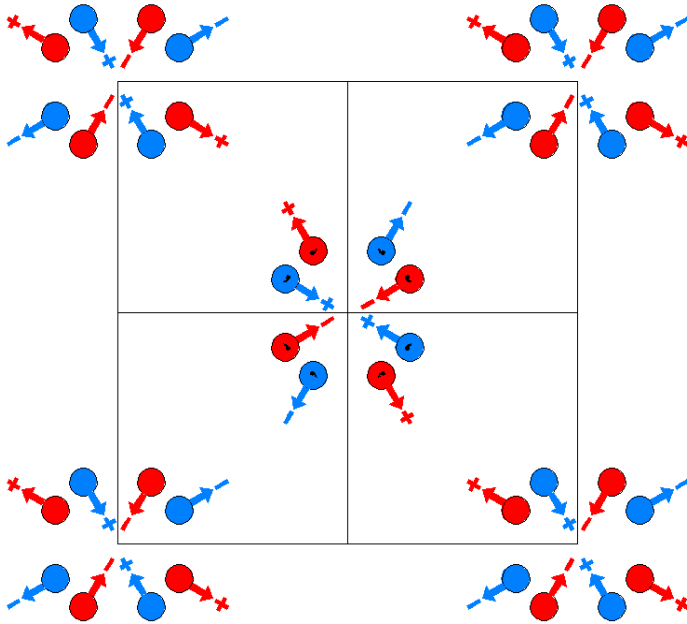
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_{2c} 4'/nbm'$   
125.12.1042

$4/mmm1'$   
 $P_{2c} 4'/n2/b2'/m'$

Tetragonal



**Origin** at 4'22' at 4'/n22'/g', at -1/4,-1/4,0 from center ( 2'/m' )

**Asymmetric unit**  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 <sub>0,0,z</sub> (2 <sub>z</sub>  0,0,0)	(3) 4 <sup>+</sup> <sub>0,0,z</sub> (4 <sub>z</sub>  0,0,0)'	(4) 4 <sup>-</sup> <sub>0,0,z</sub> (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(5) 2 <sub>0,y,0</sub> (2 <sub>y</sub>  0,0,0)	(6) 2 <sub>x,0,0</sub> (2 <sub>x</sub>  0,0,0)	(7) 2' <sub>x,x,0</sub> (2 <sub>xy</sub>  0,0,0)'	(8) 2' <sub>x,x̄,0</sub> (2 <sub>xy</sub> <sup>-</sup>  0,0,0)'
(9) $\bar{1}$ <sub>1/4,1/4,0</sub> ( $\bar{1}$  1/2,1/2,0)	(10) n <sub>(1/2,1/2,0)</sub> x,y,0 (m <sub>z</sub>  1/2,1/2,0)	(11) $\bar{4}^+$ <sub>1/2,0,z; 1/2,0,0</sub> ( $\bar{4}_z$  1/2,1/2,0)'	(12) $\bar{4}^-$ <sub>0,1/2,z; 0,1/2,0</sub> ( $\bar{4}_z$ <sup>-1</sup>  1/2,1/2,0)'
(13) a <sub>(1/2,0,0)</sub> x,1/4,z (m <sub>y</sub>  1/2,1/2,0)	(14) b <sub>(0,1/2,0)</sub> 1/4,y,z (m <sub>x</sub>  1/2,1/2,0)	(15) m' <sub>x+1/2,x̄,z</sub> (m <sub>xy</sub>  1/2,1/2,0)'	(16) g' <sub>(1/2,1/2,0)</sub> x,x,z (m <sub>xy</sub> <sup>-</sup>  1/2,1/2,0)'

For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 2' (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)'	(3) 4 <sup>+</sup> (0,0,1) 0,0,z (4 <sub>z</sub>  0,0,1)	(4) 4 <sup>-</sup> (0,0,1) 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,1)
(5) 2' (0,y,1/2) (2 <sub>y</sub>  0,0,1)'	(6) 2' (x,0,1/2) (2 <sub>x</sub>  0,0,1)'	(7) 2 (x,x,1/2) (2 <sub>xy</sub>  0,0,1)	(8) 2 (x,x̄,1/2) (2 <sub>xy</sub> <sup>-</sup>  0,0,1)
(9) $\bar{1}$ ' <sub>1/4,1/4,1/2</sub> ( $\bar{1}$ ' 1/2,1/2,1)'	(10) n' (1/2,1/2,0) x,y,1/2 (m <sub>z</sub>  1/2,1/2,1)'	(11) $\bar{4}^+$ <sub>1/2,0,z; 1/2,0,1/2</sub> ( $\bar{4}_z$  1/2,1/2,1)	(12) $\bar{4}^-$ <sub>0,1/2,z; 0,1/2,1/2</sub> ( $\bar{4}_z$ <sup>-1</sup>  1/2,1/2,1)
(13) n' (1/2,0,1) x,1/4,z (m <sub>y</sub>  1/2,1/2,1)'	(14) n' (0,1/2,1) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1)'	(15) c (0,0,1) x+1/2,x̄,z (m <sub>xy</sub>  1/2,1/2,1)	(16) n (1/2,1/2,1) x,x,z (m <sub>xy</sub> <sup>-</sup>  1/2,1/2,1)

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +		(0,0,1)' +	
32 n 1				
(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]	
(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},u,w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	
(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y+1/2,\bar{x}+1/2,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	
(13) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z$ [ $\bar{v},u,w$ ]	
16 m ..m'	$x,x+1/2,z$ [ $u,u,w$ ]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,z$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,\bar{x},z$ [ $\bar{u},u,\bar{w}$ ]
	$\bar{x},x+1/2,\bar{z}$ [ $\bar{u},u,\bar{w}$ ]	$x,\bar{x}+1/2,\bar{z}$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x,\bar{z}$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,\bar{x},\bar{z}$ [ $u,u,w$ ]

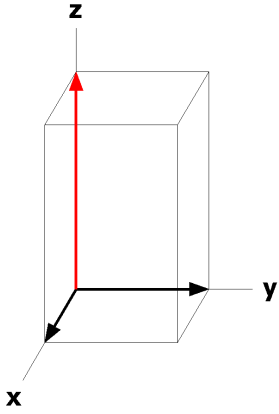
16	l	.2'	$x, 0, 1/2 [0, v, w]$	$\bar{x}, 0, 1/2 [0, \bar{v}, w]$	$0, x, 1/2 [v, 0, \bar{w}]$	$0, \bar{x}, 1/2 [\bar{v}, 0, \bar{w}]$
			$\bar{x}+1/2, 1/2, 1/2 [0, \bar{v}, \bar{w}]$	$x+1/2, 1/2, 1/2 [0, v, \bar{w}]$	$1/2, \bar{x}+1/2, 1/2 [\bar{v}, 0, w]$	$1/2, x+1/2, 1/2 [v, 0, w]$
16	k	.2.	$x, 0, 0 [u, 0, 0]$	$\bar{x}, 0, 0 [\bar{u}, 0, 0]$	$0, x, 0 [0, \bar{u}, 0]$	$0, \bar{x}, 0 [0, u, 0]$
			$\bar{x}+1/2, 1/2, 0 [\bar{u}, 0, 0]$	$x+1/2, 1/2, 0 [u, 0, 0]$	$1/2, \bar{x}+1/2, 0 [0, \bar{u}, 0]$	$1/2, x+1/2, 0 [0, u, 0]$
16	j	..2	$x, x, 1/2 [u, u, 0]$	$\bar{x}, \bar{x}, 1/2 [\bar{u}, \bar{u}, 0]$	$\bar{x}, x, 1/2 [u, \bar{u}, 0]$	$x, \bar{x}, 1/2 [\bar{u}, u, 0]$
			$\bar{x}+1/2, \bar{x}+1/2, 1/2 [\bar{u}, \bar{u}, 0]$	$x+1/2, x+1/2, 1/2 [u, u, 0]$	$x+1/2, \bar{x}+1/2, 1/2 [\bar{u}, u, 0]$	$\bar{x}+1/2, x+1/2, 1/2 [u, \bar{u}, 0]$
16	i	..2'	$x, x, 0 [\bar{u}, u, w]$	$\bar{x}, \bar{x}, 0 [u, \bar{u}, w]$	$\bar{x}, x, 0 [u, u, \bar{w}]$	$x, \bar{x}, 0 [\bar{u}, \bar{u}, \bar{w}]$
			$\bar{x}+1/2, \bar{x}+1/2, 0 [\bar{u}, u, w]$	$x+1/2, x+1/2, 0 [u, \bar{u}, w]$	$x+1/2, \bar{x}+1/2, 0 [u, u, \bar{w}]$	$\bar{x}+1/2, x+1/2, 0 [\bar{u}, \bar{u}, \bar{w}]$
8	h	2.m'm'	$0, 1/2, z [0, 0, w]$	$1/2, 0, z [0, 0, \bar{w}]$	$0, 1/2, \bar{z} [0, 0, \bar{w}]$	$1/2, 0, \bar{z} [0, 0, w]$
8	g	4'..	$0, 0, z [0, 0, 0]$	$0, 0, \bar{z} [0, 0, 0]$	$1/2, 1/2, \bar{z} [0, 0, 0]$	$1/2, 1/2, z [0, 0, 0]$
8	f	..2/m'	$1/4, 1/4, 1/2 [0, 0, 0]$	$3/4, 3/4, 1/2 [0, 0, 0]$	$3/4, 1/4, 1/2 [0, 0, 0]$	$1/4, 3/4, 1/2 [0, 0, 0]$
8	e	..2'/m'	$1/4, 1/4, 0 [u, \bar{u}, w]$	$3/4, 3/4, 0 [\bar{u}, u, w]$	$3/4, 1/4, 0 [\bar{u}, \bar{u}, \bar{w}]$	$1/4, 3/4, 0 [u, u, \bar{w}]$
4	d	$\bar{4}$ '2m'	$0, 1/2, 1/2 [0, 0, w]$	$1/2, 0, 1/2 [0, 0, \bar{w}]$		
4	c	$\bar{4}$ '2m'	$0, 1/2, 0 [0, 0, 0]$	$1/2, 0, 0 [0, 0, 0]$		
4	b	4'2'2	$0, 0, 1/2 [0, 0, 0]$	$1/2, 1/2, 1/2 [0, 0, 0]$		
4	a	4'22'	$0, 0, 0 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$		

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$   $p_c 2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 1/4, 1/2$

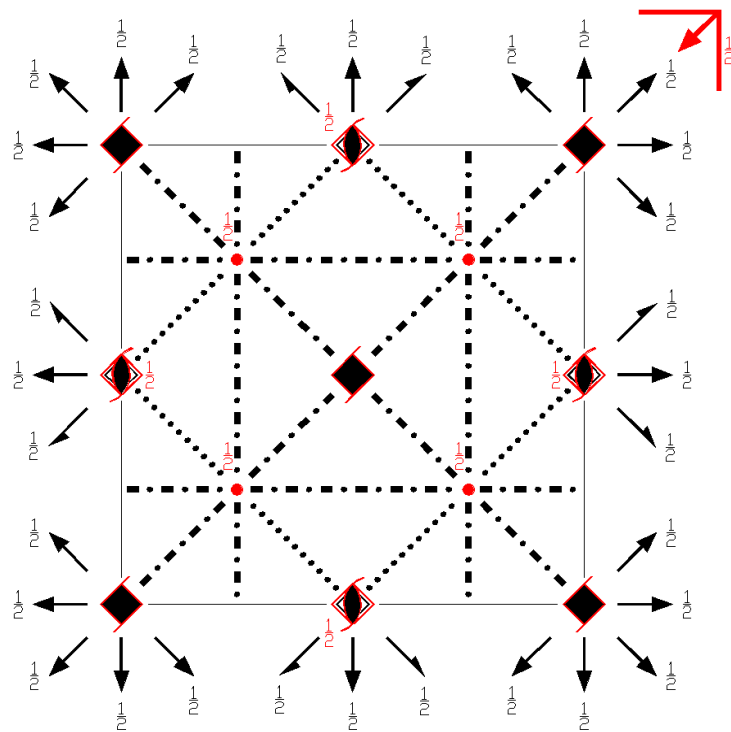
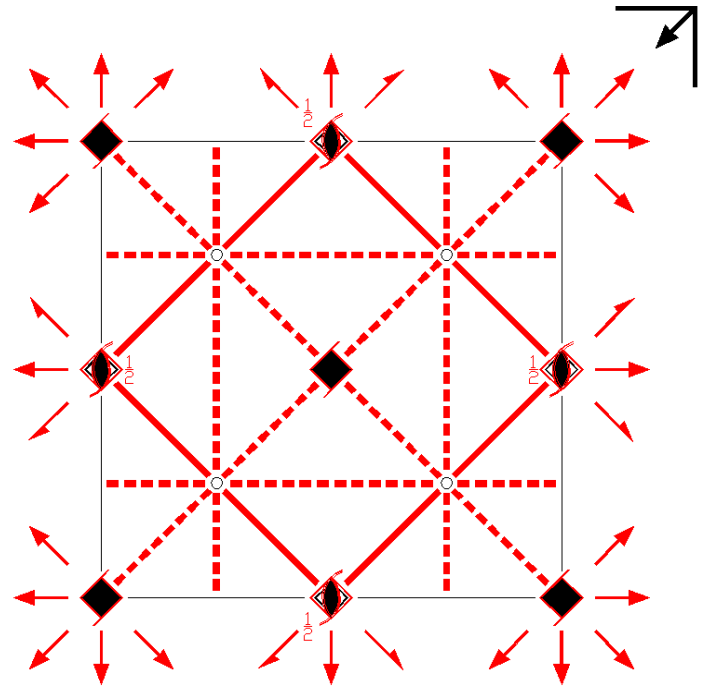
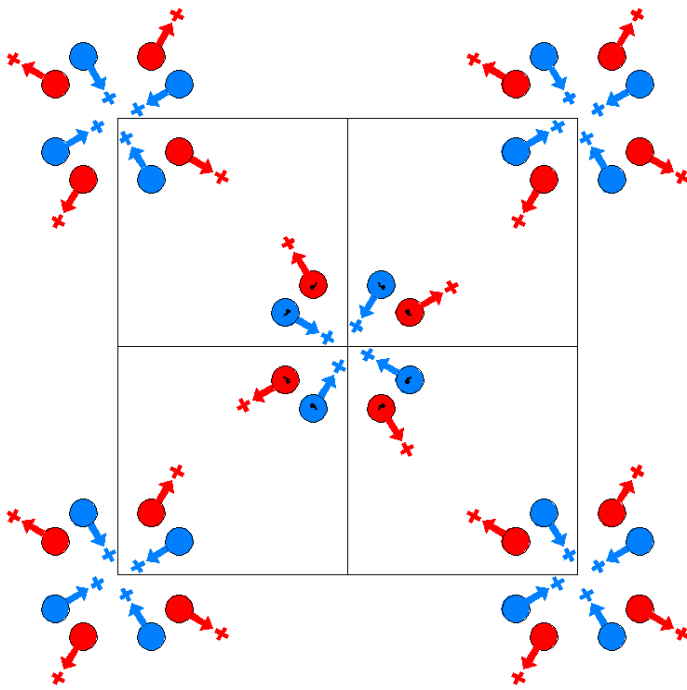
Along  $[1, 1, 0]$   $p_{2a} 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x, x, 1/2$



$P_{2c} 4/nb'm'$   
125.13.1043

$4/mmm1'$   
 $P_{2c} 4/n2'/b'2'/m'$

Tetragonal



**Origin** at 42'2' at 4/n2'2'/g', at -1/4,-1/4,0 from center ( 2'/m' )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)
(5) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(6) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'	(7) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) 2' x, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  0,0,0)'
(9) $\bar{1}$ 1/4,1/4,0 ( $\bar{1}$  1/2,1/2,0)	(10) n (1/2,1/2,0) x,y,0 (m <sub>z</sub>  1/2,1/2,0)	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,0 ( $\bar{4}_z^+$  1/2,1/2,0)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,0 ( $\bar{4}_z^-$  1/2,1/2,0)
(13) a' (1/2,0,0) x,1/4,z (m <sub>y</sub>  1/2,1/2,0)'	(14) b' (0,1/2,0) 1/4,y,z (m <sub>x</sub>  1/2,1/2,0)'	(15) m' x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,0)'	(16) g' (1/2,1/2,0) x,x,z (m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)'

For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 2' (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)'	(3) 4 <sup>+</sup> ' (0,0,1) 0,0,z (4 <sub>z</sub>  0,0,1)'	(4) 4 <sup>-</sup> ' (0,0,1) 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,1)'
(5) 2 0,y,1/2 (2 <sub>y</sub>  0,0,1)	(6) 2 x,0,1/2 (2 <sub>x</sub>  0,0,1)	(7) 2 x,x,1/2 (2 <sub>xy</sub>  0,0,1)	(8) 2 x, $\bar{x}$ ,1/2 (2 <sub><math>\bar{xy}</math></sub>  0,0,1)
(9) $\bar{1}$ ' 1/4,1/4,1/2 ( $\bar{1}$ ' 1/2,1/2,1)'	(10) n' (1/2,1/2,0) x,y,1/2 (m <sub>z</sub> ' 1/2,1/2,1)'	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/2 ( $\bar{4}_z^+$ ' 1/2,1/2,1)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/2 ( $\bar{4}_z^-$ ' 1/2,1/2,1)'
(13) n (1/2,0,1) x,1/4,z (m <sub>y</sub>  1/2,1/2,1)	(14) n (0,1/2,1) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1)	(15) c (0,0,1) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,1)	(16) n (1/2,1/2,1) x,x,z (m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1)

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +		(0,0,1)' +	
32 n 1				
(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ]	
(5) $\bar{x},y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	
(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [u,v,w]	(10) x+1/2,y+1/2, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y+1/2, $\bar{x}+1/2,\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}$ [v, $\bar{u},w$ ]	
(13) x+1/2, $\bar{y}+1/2,z$ [ $\bar{u},\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $\bar{v},\bar{u},w$ ]	(16) y+1/2,x+1/2,z [ $\bar{v},\bar{u},w$ ]	
16 m ..m'	x,x+1/2,z [u,u,w]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,z$ [ $\bar{u},u,w$ ]	x+1/2, $\bar{x},z$ [u, $\bar{u},w$ ]
	$\bar{x},x+1/2,\bar{z}$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x}+1/2,\bar{z}$ [ $\bar{u},u,w$ ]	x+1/2,x, $\bar{z}$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,\bar{x},\bar{z}$ [u,u,w]



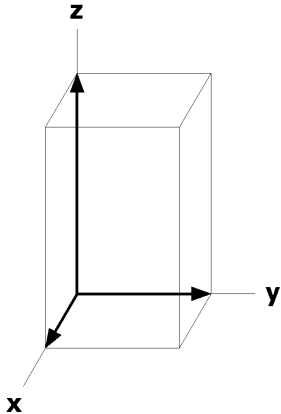
16	l	.2.	x,0,1/2 [u,0,0] $\bar{x}+1/2,1/2,1/2 [\bar{u},0,0]$	$\bar{x},0,1/2 [\bar{u},0,0]$ x+1/2,1/2,1/2 [u,0,0]	0,x,1/2 [0,u,0] 1/2, $\bar{x}+1/2,1/2 [0,\bar{u},0]$	0, $\bar{x},1/2 [0,\bar{u},0]$ 1/2,x+1/2,1/2 [0,u,0]
16	k	.2'	x,0,0 [0,v,w] $\bar{x}+1/2,1/2,0 [0,v,w]$	$\bar{x},0,0 [0,\bar{v},w]$ x+1/2,1/2,0 [0, $\bar{v},w]$	0,x,0 [ $\bar{v},0,w]$ 1/2, $\bar{x}+1/2,0 [\bar{v},0,w]$	0, $\bar{x},0 [v,0,w]$ 1/2,x+1/2,0 [v,0,w]
16	j	..2	x,x,1/2 [u,u,0] $\bar{x}+1/2,\bar{x}+1/2,1/2 [\bar{u},\bar{u},0]$	$\bar{x},\bar{x},1/2 [\bar{u},\bar{u},0]$ x+1/2,x+1/2,1/2 [u,u,0]	$\bar{x},x,1/2 [\bar{u},u,0]$ x+1/2, $\bar{x}+1/2,1/2 [u,\bar{u},0]$	x, $\bar{x},1/2 [u,\bar{u},0]$ $\bar{x}+1/2,x+1/2,1/2 [\bar{u},u,0]$
16	i	..2'	x,x,0 [ $\bar{u},u,w]$ $\bar{x}+1/2,\bar{x}+1/2,0 [\bar{u},u,w]$	$\bar{x},\bar{x},0 [u,\bar{u},w]$ x+1/2,x+1/2,0 [u, $\bar{u},w]$	$\bar{x},x,0 [\bar{u},\bar{u},w]$ x+1/2, $\bar{x}+1/2,0 [\bar{u},\bar{u},w]$	x, $\bar{x},0 [u,u,w]$ $\bar{x}+1/2,x+1/2,0 [u,u,w]$
8	h	2.m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z} [0,0,w]$	1/2,0, $\bar{z} [0,0,w]$
8	g	4..	0,0,z [0,0,w]	0,0, $\bar{z} [0,0,w]$	1/2,1/2, $\bar{z} [0,0,w]$	1/2,1/2,z [0,0,w]
8	f	..2/m	1/4,1/4,1/2 [0,0,w]	3/4,3/4,1/2 [0,0,w]	3/4,1/4,1/2 [0,0,w]	1/4,3/4,1/2 [0,0,w]
8	e	..2'/m'	1/4,1/4,0 [ $\bar{u},u,w]$	3/4,3/4,0 [u, $\bar{u},w]$	3/4,1/4,0 [ $\bar{u},\bar{u},w]$	1/4,3/4,0 [u,u,w]
4	d	$\bar{4}'2m'$	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
4	c	$\bar{4}'2m'$	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]		
4	b	422	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4	a	42'2'	0,0,0 [0,0,w]	1/2,1/2,0 [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'-2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,1/2

Along [1,1,0] p<sub>2a</sub>'-2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/2



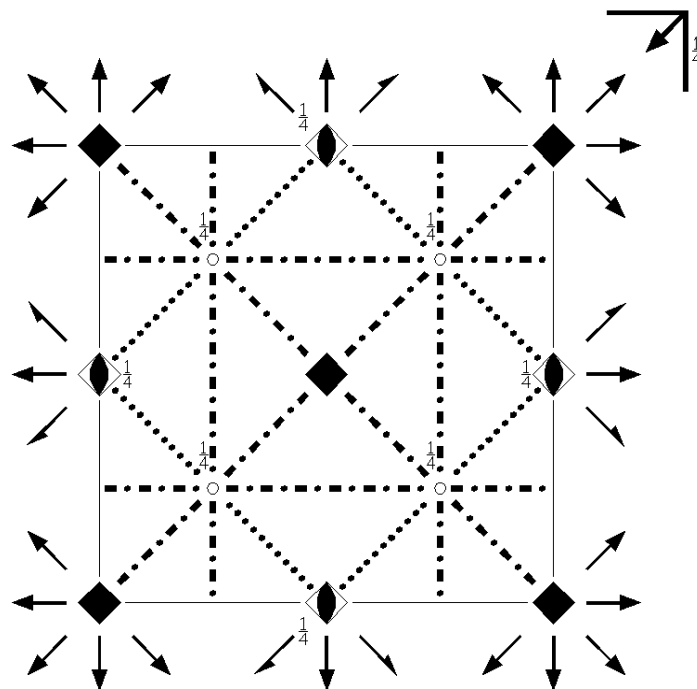
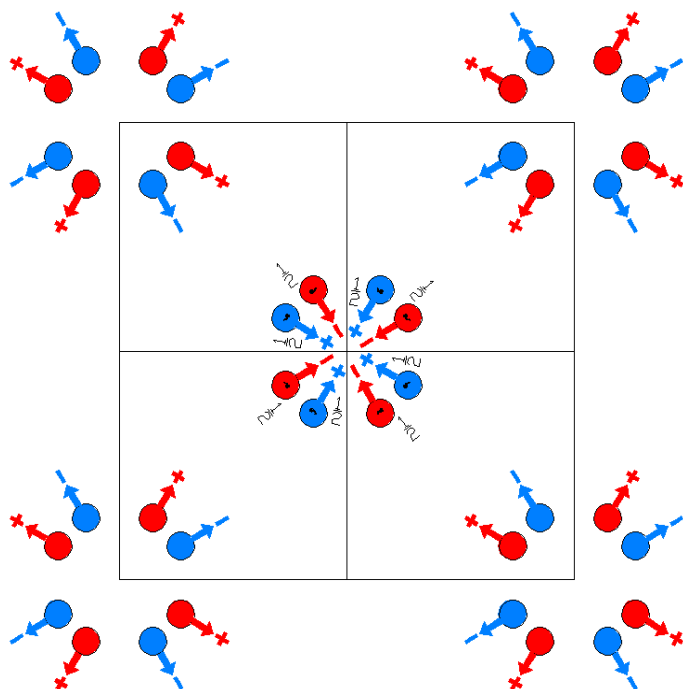
P4/nnc

126.1.1044

4/mmm

P4/n2/n2/c

Tetragonal



Origin at 422/n, at  $-1/4, -1/4, -1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                    | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)               |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                      | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                      | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)            |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)      | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2)   | (12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2)            |
| (13) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (14) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (15) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (16) n (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

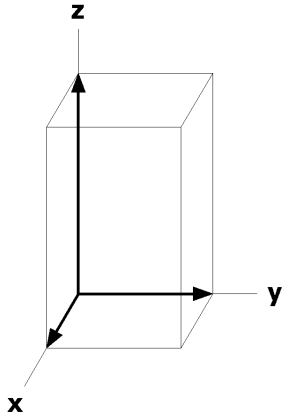
			Coordinates															
Multiplicity, Wyckoff letter, Site Symmetry.																		
16	k	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [v, $\bar{u},w$ ]	(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}$ [v,u, $\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [u,v,w]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(11) $y+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},u,w$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [v, $\bar{u},w$ ]	(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [u, $\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [v,u, $\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	j	.2.	$x,0,1/2$ [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	$0,x,1/2$ [0,u,0]	$0,\bar{x},1/2$ [0, $\bar{u},0$ ]	$\bar{x}+1/2,1/2,0$ [u,0,0]	$x+1/2,1/2,0$ [ $\bar{u},0,0$ ]	$1/2,\bar{x}+1/2,0$ [0,u,0]	$1/2,x+1/2,0$ [0, $\bar{u},0$ ]								
8	i	.2.	$x,0,0$ [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	$0,x,0$ [0,u,0]	$0,\bar{x},0$ [0, $\bar{u},0$ ]	$\bar{x}+1/2,1/2,1/2$ [u,0,0]	$x+1/2,1/2,1/2$ [ $\bar{u},0,0$ ]	$1/2,\bar{x}+1/2,1/2$ [0,u,0]	$1/2,x+1/2,1/2$ [0, $\bar{u},0$ ]								
8	h	..2	$x,x,0$ [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]	$x,\bar{x},0$ [u, $\bar{u},0$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [u,u,0]	$x+1/2,x+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,x+1/2,1/2$ [u, $\bar{u},0$ ]								
8	g	2..	$1/2,0,z$ [0,0,w]	$0,1/2,z$ [0,0,w]	$1/2,0,\bar{z}$ [0,0, $\bar{w}$ ]	$0,1/2,\bar{z}$ [0,0, $\bar{w}$ ]	$0,1/2,\bar{z}+1/2$ [0,0,w]	$1/2,0,\bar{z}+1/2$ [0,0,w]	$0,1/2,z+1/2$ [0,0, $\bar{w}$ ]	$1/2,0,z+1/2$ [0,0, $\bar{w}$ ]								
8	f	$\bar{1}$	$1/4,1/4,1/4$ [u,v,w]	$3/4,3/4,1/4$ [ $\bar{u},\bar{v},w$ ]	$3/4,1/4,1/4$ [ $\bar{v},u,w$ ]	$1/4,3/4,1/4$ [v, $\bar{u},w$ ]	$3/4,1/4,3/4$ [ $\bar{u},v,\bar{w}$ ]	$1/4,3/4,3/4$ [u, $\bar{v},\bar{w}$ ]	$1/4,1/4,3/4$ [v,u, $\bar{w}$ ]	$3/4,3/4,3/4$ [ $\bar{v},\bar{u},\bar{w}$ ]								
4	e	4..	$0,0,z$ [0,0,w]	$0,0,\bar{z}$ [0,0, $\bar{w}$ ]	$1/2,1/2,\bar{z}+1/2$ [0,0,w]	$1/2,1/2,z+1/2$ [0,0, $\bar{w}$ ]												
4	d	$\bar{4}$ ..	$1/2,0,1/4$ [0,0,w]	$0,1/2,1/4$ [0,0,w]	$1/2,0,3/4$ [0,0, $\bar{w}$ ]	$0,1/2,3/4$ [0,0, $\bar{w}$ ]												
4	c	222.	$1/2,0,0$ [0,0,0]	$0,1/2,0$ [0,0,0]	$0,1/2,1/2$ [0,0,0]	$1/2,0,1/2$ [0,0,0]												
2	b	422	$0,0,1/2$ [0,0,0]	$1/2,1/2,0$ [0,0,0]														
2	a	422	$0,0,0$ [0,0,0]	$1/2,1/2,1/2$ [0,0,0]														

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_p \cdot 4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,0,0$

Along  $[1,1,0]$   $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at  $x,x,0$

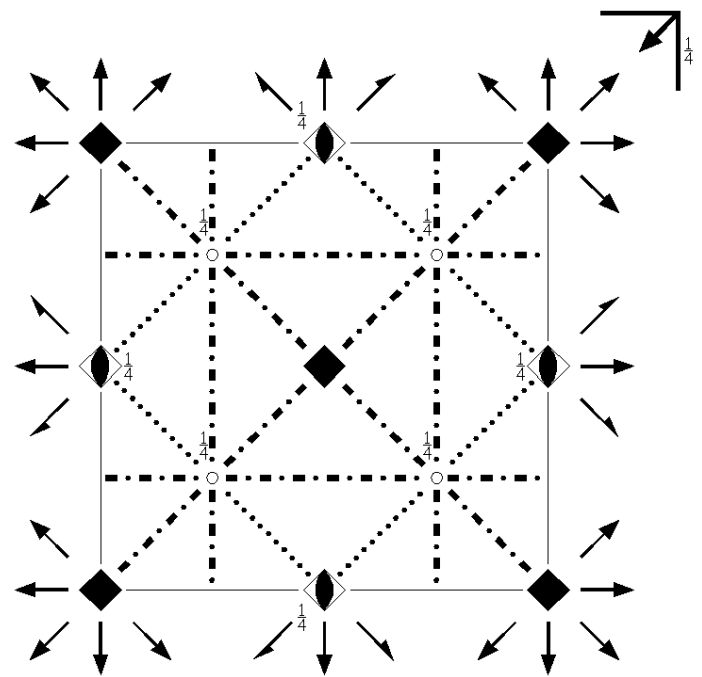
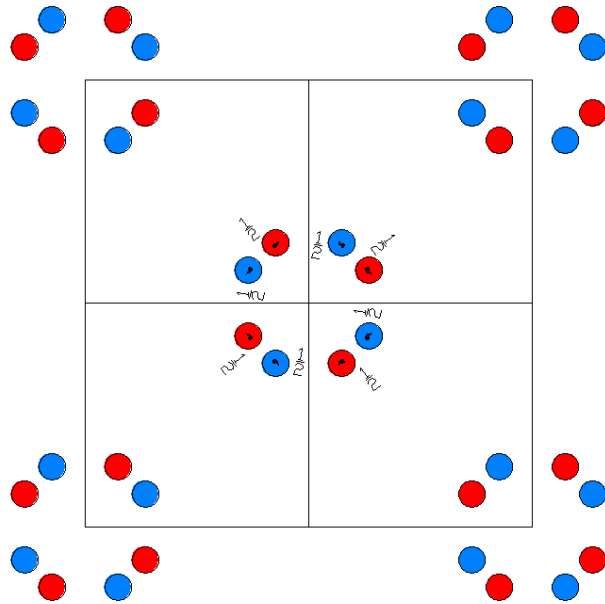


P4/nnc1'  
126.2.1045

4/mmm1'  
P4/n2/n2/c1'

Tetragonal

1'



Origin at 422/n1', at -1/4,-1/4,-1/4 from  $\bar{1}11'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

**Symmetry Operations**

For 1 + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                    | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)               |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                      | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                      | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)            |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)      | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2)   | (12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2)            |
| (13) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (14) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (15) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (16) n (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2) |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)'	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(5) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(6) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'	(7) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) 2' x, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  0,0,0)'
(9) $\bar{1}$ ' 1/4,1/4,1/4 ( $\bar{1}$  1/2,1/2,1/2)'	(10) n' (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>  1/2,1/2,1/2)'	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z^+$  1/2,1/2,1/2)'	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^-$  1/2,1/2,1/2)'
(13) n' (1/2,0,1/2) x,1/4,z (m <sub>y</sub>  1/2,1/2,1/2)'	(14) n' (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1/2)'	(15) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,1/2)'	(16) n' (1/2,1/2,1/2) x,x,z (m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

**Positions**

			Coordinates															
			1 +		1' +													
Multiplicity,	Wyckoff letter,	Site Symmetry.																
16	k	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z$ [0,0,0]	(4) y, $\bar{x},z$ [0,0,0]	(5) $\bar{x},y,\bar{z}$ [0,0,0]	(6) x, $\bar{y},\bar{z}$ [0,0,0]	(7) y,x, $\bar{z}$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}$ [0,0,0]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [0,0,0]	(10) x+1/2,y+1/2, $\bar{z}+1/2$ [0,0,0]	(11) y+1/2, $\bar{x}+1/2,\bar{z}+1/2$ [0,0,0]	(12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [0,0,0]	(13) x+1/2, $\bar{y}+1/2,z+1/2$ [0,0,0]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [0,0,0]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [0,0,0]	(16) y+1/2,x+1/2,z+1/2 [0,0,0]
8	j	.2.1'	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]	0,x,1/2 [0,0,0]	0, $\bar{x},1/2$ [0,0,0]	$\bar{x}+1/2,1/2,0$ [0,0,0]	x+1/2,1/2,0 [0,0,0]	1/2, $\bar{x}+1/2,0$ [0,0,0]	1/2,x+1/2,0 [0,0,0]								
8	i	.2.1'	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x},0$ [0,0,0]	$\bar{x}+1/2,1/2,1/2$ [0,0,0]	x+1/2,1/2,1/2 [0,0,0]	1/2, $\bar{x}+1/2,1/2$ [0,0,0]	1/2,x+1/2,1/2 [0,0,0]								
8	h	..21'	x,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x},x,0$ [0,0,0]	x, $\bar{x},0$ [0,0,0]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [0,0,0]	x+1/2,x+1/2,1/2 [0,0,0]	x+1/2, $\bar{x}+1/2,1/2$ [0,0,0]	$\bar{x}+1/2,x+1/2,1/2$ [0,0,0]								
8	g	2..1'	1/2,0,z [0,0,0]	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	0,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0,z+1/2 [0,0,0]								

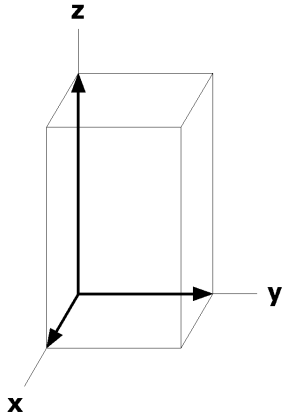
8	f	$\bar{1}1'$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]
			3/4,1/4,3/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]
4	e	4..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,1/2,z+1/2 [0,0,0]
4	d	$\bar{4}..1'$	1/2,0,1/4 [0,0,0]	0,1/2,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]	0,1/2,3/4 [0,0,0]
4	c	222.1'	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]
2	b	4221'	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a	4221'	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

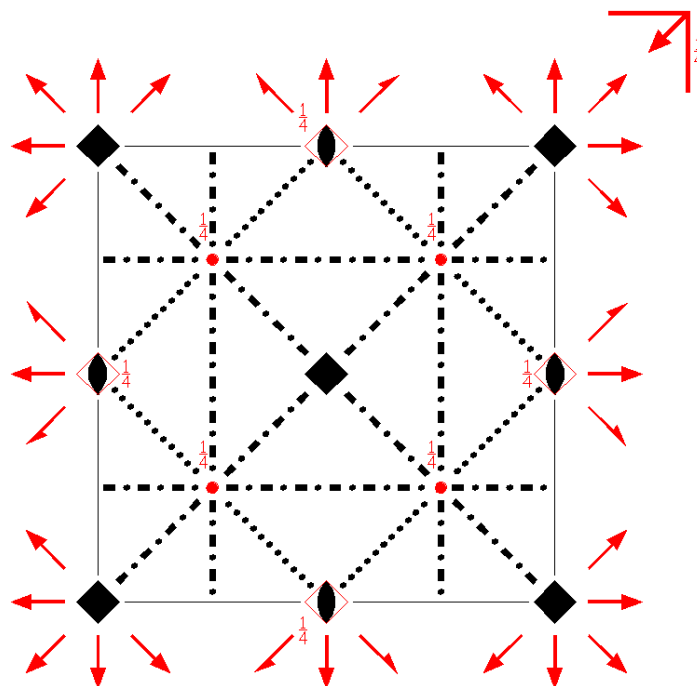
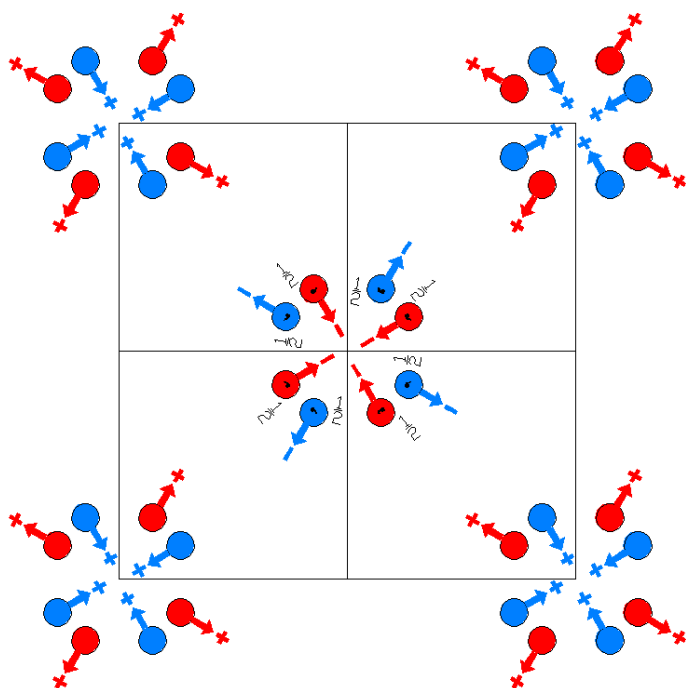
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



P4/n'nc  
126.3.1046

4/m'mm  
P4/n'2'/n2'/c

Tetragonal



Origin at  $42'2'/n$ , at  $-1/4, -1/4, -1/4$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) $1$<br>( $1 0,0,0$ )                                    | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                            | (3) $4^+$ $0,0,z$<br>( $4_z 0,0,0$ )                                    | (4) $4^-$ $0,0,z$<br>( $4_z^{-1} 0,0,0$ )                               |
| (5) $2'$ $0,y,0$<br>( $2_y 0,0,0$ )'                        | (6) $2'$ $x,0,0$<br>( $2_x 0,0,0$ )'                          | (7) $2'$ $x,x,0$<br>( $2_{xy} 0,0,0$ )'                                 | (8) $2'$ $x,\bar{x},0$<br>( $2_{\bar{xy}} 0,0,0$ )'                     |
| (9) $\bar{1}'$ $1/4,1/4,1/4$<br>( $\bar{1}' 1/2,1/2,1/2$ )' | (10) $n'$ ( $1/2,1/2,0$ ) $x,y,1/4$<br>( $m_z 1/2,1/2,1/2$ )' | (11) $\bar{4}^+$ $1/2,0,z; 1/2,0,1/4$<br>( $\bar{4}_z^+ 1/2,1/2,1/2$ )' | (12) $\bar{4}^-$ $0,1/2,z; 0,1/2,1/4$<br>( $\bar{4}_z^- 1/2,1/2,1/2$ )' |
| (13) $n$ ( $1/2,0,1/2$ ) $x,1/4,z$<br>( $m_y 1/2,1/2,1/2$ ) | (14) $n$ ( $0,1/2,1/2$ ) $1/4,y,z$<br>( $m_x 1/2,1/2,1/2$ )   | (15) $c$ ( $0,0,1/2$ ) $x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,1/2$ )    | (16) $n$ ( $1/2,1/2,1/2$ ) $x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,1/2$ )    |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

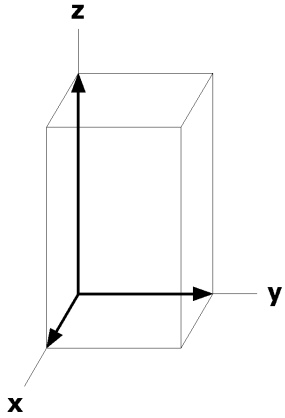
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	k	1	(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $\bar{y},x,z [\bar{v},u,w]$	(4) $y,\bar{x},z [v,\bar{u},w]$	(5) $\bar{x},y,\bar{z} [\bar{u},\bar{v},w]$	(6) $x,\bar{y},\bar{z} [\bar{u},v,w]$	(7) $y,x,\bar{z} [\bar{v},\bar{u},w]$	(8) $\bar{y},\bar{x},\bar{z} [v,u,w]$	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2 [\bar{u},\bar{v},\bar{w}]$	(10) $x+1/2,y+1/2,\bar{z}+1/2 [u,v,\bar{w}]$	(11) $y+1/2,\bar{x}+1/2,\bar{z}+1/2 [v,\bar{u},\bar{w}]$	(12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2 [\bar{v},u,\bar{w}]$	(13) $x+1/2,\bar{y}+1/2,z+1/2 [\bar{u},v,\bar{w}]$	(14) $\bar{x}+1/2,y+1/2,z+1/2 [u,\bar{v},\bar{w}]$	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2 [v,u,\bar{w}]$	(16) $y+1/2,x+1/2,z+1/2 [\bar{v},\bar{u},\bar{w}]$
8	j	.2'	$x,0,1/2 [0,v,w]$	$\bar{x},0,1/2 [0,\bar{v},w]$	$0,x,1/2 [\bar{v},0,w]$	$0,\bar{x},1/2 [v,0,w]$	$\bar{x}+1/2,1/2,0 [0,\bar{v},\bar{w}]$	$x+1/2,1/2,0 [0,v,\bar{w}]$	$1/2,\bar{x}+1/2,0 [v,0,\bar{w}]$	$1/2,x+1/2,0 [\bar{v},0,\bar{w}]$								
8	i	.2'	$x,0,0 [0,v,w]$	$\bar{x},0,0 [0,\bar{v},w]$	$0,x,0 [\bar{v},0,w]$	$0,\bar{x},0 [v,0,w]$	$\bar{x}+1/2,1/2,1/2 [0,\bar{v},\bar{w}]$	$x+1/2,1/2,1/2 [0,v,\bar{w}]$	$1/2,\bar{x}+1/2,1/2 [v,0,\bar{w}]$	$1/2,x+1/2,1/2 [\bar{v},0,\bar{w}]$								
8	h	..2'	$x,x,0 [\bar{u},u,w]$	$\bar{x},\bar{x},0 [u,\bar{u},w]$	$\bar{x},x,0 [\bar{u},\bar{u},w]$	$x,\bar{x},0 [u,u,w]$	$\bar{x}+1/2,\bar{x}+1/2,1/2 [u,\bar{u},\bar{w}]$	$x+1/2,x+1/2,1/2 [\bar{u},u,\bar{w}]$	$x+1/2,\bar{x}+1/2,1/2 [u,u,\bar{w}]$	$\bar{x}+1/2,x+1/2,1/2 [\bar{u},\bar{u},\bar{w}]$								
8	g	2..	$1/2,0,z [0,0,w]$	$0,1/2,z [0,0,w]$	$1/2,0,\bar{z} [0,0,w]$	$0,1/2,\bar{z} [0,0,w]$	$0,1/2,\bar{z}+1/2 [0,0,\bar{w}]$	$1/2,0,\bar{z}+1/2 [0,0,\bar{w}]$	$0,1/2,z+1/2 [0,0,\bar{w}]$	$1/2,0,z+1/2 [0,0,\bar{w}]$								
8	f	$\bar{1}'$	$1/4,1/4,1/4 [0,0,0]$	$3/4,3/4,1/4 [0,0,0]$	$3/4,1/4,1/4 [0,0,0]$	$1/4,3/4,1/4 [0,0,0]$	$3/4,1/4,3/4 [0,0,0]$	$1/4,3/4,3/4 [0,0,0]$	$1/4,1/4,3/4 [0,0,0]$	$3/4,3/4,3/4 [0,0,0]$								
4	e	4..	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,w]$	$1/2,1/2,\bar{z}+1/2 [0,0,\bar{w}]$	$1/2,1/2,z+1/2 [0,0,\bar{w}]$												
4	d	$\bar{4}'..$	$1/2,0,1/4 [0,0,0]$	$0,1/2,1/4 [0,0,0]$	$1/2,0,3/4 [0,0,0]$	$0,1/2,3/4 [0,0,0]$												
4	c	22'2'	$1/2,0,0 [0,0,w]$	$0,1/2,0 [0,0,w]$	$0,1/2,1/2 [0,0,\bar{w}]$	$1/2,0,1/2 [0,0,\bar{w}]$												
2	b	42'2'	$0,0,1/2 [0,0,w]$	$1/2,1/2,0 [0,0,\bar{w}]$														
2	a	42'2'	$0,0,0 [0,0,w]$	$1/2,1/2,1/2 [0,0,\bar{w}]$														

**Symmetry of Special Projections**

Along [0,0,1]  $p4mm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at x,0,0

Along [1,1,0]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at x,x,0



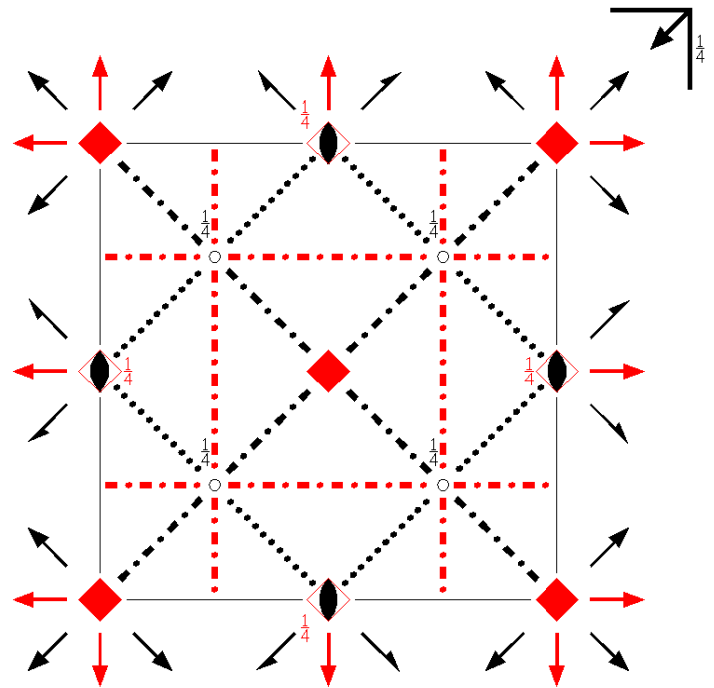
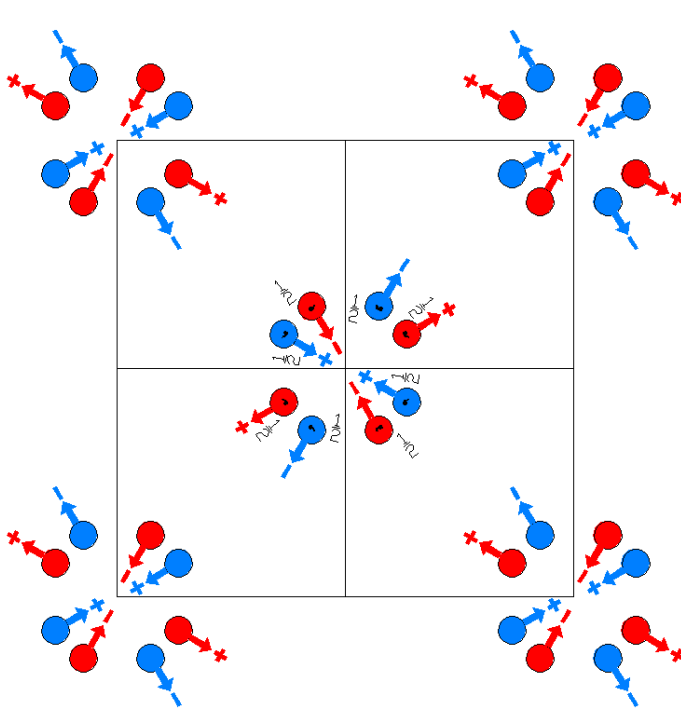
P4'/nn'c

126.4.1047

4'/mm'm

P4'/n2'/n'2/c

Tetragonal



Origin at 4'2'2/n, at  $-1/4, -1/4, -1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

**Symmetry Operations**

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                        | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)'      | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'               |
| (5) 2' 0,y,0<br>(2 <sub>y</sub> ' 0,0,0)'                     | (6) 2' x,0,0<br>(2 <sub>x</sub> ' 0,0,0)'                     | (7) 2 x,x,0<br>(2 <sub>xy</sub> ' 0,0,0)                               | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub> ' 0,0,0)           |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)        | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)   | (11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2)'  | (12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2)'           |
| (13) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (14) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (15) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (16) n (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

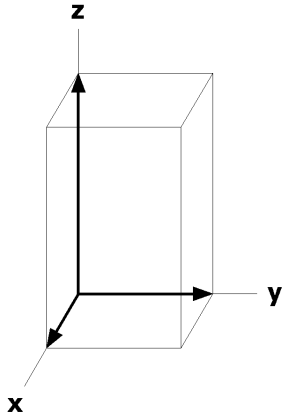
16	k	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x,z$ [ $v,\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]		
			(7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	j	.2'	$x,0,1/2$ [ $0,v,w$ ]	$\bar{x},0,1/2$ [ $0,\bar{v},w$ ]	$0,x,1/2$ [ $v,0,\bar{w}$ ]	$0,\bar{x},1/2$ [ $\bar{v},0,\bar{w}$ ]
			$\bar{x}+1/2,1/2,0$ [ $0,v,w$ ]	$x+1/2,1/2,0$ [ $0,\bar{v},w$ ]	$1/2,\bar{x}+1/2,0$ [ $v,0,\bar{w}$ ]	$1/2,x+1/2,0$ [ $\bar{v},0,\bar{w}$ ]
8	i	.2'	$x,0,0$ [ $0,v,w$ ]	$\bar{x},0,0$ [ $0,\bar{v},w$ ]	$0,x,0$ [ $v,0,\bar{w}$ ]	$0,\bar{x},0$ [ $\bar{v},0,\bar{w}$ ]
			$\bar{x}+1/2,1/2,1/2$ [ $0,v,w$ ]	$x+1/2,1/2,1/2$ [ $0,\bar{v},w$ ]	$1/2,\bar{x}+1/2,1/2$ [ $v,0,\bar{w}$ ]	$1/2,x+1/2,1/2$ [ $\bar{v},0,\bar{w}$ ]
8	h	..2	$x,x,0$ [ $u,u,0$ ]	$\bar{x},\bar{x},0$ [ $u,\bar{u},0$ ]	$\bar{x},x,0$ [ $u,\bar{u},0$ ]	$x,\bar{x},0$ [ $\bar{u},u,0$ ]
			$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $u,u,0$ ]	$x+1/2,x+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $\bar{u},u,0$ ]
8	g	2..	$1/2,0,z$ [ $0,0,w$ ]	$0,1/2,z$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}$ [ $0,0,w$ ]	$0,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]
			$0,1/2,\bar{z}+1/2$ [ $0,0,w$ ]	$1/2,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,z+1/2$ [ $0,0,w$ ]	$1/2,0,z+1/2$ [ $0,0,\bar{w}$ ]
8	f	$\bar{1}$	$1/4,1/4,1/4$ [ $u,v,w$ ]	$3/4,3/4,1/4$ [ $\bar{u},\bar{v},w$ ]	$3/4,1/4,1/4$ [ $v,\bar{u},\bar{w}$ ]	$1/4,3/4,1/4$ [ $\bar{v},u,\bar{w}$ ]
			$3/4,1/4,3/4$ [ $u,\bar{v},w$ ]	$1/4,3/4,3/4$ [ $\bar{u},v,w$ ]	$1/4,1/4,3/4$ [ $v,u,\bar{w}$ ]	$3/4,3/4,3/4$ [ $\bar{v},\bar{u},\bar{w}$ ]
4	e	4'..	$0,0,z$ [ $0,0,0$ ]	$0,0,\bar{z}$ [ $0,0,0$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,0$ ]	$1/2,1/2,z+1/2$ [ $0,0,0$ ]
4	d	$\bar{4}'..$	$1/2,0,1/4$ [ $0,0,0$ ]	$0,1/2,1/4$ [ $0,0,0$ ]	$1/2,0,3/4$ [ $0,0,0$ ]	$0,1/2,3/4$ [ $0,0,0$ ]
4	c	22'2'	$1/2,0,0$ [ $0,0,w$ ]	$0,1/2,0$ [ $0,0,\bar{w}$ ]	$0,1/2,1/2$ [ $0,0,w$ ]	$1/2,0,1/2$ [ $0,0,\bar{w}$ ]
2	b	4'2'2	$0,0,1/2$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]		
2	a	4'2'2	$0,0,0$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_4$ -4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $1/2, 0, z$

Along [1,0,0]  $c2'$ -mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $x, 0, 0$

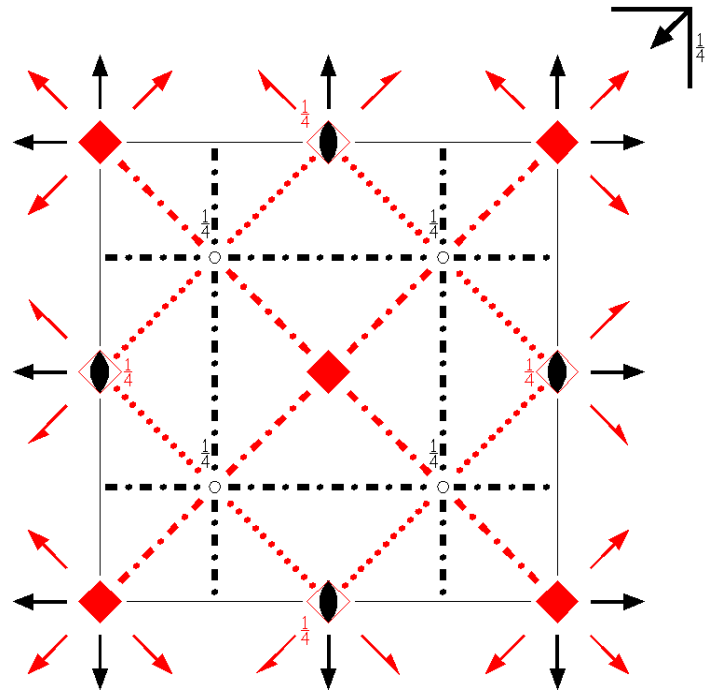
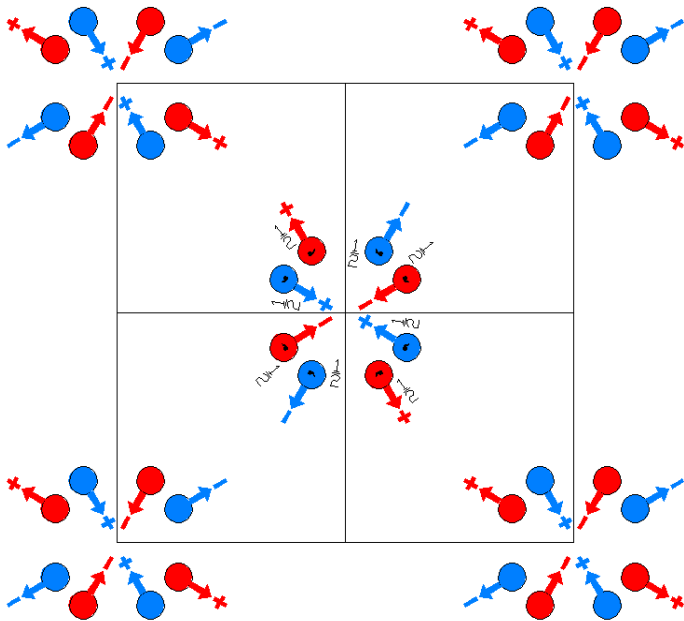
Along [1,1,0]  $p_{2a}$ -2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at  $x, x, 0$



P4'/nnc'  
126.5.1048

4'/mmm'  
P4'/n2/n2'/c'

Tetragonal



Origin at 4'22'/n', at  $-1/4, -1/4, -1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)'        | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'                  |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                      | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                      | (7) 2' x,x,0<br>(2 <sub>xy</sub> ' 0,0,0)'                               | (8) 2' x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub> ' 0,0,0)'            |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)      | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2)'    | (12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2)'              |
| (13) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (14) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (15) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)' | (16) n' (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub> ' 1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates															
Multiplicity,	Wyckoff letter,	Site Symmetry.																
16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]	(5) $\bar{x},y,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [v,u,w]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [u,v,w]	(10) x+1/2,y+1/2, $\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(11) y+1/2, $\bar{x}+1/2,\bar{z}+1/2$ [v, $\bar{u},\bar{w}$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]	(13) x+1/2, $\bar{y}+1/2,z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [u, $\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) y+1/2,x+1/2,z+1/2 [v,u,w]
8	j	.2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,1/2 [0, $\bar{u},0$ ]	0, $\bar{x},1/2$ [0,u,0]	$\bar{x}+1/2,1/2,0$ [u,0,0]	x+1/2,1/2,0 [ $\bar{u},0,0$ ]	1/2, $\bar{x}+1/2,0$ [0, $\bar{u},0$ ]	1/2,x+1/2,0 [0,u,0]								
8	i	.2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0, $\bar{u},0$ ]	0, $\bar{x},0$ [0,u,0]	$\bar{x}+1/2,1/2,1/2$ [u,0,0]	x+1/2,1/2,1/2 [ $\bar{u},0,0$ ]	1/2, $\bar{x}+1/2,1/2$ [0, $\bar{u},0$ ]	1/2,x+1/2,1/2 [0,u,0]								
8	h	..2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,0$ [u, $\bar{u},\bar{w}$ ]	x, $\bar{x},0$ [ $\bar{u},\bar{u},\bar{w}$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},u,w$ ]	x+1/2,x+1/2,1/2 [u, $\bar{u},w$ ]	x+1/2, $\bar{x}+1/2,1/2$ [u, $\bar{u},\bar{w}$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]								
8	g	2..	1/2,0,z [0,0,w]	0,1/2,z [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0,w]								
8	f	$\bar{1}$	1/4,1/4,1/4 [u,v,w]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	3/4,1/4,1/4 [v, $\bar{u},\bar{w}$ ]	1/4,3/4,1/4 [ $\bar{v},u,\bar{w}$ ]	3/4,1/4,3/4 [ $\bar{u},v,\bar{w}$ ]	1/4,3/4,3/4 [u, $\bar{v},\bar{w}$ ]	1/4,1/4,3/4 [ $\bar{v},\bar{u},w$ ]	3/4,3/4,3/4 [v,u,w]								
4	e	4'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,1/2,z+1/2 [0,0,0]												
4	d	$\bar{4}'..$	1/2,0,1/4 [0,0,0]	0,1/2,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]	0,1/2,3/4 [0,0,0]												
4	c	222.	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]												
2	b	4'22'	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]														
2	a	4'22'	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]														

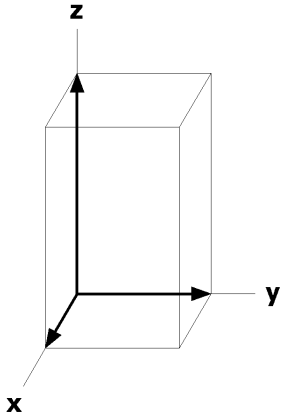
**Symmetry of Special Projections**

Along [0,0,1]  $p_4'$  4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $1/2, 0, z$

Along [1,0,0]  $c_2'$  2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x, 0, 0$

Along [1,1,0]  $p_2'$  mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at  $x, x, 0$

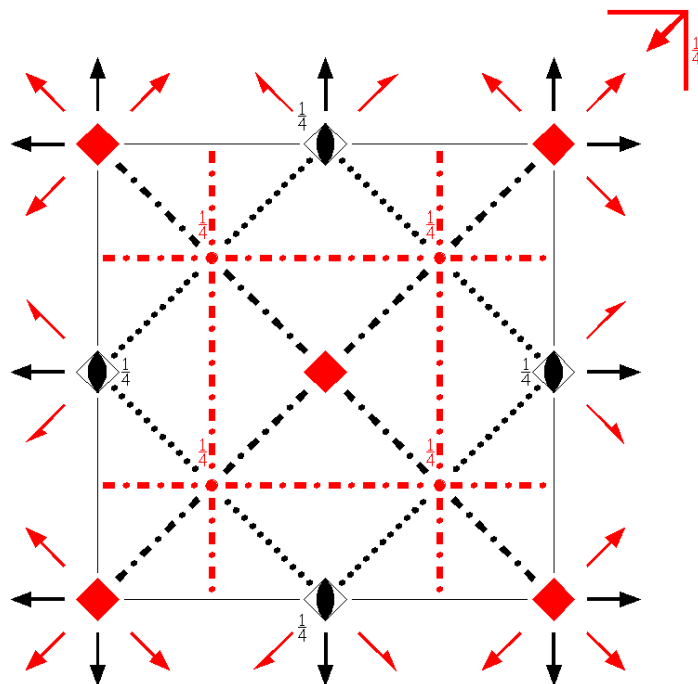
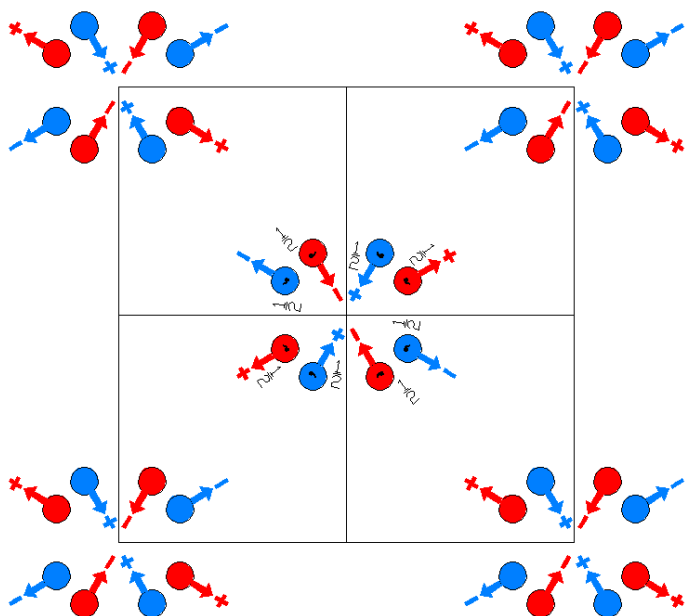




P4'/n'n'c  
126.6.1049

4'/m'm'm  
P4'/n'2/n'2'/c

Tetragonal



Origin at 4'22'n, at  $-1/4, -1/4, -1/4$  from  $\bar{1}$ '

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                         | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)'                                     | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'                                     |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                         | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                         | (7) 2' x,x,0<br>(2 <sub>xy</sub> ' 0,0,0)'  | (8) 2' x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub> ' 0,0,0)'                               |
| (9) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$ ' 1/2,1/2,1/2)'     | (10) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub> ' 1/2,1/2,1/2)' | (11) $\bar{4}$ <sup>+</sup> 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}$ <sub>z</sub> <sup>+</sup>  1/2,1/2,1/2) | (12) $\bar{4}$ <sup>-</sup> 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}$ <sub>z</sub> <sup>-</sup>  1/2,1/2,1/2) |
| (13) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub> ' 1/2,1/2,1/2)' | (14) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub> ' 1/2,1/2,1/2)' | (15) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub> ' 1/2,1/2,1/2)                               | (16) n (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

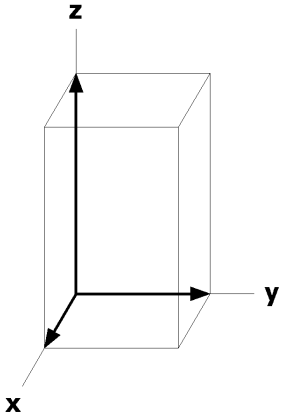
			Coordinates															
			Multiplicity, Wyckoff letter, Site Symmetry.															
16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]	(5) $\bar{x},y,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [v,u,w]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x+1/2,y+1/2, $\bar{z}+1/2$ [u, $\bar{v},\bar{w}$ ]	(11) y+1/2, $\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},u,w$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [v, $\bar{u},\bar{w}$ ]	(13) x+1/2, $\bar{y}+1/2,z+1/2$ [u, $\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [v,u, $\bar{w}$ ]	(16) y+1/2,x+1/2,z+1/2 [ $\bar{v},\bar{u},\bar{w}$ ]
8	j	.2.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,1/2 [0, $\bar{u},0$ ]	0, $\bar{x},1/2$ [0,u,0]	$\bar{x}+1/2,1/2,0$ [ $\bar{u},0,0$ ]	x+1/2,1/2,0 [u,0,0]	1/2, $\bar{x}+1/2,0$ [0,u,0]	1/2,x+1/2,0 [0, $\bar{u},0$ ]								
8	i	.2.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0, $\bar{u},0$ ]	0, $\bar{x},0$ [0,u,0]	$\bar{x}+1/2,1/2,1/2$ [ $\bar{u},0,0$ ]	x+1/2,1/2,1/2 [u,0,0]	1/2, $\bar{x}+1/2,1/2$ [0,u,0]	1/2,x+1/2,1/2 [0, $\bar{u},0$ ]								
8	h	..2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,0$ [u, $\bar{u},\bar{w}$ ]	x, $\bar{x},0$ [ $\bar{u},\bar{u},\bar{w}$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [u, $\bar{u},\bar{w}$ ]	x+1/2,x+1/2,1/2 [ $\bar{u},u,\bar{w}$ ]	x+1/2, $\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,1/2$ [u,u,w]								
8	g	2..	1/2,0,z [0,0,w]	0,1/2,z [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]								
8	f	$\bar{1}'$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]								
4	e	4'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,1/2,z+1/2 [0,0,0]												
4	d	$\bar{4}$ ..	1/2,0,1/4 [0,0,w]	0,1/2,1/4 [0,0, $\bar{w}$ ]	1/2,0,3/4 [0,0, $\bar{w}$ ]	0,1/2,3/4 [0,0,w]												
4	c	222.	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]												
2	b	4'22'	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]														
2	a	4'22'	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]														

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4'mm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $c2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,0,0$

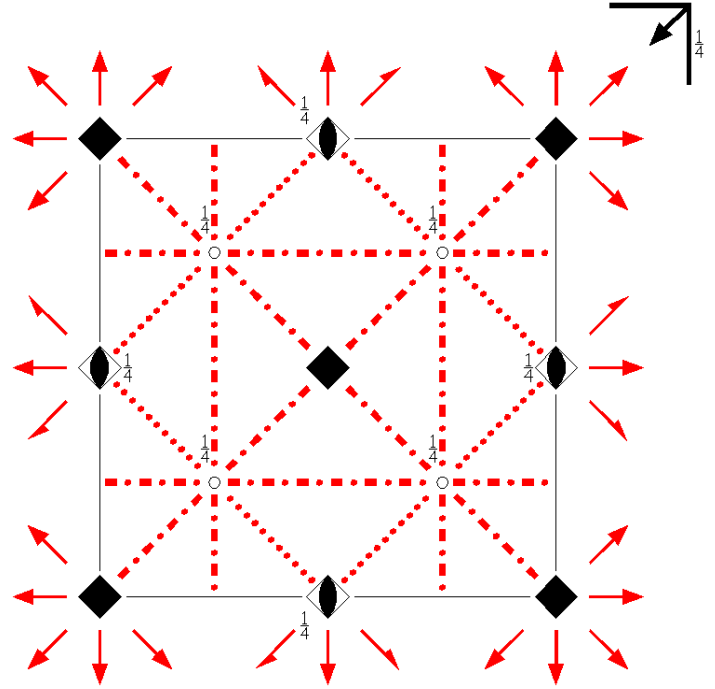
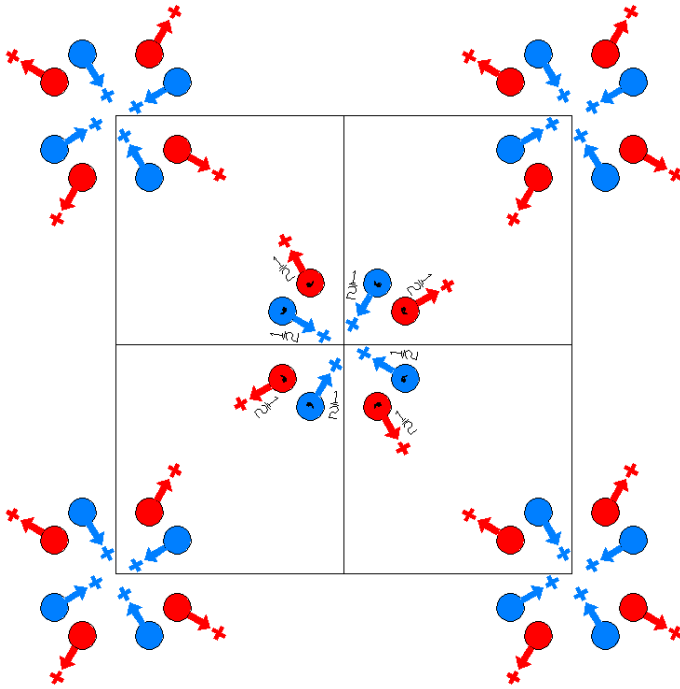
Along  $[1,1,0]$   $p_{2a}2mm$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at  $x-1/4, x+1/4, 0$



P4/nn'c'  
126.7.1050

4/mm'm'  
P4/n2'/n2'/c'

Tetragonal



Origin at  $42'2'/n'$ , at  $-1/4, -1/4, -1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |   |
|---|---|--|---|
| (1) $1$<br>( $1 0,0,0$ )                                      | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                            | (3) $4^+$ $0,0,z$<br>( $4_z 0,0,0$ )                                   | (4) $4^-$ $0,0,z$<br>( $4_z^{-1} 0,0,0$ )                                 |
| (5) $2'$ $0,y,0$<br>( $2_y 0,0,0$ )'                          | (6) $2'$ $x,0,0$<br>( $2_x 0,0,0$ )'                          | (7) $2'$ $x,x,0$<br>( $2_{xy} 0,0,0$ )'                                | (8) $2'$ $x,\bar{x},0$<br>( $2_{\bar{xy}} 0,0,0$ )'                       |
| (9) $\bar{1}$ $1/4,1/4,1/4$<br>( $\bar{1} 1/2,1/2,1/2$ )      | (10) $n$ ( $1/2,1/2,0$ ) $x,y,1/4$<br>( $m_z 1/2,1/2,1/2$ )   | (11) $\bar{4}^+$ $1/2,0,z; 1/2,0,1/4$<br>( $\bar{4}_z 1/2,1/2,1/2$ )   | (12) $\bar{4}^-$ $0,1/2,z; 0,1/2,1/4$<br>( $\bar{4}_z^{-1} 1/2,1/2,1/2$ ) |
| (13) $n'$ ( $1/2,0,1/2$ ) $x,1/4,z$<br>( $m_y 1/2,1/2,1/2$ )' | (14) $n'$ ( $0,1/2,1/2$ ) $1/4,y,z$<br>( $m_x 1/2,1/2,1/2$ )' | (15) $c'$ ( $0,0,1/2$ ) $x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,1/2$ )' | (16) $n'$ ( $1/2,1/2,1/2$ ) $x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,1/2$ )'    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

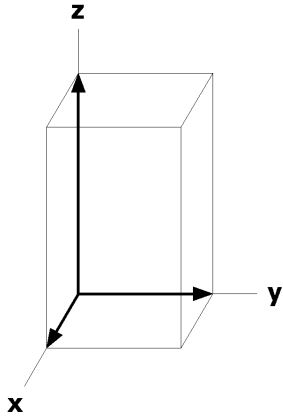
16	k	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]		
			(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [u,v,w]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},u,w$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [ $v,\bar{u},w$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $v,u,w$ ]		
8	j	.2'	$x,0,1/2$ [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	$0,x,1/2$ [ $\bar{v},0,w$ ]	$0,\bar{x},1/2$ [v,0,w]
			$\bar{x}+1/2,1/2,0$ [0,v,w]	$x+1/2,1/2,0$ [0, $\bar{v},w$ ]	$1/2,\bar{x}+1/2,0$ [ $\bar{v},0,w$ ]	$1/2,x+1/2,0$ [v,0,w]
8	i	.2'	$x,0,0$ [0,v,w]	$\bar{x},0,0$ [0, $\bar{v},w$ ]	$0,x,0$ [ $\bar{v},0,w$ ]	$0,\bar{x},0$ [v,0,w]
			$\bar{x}+1/2,1/2,1/2$ [0,v,w]	$x+1/2,1/2,1/2$ [0, $\bar{v},w$ ]	$1/2,\bar{x}+1/2,1/2$ [ $\bar{v},0,w$ ]	$1/2,x+1/2,1/2$ [v,0,w]
8	h	..2'	$x,x,0$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [ $u,\bar{u},w$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x},0$ [u,u,w]
			$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},u,w$ ]	$x+1/2,x+1/2,1/2$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,1/2$ [u,u,w]
8	g	2..	$1/2,0,z$ [0,0,w]	$0,1/2,z$ [0,0,w]	$1/2,0,\bar{z}$ [0,0,w]	$0,1/2,\bar{z}$ [0,0,w]
			$0,1/2,\bar{z}+1/2$ [0,0,w]	$1/2,0,\bar{z}+1/2$ [0,0,w]	$0,1/2,z+1/2$ [0,0,w]	$1/2,0,z+1/2$ [0,0,w]
8	f	$\bar{1}$	$1/4,1/4,1/4$ [u,v,w]	$3/4,3/4,1/4$ [ $\bar{u},\bar{v},w$ ]	$3/4,1/4,1/4$ [ $\bar{v},u,w$ ]	$1/4,3/4,1/4$ [v, $\bar{u},w$ ]
			$3/4,1/4,3/4$ [ $u,\bar{v},w$ ]	$1/4,3/4,3/4$ [ $\bar{u},v,w$ ]	$1/4,1/4,3/4$ [ $\bar{v},\bar{u},w$ ]	$3/4,3/4,3/4$ [v,u,w]
4	e	4..	$0,0,z$ [0,0,0]	$0,0,\bar{z}$ [0,0,0]	$1/2,1/2,\bar{z}+1/2$ [0,0,0]	$1/2,1/2,z+1/2$ [0,0,0]
4	d	$\bar{4}..$	$1/2,0,1/4$ [0,0,0]	$0,1/2,1/4$ [0,0,0]	$1/2,0,3/4$ [0,0,0]	$0,1/2,3/4$ [0,0,0]
4	c	22'2'	$1/2,0,0$ [0,0,0]	$0,1/2,0$ [0,0,0]	$0,1/2,1/2$ [0,0,0]	$1/2,0,1/2$ [0,0,0]
2	b	42'2'	$0,0,1/2$ [0,0,0]	$1/2,1/2,0$ [0,0,0]		
2	a	42'2'	$0,0,0$ [0,0,0]	$1/2,1/2,1/2$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p_4$  4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 0,0,z

Along [1,0,0]  $c2'$  mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at x,0,0

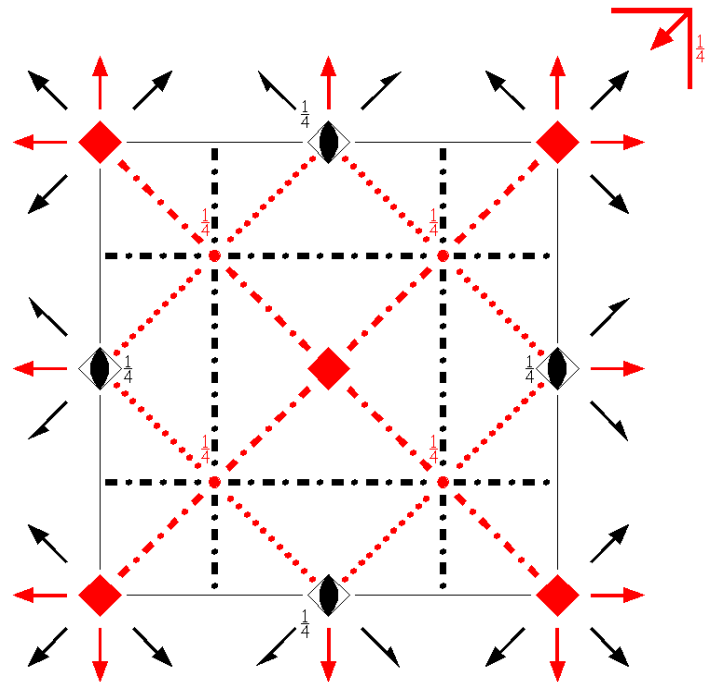
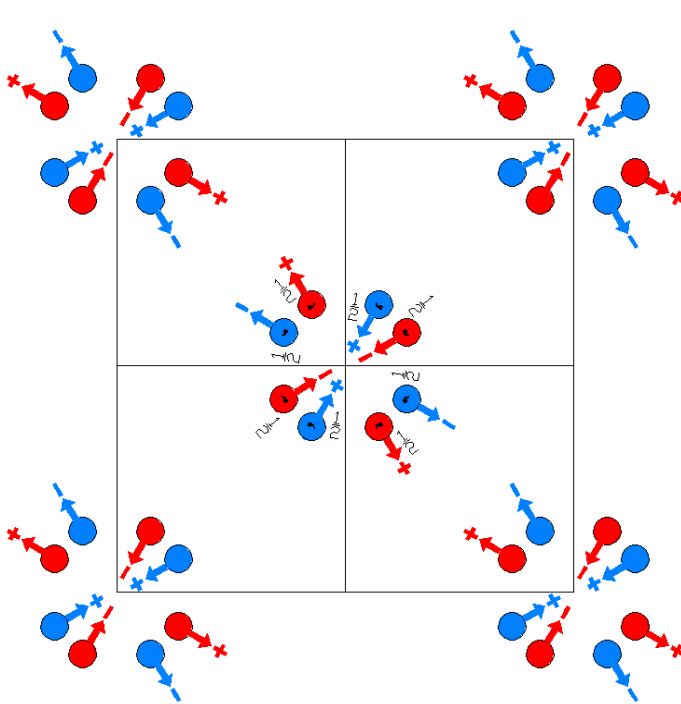
Along [1,1,0]  $p2m'$  m'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,x,0



P4'/n'nc'  
126.8.1051

4'/m'mm'  
P4'/n'2'/n2'/c'

Tetragonal



Origin at 4'2'2/n', at  $-1/4, -1/4, -1/4$  from  $\bar{1}$ '

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)           | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)'                                     | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'                                     |
| (5) 2' <sub>y</sub> 0,y,0<br>(2 <sub>y</sub> ' 0,0,0)'      | (6) 2' <sub>x</sub> x,0,0<br>(2 <sub>x</sub> ' 0,0,0)'        | (7) 2 <sub>xy</sub> x,x,0<br>(2 <sub>xy</sub>  0,0,0)   | (8) 2 <sub>xy</sub> x,x̄,0<br>(2 <sub>xy</sub> ' 0,0,0)   |
| (9) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$ ' 1/2,1/2,1/2)'  | (10) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (11) $\bar{4}$ <sup>+</sup> 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}$ <sub>z</sub> <sup>+</sup>  1/2,1/2,1/2) | (12) $\bar{4}$ <sup>-</sup> 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}$ <sub>z</sub> <sup>-</sup>  1/2,1/2,1/2) |
| (13) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (14) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)   | (15) c' (0,0,1/2) x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)'                                       | (16) n' (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub> ' 1/2,1/2,1/2)'                                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	k	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]	(5) $\bar{x},y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]	(11) $y+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},u,w$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $v,u,w$ ]
8	j	.2'	$x,0,1/2$ [ $0,v,w$ ]	$\bar{x},0,1/2$ [ $0,\bar{v},w$ ]	$0,x,1/2$ [ $v,0,\bar{w}$ ]	$0,\bar{x},1/2$ [ $\bar{v},0,\bar{w}$ ]	$\bar{x}+1/2,1/2,0$ [ $0,\bar{v},\bar{w}$ ]	$x+1/2,1/2,0$ [ $0,v,\bar{w}$ ]	$1/2,\bar{x}+1/2,0$ [ $\bar{v},0,w$ ]	$1/2,x+1/2,0$ [ $v,0,w$ ]								
8	i	.2'	$x,0,0$ [ $0,v,w$ ]	$\bar{x},0,0$ [ $0,\bar{v},w$ ]	$0,x,0$ [ $v,0,\bar{w}$ ]	$0,\bar{x},0$ [ $\bar{v},0,\bar{w}$ ]	$\bar{x}+1/2,1/2,1/2$ [ $0,\bar{v},\bar{w}$ ]	$x+1/2,1/2,1/2$ [ $0,v,\bar{w}$ ]	$1/2,\bar{x}+1/2,1/2$ [ $\bar{v},0,w$ ]	$1/2,x+1/2,1/2$ [ $v,0,w$ ]								
8	h	..2	$x,x,0$ [ $u,u,0$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [ $u,\bar{u},0$ ]	$x,\bar{x},0$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x+1/2,1/2$ [ $u,u,0$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $u,\bar{u},0$ ]								
8	g	2..	$1/2,0,z$ [ $0,0,w$ ]	$0,1/2,z$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}$ [ $0,0,w$ ]	$0,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}+1/2$ [ $0,0,w$ ]	$0,1/2,z+1/2$ [ $0,0,\bar{w}$ ]	$1/2,0,z+1/2$ [ $0,0,w$ ]								
8	f	$\bar{1}'$	$1/4,1/4,1/4$ [ $0,0,0$ ]	$3/4,3/4,1/4$ [ $0,0,0$ ]	$3/4,1/4,1/4$ [ $0,0,0$ ]	$1/4,3/4,1/4$ [ $0,0,0$ ]	$3/4,1/4,3/4$ [ $0,0,0$ ]	$1/4,3/4,3/4$ [ $0,0,0$ ]	$1/4,1/4,3/4$ [ $0,0,0$ ]	$3/4,3/4,3/4$ [ $0,0,0$ ]								
4	e	4'..	$0,0,z$ [ $0,0,0$ ]	$0,0,\bar{z}$ [ $0,0,0$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,0$ ]	$1/2,1/2,z+1/2$ [ $0,0,0$ ]												
4	d	$\bar{4}$ ..	$1/2,0,1/4$ [ $0,0,w$ ]	$0,1/2,1/4$ [ $0,0,\bar{w}$ ]	$1/2,0,3/4$ [ $0,0,w$ ]	$0,1/2,3/4$ [ $0,0,\bar{w}$ ]												
4	c	22'2'.	$1/2,0,0$ [ $0,0,w$ ]	$0,1/2,0$ [ $0,0,\bar{w}$ ]	$0,1/2,1/2$ [ $0,0,\bar{w}$ ]	$1/2,0,1/2$ [ $0,0,w$ ]												
2	b	4'2'2	$0,0,1/2$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]														
2	a	4'2'2	$0,0,0$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]														

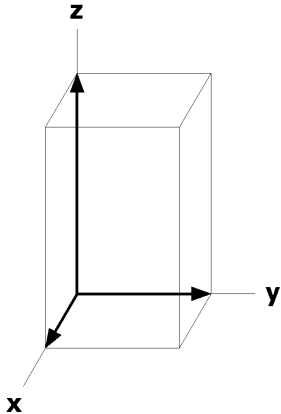


**Symmetry of Special Projections**

Along [0,0,1]  $p4'm'm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at x,0,0

Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,x,0



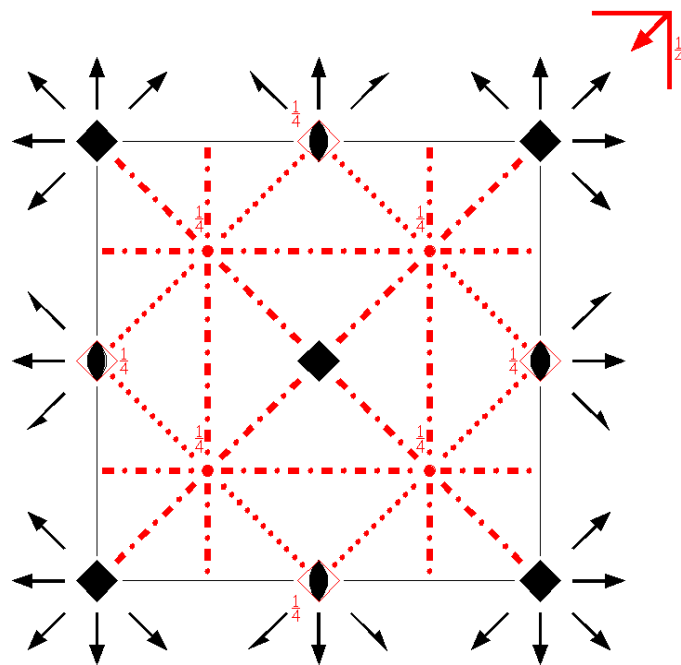
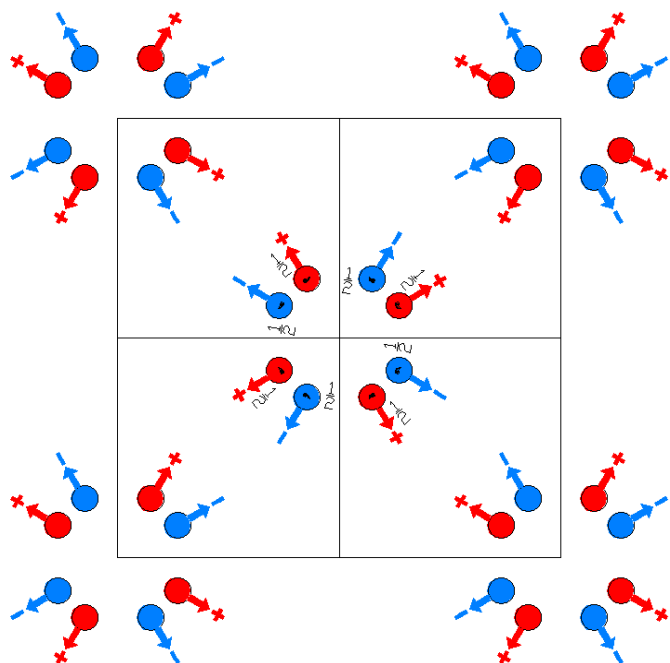
P4/n'n'c'

126.9.1052

4/m'm'm'

P4/n'2/n'2/c'

Tetragonal



Origin at  $422/n'$ , at  $-1/4, -1/4, -1/4$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                        | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                      | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)                 |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                        | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                        | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                  | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)              |
| (9) $\bar{1}'$ 1/4,1/4,1/4<br>( $\bar{1}'$  1/2,1/2,1/2)'     | (10) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2)'    | (12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2)'             |
| (13) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (14) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (15) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)' | (16) n' (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

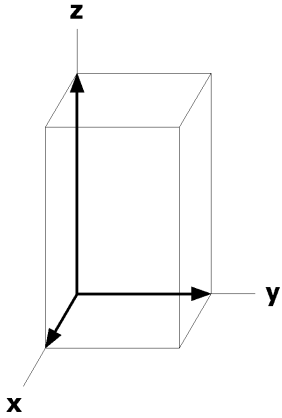
			Coordinates															
Multiplicity, Wyckoff letter, Site Symmetry.																		
16	k	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]	(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]	(11) $y+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]	(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $v,u,w$ ]
8	j	.2.	$x,0,1/2$ [ $u,0,0$ ]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	$0,x,1/2$ [ $0,u,0$ ]	$0,\bar{x},1/2$ [ $0,\bar{u},0$ ]	$\bar{x}+1/2,1/2,0$ [ $\bar{u},0,0$ ]	$x+1/2,1/2,0$ [ $u,0,0$ ]	$1/2,\bar{x}+1/2,0$ [ $0,\bar{u},0$ ]	$1/2,x+1/2,0$ [ $0,u,0$ ]								
8	i	.2.	$x,0,0$ [ $u,0,0$ ]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	$0,x,0$ [ $0,u,0$ ]	$0,\bar{x},0$ [ $0,\bar{u},0$ ]	$\bar{x}+1/2,1/2,1/2$ [ $\bar{u},0,0$ ]	$x+1/2,1/2,1/2$ [ $u,0,0$ ]	$1/2,\bar{x}+1/2,1/2$ [ $0,\bar{u},0$ ]	$1/2,x+1/2,1/2$ [ $0,u,0$ ]								
8	h	..2	$x,x,0$ [ $u,u,0$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]	$x,\bar{x},0$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x+1/2,1/2$ [ $u,u,0$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $\bar{u},u,0$ ]								
8	g	2..	$1/2,0,z$ [ $0,0,w$ ]	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,z+1/2$ [ $0,0,w$ ]	$1/2,0,z+1/2$ [ $0,0,w$ ]								
8	f	$\bar{1}'$	$1/4,1/4,1/4$ [ $0,0,0$ ]	$3/4,3/4,1/4$ [ $0,0,0$ ]	$3/4,1/4,1/4$ [ $0,0,0$ ]	$1/4,3/4,1/4$ [ $0,0,0$ ]	$3/4,1/4,3/4$ [ $0,0,0$ ]	$1/4,3/4,3/4$ [ $0,0,0$ ]	$1/4,1/4,3/4$ [ $0,0,0$ ]	$3/4,3/4,3/4$ [ $0,0,0$ ]								
4	e	4..	$0,0,z$ [ $0,0,w$ ]	$0,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$1/2,1/2,z+1/2$ [ $0,0,w$ ]												
4	d	$\bar{4}'..$	$1/2,0,1/4$ [ $0,0,0$ ]	$0,1/2,1/4$ [ $0,0,0$ ]	$1/2,0,3/4$ [ $0,0,0$ ]	$0,1/2,3/4$ [ $0,0,0$ ]												
4	c	222.	$1/2,0,0$ [ $0,0,0$ ]	$0,1/2,0$ [ $0,0,0$ ]	$0,1/2,1/2$ [ $0,0,0$ ]	$1/2,0,1/2$ [ $0,0,0$ ]												
2	b	422	$0,0,1/2$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]														
2	a	422	$0,0,0$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]														

**Symmetry of Special Projections**

Along [0,0,1]  $p4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 0,0,z

Along [1,0,0]  $c2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,0,0

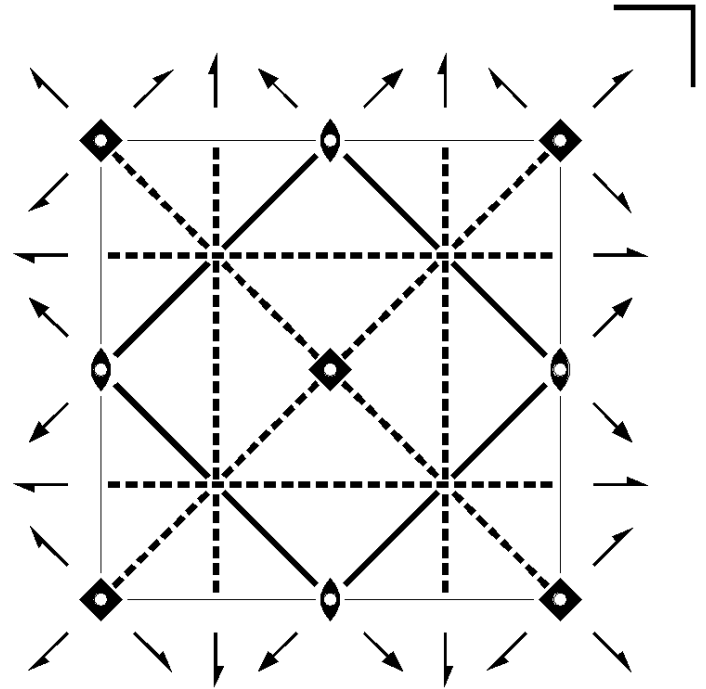
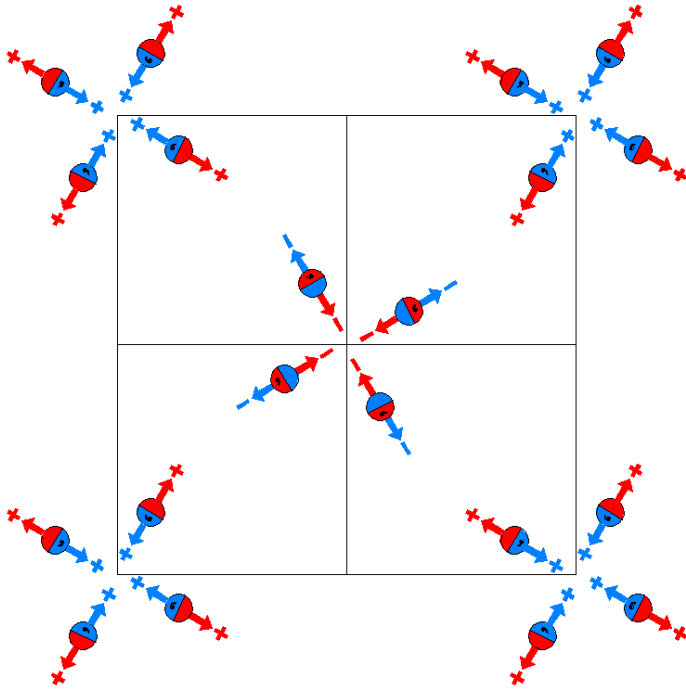
Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,x,0



P4/mbm  
127.1.1053

4/mmm  
P4/m2<sub>1</sub>/b2/m

Tetragonal



Origin at center ( 4/m ) at 4/m12<sub>1</sub>/g

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)        | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)            |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)  | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)  | (7) 2 (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)    | (8) 2 x, $\bar{x}$ +1/2,0<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,0) |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)              | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)                 | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)   | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                     |
| (13) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (14) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (15) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0) | (16) g (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

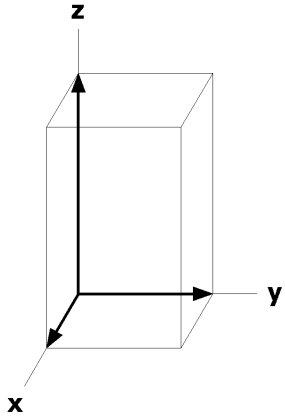
			Coordinates								
			Multiplicity, Wyckoff letter, Site Symmetry.								
16	I	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y},x,z$	$[\bar{v},u,w]$	(4)	$y,\bar{x},z$	$[v,\bar{u},w]$
(5)	$\bar{x}+1/2,y+1/2,\bar{z}$	$[\bar{u},v,\bar{w}]$	(6)	$x+1/2,\bar{y}+1/2,\bar{z}$	$[u,\bar{v},\bar{w}]$	(7)	$y+1/2,x+1/2,\bar{z}$	$[v,u,\bar{w}]$	(8)	$\bar{y}+1/2,\bar{x}+1/2,\bar{z}$	$[\bar{v},\bar{u},\bar{w}]$
(9)	$\bar{x},\bar{y},\bar{z}$	$[u,v,w]$	(10)	$x,y,\bar{z}$	$[\bar{u},\bar{v},w]$	(11)	$y,\bar{x},\bar{z}$	$[\bar{v},u,w]$	(12)	$\bar{y},x,\bar{z}$	$[v,\bar{u},w]$
(13)	$x+1/2,\bar{y}+1/2,z$	$[\bar{u},v,\bar{w}]$	(14)	$\bar{x}+1/2,y+1/2,z$	$[u,\bar{v},\bar{w}]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[v,u,\bar{w}]$	(16)	$y+1/2,x+1/2,z$	$[\bar{v},\bar{u},\bar{w}]$
8	k	..m	$x,x+1/2,z$	$[\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,z$	$[u,\bar{u},0]$	$\bar{x}+1/2,x,z$	$[\bar{u},\bar{u},0]$	$x+1/2,\bar{x},z$	$[u,u,0]$	
			$\bar{x}+1/2,x,\bar{z}$	$[u,u,0]$	$x+1/2,\bar{x},\bar{z}$	$[u,\bar{u},0]$	$x,x+1/2,\bar{z}$	$[u,\bar{u},0]$	$\bar{x},\bar{x}+1/2,\bar{z}$	$[\bar{u},\bar{u},0]$	
8	j	m..	$x,y,1/2$	$[0,0,w]$	$\bar{x},\bar{y},1/2$	$[0,0,w]$	$\bar{y},x,1/2$	$[0,0,w]$	$y,\bar{x},1/2$	$[0,0,w]$	
			$\bar{x}+1/2,y+1/2,1/2$	$[0,0,\bar{w}]$	$x+1/2,\bar{y}+1/2,1/2$	$[0,0,\bar{w}]$	$y+1/2,x+1/2,1/2$	$[0,0,\bar{w}]$	$\bar{y}+1/2,\bar{x}+1/2,1/2$	$[0,0,\bar{w}]$	
8	i	m..	$x,y,0$	$[0,0,w]$	$\bar{x},\bar{y},0$	$[0,0,w]$	$\bar{y},x,0$	$[0,0,w]$	$y,\bar{x},0$	$[0,0,w]$	
			$\bar{x}+1/2,y+1/2,0$	$[0,0,\bar{w}]$	$x+1/2,\bar{y}+1/2,0$	$[0,0,\bar{w}]$	$y+1/2,x+1/2,0$	$[0,0,\bar{w}]$	$\bar{y}+1/2,\bar{x}+1/2,0$	$[0,0,\bar{w}]$	
4	h	m.2m	$x,x+1/2,1/2$	$[0,0,0]$	$\bar{x},\bar{x}+1/2,1/2$	$[0,0,0]$	$\bar{x}+1/2,x,1/2$	$[0,0,0]$	$x+1/2,\bar{x},1/2$	$[0,0,0]$	
4	g	m.2m	$x,x+1/2,0$	$[0,0,0]$	$\bar{x},\bar{x}+1/2,0$	$[0,0,0]$	$\bar{x}+1/2,x,0$	$[0,0,0]$	$x+1/2,\bar{x},0$	$[0,0,0]$	
4	f	2.mm	$0,1/2,z$	$[0,0,0]$	$1/2,0,z$	$[0,0,0]$	$1/2,0,\bar{z}$	$[0,0,0]$	$0,1/2,\bar{z}$	$[0,0,0]$	
4	e	4..	$0,0,z$	$[0,0,w]$	$1/2,1/2,\bar{z}$	$[0,0,\bar{w}]$	$0,0,\bar{z}$	$[0,0,w]$	$1/2,1/2,z$	$[0,0,\bar{w}]$	
2	d	m.mm	$0,1/2,0$	$[0,0,0]$	$1/2,0,0$	$[0,0,0]$					
2	c	m.mm	$0,1/2,1/2$	$[0,0,0]$	$1/2,0,1/2$	$[0,0,0]$					
2	b	4/m..	$0,0,1/2$	$[0,0,w]$	$1/2,1/2,1/2$	$[0,0,\bar{w}]$					
2	a	4/m..	$0,0,0$	$[0,0,w]$	$1/2,1/2,0$	$[0,0,\bar{w}]$					

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4gm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a^*}2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,1/4,0$

Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$



P4/mbm1'

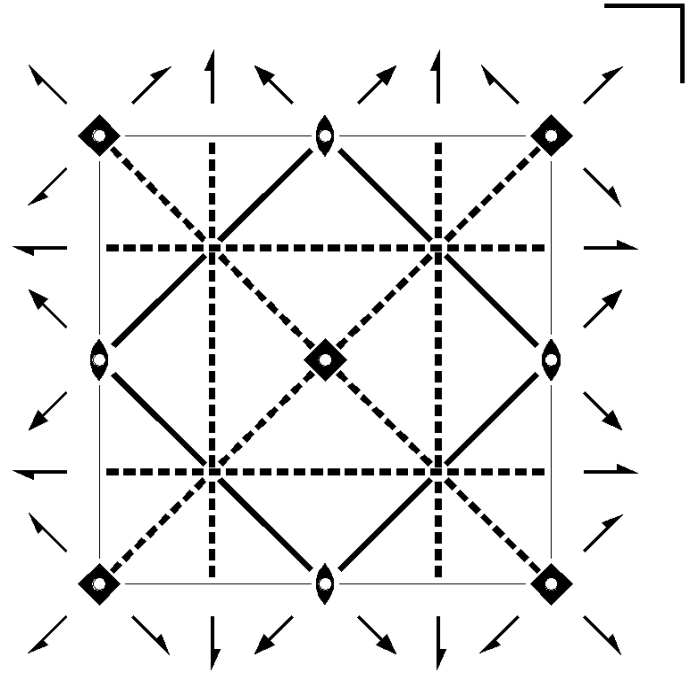
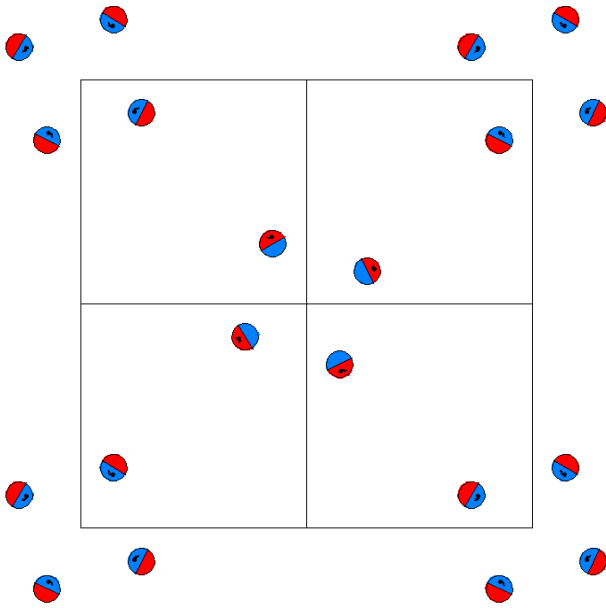
127.2.1054

4/mmm1'

P4/m2<sub>1</sub>/b2/m1'

Tetragonal

1'



Origin at center ( 4/m1' ) at 4/m12<sub>1</sub>/g1'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

Symmetry Operations

For 1 + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)        | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)            |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)  | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)  | (7) 2 (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)    | (8) 2 x, $\bar{x}$ +1/2,0<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,0) |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)              | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)                 | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)   | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                     |
| (13) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (14) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (15) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0) | (16) g (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)  |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)'	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(5) 2' (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>  1/2,1/2,0)'	(6) 2' (1/2,0,0) x,1/4,0 (2 <sub>x</sub>  1/2,1/2,0)'	(7) 2' (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>  1/2,1/2,0)'	(8) 2' x, $\bar{x}$ +1/2,0 (2 <sub>xy</sub> <sup>-</sup>  1/2,1/2,0)'
(9) $\bar{1}$ ' 0,0,0 ( $\bar{1}$  0,0,0)'	(10) m' x,y,0 (m <sub>z</sub>  0,0,0)'	(11) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'	(12) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z^{-1}$  0,0,0)'
(13) a' (1/2,0,0) x,1/4,z (m <sub>y</sub>  1/2,1/2,0)'	(14) b' (0,1/2,0) 1/4,y,z (m <sub>x</sub>  1/2,1/2,0)'	(15) m' x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,0)'	(16) g' (1/2,1/2,0) x,x,z (m <sub>xy</sub> <sup>-</sup>  1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

**Positions**

		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.		1 +		1' +	
16	l 11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z$ [0,0,0]	(4) y, $\bar{x},z$ [0,0,0]
		(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [0,0,0]	(6) x+1/2, $\bar{y}+1/2,\bar{z}$ [0,0,0]	(7) y+1/2,x+1/2, $\bar{z}$ [0,0,0]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}$ [0,0,0]
		(9) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(10) x,y, $\bar{z}$ [0,0,0]	(11) y, $\bar{x},\bar{z}$ [0,0,0]	(12) $\bar{y},x,\bar{z}$ [0,0,0]
		(13) x+1/2, $\bar{y}+1/2,z$ [0,0,0]	(14) $\bar{x}+1/2,y+1/2,z$ [0,0,0]	(15) $\bar{y}+1/2,\bar{x}+1/2,z$ [0,0,0]	(16) y+1/2,x+1/2,z [0,0,0]
8	k ..m1'	x,x+1/2,z [0,0,0]	$\bar{x},\bar{x}+1/2,z$ [0,0,0]	$\bar{x}+1/2,x,z$ [0,0,0]	x+1/2, $\bar{x},z$ [0,0,0]
		$\bar{x}+1/2,x,\bar{z}$ [0,0,0]	x+1/2, $\bar{x},\bar{z}$ [0,0,0]	x,x+1/2, $\bar{z}$ [0,0,0]	$\bar{x},\bar{x}+1/2,\bar{z}$ [0,0,0]
8	j m..1'	x,y,1/2 [0,0,0]	$\bar{x},\bar{y},1/2$ [0,0,0]	$\bar{y},x,1/2$ [0,0,0]	y, $\bar{x},1/2$ [0,0,0]
		$\bar{x}+1/2,y+1/2,1/2$ [0,0,0]	x+1/2, $\bar{y}+1/2,1/2$ [0,0,0]	y+1/2,x+1/2,1/2 [0,0,0]	$\bar{y}+1/2,\bar{x}+1/2,1/2$ [0,0,0]
8	i m..1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{y},x,0$ [0,0,0]	y, $\bar{x},0$ [0,0,0]
		$\bar{x}+1/2,y+1/2,0$ [0,0,0]	x+1/2, $\bar{y}+1/2,0$ [0,0,0]	y+1/2,x+1/2,0 [0,0,0]	$\bar{y}+1/2,\bar{x}+1/2,0$ [0,0,0]
4	h m.2m1'	x,x+1/2,1/2 [0,0,0]	$\bar{x},\bar{x}+1/2,1/2$ [0,0,0]	$\bar{x}+1/2,x,1/2$ [0,0,0]	x+1/2, $\bar{x},1/2$ [0,0,0]
4	g m.2m1'	x,x+1/2,0 [0,0,0]	$\bar{x},\bar{x}+1/2,0$ [0,0,0]	$\bar{x}+1/2,x,0$ [0,0,0]	x+1/2, $\bar{x},0$ [0,0,0]
4	f 2.mm1'	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]
4	e 4..1'	0,0,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2,z [0,0,0]
2	d m.mm1'	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
2	c m.mm1'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		



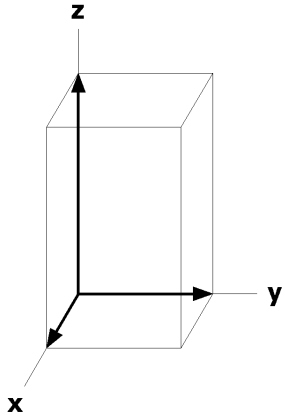
2	b	4/m..1'	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]
2	a	4/m..1'	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

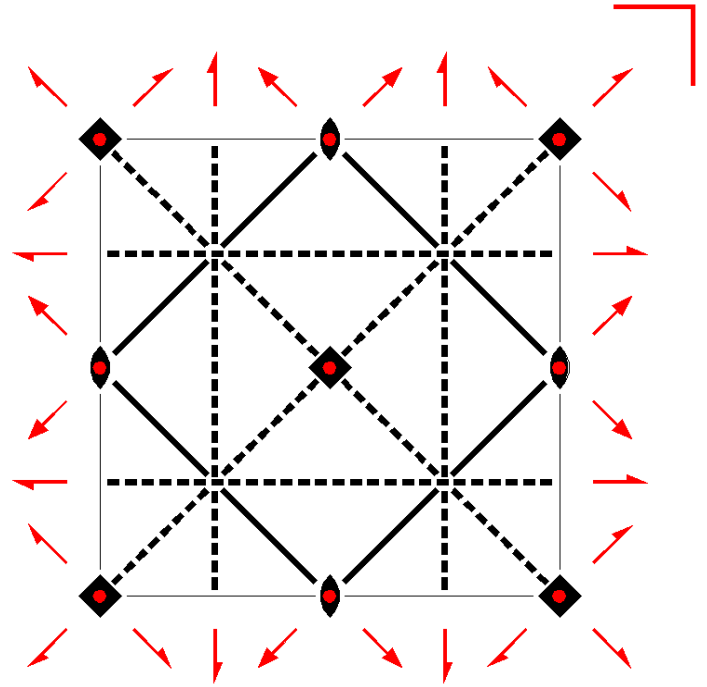
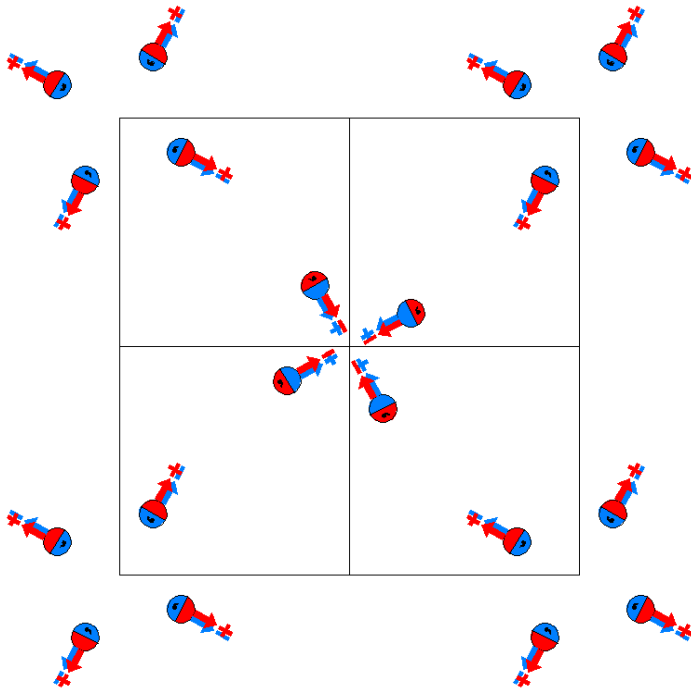
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4/m'bm  
127.3.1055

4/m'mm  
P4/m'2<sub>1</sub>'/b2'/m

Tetragonal



Origin at center ( 4/m' ) at 4/m'12<sub>1</sub>'/g

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)                   | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                     | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (5) 2' <sub>y</sub> (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (6) 2' <sub>x</sub> (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' | (7) 2' <sub>xy</sub> (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)' | (8) 2' <sub>xy</sub> x,x+1/2,0<br>(2 <sub>xy</sub>  1/2,1/2,0)'   |
| (9) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$ ' 0,0,0)'                        | (10) m' <sub>z</sub> x,y,0<br>(m' <sub>z</sub>  0,0,0)'               | (11) $\bar{4}^+$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^+$ ' 0,0,0)'            | (12) $\bar{4}^-$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^-$ ' 0,0,0)'      |
| (13) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)               | (14) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)               | (15) m (x+1/2,x,z)<br>(m <sub>xy</sub>  1/2,1/2,0)                      | (16) g (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

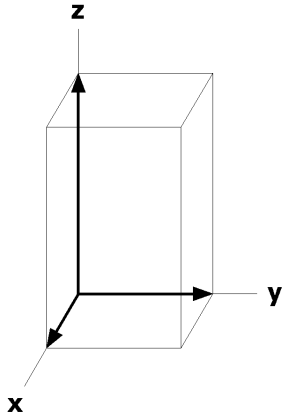
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates								
16	I	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y},x,z$	$[\bar{v},u,w]$	(4)	$y,\bar{x},z$	$[v,\bar{u},w]$
(5)	$\bar{x}+1/2,y+1/2,\bar{z}$	$[u,\bar{v},w]$	(6)	$x+1/2,\bar{y}+1/2,\bar{z}$	$[\bar{u},v,w]$	(7)	$y+1/2,x+1/2,\bar{z}$	$[\bar{v},\bar{u},w]$	(8)	$\bar{y}+1/2,\bar{x}+1/2,\bar{z}$	$[v,u,w]$
(9)	$\bar{x},\bar{y},\bar{z}$	$[\bar{u},\bar{v},\bar{w}]$	(10)	$x,y,\bar{z}$	$[u,v,\bar{w}]$	(11)	$y,\bar{x},\bar{z}$	$[v,\bar{u},\bar{w}]$	(12)	$\bar{y},x,\bar{z}$	$[\bar{v},u,\bar{w}]$
(13)	$x+1/2,\bar{y}+1/2,z$	$[\bar{u},v,\bar{w}]$	(14)	$\bar{x}+1/2,y+1/2,z$	$[u,\bar{v},\bar{w}]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[v,u,\bar{w}]$	(16)	$y+1/2,x+1/2,z$	$[\bar{v},\bar{u},\bar{w}]$
8	k	..m	$x,x+1/2,z$	$[\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,z$	$[u,\bar{u},0]$	$\bar{x}+1/2,x,z$	$[\bar{u},\bar{u},0]$	$x+1/2,\bar{x},z$	$[u,u,0]$	
			$\bar{x}+1/2,x,\bar{z}$	$[\bar{u},\bar{u},0]$	$x+1/2,\bar{x},\bar{z}$	$[u,u,0]$	$x,x+1/2,\bar{z}$	$[\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,\bar{z}$	$[u,\bar{u},0]$	
8	j	m'..	$x,y,1/2$	$[u,v,0]$	$\bar{x},\bar{y},1/2$	$[\bar{u},\bar{v},0]$	$\bar{y},x,1/2$	$[\bar{v},u,0]$	$y,\bar{x},1/2$	$[v,\bar{u},0]$	
			$\bar{x}+1/2,y+1/2,1/2$	$[u,\bar{v},0]$	$x+1/2,\bar{y}+1/2,1/2$	$[\bar{u},v,0]$	$y+1/2,x+1/2,1/2$	$[\bar{v},\bar{u},0]$	$\bar{y}+1/2,\bar{x}+1/2,1/2$	$[v,u,0]$	
8	i	m'..	$x,y,0$	$[u,v,0]$	$\bar{x},\bar{y},0$	$[\bar{u},\bar{v},0]$	$\bar{y},x,0$	$[\bar{v},u,0]$	$y,\bar{x},0$	$[v,\bar{u},0]$	
			$\bar{x}+1/2,y+1/2,0$	$[u,\bar{v},0]$	$x+1/2,\bar{y}+1/2,0$	$[\bar{u},v,0]$	$y+1/2,x+1/2,0$	$[\bar{v},\bar{u},0]$	$\bar{y}+1/2,\bar{x}+1/2,0$	$[v,u,0]$	
4	h	m'.2'm	$x,x+1/2,1/2$	$[\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,1/2$	$[u,\bar{u},0]$	$\bar{x}+1/2,x,1/2$	$[\bar{u},\bar{u},0]$	$x+1/2,\bar{x},1/2$	$[u,u,0]$	
4	g	m'.2'm	$x,x+1/2,0$	$[\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,0$	$[u,\bar{u},0]$	$\bar{x}+1/2,x,0$	$[\bar{u},\bar{u},0]$	$x+1/2,\bar{x},0$	$[u,u,0]$	
4	f	2.mm	$0,1/2,z$	$[0,0,0]$	$1/2,0,z$	$[0,0,0]$	$1/2,0,\bar{z}$	$[0,0,0]$	$0,1/2,\bar{z}$	$[0,0,0]$	
4	e	4..	$0,0,z$	$[0,0,w]$	$1/2,1/2,\bar{z}$	$[0,0,w]$	$0,0,\bar{z}$	$[0,0,\bar{w}]$	$1/2,1/2,z$	$[0,0,\bar{w}]$	
2	d	m'.mm	$0,1/2,0$	$[0,0,0]$	$1/2,0,0$	$[0,0,0]$					
2	c	m'.mm	$0,1/2,1/2$	$[0,0,0]$	$1/2,0,1/2$	$[0,0,0]$					
2	b	4/m'..	$0,0,1/2$	$[0,0,0]$	$1/2,1/2,1/2$	$[0,0,0]$					
2	a	4/m'..	$0,0,0$	$[0,0,0]$	$1/2,1/2,0$	$[0,0,0]$					

### Symmetry of Special Projections

Along  $[0,0,1]$  p4gm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p<sub>2a</sub>'2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

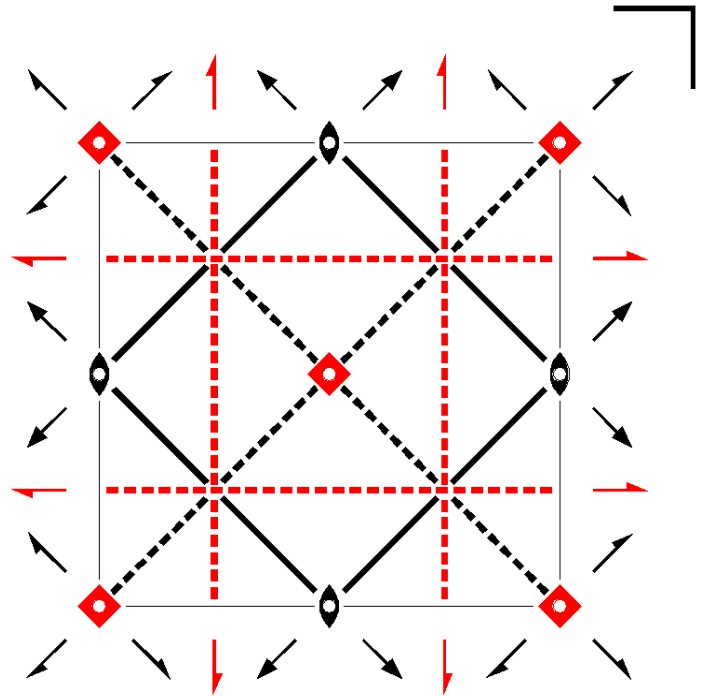
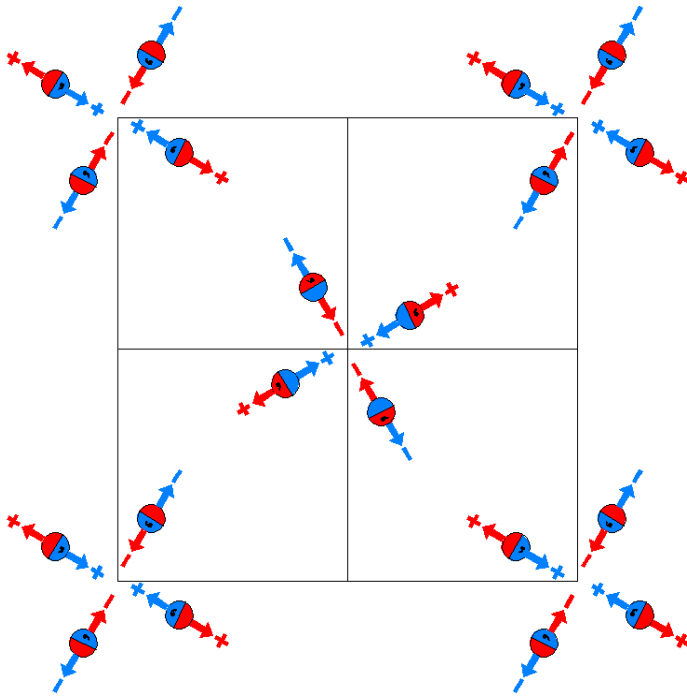
Along  $[1,1,0]$  p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$



P4'/mb'm  
127.4.1056

4'/mm'm  
P4'/m2<sub>1</sub>'/b2'/m

Tetragonal



Origin at center ( $4'/m$ ) at  $4'/m\bar{2}_1/g$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'       | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'           |
| (5) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)'  | (6) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)'  | (7) 2 (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)    | (8) 2 x, $\bar{x}$ +1/2,0<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,0) |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)                | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)                   | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'  | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                    |
| (13) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (14) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' | (15) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0) | (16) g (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

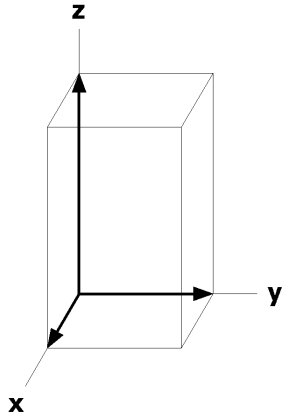
			Coordinates								
			Multiplicity, Wyckoff letter, Site Symmetry.								
16	I	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y},x,z$	$[v,\bar{u},\bar{w}]$	(4)	$y,\bar{x},z$	$[\bar{v},u,\bar{w}]$
(5)	$\bar{x}+1/2,y+1/2,\bar{z}$	$[u,\bar{v},w]$	(6)	$x+1/2,\bar{y}+1/2,\bar{z}$	$[\bar{u},v,w]$	(7)	$y+1/2,x+1/2,\bar{z}$	$[v,u,\bar{w}]$	(8)	$\bar{y}+1/2,\bar{x}+1/2,\bar{z}$	$[\bar{v},\bar{u},\bar{w}]$
(9)	$\bar{x},\bar{y},\bar{z}$	$[u,v,w]$	(10)	$x,y,\bar{z}$	$[\bar{u},\bar{v},w]$	(11)	$y,\bar{x},\bar{z}$	$[v,\bar{u},\bar{w}]$	(12)	$\bar{y},x,\bar{z}$	$[\bar{v},u,\bar{w}]$
(13)	$x+1/2,\bar{y}+1/2,z$	$[u,\bar{v},w]$	(14)	$\bar{x}+1/2,y+1/2,z$	$[\bar{u},v,w]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[v,u,\bar{w}]$	(16)	$y+1/2,x+1/2,z$	$[\bar{v},\bar{u},\bar{w}]$
8	k	..m	$x,x+1/2,z$	$[\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,z$	$[u,\bar{u},0]$	$\bar{x}+1/2,x,z$	$[u,u,0]$	$x+1/2,\bar{x},z$	$[\bar{u},\bar{u},0]$	
			$\bar{x}+1/2,x,\bar{z}$	$[\bar{u},\bar{u},0]$	$x+1/2,\bar{x},\bar{z}$	$[u,u,0]$	$x,x+1/2,\bar{z}$	$[u,\bar{u},0]$	$\bar{x},\bar{x}+1/2,\bar{z}$	$[\bar{u},u,0]$	
8	j	m..	$x,y,1/2$	$[0,0,w]$	$\bar{x},\bar{y},1/2$	$[0,0,w]$	$\bar{y},x,1/2$	$[0,0,\bar{w}]$	$y,\bar{x},1/2$	$[0,0,\bar{w}]$	
			$\bar{x}+1/2,y+1/2,1/2$	$[0,0,w]$	$x+1/2,\bar{y}+1/2,1/2$	$[0,0,w]$	$y+1/2,x+1/2,1/2$	$[0,0,\bar{w}]$	$\bar{y}+1/2,\bar{x}+1/2,1/2$	$[0,0,\bar{w}]$	
8	i	m..	$x,y,0$	$[0,0,w]$	$\bar{x},\bar{y},0$	$[0,0,w]$	$\bar{y},x,0$	$[0,0,\bar{w}]$	$y,\bar{x},0$	$[0,0,\bar{w}]$	
			$\bar{x}+1/2,y+1/2,0$	$[0,0,w]$	$x+1/2,\bar{y}+1/2,0$	$[0,0,w]$	$y+1/2,x+1/2,0$	$[0,0,\bar{w}]$	$\bar{y}+1/2,\bar{x}+1/2,0$	$[0,0,\bar{w}]$	
4	h	m.2m	$x,x+1/2,1/2$	$[0,0,0]$	$\bar{x},\bar{x}+1/2,1/2$	$[0,0,0]$	$\bar{x}+1/2,x,1/2$	$[0,0,0]$	$x+1/2,\bar{x},1/2$	$[0,0,0]$	
4	g	m.2m	$x,x+1/2,0$	$[0,0,0]$	$\bar{x},\bar{x}+1/2,0$	$[0,0,0]$	$\bar{x}+1/2,x,0$	$[0,0,0]$	$x+1/2,\bar{x},0$	$[0,0,0]$	
4	f	2.mm	$0,1/2,z$	$[0,0,0]$	$1/2,0,z$	$[0,0,0]$	$1/2,0,\bar{z}$	$[0,0,0]$	$0,1/2,\bar{z}$	$[0,0,0]$	
4	e	4'..	$0,0,z$	$[0,0,0]$	$1/2,1/2,\bar{z}$	$[0,0,0]$	$0,0,\bar{z}$	$[0,0,0]$	$1/2,1/2,z$	$[0,0,0]$	
2	d	m.mm	$0,1/2,0$	$[0,0,0]$	$1/2,0,0$	$[0,0,0]$					
2	c	m.mm	$0,1/2,1/2$	$[0,0,0]$	$1/2,0,1/2$	$[0,0,0]$					
2	b	4'/m..	$0,0,1/2$	$[0,0,0]$	$1/2,1/2,1/2$	$[0,0,0]$					
2	a	4'/m..	$0,0,0$	$[0,0,0]$	$1/2,1/2,0$	$[0,0,0]$					

**Symmetry of Special Projections**

Along  $[0,0,1]$  p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along  $[1,0,0]$  p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

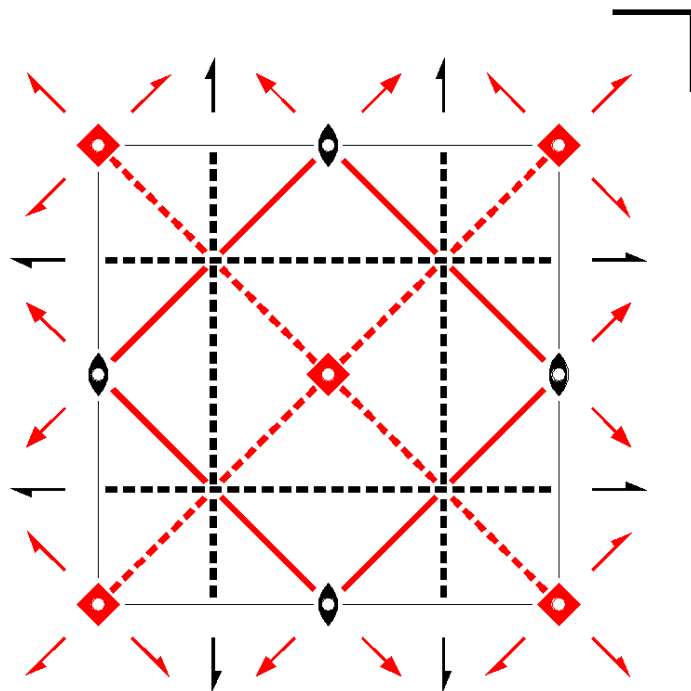
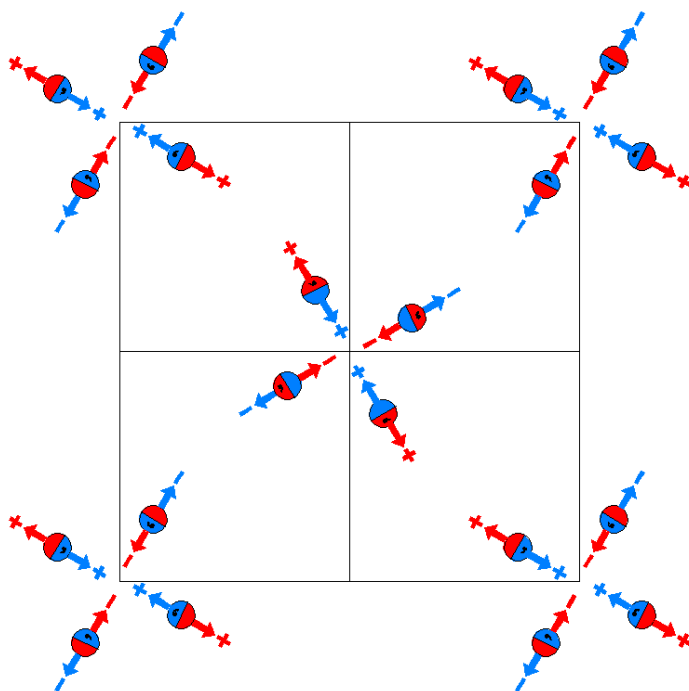
Along  $[1,1,0]$  p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4'/mbm'  
127.5.1057

4'/mmm'  
P4'/m2<sub>1</sub>/b2'/m'

Tetragonal



Origin at center ( $4'/m$ ) at  $4'/m2_1, 'g'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'      | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)  | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)  | (7) 2' (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)' | (8) 2' x,x+1/2,0<br>(2 <sub>xy</sub>  1/2,1/2,0)'                  |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)              | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)                 | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)' | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'          |
| (13) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (14) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (15) m' x+1/2,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)'        | (16) g' (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)'         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

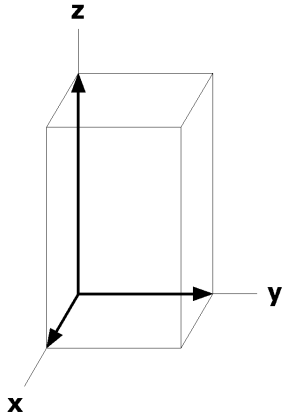
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates								
16	I	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y},x,z$	$[v,\bar{u},\bar{w}]$	(4)	$y,\bar{x},z$	$[\bar{v},u,\bar{w}]$
(5)	$\bar{x}+1/2,y+1/2,\bar{z}$	$[\bar{u},v,\bar{w}]$	(6)	$x+1/2,\bar{y}+1/2,\bar{z}$	$[u,\bar{v},\bar{w}]$	(7)	$y+1/2,x+1/2,\bar{z}$	$[\bar{v},\bar{u},w]$	(8)	$\bar{y}+1/2,\bar{x}+1/2,\bar{z}$	$[v,u,w]$
(9)	$\bar{x},\bar{y},\bar{z}$	$[u,v,w]$	(10)	$x,y,\bar{z}$	$[\bar{u},\bar{v},w]$	(11)	$y,\bar{x},\bar{z}$	$[v,\bar{u},\bar{w}]$	(12)	$\bar{y},x,\bar{z}$	$[\bar{v},u,\bar{w}]$
(13)	$x+1/2,\bar{y}+1/2,z$	$[\bar{u},v,\bar{w}]$	(14)	$\bar{x}+1/2,y+1/2,z$	$[u,\bar{v},\bar{w}]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[\bar{v},\bar{u},w]$	(16)	$y+1/2,x+1/2,z$	$[v,u,w]$
8	k	..m'	$x,x+1/2,z$	$[\bar{x},\bar{x}+1/2,z$	$[\bar{u},\bar{u},w]$	$\bar{x}+1/2,x,z$	$[u,\bar{u},\bar{w}]$	$x+1/2,\bar{x},z$	$[\bar{u},u,\bar{w}]$		
			$\bar{x}+1/2,x,\bar{z}$	$[\bar{u},\bar{u},\bar{w}]$	$x+1/2,\bar{x},\bar{z}$	$[u,\bar{u},\bar{w}]$	$x,x+1/2,\bar{z}$	$[\bar{u},\bar{u},w]$	$\bar{x},\bar{x}+1/2,\bar{z}$	$[u,u,w]$	
8	j	m..	$x,y,1/2$	$[0,0,w]$	$\bar{x},\bar{y},1/2$	$[0,0,w]$	$\bar{y},x,1/2$	$[0,0,\bar{w}]$	$y,\bar{x},1/2$	$[0,0,\bar{w}]$	
			$\bar{x}+1/2,y+1/2,1/2$	$[0,0,\bar{w}]$	$x+1/2,\bar{y}+1/2,1/2$	$[0,0,\bar{w}]$	$y+1/2,x+1/2,1/2$	$[0,0,w]$	$\bar{y}+1/2,\bar{x}+1/2,1/2$	$[0,0,w]$	
8	i	m..	$x,y,0$	$[0,0,w]$	$\bar{x},\bar{y},0$	$[0,0,w]$	$\bar{y},x,0$	$[0,0,\bar{w}]$	$y,\bar{x},0$	$[0,0,\bar{w}]$	
			$\bar{x}+1/2,y+1/2,0$	$[0,0,\bar{w}]$	$x+1/2,\bar{y}+1/2,0$	$[0,0,\bar{w}]$	$y+1/2,x+1/2,0$	$[0,0,w]$	$\bar{y}+1/2,\bar{x}+1/2,0$	$[0,0,w]$	
4	h	m.2'm'	$x,x+1/2,1/2$	$[0,0,w]$	$\bar{x},\bar{x}+1/2,1/2$	$[0,0,w]$	$\bar{x}+1/2,x,1/2$	$[0,0,\bar{w}]$	$x+1/2,\bar{x},1/2$	$[0,0,\bar{w}]$	
4	g	m.2'm'	$x,x+1/2,0$	$[0,0,w]$	$\bar{x},\bar{x}+1/2,0$	$[0,0,w]$	$\bar{x}+1/2,x,0$	$[0,0,\bar{w}]$	$x+1/2,\bar{x},0$	$[0,0,\bar{w}]$	
4	f	2.m'm'	$0,1/2,z$	$[0,0,w]$	$1/2,0,z$	$[0,0,\bar{w}]$	$1/2,0,\bar{z}$	$[0,0,w]$	$0,1/2,\bar{z}$	$[0,0,\bar{w}]$	
4	e	4'..	$0,0,z$	$[0,0,0]$	$1/2,1/2,\bar{z}$	$[0,0,0]$	$0,0,\bar{z}$	$[0,0,0]$	$1/2,1/2,z$	$[0,0,0]$	
2	d	m.m'm'	$0,1/2,0$	$[0,0,w]$	$1/2,0,0$	$[0,0,\bar{w}]$					
2	c	m.m'm'	$0,1/2,1/2$	$[0,0,w]$	$1/2,0,1/2$	$[0,0,\bar{w}]$					
2	b	4'/m..	$0,0,1/2$	$[0,0,0]$	$1/2,1/2,1/2$	$[0,0,0]$					
2	a	4'/m..	$0,0,0$	$[0,0,0]$	$1/2,1/2,0$	$[0,0,0]$					

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4gm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a'}2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,1/4,0$

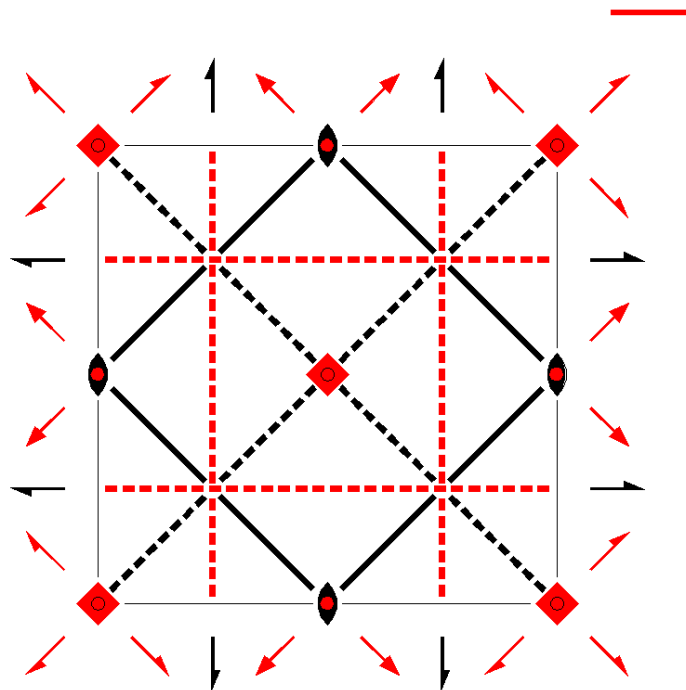
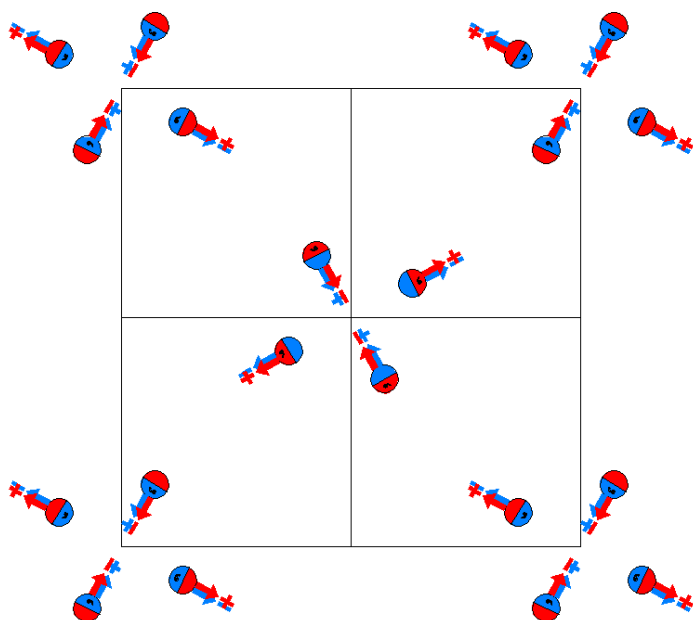
Along  $[1,1,0]$   $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,0$



P4'/m'b'm  
127.6.1058

4'/m'm'm  
P4'/m'2<sub>1</sub>/b'2'/m

Tetragonal



Origin at center ( $4'/m'$ ) at  $4'/m'12_1'/g$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'       | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'             |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)    | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)    | (7) 2' (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)'  | (8) 2' x, $\bar{x}$ +1/2,0<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)' |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)'               | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'                 | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)   | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                       |
| (13) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (14) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' | (15) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0) | (16) g (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)    |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

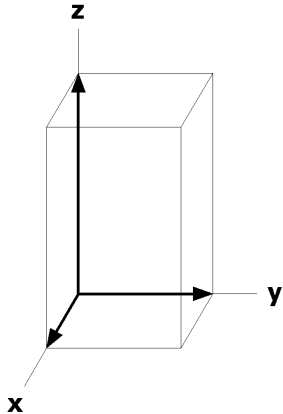
		Coordinates									
		Multiplicity, Wyckoff letter, Site Symmetry.									
16	I	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y},x,z$	$[v,\bar{u},\bar{w}]$	(4)	$y,\bar{x},z$	$[\bar{v},u,\bar{w}]$
(5)	$\bar{x}+1/2,y+1/2,\bar{z}$	$[\bar{u},v,\bar{w}]$	(6)	$x+1/2,\bar{y}+1/2,\bar{z}$	$[u,\bar{v},\bar{w}]$	(7)	$y+1/2,x+1/2,\bar{z}$	$[\bar{v},\bar{u},w]$	(8)	$\bar{y}+1/2,\bar{x}+1/2,\bar{z}$	$[v,u,w]$
(9)	$\bar{x},\bar{y},\bar{z}$	$[\bar{u},\bar{v},\bar{w}]$	(10)	$x,y,\bar{z}$	$[u,v,\bar{w}]$	(11)	$y,\bar{x},\bar{z}$	$[\bar{v},u,w]$	(12)	$\bar{y},x,\bar{z}$	$[v,\bar{u},w]$
(13)	$x+1/2,\bar{y}+1/2,z$	$[u,\bar{v},w]$	(14)	$\bar{x}+1/2,y+1/2,z$	$[\bar{u},v,w]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[v,u,\bar{w}]$	(16)	$y+1/2,x+1/2,z$	$[\bar{v},\bar{u},\bar{w}]$
8	k	..m	$x,x+1/2,z$	$[\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,z$	$[u,\bar{u},0]$	$\bar{x}+1/2,x,z$	$[u,u,0]$	$x+1/2,\bar{x},z$	$[\bar{u},\bar{u},0]$	
			$\bar{x}+1/2,x,\bar{z}$	$[u,u,0]$	$x+1/2,\bar{x},\bar{z}$	$[\bar{u},\bar{u},0]$	$x,x+1/2,\bar{z}$	$[\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,\bar{z}$	$[u,\bar{u},0]$	
8	j	m'..	$x,y,1/2$	$[u,v,0]$	$\bar{x},\bar{y},1/2$	$[\bar{u},\bar{v},0]$	$\bar{y},x,1/2$	$[v,\bar{u},0]$	$y,\bar{x},1/2$	$[\bar{v},u,0]$	
			$\bar{x}+1/2,y+1/2,1/2$	$[\bar{u},v,0]$	$x+1/2,\bar{y}+1/2,1/2$	$[u,\bar{v},0]$	$y+1/2,x+1/2,1/2$	$[\bar{v},\bar{u},0]$	$\bar{y}+1/2,\bar{x}+1/2,1/2$	$[v,u,0]$	
8	i	m'..	$x,y,0$	$[u,v,0]$	$\bar{x},\bar{y},0$	$[\bar{u},\bar{v},0]$	$\bar{y},x,0$	$[v,\bar{u},0]$	$y,\bar{x},0$	$[\bar{v},u,0]$	
			$\bar{x}+1/2,y+1/2,0$	$[\bar{u},v,0]$	$x+1/2,\bar{y}+1/2,0$	$[u,\bar{v},0]$	$y+1/2,x+1/2,0$	$[\bar{v},\bar{u},0]$	$\bar{y}+1/2,\bar{x}+1/2,0$	$[v,u,0]$	
4	h	m'.2'm	$x,x+1/2,1/2$	$[\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,1/2$	$[u,\bar{u},0]$	$\bar{x}+1/2,x,1/2$	$[u,u,0]$	$x+1/2,\bar{x},1/2$	$[\bar{u},\bar{u},0]$	
4	g	m'.2'm	$x,x+1/2,0$	$[\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,0$	$[u,\bar{u},0]$	$\bar{x}+1/2,x,0$	$[u,u,0]$	$x+1/2,\bar{x},0$	$[\bar{u},\bar{u},0]$	
4	f	2.mm	$0,1/2,z$	$[0,0,0]$	$1/2,0,z$	$[0,0,0]$	$1/2,0,\bar{z}$	$[0,0,0]$	$0,1/2,\bar{z}$	$[0,0,0]$	
4	e	4'..	$0,0,z$	$[0,0,0]$	$1/2,1/2,\bar{z}$	$[0,0,0]$	$0,0,\bar{z}$	$[0,0,0]$	$1/2,1/2,z$	$[0,0,0]$	
2	d	m'.mm	$0,1/2,0$	$[0,0,0]$	$1/2,0,0$	$[0,0,0]$					
2	c	m'.mm	$0,1/2,1/2$	$[0,0,0]$	$1/2,0,1/2$	$[0,0,0]$					
2	b	4'/m'..	$0,0,1/2$	$[0,0,0]$	$1/2,1/2,1/2$	$[0,0,0]$					
2	a	4'/m'..	$0,0,0$	$[0,0,0]$	$1/2,1/2,0$	$[0,0,0]$					

**Symmetry of Special Projections**

Along [0,0,1] p4'g'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

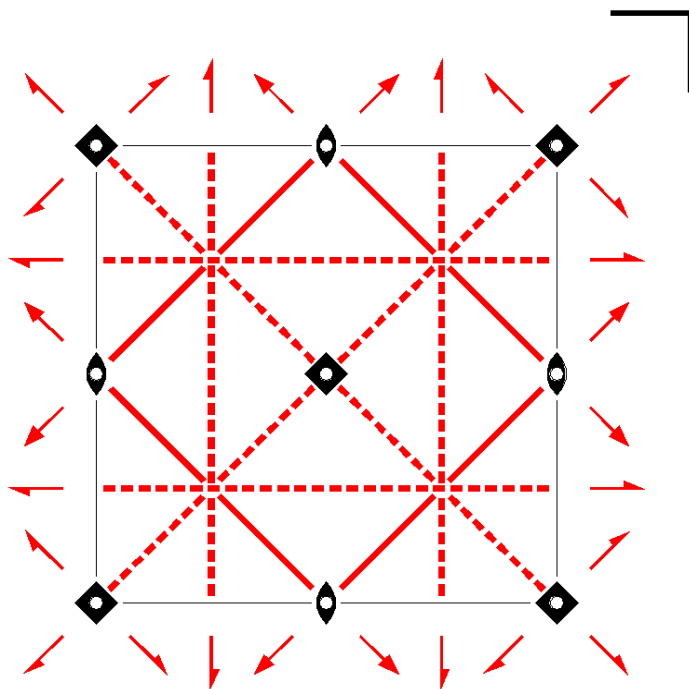
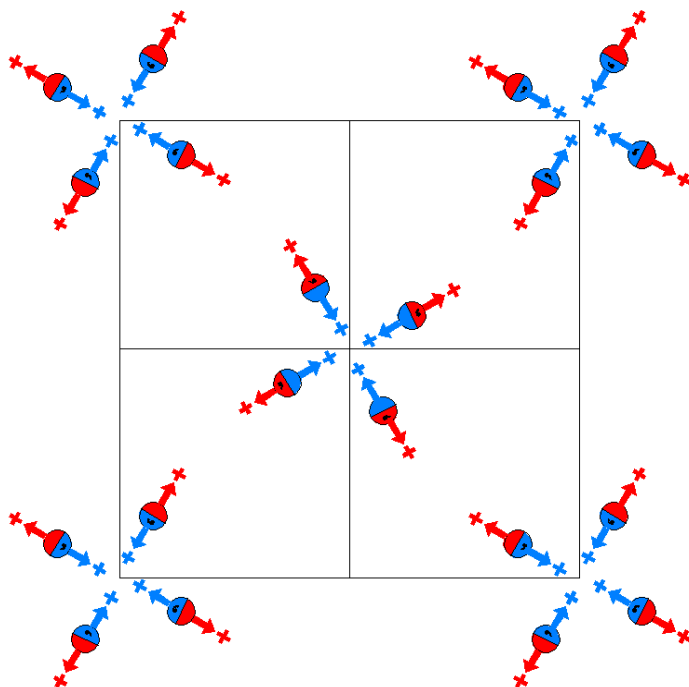
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4/mb'm'  
127.7.1059

4/mm'm'  
P4/m2<sub>1</sub>'/b'2'/m'

Tetragonal



Origin at center ( 4/m ) at 4/m12<sub>1</sub>'/g'

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x$

### Symmetry Operations

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)       | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)        |
| (5) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)'  | (6) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)'  | (7) 2' (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)' | (8) 2' x,x̄+1/2,0<br>(2 <sub>xy</sub> <sup>-1</sup>  1/2,1/2,0)'         |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)                | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)                   | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)  | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                 |
| (13) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (14) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' | (15) m' x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)'       | (16) g' (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub> <sup>-1</sup>  1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

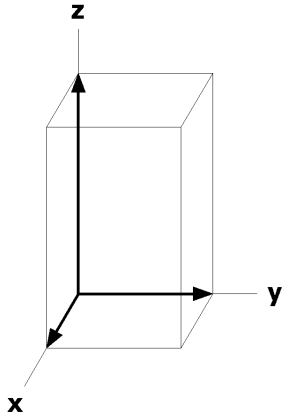
			Coordinates								
Multiplicity, Wyckoff letter, Site Symmetry.											
16	l	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y},x,z$	$[\bar{v},u,w]$	(4)	$y,\bar{x},z$	$[v,\bar{u},w]$
(5)	$\bar{x}+1/2,y+1/2,\bar{z}$	$[u,\bar{v},w]$	(6)	$x+1/2,\bar{y}+1/2,\bar{z}$	$[\bar{u},v,w]$	(7)	$y+1/2,x+1/2,\bar{z}$	$[\bar{v},\bar{u},w]$	(8)	$\bar{y}+1/2,\bar{x}+1/2,\bar{z}$	$[v,u,w]$
(9)	$\bar{x},\bar{y},\bar{z}$	$[u,v,w]$	(10)	$x,y,\bar{z}$	$[\bar{u},\bar{v},w]$	(11)	$y,\bar{x},\bar{z}$	$[\bar{v},u,w]$	(12)	$\bar{y},x,\bar{z}$	$[v,\bar{u},w]$
(13)	$x+1/2,\bar{y}+1/2,z$	$[u,\bar{v},w]$	(14)	$\bar{x}+1/2,y+1/2,z$	$[\bar{u},v,w]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[\bar{v},\bar{u},w]$	(16)	$y+1/2,x+1/2,z$	$[v,u,w]$
8	k	..m'	$x,x+1/2,z$	$[\bar{x},\bar{x}+1/2,z$	$[\bar{u},\bar{u},w]$	$\bar{x}+1/2,x,z$	$[\bar{u},u,w]$	$x+1/2,\bar{x},z$	$[u,\bar{u},w]$		
			$\bar{x}+1/2,x,\bar{z}$	$[u,\bar{u},w]$	$x+1/2,\bar{x},\bar{z}$	$[u,u,w]$	$x,x+1/2,\bar{z}$	$[u,\bar{u},w]$	$\bar{x},\bar{x}+1/2,\bar{z}$	$[u,u,w]$	
8	j	m..	$x,y,1/2$	$[0,0,w]$	$\bar{x},\bar{y},1/2$	$[0,0,w]$	$\bar{y},x,1/2$	$[0,0,w]$	$y,\bar{x},1/2$	$[0,0,w]$	
			$\bar{x}+1/2,y+1/2,1/2$	$[0,0,w]$	$x+1/2,\bar{y}+1/2,1/2$	$[0,0,w]$	$y+1/2,x+1/2,1/2$	$[0,0,w]$	$\bar{y}+1/2,\bar{x}+1/2,1/2$	$[0,0,w]$	
8	i	m..	$x,y,0$	$[0,0,w]$	$\bar{x},\bar{y},0$	$[0,0,w]$	$\bar{y},x,0$	$[0,0,w]$	$y,\bar{x},0$	$[0,0,w]$	
			$\bar{x}+1/2,y+1/2,0$	$[0,0,w]$	$x+1/2,\bar{y}+1/2,0$	$[0,0,w]$	$y+1/2,x+1/2,0$	$[0,0,w]$	$\bar{y}+1/2,\bar{x}+1/2,0$	$[0,0,w]$	
4	h	m.2'm'	$x,x+1/2,1/2$	$[0,0,w]$	$\bar{x},\bar{x}+1/2,1/2$	$[0,0,w]$	$\bar{x}+1/2,x,1/2$	$[0,0,w]$	$x+1/2,\bar{x},1/2$	$[0,0,w]$	
4	g	m.2'm'	$x,x+1/2,0$	$[0,0,w]$	$\bar{x},\bar{x}+1/2,0$	$[0,0,w]$	$\bar{x}+1/2,x,0$	$[0,0,w]$	$x+1/2,\bar{x},0$	$[0,0,w]$	
4	f	2.m'm'	$0,1/2,z$	$[0,0,w]$	$1/2,0,z$	$[0,0,w]$	$1/2,0,\bar{z}$	$[0,0,w]$	$0,1/2,\bar{z}$	$[0,0,w]$	
4	e	4..	$0,0,z$	$[0,0,w]$	$1/2,1/2,\bar{z}$	$[0,0,w]$	$0,0,\bar{z}$	$[0,0,w]$	$1/2,1/2,z$	$[0,0,w]$	
2	d	m.m'm'	$0,1/2,0$	$[0,0,w]$	$1/2,0,0$	$[0,0,w]$					
2	c	m.m'm'	$0,1/2,1/2$	$[0,0,w]$	$1/2,0,1/2$	$[0,0,w]$					
2	b	4/m..	$0,0,1/2$	$[0,0,w]$	$1/2,1/2,1/2$	$[0,0,w]$					
2	a	4/m..	$0,0,0$	$[0,0,w]$	$1/2,1/2,0$	$[0,0,w]$					

### Symmetry of Special Projections

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



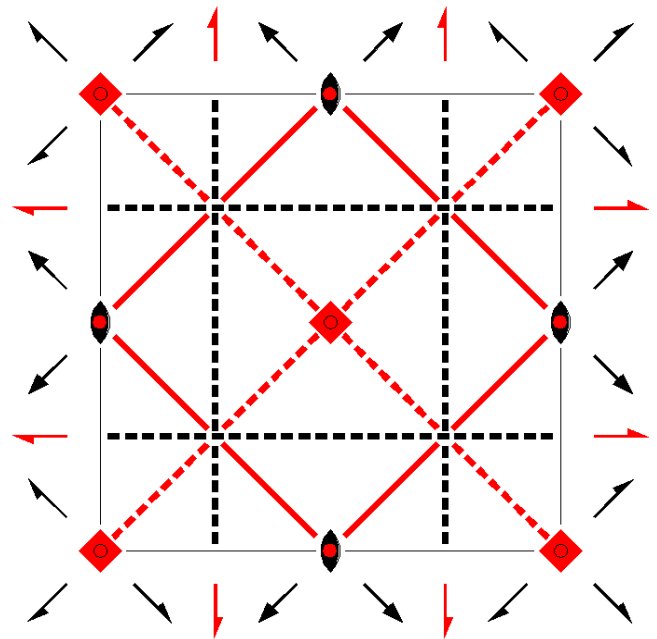
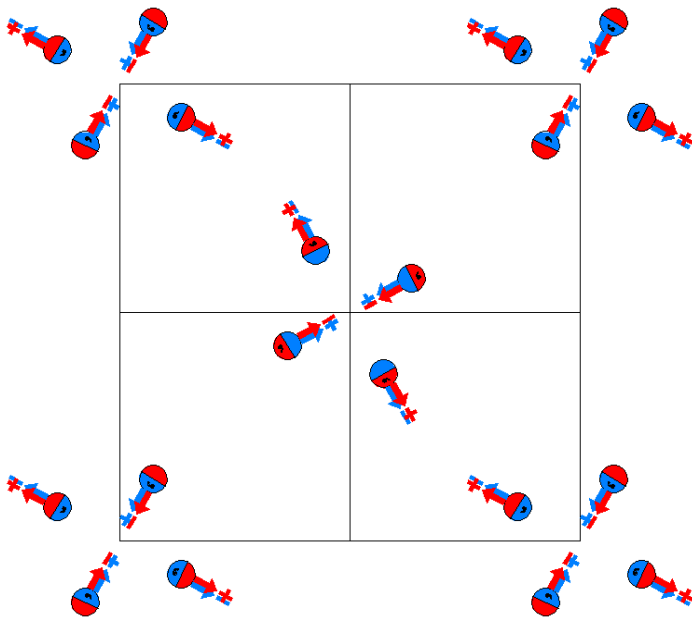
P4'/m'bm'

127.8.1060

4'/m'mm'

P4'/m'2<sub>1</sub>'/b2/m'

Tetragonal



Origin at center ( $4'/m'$ ) at  $4'/m'12_1/g'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                   | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'                         | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'                         |
| (5) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (6) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' | (7) 2 (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)                      | (8) 2 x, $\bar{x}$ +1/2,0<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)               |
| (9) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)'            | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'                | (11) $\bar{4}$ <sup>+</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub>  0,0,0) | (12) $\bar{4}$ <sup>-</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)  | (14) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)  | (15) m' x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0)'                 | (16) g' (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)'              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

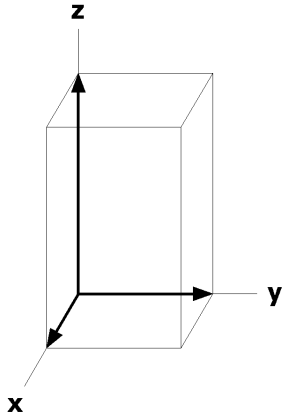
			Coordinates								
Multiplicity,	Wyckoff letter,	Site Symmetry.									
16	l	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y},x,z$	$[v,\bar{u},\bar{w}]$	(4)	$y,\bar{x},z$	$[\bar{v},u,\bar{w}]$
(5)	$\bar{x}+1/2,y+1/2,\bar{z}$	$[u,\bar{v},w]$	(6)	$x+1/2,\bar{y}+1/2,\bar{z}$	$[\bar{u},v,w]$	(7)	$y+1/2,x+1/2,\bar{z}$	$[v,u,\bar{w}]$	(8)	$\bar{y}+1/2,\bar{x}+1/2,\bar{z}$	$[\bar{v},\bar{u},\bar{w}]$
(9)	$\bar{x},\bar{y},\bar{z}$	$[\bar{u},\bar{v},\bar{w}]$	(10)	$x,y,\bar{z}$	$[u,v,\bar{w}]$	(11)	$y,\bar{x},\bar{z}$	$[\bar{v},u,w]$	(12)	$\bar{y},x,\bar{z}$	$[v,\bar{u},w]$
(13)	$x+1/2,\bar{y}+1/2,z$	$[\bar{u},v,\bar{w}]$	(14)	$\bar{x}+1/2,y+1/2,z$	$[u,\bar{v},\bar{w}]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[\bar{v},\bar{u},w]$	(16)	$y+1/2,x+1/2,z$	$[v,u,w]$
8	k	..m'	$x,x+1/2,z$	$[\bar{x},\bar{x}+1/2,z$	$[\bar{u},\bar{u},w]$	$\bar{x}+1/2,x,z$	$[u,\bar{u},\bar{w}]$	$x+1/2,\bar{x},z$	$[\bar{u},u,\bar{w}]$	$\bar{x},\bar{x}+1/2,z$	$[\bar{u},\bar{u},\bar{w}]$
8	j	m'..	$x,y,1/2$	$[u,v,0]$	$\bar{x},\bar{y},1/2$	$[\bar{u},\bar{v},0]$	$\bar{y},x,1/2$	$[v,\bar{u},0]$	$y,\bar{x},1/2$	$[\bar{v},u,0]$	
8	i	m'..	$\bar{x}+1/2,y+1/2,1/2$	$[u,\bar{v},0]$	$x+1/2,\bar{y}+1/2,1/2$	$[\bar{u},v,0]$	$y+1/2,x+1/2,1/2$	$[v,u,0]$	$\bar{y}+1/2,\bar{x}+1/2,1/2$	$[\bar{v},\bar{u},0]$	
4	h	m'.2m'	$x,x+1/2,1/2$	$[u,u,0]$	$\bar{x},\bar{x}+1/2,1/2$	$[\bar{u},\bar{u},0]$	$\bar{x}+1/2,x,1/2$	$[u,\bar{u},0]$	$x+1/2,\bar{x},1/2$	$[\bar{u},u,0]$	
4	g	m'.2m'	$x,x+1/2,0$	$[u,u,0]$	$\bar{x},\bar{x}+1/2,0$	$[\bar{u},\bar{u},0]$	$\bar{x}+1/2,x,0$	$[u,\bar{u},0]$	$x+1/2,\bar{x},0$	$[\bar{u},u,0]$	
4	f	2.m'm'	$0,1/2,z$	$[0,0,w]$	$1/2,0,z$	$[0,0,\bar{w}]$	$1/2,0,\bar{z}$	$[0,0,w]$	$0,1/2,\bar{z}$	$[0,0,\bar{w}]$	
4	e	4'..	$0,0,z$	$[0,0,0]$	$1/2,1/2,\bar{z}$	$[0,0,0]$	$0,0,\bar{z}$	$[0,0,0]$	$1/2,1/2,z$	$[0,0,0]$	
2	d	m'.m'm'	$0,1/2,0$	$[0,0,0]$	$1/2,0,0$	$[0,0,0]$					
2	c	m'.m'm'	$0,1/2,1/2$	$[0,0,0]$	$1/2,0,1/2$	$[0,0,0]$					
2	b	4'/m'..	$0,0,1/2$	$[0,0,0]$	$1/2,1/2,1/2$	$[0,0,0]$					
2	a	4'/m'..	$0,0,0$	$[0,0,0]$	$1/2,1/2,0$	$[0,0,0]$					

### Symmetry of Special Projections

Along [0,0,1] p4'gm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

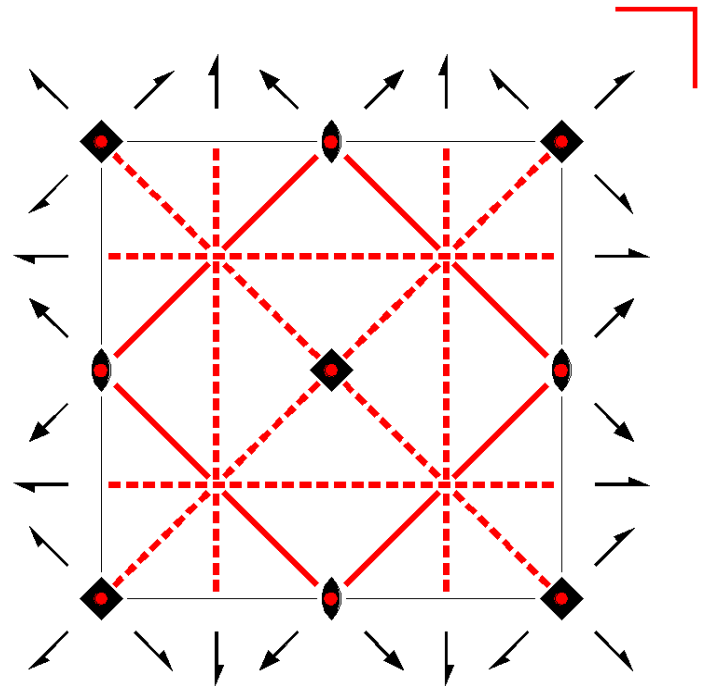
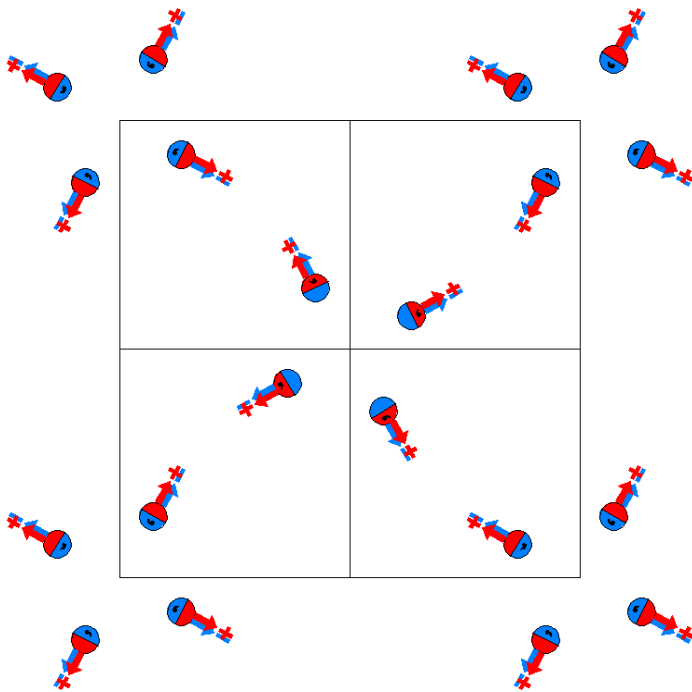
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4/m'b'm'  
127.9.1061

4/m'm'm'  
P4/m'2<sub>1</sub>/b'2/m'

Tetragonal



Origin at center ( 4/m' ) at 4/m'12<sub>1</sub>/g'

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x$

### Symmetry Operations

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)           | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)              |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)     | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)     | (7) 2 (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)       | (8) 2 x, $\bar{x}$ +1/2,0<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)   |
| (9) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$ ' 0,0,0)'             | (10) m' x,y,0<br>(m <sub>z</sub> ' 0,0,0)'                 | (11) $\bar{4}^+$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^+$ ' 0,0,0)'  | (12) $\bar{4}^-$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^-$ ' 0,0,0)'                   |
| (13) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub> ' 1/2,1/2,0)' | (14) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub> ' 1/2,1/2,0)' | (15) m' x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub> ' 1/2,1/2,0)' | (16) g' (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub> ' 1/2,1/2,0)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

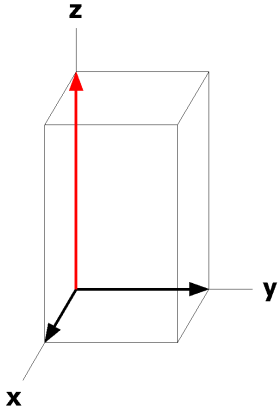
		Coordinates																							
Multiplicity,	Wyckoff letter,	Site Symmetry.																							
16	l	1																							
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y},x,z$	$[\bar{v},u,w]$	(4)	$y,\bar{x},z$	$[v,\bar{u},w]$														
(5)	$\bar{x}+1/2,y+1/2,\bar{z}$	$[\bar{u},v,\bar{w}]$	(6)	$x+1/2,\bar{y}+1/2,\bar{z}$	$[u,\bar{v},\bar{w}]$	(7)	$y+1/2,x+1/2,\bar{z}$	$[v,u,\bar{w}]$	(8)	$\bar{y}+1/2,\bar{x}+1/2,\bar{z}$	$[\bar{v},\bar{u},\bar{w}]$														
(9)	$\bar{x},\bar{y},\bar{z}$	$[\bar{u},\bar{v},\bar{w}]$	(10)	$x,y,\bar{z}$	$[u,v,\bar{w}]$	(11)	$y,\bar{x},\bar{z}$	$[v,\bar{u},\bar{w}]$	(12)	$\bar{y},x,\bar{z}$	$[\bar{v},u,\bar{w}]$														
(13)	$x+1/2,\bar{y}+1/2,z$	$[u,\bar{v},w]$	(14)	$\bar{x}+1/2,y+1/2,z$	$[\bar{u},v,w]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[\bar{v},\bar{u},w]$	(16)	$y+1/2,x+1/2,z$	$[v,u,w]$														
8	k	..m'	$x,x+1/2,z$	$[\bar{x},\bar{x}+1/2,z$	$[\bar{u},\bar{u},w]$	$\bar{x}+1/2,x,z$	$[\bar{u},u,w]$	$x+1/2,\bar{x},z$	$[u,\bar{u},w]$	$\bar{x},\bar{x}+1/2,z$	$[\bar{u},\bar{u},\bar{w}]$														
8	j	m'..	$x,y,1/2$	$[u,v,0]$	$[\bar{x},\bar{y},1/2$	$[\bar{u},\bar{v},0]$	$\bar{y},x,1/2$	$[\bar{v},u,0]$	$y,\bar{x},1/2$	$[v,\bar{u},0]$	$\bar{x}+1/2,y+1/2,1/2$	$[\bar{u},v,0]$	$x+1/2,\bar{y}+1/2,1/2$	$[u,\bar{v},0]$	$y+1/2,x+1/2,1/2$	$[v,u,0]$	$\bar{y}+1/2,\bar{x}+1/2,1/2$	$[\bar{v},\bar{u},0]$							
8	i	m'..	$x,y,0$	$[u,v,0]$	$[\bar{x},\bar{y},0$	$[\bar{u},\bar{v},0]$	$\bar{y},x,0$	$[\bar{v},u,0]$	$y,\bar{x},0$	$[v,\bar{u},0]$	$\bar{x}+1/2,y+1/2,0$	$[\bar{u},v,0]$	$x+1/2,\bar{y}+1/2,0$	$[u,\bar{v},0]$	$y+1/2,x+1/2,0$	$[v,u,0]$	$\bar{y}+1/2,\bar{x}+1/2,0$	$[\bar{v},\bar{u},0]$							
4	h	m'.2m'	$x,x+1/2,1/2$	$[u,u,0]$	$[\bar{x},\bar{x}+1/2,1/2$	$[\bar{u},\bar{u},0]$	$\bar{x}+1/2,x,1/2$	$[\bar{u},u,0]$	$x+1/2,\bar{x},1/2$	$[u,\bar{u},0]$	4	g	m'.2m'	$x,x+1/2,0$	$[u,u,0]$	$[\bar{x},\bar{x}+1/2,0$	$[\bar{u},\bar{u},0]$	$\bar{x}+1/2,x,0$	$[\bar{u},u,0]$	$x+1/2,\bar{x},0$	$[u,\bar{u},0]$				
4	f	2.m'm'	$0,1/2,z$	$[0,0,w]$	$1/2,0,z$	$[0,0,w]$	$1/2,0,\bar{z}$	$[0,0,\bar{w}]$	$0,1/2,\bar{z}$	$[0,0,\bar{w}]$	4	e	4..	$0,0,z$	$[0,0,w]$	$1/2,1/2,\bar{z}$	$[0,0,\bar{w}]$	$0,0,\bar{z}$	$[0,0,\bar{w}]$	$1/2,1/2,z$	$[0,0,w]$				
2	d	m'.m'm'	$0,1/2,0$	$[0,0,0]$	$1/2,0,0$	$[0,0,0]$	2	c	m'.m'm'	$0,1/2,1/2$	$[0,0,0]$	2	b	4/m'..	$0,0,1/2$	$[0,0,0]$	$1/2,1/2,1/2$	$[0,0,0]$	2	a	4/m'..	$0,0,0$	$[0,0,0]$	$1/2,1/2,0$	$[0,0,0]$

### Symmetry of Special Projections

Along [0,0,1] p4g'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

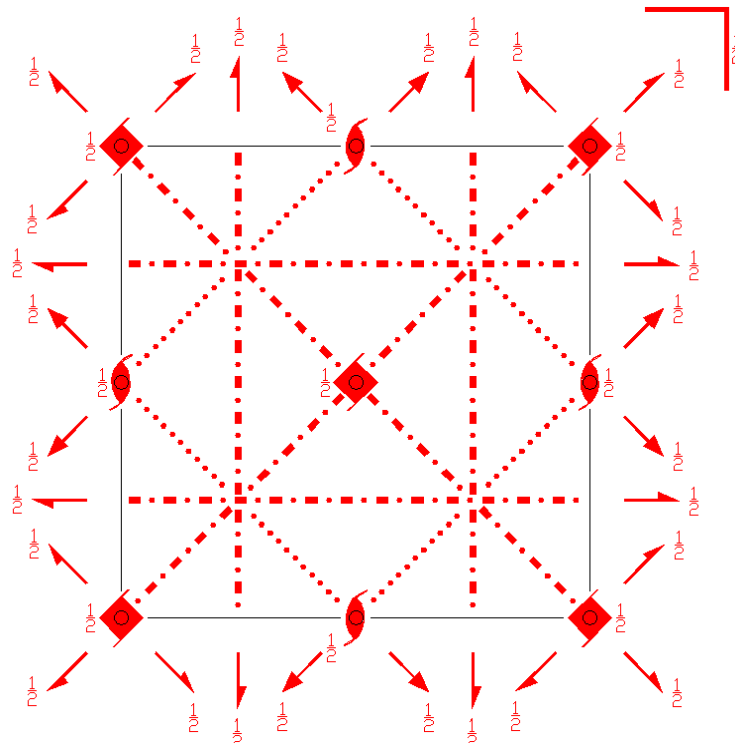
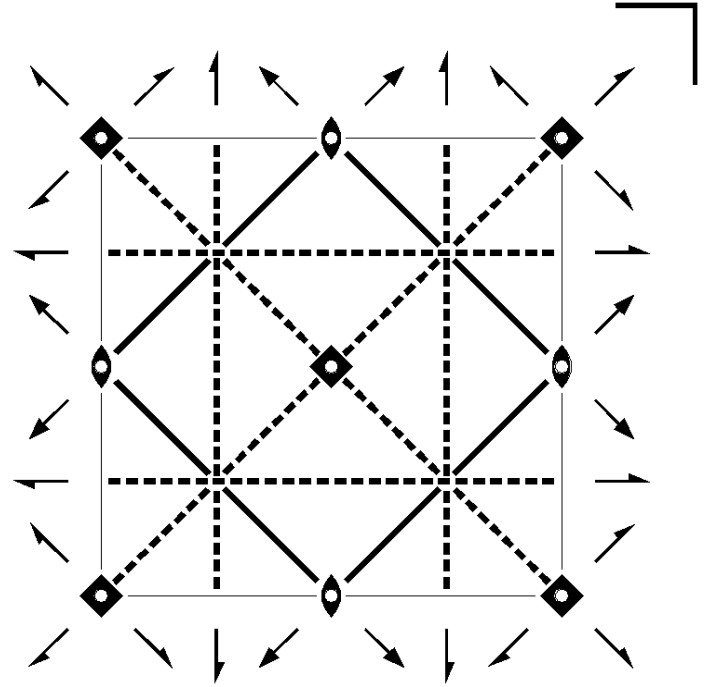
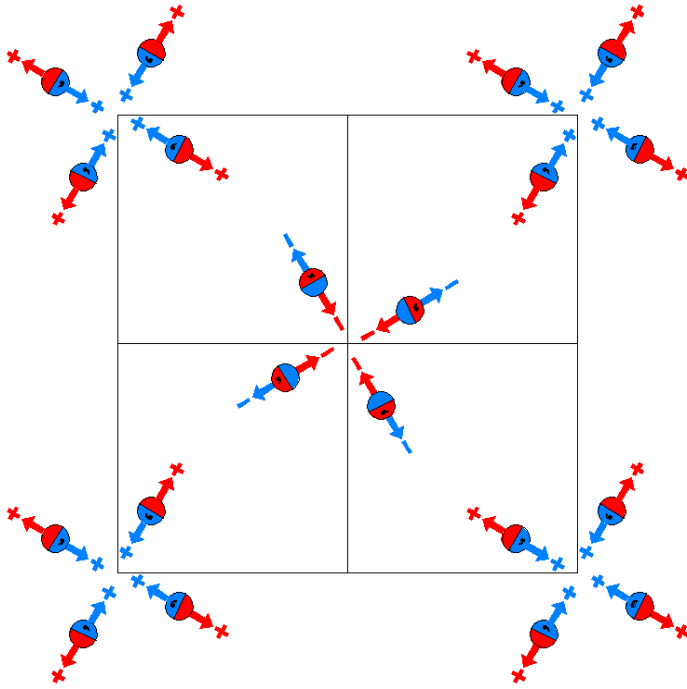
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_{2c} 4/m\bar{b}m$   
127.10.1062

$4/m\bar{m}m1'$   
 $P_{2c} 4/m\bar{2}_1/b\bar{2}/m$

Tetragonal





**Origin** at center ( 4/m ) at 4/m12<sub>1</sub>/g

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)        | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)            |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)  | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)  | (7) 2 (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)    | (8) 2 x, $\bar{x}$ +1/2,0<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,0) |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)              | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)                 | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)     | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z$ <sup>-1</sup>  0,0,0)         |
| (13) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (14) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (15) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0) | (16) g (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)  |

For (0,0,1)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (0,0,1)<br>(1 0,0,1)'                               | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)'           | (3) 4 <sup>+</sup> ' (0,0,1) 0,0,z<br>(4 <sub>z</sub>  0,0,1)'       | (4) 4 <sup>-</sup> ' (0,0,1) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1)'     |
| (5) 2' (0,1/2,0) 1/4,y,1/2<br>(2 <sub>y</sub>  1/2,1/2,1)' | (6) 2' (1/2,0,0) x,1/4,1/2<br>(2 <sub>x</sub>  1/2,1/2,1)' | (7) 2' (1/2,1/2,0) x,x,1/2<br>(2 <sub>xy</sub>  1/2,1/2,1)'          | (8) 2' x, $\bar{x}$ +1/2,1/2<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1)' |
| (9) $\bar{1}$ ' 0,0,1/2<br>( $\bar{1}$  0,0,1)'            | (10) m' x,y,1/2<br>(m <sub>z</sub>  0,0,1)'                | (11) $\bar{4}^+$ ' 0,0,z; 0,0,1/2<br>( $\bar{4}_z$  0,0,1)'          | (12) $\bar{4}^-$ ' 0,0,z; 0,0,1/2<br>( $\bar{4}_z$ <sup>-1</sup>  0,0,1)'        |
| (13) n' (1/2,0,1) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1)'  | (14) n' (0,1/2,1) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1)'  | (15) c' (0,0,1) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1)' | (16) n' (1/2,1/2,1) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1)'    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (0,0,1)' +

32 | 1

- |   |  |   |   |   |
|---|--|---|---|---|
| (1) x,y,z [u,v,w]   | (2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]              | (3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]                     | (4) y, $\bar{x},z$ [ $v,\bar{u},w$ ]  |   |
| (5) $\bar{x}$ +1/2,y+1/2, $\bar{z}$ [ $\bar{u},v,\bar{w}$ ] | (6) x+1/2, $\bar{y}$ +1/2, $\bar{z}$ [ $u,\bar{v},\bar{w}$ ] | (7) y+1/2,x+1/2, $\bar{z}$ [ $v,u,\bar{w}$ ]            | (8) $\bar{y}$ +1/2, $\bar{x}$ +1/2, $\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ] |   |
| (9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]             | (10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]                  | (11) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]             | (12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]                                  |   |
| (13) x+1/2, $\bar{y}$ +1/2,z [ $\bar{u},v,\bar{w}$ ]        | (14) $\bar{x}$ +1/2,y+1/2,z [ $u,\bar{v},\bar{w}$ ]          | (15) $\bar{y}$ +1/2, $\bar{x}$ +1/2,z [ $v,u,\bar{w}$ ] | (16) y+1/2,x+1/2,z [ $\bar{v},\bar{u},\bar{w}$ ]                            |   |
| 16 k ..m  | x,x+1/2,z [ $\bar{u},u,0$ ]                                  | $\bar{x},\bar{x}$ +1/2,z [ $u,\bar{u},0$ ]              | $\bar{x}$ +1/2,x,z [ $\bar{u},\bar{u},0$ ]                                  | x+1/2, $\bar{x},z$ [ $u,u,0$ ]                      |
|   | $\bar{x}$ +1/2,x, $\bar{z}$ [ $u,u,0$ ]                      | x+1/2, $\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]        | x,x+1/2, $\bar{z}$ [ $u,\bar{u},0$ ]  | $\bar{x},\bar{x}$ +1/2, $\bar{z}$ [ $\bar{u},u,0$ ] |

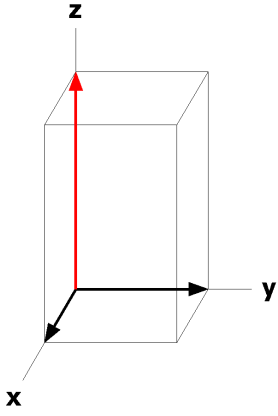
16	j	m'..	$x,y,1/2 [u,v,0]$	$\bar{x},\bar{y},1/2 [\bar{u},\bar{v},0]$	$\bar{y},x,1/2 [\bar{v},u,0]$	$y,\bar{x},1/2 [v,\bar{u},0]$
			$\bar{x}+1/2,y+1/2,1/2 [u,\bar{v},0]$	$x+1/2,\bar{y}+1/2,1/2 [\bar{u},v,0]$	$y+1/2,x+1/2,1/2 [\bar{v},\bar{u},0]$	$\bar{y}+1/2,\bar{x}+1/2,1/2 [v,u,0]$
16	i	m..	$x,y,0 [0,0,w]$	$\bar{x},\bar{y},0 [0,0,w]$	$\bar{y},x,0 [0,0,w]$	$y,\bar{x},0 [0,0,w]$
			$\bar{x}+1/2,y+1/2,0 [0,0,\bar{w}]$	$x+1/2,\bar{y}+1/2,0 [0,0,\bar{w}]$	$y+1/2,x+1/2,0 [0,0,\bar{w}]$	$\bar{y}+1/2,\bar{x}+1/2,0 [0,0,\bar{w}]$
8	h	m'.2'm	$x,x+1/2,1/2 [\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,1/2 [u,\bar{u},0]$	$\bar{x}+1/2,x,1/2 [\bar{u},\bar{u},0]$	$x+1/2,\bar{x},1/2 [u,u,0]$
8	g	m.2m	$x,x+1/2,0 [0,0,0]$	$\bar{x},\bar{x}+1/2,0 [0,0,0]$	$\bar{x}+1/2,x,0 [0,0,0]$	$x+1/2,\bar{x},0 [0,0,0]$
8	f	2.mm	$0,1/2,z [0,0,0]$	$1/2,0,z [0,0,0]$	$1/2,0,\bar{z} [0,0,0]$	$0,1/2,\bar{z} [0,0,0]$
8	e	4..	$0,0,z [0,0,w]$	$1/2,1/2,\bar{z} [0,0,\bar{w}]$	$0,0,\bar{z} [0,0,w]$	$1/2,1/2,z [0,0,\bar{w}]$
4	d	m.mm	$0,1/2,0 [0,0,0]$	$1/2,0,0 [0,0,0]$		
4	c	m'.mm	$0,1/2,1/2 [0,0,0]$	$1/2,0,1/2 [0,0,0]$		
4	b	4/m'..	$0,0,1/2 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$		
4	a	4/m..	$0,0,0 [0,0,w]$	$1/2,1/2,0 [0,0,\bar{w}]$		

### Symmetry of Special Projections

Along  $[0,0,1]$  p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p<sub>c</sub>.2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,1/4,0$

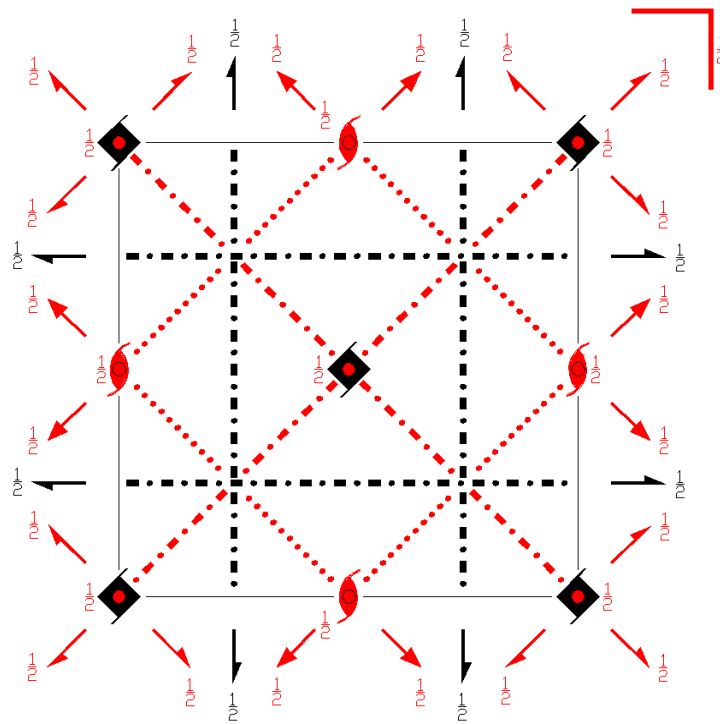
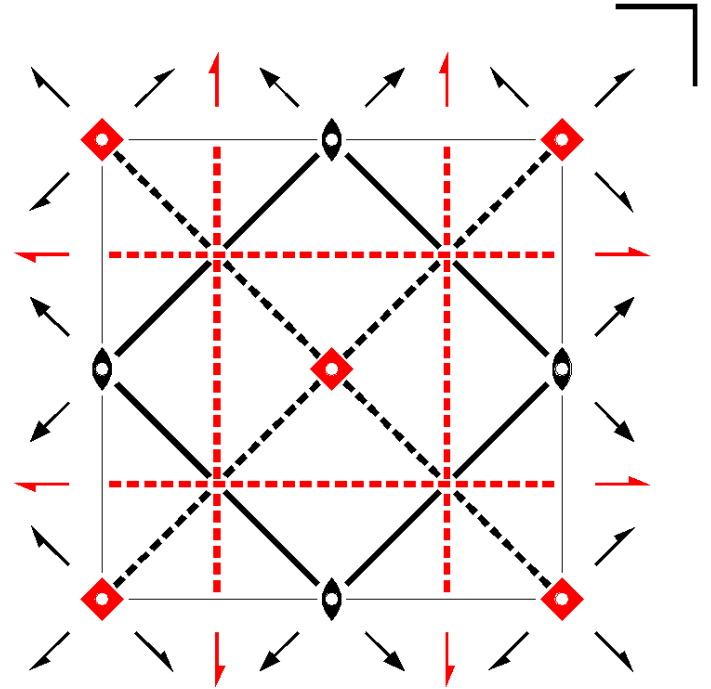
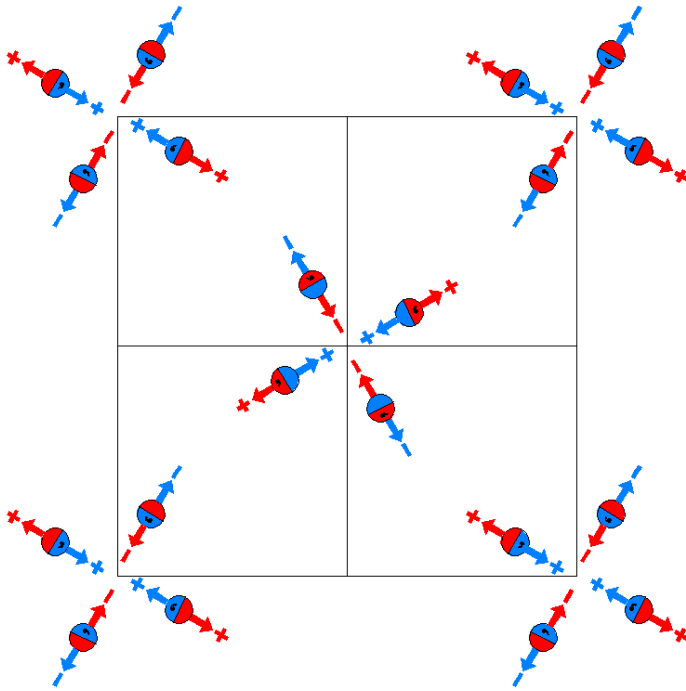
Along  $[1,1,0]$  p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$



$P_{2c} 4'/mb'm$   
127.11.1063

$4/mmm1'$   
 $P_{2c} 4'/m2_1'/b'2/m$

Tetragonal



**Origin** at center ( 4'/m ) at 4'/m12, /g

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 <sub>0,0,z</sub><br>(2 <sub>z</sub>  0,0,0)                    | (3) 4 <sup>+</sup> <sub>0,0,z</sub><br>(4 <sub>z</sub>  0,0,0)'         | (4) 4 <sup>-</sup> <sub>0,0,z</sub><br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'         |
| (5) 2' <sub>(0,1/2,0)</sub> 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)'  | (6) 2' <sub>(1/2,0,0)</sub> x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)'  | (7) 2 <sub>(1/2,1/2,0)</sub> x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)      | (8) 2 <sub>x, x̄+1/2,0</sub><br>(2 <sub>xy</sub>  1/2,1/2,0)                          |
| (9) 1̄ <sub>0,0,0</sub><br>(1̄ 0,0,0)                                | (10) m <sub>x,y,0</sub><br>(m <sub>z</sub>  0,0,0)                   | (11) 4 <sup>+</sup> <sub>0,0,z; 0,0,0</sub><br>(4 <sub>z</sub>  0,0,0)' | (12) 4 <sup>-</sup> <sub>0,0,z; 0,0,0</sub><br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (13) a' <sub>(1/2,0,0)</sub> x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (14) b' <sub>(0,1/2,0)</sub> 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' | (15) m <sub>x+1/2, x̄,z</sub><br>(m <sub>xy</sub>  1/2,1/2,0)           | (16) g <sub>(1/2,1/2,0)</sub> x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)                   |

For (0,0,1)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) t' (0,0,1)<br>(1 0,0,1)'  | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)'                    | (3) 4 <sup>+</sup> (0,0,1) 0,0,z<br>(4 <sub>z</sub>  0,0,1)   | (4) 4 <sup>-</sup> (0,0,1) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1)   |
| (5) 2 <sub>(0,1/2,0)</sub> 1/4,y,1/2<br>(2 <sub>y</sub>  1/2,1/2,1) | (6) 2 <sub>(1/2,0,0)</sub> x,1/4,1/2<br>(2 <sub>x</sub>  1/2,1/2,1) | (7) 2' (1/2,1/2,0) x,x,1/2<br>(2 <sub>xy</sub>  1/2,1/2,1)'   | (8) 2' x, x̄+1/2,1/2<br>(2 <sub>xy</sub>  1/2,1/2,1)'                       |
| (9) 1̄' 0,0,1/2<br>(1̄ 0,0,1)'                                      | (10) m' x,y,1/2<br>(m <sub>z</sub>  0,0,1)'                         | (11) 4 <sup>+</sup> 0,0,z; 0,0,1/2<br>(4 <sub>z</sub>  0,0,1) | (12) 4 <sup>-</sup> 0,0,z; 0,0,1/2<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1) |
| (13) n (1/2,0,1) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1)             | (14) n (0,1/2,1) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1)             | (15) c' (0,0,1) x+1/2, x̄,z<br>(m <sub>xy</sub>  1/2,1/2,1)'  | (16) n' (1/2,1/2,1) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1)'                  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) +      (0,0,1)' +

32    |    1

- |                              |                              |                                |                                |
|------------------------------|------------------------------|--------------------------------|--------------------------------|
| (1) x,y,z [u,v,w]            | (2) x̄,ȳ,z [ū,v̄,w]         | (3) ȳ,x̄,z [v̄,ū,w̄]          | (4) y,x,z [v̄,u,w̄]            |
| (5) x̄+1/2,y+1/2,z̄ [ū,v̄,w] | (6) x+1/2,ȳ+1/2,z̄ [ū,v̄,w] | (7) y+1/2,x+1/2,z̄ [v̄,u,w̄]   | (8) ȳ+1/2,x̄+1/2,z̄ [v̄,ū,w̄] |
| (9) x̄,ȳ,z̄ [ū,v̄,w]        | (10) x,y,z̄ [ū,v̄,w]         | (11) y,x,z̄ [v̄,ū,w̄]          | (12) ȳ,x̄,z̄ [v̄,u,w̄]        |
| (13) x+1/2,ȳ+1/2,z [ū,v̄,w] | (14) x̄+1/2,y+1/2,z [ū,v̄,w] | (15) ȳ+1/2,x̄+1/2,z [v̄,u,w̄] | (16) y+1/2,x+1/2,z [v̄,ū,w̄]   |
| 16    k    ..m               | x,x+1/2,z [ū,u,0]            | x̄,x̄+1/2,z [ū,ū,0]            | x̄+1/2,x,z [u,u,0]             |
|                              | x̄+1/2,x,z̄ [ū,ū,0]          | x+1/2,x̄,z̄ [u,u,0]            | x,x+1/2,z̄ [u,ū,0]             |
|                              |                              |                                | x̄,x̄+1/2,z̄ [ū,ū,0]           |

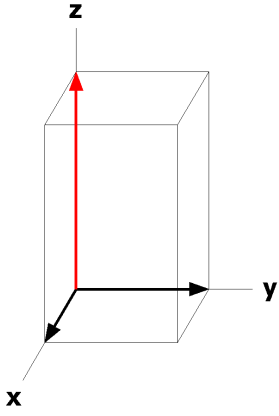
16	j	m'..	x,y,1/2 [u,v,0] $\bar{x}+1/2,y+1/2,1/2 [\bar{u},v,0]$	$\bar{x},\bar{y},1/2 [\bar{u},\bar{v},0]$ x+1/2, $\bar{y}+1/2,1/2 [u,\bar{v},0]$	$\bar{y},x,1/2 [v,\bar{u},0]$ y+1/2,x+1/2,1/2 [ $\bar{v},\bar{u},0]$	y, $\bar{x},1/2 [\bar{v},u,0]$ $\bar{y}+1/2,\bar{x}+1/2,1/2 [v,u,0]$
16	i	m..	x,y,0 [0,0,w] $\bar{x}+1/2,y+1/2,0 [0,0,w]$	$\bar{x},\bar{y},0 [0,0,w]$ x+1/2, $\bar{y}+1/2,0 [0,0,w]$	$\bar{y},x,0 [0,0,\bar{w}]$ y+1/2,x+1/2,0 [0,0, $\bar{w}$ ]	y, $\bar{x},0 [0,0,\bar{w}]$ $\bar{y}+1/2,\bar{x}+1/2,0 [0,0,\bar{w}]$
8	h	m'.2'm	x,x+1/2,1/2 [ $\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,1/2 [u,\bar{u},0]$	$\bar{x}+1/2,x,1/2 [u,u,0]$	x+1/2, $\bar{x},1/2 [\bar{u},\bar{u},0]$
8	g	m.2m	x,x+1/2,0 [0,0,0]	$\bar{x},\bar{x}+1/2,0 [0,0,0]$	$\bar{x}+1/2,x,0 [0,0,0]$	x+1/2, $\bar{x},0 [0,0,0]$
8	f	2.mm	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	1/2,0, $\bar{z} [0,0,0]$	0,1/2, $\bar{z} [0,0,0]$
8	e	4'..	0,0,z [0,0,0]	1/2,1/2, $\bar{z} [0,0,0]$	0,0, $\bar{z} [0,0,0]$	1/2,1/2,z [0,0,0]
4	d	m.mm	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		
4	c	m'.mm	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
4	b	4'/m'..	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4	a	4'/m..	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

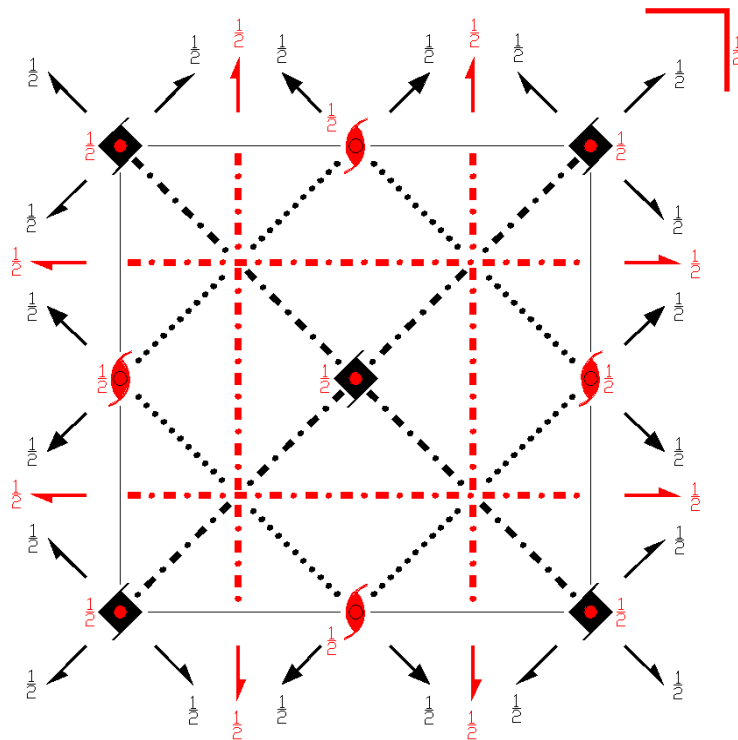
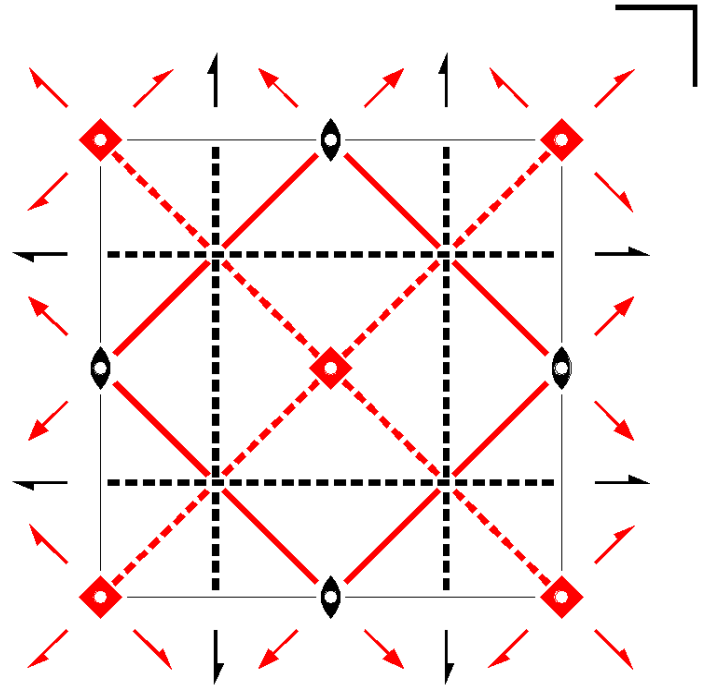
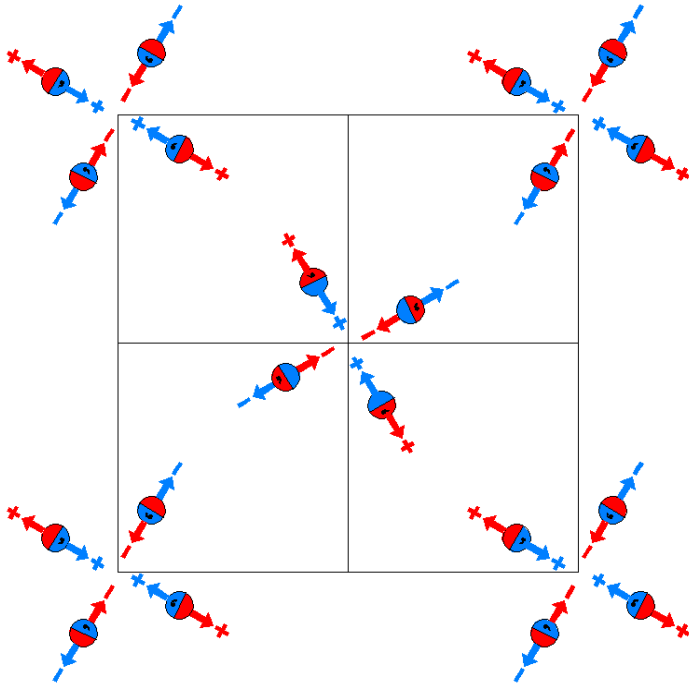
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_{2c} 4'/mbm'$   
127.12.1064

$4/mmm1'$   
 $P_{2c} 4'/m2_1/b2'/m'$

Tetragonal



**Origin** at center ( 4'/m ) at 4'/m12, 'g'

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 4 <sup>+</sup> ' 0,0,z (4 <sub>z</sub>  0,0,0)'	(4) 4 <sup>-</sup> ' 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(5) 2 (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>  1/2,1/2,0)	(6) 2 (1/2,0,0) x,1/4,0 (2 <sub>x</sub>  1/2,1/2,0)	(7) 2' (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>  1/2,1/2,0)'	(8) 2' x, $\bar{x}$ +1/2,0 (2 <sub>xy</sub> <sup>-</sup>  1/2,1/2,0)'
(9) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(10) m x,y,0 (m <sub>z</sub>  0,0,0)	(11) $\bar{4}^+$ ' 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'	(12) $\bar{4}^-$ ' 0,0,z; 0,0,0 ( $\bar{4}_z$ <sup>-1</sup>  0,0,0)'
(13) a (1/2,0,0) x,1/4,z (m <sub>y</sub>  1/2,1/2,0)	(14) b (0,1/2,0) 1/4,y,z (m <sub>x</sub>  1/2,1/2,0)	(15) m' x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,0)'	(16) g' (1/2,1/2,0) x,x,z (m <sub>xy</sub> <sup>-</sup>  1/2,1/2,0)'

For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 2' (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)'	(3) 4 <sup>+</sup> (0,0,1) 0,0,z (4 <sub>z</sub>  0,0,1)	(4) 4 <sup>-</sup> (0,0,1) 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,1)
(5) 2' (0,1/2,0) 1/4,y,1/2 (2 <sub>y</sub>  1/2,1/2,1)'	(6) 2' (1/2,0,0) x,1/4,1/2 (2 <sub>x</sub>  1/2,1/2,1)'	(7) 2 (1/2,1/2,0) x,x,1/2 (2 <sub>xy</sub>  1/2,1/2,1)	(8) 2 x, $\bar{x}$ +1/2,1/2 (2 <sub>xy</sub> <sup>-</sup>  1/2,1/2,1)
(9) $\bar{1}$ ' 0,0,1/2 ( $\bar{1}$  0,0,1)'	(10) m' x,y,1/2 (m <sub>z</sub>  0,0,1)'	(11) $\bar{4}^+$ 0,0,z; 0,0,1/2 ( $\bar{4}_z$  0,0,1)	(12) $\bar{4}^-$ 0,0,z; 0,0,1/2 ( $\bar{4}_z$ <sup>-1</sup>  0,0,1)
(13) n' (1/2,0,1) x,1/4,z (m <sub>y</sub>  1/2,1/2,1)'	(14) n' (0,1/2,1) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1)'	(15) c (0,0,1) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,1)	(16) n (1/2,1/2,1) x,x,z (m <sub>xy</sub> <sup>-</sup>  1/2,1/2,1)

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
32 I 1				
(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]	
(5) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x+1/2, $\bar{y}+1/2,z$ [ $u,\bar{v},\bar{w}$ ]	(7) y+1/2,x+1/2,z [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $v,u,w$ ]	
(9) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(10) x,y,z [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,z$ [ $\bar{v},u,\bar{w}$ ]	
(13) x+1/2, $\bar{y}+1/2,z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $\bar{v},\bar{u},w$ ]	(16) y+1/2,x+1/2,z [ $v,u,w$ ]	
16 k ..m'	x,x+1/2,z [u,u,w]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,z$ [ $u,\bar{u},\bar{w}$ ]	x+1/2, $\bar{x},z$ [ $\bar{u},u,\bar{w}$ ]
	$\bar{x}+1/2,x,z$ [ $\bar{u},u,\bar{w}$ ]	x+1/2, $\bar{x},z$ [ $u,\bar{u},\bar{w}$ ]	x,x+1/2,z [ $\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x}+1/2,z$ [ $u,u,w$ ]

16	j	m'..	x,y,1/2 [u,v,0] $\bar{x}+1/2,y+1/2,1/2$ [u, $\bar{v}$ ,0]	$\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v}$ ,0] x+1/2, $\bar{y}+1/2,1/2$ [ $\bar{u},v,0$ ]	$\bar{y},x,1/2$ [v, $\bar{u}$ ,0] y+1/2,x+1/2,1/2 [v,u,0]	y, $\bar{x},1/2$ [ $\bar{v},u,0$ ] $\bar{y}+1/2,\bar{x}+1/2,1/2$ [ $\bar{v},\bar{u},0$ ]
16	i	m..	x,y,0 [0,0,w] $\bar{x}+1/2,y+1/2,0$ [0,0, $\bar{w}$ ]	$\bar{x},\bar{y},0$ [0,0,w] x+1/2, $\bar{y}+1/2,0$ [0,0, $\bar{w}$ ]	$\bar{y},x,0$ [0,0, $\bar{w}$ ] y+1/2,x+1/2,0 [0,0,w]	y, $\bar{x},0$ [0,0, $\bar{w}$ ] $\bar{y}+1/2,\bar{x}+1/2,0$ [0,0,w]
8	h	m'.2m'	x,x+1/2,1/2 [u,u,0]	$\bar{x},\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,1/2$ [u, $\bar{u},0$ ]	x+1/2, $\bar{x},1/2$ [ $\bar{u},u,0$ ]
8	g	m.2'm'	x,x+1/2,0 [0,0,w]	$\bar{x},\bar{x}+1/2,0$ [0,0,w]	$\bar{x}+1/2,x,0$ [0,0, $\bar{w}$ ]	x+1/2, $\bar{x},0$ [0,0, $\bar{w}$ ]
8	f	2.m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]
8	e	4'..	0,0,z [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2,z [0,0,0]
4	d	m.m'm'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]		
4	c	m'.mm	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
4	b	4'/m'..	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4	a	4'/m..	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

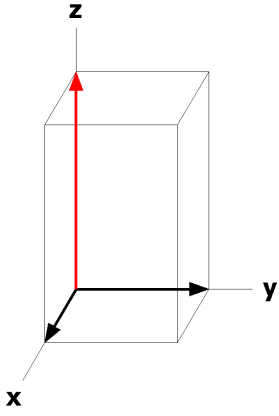
### Symmetry of Special Projections

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>c</sub>·2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [1,1,0] p<sub>2a</sub>·2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/2

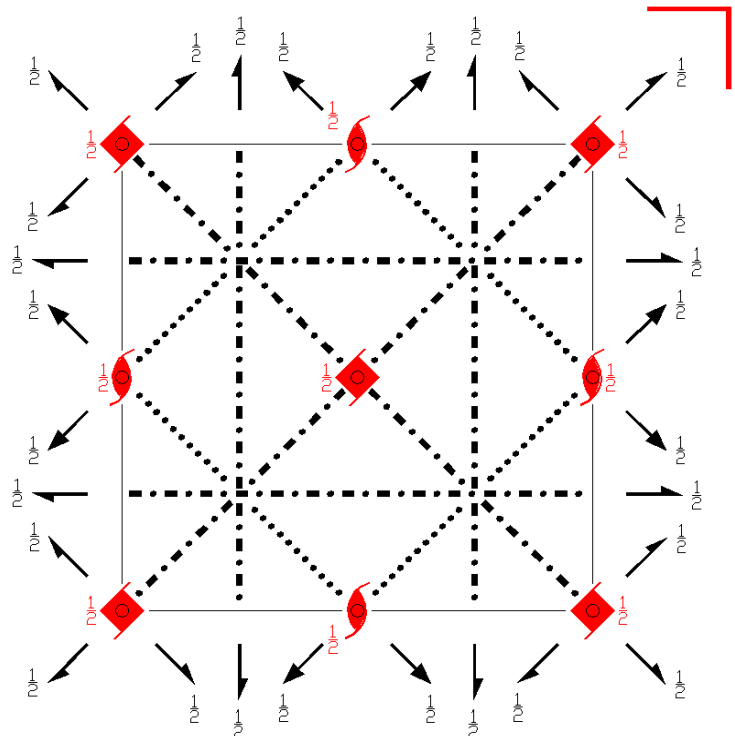
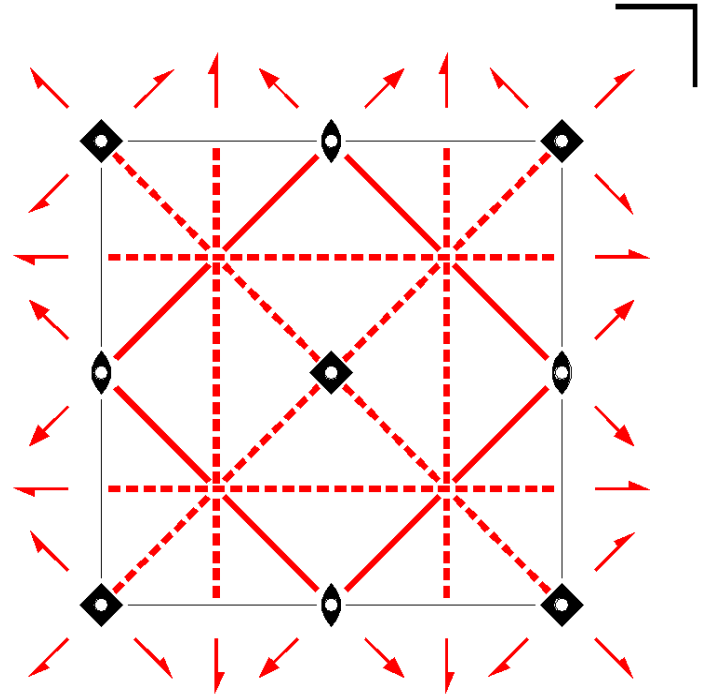
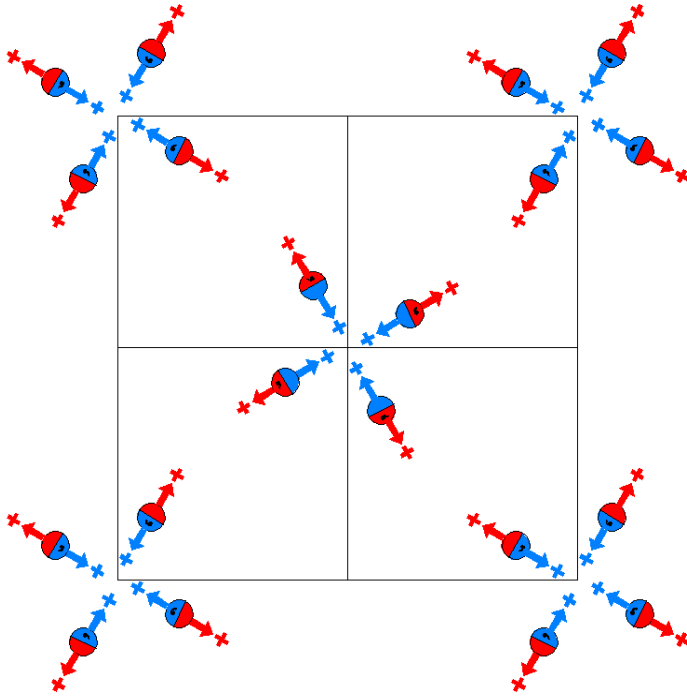




$P_{2c} 4/m\bar{b}'m'$   
127.13.1065

$4/mmm1'$   
 $P_{2c} 4/m2_1'b'2'/m'$

Tetragonal



**Origin** at center ( 4/m ) at 4/m12, 'g'

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)	(4) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)
(5) 2' (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>  1/2,1/2,0)'	(6) 2' (1/2,0,0) x,1/4,0 (2 <sub>x</sub>  1/2,1/2,0)'	(7) 2' (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>  1/2,1/2,0)'	(8) 2' x, $\bar{x}$ +1/2,0 (2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)'
(9) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(10) m x,y,0 (m <sub>z</sub>  0,0,0)	(11) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)	(12) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z$ <sup>-1</sup>  0,0,0)
(13) a' (1/2,0,0) x,1/4,z (m <sub>y</sub>  1/2,1/2,0)'	(14) b' (0,1/2,0) 1/4,y,z (m <sub>x</sub>  1/2,1/2,0)'	(15) m' x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,0)'	(16) g' (1/2,1/2,0) x,x,z (m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)'

For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 2' (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)'	(3) 4 <sup>+</sup> ' (0,0,1) 0,0,z (4 <sub>z</sub>  0,0,1)'	(4) 4 <sup>-</sup> ' (0,0,1) 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,1)'
(5) 2 (0,1/2,0) 1/4,y,1/2 (2 <sub>y</sub>  1/2,1/2,1)	(6) 2 (1/2,0,0) x,1/4,1/2 (2 <sub>x</sub>  1/2,1/2,1)	(7) 2 (1/2,1/2,0) x,x,1/2 (2 <sub>xy</sub>  1/2,1/2,1)	(8) 2 x, $\bar{x}$ +1/2,1/2 (2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1)
(9) $\bar{1}$ ' 0,0,1/2 ( $\bar{1}$  0,0,1)'	(10) m' x,y,1/2 (m <sub>z</sub>  0,0,1)'	(11) $\bar{4}^+$ ' 0,0,z; 0,0,1/2 ( $\bar{4}_z$  0,0,1)'	(12) $\bar{4}^-$ ' 0,0,z; 0,0,1/2 ( $\bar{4}_z$ <sup>-1</sup>  0,0,1)'
(13) n (1/2,0,1) x,1/4,z (m <sub>y</sub>  1/2,1/2,1)	(14) n (0,1/2,1) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1)	(15) c (0,0,1) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,1)	(16) n (1/2,1/2,1) x,x,z (m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1)

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(0,0,1)' +		
32 I 1				
(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [ $v,\bar{u},w$ ]	
(5) $\bar{x}$ +1/2,y+1/2, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) x+1/2, $\bar{y}$ +1/2, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) y+1/2,x+1/2, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y}$ +1/2, $\bar{x}$ +1/2, $\bar{z}$ [ $v,u,w$ ]	
(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]	
(13) x+1/2, $\bar{y}$ +1/2,z [ $\bar{u},\bar{v},w$ ]	(14) $\bar{x}$ +1/2,y+1/2,z [ $\bar{u},\bar{v},w$ ]	(15) $\bar{y}$ +1/2, $\bar{x}$ +1/2,z [ $\bar{v},\bar{u},w$ ]	(16) y+1/2,x+1/2,z [ $v,u,w$ ]	
16 k ..m'	x,x+1/2,z [u,u,w]	$\bar{x},\bar{x}$ +1/2,z [ $\bar{u},\bar{u},w$ ]	$\bar{x}$ +1/2,x,z [ $\bar{u},u,w$ ]	x+1/2, $\bar{x},z$ [ $u,\bar{u},w$ ]
	$\bar{x}$ +1/2,x, $\bar{z}$ [ $\bar{u},\bar{u},w$ ]	x+1/2, $\bar{x},\bar{z}$ [ $\bar{u},u,w$ ]	x,x+1/2, $\bar{z}$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x}$ +1/2, $\bar{z}$ [ $u,u,w$ ]

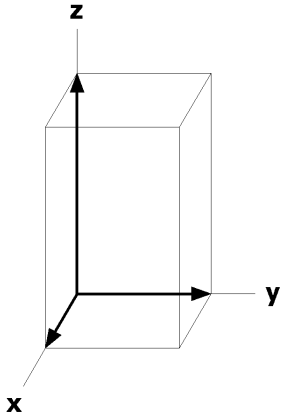
16	j	m'..	x,y,1/2 [u,v,0] $\bar{x}+1/2,y+1/2,1/2 [\bar{u},v,0]$	$\bar{x},\bar{y},1/2 [\bar{u},\bar{v},0]$ x+1/2, $\bar{y}+1/2,1/2 [u,\bar{v},0]$	$\bar{y},x,1/2 [\bar{v},u,0]$ y+1/2,x+1/2,1/2 [v,u,0]	y, $\bar{x},1/2 [v,\bar{u},0]$ $\bar{y}+1/2,\bar{x}+1/2,1/2 [\bar{v},\bar{u},0]$
16	i	m..	x,y,0 [0,0,w] $\bar{x}+1/2,y+1/2,0 [0,0,w]$	$\bar{x},\bar{y},0 [0,0,w]$ x+1/2, $\bar{y}+1/2,0 [0,0,w]$	$\bar{y},x,0 [0,0,w]$ y+1/2,x+1/2,0 [0,0,w]	y, $\bar{x},0 [0,0,w]$ $\bar{y}+1/2,\bar{x}+1/2,0 [0,0,w]$
8	h	m'.2m'	x,x+1/2,1/2 [u,u,0]	$\bar{x},\bar{x}+1/2,1/2 [\bar{u},\bar{u},0]$	$\bar{x}+1/2,x,1/2 [\bar{u},u,0]$	x+1/2, $\bar{x},1/2 [u,\bar{u},0]$
8	g	m.2'm'	x,x+1/2,0 [0,0,w]	$\bar{x},\bar{x}+1/2,0 [0,0,w]$	$\bar{x}+1/2,x,0 [0,0,w]$	x+1/2, $\bar{x},0 [0,0,w]$
8	f	2.m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	1/2,0, $\bar{z} [0,0,w]$	0,1/2, $\bar{z} [0,0,w]$
8	e	4..	0,0,z [0,0,w]	1/2,1/2, $\bar{z} [0,0,w]$	0,0, $\bar{z} [0,0,w]$	1/2,1/2,z [0,0,w]
4	d	m.m'm'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]		
4	c	m'.m'm'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		
4	b	4/m'..	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4	a	4/m..	0,0,0 [0,0,w]	1/2,1/2,0 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,1/2

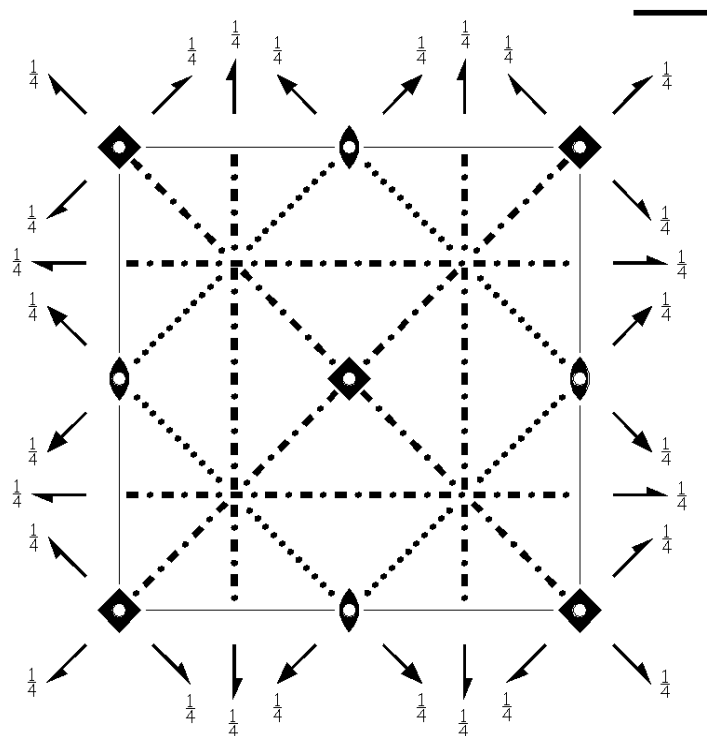
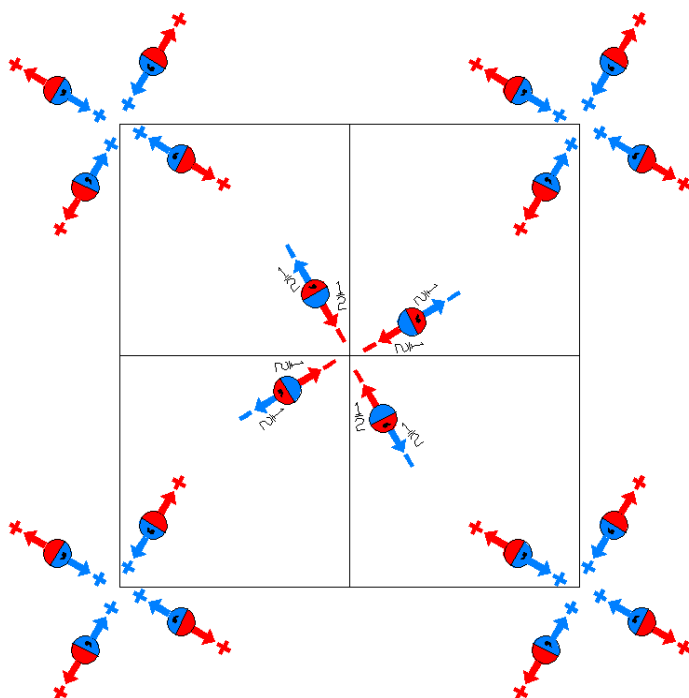
Along [1,1,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/2



P4/mnc  
128.1.1066

4/mmm  
P4/m2<sub>1</sub>/n2/c

Tetragonal



Origin at center ( 4/m ) at 4/m1n

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                    | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)                |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)  | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)  | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)            | (8) 2 x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2) |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)                  | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)                     | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)               | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                         |
| (13) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (14) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (15) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (16) n (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

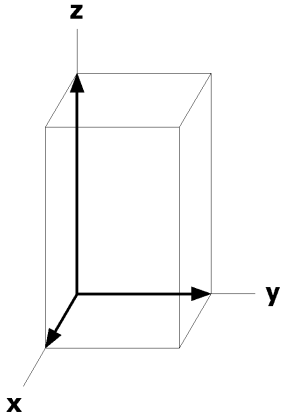
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	i	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(10) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]	(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	h	m..	$x,y,0$ [ $0,0,w$ ]	$\bar{x},\bar{y},0$ [ $0,0,w$ ]	$\bar{y},x,0$ [ $0,0,w$ ]	$y,\bar{x},0$ [ $0,0,w$ ]	$\bar{x}+1/2,y+1/2,1/2$ [ $0,0,\bar{w}$ ]	$x+1/2,\bar{y}+1/2,1/2$ [ $0,0,\bar{w}$ ]	$y+1/2,x+1/2,1/2$ [ $0,0,\bar{w}$ ]	$\bar{y}+1/2,\bar{x}+1/2,1/2$ [ $0,0,\bar{w}$ ]								
8	g	..2	$x,x+1/2,1/4$ [ $u,u,0$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},u,0$ ]	$x+1/2,\bar{x},1/4$ [ $u,\bar{u},0$ ]	$\bar{x},\bar{x}+1/2,3/4$ [ $u,u,0$ ]	$x,x+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},3/4$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,x,3/4$ [ $u,\bar{u},0$ ]								
8	f	2..	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,w$ ]	$1/2,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}$ [ $0,0,w$ ]	$1/2,0,\bar{z}$ [ $0,0,w$ ]	$1/2,0,z+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,z+1/2$ [ $0,0,\bar{w}$ ]								
4	e	4..	$0,0,z$ [ $0,0,w$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,0,\bar{z}$ [ $0,0,w$ ]	$1/2,1/2,z+1/2$ [ $0,0,\bar{w}$ ]												
4	d	2.22	$0,1/2,1/4$ [ $0,0,0$ ]	$1/2,0,1/4$ [ $0,0,0$ ]	$0,1/2,3/4$ [ $0,0,0$ ]	$1/2,0,3/4$ [ $0,0,0$ ]												
4	c	2/m..	$0,1/2,0$ [ $0,0,w$ ]	$1/2,0,0$ [ $0,0,w$ ]	$1/2,0,1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,1/2$ [ $0,0,\bar{w}$ ]												
2	b	4/m..	$0,0,1/2$ [ $0,0,w$ ]	$1/2,1/2,0$ [ $0,0,\bar{w}$ ]														
2	a	4/m..	$0,0,0$ [ $0,0,w$ ]	$1/2,1/2,1/2$ [ $0,0,\bar{w}$ ]														

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4gm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c_{2v}2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p_{2a}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,1/4$

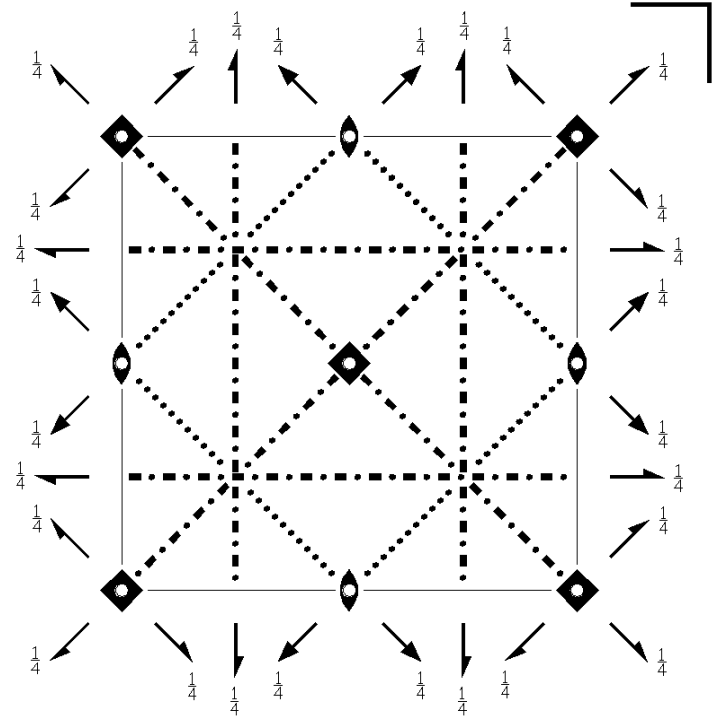
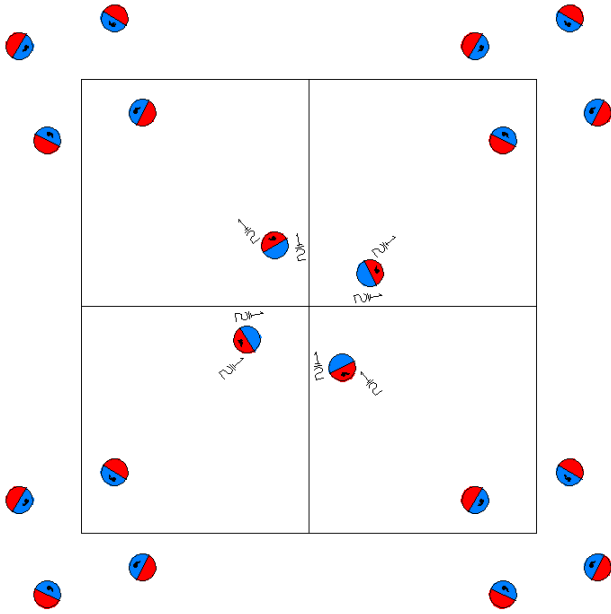


P4/mnc1'  
128.2.1067

4/mmm1'  
P4/m2<sub>1</sub>/n2/c1'

Tetragonal

1'



Origin at center ( 4/m1' ) at 4/m1n1'

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For 1 + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                    | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)                |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)  | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)  | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)            | (8) 2 x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2) |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)                  | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)                     | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)               | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                         |
| (13) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (14) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (15) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (16) n (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)  |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)'	(4) 4' 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(5) 2' (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>  1/2,1/2,1/2)'	(6) 2' (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>  1/2,1/2,1/2)'	(7) 2' (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(8) 2' x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub> <sup>-</sup>  1/2,1/2,1/2)'
(9) $\bar{1}$ ' 0,0,0 ( $\bar{1}$  0,0,0)'	(10) m' x,y,0 (m <sub>z</sub>  0,0,0)'	(11) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'	(12) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z$ <sup>-1</sup>  0,0,0)'
(13) n' (1/2,0,1/2) x,1/4,z (m <sub>y</sub>  1/2,1/2,1/2)'	(14) n' (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1/2)'	(15) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,1/2)'	(16) n' (1/2,1/2,1/2) x,x,z (m <sub>xy</sub> <sup>-</sup>  1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

**Positions**

			Coordinates															
Multiplicity, Wyckoff letter, Site Symmetry.			1 +	1' +														
16	i	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z$ [0,0,0]	(4) y, $\bar{x},z$ [0,0,0]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [0,0,0]	(6) x+1/2, $\bar{y}+1/2,\bar{z}+1/2$ [0,0,0]	(7) y+1/2,x+1/2, $\bar{z}+1/2$ [0,0,0]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [0,0,0]	(9) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(10) x,y, $\bar{z}$ [0,0,0]	(11) y, $\bar{x},\bar{z}$ [0,0,0]	(12) $\bar{y},x,\bar{z}$ [0,0,0]	(13) x+1/2, $\bar{y}+1/2,z+1/2$ [0,0,0]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [0,0,0]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [0,0,0]	(16) y+1/2,x+1/2,z+1/2 [0,0,0]
8	h	m..1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{y},x,0$ [0,0,0]	y, $\bar{x},0$ [0,0,0]	$\bar{x}+1/2,y+1/2,1/2$ [0,0,0]	x+1/2, $\bar{y}+1/2,1/2$ [0,0,0]	y+1/2,x+1/2,1/2 [0,0,0]	$\bar{y}+1/2,\bar{x}+1/2,1/2$ [0,0,0]								
8	g	..21'	x,x+1/2,1/4 [0,0,0]	$\bar{x},\bar{x}+1/2,1/4$ [0,0,0]	$\bar{x}+1/2,x,1/4$ [0,0,0]	x+1/2, $\bar{x},1/4$ [0,0,0]	$\bar{x},\bar{x}+1/2,3/4$ [0,0,0]	x,x+1/2,3/4 [0,0,0]	x+1/2, $\bar{x},3/4$ [0,0,0]	$\bar{x}+1/2,x,3/4$ [0,0,0]								
8	f	2..1'	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	0,1/2, $\bar{z}+1/2$ [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	1/2,0,z+1/2 [0,0,0]	0,1/2,z+1/2 [0,0,0]								
4	e	4..1'	0,0,z [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2,z+1/2 [0,0,0]												
4	d	2.221'	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,3/4 [0,0,0]												
4	c	2/m..1'	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]												

2	b	4/m..1'	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
2	a	4/m..1'	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]

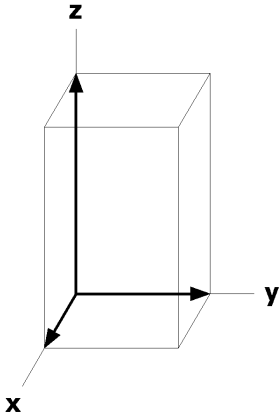
### Symmetry of Special Projections

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

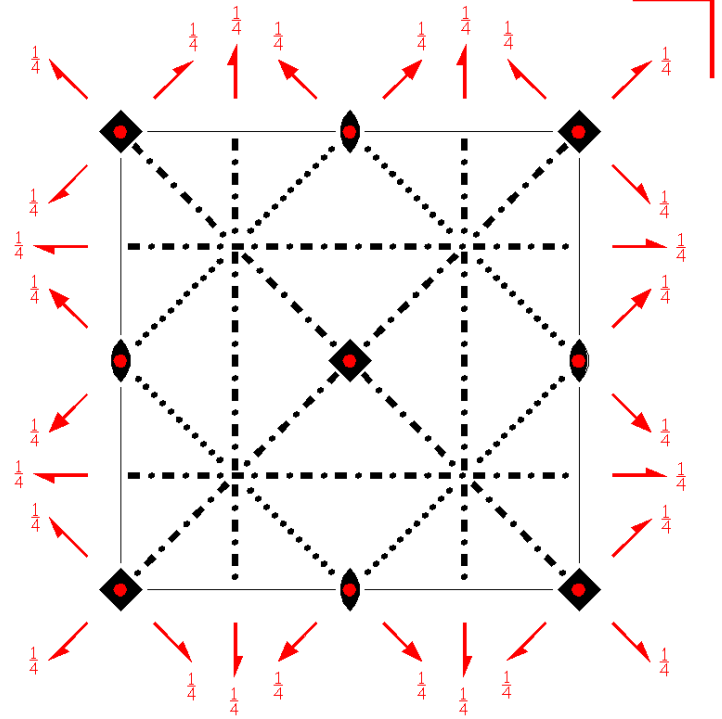
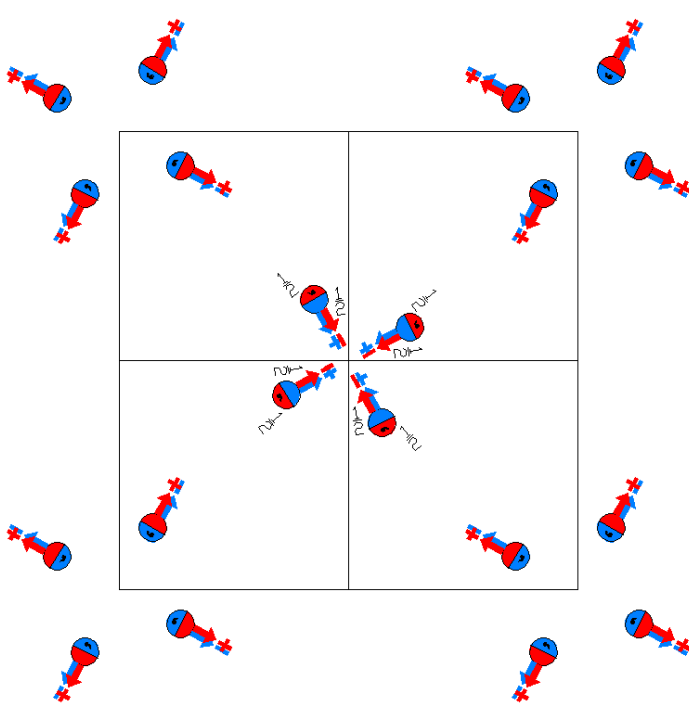




P4/m'nc  
128.3.1068

4/m'mm  
P4/m'2<sub>1</sub>'/n2'/c

Tetragonal



Origin at center ( 4/m' ) at 4/m'1n

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                       | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                         | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)           |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'               | (8) 2' x,x̄+1/2,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'                      |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'                                  | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'                    | (11) 4̄ <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (12) 4̄ <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (13) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)  | (14) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)  | (15) c (0,0,1/2) x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)               | (16) n (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)                |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

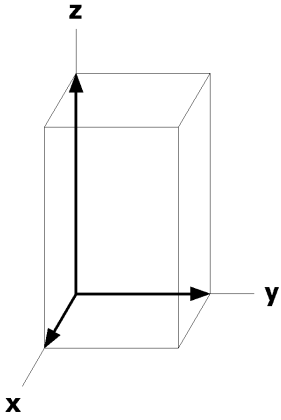
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	i	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $v,u,w$ ]	(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	h	m'..	$x,y,0$ [ $u,v,0$ ]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},u,0$ ]	$y,\bar{x},0$ [ $v,\bar{u},0$ ]	$\bar{x}+1/2,y+1/2,1/2$ [ $u,\bar{v},0$ ]	$x+1/2,\bar{y}+1/2,1/2$ [ $\bar{u},v,0$ ]	$y+1/2,x+1/2,1/2$ [ $\bar{v},\bar{u},0$ ]	$\bar{y}+1/2,\bar{x}+1/2,1/2$ [ $v,u,0$ ]								
8	g	..2'	$x,x+1/2,1/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},\bar{u},w$ ]	$x+1/2,\bar{x},1/4$ [ $u,u,w$ ]	$\bar{x},\bar{x}+1/2,3/4$ [ $u,\bar{u},\bar{w}$ ]	$x,x+1/2,3/4$ [ $\bar{u},u,\bar{w}$ ]	$x+1/2,\bar{x},3/4$ [ $u,u,\bar{w}$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]								
8	f	2..	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,w$ ]	$1/2,0,\bar{z}+1/2$ [ $0,0,w$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,w$ ]	$0,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,0,z+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,z+1/2$ [ $0,0,\bar{w}$ ]								
4	e	4..	$0,0,z$ [ $0,0,w$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,w$ ]	$0,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,1/2,z+1/2$ [ $0,0,\bar{w}$ ]												
4	d	2.2'2'	$0,1/2,1/4$ [ $0,0,w$ ]	$1/2,0,1/4$ [ $0,0,w$ ]	$0,1/2,3/4$ [ $0,0,\bar{w}$ ]	$1/2,0,3/4$ [ $0,0,\bar{w}$ ]												
4	c	2/m'..	$0,1/2,0$ [ $0,0,0$ ]	$1/2,0,0$ [ $0,0,0$ ]	$1/2,0,1/2$ [ $0,0,0$ ]	$0,1/2,1/2$ [ $0,0,0$ ]												
2	b	4/m'..	$0,0,1/2$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]														
2	a	4/m'..	$0,0,0$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]														

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4gm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c_{2v}2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

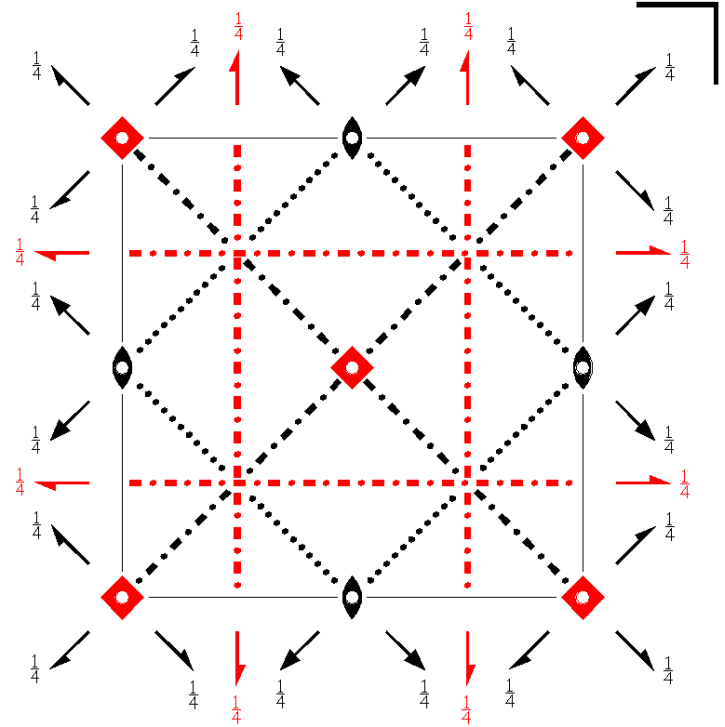
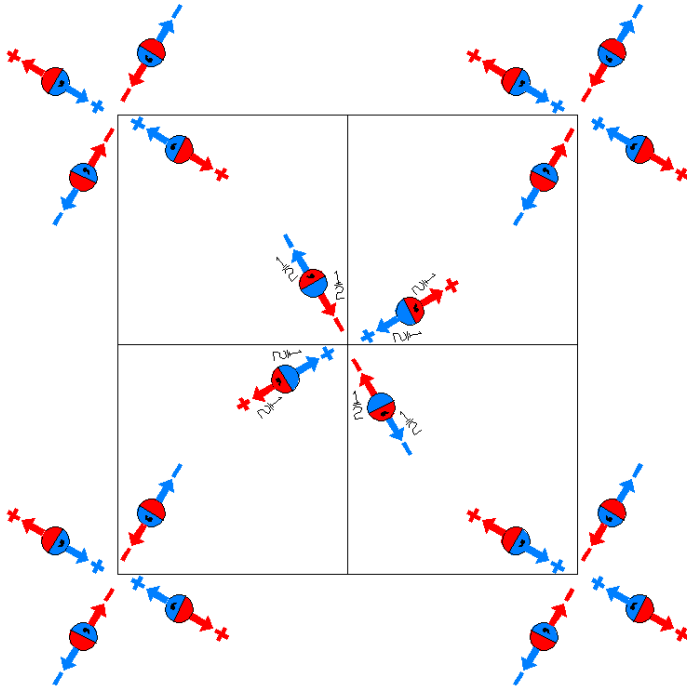
Along  $[1,1,0]$   $p_{2a}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,0$



P4'/mn'c  
128.4.1069

4'/mm'm  
P4'/m2<sub>1</sub>'/n'2/c

Tetragonal



Origin at center ( 4'/m ) at 4'/m1n

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                         | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)'      | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'                |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub> ' 1/2,1/2,1/2)'  | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub> ' 1/2,1/2,1/2)'  | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)            | (8) 2 x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2) |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)                     | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)                        | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'              | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                        |
| (13) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub> ' 1/2,1/2,1/2)' | (14) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub> ' 1/2,1/2,1/2)' | (15) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (16) n (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

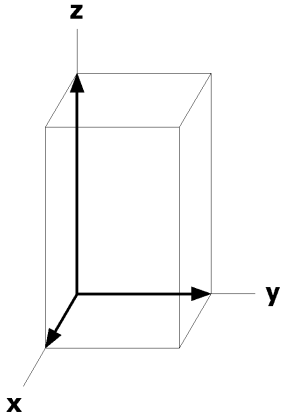
			Coordinates															
Multiplicity,	Wyckoff letter,	Site Symmetry.																
16	i	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $v,\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(10) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	h	m..	$x,y,0$ [ $0,0,w$ ]	$\bar{x},\bar{y},0$ [ $0,0,w$ ]	$\bar{y},x,0$ [ $0,0,\bar{w}$ ]	$y,\bar{x},0$ [ $0,0,\bar{w}$ ]	$\bar{x}+1/2,y+1/2,1/2$ [ $0,0,w$ ]	$x+1/2,\bar{y}+1/2,1/2$ [ $0,0,w$ ]	$y+1/2,x+1/2,1/2$ [ $0,0,\bar{w}$ ]	$\bar{y}+1/2,\bar{x}+1/2,1/2$ [ $0,0,\bar{w}$ ]								
8	g	..2	$x,x+1/2,1/4$ [ $u,u,0$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,1/4$ [ $u,\bar{u},0$ ]	$x+1/2,\bar{x},1/4$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}+1/2,3/4$ [ $u,u,0$ ]	$x,x+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},3/4$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},u,0$ ]								
8	f	2..	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}+1/2$ [ $0,0,w$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}$ [ $0,0,w$ ]	$1/2,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,0,z+1/2$ [ $0,0,w$ ]	$0,1/2,z+1/2$ [ $0,0,\bar{w}$ ]								
4	e	4'..	$0,0,z$ [ $0,0,0$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,0$ ]	$0,0,\bar{z}$ [ $0,0,0$ ]	$1/2,1/2,z+1/2$ [ $0,0,0$ ]												
4	d	2.22	$0,1/2,1/4$ [ $0,0,0$ ]	$1/2,0,1/4$ [ $0,0,0$ ]	$0,1/2,3/4$ [ $0,0,0$ ]	$1/2,0,3/4$ [ $0,0,0$ ]												
4	c	2/m..	$0,1/2,0$ [ $0,0,w$ ]	$1/2,0,0$ [ $0,0,\bar{w}$ ]	$1/2,0,1/2$ [ $0,0,w$ ]	$0,1/2,1/2$ [ $0,0,\bar{w}$ ]												
2	b	4'/m..	$0,0,1/2$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]														
2	a	4'/m..	$0,0,0$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]														

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4gm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $x,0,0$

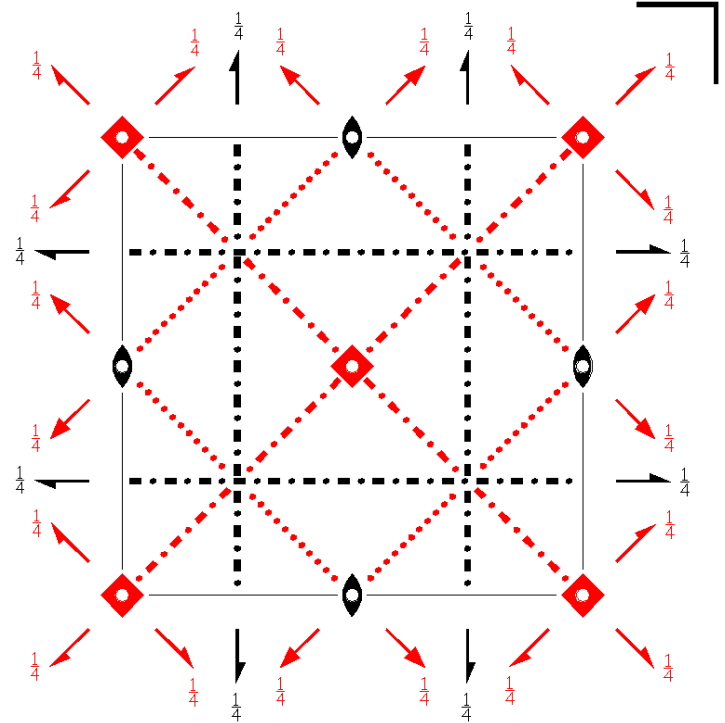
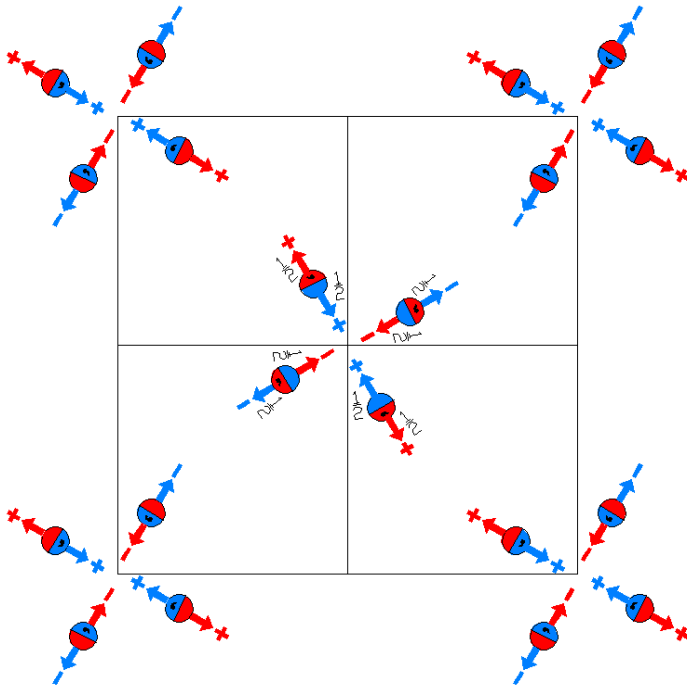
Along  $[1,1,0]$   $p_{2a'}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,1/4$



P4'/mnc'  
128.5.1070

4'/mmm'  
P4'/m2<sub>1</sub>/n2'/c'

Tetragonal



Origin at center ( 4'/m ) at 4'/m1n'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'           |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)  | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)  | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'     | (8) 2' x,x+1/2,1/4<br>(2 <sub>xy</sub> <sup>-</sup>  1/2,1/2,1/2)'          |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)                  | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)                     | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'         | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                   |
| (13) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (14) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (15) c' (0,0,1/2) x+1/2,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)'    | (16) n' (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub> <sup>-</sup>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

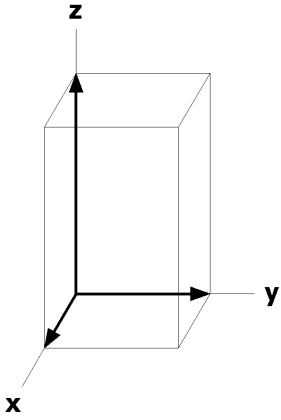
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
16	i	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $v,\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
			(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $v,u,w$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(10) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $v,u,w$ ]
8	h	m..	$x,y,0$ [ $0,0,w$ ]	$\bar{x},\bar{y},0$ [ $0,0,w$ ]	$\bar{y},x,0$ [ $0,0,\bar{w}$ ]	$y,\bar{x},0$ [ $0,0,\bar{w}$ ]
			$\bar{x}+1/2,y+1/2,1/2$ [ $0,0,\bar{w}$ ]	$x+1/2,\bar{y}+1/2,1/2$ [ $0,0,\bar{w}$ ]	$y+1/2,x+1/2,1/2$ [ $0,0,w$ ]	$\bar{y}+1/2,\bar{x}+1/2,1/2$ [ $0,0,w$ ]
8	g	..2'	$x,x+1/2,1/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x,1/4$ [ $u,u,\bar{w}$ ]	$x+1/2,\bar{x},1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x},\bar{x}+1/2,3/4$ [ $\bar{u},u,w$ ]	$x,x+1/2,3/4$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x},3/4$ [ $u,u,\bar{w}$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	f	2..	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,w$ ]
			$0,1/2,\bar{z}$ [ $0,0,w$ ]	$1/2,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,0,z+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,z+1/2$ [ $0,0,w$ ]
4	e	4'..	$0,0,z$ [ $0,0,0$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,0$ ]	$0,0,\bar{z}$ [ $0,0,0$ ]	$1/2,1/2,z+1/2$ [ $0,0,0$ ]
4	d	2.2'2'	$0,1/2,1/4$ [ $0,0,w$ ]	$1/2,0,1/4$ [ $0,0,\bar{w}$ ]	$0,1/2,3/4$ [ $0,0,w$ ]	$1/2,0,3/4$ [ $0,0,\bar{w}$ ]
4	c	2/m..	$0,1/2,0$ [ $0,0,w$ ]	$1/2,0,0$ [ $0,0,\bar{w}$ ]	$1/2,0,1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,1/2$ [ $0,0,w$ ]
2	b	4'/m..	$0,0,1/2$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]		
2	a	4'/m..	$0,0,0$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4gm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c_p \cdot 2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $x,0,0$

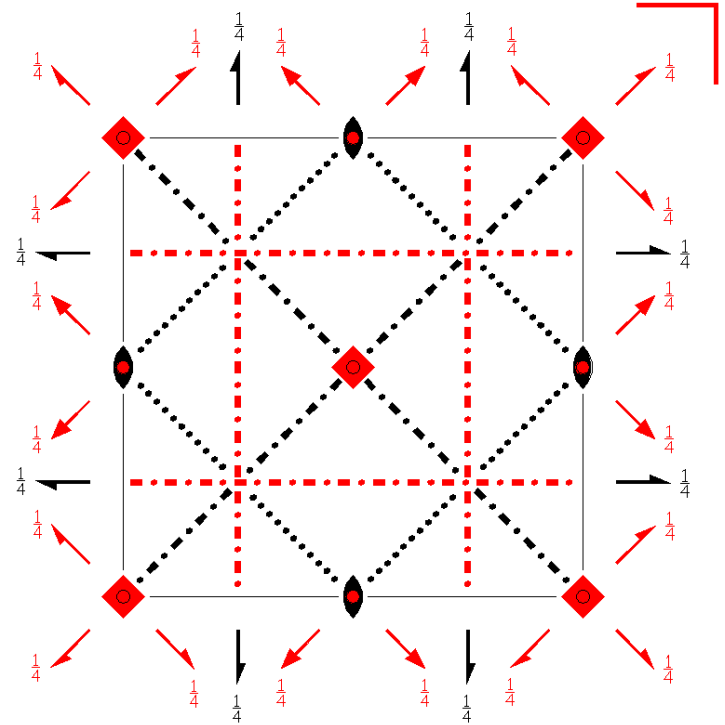
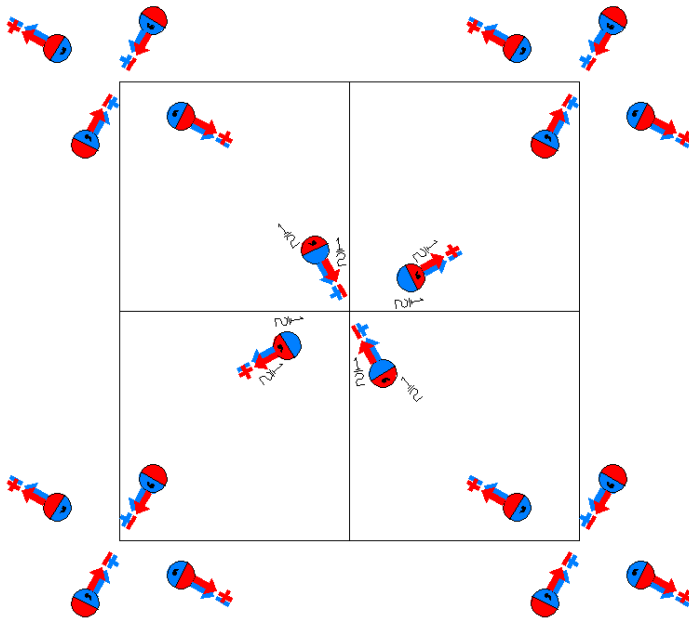
Along  $[1,1,0]$   $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,0$



P4'/m'n'c  
128.6.1071

4'/m'm'm  
P4'/m'2<sub>1</sub>/n'2'/c

Tetragonal



Origin at center ( $4'/m'$ ) at  $4'/m'1n$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                         | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)'          | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'          |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)     | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)     | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub> ' 1/2,1/2,1/2)'             | (8) 2' x,x̄+1/2,1/4<br>(2 <sub>xy</sub> ' 1/2,1/2,1/2)'                    |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'                                    | (10) m' x,y,0<br>(m <sub>z</sub> ' 0,0,0)'                     | (11) 4̄ <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup> ̄ 0,0,0) | (12) 4̄ <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-</sup> ̄ 0,0,0) |
| (13) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub> ' 1/2,1/2,1/2)' | (14) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub> ' 1/2,1/2,1/2)' | (15) c (0,0,1/2) x+1/2,x̄,z<br>(m <sub>xy</sub> ' 1/2,1/2,1/2)             | (16) n (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	i	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $v,\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $v,u,w$ ]	(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]	(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	h	m'..	$x,y,0$ [ $u,v,0$ ]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $v,\bar{u},0$ ]	$y,\bar{x},0$ [ $\bar{v},u,0$ ]	$\bar{x}+1/2,y+1/2,1/2$ [ $\bar{u},v,0$ ]	$x+1/2,\bar{y}+1/2,1/2$ [ $u,\bar{v},0$ ]	$y+1/2,x+1/2,1/2$ [ $\bar{v},\bar{u},0$ ]	$\bar{y}+1/2,\bar{x}+1/2,1/2$ [ $v,u,0$ ]								
8	g	..2'	$x,x+1/2,1/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x,1/4$ [ $u,u,\bar{w}$ ]	$x+1/2,\bar{x},1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	$\bar{x},\bar{x}+1/2,3/4$ [ $u,\bar{u},\bar{w}$ ]	$x,x+1/2,3/4$ [ $\bar{u},u,\bar{w}$ ]	$x+1/2,\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,3/4$ [ $u,u,w$ ]								
8	f	2..	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,w$ ]	$0,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}$ [ $0,0,w$ ]	$1/2,0,z+1/2$ [ $0,0,w$ ]	$0,1/2,z+1/2$ [ $0,0,\bar{w}$ ]								
4	e	4'..	$0,0,z$ [ $0,0,0$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,0$ ]	$0,0,\bar{z}$ [ $0,0,0$ ]	$1/2,1/2,z+1/2$ [ $0,0,0$ ]												
4	d	2.2'2'	$0,1/2,1/4$ [ $0,0,w$ ]	$1/2,0,1/4$ [ $0,0,\bar{w}$ ]	$0,1/2,3/4$ [ $0,0,\bar{w}$ ]	$1/2,0,3/4$ [ $0,0,w$ ]												
4	c	2/m'..	$0,1/2,0$ [ $0,0,0$ ]	$1/2,0,0$ [ $0,0,0$ ]	$1/2,0,1/2$ [ $0,0,0$ ]	$0,1/2,1/2$ [ $0,0,0$ ]												
2	b	4'/m'..	$0,0,1/2$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]														
2	a	4'/m'..	$0,0,0$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]														

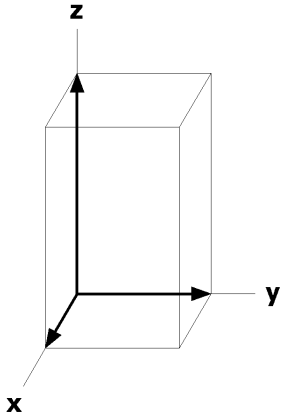
**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4'g'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p_{2a'}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,0$

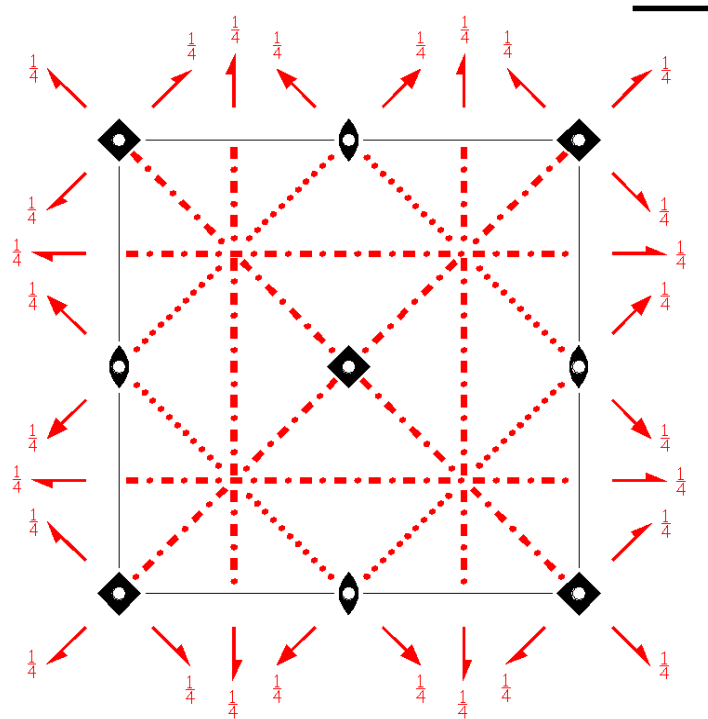
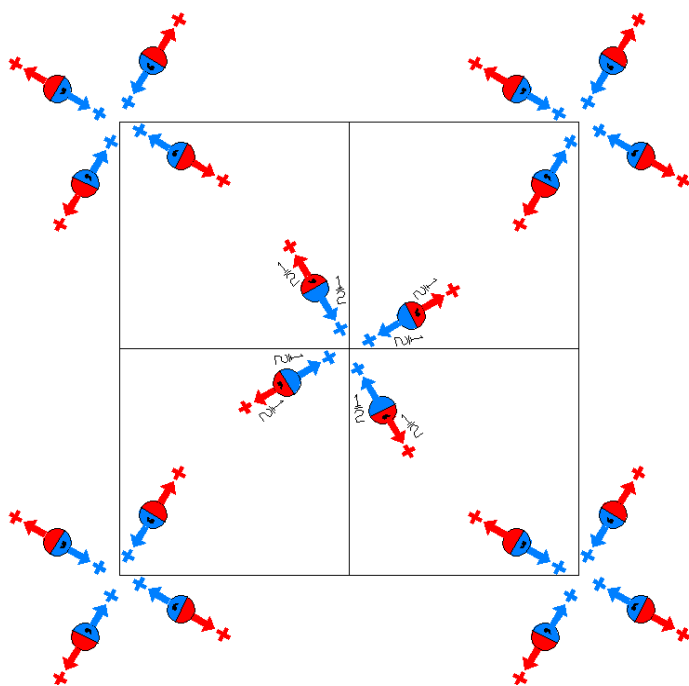




P4/mn'c'  
128.7.1072

4/mm'm'  
P4/m2<sub>1</sub>'n'2'/c'

Tetragonal



Origin at center ( 4/m ) at 4/m1n'

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                        | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)             | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)            |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)'  | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)'  | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'   | (8) 2' x,x̄+1/2,1/4<br>(2 <sub>xy</sub> <sup>-1</sup>  1/2,1/2,1/2)'         |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)                    | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)                       | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)          | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)                  |
| (13) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (14) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (15) c' (0,0,1/2) x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)' | (16) n' (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub> <sup>-1</sup>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

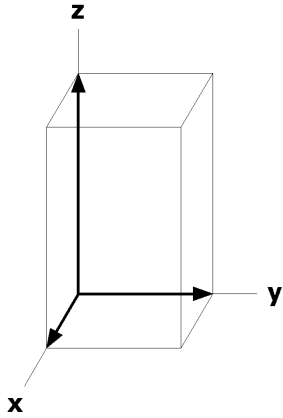
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	i	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z$ [ $\bar{v}, u, w$ ]	(4) $y, \bar{x}, z$ [v, $\bar{u}$ ,w]	(5) $\bar{x}+1/2, y+1/2, \bar{z}+1/2$ [u, $\bar{v}, w$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]	(7) $y+1/2, x+1/2, \bar{z}+1/2$ [ $\bar{v}, \bar{u}, w$ ]	(8) $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2$ [v,u,w]	(9) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(10) $x, y, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(11) $y, \bar{x}, \bar{z}$ [ $\bar{v}, u, w$ ]	(12) $\bar{y}, x, \bar{z}$ [v, $\bar{u}$ ,w]	(13) $x+1/2, \bar{y}+1/2, z+1/2$ [u, $\bar{v}, w$ ]	(14) $\bar{x}+1/2, y+1/2, z+1/2$ [ $\bar{u}, v, w$ ]	(15) $\bar{y}+1/2, \bar{x}+1/2, z+1/2$ [ $\bar{v}, \bar{u}, w$ ]	(16) $y+1/2, x+1/2, z+1/2$ [v,u,w]
8	h	m..	$x, y, 0$ [0,0,w]	$\bar{x}, \bar{y}, 0$ [0,0,w]	$\bar{y}, x, 0$ [0,0,w]	$y, \bar{x}, 0$ [0,0,w]	$\bar{x}+1/2, y+1/2, 1/2$ [0,0,w]	$x+1/2, \bar{y}+1/2, 1/2$ [0,0,w]	$y+1/2, x+1/2, 1/2$ [0,0,w]	$\bar{y}+1/2, \bar{x}+1/2, 1/2$ [0,0,w]								
8	g	..2'	$x, x+1/2, 1/4$ [ $\bar{u}, u, w$ ]	$\bar{x}, \bar{x}+1/2, 1/4$ [ $u, \bar{u}, w$ ]	$\bar{x}+1/2, x, 1/4$ [ $\bar{u}, \bar{u}, w$ ]	$x+1/2, \bar{x}, 1/4$ [ $u, u, w$ ]	$\bar{x}, \bar{x}+1/2, 3/4$ [ $\bar{u}, u, w$ ]	$x, x+1/2, 3/4$ [ $u, \bar{u}, w$ ]	$x+1/2, \bar{x}, 3/4$ [ $\bar{u}, \bar{u}, w$ ]	$\bar{x}+1/2, x, 3/4$ [ $u, u, w$ ]								
8	f	2..	$0, 1/2, z$ [0,0,w]	$1/2, 0, z$ [0,0,w]	$1/2, 0, \bar{z}+1/2$ [0,0,w]	$0, 1/2, \bar{z}+1/2$ [0,0,w]	$0, 1/2, \bar{z}$ [0,0,w]	$1/2, 0, \bar{z}$ [0,0,w]	$1/2, 0, z+1/2$ [0,0,w]	$0, 1/2, z+1/2$ [0,0,w]								
4	e	4..	$0, 0, z$ [0,0,w]	$1/2, 1/2, \bar{z}+1/2$ [0,0,w]	$0, 0, \bar{z}$ [0,0,w]	$1/2, 1/2, z+1/2$ [0,0,w]												
4	d	2.2'2'	$0, 1/2, 1/4$ [0,0,w]	$1/2, 0, 1/4$ [0,0,w]	$0, 1/2, 3/4$ [0,0,w]	$1/2, 0, 3/4$ [0,0,w]												
4	c	2/m..	$0, 1/2, 0$ [0,0,w]	$1/2, 0, 0$ [0,0,w]	$1/2, 0, 1/2$ [0,0,w]	$0, 1/2, 1/2$ [0,0,w]												
2	b	4/m..	$0, 0, 1/2$ [0,0,w]	$1/2, 1/2, 0$ [0,0,w]														
2	a	4/m..	$0, 0, 0$ [0,0,w]	$1/2, 1/2, 1/2$ [0,0,w]														

### Symmetry of Special Projections

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

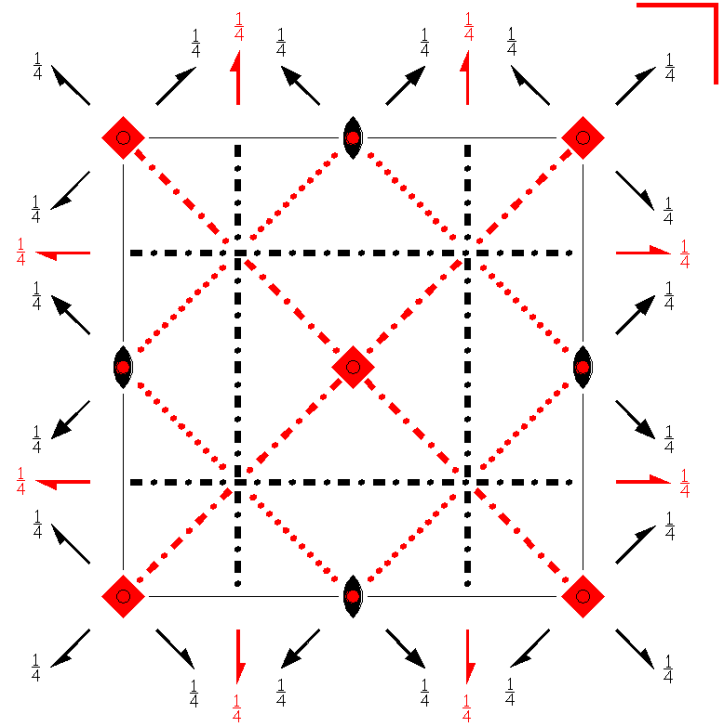
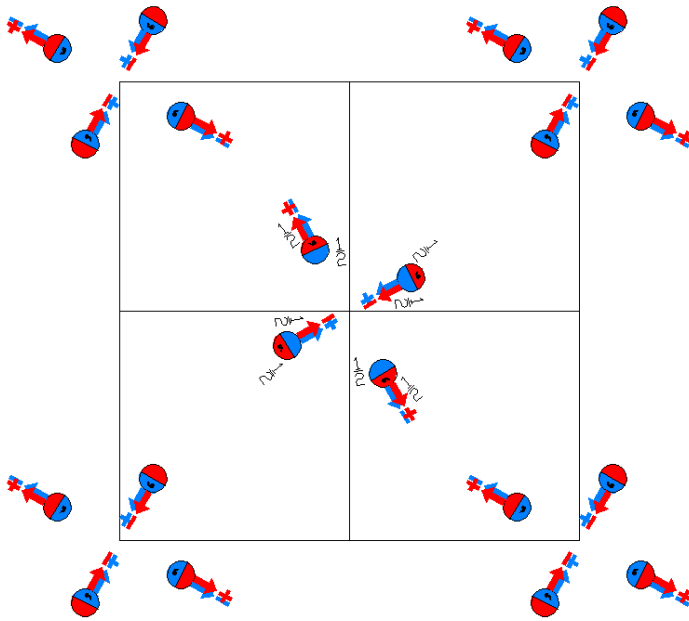
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



P4'/m'nc'  
128.8.1073

4'/m'mm'  
P4'/m'2<sub>1</sub>'/n2/c'

Tetragonal



Origin at center ( 4'/m' ) at 4'/m'1n'

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                        | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)'                         | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'                         |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub> ' 1/2,1/2,1/2)' | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub> ' 1/2,1/2,1/2)' | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)                               | (8) 2 x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)          |
| (9) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$ ' 0,0,0)'                | (10) m' x,y,0<br>(m <sub>z</sub> ' 0,0,0)'                    | (11) $\bar{4}$ <sup>+</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>+</sup>  0,0,0) | (12) $\bar{4}$ <sup>-</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>-</sup>  0,0,0) |
| (13) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)   | (14) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)   | (15) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)'                  | (16) n' (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)'         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

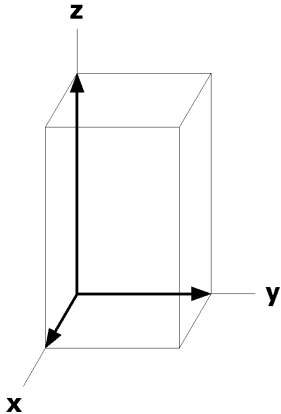
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	i	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [u,v,w]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [u,v,w]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [u,v,w]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [v,u,w]
8	h	m'..	$x,y,0$ [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},\bar{u},0$ ]	$y,\bar{x},0$ [ $\bar{v},u,0$ ]	$\bar{x}+1/2,y+1/2,1/2$ [ $\bar{u},\bar{v},0$ ]	$x+1/2,\bar{y}+1/2,1/2$ [ $\bar{u},v,0$ ]	$y+1/2,x+1/2,1/2$ [v,u,0]	$\bar{y}+1/2,\bar{x}+1/2,1/2$ [ $\bar{v},\bar{u},0$ ]								
8	g	..2	$x,x+1/2,1/4$ [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,1/4$ [u,u,0]	$x+1/2,\bar{x},1/4$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$x,x+1/2,3/4$ [u,u,0]	$x+1/2,\bar{x},3/4$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,x,3/4$ [u,u,0]								
8	f	2..	$0,1/2,z$ [0,0,w]	$1/2,0,z$ [0,0,w]	$1/2,0,\bar{z}+1/2$ [0,0,w]	$0,1/2,\bar{z}+1/2$ [0,0,w]	$0,1/2,\bar{z}$ [0,0,w]	$1/2,0,\bar{z}$ [0,0,w]	$1/2,0,z+1/2$ [0,0,w]	$0,1/2,z+1/2$ [0,0,w]								
4	e	4'..	$0,0,z$ [0,0,0]	$1/2,1/2,\bar{z}+1/2$ [0,0,0]	$0,0,\bar{z}$ [0,0,0]	$1/2,1/2,z+1/2$ [0,0,0]												
4	d	2.22	$0,1/2,1/4$ [0,0,0]	$1/2,0,1/4$ [0,0,0]	$0,1/2,3/4$ [0,0,0]	$1/2,0,3/4$ [0,0,0]												
4	c	2/m'..	$0,1/2,0$ [0,0,0]	$1/2,0,0$ [0,0,0]	$1/2,0,1/2$ [0,0,0]	$0,1/2,1/2$ [0,0,0]												
2	b	4'/m'..	$0,0,1/2$ [0,0,0]	$1/2,1/2,0$ [0,0,0]														
2	a	4'/m'..	$0,0,0$ [0,0,0]	$1/2,1/2,1/2$ [0,0,0]														

### Symmetry of Special Projections

Along [0,0,1]  $p4'gm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

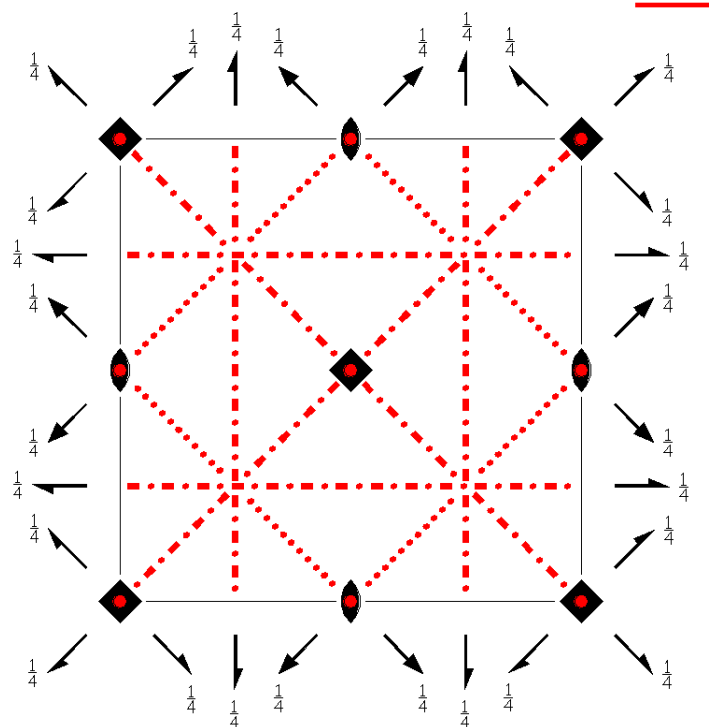
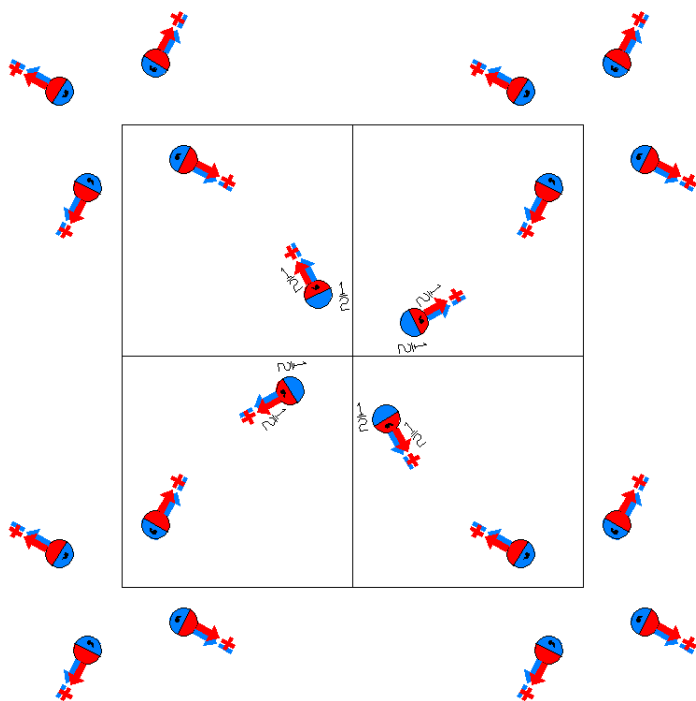
Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



P4/m'n'c'  
128.9.1074

4/m'm'm'  
P4/m'2<sub>1</sub>/n'2/c'

Tetragonal



Origin at center ( 4/m' ) at 4/m'1n'

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                        | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                      | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)                 |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)    | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)    | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)              | (8) 2 x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)  |
| (9) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$ ' 0,0,0)'                | (10) m' x,y,0<br>(m <sub>z</sub> ' 0,0,0)'                    | (11) $\bar{4}^+$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^+$ ' 0,0,0)'             | (12) $\bar{4}^-$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^-$ ' 0,0,0)'                      |
| (13) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (14) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (15) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)' | (16) n' (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

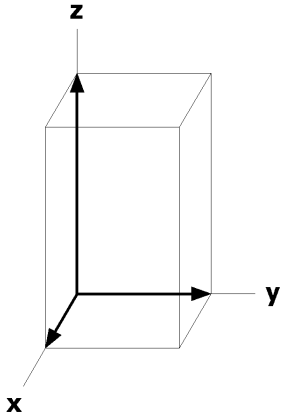
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	i	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z$ [ $v,\bar{u},w$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},z$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,z$ [ $\bar{v},u,\bar{w}$ ]	(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $v,u,w$ ]
8	h	m'..	$x,y,0$ [ $u,v,0$ ]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},u,0$ ]	$y,\bar{x},0$ [ $v,\bar{u},0$ ]	$\bar{x}+1/2,y+1/2,1/2$ [ $\bar{u},\bar{v},0$ ]	$x+1/2,\bar{y}+1/2,1/2$ [ $u,\bar{v},0$ ]	$y+1/2,x+1/2,1/2$ [ $v,u,0$ ]	$\bar{y}+1/2,\bar{x}+1/2,1/2$ [ $\bar{v},\bar{u},0$ ]								
8	g	..2	$x,x+1/2,1/4$ [ $u,u,0$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},u,0$ ]	$x+1/2,\bar{x},1/4$ [ $u,\bar{u},0$ ]	$\bar{x},\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$x,x+1/2,3/4$ [ $u,u,0$ ]	$x+1/2,\bar{x},3/4$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},u,0$ ]								
8	f	2..	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,w$ ]	$1/2,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,0,z+1/2$ [ $0,0,w$ ]	$0,1/2,z+1/2$ [ $0,0,w$ ]								
4	e	4..	$0,0,z$ [ $0,0,w$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,1/2,z+1/2$ [ $0,0,w$ ]												
4	d	2.22	$0,1/2,1/4$ [ $0,0,0$ ]	$1/2,0,1/4$ [ $0,0,0$ ]	$0,1/2,3/4$ [ $0,0,0$ ]	$1/2,0,3/4$ [ $0,0,0$ ]												
4	c	2/m'..	$0,1/2,0$ [ $0,0,0$ ]	$1/2,0,0$ [ $0,0,0$ ]	$1/2,0,1/2$ [ $0,0,0$ ]	$0,1/2,1/2$ [ $0,0,0$ ]												
2	b	4/m'..	$0,0,1/2$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]														
2	a	4/m'..	$0,0,0$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]														

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4g'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

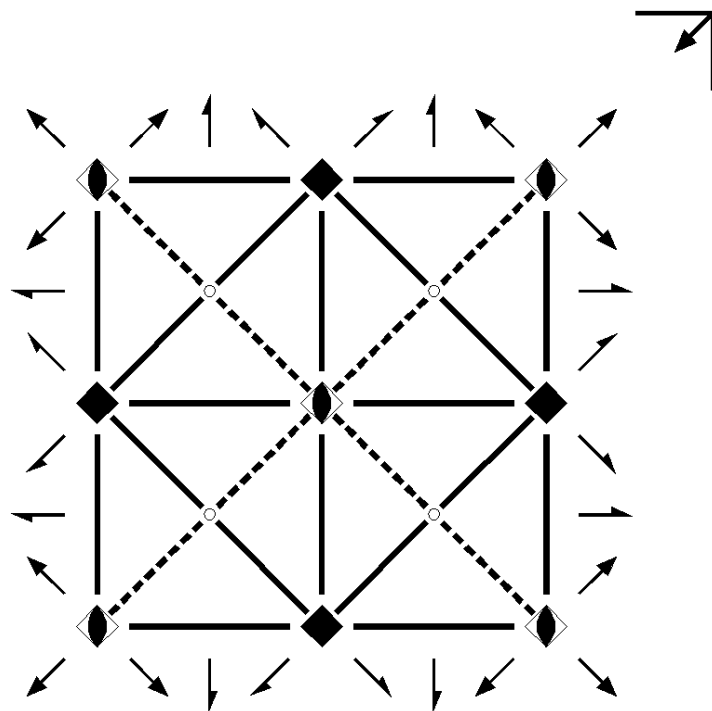
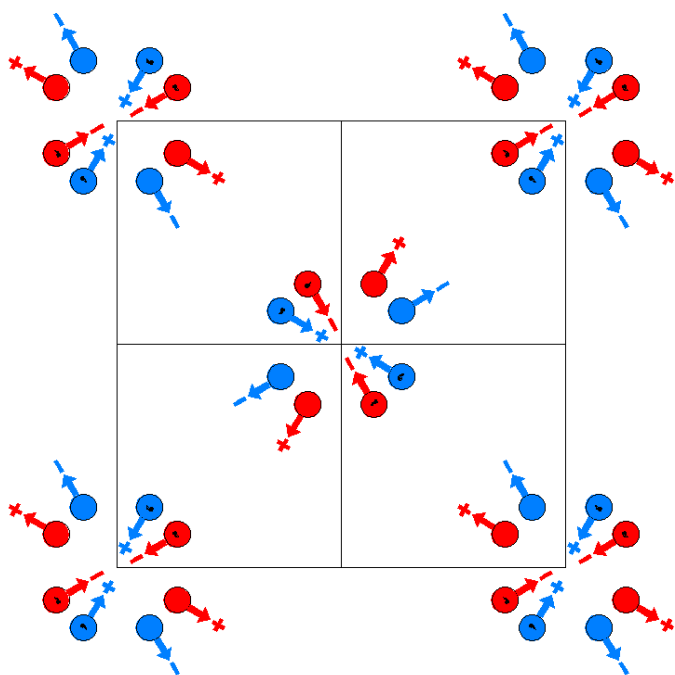
Along  $[1,1,0]$   $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



P4/nmm  
129.1.1075

4/mmm  
P4/n<sub>2</sub><sub>1</sub>/m2/m

Tetragonal



Origin at center  $\bar{4}m2$  at  $\bar{4}/nm2/g$ , at  $-1/4, 1/4, 0$  from center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |   |  |   |  |
|---|--|---|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                               | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub> <sup>+</sup>  1/2,1/2,0)  | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-</sup>  1/2,1/2,0) |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub> <sup>+</sup>  1/2,1/2,0) | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub> <sup>+</sup>  1/2,1/2,0)  | (7) 2 x,x,0<br>(2 <sub>xy</sub> <sup>+</sup>  0,0,0)                    | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,0)         |
| (9) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)                  | (10) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub> <sup>+</sup>  1/2,1/2,0) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)                | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)               |
| (13) m x,0,z<br>(m <sub>y</sub> <sup>+</sup>  0,0,0)                | (14) m 0,y,z<br>(m <sub>x</sub> <sup>+</sup>  0,0,0)                 | (15) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub> <sup>+</sup>  1/2,1/2,0) | (16) g (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub> <sup>-</sup>  1/2,1/2,0)  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

		Coordinates									
		Multiplicity, Wyckoff letter, Site Symmetry.									
16	k	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}, \bar{y}, z$	$[\bar{u}, \bar{v}, w]$	(3)	$\bar{y}+1/2, x+1/2, z$	$[\bar{v}, u, w]$	(4)	$y+1/2, \bar{x}+1/2, z$	$[v, \bar{u}, w]$
(5)	$\bar{x}+1/2, y+1/2, \bar{z}$	$[\bar{u}, v, \bar{w}]$	(6)	$x+1/2, \bar{y}+1/2, \bar{z}$	$[u, \bar{v}, \bar{w}]$	(7)	$y, x, \bar{z}$	$[v, u, \bar{w}]$	(8)	$\bar{y}, \bar{x}, \bar{z}$	$[\bar{v}, \bar{u}, \bar{w}]$
(9)	$\bar{x}+1/2, \bar{y}+1/2, \bar{z}$	$[\bar{u}, v, w]$	(10)	$x+1/2, y+1/2, \bar{z}$	$[\bar{u}, \bar{v}, w]$	(11)	$y, \bar{x}, \bar{z}$	$[\bar{v}, u, w]$	(12)	$\bar{y}, x, \bar{z}$	$[v, \bar{u}, w]$
(13)	$x, \bar{y}, z$	$[\bar{u}, v, \bar{w}]$	(14)	$\bar{x}, y, z$	$[u, \bar{v}, \bar{w}]$	(15)	$\bar{y}+1/2, \bar{x}+1/2, z$	$[v, u, \bar{w}]$	(16)	$y+1/2, x+1/2, z$	$[\bar{v}, \bar{u}, \bar{w}]$
8	j	..m	$x, x+1/2, z$	$[\bar{u}, u, 0]$	$\bar{x}, \bar{x}+1/2, z$	$[u, \bar{u}, 0]$	$\bar{x}, x+1/2, z$	$[u, \bar{u}, 0]$	$x, \bar{x}+1/2, z$	$[u, u, 0]$	
			$\bar{x}+1/2, x, \bar{z}$	$[u, u, 0]$	$x+1/2, \bar{x}, \bar{z}$	$[u, \bar{u}, 0]$	$x+1/2, x, \bar{z}$	$[u, \bar{u}, 0]$	$\bar{x}+1/2, \bar{x}, \bar{z}$	$[u, u, 0]$	
8	i	.m.	$0, y, z$	$[u, 0, 0]$	$0, \bar{y}, z$	$[\bar{u}, 0, 0]$	$\bar{y}+1/2, 1/2, z$	$[0, u, 0]$	$y+1/2, 1/2, z$	$[0, \bar{u}, 0]$	
			$1/2, y+1/2, \bar{z}$	$[\bar{u}, 0, 0]$	$1/2, \bar{y}+1/2, \bar{z}$	$[u, 0, 0]$	$y, 0, \bar{z}$	$[0, u, 0]$	$\bar{y}, 0, \bar{z}$	$[0, \bar{u}, 0]$	
8	h	..2	$x, x, 1/2$	$[u, u, 0]$	$\bar{x}, \bar{x}, 1/2$	$[\bar{u}, \bar{u}, 0]$	$\bar{x}+1/2, x+1/2, 1/2$	$[\bar{u}, u, 0]$	$x+1/2, \bar{x}+1/2, 1/2$	$[u, \bar{u}, 0]$	
			$\bar{x}+1/2, \bar{x}+1/2, 1/2$	$[u, u, 0]$	$x+1/2, x+1/2, 1/2$	$[\bar{u}, \bar{u}, 0]$	$x, \bar{x}, 1/2$	$[\bar{u}, u, 0]$	$\bar{x}, x, 1/2$	$[u, \bar{u}, 0]$	
8	g	..2	$x, x, 0$	$[u, u, 0]$	$\bar{x}, \bar{x}, 0$	$[\bar{u}, \bar{u}, 0]$	$\bar{x}+1/2, x+1/2, 0$	$[\bar{u}, u, 0]$	$x+1/2, \bar{x}+1/2, 0$	$[u, \bar{u}, 0]$	
			$\bar{x}+1/2, \bar{x}+1/2, 0$	$[u, u, 0]$	$x+1/2, x+1/2, 0$	$[\bar{u}, \bar{u}, 0]$	$x, \bar{x}, 0$	$[\bar{u}, u, 0]$	$\bar{x}, x, 0$	$[u, \bar{u}, 0]$	
4	f	2mm.	$0, 0, z$	$[0, 0, 0]$	$1/2, 1/2, z$	$[0, 0, 0]$	$1/2, 1/2, \bar{z}$	$[0, 0, 0]$	$0, 0, \bar{z}$	$[0, 0, 0]$	
4	e	..2/m	$1/4, 1/4, 1/2$	$[u, u, 0]$	$3/4, 3/4, 1/2$	$[\bar{u}, \bar{u}, 0]$	$1/4, 3/4, 1/2$	$[\bar{u}, u, 0]$	$3/4, 1/4, 1/2$	$[u, \bar{u}, 0]$	
4	d	..2/m	$1/4, 1/4, 0$	$[u, u, 0]$	$3/4, 3/4, 0$	$[\bar{u}, \bar{u}, 0]$	$1/4, 3/4, 0$	$[\bar{u}, u, 0]$	$3/4, 1/4, 0$	$[u, \bar{u}, 0]$	
2	c	4mm	$0, 1/2, z$	$[0, 0, 0]$	$1/2, 0, \bar{z}$	$[0, 0, 0]$					
2	b	$\bar{4}m2$	$0, 0, 1/2$	$[0, 0, 0]$	$1/2, 1/2, 1/2$	$[0, 0, 0]$					
2	a	$\bar{4}m2$	$0, 0, 0$	$[0, 0, 0]$	$1/2, 1/2, 0$	$[0, 0, 0]$					

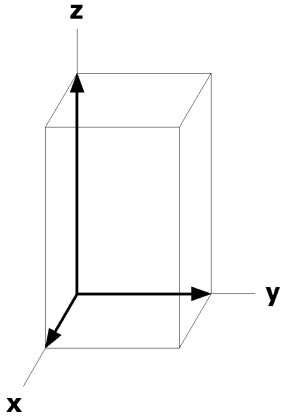
**Symmetry of Special Projections**

Along  $[0, 0, 1]$   $p_2, 4mm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0, 1/2, z$

Along  $[1, 0, 0]$   $p2'm'g$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 1/4, 0$

Along  $[1, 1, 0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 0$





P4/nmm1'

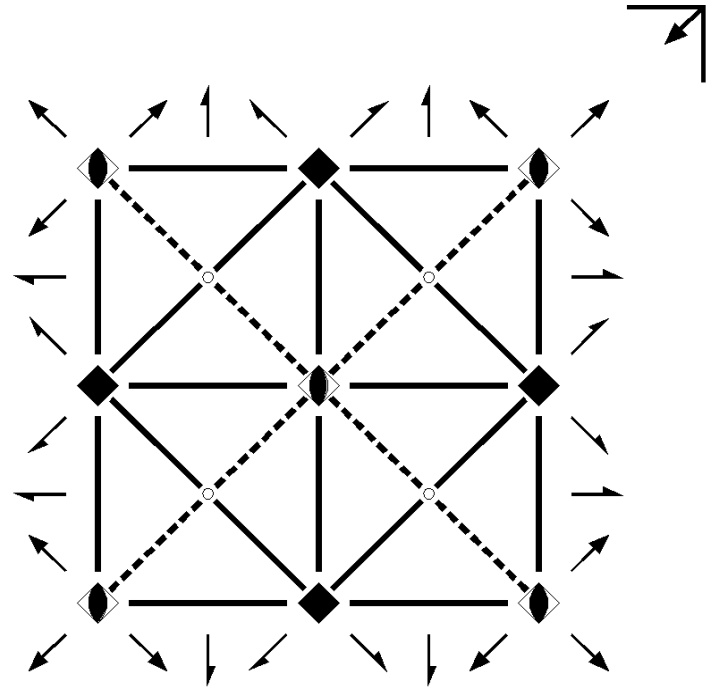
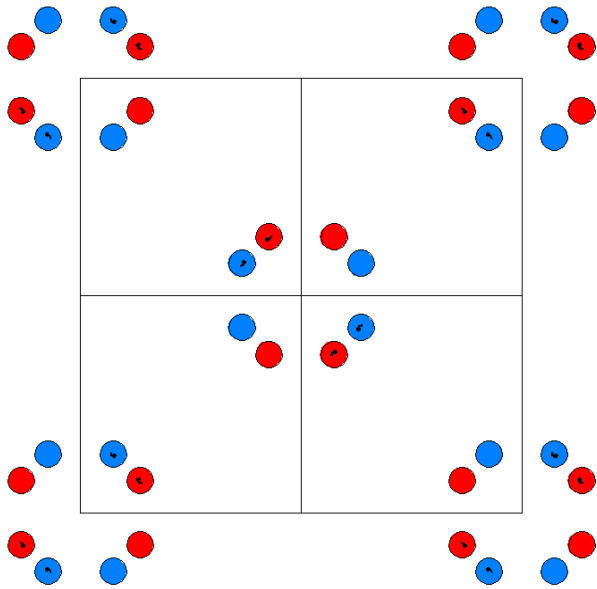
129.2.1076

4/mmm1'

P4/n2<sub>1</sub>/m2/m1'

Tetragonal

1'



Origin at center  $\bar{4}m21'$  at  $\bar{4}/nm2/g1'$ , at  $-1/4, 1/4, 0$  from center ( $2/m1'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

**Symmetry Operations**

For 1 + set

- |  |   |  |   |
|--|---|--|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                  | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0)  | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)     |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                    | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)        |
| (9) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)     | (10) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)   | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                    |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)                | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)                 | (15) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0) | (16) g (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0) |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> 0,1/2,z (4 <sub>z</sub>  1/2,1/2,0)'	(4) 4 <sup>-</sup> 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)'
(5) 2' (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>  1/2,1/2,0)'	(6) 2' (1/2,0,0) x,1/4,0 (2 <sub>x</sub>  1/2,1/2,0)'	(7) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) 2' x,x̄,0 (2 <sub>xy</sub>  0,0,0)'
(9) 1̄' 1/4,1/4,0 (1̄ 1/2,1/2,0)'	(10) n' (1/2,1/2,0) x,y,0 (m <sub>z</sub>  1/2,1/2,0)'	(11) 4 <sup>+</sup> 0,0,z; 0,0,0 (4 <sub>z</sub>  0,0,0)'	(12) 4 <sup>-</sup> 0,0,z; 0,0,0 (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(13) m' x,0,z (m <sub>y</sub>  0,0,0)'	(14) m' 0,y,z (m <sub>x</sub>  0,0,0)'	(15) m' x+1/2,x̄,z (m <sub>xy</sub>  1/2,1/2,0)'	(16) g' (1/2,1/2,0) x,x,z (m <sub>xy</sub>  1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

16	k	11'									
(1)	x,y,z	[0,0,0]	(2)	x̄,ȳ,z	[0,0,0]	(3)	ȳ+1/2,x+1/2,z	[0,0,0]	(4)	y+1/2,x̄+1/2,z	[0,0,0]
(5)	x̄+1/2,y+1/2,z̄	[0,0,0]	(6)	x+1/2,ȳ+1/2,z̄	[0,0,0]	(7)	y,x,z̄	[0,0,0]	(8)	ȳ,x̄,z̄	[0,0,0]
(9)	x̄+1/2,ȳ+1/2,z̄	[0,0,0]	(10)	x+1/2,y+1/2,z̄	[0,0,0]	(11)	y,x̄,z̄	[0,0,0]	(12)	ȳ,x,z̄	[0,0,0]
(13)	x,ȳ,z	[0,0,0]	(14)	x̄,y,z	[0,0,0]	(15)	ȳ+1/2,x̄+1/2,z	[0,0,0]	(16)	y+1/2,x+1/2,z	[0,0,0]
8	j	..m1'	x,x+1/2,z	[0,0,0]	x̄,x̄+1/2,z	[0,0,0]	x̄,x+1/2,z	[0,0,0]	x,x̄+1/2,z	[0,0,0]	
			x̄+1/2,x,z̄	[0,0,0]	x+1/2,x̄,z̄	[0,0,0]	x+1/2,x,z̄	[0,0,0]	x̄+1/2,x̄,z̄	[0,0,0]	
8	i	.m.1'	0,y,z	[0,0,0]	0,ȳ,z	[0,0,0]	ȳ+1/2,1/2,z	[0,0,0]	y+1/2,1/2,z	[0,0,0]	
			1/2,y+1/2,z̄	[0,0,0]	1/2,ȳ+1/2,z̄	[0,0,0]	y,0,z̄	[0,0,0]	ȳ,0,z̄	[0,0,0]	
8	h	..21'	x,x,1/2	[0,0,0]	x̄,x̄,1/2	[0,0,0]	x̄+1/2,x+1/2,1/2	[0,0,0]	x+1/2,x̄+1/2,1/2	[0,0,0]	
			x̄+1/2,x̄+1/2,1/2	[0,0,0]	x+1/2,x+1/2,1/2	[0,0,0]	x,x̄,1/2	[0,0,0]	x̄,x,1/2	[0,0,0]	
8	g	..21'	x,x,0	[0,0,0]	x̄,x̄,0	[0,0,0]	x̄+1/2,x+1/2,0	[0,0,0]	x+1/2,x̄+1/2,0	[0,0,0]	
			x̄+1/2,x̄+1/2,0	[0,0,0]	x+1/2,x+1/2,0	[0,0,0]	x,x̄,0	[0,0,0]	x̄,x,0	[0,0,0]	
4	f	2mm.1'	0,0,z	[0,0,0]	1/2,1/2,z	[0,0,0]	1/2,1/2,z̄	[0,0,0]	0,0,z̄	[0,0,0]	
4	e	..2/m1'	1/4,1/4,1/2	[0,0,0]	3/4,3/4,1/2	[0,0,0]	1/4,3/4,1/2	[0,0,0]	3/4,1/4,1/2	[0,0,0]	
4	d	..2/m1'	1/4,1/4,0	[0,0,0]	3/4,3/4,0	[0,0,0]	1/4,3/4,0	[0,0,0]	3/4,1/4,0	[0,0,0]	
2	c	4mm1'	0,1/2,z	[0,0,0]	1/2,0,z̄	[0,0,0]					

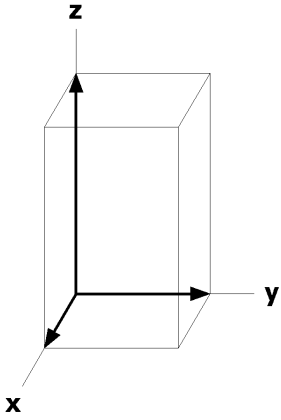
2	b	$\bar{4}m21'$	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]
2	a	$\bar{4}m21'$	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p2mg1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

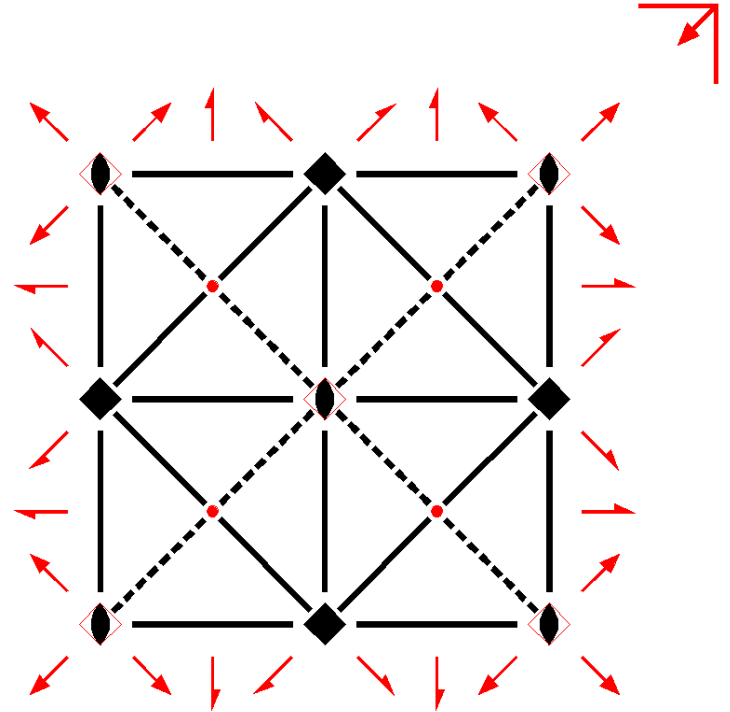
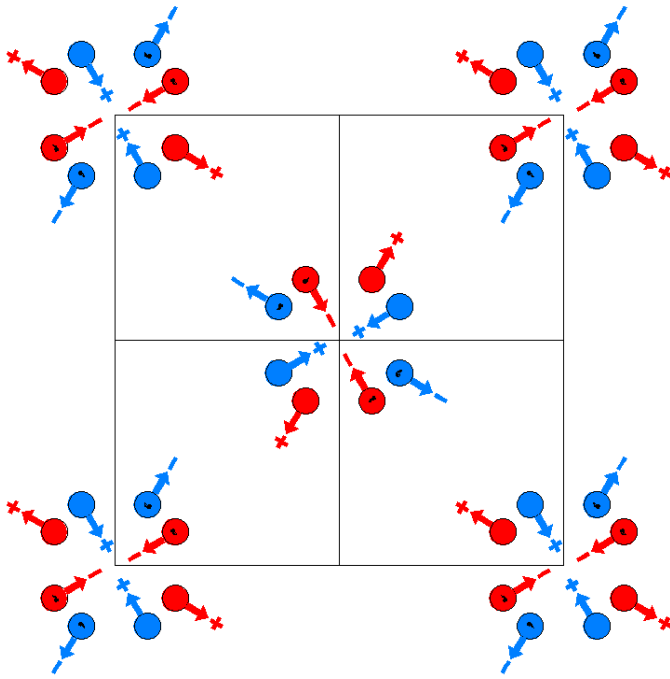
Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4/n'mm  
129.3.1077

4/m'mm  
P4/n'2<sub>1</sub>'/m2'/m

Tetragonal



Origin at center  $\bar{4}'m2'$  at  $\bar{4}'/nm2'/g$ , at  $-1/4, 1/4, 0$  from center ( $2'/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

**Symmetry Operations**

- |  |   |  |   |
|--|---|--|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                    | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0)  | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)     |
| (5) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (6) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)'  | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                  | (8) 2' x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)'      |
| (9) $\bar{1}'$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)'     | (10) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'  | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                   |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)                  | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)                   | (15) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0) | (16) g (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

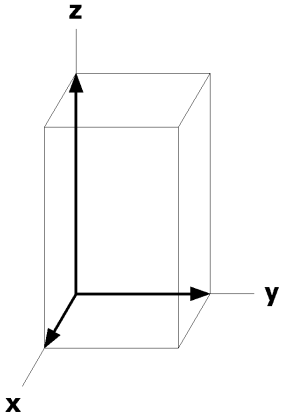
		Coordinates										
		Multiplicity, Wyckoff letter, Site Symmetry.										
16	k	1										
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y}+1/2,x+1/2,z$	$[\bar{v},u,w]$	(4)	$y+1/2,\bar{x}+1/2,z$	$[v,\bar{u},w]$	
(5)	$\bar{x}+1/2,y+1/2,\bar{z}$	$[\bar{u},\bar{v},w]$	(6)	$x+1/2,\bar{y}+1/2,\bar{z}$	$[\bar{u},v,w]$	(7)	$y,x,\bar{z}$	$[\bar{v},\bar{u},w]$	(8)	$\bar{y},\bar{x},\bar{z}$	$[v,u,w]$	
(9)	$\bar{x}+1/2,\bar{y}+1/2,\bar{z}$	$[\bar{u},\bar{v},\bar{w}]$	(10)	$x+1/2,y+1/2,\bar{z}$	$[\bar{u},v,\bar{w}]$	(11)	$y,\bar{x},\bar{z}$	$[v,\bar{u},\bar{w}]$	(12)	$\bar{y},x,\bar{z}$	$[\bar{v},u,\bar{w}]$	
(13)	$x,\bar{y},z$	$[\bar{u},v,\bar{w}]$	(14)	$\bar{x},y,z$	$[u,\bar{v},\bar{w}]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[v,u,\bar{w}]$	(16)	$y+1/2,x+1/2,z$	$[\bar{v},\bar{u},\bar{w}]$	
8	j	..m	$x,x+1/2,z$	$[\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,z$	$[u,\bar{u},0]$	$\bar{x},x+1/2,z$	$[u,\bar{u},0]$	$x,\bar{x}+1/2,z$	$[u,u,0]$	$\bar{x}+1/2,\bar{x},\bar{z}$	$[u,\bar{u},0]$
8	i	.m.	$0,y,z$	$[u,0,0]$	$0,\bar{y},z$	$[\bar{u},0,0]$	$\bar{y}+1/2,1/2,z$	$[0,u,0]$	$y+1/2,1/2,z$	$[0,\bar{u},0]$	$1/2,y+1/2,\bar{z}$	$[u,0,0]$
8	h	..2'	$x,x,1/2$	$[\bar{u},u,w]$	$\bar{x},\bar{x},1/2$	$[u,\bar{u},w]$	$\bar{x}+1/2,x+1/2,1/2$	$[\bar{u},\bar{u},w]$	$x+1/2,\bar{x}+1/2,1/2$	$[u,u,w]$	$\bar{x}+1/2,\bar{x}+1/2,1/2$	$[u,\bar{u},\bar{w}]$
8	g	..2'	$x,x,0$	$[\bar{u},u,w]$	$\bar{x},\bar{x},0$	$[u,\bar{u},w]$	$\bar{x}+1/2,x+1/2,0$	$[\bar{u},\bar{u},w]$	$x+1/2,\bar{x}+1/2,0$	$[u,u,w]$	$\bar{x}+1/2,\bar{x}+1/2,0$	$[u,\bar{u},\bar{w}]$
4	f	2mm.	$0,0,z$	$[0,0,0]$	$1/2,1/2,z$	$[0,0,0]$	$1/2,1/2,\bar{z}$	$[0,0,0]$	$0,0,\bar{z}$	$[0,0,0]$		
4	e	..2'/m	$1/4,1/4,1/2$	$[0,0,0]$	$3/4,3/4,1/2$	$[0,0,0]$	$1/4,3/4,1/2$	$[0,0,0]$	$3/4,1/4,1/2$	$[0,0,0]$		
4	d	..2'/m	$1/4,1/4,0$	$[0,0,0]$	$3/4,3/4,0$	$[0,0,0]$	$1/4,3/4,0$	$[0,0,0]$	$3/4,1/4,0$	$[0,0,0]$		
2	c	4mm	$0,1/2,z$	$[0,0,0]$	$1/2,0,\bar{z}$	$[0,0,0]$						
2	b	$\bar{4}'m2'$	$0,0,1/2$	$[0,0,0]$	$1/2,1/2,1/2$	$[0,0,0]$						
2	a	$\bar{4}'m2'$	$0,0,0$	$[0,0,0]$	$1/2,1/2,0$	$[0,0,0]$						

**Symmetry of Special Projections**

Along [0,0,1]  $p4'mm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p2mg1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

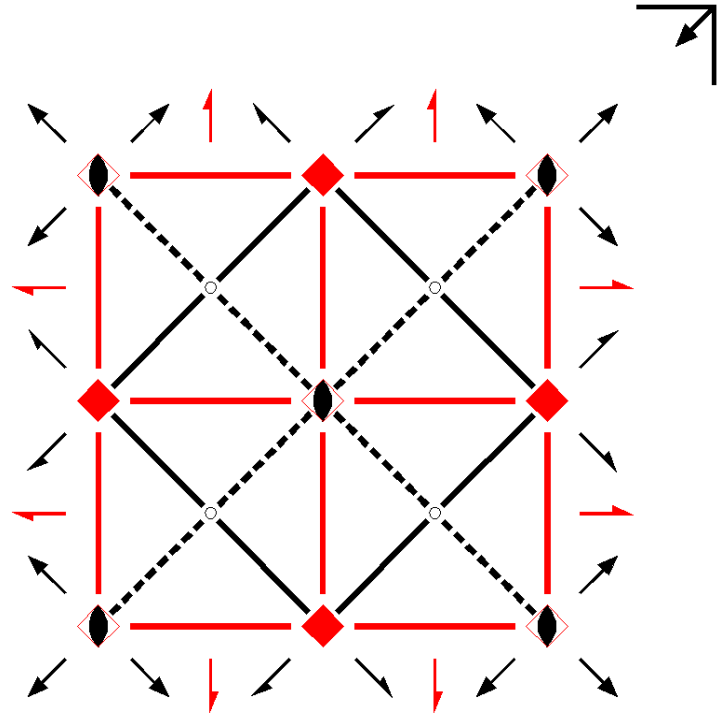
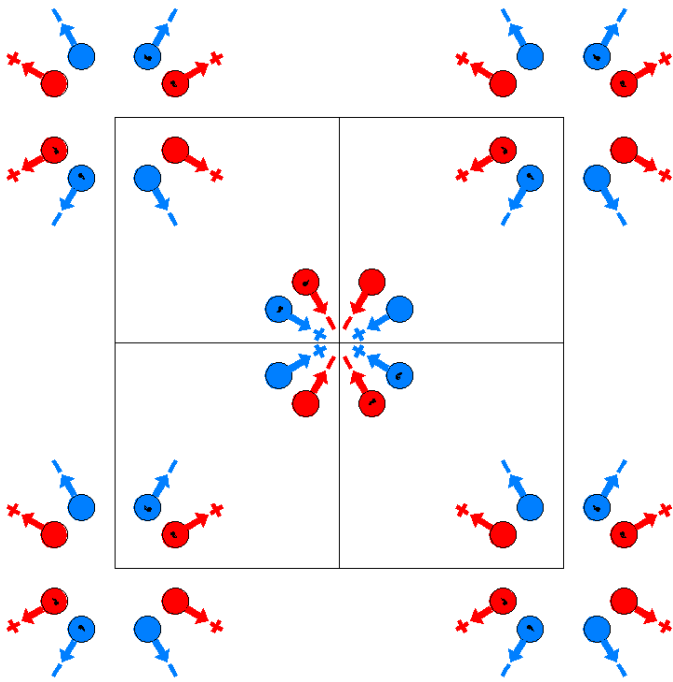
Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4'/nm'm  
129.4.1078

4'/mm'm  
P4'/n2<sub>1</sub>'/m'2/m

Tetragonal



Origin at center  $\bar{4}'m'2$  at  $\bar{4}'/nm'2/g$ , at  $-1/4, 1/4, 0$  from center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                   | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0)' | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)'    |
| (5) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (6) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                    | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)        |
| (9) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)       | (10) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)  | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'  | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                   |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)'                | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)'                | (15) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0) | (16) g (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

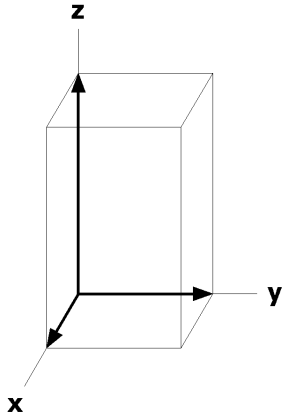
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
16	k	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{y}+1/2, x+1/2, z [v, \bar{u}, \bar{w}]$	(4) $y+1/2, \bar{x}+1/2, z [\bar{v}, u, \bar{w}]$
			(5) $\bar{x}+1/2, y+1/2, \bar{z} [u, \bar{v}, w]$	(6) $x+1/2, \bar{y}+1/2, \bar{z} [\bar{u}, v, w]$	(7) $y, x, \bar{z} [v, u, \bar{w}]$	(8) $\bar{y}, \bar{x}, \bar{z} [\bar{v}, \bar{u}, \bar{w}]$
			(9) $\bar{x}+1/2, \bar{y}+1/2, \bar{z} [u, v, w]$	(10) $x+1/2, y+1/2, \bar{z} [\bar{u}, \bar{v}, w]$	(11) $y, \bar{x}, \bar{z} [v, \bar{u}, \bar{w}]$	(12) $\bar{y}, x, \bar{z} [\bar{v}, u, \bar{w}]$
			(13) $x, \bar{y}, z [u, \bar{v}, w]$	(14) $\bar{x}, y, z [\bar{u}, v, w]$	(15) $\bar{y}+1/2, \bar{x}+1/2, z [v, u, \bar{w}]$	(16) $y+1/2, x+1/2, z [\bar{v}, \bar{u}, \bar{w}]$
8	j	..m	$x, x+1/2, z [\bar{u}, u, 0]$	$\bar{x}, \bar{x}+1/2, z [u, \bar{u}, 0]$	$\bar{x}, x+1/2, z [u, u, 0]$	$x, \bar{x}+1/2, z [\bar{u}, \bar{u}, 0]$
			$\bar{x}+1/2, x, \bar{z} [\bar{u}, \bar{u}, 0]$	$x+1/2, \bar{x}, \bar{z} [u, u, 0]$	$x+1/2, x, \bar{z} [u, \bar{u}, 0]$	$\bar{x}+1/2, \bar{x}, \bar{z} [\bar{u}, u, 0]$
8	i	.m'	$0, y, z [0, v, w]$	$0, \bar{y}, z [0, \bar{v}, w]$	$\bar{y}+1/2, 1/2, z [v, 0, \bar{w}]$	$y+1/2, 1/2, z [\bar{v}, 0, \bar{w}]$
			$1/2, y+1/2, \bar{z} [0, \bar{v}, w]$	$1/2, \bar{y}+1/2, \bar{z} [0, v, w]$	$y, 0, \bar{z} [v, 0, \bar{w}]$	$\bar{y}, 0, \bar{z} [\bar{v}, 0, \bar{w}]$
8	h	..2	$x, x, 1/2 [u, u, 0]$	$\bar{x}, \bar{x}, 1/2 [\bar{u}, \bar{u}, 0]$	$\bar{x}+1/2, x+1/2, 1/2 [u, \bar{u}, 0]$	$x+1/2, \bar{x}+1/2, 1/2 [\bar{u}, u, 0]$
			$\bar{x}+1/2, \bar{x}+1/2, 1/2 [u, u, 0]$	$x+1/2, x+1/2, 1/2 [\bar{u}, \bar{u}, 0]$	$x, \bar{x}, 1/2 [u, \bar{u}, 0]$	$\bar{x}, x, 1/2 [\bar{u}, u, 0]$
8	g	..2	$x, x, 0 [u, u, 0]$	$\bar{x}, \bar{x}, 0 [\bar{u}, \bar{u}, 0]$	$\bar{x}+1/2, x+1/2, 0 [u, \bar{u}, 0]$	$x+1/2, \bar{x}+1/2, 0 [\bar{u}, u, 0]$
			$\bar{x}+1/2, \bar{x}+1/2, 0 [u, u, 0]$	$x+1/2, x+1/2, 0 [\bar{u}, \bar{u}, 0]$	$x, \bar{x}, 0 [u, \bar{u}, 0]$	$\bar{x}, x, 0 [\bar{u}, u, 0]$
4	f	2m'm'	$0, 0, z [0, 0, w]$	$1/2, 1/2, z [0, 0, \bar{w}]$	$1/2, 1/2, \bar{z} [0, 0, w]$	$0, 0, \bar{z} [0, 0, \bar{w}]$
4	e	..2/m	$1/4, 1/4, 1/2 [u, u, 0]$	$3/4, 3/4, 1/2 [\bar{u}, \bar{u}, 0]$	$1/4, 3/4, 1/2 [u, \bar{u}, 0]$	$3/4, 1/4, 1/2 [\bar{u}, u, 0]$
4	d	..2/m	$1/4, 1/4, 0 [u, u, 0]$	$3/4, 3/4, 0 [\bar{u}, \bar{u}, 0]$	$1/4, 3/4, 0 [u, \bar{u}, 0]$	$3/4, 1/4, 0 [\bar{u}, u, 0]$
2	c	4'm'm	$0, 1/2, z [0, 0, 0]$	$1/2, 0, \bar{z} [0, 0, 0]$		
2	b	$\bar{4}$ 'm'2	$0, 0, 1/2 [0, 0, 0]$	$1/2, 1/2, 1/2 [0, 0, 0]$		
2	a	$\bar{4}$ 'm'2	$0, 0, 0 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$		

### Symmetry of Special Projections

Along [0,0,1]  $p_p$ -4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

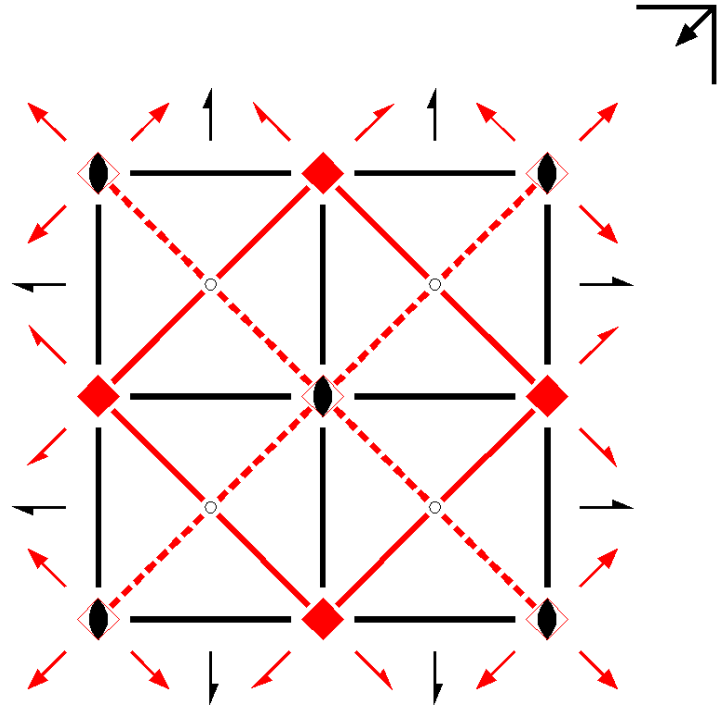
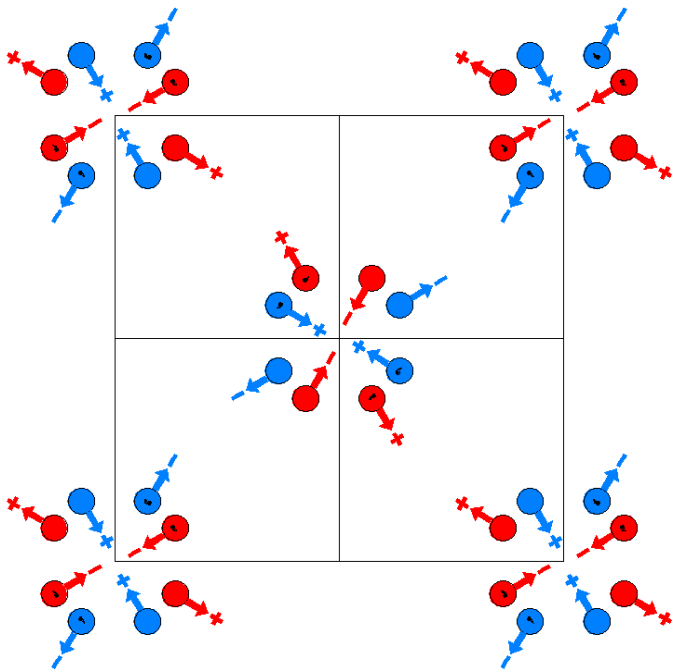
Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4'/nmm'  
129.5.1079

4'/mmm'  
P4'/n2<sub>1</sub>/m2'/m'

Tetragonal



Origin at center  $\bar{4}'m2'$  at  $\bar{4}'/nm2'/g'$ , at  $-1/4, 1/4, 0$  from center ( $2'/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |  |   |  |   |
|--|---|--|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                  | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0)'   | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)'      |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)  | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                    | (8) 2' x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)'        |
| (9) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)     | (10) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'    | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                     |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)                | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)                 | (15) m' x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0)' | (16) g' (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

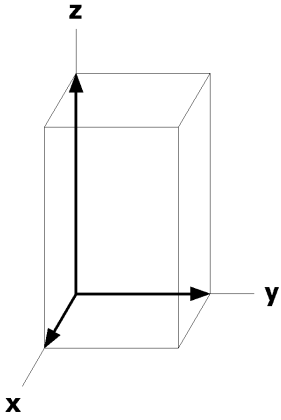
		Coordinates									
		Multiplicity, Wyckoff letter, Site Symmetry.									
16	k	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y}+1/2,x+1/2,z$	$[v,\bar{u},\bar{w}]$	(4)	$y+1/2,\bar{x}+1/2,z$	$[\bar{v},u,\bar{w}]$
(5)	$\bar{x}+1/2,y+1/2,\bar{z}$	$[\bar{u},v,\bar{w}]$	(6)	$x+1/2,\bar{y}+1/2,\bar{z}$	$[u,\bar{v},\bar{w}]$	(7)	$y,x,\bar{z}$	$[\bar{v},\bar{u},w]$	(8)	$\bar{y},\bar{x},\bar{z}$	$[v,u,w]$
(9)	$\bar{x}+1/2,\bar{y}+1/2,\bar{z}$	$[u,v,w]$	(10)	$x+1/2,y+1/2,\bar{z}$	$[\bar{u},\bar{v},w]$	(11)	$y,\bar{x},\bar{z}$	$[v,\bar{u},\bar{w}]$	(12)	$\bar{y},x,\bar{z}$	$[\bar{v},u,\bar{w}]$
(13)	$x,\bar{y},z$	$[\bar{u},v,\bar{w}]$	(14)	$\bar{x},y,z$	$[u,\bar{v},\bar{w}]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[\bar{v},\bar{u},w]$	(16)	$y+1/2,x+1/2,z$	$[v,u,w]$
8	j	..m'	$x,x+1/2,z$	$[\bar{u},u,w]$	$\bar{x},\bar{x}+1/2,z$	$[\bar{u},\bar{u},w]$	$\bar{x},x+1/2,z$	$[u,\bar{u},\bar{w}]$	$x,\bar{x}+1/2,z$	$[\bar{u},u,\bar{w}]$	
			$\bar{x}+1/2,x,\bar{z}$	$[\bar{u},u,\bar{w}]$	$x+1/2,\bar{x},\bar{z}$	$[u,\bar{u},\bar{w}]$	$x+1/2,x,\bar{z}$	$[u,\bar{u},w]$	$\bar{x}+1/2,\bar{x},\bar{z}$	$[u,u,w]$	
8	i	.m.	0,y,z	$[u,0,0]$	0, $\bar{y},z$	$[\bar{u},0,0]$	$\bar{y}+1/2,1/2,z$	$[0,\bar{u},0]$	$y+1/2,1/2,z$	$[0,u,0]$	
			1/2,y+1/2, $\bar{z}$	$[\bar{u},0,0]$	1/2, $\bar{y}+1/2,\bar{z}$	$[u,0,0]$	y,0, $\bar{z}$	$[0,\bar{u},0]$	$\bar{y},0,\bar{z}$	$[0,u,0]$	
8	h	..2'	$x,x,1/2$	$[\bar{u},u,w]$	$\bar{x},\bar{x},1/2$	$[u,\bar{u},w]$	$\bar{x}+1/2,x+1/2,1/2$	$[u,u,\bar{w}]$	$x+1/2,\bar{x}+1/2,1/2$	$[\bar{u},\bar{u},\bar{w}]$	
			$\bar{x}+1/2,\bar{x}+1/2,1/2$	$[\bar{u},u,w]$	$x+1/2,x+1/2,1/2$	$[u,\bar{u},w]$	$x,\bar{x},1/2$	$[u,u,\bar{w}]$	$\bar{x},x,1/2$	$[\bar{u},\bar{u},\bar{w}]$	
8	g	..2'	$x,x,0$	$[\bar{u},u,w]$	$\bar{x},\bar{x},0$	$[u,\bar{u},w]$	$\bar{x}+1/2,x+1/2,0$	$[u,u,\bar{w}]$	$x+1/2,\bar{x}+1/2,0$	$[\bar{u},\bar{u},\bar{w}]$	
			$\bar{x}+1/2,\bar{x}+1/2,0$	$[\bar{u},u,w]$	$x+1/2,x+1/2,0$	$[u,\bar{u},w]$	$x,\bar{x},0$	$[u,u,\bar{w}]$	$\bar{x},x,0$	$[\bar{u},\bar{u},\bar{w}]$	
4	f	2mm.	0,0,z	$[0,0,0]$	1/2,1/2,z	$[0,0,0]$	1/2,1/2, $\bar{z}$	$[0,0,0]$	0,0, $\bar{z}$	$[0,0,0]$	
4	e	..2'/m'	1/4,1/4,1/2	$[\bar{u},u,w]$	3/4,3/4,1/2	$[u,\bar{u},w]$	1/4,3/4,1/2	$[u,u,\bar{w}]$	3/4,1/4,1/2	$[\bar{u},\bar{u},\bar{w}]$	
4	d	..2'/m'	1/4,1/4,0	$[\bar{u},u,w]$	3/4,3/4,0	$[u,\bar{u},w]$	1/4,3/4,0	$[u,u,\bar{w}]$	3/4,1/4,0	$[\bar{u},\bar{u},\bar{w}]$	
2	c	4'mm'	0,1/2,z	$[0,0,0]$	1/2,0, $\bar{z}$	$[0,0,0]$					
2	b	$\bar{4}'m2'$	0,0,1/2	$[0,0,0]$	1/2,1/2,1/2	$[0,0,0]$					
2	a	$\bar{4}'m2'$	0,0,0	$[0,0,0]$	1/2,1/2,0	$[0,0,0]$					

**Symmetry of Special Projections**

Along [0,0,1]  $p_2$ .4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p2mg1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [1,1,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



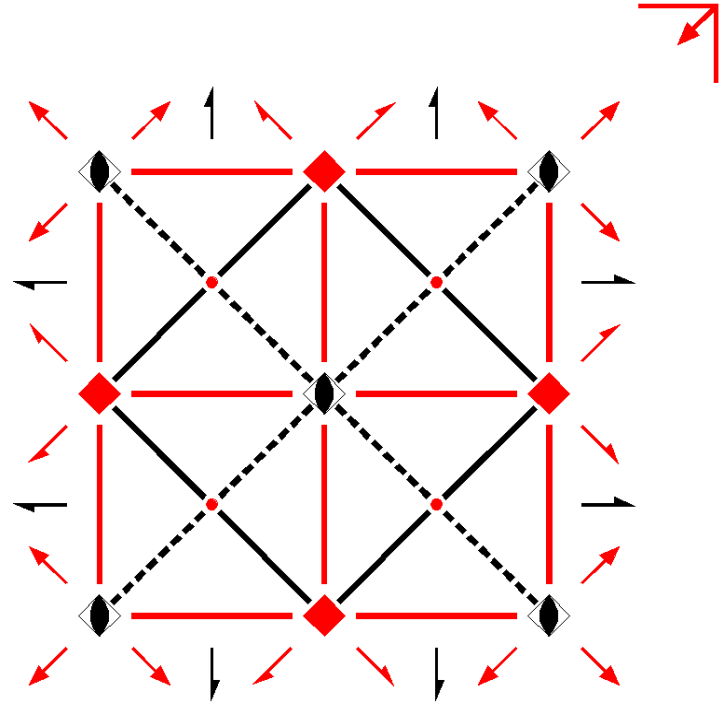
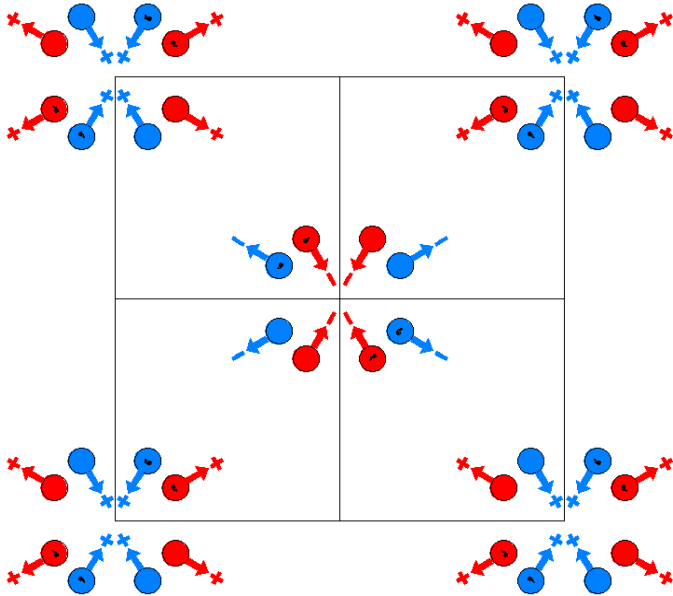
P4'/n'm'm

129.6.1080

4'/m'm'm

P4'/n'2<sub>1</sub>/m'2'/m

Tetragonal



Origin at center  $\bar{4}m'2'$  at  $\bar{4}/n'm'2'/g$ , at  $-1/4, 1/4, 0$  from center ( $2'/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |  |   |   |  |
|--|---|---|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                    | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0)'                                | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)'                   |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)    | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'   | (8) 2' x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)'                     |
| (9) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$ ' 1/2,1/2,0)' | (10) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (11) $\bar{4}$ <sup>+</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>+</sup>  0,0,0) | (12) $\bar{4}$ <sup>-</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)'              | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)'                 | (15) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0)                                | (16) g (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)                |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

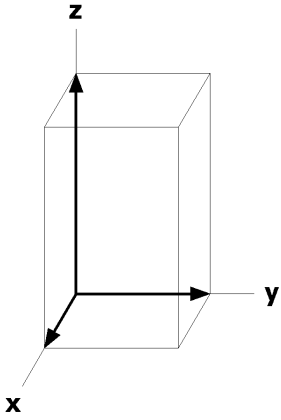
		Coordinates									
		Multiplicity, Wyckoff letter, Site Symmetry.									
16	k	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y}+1/2,x+1/2,z$	$[v,\bar{u},\bar{w}]$	(4)	$y+1/2,\bar{x}+1/2,z$	$[\bar{v},u,\bar{w}]$
(5)	$\bar{x}+1/2,y+1/2,\bar{z}$	$[\bar{u},v,\bar{w}]$	(6)	$x+1/2,\bar{y}+1/2,\bar{z}$	$[u,\bar{v},\bar{w}]$	(7)	$y,x,\bar{z}$	$[\bar{v},\bar{u},w]$	(8)	$\bar{y},\bar{x},\bar{z}$	$[v,u,w]$
(9)	$\bar{x}+1/2,\bar{y}+1/2,\bar{z}$	$[\bar{u},\bar{v},\bar{w}]$	(10)	$x+1/2,y+1/2,\bar{z}$	$[u,v,\bar{w}]$	(11)	$y,\bar{x},\bar{z}$	$[\bar{v},u,w]$	(12)	$\bar{y},x,\bar{z}$	$[v,\bar{u},w]$
(13)	$x,\bar{y},z$	$[u,\bar{v},w]$	(14)	$\bar{x},y,z$	$[\bar{u},v,w]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[v,u,\bar{w}]$	(16)	$y+1/2,x+1/2,z$	$[\bar{v},\bar{u},\bar{w}]$
8	j	..m	$x,x+1/2,z$	$[\bar{u},u,0]$	$\bar{x},\bar{x}+1/2,z$	$[u,\bar{u},0]$	$\bar{x},x+1/2,z$	$[u,u,0]$	$x,\bar{x}+1/2,z$	$[\bar{u},\bar{u},0]$	
			$\bar{x}+1/2,x,\bar{z}$	$[u,u,0]$	$x+1/2,\bar{x},\bar{z}$	$[u,\bar{u},0]$	$x+1/2,x,\bar{z}$	$[u,u,0]$	$\bar{x}+1/2,\bar{x},\bar{z}$	$[u,\bar{u},0]$	
8	i	.m'	$0,y,z$	$[0,v,w]$	$0,\bar{y},z$	$[0,\bar{v},w]$	$\bar{y}+1/2,1/2,z$	$[v,0,\bar{w}]$	$y+1/2,1/2,z$	$[\bar{v},0,\bar{w}]$	
			$1/2,y+1/2,\bar{z}$	$[0,v,\bar{w}]$	$1/2,\bar{y}+1/2,\bar{z}$	$[0,\bar{v},\bar{w}]$	$y,0,\bar{z}$	$[\bar{v},0,w]$	$\bar{y},0,\bar{z}$	$[v,0,w]$	
8	h	..2'	$x,x,1/2$	$[\bar{u},u,w]$	$\bar{x},\bar{x},1/2$	$[u,\bar{u},w]$	$\bar{x}+1/2,x+1/2,1/2$	$[u,u,\bar{w}]$	$x+1/2,\bar{x}+1/2,1/2$	$[\bar{u},\bar{u},\bar{w}]$	
			$\bar{x}+1/2,\bar{x}+1/2,1/2$	$[u,\bar{u},\bar{w}]$	$x+1/2,x+1/2,1/2$	$[\bar{u},u,\bar{w}]$	$x,\bar{x},1/2$	$[\bar{u},\bar{u},w]$	$\bar{x},x,1/2$	$[u,u,w]$	
8	g	..2'	$x,x,0$	$[\bar{u},u,w]$	$\bar{x},\bar{x},0$	$[u,\bar{u},w]$	$\bar{x}+1/2,x+1/2,0$	$[u,u,\bar{w}]$	$x+1/2,\bar{x}+1/2,0$	$[\bar{u},\bar{u},\bar{w}]$	
			$\bar{x}+1/2,\bar{x}+1/2,0$	$[u,\bar{u},\bar{w}]$	$x+1/2,x+1/2,0$	$[\bar{u},u,\bar{w}]$	$x,\bar{x},0$	$[\bar{u},\bar{u},w]$	$\bar{x},x,0$	$[u,u,w]$	
4	f	2m'm'	$0,0,z$	$[0,0,w]$	$1/2,1/2,z$	$[0,0,\bar{w}]$	$1/2,1/2,\bar{z}$	$[0,0,\bar{w}]$	$0,0,\bar{z}$	$[0,0,w]$	
4	e	..2'/m	$1/4,1/4,1/2$	$[0,0,0]$	$3/4,3/4,1/2$	$[0,0,0]$	$1/4,3/4,1/2$	$[0,0,0]$	$3/4,1/4,1/2$	$[0,0,0]$	
4	d	..2'/m	$1/4,1/4,0$	$[0,0,0]$	$3/4,3/4,0$	$[0,0,0]$	$1/4,3/4,0$	$[0,0,0]$	$3/4,1/4,0$	$[0,0,0]$	
2	c	4m'm	$0,1/2,z$	$[0,0,0]$	$1/2,0,\bar{z}$	$[0,0,0]$					
2	b	$\bar{4}m'2'$	$0,0,1/2$	$[0,0,w]$	$1/2,1/2,1/2$	$[0,0,\bar{w}]$					
2	a	$\bar{4}m'2'$	$0,0,0$	$[0,0,w]$	$1/2,1/2,0$	$[0,0,\bar{w}]$					

**Symmetry of Special Projections**

Along [0,0,1] p4'm'm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

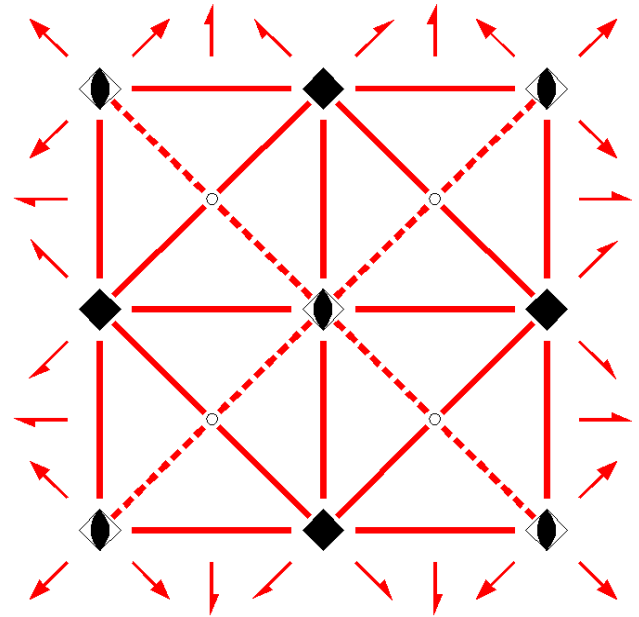
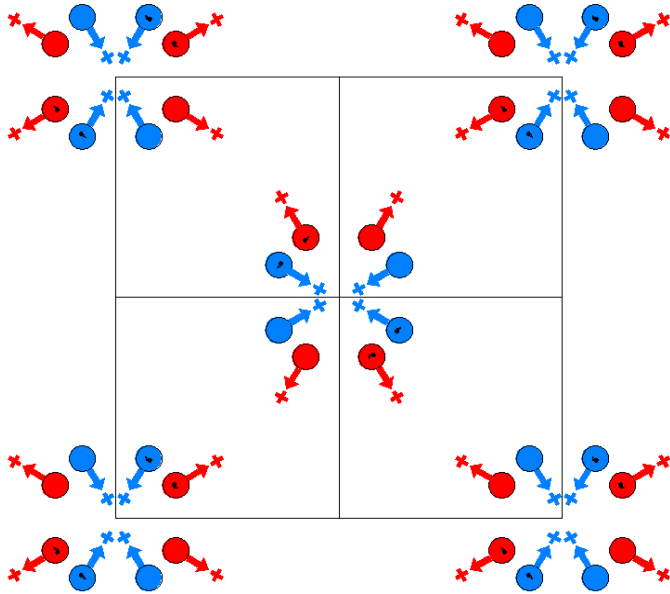
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4/nm'm'  
129.7.1081

4/mm'm'  
P4/n2<sub>1</sub>'/m'2'/m'

Tetragonal



Origin at center  $\bar{4}m'2'$  at  $\bar{4}/nm'2'/g'$ , at  $-1/4, 1/4, 0$  from center ( $2'/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 <sub>0,0,z</sub><br>(2 <sub>z</sub>  0,0,0)            | (3) 4 <sup>+</sup> <sub>0,1/2,z</sub><br>(4 <sub>z</sub>  1/2,1/2,0) | (4) 4 <sup>-</sup> <sub>1/2,0,z</sub><br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0) |
| (5) 2' <sub>(0,1/2,0)</sub><br>(2 <sub>y</sub>  1/2,1/2,0)'   | (6) 2' <sub>(1/2,0,0)</sub><br>(2 <sub>x</sub>  1/2,1/2,0)'  | (7) 2' <sub>x,x,0</sub><br>(2 <sub>xy</sub>  0,0,0)'                 | (8) 2' <sub>x,x̄,0</sub><br>(2 <sub>xȳ</sub>  0,0,0)'                             |
| (9) $\bar{1}$ <sub>1/4,1/4,0</sub><br>( $\bar{1}$  1/2,1/2,0) | (10) n <sub>(1/2,1/2,0)</sub><br>(m <sub>z</sub>  1/2,1/2,0) | (11) $\bar{4}^+$ <sub>0,0,z</sub><br>( $\bar{4}_z$  0,0,0)           | (12) $\bar{4}^-$ <sub>0,0,z</sub><br>( $\bar{4}_z$ <sup>-1</sup>  0,0,0)           |
| (13) m' <sub>x,0,z</sub><br>(m <sub>y</sub>  0,0,0)'          | (14) m' <sub>0,y,z</sub><br>(m <sub>x</sub>  0,0,0)'         | (15) m' <sub>x+1/2,x̄,z</sub><br>(m <sub>xy</sub>  1/2,1/2,0)'       | (16) g' <sub>(1/2,1/2,0)</sub><br>(m <sub>xȳ</sub>  1/2,1/2,0)'                   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

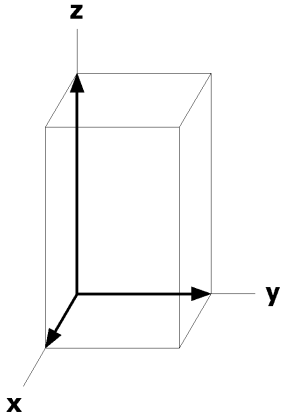
		Coordinates					
Multiplicity, Wyckoff letter, Site Symmetry.							
16	k 1						
(1)	x,y,z [u,v,w]	(2)	$\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3)	$\bar{y}+1/2, x+1/2, z$ [ $\bar{v}, u, w$ ]	(4)	$y+1/2, \bar{x}+1/2, z$ [ $v, \bar{u}, w$ ]
(5)	$\bar{x}+1/2, y+1/2, \bar{z}$ [ $u, \bar{v}, w$ ]	(6)	$x+1/2, \bar{y}+1/2, \bar{z}$ [ $\bar{u}, v, w$ ]	(7)	$y, x, \bar{z}$ [ $\bar{v}, \bar{u}, w$ ]	(8)	$\bar{y}, \bar{x}, \bar{z}$ [ $v, u, w$ ]
(9)	$\bar{x}+1/2, \bar{y}+1/2, \bar{z}$ [ $u, v, w$ ]	(10)	$x+1/2, y+1/2, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(11)	$y, \bar{x}, \bar{z}$ [ $\bar{v}, u, w$ ]	(12)	$\bar{y}, x, \bar{z}$ [ $v, \bar{u}, w$ ]
(13)	$x, \bar{y}, z$ [ $u, \bar{v}, w$ ]	(14)	$\bar{x}, y, z$ [ $\bar{u}, v, w$ ]	(15)	$\bar{y}+1/2, \bar{x}+1/2, z$ [ $\bar{v}, \bar{u}, w$ ]	(16)	$y+1/2, x+1/2, z$ [ $v, u, w$ ]
8	j ..m'	$x, x+1/2, z$ [ $u, u, w$ ]	$\bar{x}, \bar{x}+1/2, z$ [ $\bar{u}, \bar{u}, w$ ]	$\bar{x}, x+1/2, z$ [ $\bar{u}, u, w$ ]	$x, \bar{x}+1/2, z$ [ $u, \bar{u}, w$ ]		
		$\bar{x}+1/2, x, \bar{z}$ [ $u, \bar{u}, w$ ]	$x+1/2, \bar{x}, \bar{z}$ [ $\bar{u}, u, w$ ]	$x+1/2, x, \bar{z}$ [ $\bar{u}, \bar{u}, w$ ]	$\bar{x}+1/2, \bar{x}, \bar{z}$ [ $u, u, w$ ]		
8	i .m'	$0, y, z$ [ $0, v, w$ ]	$0, \bar{y}, z$ [ $0, \bar{v}, w$ ]	$\bar{y}+1/2, 1/2, z$ [ $\bar{v}, 0, w$ ]	$y+1/2, 1/2, z$ [ $v, 0, w$ ]		
		$1/2, y+1/2, \bar{z}$ [ $0, \bar{v}, w$ ]	$1/2, \bar{y}+1/2, \bar{z}$ [ $0, v, w$ ]	$y, 0, \bar{z}$ [ $\bar{v}, 0, w$ ]	$\bar{y}, 0, \bar{z}$ [ $v, 0, w$ ]		
8	h ..2'	$x, x, 1/2$ [ $\bar{u}, u, w$ ]	$\bar{x}, \bar{x}, 1/2$ [ $u, \bar{u}, w$ ]	$\bar{x}+1/2, x+1/2, 1/2$ [ $\bar{u}, \bar{u}, w$ ]	$x+1/2, \bar{x}+1/2, 1/2$ [ $u, u, w$ ]		
		$\bar{x}+1/2, \bar{x}+1/2, 1/2$ [ $\bar{u}, u, w$ ]	$x+1/2, x+1/2, 1/2$ [ $u, \bar{u}, w$ ]	$x, \bar{x}, 1/2$ [ $\bar{u}, \bar{u}, w$ ]	$\bar{x}, x, 1/2$ [ $u, u, w$ ]		
8	g ..2'	$x, x, 0$ [ $\bar{u}, u, w$ ]	$\bar{x}, \bar{x}, 0$ [ $u, \bar{u}, w$ ]	$\bar{x}+1/2, x+1/2, 0$ [ $\bar{u}, \bar{u}, w$ ]	$x+1/2, \bar{x}+1/2, 0$ [ $u, u, w$ ]		
		$\bar{x}+1/2, \bar{x}+1/2, 0$ [ $\bar{u}, u, w$ ]	$x+1/2, x+1/2, 0$ [ $u, \bar{u}, w$ ]	$x, \bar{x}, 0$ [ $\bar{u}, \bar{u}, w$ ]	$\bar{x}, x, 0$ [ $u, u, w$ ]		
4	f 2m'm'	$0, 0, z$ [ $0, 0, w$ ]	$1/2, 1/2, z$ [ $0, 0, w$ ]	$1/2, 1/2, \bar{z}$ [ $0, 0, w$ ]	$0, 0, \bar{z}$ [ $0, 0, w$ ]		
4	e ..2'/m'	$1/4, 1/4, 1/2$ [ $\bar{u}, u, w$ ]	$3/4, 3/4, 1/2$ [ $u, \bar{u}, w$ ]	$1/4, 3/4, 1/2$ [ $\bar{u}, \bar{u}, w$ ]	$3/4, 1/4, 1/2$ [ $u, u, w$ ]		
4	d ..2'/m'	$1/4, 1/4, 0$ [ $\bar{u}, u, w$ ]	$3/4, 3/4, 0$ [ $u, \bar{u}, w$ ]	$1/4, 3/4, 0$ [ $\bar{u}, \bar{u}, w$ ]	$3/4, 1/4, 0$ [ $u, u, w$ ]		
2	c 4m'm'	$0, 1/2, z$ [ $0, 0, w$ ]	$1/2, 0, \bar{z}$ [ $0, 0, w$ ]				
2	b $\bar{4}m'2'$	$0, 0, 1/2$ [ $0, 0, w$ ]	$1/2, 1/2, 1/2$ [ $0, 0, w$ ]				
2	a $\bar{4}m'2'$	$0, 0, 0$ [ $0, 0, w$ ]	$1/2, 1/2, 0$ [ $0, 0, w$ ]				

**Symmetry of Special Projections**

Along [0,0,1]  $p_2, 4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $1/2, 0, z$

Along [1,0,0]  $p2'm'g$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 1/4, 0$

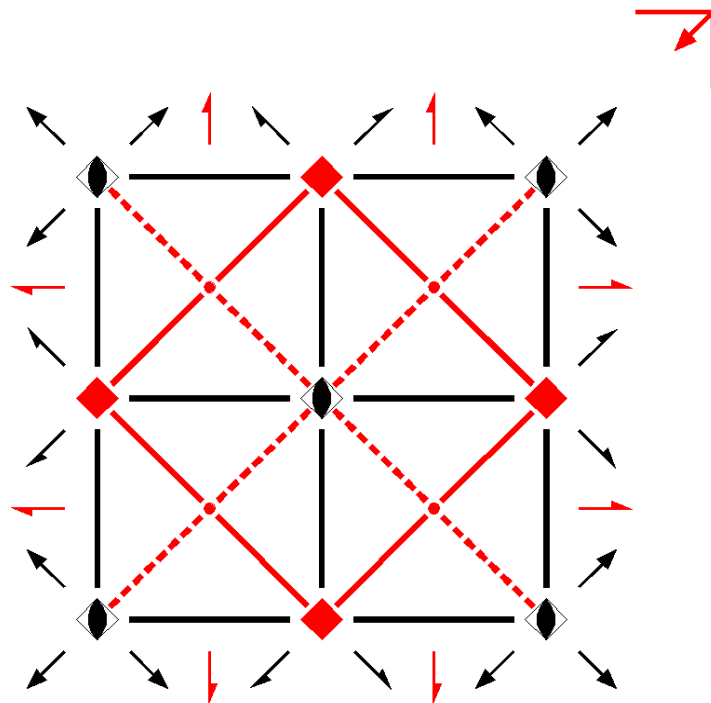
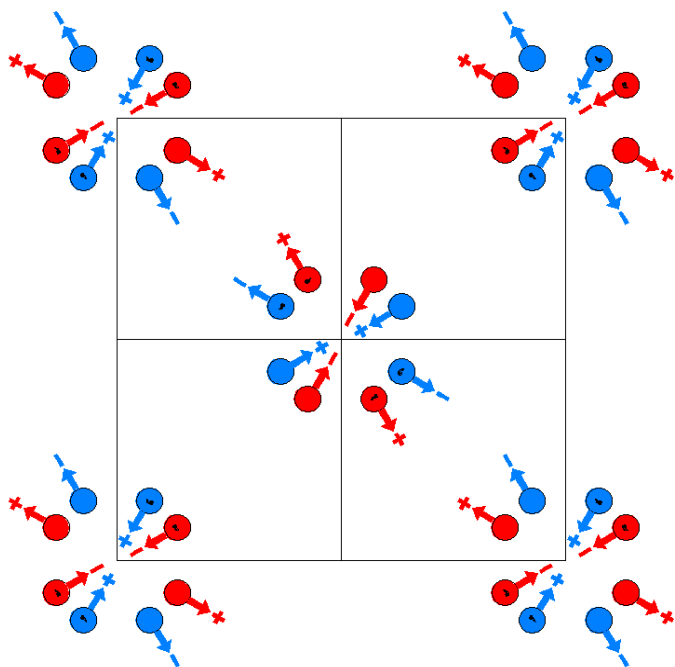
Along [1,1,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x, x, 0$



P4'/n'mm'  
129.8.1082

4'/m'mm'  
P4'/n'2<sub>1</sub>'/m2/m'

Tetragonal



Origin at center  $\bar{4}m2$  at  $\bar{4}/n'm2/g'$ , at  $-1/4, 1/4, 0$  from center ( $2/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$ ;  $y \leq 1/2 - x$

### Symmetry Operations

- |  |   |  |  |
|--|---|--|--|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                    | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0)'                   | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)'                   |
| (5) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (6) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)'  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                      | (8) 2 x,x̄,0<br>(2 <sub>xy</sub>  0,0,0)   |
| (9) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$ ' 1/2,1/2,0)'   | (10) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (11) $\bar{4}$ <sup>+</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub>  0,0,0) | (12) $\bar{4}$ <sup>-</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)                  | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)                   | (15) m' x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,0)'                          | (16) g' (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)'                                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

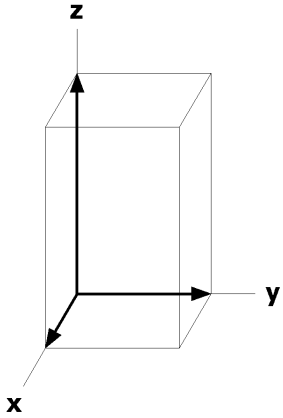
		Coordinates										
Multiplicity,	Wyckoff letter,	Site Symmetry.										
16	k	1										
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{y}+1/2,x+1/2,z$	$[v,\bar{u},\bar{w}]$	(4)	$y+1/2,\bar{x}+1/2,z$	$[\bar{v},u,\bar{w}]$	
(5)	$\bar{x}+1/2,y+1/2,\bar{z}$	$[\bar{u},\bar{v},w]$	(6)	$x+1/2,\bar{y}+1/2,\bar{z}$	$[\bar{u},v,w]$	(7)	$y,x,\bar{z}$	$[v,u,\bar{w}]$	(8)	$\bar{y},\bar{x},\bar{z}$	$[\bar{v},\bar{u},\bar{w}]$	
(9)	$\bar{x}+1/2,\bar{y}+1/2,\bar{z}$	$[\bar{u},\bar{v},\bar{w}]$	(10)	$x+1/2,y+1/2,\bar{z}$	$[u,v,\bar{w}]$	(11)	$y,\bar{x},\bar{z}$	$[\bar{v},u,w]$	(12)	$\bar{y},x,\bar{z}$	$[v,\bar{u},w]$	
(13)	$x,\bar{y},z$	$[\bar{u},v,\bar{w}]$	(14)	$\bar{x},y,z$	$[u,\bar{v},\bar{w}]$	(15)	$\bar{y}+1/2,\bar{x}+1/2,z$	$[\bar{v},\bar{u},w]$	(16)	$y+1/2,x+1/2,z$	$[v,u,w]$	
8	j	..m'	$x,x+1/2,z$	$[\bar{x},\bar{x}+1/2,z$	$[\bar{u},\bar{u},w]$	$\bar{x},x+1/2,z$	$[u,\bar{u},\bar{w}]$	$x,\bar{x}+1/2,z$	$[\bar{u},u,\bar{w}]$	$\bar{x}+1/2,\bar{x},\bar{z}$	$[\bar{u},\bar{u},\bar{w}]$	
8	i	.m.	$0,y,z$	$[u,0,0]$	$0,\bar{y},z$	$[\bar{u},0,0]$	$\bar{y}+1/2,1/2,z$	$[0,\bar{u},0]$	$y+1/2,1/2,z$	$[0,u,0]$	$\bar{y},0,\bar{z}$	$[0,\bar{u},0]$
8	h	..2	$x,x,1/2$	$[u,u,0]$	$\bar{x},\bar{x},1/2$	$[\bar{u},\bar{u},0]$	$\bar{x}+1/2,x+1/2,1/2$	$[u,\bar{u},0]$	$x+1/2,\bar{x}+1/2,1/2$	$[\bar{u},u,0]$	$\bar{x},x,1/2$	$[u,\bar{u},0]$
8	g	..2	$x,x,0$	$[u,u,0]$	$\bar{x},\bar{x},0$	$[\bar{u},\bar{u},0]$	$\bar{x}+1/2,x+1/2,0$	$[u,\bar{u},0]$	$x+1/2,\bar{x}+1/2,0$	$[\bar{u},u,0]$	$\bar{x},x,0$	$[u,\bar{u},0]$
4	f	2mm.	$0,0,z$	$[0,0,0]$	$1/2,1/2,z$	$[0,0,0]$	$1/2,1/2,\bar{z}$	$[0,0,0]$	$0,0,\bar{z}$	$[0,0,0]$		
4	e	..2/m'	$1/4,1/4,1/2$	$[0,0,0]$	$3/4,3/4,1/2$	$[0,0,0]$	$1/4,3/4,1/2$	$[0,0,0]$	$3/4,1/4,1/2$	$[0,0,0]$		
4	d	..2/m'	$1/4,1/4,0$	$[0,0,0]$	$3/4,3/4,0$	$[0,0,0]$	$1/4,3/4,0$	$[0,0,0]$	$3/4,1/4,0$	$[0,0,0]$		
2	c	4'mm	$0,1/2,z$	$[0,0,0]$	$1/2,0,\bar{z}$	$[0,0,0]$						
2	b	$\bar{4}m2$	$0,0,1/2$	$[0,0,0]$	$1/2,1/2,1/2$	$[0,0,0]$						
2	a	$\bar{4}m2$	$0,0,0$	$[0,0,0]$	$1/2,1/2,0$	$[0,0,0]$						

**Symmetry of Special Projections**

Along [0,0,1] p4'm'm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



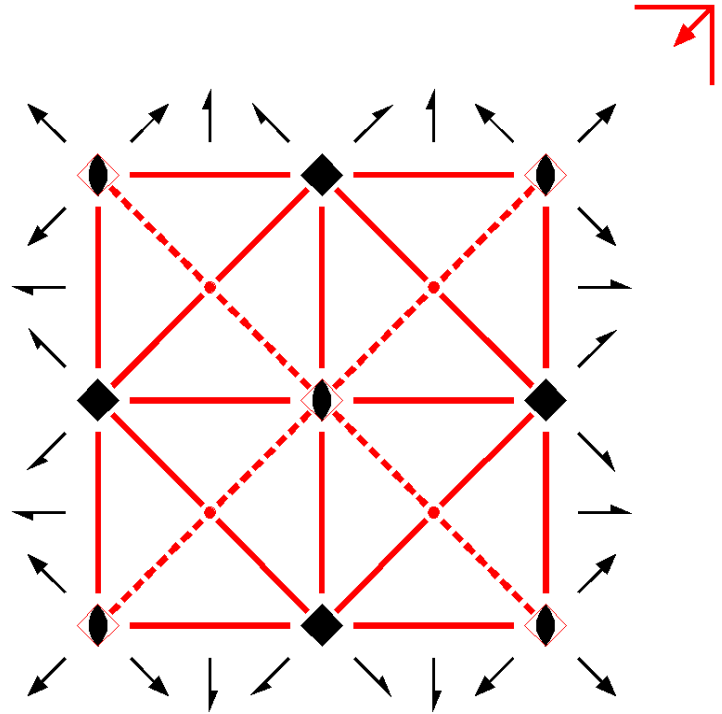
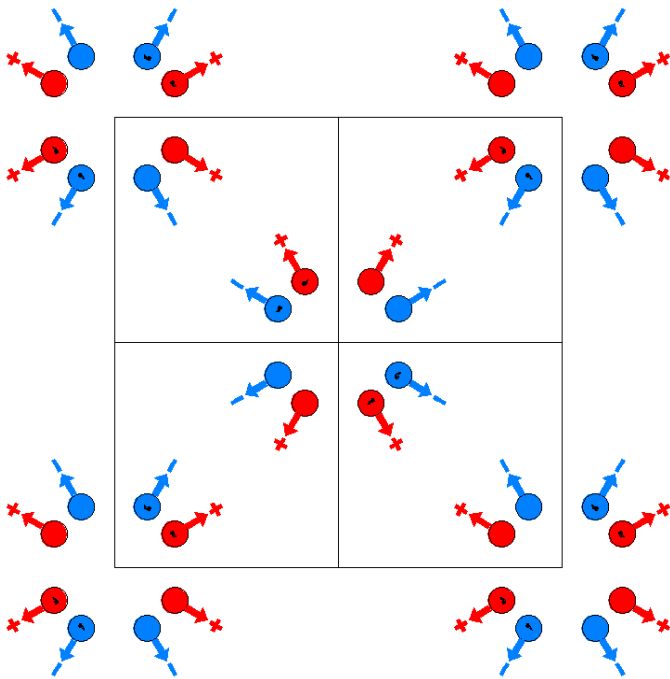
P4/n'm'm'

129.9.1083

4/m'm'm'

P4/n'2<sub>1</sub>/m'2/m'

Tetragonal



Origin at center  $\bar{4}'m'2$  at  $\bar{4}'n'm'2/g'$ , at  $-1/4, 1/4, 0$  from center ( $2/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

- |  |   |  |   |
|--|---|--|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                    | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0)    | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)       |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)    | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                      | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)          |
| (9) $\bar{1}'$ 1/4,1/4,0<br>( $\bar{1}'$  1/2,1/2,0)'  | (10) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)' | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'    | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                     |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)'              | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)'                 | (15) m' x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0)' | (16) g' (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

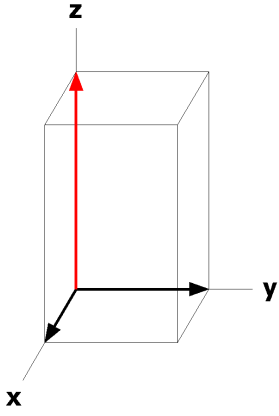
		Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.					
16	k 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z$ [ $v,\bar{u},w$ ]
		(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
		(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
		(13) $x,\bar{y},z$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z$ [ $v,u,w$ ]
8	j ..m'	$x,x+1/2,z$ [ $u,u,w$ ]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x+1/2,z$ [ $\bar{u},u,w$ ]	$x,\bar{x}+1/2,z$ [ $u,\bar{u},w$ ]
		$\bar{x}+1/2,x,\bar{z}$ [ $\bar{u},u,\bar{w}$ ]	$x+1/2,\bar{x},\bar{z}$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x,\bar{z}$ [ $u,u,\bar{w}$ ]	$\bar{x}+1/2,\bar{x},\bar{z}$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	i .m'	$0,y,z$ [ $0,v,w$ ]	$0,\bar{y},z$ [ $0,\bar{v},w$ ]	$\bar{y}+1/2,1/2,z$ [ $\bar{v},0,w$ ]	$y+1/2,1/2,z$ [ $v,0,w$ ]
		$1/2,y+1/2,\bar{z}$ [ $0,v,\bar{w}$ ]	$1/2,\bar{y}+1/2,\bar{z}$ [ $0,\bar{v},\bar{w}$ ]	$y,0,\bar{z}$ [ $v,0,\bar{w}$ ]	$\bar{y},0,\bar{z}$ [ $\bar{v},0,\bar{w}$ ]
8	h ..2	$x,x,1/2$ [ $u,u,0$ ]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $\bar{u},u,0$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $u,\bar{u},0$ ]
		$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x+1/2,1/2$ [ $u,u,0$ ]	$x,\bar{x},1/2$ [ $u,\bar{u},0$ ]	$\bar{x},x,1/2$ [ $\bar{u},u,0$ ]
8	g ..2	$x,x,0$ [ $u,u,0$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,0$ [ $\bar{u},u,0$ ]	$x+1/2,\bar{x}+1/2,0$ [ $u,\bar{u},0$ ]
		$\bar{x}+1/2,\bar{x}+1/2,0$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x+1/2,0$ [ $u,u,0$ ]	$x,\bar{x},0$ [ $u,\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]
4	f 2m'm'	$0,0,z$ [ $0,0,w$ ]	$1/2,1/2,z$ [ $0,0,w$ ]	$1/2,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]	$0,0,\bar{z}$ [ $0,0,\bar{w}$ ]
4	e ..2/m'	$1/4,1/4,1/2$ [ $0,0,0$ ]	$3/4,3/4,1/2$ [ $0,0,0$ ]	$1/4,3/4,1/2$ [ $0,0,0$ ]	$3/4,1/4,1/2$ [ $0,0,0$ ]
4	d ..2/m'	$1/4,1/4,0$ [ $0,0,0$ ]	$3/4,3/4,0$ [ $0,0,0$ ]	$1/4,3/4,0$ [ $0,0,0$ ]	$3/4,1/4,0$ [ $0,0,0$ ]
2	c 4m'm'	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,\bar{z}$ [ $0,0,\bar{w}$ ]		
2	b $\bar{4}$ 'm'2	$0,0,1/2$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]		
2	a $\bar{4}$ 'm'2	$0,0,0$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

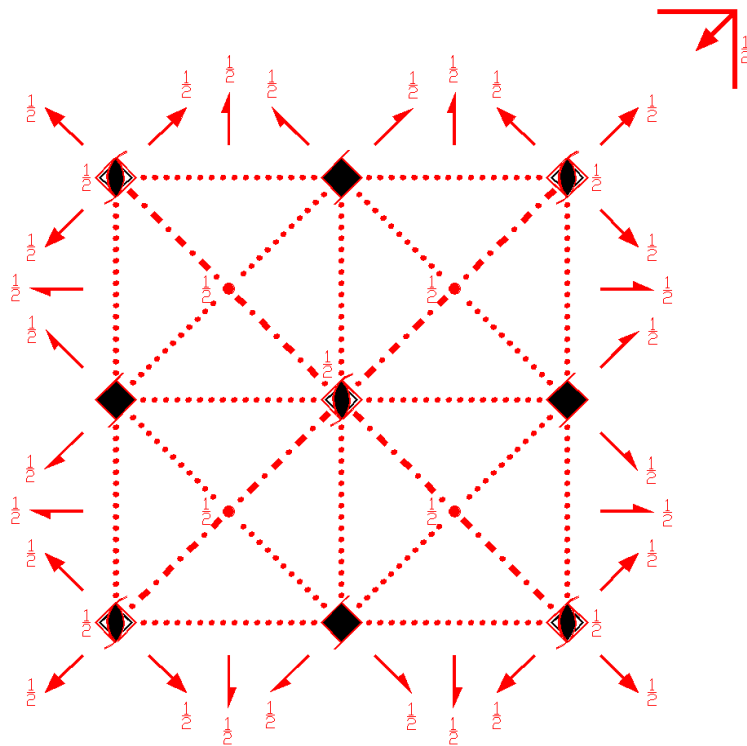
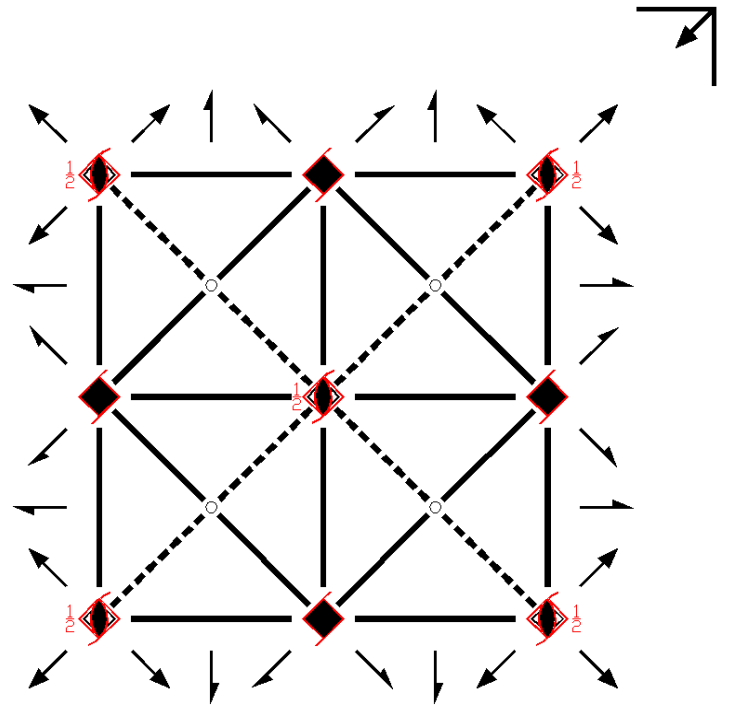
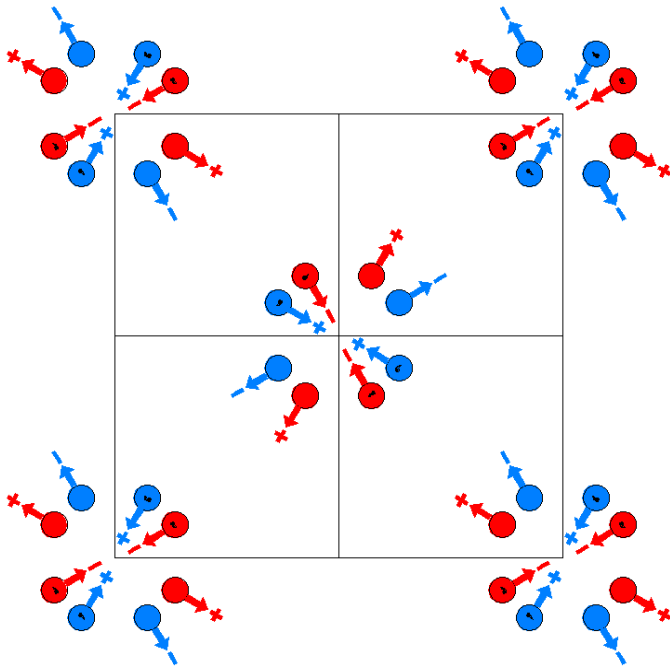
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$P_{2c} 4/nmm$   
129.10.1084

$4/mmm1'$   
 $P_{2c} 4/n2_1/m2/m$

Tetragonal



**Origin** at center  $\bar{4}m2$  at  $\bar{4}/nm2/g$ , at  $-1/4, 1/4, 0$  from center ( $2/m$ )

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |  |   |  |   |
|--|---|--|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                  | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0)  | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0) |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                    | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,0)          |
| (9) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)     | (10) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)     | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z$ <sup>-1</sup>  0,0,0)    |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)                | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)                 | (15) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0) | (16) g (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub> <sup>-</sup>  1/2,1/2,0)   |

For (0,0,1)' + set

- |  |   |  |  |
|--|---|--|--|
| (1) t' (0,0,1)<br>(1 0,0,1)'                               | (2) 2' (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)'            | (3) 4 <sup>+</sup> ' (0,0,1) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1)' | (4) 4 <sup>-</sup> ' (0,0,1) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1)' |
| (5) 2' (0,1/2,0) 1/4,y,1/2<br>(2 <sub>y</sub>  1/2,1/2,1)' | (6) 2' (1/2,0,0) x,1/4,1/2<br>(2 <sub>x</sub>  1/2,1/2,1)'  | (7) 2' x,x,1/2<br>(2 <sub>xy</sub>  0,0,1)'                          | (8) 2' x, $\bar{x}$ ,1/2<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,1)'                 |
| (9) $\bar{1}$ ' 1/4,1/4,1/2<br>( $\bar{1}$  1/2,1/2,1)'    | (10) n' (1/2,1/2,0) x,y,1/2<br>(m <sub>z</sub>  1/2,1/2,1)' | (11) $\bar{4}^+$ ' 0,0,z; 0,0,1/2<br>( $\bar{4}_z$  0,0,1)'          | (12) $\bar{4}^-$ ' 0,0,z; 0,0,1/2<br>( $\bar{4}_z$ <sup>-1</sup>  0,0,1)'          |
| (13) c' (0,0,1) x,0,z<br>(m <sub>y</sub>  0,0,1)'          | (14) c' (0,0,1) 0,y,z<br>(m <sub>x</sub>  0,0,1)'           | (15) c' (0,0,1) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1)' | (16) n' (1/2,1/2,1) x,x,z<br>(m <sub>xy</sub> <sup>-</sup>  1/2,1/2,1)'            |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (0,0,1)' +

32 k 1

- |   |   |  |   |
|---|---|--|---|
| (1) x,y,z [u,v,w]   | (2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]         | (3) $\bar{y}+1/2, x+1/2, z$ [ $\bar{v}, u, w$ ]        | (4) $y+1/2, \bar{x}+1/2, z$ [ $v, \bar{u}, w$ ]                 |
| (5) $\bar{x}+1/2, y+1/2, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ] | (6) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ] | (7) $y, x, \bar{z}$ [ $v, u, \bar{w}$ ]                | (8) $\bar{y}, \bar{x}, \bar{z}$ [ $\bar{v}, \bar{u}, \bar{w}$ ] |
| (9) $\bar{x}+1/2, \bar{y}+1/2, \bar{z}$ [ $u, v, w$ ]       | (10) $x+1/2, y+1/2, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]      | (11) $y, \bar{x}, \bar{z}$ [ $\bar{v}, u, w$ ]         | (12) $\bar{y}, x, \bar{z}$ [ $v, \bar{u}, w$ ]                  |
| (13) $x, \bar{y}, z$ [ $\bar{u}, v, \bar{w}$ ]              | (14) $\bar{x}, y, z$ [ $u, \bar{v}, \bar{w}$ ]              | (15) $\bar{y}+1/2, \bar{x}+1/2, z$ [ $v, u, \bar{w}$ ] | (16) $y+1/2, x+1/2, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]          |
| 16 j ..m  | $x, x+1/2, z$ [ $\bar{u}, u, 0$ ]                           | $\bar{x}, \bar{x}+1/2, z$ [ $u, \bar{u}, 0$ ]          | $\bar{x}, x+1/2, z$ [ $\bar{u}, \bar{u}, 0$ ]                   |
|   | $\bar{x}+1/2, x, \bar{z}$ [ $u, u, 0$ ]                     | $x+1/2, \bar{x}, \bar{z}$ [ $\bar{u}, \bar{u}, 0$ ]    | $x+1/2, x, \bar{z}$ [ $u, \bar{u}, 0$ ]                         |
|   |   |  | $\bar{x}+1/2, \bar{x}, \bar{z}$ [ $\bar{u}, u, 0$ ]             |

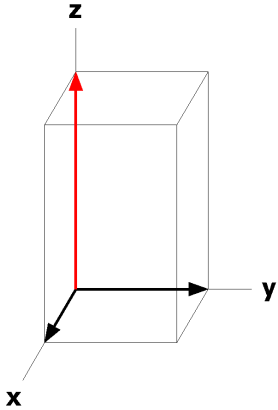
16	i	.m.	0,y,z [u,0,0] 1/2,y+1/2,z̄ [ū,0,0]	0,ȳ,z [ū,0,0] 1/2,ȳ+1/2,z̄ [u,0,0]	ȳ+1/2,1/2,z [0,u,0] y,0,z̄ [0,u,0]	y+1/2,1/2,z [0,ū,0] ȳ,0,z̄ [0,ū,0]
16	h	..2'	x,x,1/2 [ū,u,w] x̄+1/2,x̄+1/2,1/2 [u,ū,w̄]	x̄,x̄,1/2 [u,ū,w] x̄+1/2,x̄+1/2,1/2 [ū,u,w̄]	x̄+1/2,x+1/2,1/2 [ū,ū,w] x̄,x̄,1/2 [u,u,w̄]	x+1/2,x̄+1/2,1/2 [u,u,w] x̄,x,1/2 [ū,ū,w̄]
16	g	..2	x,x,0 [u,u,0] x̄+1/2,x̄+1/2,0 [u,u,0]	x̄,x̄,0 [ū,ū,0] x+1/2,x+1/2,0 [ū,ū,0]	x̄+1/2,x+1/2,0 [ū,u,0] x̄,x̄,0 [ū,u,0]	x+1/2,x̄+1/2,0 [u,ū,0] x̄,x,0 [u,ū,0]
8	f	2mm.	0,0,z [0,0,0]	1/2,1/2,z [0,0,0]	1/2,1/2,z̄ [0,0,0]	0,0,z̄ [0,0,0]
8	e	..2'/m	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]
8	d	..2'/m	1/4,1/4,0 [u,u,0]	3/4,3/4,0 [ū,ū,0]	1/4,3/4,0 [ū,u,0]	3/4,1/4,0 [u,ū,0]
4	c	4mm	0,1/2,z [0,0,0]	1/2,0,z̄ [0,0,0]		
4	b	4̄m2'	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4	a	4̄m2	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



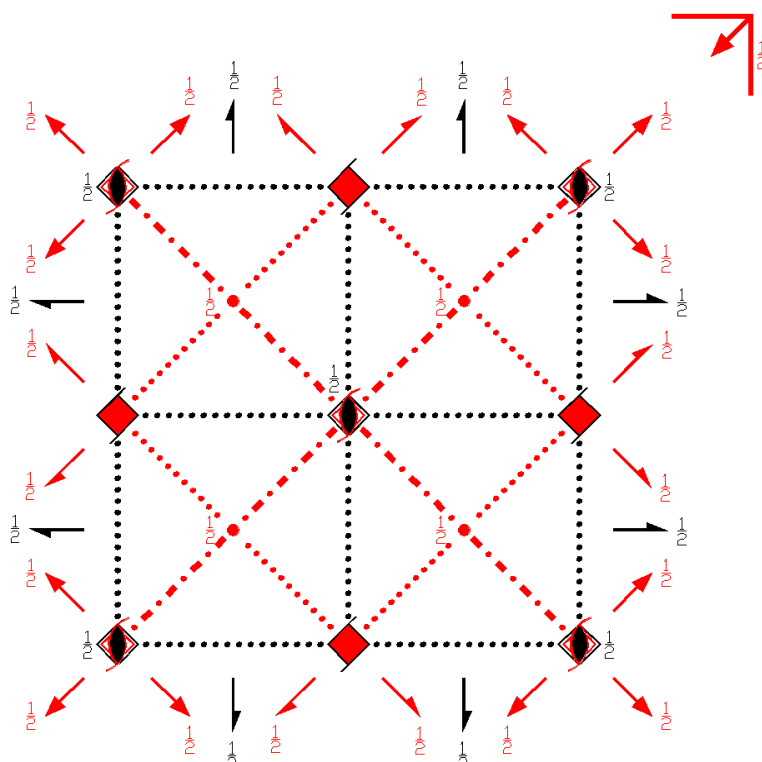
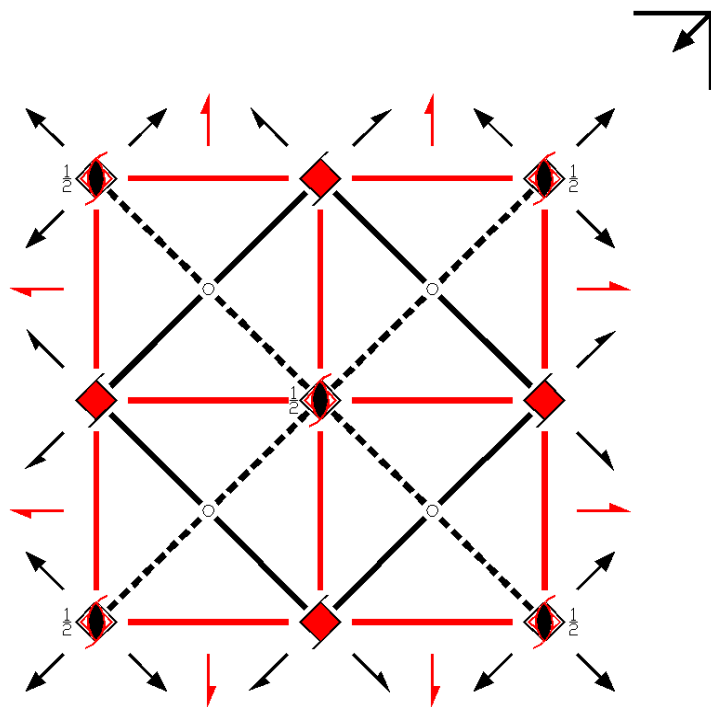
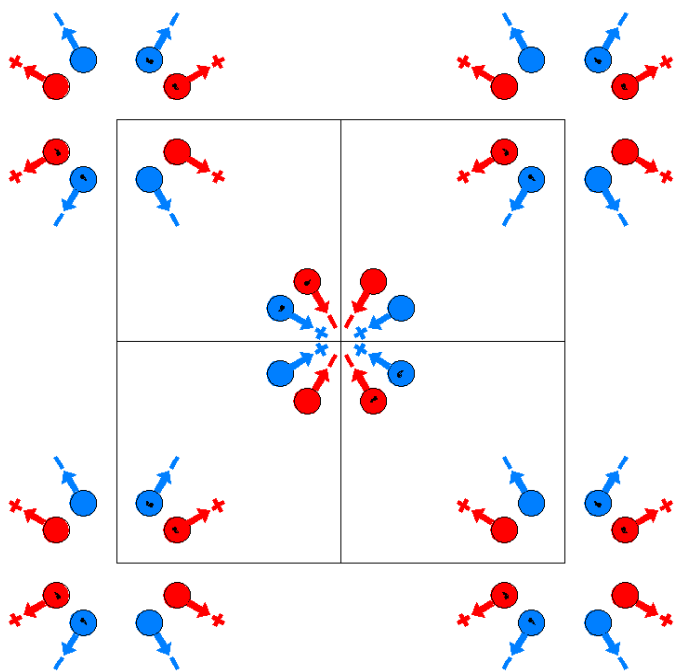
$P_{2c} 4'/nm'm$

129.11.1085

$4/mmm1'$

$P_{2c} 4'/n2_1'/m'2/m$

Tetragonal



**Origin** at center  $\bar{4}'m'2$  at  $\bar{4}'/nm'2/g$ , at  $-1/4, 1/4, 0$  from center (  $2/m$  )

**Asymmetric unit**  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 4 <sup>+</sup> 0,1/2,z (4 <sub>z</sub>  1/2,1/2,0)'	(4) 4 <sup>-</sup> 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)'
(5) 2' (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>  1/2,1/2,0)'	(6) 2' (1/2,0,0) x,1/4,0 (2 <sub>x</sub>  1/2,1/2,0)'	(7) 2 x,x,0 (2 <sub>xy</sub>  0,0,0)	(8) 2 x, $\bar{x}$ ,0 (2 <sub>xy</sub>  0,0,0)
(9) $\bar{1}$ 1/4,1/4,0 ( $\bar{1}$  1/2,1/2,0)	(10) n (1/2,1/2,0) x,y,0 (m <sub>z</sub>  1/2,1/2,0)	(11) $\bar{4}^+$ 0,0,z; 0,0,0 (4 <sub>z</sub>  0,0,0)'	(12) $\bar{4}^-$ 0,0,z; 0,0,0 (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(13) m' x,0,z (m <sub>y</sub>  0,0,0)'	(14) m' 0,y,z (m <sub>x</sub>  0,0,0)'	(15) m x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,0)	(16) g (1/2,1/2,0) x,x,z (m <sub>xy</sub>  1/2,1/2,0)

For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 2' (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)'	(3) 4 <sup>+</sup> (0,0,1) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1)	(4) 4 <sup>-</sup> (0,0,1) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1)
(5) 2 (0,1/2,0) 1/4,y,1/2 (2 <sub>y</sub>  1/2,1/2,1)	(6) 2 (1/2,0,0) x,1/4,1/2 (2 <sub>x</sub>  1/2,1/2,1)	(7) 2' x,x,1/2 (2 <sub>xy</sub>  0,0,1)'	(8) 2' x, $\bar{x}$ ,1/2 (2 <sub>xy</sub>  0,0,1)'
(9) $\bar{1}$ ' 1/4,1/4,1/2 ( $\bar{1}$ ' 1/2,1/2,1)'	(10) n' (1/2,1/2,0) x,y,1/2 (m <sub>z</sub>  1/2,1/2,1)'	(11) $\bar{4}^+$ 0,0,z; 0,0,1/2 (4 <sub>z</sub>  0,0,1)	(12) $\bar{4}^-$ 0,0,z; 0,0,1/2 (4 <sub>z</sub> <sup>-1</sup>  0,0,1)
(13) c (0,0,1) x,0,z (m <sub>y</sub>  0,0,1)	(14) c (0,0,1) 0,y,z (m <sub>x</sub>  0,0,1)	(15) c' (0,0,1) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,1)'	(16) n' (1/2,1/2,1) x,x,z (m <sub>xy</sub>  1/2,1/2,1)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) +      (0,0,1)' +

32    k    1

(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}+1/2, x+1/2, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(4) $y+1/2, \bar{x}+1/2, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]
(5) $\bar{x}+1/2, y+1/2, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(7) $y, x, \bar{z}$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(8) $\bar{y}, \bar{x}, \bar{z}$ [ $\bar{v}, \bar{u}, \bar{w}$ ]
(9) $\bar{x}+1/2, \bar{y}+1/2, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(10) $x+1/2, y+1/2, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(11) $y, \bar{x}, \bar{z}$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(12) $\bar{y}, x, \bar{z}$ [ $\bar{v}, \bar{u}, \bar{w}$ ]
(13) $x, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(14) $\bar{x}, y, z$ [ $\bar{u}, \bar{v}, w$ ]	(15) $\bar{y}+1/2, \bar{x}+1/2, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(16) $y+1/2, x+1/2, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]
16    j    ..m	$x, x+1/2, z$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}, \bar{x}+1/2, z$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}, x+1/2, z$ [ $\bar{u}, \bar{u}, 0$ ]
	$\bar{x}+1/2, x, \bar{z}$ [ $\bar{u}, \bar{u}, 0$ ]	$x+1/2, \bar{x}, \bar{z}$ [ $\bar{u}, \bar{u}, 0$ ]	$x+1/2, x, \bar{z}$ [ $\bar{u}, \bar{u}, 0$ ]
		$\bar{x}, x+1/2, z$ [ $\bar{u}, \bar{u}, 0$ ]	$x, \bar{x}+1/2, z$ [ $\bar{u}, \bar{u}, 0$ ]
		$x+1/2, x, \bar{z}$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}+1/2, \bar{x}, \bar{z}$ [ $\bar{u}, \bar{u}, 0$ ]

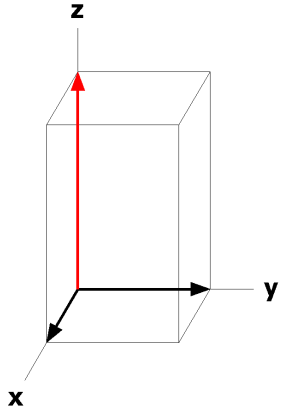
16	i	.m'	0,y,z [0,v,w]	0, $\bar{y}$ ,z [0, $\bar{v}$ ,w]	$\bar{y}+1/2,1/2,z$ [v,0, $\bar{w}$ ]	y+1/2,1/2,z [ $\bar{v}$ ,0, $\bar{w}$ ]
			1/2,y+1/2, $\bar{z}$ [0, $\bar{v}$ ,w]	1/2, $\bar{y}+1/2,\bar{z}$ [0,v,w]	y,0, $\bar{z}$ [v,0, $\bar{w}$ ]	$\bar{y}$ ,0, $\bar{z}$ [ $\bar{v}$ ,0, $\bar{w}$ ]
16	h	..2'	x,x,1/2 [ $\bar{u}$ ,u,w]	$\bar{x},\bar{x},1/2$ [u, $\bar{u}$ ,w]	$\bar{x}+1/2,x+1/2,1/2$ [u,u, $\bar{w}$ ]	x+1/2, $\bar{x}+1/2,1/2$ [ $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]
			$\bar{x}+1/2,\bar{x}+1/2,1/2$ [u, $\bar{u}$ , $\bar{w}$ ]	x+1/2,x+1/2,1/2 [ $\bar{u}$ ,u, $\bar{w}$ ]	x, $\bar{x},1/2$ [ $\bar{u}$ , $\bar{u}$ ,w]	$\bar{x},x,1/2$ [u,u,w]
16	g	..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u}$ , $\bar{u}$ ,0]	$\bar{x}+1/2,x+1/2,0$ [u, $\bar{u}$ ,0]	x+1/2, $\bar{x}+1/2,0$ [ $\bar{u}$ ,u,0]
			$\bar{x}+1/2,\bar{x}+1/2,0$ [u,u,0]	x+1/2,x+1/2,0 [ $\bar{u}$ , $\bar{u}$ ,0]	x, $\bar{x},0$ [u, $\bar{u}$ ,0]	$\bar{x},x,0$ [ $\bar{u}$ ,u,0]
8	f	2m'm'	0,0,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
8	e	..2'/m	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]
8	d	..2/m	1/4,1/4,0 [u,u,0]	3/4,3/4,0 [ $\bar{u}$ , $\bar{u}$ ,0]	1/4,3/4,0 [u, $\bar{u}$ ,0]	3/4,1/4,0 [ $\bar{u}$ ,u,0]
4	c	4'm'm	0,1/2,z [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]		
4	b	$\bar{4}$ m'2'	0,0,1/2 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		
4	a	$\bar{4}$ 'm'2	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub> 2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/2

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



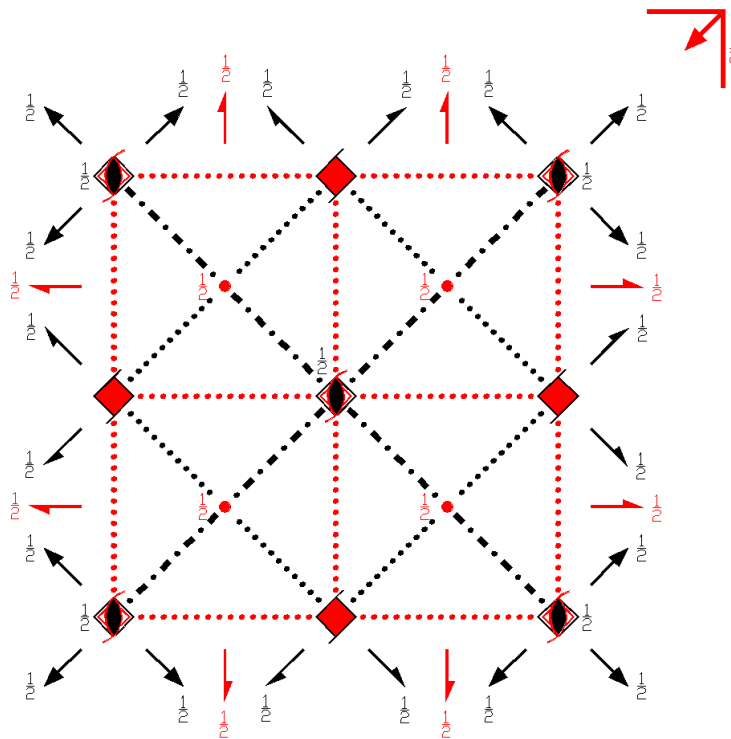
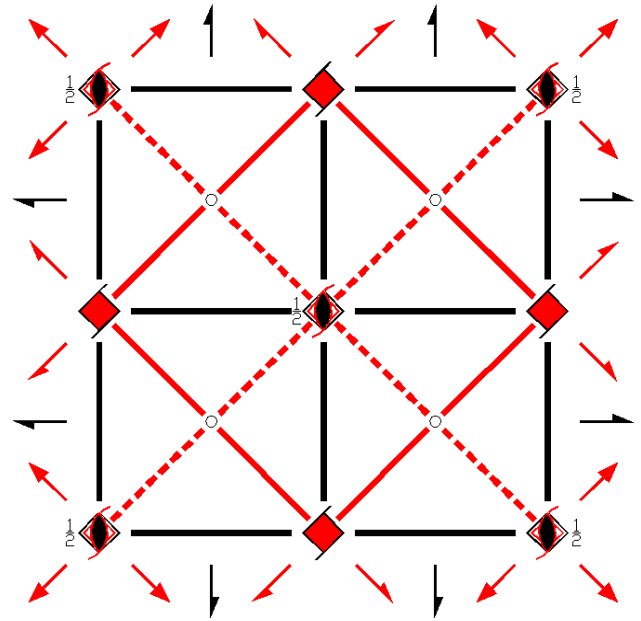
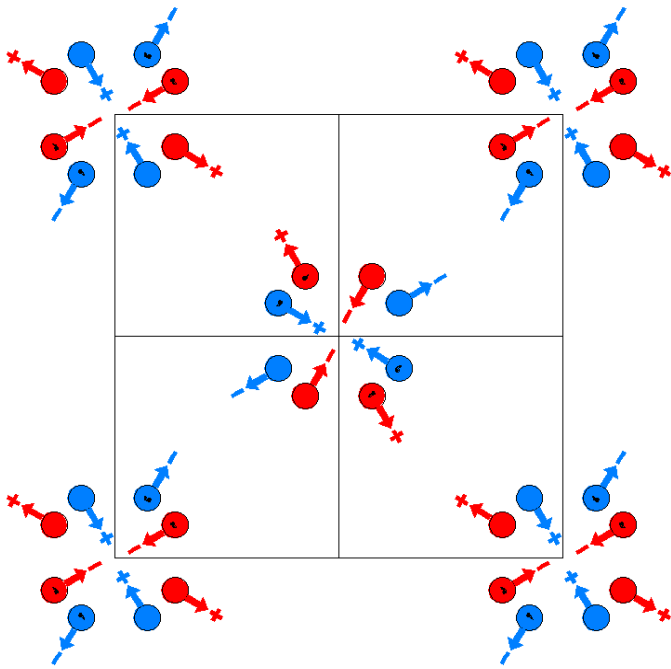
$P_{2c} 4'/nmm'$

129.12.1086

$4/mmm1'$

$P_{2c} 4'/n2_1/m2'/m'$

Tetragonal





**Origin** at center  $\bar{4}'m2'$  at  $\bar{4}'/nm2'/g'$ , at -1/4, 1/4, 0 from center (  $2'/m'$  )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 4 <sup>+</sup> ' 0,1/2,z (4 <sub>z</sub>  1/2,1/2,0)'	(4) 4 <sup>-</sup> ' 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)'
(5) 2 (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>  1/2,1/2,0)	(6) 2 (1/2,0,0) x,1/4,0 (2 <sub>x</sub>  1/2,1/2,0)	(7) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) 2' x, $\bar{x}$ ,0 (2 <sub>xy</sub>  0,0,0)'
(9) $\bar{1}$ 1/4,1/4,0 ( $\bar{1}$  1/2,1/2,0)	(10) n (1/2,1/2,0) x,y,0 (m <sub>z</sub>  1/2,1/2,0)	(11) $\bar{4}^+$ ' 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'	(12) $\bar{4}^-$ ' 0,0,z; 0,0,0 ( $\bar{4}_z$ <sup>-1</sup>  0,0,0)'
(13) m x,0,z (m <sub>y</sub>  0,0,0)	(14) m 0,y,z (m <sub>x</sub>  0,0,0)	(15) m' x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,0)'	(16) g' (1/2,1/2,0) x,x,z (m <sub>xy</sub>  1/2,1/2,0)'

For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 2' (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)'	(3) 4 <sup>+</sup> (0,0,1) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1)	(4) 4 <sup>-</sup> (0,0,1) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1)
(5) 2' (0,1/2,0) 1/4,y,1/2 (2 <sub>y</sub>  1/2,1/2,1)'	(6) 2' (1/2,0,0) x,1/4,1/2 (2 <sub>x</sub>  1/2,1/2,1)'	(7) 2 x,x,1/2 (2 <sub>xy</sub>  0,0,1)	(8) 2 x, $\bar{x}$ ,1/2 (2 <sub>xy</sub>  0,0,1)
(9) $\bar{1}$ ' 1/4,1/4,1/2 ( $\bar{1}$  1/2,1/2,1)'	(10) n' (1/2,1/2,0) x,y,1/2 (m <sub>z</sub>  1/2,1/2,1)'	(11) $\bar{4}^+$ 0,0,z; 0,0,1/2 ( $\bar{4}_z$  0,0,1)	(12) $\bar{4}^-$ 0,0,z; 0,0,1/2 ( $\bar{4}_z$ <sup>-1</sup>  0,0,1)
(13) c' (0,0,1) x,0,z (m <sub>y</sub>  0,0,1)'	(14) c' (0,0,1) 0,y,z (m <sub>x</sub>  0,0,1)'	(15) c (0,0,1) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,1)	(16) n (1/2,1/2,1) x,x,z (m <sub>xy</sub>  1/2,1/2,1)

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (0,0,1)' +

32 k 1

(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z$ [ $\bar{v},u,\bar{w}$ ]
(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},u,w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]
(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
(13) $x,\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z$ [ $v,u,w$ ]
16 j ..m'	$x,x+1/2,z$ [ $u,u,w$ ]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x+1/2,z$ [ $u,\bar{u},\bar{w}$ ]
	$\bar{x}+1/2,x,\bar{z}$ [ $\bar{u},u,\bar{w}$ ]	$x+1/2,\bar{x},\bar{z}$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x,\bar{z}$ [ $\bar{u},\bar{u},\bar{w}$ ]
		$\bar{x},x+1/2,z$ [ $u,\bar{u},\bar{w}$ ]	$x,\bar{x}+1/2,z$ [ $\bar{u},u,\bar{w}$ ]
		$x+1/2,x,\bar{z}$ [ $\bar{u},\bar{u},\bar{w}$ ]	$\bar{x}+1/2,\bar{x},\bar{z}$ [ $u,u,\bar{w}$ ]

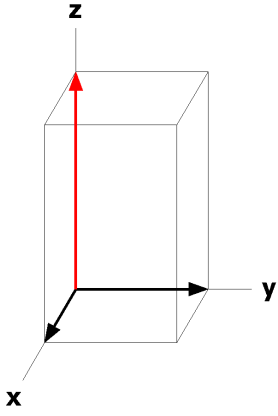
16	i	.m.	0,y,z [u,0,0] 1/2,y+1/2,z̄ [ū,0,0]	0,ȳ,z [ū,0,0] 1/2,ȳ+1/2,z̄ [u,0,0]	ȳ+1/2,1/2,z [0,ū,0] y,0,z̄ [0,ū,0]	y+1/2,1/2,z [0,u,0] ȳ,0,z̄ [0,u,0]
16	h	..2	x,x,1/2 [u,u,0] x̄+1/2,x̄+1/2,1/2 [ū,ū,0]	x̄,x̄,1/2 [ū,ū,0] x̄+1/2,x̄+1/2,1/2 [u,u,0]	x̄+1/2,x+1/2,1/2 [u,ū,0] x,x̄,1/2 [ū,u,0]	x+1/2,x̄+1/2,1/2 [ū,u,0] x̄,x,1/2 [u,ū,0]
16	g	..2'	x,x,0 [ū,u,w] x̄+1/2,x̄+1/2,0 [ū,ū,w]	x̄,x̄,0 [u,ū,w] x+1/2,x+1/2,0 [u,ū,w]	x̄+1/2,x+1/2,0 [u,u,w̄] x,x̄,0 [u,u,w̄]	x+1/2,x̄+1/2,0 [ū,ū,w̄] x̄,x,0 [ū,ū,w̄]
8	f	2mm.	0,0,z [0,0,0]	1/2,1/2,z [0,0,0]	1/2,1/2,z̄ [0,0,0]	0,0,z̄ [0,0,0]
8	e	..2/m	1/4,1/4,1/2 [u,u,0]	3/4,3/4,1/2 [ū,ū,0]	1/4,3/4,1/2 [u,ū,0]	3/4,1/4,1/2 [ū,u,0]
8	d	..2'/m'	1/4,1/4,0 [ū,u,w]	3/4,3/4,0 [u,ū,w]	1/4,3/4,0 [u,u,w̄]	3/4,1/4,0 [ū,ū,w̄]
4	c	4'mm'	0,1/2,z [0,0,0]	1/2,0,z̄ [0,0,0]		
4	b	4̄m2	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4	a	4̄'m2'	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

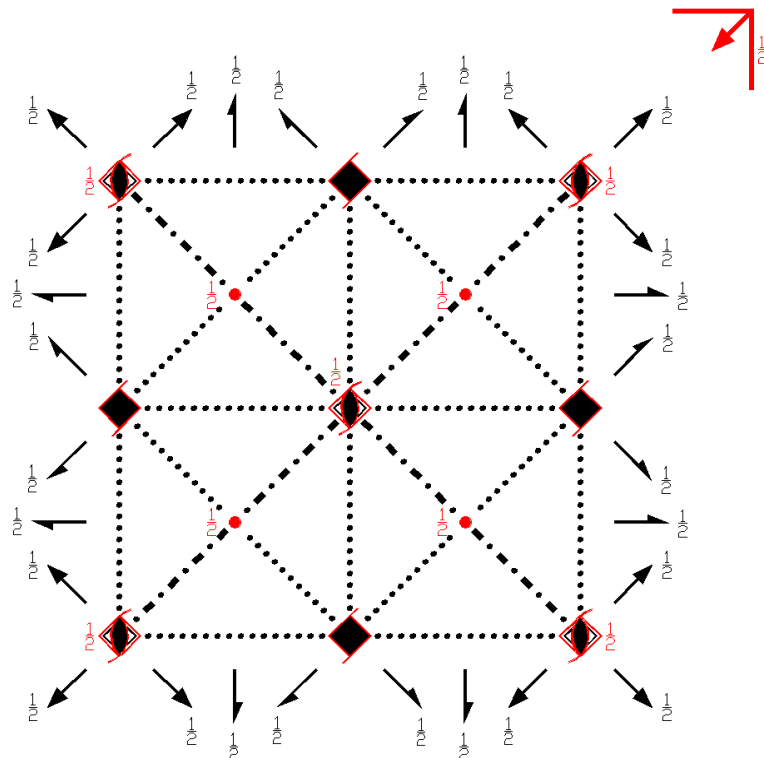
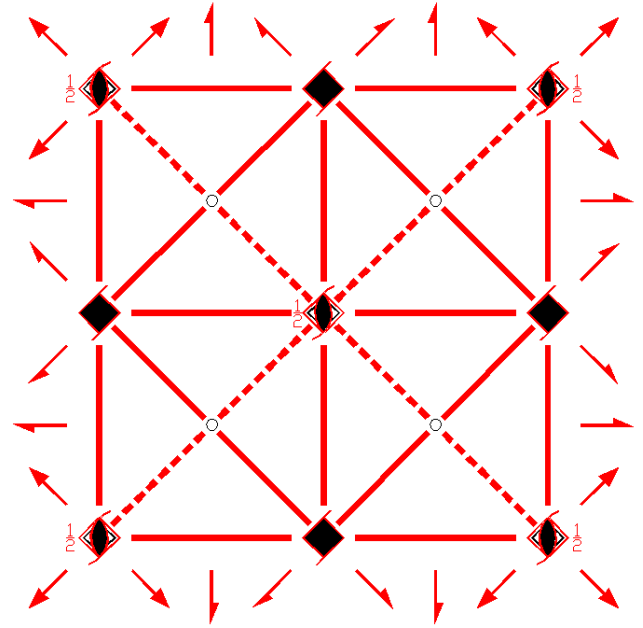
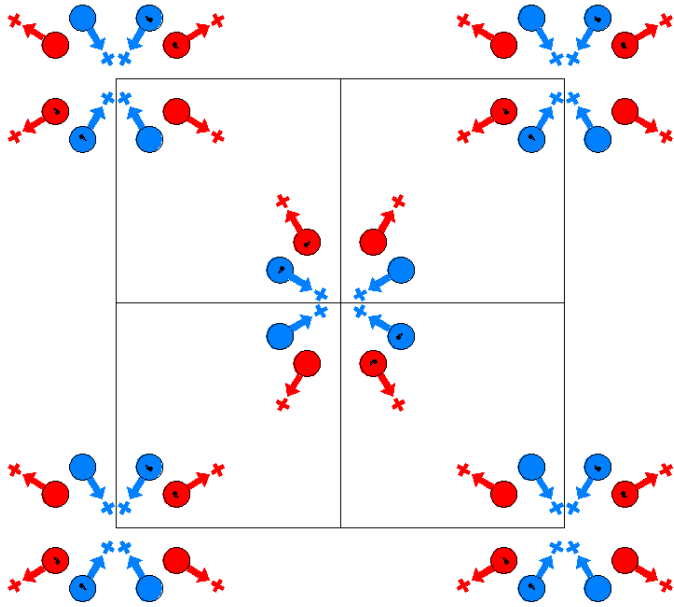
Along [1,1,0] p<sub>2a</sub>\* 2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/2



$P_{2c} 4/nm'm'$   
129.13.1087

$4/mmm1'$   
 $P_{2c} 4/n2_1'/m'2'/m'$

Tetragonal



**Origin** at center  $\bar{4}m'2'$  at  $\bar{4}/nm'2'/g'$ , at -1/4, 1/4, 0 from center (  $2'/m'$  )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 4 <sup>+</sup> 0,1/2,z (4 <sub>z</sub>  1/2,1/2,0)	(4) 4 <sup>-</sup> 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)
(5) 2' (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>  1/2,1/2,0)'	(6) 2' (1/2,0,0) x,1/4,0 (2 <sub>x</sub>  1/2,1/2,0)'	(7) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) 2' x, $\bar{x}$ ,0 (2 <sub>xy</sub> <sup>-</sup>  0,0,0)'
(9) $\bar{1}$ 1/4,1/4,0 ( $\bar{1}$  1/2,1/2,0)	(10) n (1/2,1/2,0) x,y,0 (m <sub>z</sub>  1/2,1/2,0)	(11) $\bar{4}^+$ 0,0,z; 0,0,0 (4 <sub>z</sub>  0,0,0)	(12) $\bar{4}^-$ 0,0,z; 0,0,0 (4 <sub>z</sub> <sup>-1</sup>  0,0,0)
(13) m' x,0,z (m <sub>y</sub>  0,0,0)'	(14) m' 0,y,z (m <sub>x</sub>  0,0,0)'	(15) m' x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,0)'	(16) g' (1/2,1/2,0) x,x,z (m <sub>xy</sub> <sup>-</sup>  1/2,1/2,0)'

For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 2' (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)'	(3) 4 <sup>+</sup> ' (0,0,1) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1)'	(4) 4 <sup>-</sup> ' (0,0,1) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1)'
(5) 2 (0,1/2,0) 1/4,y,1/2 (2 <sub>y</sub>  1/2,1/2,1)	(6) 2 (1/2,0,0) x,1/4,1/2 (2 <sub>x</sub>  1/2,1/2,1)	(7) 2 x,x,1/2 (2 <sub>xy</sub>  0,0,1)	(8) 2 x, $\bar{x}$ ,1/2 (2 <sub>xy</sub> <sup>-</sup>  0,0,1)
(9) $\bar{1}$ ' 1/4,1/4,1/2 ( $\bar{1}$  1/2,1/2,1)'	(10) n' (1/2,1/2,0) x,y,1/2 (m <sub>z</sub>  1/2,1/2,1)'	(11) $\bar{4}^+$ ' 0,0,z; 0,0,1/2 (4 <sub>z</sub>  0,0,1)'	(12) $\bar{4}^-$ ' 0,0,z; 0,0,1/2 (4 <sub>z</sub> <sup>-1</sup>  0,0,1)'
(13) c (0,0,1) x,0,z (m <sub>y</sub>  0,0,1)	(14) c (0,0,1) 0,y,z (m <sub>x</sub>  0,0,1)	(15) c (0,0,1) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,1)	(16) n (1/2,1/2,1) x,x,z (m <sub>xy</sub> <sup>-</sup>  1/2,1/2,1)

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) +      (0,0,1)' +

32    k    1

(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z$ [ $v,\bar{u},w$ ]
(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},u,w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]
(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
(13) $x,\bar{y},z$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z$ [ $v,u,w$ ]
16    j    ..m'	$x,x+1/2,z$ [ $u,u,w$ ]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x+1/2,z$ [ $\bar{u},u,w$ ]
	$\bar{x}+1/2,x,\bar{z}$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x},\bar{z}$ [ $\bar{u},u,w$ ]	$\bar{x}+1/2,\bar{x},\bar{z}$ [ $u,u,w$ ]

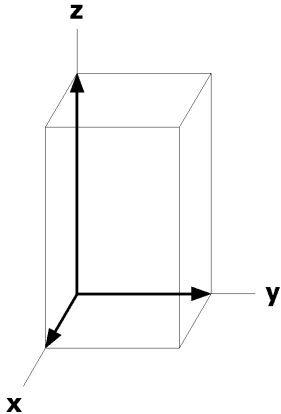
16	i	.m'	0,y,z [0,v,w]	0, $\bar{y}$ ,z [0, $\bar{v}$ ,w]	$\bar{y}+1/2,1/2,z$ [ $\bar{v}$ ,0,w]	y+1/2,1/2,z [v,0,w]
			1/2,y+1/2, $\bar{z}$ [0, $\bar{v}$ ,w]	1/2, $\bar{y}+1/2,\bar{z}$ [0,v,w]	y,0, $\bar{z}$ [ $\bar{v}$ ,0,w]	$\bar{y}$ ,0, $\bar{z}$ [v,0,w]
16	h	..2	x,x,1/2 [u,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $\bar{u},u,0$ ]	x+1/2, $\bar{x}+1/2,1/2$ [u, $\bar{u},0$ ]
			$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]	x+1/2,x+1/2,1/2 [u,u,0]	x, $\bar{x},1/2$ [u, $\bar{u},0$ ]	$\bar{x},x,1/2$ [ $\bar{u},u,0$ ]
16	g	..2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [u, $\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,0$ [ $\bar{u},\bar{u},w$ ]	x+1/2, $\bar{x}+1/2,0$ [u,u,w]
			$\bar{x}+1/2,\bar{x}+1/2,0$ [ $\bar{u},u,w$ ]	x+1/2,x+1/2,0 [u, $\bar{u},w$ ]	x, $\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,0$ [u,u,w]
8	f	2m'm'	0,0,z [0,0,w]	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]
8	e	..2/m'	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]	1/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]
8	d	..2'/m'	1/4,1/4,0 [ $\bar{u},u,w$ ]	3/4,3/4,0 [u, $\bar{u},w$ ]	1/4,3/4,0 [ $\bar{u},\bar{u},w$ ]	3/4,1/4,0 [u,u,w]
4	c	4m'm'	0,1/2,z [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]		
4	b	$\bar{4}$ 'm'2	0,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4	a	$\bar{4}$ m'2'	0,0,0 [0,0,w]	1/2,1/2,0 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

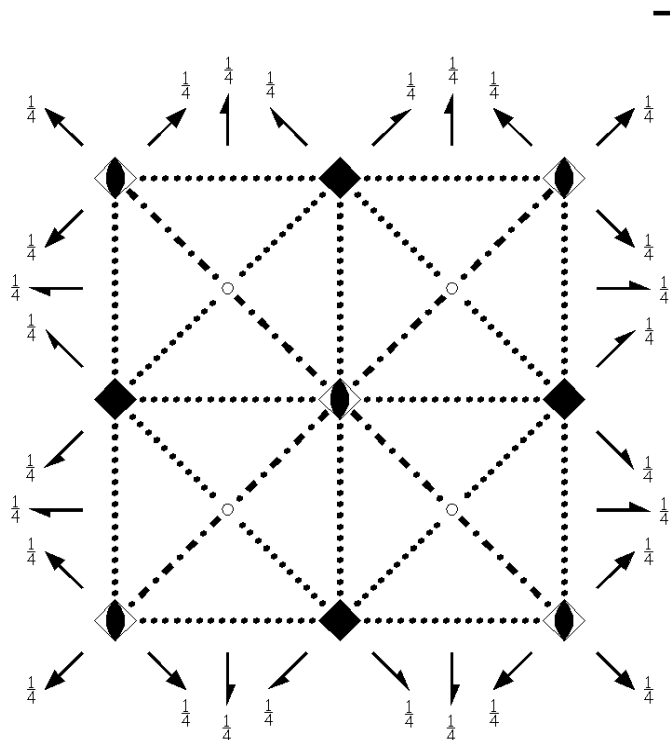
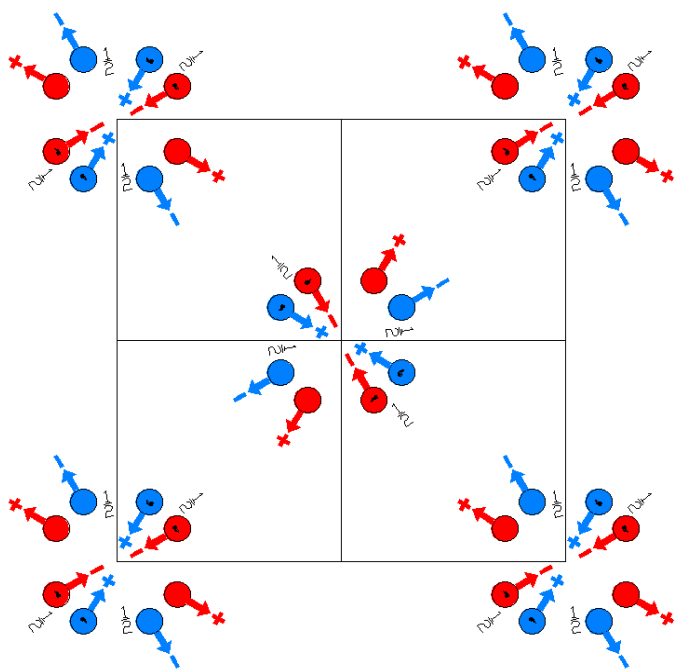
Along [1,1,0] p<sub>2a</sub>\* 2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/2



P4/ncc  
130.1.1088

4/mmm  
P4/n<sub>2</sub><sub>1</sub>/c2/c

Tetragonal



Origin at  $\bar{4}/ncn$ , at  $-1/4, 1/4, 0$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0)              | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)         |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                            | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)        |
| (9) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)         | (10) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)    | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)               | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                        |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)        | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)        | (15) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (16) n (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

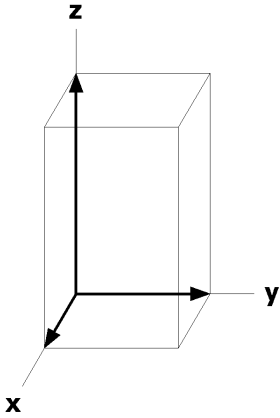
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z$ [ $v,\bar{u},w$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]	(13) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	f	.2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/4$ [ $\bar{u},u,0$ ]	$x+1/2,\bar{x}+1/2,1/4$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,\bar{x}+1/2,3/4$ [u,u,0]	$x+1/2,x+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},3/4$ [ $\bar{u},u,0$ ]	$\bar{x},x,3/4$ [ $u,\bar{u},0$ ]								
8	e	2..	0,0,z [0,0,w]	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]								
8	d	$\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,0 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,0 [ $\bar{v},u,w$ ]	3/4,1/4,0 [ $v,\bar{u},w$ ]	1/4,3/4,1/2 [ $\bar{u},v,\bar{w}$ ]	3/4,1/4,1/2 [ $u,\bar{v},\bar{w}$ ]	1/4,1/4,1/2 [ $v,u,\bar{w}$ ]	3/4,3/4,1/2 [ $\bar{v},\bar{u},\bar{w}$ ]								
4	c	4..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]												
4	b	$\bar{4}..$	0,0,0 [0,0,w]	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]	0,0,1/2 [0,0, $\bar{w}$ ]												
4	a	2.22	0,0,1/4 [0,0,0]	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]	0,0,3/4 [0,0,0]												

**Symmetry of Special Projections**

Along [0,0,1]  $p_p$ , 4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/2,0,z

Along [1,0,0]  $p_{2b}$ , 2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,0

Along [1,1,0]  $p_{2a}$ , 2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0

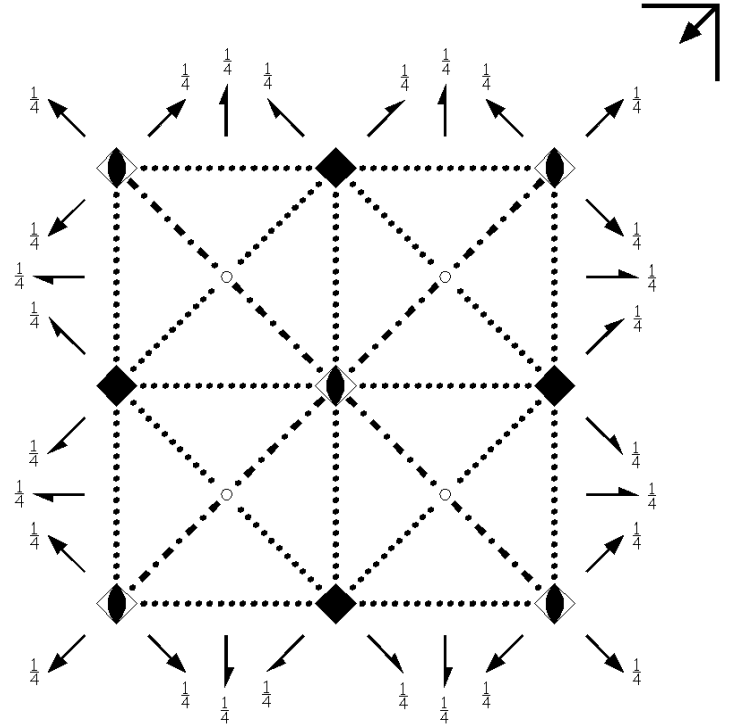
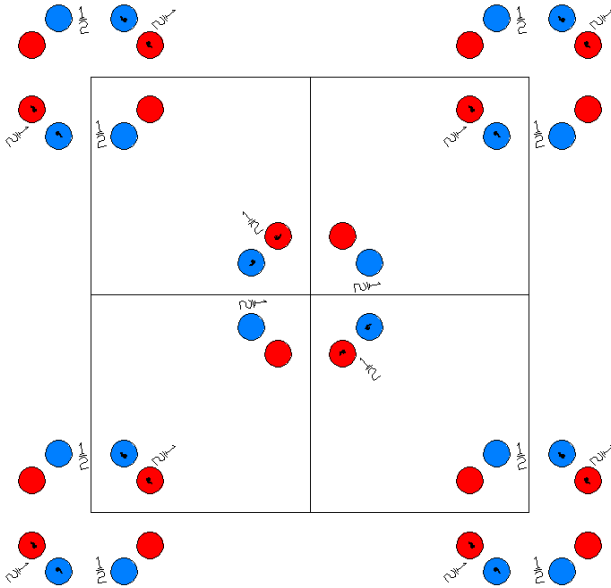


P4/ncc1'  
130.2.1089

4/mmm1'  
P4/n2<sub>1</sub>/c2/c1'

Tetragonal

1'



Origin at  $\bar{4}/ncn1'$ , at  $-1/4, 1/4, 0$  from  $\bar{1}1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For 1 + set

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0)              | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)         |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                            | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)        |
| (9) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)         | (10) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)    | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)               | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                        |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)        | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)        | (15) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (16) n (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2) |



## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> 0,1/2,z (4 <sub>z</sub>  1/2,1/2,0)'	(4) 4 <sup>-</sup> 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)'
(5) 2' (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>  1/2,1/2,1/2)'	(6) 2' (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>  1/2,1/2,1/2)'	(7) 2' x,x,1/4 (2 <sub>xy</sub>  0,0,1/2)'	(8) 2' x, $\bar{x}$ ,1/4 (2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)'
(9) $\bar{1}$ ' 1/4,1/4,0 ( $\bar{1}$  1/2,1/2,0)'	(10) n' (1/2,1/2,0) x,y,0 (m <sub>z</sub>  1/2,1/2,0)'	(11) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z^+$  0,0,0)'	(12) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z^-$  0,0,0)'
(13) c' (0,0,1/2) x,0,z (m <sub>y</sub>  0,0,1/2)'	(14) c' (0,0,1/2) 0,y,z (m <sub>x</sub>  0,0,1/2)'	(15) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,1/2)'	(16) n' (1/2,1/2,1/2) x,x,z (m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			1 +		1' +	
16	g	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y}+1/2,x+1/2,z$ [0,0,0]	(4) $y+1/2,\bar{x}+1/2,z$ [0,0,0]
			(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [0,0,0]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [0,0,0]	(7) $y,x,\bar{z}+1/2$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [0,0,0]
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [0,0,0]	(10) $x+1/2,y+1/2,\bar{z}$ [0,0,0]	(11) $y,\bar{x},\bar{z}$ [0,0,0]	(12) $\bar{y},x,\bar{z}$ [0,0,0]
			(13) $x,\bar{y},z+1/2$ [0,0,0]	(14) $\bar{x},y,z+1/2$ [0,0,0]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [0,0,0]	(16) $y+1/2,x+1/2,z+1/2$ [0,0,0]
8	f	..21'	x,x,1/4 [0,0,0]	$\bar{x},\bar{x},1/4$ [0,0,0]	$\bar{x}+1/2,x+1/2,1/4$ [0,0,0]	$x+1/2,\bar{x}+1/2,1/4$ [0,0,0]
			$\bar{x}+1/2,\bar{x}+1/2,3/4$ [0,0,0]	$x+1/2,x+1/2,3/4$ [0,0,0]	$x,\bar{x},3/4$ [0,0,0]	$\bar{x},x,3/4$ [0,0,0]
8	e	2..1'	0,0,z [0,0,0]	1/2,1/2,z [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]
			1/2,1/2, $\bar{z}$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0,z+1/2 [0,0,0]	1/2,1/2,z+1/2 [0,0,0]
8	d	$\bar{1}$ 1'	1/4,1/4,0 [0,0,0]	3/4,3/4,0 [0,0,0]	1/4,3/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]
			1/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]
4	c	4..1'	0,1/2,z [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	0,1/2,z+1/2 [0,0,0]
4	b	$\bar{4}$ ..1'	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	0,0,1/2 [0,0,0]

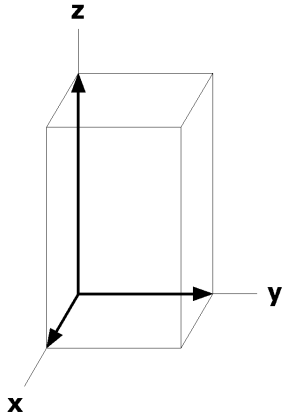
4 a 2.221' 0,0,1/4 [0,0,0] 1/2,1/2,1/4 [0,0,0] 1/2,1/2,3/4 [0,0,0] 0,0,3/4 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,0

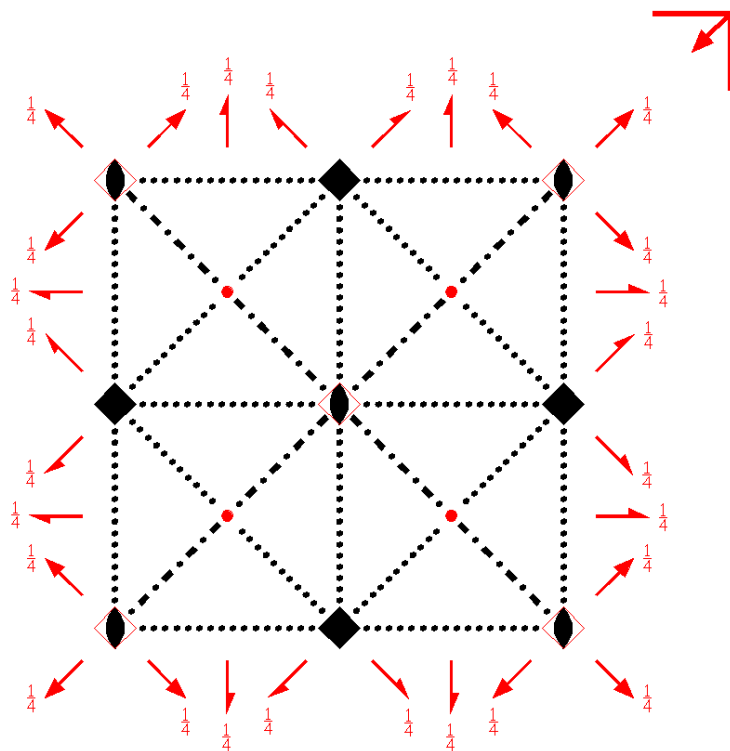
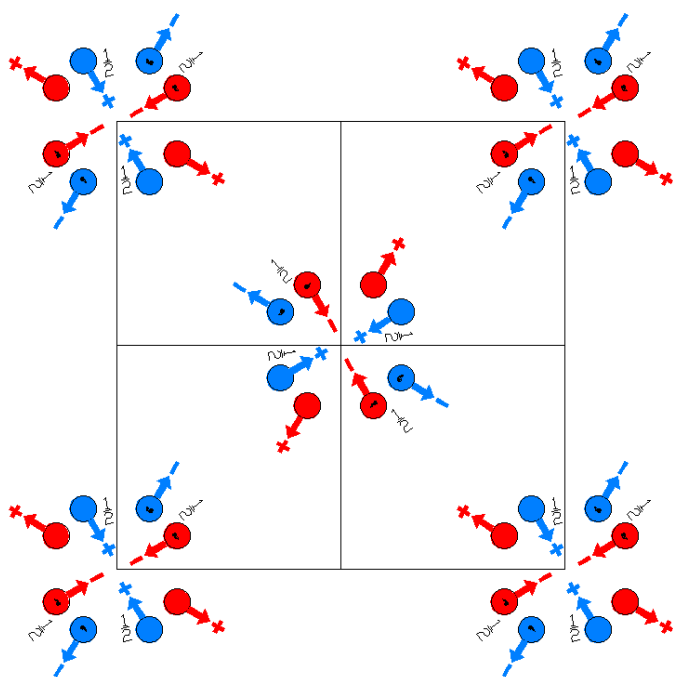
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



P4/n'cc  
130.3.1090

4/m'mm  
P4/n'2<sub>1</sub>'/c2'/c

Tetragonal



Origin at  $\bar{4}'/n'cn$ , at  $-1/4, 1/4, 0$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) $1$<br>( $1 0,0,0$ )                                   | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                         | (3) $4^+$ $0,1/2,z$<br>( $4_z 1/2,1/2,0$ )                         | (4) $4^-$ $1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,0$ )                    |
| (5) $2'$ $(0,1/2,0)$ $1/4,y,1/4$<br>( $2_y 1/2,1/2,1/2$ )' | (6) $2'$ $(1/2,0,0)$ $x,1/4,1/4$<br>( $2_x 1/2,1/2,1/2$ )' | (7) $2'$ $x,x,1/4$<br>( $2_{xy} 0,0,1/2$ )'                        | (8) $2'$ $x,\bar{x},1/4$<br>( $2_{\bar{xy}} 0,0,1/2$ )'            |
| (9) $\bar{1}'$ $1/4,1/4,0$<br>( $\bar{1} 1/2,1/2,0$ )'     | (10) $n'$ $(1/2,1/2,0)$ $x,y,0$<br>( $m_z 1/2,1/2,0$ )'    | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )'          | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ )'     |
| (13) $c$ $(0,0,1/2)$ $x,0,z$<br>( $m_y 0,0,1/2$ )          | (14) $c$ $(0,0,1/2)$ $0,y,z$<br>( $m_x 0,0,1/2$ )          | (15) $c$ $(0,0,1/2)$ $x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,1/2$ ) | (16) $n$ $(1/2,1/2,1/2)$ $x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,1/2$ ) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

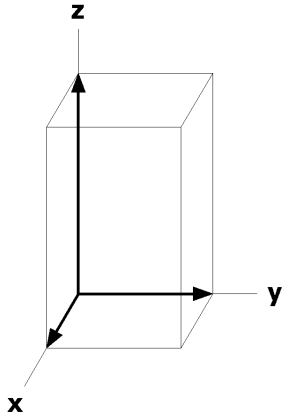
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z$ [v, $\bar{u},w$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [u, $\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(7) y,x, $\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [v,u,w]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}$ [u,v, $\bar{w}$ ]	(11) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(13) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [u, $\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [v,u, $\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	f	..2'	x,x,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [u, $\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,1/4$ [ $\bar{u},\bar{u},w$ ]	$x+1/2,\bar{x}+1/2,1/4$ [u,u,w]	$\bar{x}+1/2,\bar{x}+1/2,3/4$ [u, $\bar{u},\bar{w}$ ]	$x+1/2,x+1/2,3/4$ [ $\bar{u},u,\bar{w}$ ]	$x,\bar{x},3/4$ [u,u, $\bar{w}$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]								
8	e	2..	0,0,z [0,0,w]	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]								
8	d	$\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,0 [0,0,0]	1/4,3/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]	1/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]								
4	c	4..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]												
4	b	$\bar{4}'..$	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	0,0,1/2 [0,0,0]												
4	a	2.2'2'	0,0,1/4 [0,0,w]	1/2,1/2,1/4 [0,0,w]	1/2,1/2,3/4 [0,0, $\bar{w}$ ]	0,0,3/4 [0,0, $\bar{w}$ ]												

**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b} \cdot 2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,1/4

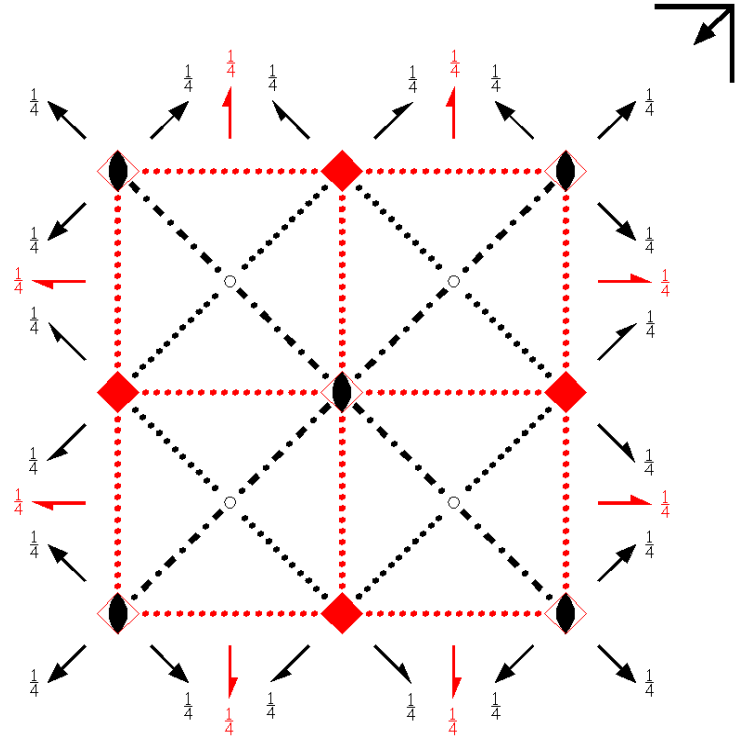
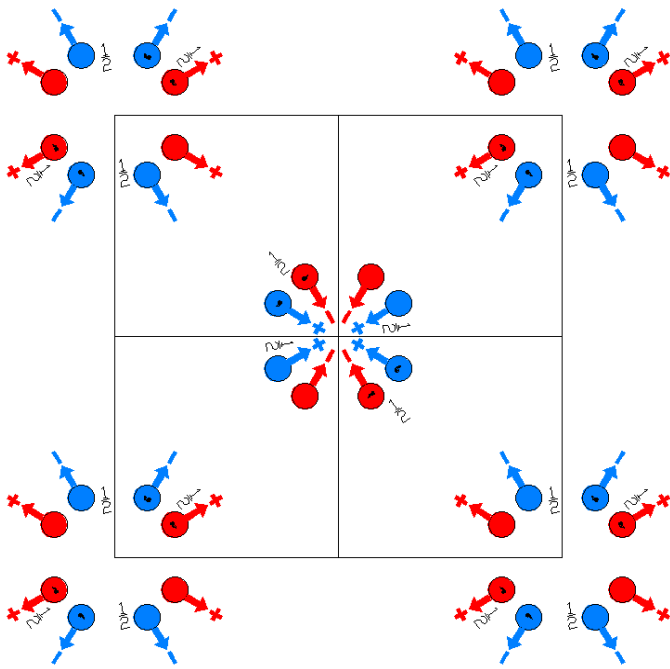
Along [1,1,0]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



P4'/nc'c  
130.4.1091

4'/mm'm  
P4'/n2<sub>1</sub>'/c'2/c

Tetragonal



Origin at  $\bar{4}'/nc'n$ , at  $-1/4, 1/4, 0$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                       | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0)'             | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)'        |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                            | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)        |
| (9) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)           | (10) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)      | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'              | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                       |
| (13) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)'        | (14) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)'        | (15) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (16) n (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

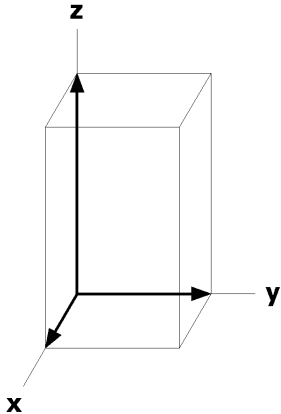
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z$ [ $\bar{v},u,\bar{w}$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(13) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	f	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/4$ [ $u,\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,1/4$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,\bar{x}+1/2,3/4$ [ $u,u,0$ ]	$x+1/2,x+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},3/4$ [ $u,\bar{u},0$ ]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]								
8	e	2..	0,0,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]								
8	d	$\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,0 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,0 [ $v,\bar{u},\bar{w}$ ]	3/4,1/4,0 [ $\bar{v},u,\bar{w}$ ]	1/4,3/4,1/2 [u, $\bar{v},w$ ]	3/4,1/4,1/2 [ $\bar{u},v,w$ ]	1/4,1/4,1/2 [ $v,u,\bar{w}$ ]	3/4,3/4,1/2 [ $\bar{v},\bar{u},\bar{w}$ ]								
4	c	4'..	0,1/2,z [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	0,1/2,z+1/2 [0,0,0]												
4	b	$\bar{4}'..$	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	0,0,1/2 [0,0,0]												
4	a	2.22	0,0,1/4 [0,0,0]	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]	0,0,3/4 [0,0,0]												

**Symmetry of Special Projections**

Along [0,0,1]  $p_p, 4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p 2'm'g$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,0

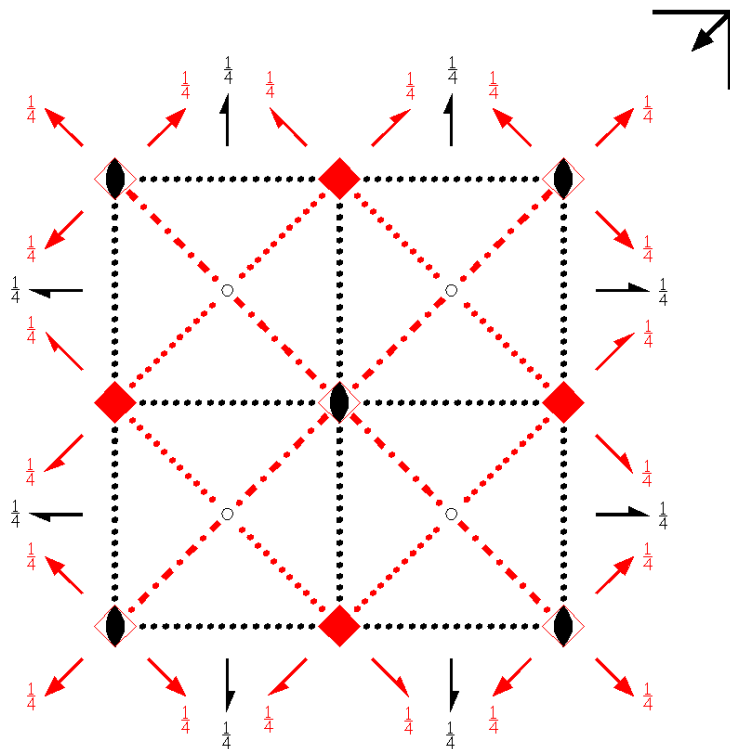
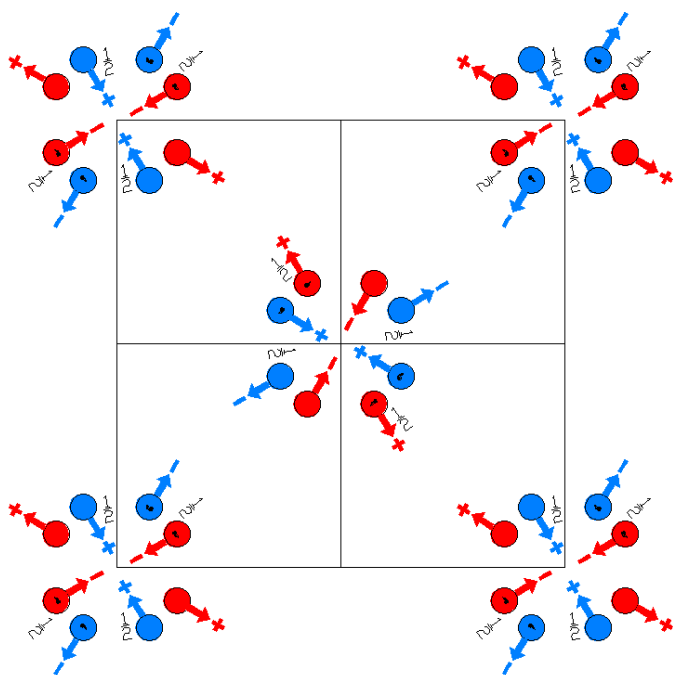
Along [1,1,0]  $p_{2a}, 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



P4'/ncc'  
130.5.1092

4'/mmm'  
P4'/n2<sub>1</sub>/c2'/c'

Tetragonal



Origin at  $\bar{4}'/ncn'$ , at  $-1/4, 1/4, 0$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |  |   |
|--|--|--|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                     | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0)'               | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)'          |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2) | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                            | (8) 2' x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)'        |
| (9) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)         | (10) n (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)    | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'                | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                         |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)        | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)        | (15) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)' | (16) n' (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	g	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z$ [ $\bar{v},u,\bar{w}$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $v,u,w$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(13) $x,\bar{y},z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $v,u,w$ ]
8	f	..2'	$x,x,1/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,1/4$ [ $u,u,\bar{w}$ ]	$x+1/2,\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	$\bar{x}+1/2,\bar{x}+1/2,3/4$ [ $\bar{u},u,w$ ]	$x+1/2,x+1/2,3/4$ [ $u,\bar{u},w$ ]	$x,\bar{x},3/4$ [ $u,u,\bar{w}$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]								
8	e	2..	$0,0,z$ [ $0,0,w$ ]	$1/2,1/2,z$ [ $0,0,\bar{w}$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,0,\bar{z}+1/2$ [ $0,0,w$ ]	$1/2,1/2,\bar{z}$ [ $0,0,w$ ]	$0,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$0,0,z+1/2$ [ $0,0,\bar{w}$ ]	$1/2,1/2,z+1/2$ [ $0,0,w$ ]								
8	d	$\bar{1}$	$1/4,1/4,0$ [ $u,v,w$ ]	$3/4,3/4,0$ [ $\bar{u},\bar{v},w$ ]	$1/4,3/4,0$ [ $v,\bar{u},\bar{w}$ ]	$3/4,1/4,0$ [ $\bar{v},u,\bar{w}$ ]	$1/4,3/4,1/2$ [ $\bar{u},v,\bar{w}$ ]	$3/4,1/4,1/2$ [ $u,\bar{v},\bar{w}$ ]	$1/4,1/4,1/2$ [ $\bar{v},\bar{u},w$ ]	$3/4,3/4,1/2$ [ $v,u,w$ ]								
4	c	4'..	$0,1/2,z$ [ $0,0,0$ ]	$1/2,0,\bar{z}+1/2$ [ $0,0,0$ ]	$1/2,0,\bar{z}$ [ $0,0,0$ ]	$0,1/2,z+1/2$ [ $0,0,0$ ]												
4	b	$\bar{4}'..$	$0,0,0$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]	$0,0,1/2$ [ $0,0,0$ ]												
4	a	2.2'2'	$0,0,1/4$ [ $0,0,w$ ]	$1/2,1/2,1/4$ [ $0,0,\bar{w}$ ]	$1/2,1/2,3/4$ [ $0,0,w$ ]	$0,0,3/4$ [ $0,0,\bar{w}$ ]												

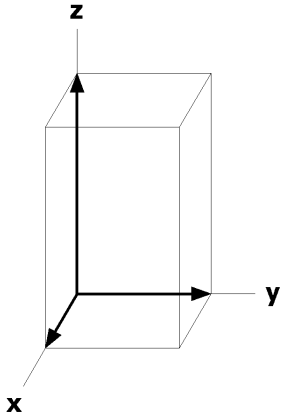
**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_p$ , 4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2b}$ , 2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,1/4,0$

Along  $[1,1,0]$   $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,0$

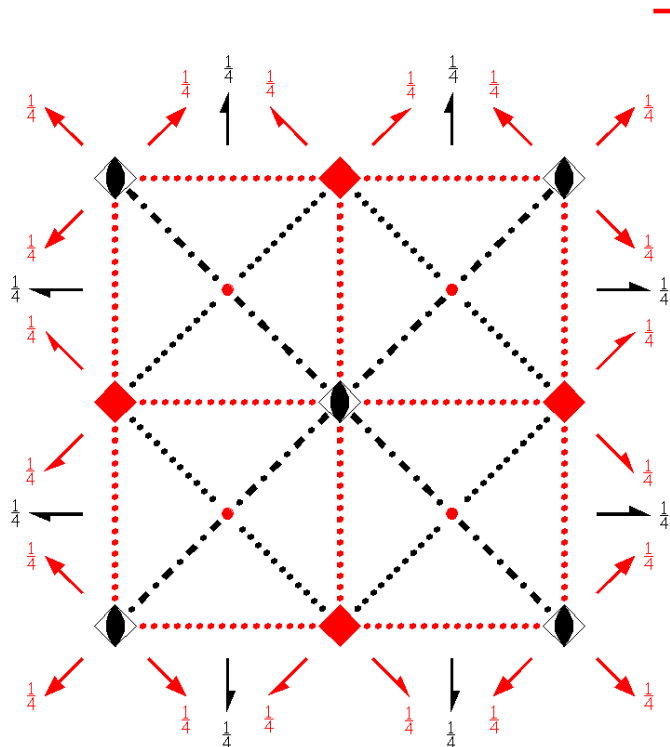
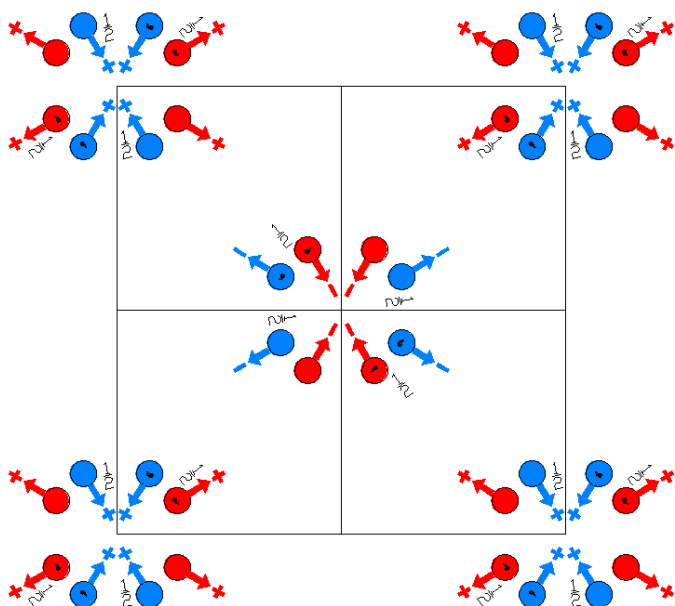




P4'/n'c'c  
130.6.1093

4'/m'm'm  
P4'/n'2<sub>1</sub>/c'2'/c

Tetragonal



Origin at  $\bar{4}/n'c'n'$ , at  $-1/4, 1/4, 0$  from  $\bar{1}$ '

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) $1$<br>( $1 0,0,0$ )                                 | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                       | (3) $4^+$ $0,1/2,z$<br>( $4_z 1/2,1/2,0$ )'                        | (4) $4^-$ $1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,0$ )'                   |
| (5) $2$ $(0,1/2,0)$ $1/4,y,1/4$<br>( $2_y 1/2,1/2,1/2$ ) | (6) $2$ $(1/2,0,0)$ $x,1/4,1/4$<br>( $2_x 1/2,1/2,1/2$ ) | (7) $2'$ $x,x,1/4$<br>( $2_{xy} 0,0,1/2$ )'                        | (8) $2'$ $x,\bar{x},1/4$<br>( $2_{\bar{xy}} 0,0,1/2$ )'            |
| (9) $\bar{1}$ ' $1/4,1/4,0$<br>( $\bar{1} 1/2,1/2,0$ )'  | (10) $n'$ $(1/2,1/2,0)$ $x,y,0$<br>( $m_z 1/2,1/2,0$ )'  | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )           | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ )      |
| (13) $c'$ $(0,0,1/2)$ $x,0,z$<br>( $m_y 0,0,1/2$ )'      | (14) $c'$ $(0,0,1/2)$ $0,y,z$<br>( $m_x 0,0,1/2$ )'      | (15) $c$ $(0,0,1/2)$ $x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,1/2$ ) | (16) $n$ $(1/2,1/2,1/2)$ $x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,1/2$ ) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

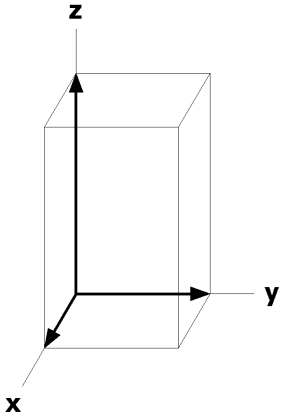
16	g	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $v,u,w$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}$ [ $u,v,\bar{w}$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]		
			(13) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	f	..2'	$x,x,1/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,1/4$ [ $u,u,\bar{w}$ ]	$x+1/2,\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x}+1/2,\bar{x}+1/2,3/4$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x+1/2,3/4$ [ $\bar{u},u,\bar{w}$ ]	$x,\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,3/4$ [ $u,u,w$ ]
8	e	2..	$0,0,z$ [ $0,0,w$ ]	$1/2,1/2,z$ [ $0,0,\bar{w}$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,0,\bar{z}+1/2$ [ $0,0,w$ ]
			$1/2,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]	$0,0,\bar{z}$ [ $0,0,w$ ]	$0,0,z+1/2$ [ $0,0,w$ ]	$1/2,1/2,z+1/2$ [ $0,0,\bar{w}$ ]
8	d	$\bar{1}'$	$1/4,1/4,0$ [ $0,0,0$ ]	$3/4,3/4,0$ [ $0,0,0$ ]	$1/4,3/4,0$ [ $0,0,0$ ]	$3/4,1/4,0$ [ $0,0,0$ ]
			$1/4,3/4,1/2$ [ $0,0,0$ ]	$3/4,1/4,1/2$ [ $0,0,0$ ]	$1/4,1/4,1/2$ [ $0,0,0$ ]	$3/4,3/4,1/2$ [ $0,0,0$ ]
4	c	4'..	$0,1/2,z$ [ $0,0,0$ ]	$1/2,0,\bar{z}+1/2$ [ $0,0,0$ ]	$1/2,0,\bar{z}$ [ $0,0,0$ ]	$0,1/2,z+1/2$ [ $0,0,0$ ]
4	b	$\bar{4}$ ..	$0,0,0$ [ $0,0,w$ ]	$1/2,1/2,0$ [ $0,0,\bar{w}$ ]	$1/2,1/2,1/2$ [ $0,0,\bar{w}$ ]	$0,0,1/2$ [ $0,0,w$ ]
4	a	2.2'2'	$0,0,1/4$ [ $0,0,w$ ]	$1/2,1/2,1/4$ [ $0,0,\bar{w}$ ]	$1/2,1/2,3/4$ [ $0,0,\bar{w}$ ]	$0,0,3/4$ [ $0,0,w$ ]

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4'mm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,1/4,0$

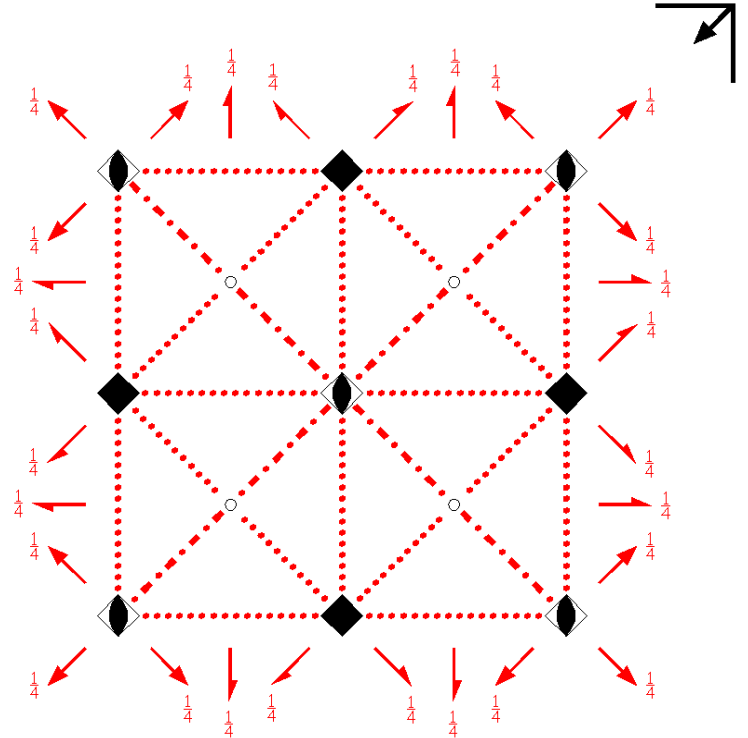
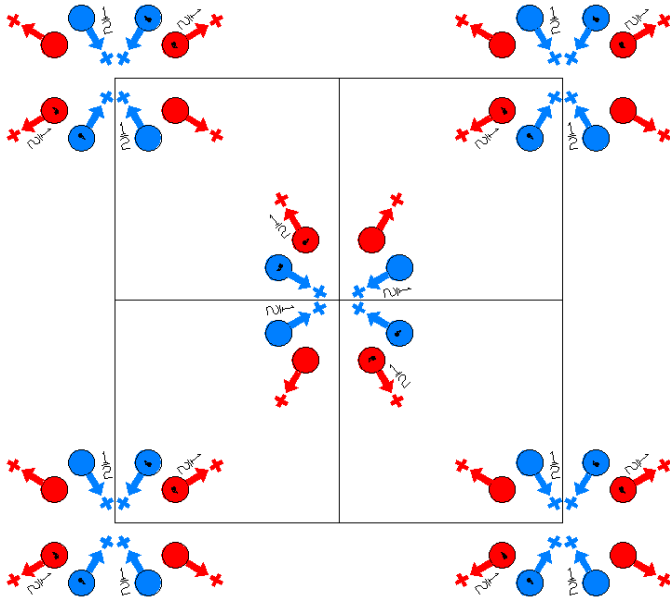
Along  $[1,1,0]$   $p_{2a'}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,0$



P4/nc'c'  
130.7.1094

4/mm'm'  
P4/n2<sub>1</sub>'/c<sub>2</sub>'/c'

Tetragonal



Origin at  $\bar{4}/nc'n'$ , at  $-1/4, 1/4, 0$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) $1$<br>( $1 0,0,0$ )                                   | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                         | (3) $4^+$ $0,1/2,z$<br>( $4_z 1/2,1/2,0$ )                           | (4) $4^-$ $1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,0$ )                      |
| (5) $2'$ $(0,1/2,0)$ $1/4,y,1/4$<br>( $2_y 1/2,1/2,1/2$ )' | (6) $2'$ $(1/2,0,0)$ $x,1/4,1/4$<br>( $2_x 1/2,1/2,1/2$ )' | (7) $2'$ $x,x,1/4$<br>( $2_{xy} 0,0,1/2$ )'                          | (8) $2'$ $x,\bar{x},1/4$<br>( $2_{\bar{xy}} 0,0,1/2$ )'              |
| (9) $\bar{1}$ $1/4,1/4,0$<br>( $\bar{1} 1/2,1/2,0$ )       | (10) $n$ $(1/2,1/2,0)$ $x,y,0$<br>( $m_z 1/2,1/2,0$ )      | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )             | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ )        |
| (13) $c'$ $(0,0,1/2)$ $x,0,z$<br>( $m_y 0,0,1/2$ )'        | (14) $c'$ $(0,0,1/2)$ $0,y,z$<br>( $m_x 0,0,1/2$ )'        | (15) $c'$ $(0,0,1/2)$ $x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,1/2$ )' | (16) $n'$ $(1/2,1/2,1/2)$ $x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,1/2$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

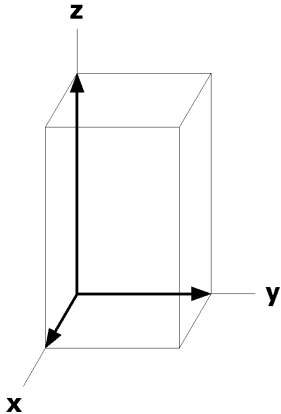
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	g	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z$ [v, $\bar{u},w$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [u, $\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [v,u,w]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [u,v,w]	(10) $x+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [v, $\bar{u},w$ ]	(13) $x,\bar{y},z+1/2$ [u, $\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z+1/2$ [v,u,w]
8	f	..2'	$x,x,1/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [u, $\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,1/4$ [ $\bar{u},\bar{u},w$ ]	$x+1/2,\bar{x}+1/2,1/4$ [u,u,w]	$\bar{x}+1/2,\bar{x}+1/2,3/4$ [ $\bar{u},u,w$ ]	$x+1/2,x+1/2,3/4$ [u, $\bar{u},w$ ]	$x,\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,3/4$ [u,u,w]								
8	e	2..	0,0,z [0,0,w]	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0,w]	1/2,1/2,z+1/2 [0,0,w]								
8	d	$\bar{1}$	1/4,1/4,0 [u,v,w]	3/4,3/4,0 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,0 [ $\bar{v},u,w$ ]	3/4,1/4,0 [v, $\bar{u},w$ ]	1/4,3/4,1/2 [u, $\bar{v},w$ ]	3/4,1/4,1/2 [ $\bar{u},v,w$ ]	1/4,1/4,1/2 [ $\bar{v},\bar{u},w$ ]	3/4,3/4,1/2 [v,u,w]								
4	c	4..	0,1/2,z [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	0,1/2,z+1/2 [0,0,0]												
4	b	$\bar{4}$ ..	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	0,0,1/2 [0,0,0]												
4	a	2.2'2'	0,0,1/4 [0,0,0]	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]	0,0,3/4 [0,0,0]												

**Symmetry of Special Projections**

Along [0,0,1]  $p_2$ , 4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/2,0,z

Along [1,0,0]  $p$  2'm'g  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,0

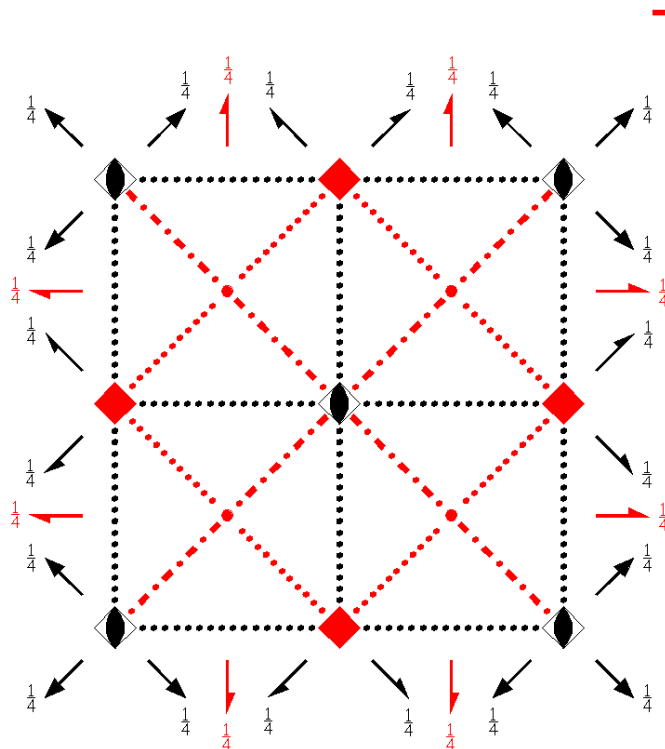
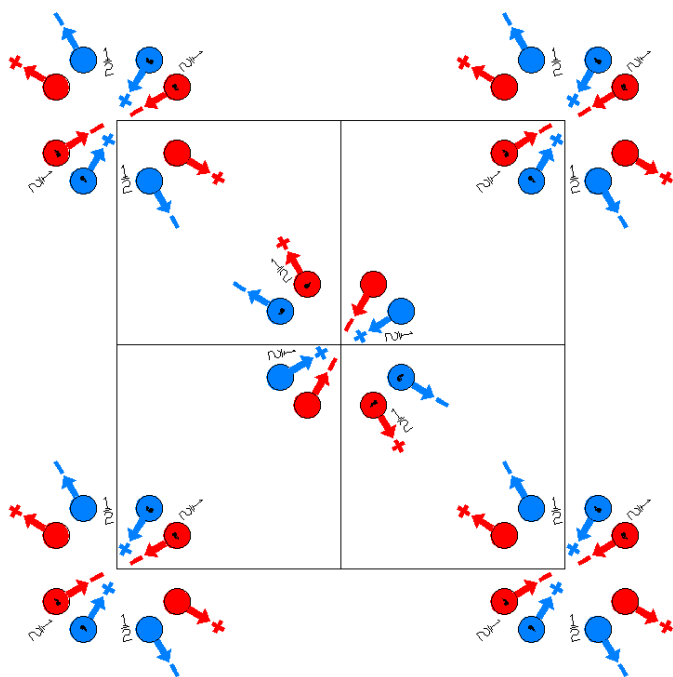
Along [1,1,0]  $p2$ 'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



P4'/n'cc'  
130.8.1095

4'/m'mm'  
P4'/n'2<sub>1</sub>'/c2/c'

Tetragonal



Origin at  $\bar{4}/n'cn'$ , at  $-1/4, 1/4, 0$  from  $\bar{1}$ '

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                       | (3) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,0)'                   | (4) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)'                   |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)' | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)' | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                                  | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)                   |
| (9) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)'        | (10) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>  1/2,1/2,0)'    | (11) $\bar{4}$ <sup>+</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub>  0,0,0) | (12) $\bar{4}$ <sup>-</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)          | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)          | (15) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)'     | (16) n' (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)'          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

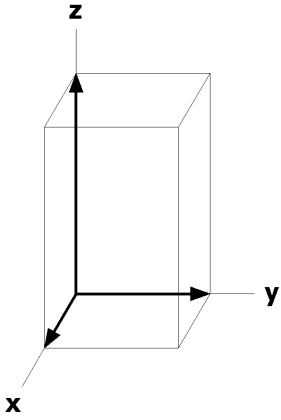
16	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]		
			(7) $y,x,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}$ [ $u,v,\bar{w}$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]		
			(13) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $v,u,w$ ]		
8	f	..2	$x,x,1/4$ [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/4$ [ $u,\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,1/4$ [ $\bar{u},u,0$ ]
			$\bar{x}+1/2,\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x+1/2,3/4$ [u,u,0]	$x,\bar{x},3/4$ [ $\bar{u},u,0$ ]	$\bar{x},x,3/4$ [ $u,\bar{u},0$ ]
8	e	2..	0,0,z [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
			1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0,w]
8	d	$\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,0 [0,0,0]	1/4,3/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]
			1/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]
4	c	4'..	0,1/2,z [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	0,1/2,z+1/2 [0,0,0]
4	b	$\bar{4}'$ ..	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	0,0,1/2 [0,0,0]
4	a	2.22	0,0,1/4 [0,0,0]	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]	0,0,3/4 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $p4'm'm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b'}2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,1/2

Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



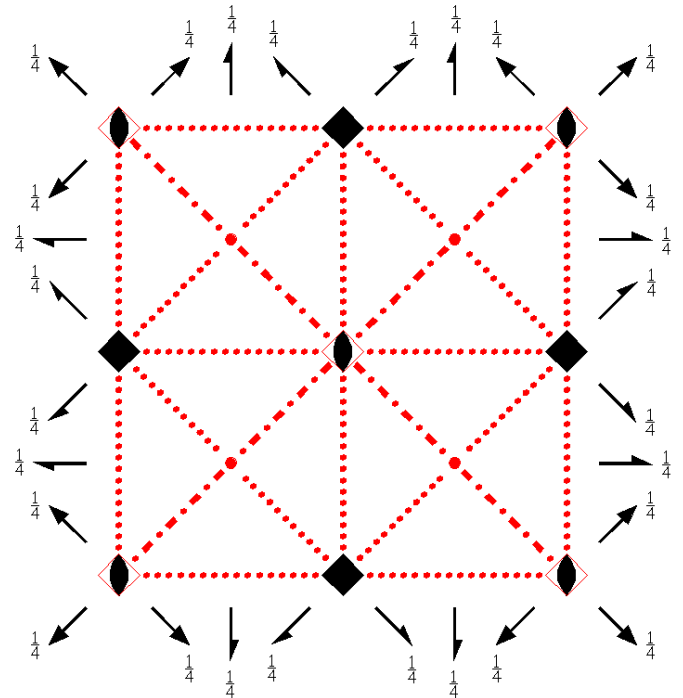
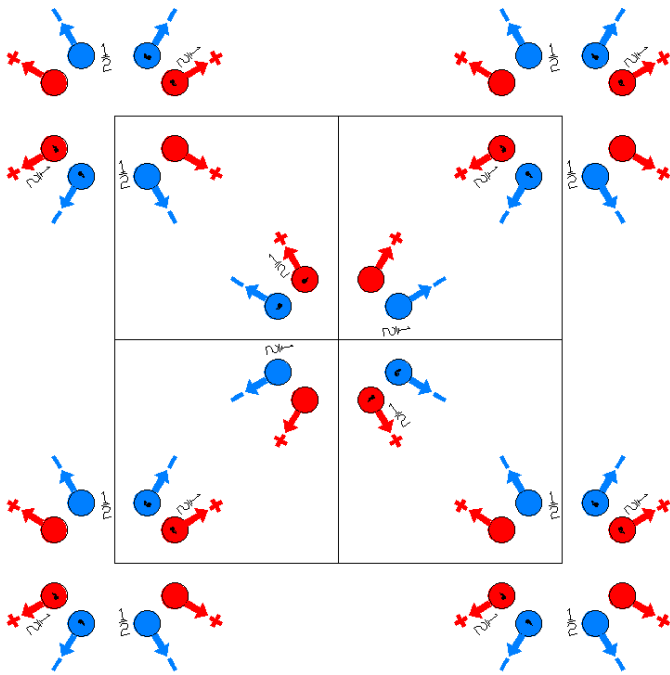
P4/n'c'c'

130.9.1096

4/m'm'm'

P4/n'2<sub>1</sub>/c'2/c'

Tetragonal



Origin at  $\bar{4}'n'c'n'$ , at  $-1/4, 1/4, 0$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) $1$<br>( $1 0,0,0$ )                                 | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                       | (3) $4^+$ $0,1/2,z$<br>( $4_z 1/2,1/2,0$ )                          | (4) $4^-$ $1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,0$ )                     |
| (5) $2$ $(0,1/2,0)$ $1/4,y,1/4$<br>( $2_y 1/2,1/2,1/2$ ) | (6) $2$ $(1/2,0,0)$ $x,1/4,1/4$<br>( $2_x 1/2,1/2,1/2$ ) | (7) $2$ $x,x,1/4$<br>( $2_{xy} 0,0,1/2$ )                           | (8) $2$ $x,\bar{x},1/4$<br>( $2_{\bar{xy}} 0,0,1/2$ )               |
| (9) $\bar{1}'$ $1/4,1/4,0$<br>( $\bar{1}' 1/2,1/2,0$ )   | (10) $n'$ $(1/2,1/2,0)$ $x,y,0$<br>( $m_z 1/2,1/2,0$ )   | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )            | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ )       |
| (13) $c'$ $(0,0,1/2)$ $x,0,z$<br>( $m_y 0,0,1/2$ )       | (14) $c'$ $(0,0,1/2)$ $0,y,z$<br>( $m_x 0,0,1/2$ )       | (15) $c'$ $(0,0,1/2)$ $x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,1/2$ ) | (16) $n'$ $(1/2,1/2,1/2)$ $x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,1/2$ ) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z$ [ $v,\bar{u},w$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(13) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $v,u,w$ ]
8	f	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/4$ [ $\bar{u},u,0$ ]	$x+1/2,\bar{x}+1/2,1/4$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x+1/2,3/4$ [ $u,u,0$ ]	$x,\bar{x},3/4$ [ $u,\bar{u},0$ ]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]								
8	e	2..	0,0,z [0,0,w]	1/2,1/2,z [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]	1/2,1/2,z+1/2 [0,0,w]								
8	d	$\bar{1}'$	1/4,1/4,0 [0,0,0]	3/4,3/4,0 [0,0,0]	1/4,3/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]	1/4,3/4,1/2 [0,0,0]	3/4,1/4,1/2 [0,0,0]	1/4,1/4,1/2 [0,0,0]	3/4,3/4,1/2 [0,0,0]								
4	c	4..	0,1/2,z [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0,w]												
4	b	$\bar{4}'..$	0,0,0 [0,0,0]	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	0,0,1/2 [0,0,0]												
4	a	2.22	0,0,1/4 [0,0,0]	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]	0,0,3/4 [0,0,0]												

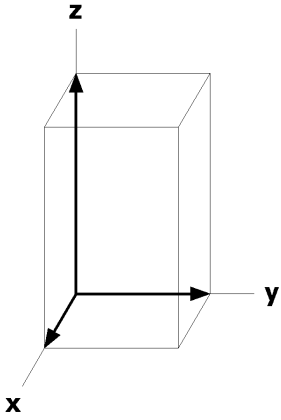
**Symmetry of Special Projections**

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p 2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0





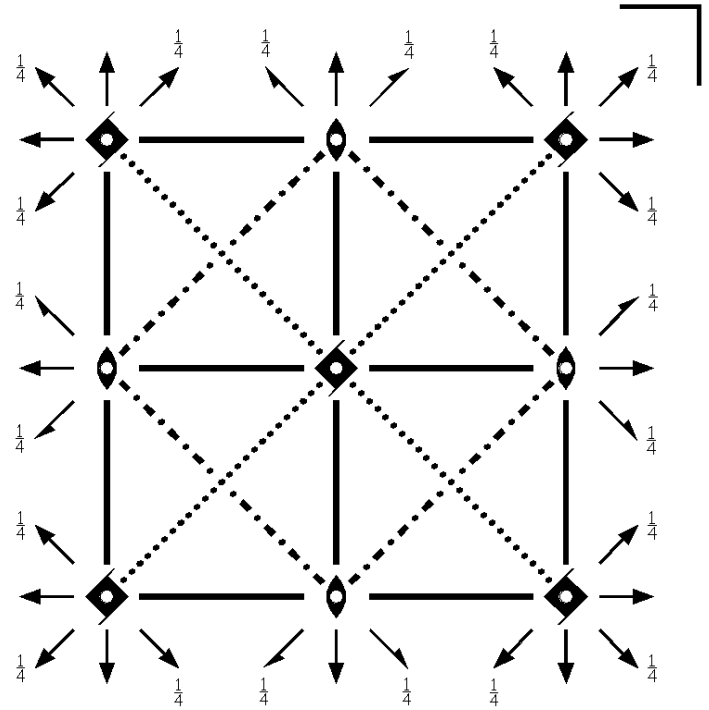
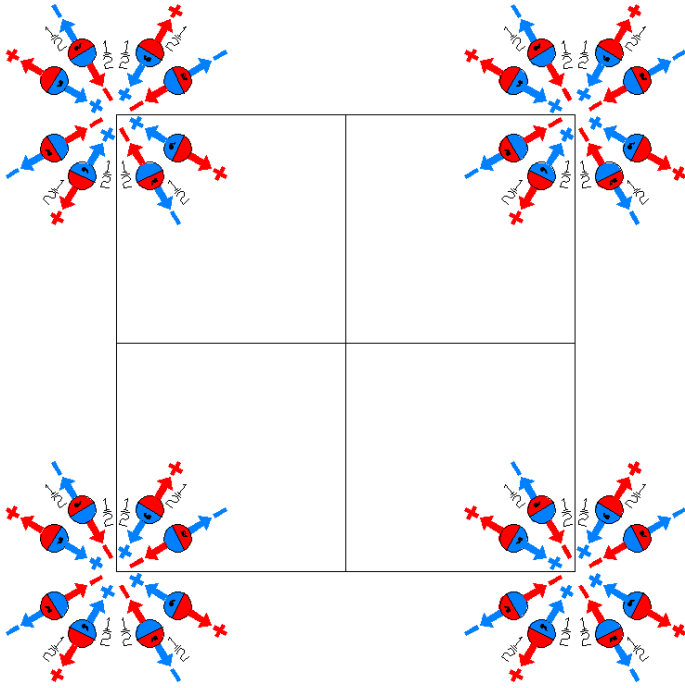
$P4_2/mmc$

131.1.1097

4/mmm

$P4_2/m2/m2/c$

Tetragonal



Origin at center ( mmm ) at  $4_2/m2/mc$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)     | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                     | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)      |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (11) $\bar{4}^+$ 0,0,z; 0,0,1/4<br>( $\bar{4}_z^+$  0,0,1/2)    | (12) $\bar{4}^-$ 0,0,z; 0,0,1/4<br>( $\bar{4}_z^-$  0,0,1/2)                  |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)    | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (15) c (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2)  | (16) c (0,0,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,1/2)       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	r	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(10) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $v,\bar{u},w$ ]
			(13) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y,x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	q	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,1/2$ [0,0,w]	$y,\bar{x},1/2$ [0,0,w]
			$\bar{x},y,0$ [0,0, $\bar{w}$ ]	$x,\bar{y},0$ [0,0, $\bar{w}$ ]	$y,x,1/2$ [0,0, $\bar{w}$ ]	$\bar{y},\bar{x},1/2$ [0,0, $\bar{w}$ ]
8	p	.m.	1/2,y,z [u,0,0]	1/2, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},1/2,z+1/2$ [0,u,0]	$y,1/2,z+1/2$ [0, $\bar{u},0$ ]
			1/2, $y,\bar{z}$ [ $\bar{u},0,0$ ]	1/2, $\bar{y},\bar{z}$ [u,0,0]	$y,1/2,\bar{z}+1/2$ [0,u,0]	$\bar{y},1/2,\bar{z}+1/2$ [0, $\bar{u},0$ ]
8	o	.m.	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},0,z+1/2$ [0,u,0]	$y,0,z+1/2$ [0, $\bar{u},0$ ]
			0, $y,\bar{z}$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]	$y,0,\bar{z}+1/2$ [0,u,0]	$\bar{y},0,\bar{z}+1/2$ [0, $\bar{u},0$ ]
8	n	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]	$x,\bar{x},3/4$ [ $u,\bar{u},0$ ]
			$\bar{x},\bar{x},3/4$ [u,u,0]	$x,x,3/4$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},1/4$ [ $\bar{u},u,0$ ]	$\bar{x},x,1/4$ [ $u,\bar{u},0$ ]
4	m	m2m.	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]	1/2,x,1/2 [0,0,0]	1/2, $\bar{x},1/2$ [0,0,0]
4	l	m2m.	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x},0$ [0,0,0]
4	k	m2m.	x,1/2,1/2 [0,0,0]	$\bar{x},1/2,1/2$ [0,0,0]	1/2,x,0 [0,0,0]	1/2, $\bar{x},0$ [0,0,0]
4	j	m2m.	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,1/2 [0,0,0]	0, $\bar{x},1/2$ [0,0,0]
4	i	2mm.	0,1/2,z [0,0,0]	1/2,0,z+1/2 [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]
4	h	2mm.	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]
4	g	2mm.	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]
2	f	$\bar{4}m2$	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	e	$\bar{4}m2$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	d	mmm.	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]		
2	c	mmm.	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	b	mmm.	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

2 a mmm. 0,0,0 [0,0,0]

0,0,1/2 [0,0,0]

**Symmetry of Special Projections**Along [0,0,1]  $p4mm1'$  $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$ 

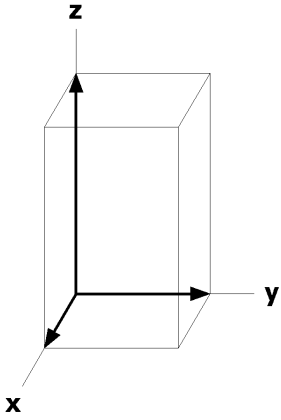
Origin at 0,0,z

Along [1,0,0]  $p2mm1'$  $\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}$ 

Origin at x,0,0

Along [1,1,0]  $p_{2a^*} 2m'm'$  $\mathbf{a}^* = -\mathbf{c}/2 \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$ 

Origin at x,x,0



$P4_2/mmc1'$

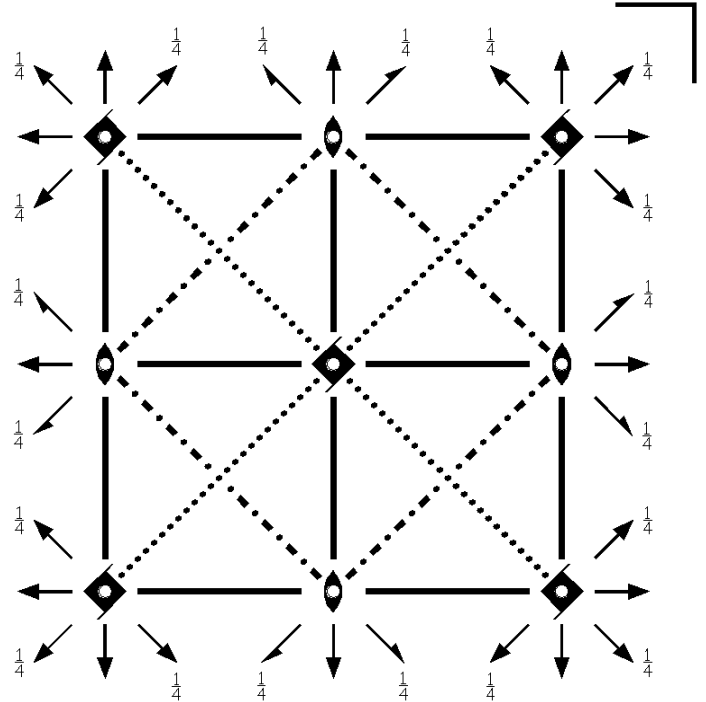
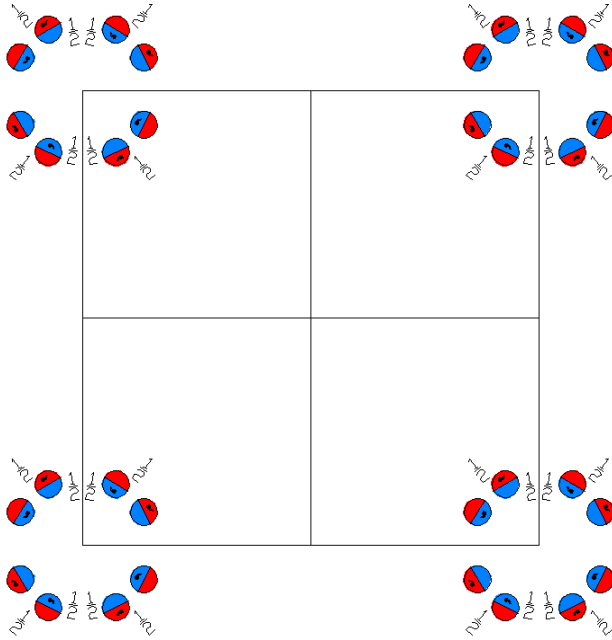
131.2.1098

$4/mmm1'$

$P4_2/m2/m2/c1'$

Tetragonal

1'



Origin at center ( $mmm1'$ ) at  $4_2/m2/mc1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For 1 + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)              | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                                  | (8) 2 x,x̄,1/4<br>(2 <sub>xȳ</sub>  0,0,1/2)                                 |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)              | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (11) 4 <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>+</sup>  0,0,1/2) | (12) 4 <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (15) c (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)                        | (16) c (0,0,1/2) x,x,z<br>(m <sub>xȳ</sub>  0,0,1/2)                         |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> ' (0,0,1/2) 0,0,z (4 <sub>z</sub>  0,0,1/2)'	(4) 4 <sup>-</sup> ' (0,0,1/2) 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)'
(5) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(6) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'	(7) 2' x,x,1/4 (2 <sub>xy</sub>  0,0,1/2)'	(8) 2' x, $\bar{x}$ ,1/4 (2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)'
(9) $\bar{1}$ ' 0,0,0 ( $\bar{1}$  0,0,0)'	(10) m' x,y,0 (m <sub>z</sub>  0,0,0)'	(11) $\bar{4}^+$ ' 0,0,z; 0,0,1/4 ( $\bar{4}_z^+$  0,0,1/2)'	(12) $\bar{4}^-$ ' 0,0,z; 0,0,1/4 ( $\bar{4}_z^-$  0,0,1/2)'
(13) m' x,0,z (m <sub>y</sub>  0,0,0)'	(14) m' 0,y,z (m <sub>x</sub>  0,0,0)'	(15) c' (0,0,1/2) x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,1/2)'	(16) c' (0,0,1/2) x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			1+	1+	1+	1+
16	r	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z+1/2$ [0,0,0]	(4) y, $\bar{x},z+1/2$ [0,0,0]
			(5) $\bar{x},y,\bar{z}$ [0,0,0]	(6) x, $\bar{y},\bar{z}$ [0,0,0]	(7) y,x, $\bar{z}+1/2$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [0,0,0]
			(9) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(10) x,y, $\bar{z}$ [0,0,0]	(11) y, $\bar{x},\bar{z}+1/2$ [0,0,0]	(12) $\bar{y},x,\bar{z}+1/2$ [0,0,0]
			(13) x, $\bar{y},z$ [0,0,0]	(14) $\bar{x},y,z$ [0,0,0]	(15) $\bar{y},\bar{x},z+1/2$ [0,0,0]	(16) y,x,z+1/2 [0,0,0]
8	q	m..1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{y},x,1/2$ [0,0,0]	y, $\bar{x},1/2$ [0,0,0]
			$\bar{x},y,0$ [0,0,0]	x, $\bar{y},0$ [0,0,0]	y,x,1/2 [0,0,0]	$\bar{y},\bar{x},1/2$ [0,0,0]
8	p	.m.1'	1/2,y,z [0,0,0]	1/2, $\bar{y},z$ [0,0,0]	$\bar{y},1/2,z+1/2$ [0,0,0]	y,1/2,z+1/2 [0,0,0]
			1/2,y, $\bar{z}$ [0,0,0]	1/2, $\bar{y},\bar{z}$ [0,0,0]	y,1/2, $\bar{z}+1/2$ [0,0,0]	$\bar{y},1/2,\bar{z}+1/2$ [0,0,0]
8	o	.m.1'	0,y,z [0,0,0]	0, $\bar{y},z$ [0,0,0]	$\bar{y},0,z+1/2$ [0,0,0]	y,0,z+1/2 [0,0,0]
			0,y, $\bar{z}$ [0,0,0]	0, $\bar{y},\bar{z}$ [0,0,0]	y,0, $\bar{z}+1/2$ [0,0,0]	$\bar{y},0,\bar{z}+1/2$ [0,0,0]
8	n	..21'	x,x,1/4 [0,0,0]	$\bar{x},\bar{x},1/4$ [0,0,0]	$\bar{x},x,3/4$ [0,0,0]	x, $\bar{x},3/4$ [0,0,0]
			$\bar{x},\bar{x},3/4$ [0,0,0]	x,x,3/4 [0,0,0]	x, $\bar{x},1/4$ [0,0,0]	$\bar{x},x,1/4$ [0,0,0]
4	m	m2m.1'	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]	1/2,x,1/2 [0,0,0]	1/2, $\bar{x},1/2$ [0,0,0]
4	l	m2m.1'	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x},0$ [0,0,0]
4	k	m2m.1'	x,1/2,1/2 [0,0,0]	$\bar{x},1/2,1/2$ [0,0,0]	1/2,x,0 [0,0,0]	1/2, $\bar{x},0$ [0,0,0]
4	j	m2m.1'	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,1/2 [0,0,0]	0, $\bar{x},1/2$ [0,0,0]

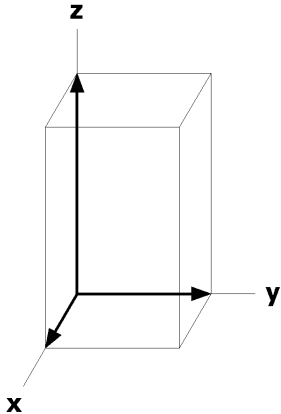
4	i	$2mm.1'$	$0,1/2,z [0,0,0]$	$1/2,0,z+1/2 [0,0,0]$	$0,1/2,\bar{z} [0,0,0]$	$1/2,0,\bar{z}+1/2 [0,0,0]$
4	h	$2mm.1'$	$1/2,1/2,z [0,0,0]$	$1/2,1/2,z+1/2 [0,0,0]$	$1/2,1/2,\bar{z} [0,0,0]$	$1/2,1/2,\bar{z}+1/2 [0,0,0]$
4	g	$2mm.1'$	$0,0,z [0,0,0]$	$0,0,z+1/2 [0,0,0]$	$0,0,\bar{z} [0,0,0]$	$0,0,\bar{z}+1/2 [0,0,0]$
2	f	$\bar{4}m21'$	$1/2,1/2,1/4 [0,0,0]$	$1/2,1/2,3/4 [0,0,0]$		
2	e	$\bar{4}m21'$	$0,0,1/4 [0,0,0]$	$0,0,3/4 [0,0,0]$		
2	d	$mmm.1'$	$0,1/2,1/2 [0,0,0]$	$1/2,0,0 [0,0,0]$		
2	c	$mmm.1'$	$0,1/2,0 [0,0,0]$	$1/2,0,1/2 [0,0,0]$		
2	b	$mmm.1'$	$1/2,1/2,0 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$		
2	a	$mmm.1'$	$0,0,0 [0,0,0]$	$0,0,1/2 [0,0,0]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



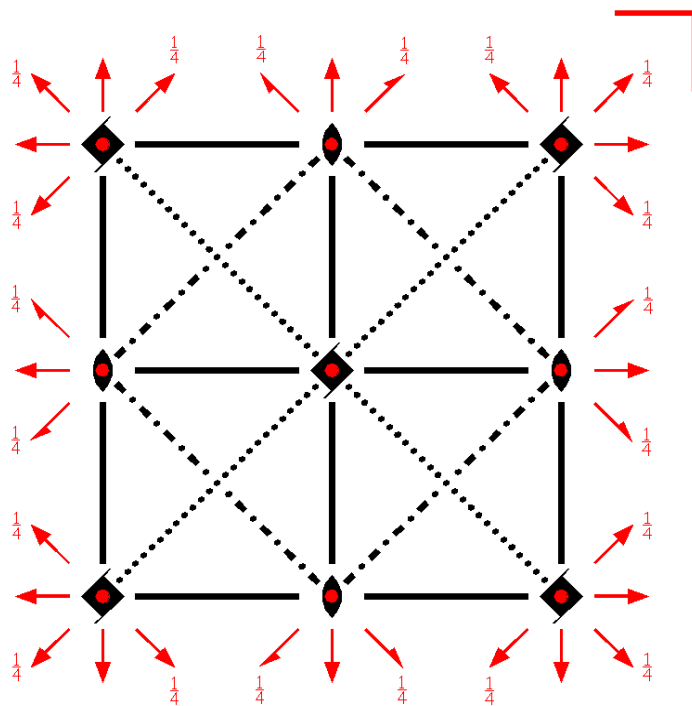
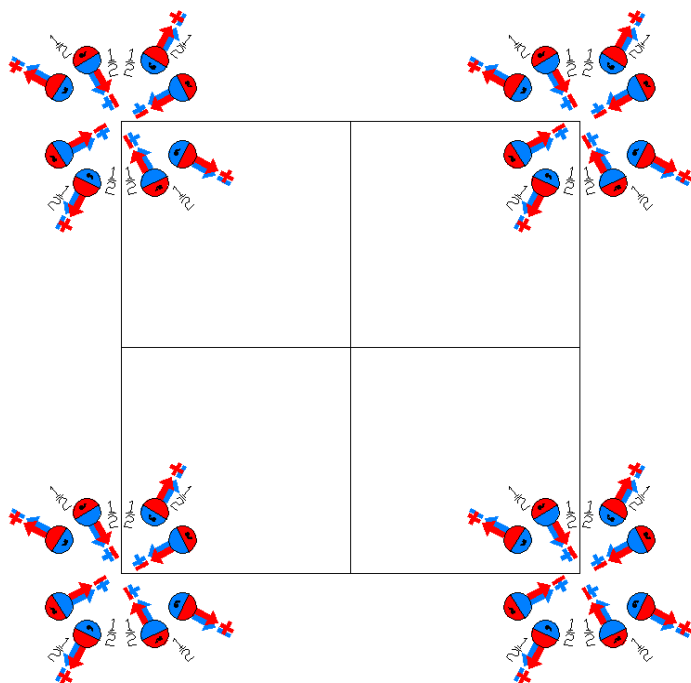
$P4_2/m'mc$

131.3.1099

$4/m'mm$

$P4_2/m'2'/m2'/c$

Tetragonal



Origin at center ( $mmm'$ ) at  $4_2/m'2'/mc$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)                 | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)   |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'  | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                                   | (8) 2' x,x̄,1/4<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,1/2)'                    |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'              | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) 4̄ <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' | (12) 4̄ <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)  | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   | (15) c (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)                           | (16) c (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)                            |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	r	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $v,u,w$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]
			(13) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y,x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	q	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},u,0$ ]	$y,\bar{x},1/2$ [ $v,\bar{u},0$ ]
			$\bar{x},y,0$ [ $u,\bar{v},0$ ]	$x,\bar{y},0$ [ $\bar{u},v,0$ ]	$y,x,1/2$ [ $\bar{v},\bar{u},0$ ]	$\bar{y},\bar{x},1/2$ [ $v,u,0$ ]
8	p	.m.	1/2,y,z [u,0,0]	1/2, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},1/2,z+1/2$ [0,u,0]	$y,1/2,z+1/2$ [0, $\bar{u},0$ ]
			1/2, $y,\bar{z}$ [u,0,0]	1/2, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]	$y,1/2,\bar{z}+1/2$ [0, $\bar{u},0$ ]	$\bar{y},1/2,\bar{z}+1/2$ [0,u,0]
8	o	.m.	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},0,z+1/2$ [0,u,0]	$y,0,z+1/2$ [0, $\bar{u},0$ ]
			0, $y,\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]	$y,0,\bar{z}+1/2$ [0, $\bar{u},0$ ]	$\bar{y},0,\bar{z}+1/2$ [0,u,0]
8	n	..2'	x,x,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [ $u,\bar{u},w$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x},3/4$ [ $u,u,w$ ]
			$\bar{x},\bar{x},3/4$ [ $u,\bar{u},\bar{w}$ ]	$x,x,3/4$ [ $\bar{u},u,\bar{w}$ ]	$x,\bar{x},1/4$ [ $u,u,\bar{w}$ ]	$\bar{x},x,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
4	m	m'2'm.	x,1/2,0 [0,v,0]	$\bar{x},1/2,0$ [0, $\bar{v},0$ ]	1/2,x,1/2 [ $\bar{v},0,0$ ]	1/2, $\bar{x},1/2$ [ $v,0,0$ ]
4	l	m'2'm.	x,0,1/2 [0,v,0]	$\bar{x},0,1/2$ [0, $\bar{v},0$ ]	0,x,0 [ $\bar{v},0,0$ ]	0, $\bar{x},0$ [ $v,0,0$ ]
4	k	m'2'm.	x,1/2,1/2 [0,v,0]	$\bar{x},1/2,1/2$ [0, $\bar{v},0$ ]	1/2,x,0 [ $\bar{v},0,0$ ]	1/2, $\bar{x},0$ [ $v,0,0$ ]
4	j	m'2'm.	x,0,0 [0,v,0]	$\bar{x},0,0$ [0, $\bar{v},0$ ]	0,x,1/2 [ $\bar{v},0,0$ ]	0, $\bar{x},1/2$ [ $v,0,0$ ]
4	i	2mm.	0,1/2,z [0,0,0]	1/2,0,z+1/2 [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]
4	h	2mm.	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]
4	g	2mm.	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]
2	f	$\bar{4}'m2'$	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	e	$\bar{4}'m2'$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	d	m'mm.	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]		
2	c	m'mm.	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	b	m'mm.	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		



2 a m'mm. 0,0,0 [0,0,0]

0,0,1/2 [0,0,0]

**Symmetry of Special Projections**Along [0,0,1]  $p4mm$  $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$ 

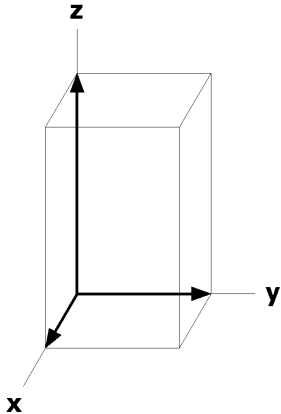
Origin at 0,0,z

Along [1,0,0]  $p2mm1'$  $\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}$ 

Origin at x,0,0

Along [1,1,0]  $p_{2a^*} 2m'm'$  $\mathbf{a}^* = -\mathbf{c}/2 \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$ 

Origin at x,x,0



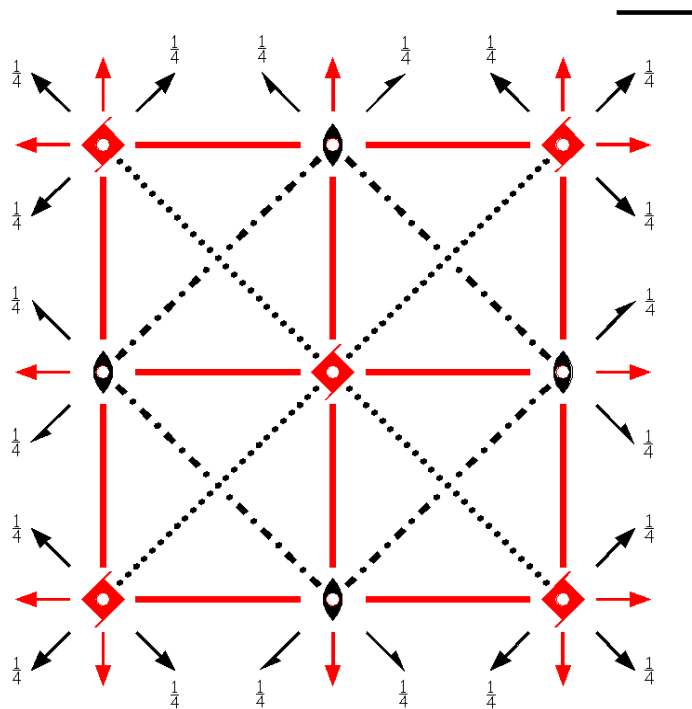
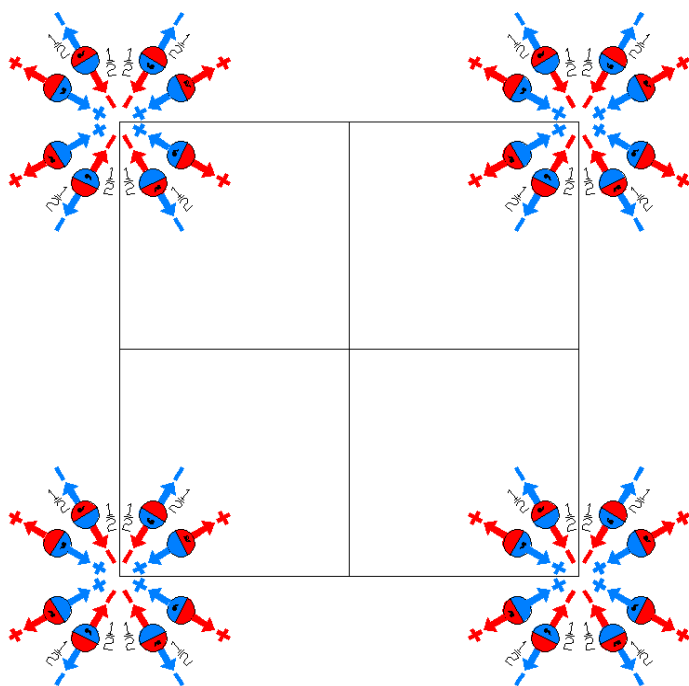
$P4_2'/mm'c$

131.4.1100

$4'/mm'm$

$P4_2'/m2'/m'2'/c$

Tetragonal



Origin at center ( $m'm'm$ ) at  $4_2'/m2'/m'c$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'  | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'  | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                      | (8) 2 x,x̄,1/4<br>(2 <sub>xȳ</sub>  0,0,1/2)                                  |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)                | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)   | (11) 4 <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub>  0,0,1/2)' | (12) 4 <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (15) c (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)            | (16) c (0,0,1/2) x,x,z<br>(m <sub>xȳ</sub>  0,0,1/2)                          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	r	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $v,\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ]
			(5) $\bar{x},\bar{y},\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(10) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]
			(13) $x,\bar{y},z$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y,x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	q	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,1/2$ [0,0, $\bar{w}$ ]	$y,\bar{x},1/2$ [0,0, $\bar{w}$ ]
			$\bar{x},y,0$ [0,0,w]	$x,\bar{y},0$ [0,0,w]	$y,x,1/2$ [0,0, $\bar{w}$ ]	$\bar{y},\bar{x},1/2$ [0,0, $\bar{w}$ ]
8	p	.m'.	1/2,y,z [0,v,w]	1/2, $\bar{y},z$ [0, $\bar{v},w$ ]	$\bar{y},1/2,z+1/2$ [ $v,0,\bar{w}$ ]	$y,1/2,z+1/2$ [ $\bar{v},0,\bar{w}$ ]
			1/2, $\bar{y},\bar{z}$ [0, $\bar{v},w$ ]	1/2, $\bar{y},z$ [0,v,w]	$y,1/2,\bar{z}+1/2$ [ $v,0,\bar{w}$ ]	$\bar{y},1/2,\bar{z}+1/2$ [ $\bar{v},0,\bar{w}$ ]
8	o	.m'.	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	$\bar{y},0,z+1/2$ [ $v,0,\bar{w}$ ]	$y,0,z+1/2$ [ $\bar{v},0,\bar{w}$ ]
			0, $\bar{y},\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},z$ [0,v,w]	$y,0,\bar{z}+1/2$ [ $v,0,\bar{w}$ ]	$\bar{y},0,\bar{z}+1/2$ [ $\bar{v},0,\bar{w}$ ]
8	n	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,3/4$ [ $u,\bar{u},0$ ]	$x,\bar{x},3/4$ [ $\bar{u},u,0$ ]
			$\bar{x},\bar{x},3/4$ [ $u,u,0$ ]	$x,x,3/4$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},1/4$ [ $u,\bar{u},0$ ]	$\bar{x},x,1/4$ [ $\bar{u},u,0$ ]
4	m	m2'm'.	x,1/2,0 [0,0,w]	$\bar{x},1/2,0$ [0,0,w]	1/2,x,1/2 [0,0, $\bar{w}$ ]	1/2, $\bar{x},1/2$ [0,0, $\bar{w}$ ]
4	l	m2'm'.	x,0,1/2 [0,0,w]	$\bar{x},0,1/2$ [0,0,w]	0,x,0 [0,0, $\bar{w}$ ]	0, $\bar{x},0$ [0,0, $\bar{w}$ ]
4	k	m2'm'.	x,1/2,1/2 [0,0,w]	$\bar{x},1/2,1/2$ [0,0,w]	1/2,x,0 [0,0, $\bar{w}$ ]	1/2, $\bar{x},0$ [0,0, $\bar{w}$ ]
4	j	m2'm'.	x,0,0 [0,0,w]	$\bar{x},0,0$ [0,0,w]	0,x,1/2 [0,0, $\bar{w}$ ]	0, $\bar{x},1/2$ [0,0, $\bar{w}$ ]
4	i	2m'm'.	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	h	2m'm'.	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	g	2m'm'.	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
2	f	$\bar{4}$ 'm'2	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	e	$\bar{4}$ 'm'2	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	d	mm'm'.	0,1/2,1/2 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]		
2	c	mm'm'.	0,1/2,0 [0,0,w]	1/2,0,1/2 [0,0, $\bar{w}$ ]		
2	b	mm'm'.	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		

2 a mm'm'. 0,0,0 [0,0,w]

0,0,1/2 [0,0, $\bar{w}$ ]

### Symmetry of Special Projections

Along [0,0,1]  $p4mm1'$

$\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$

Origin at 0,0,z

Along [1,0,0]  $p2'mm'$

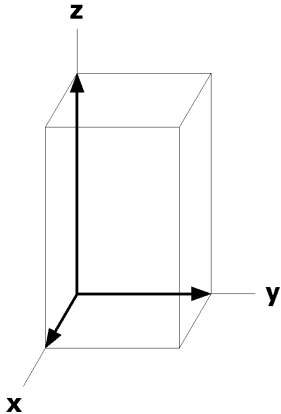
$\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$

Origin at x,0,0

Along [1,1,0]  $p_{2a'} 2m'm'$

$\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$

Origin at x,x,0



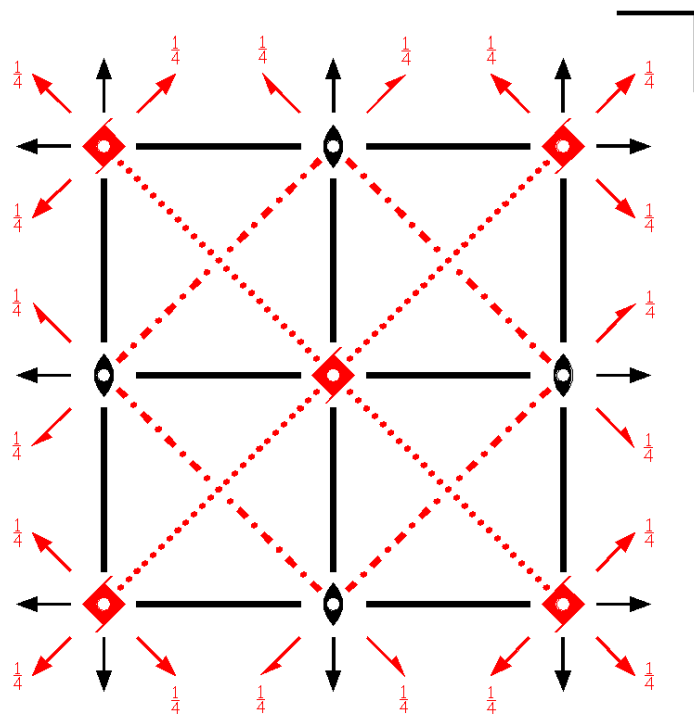
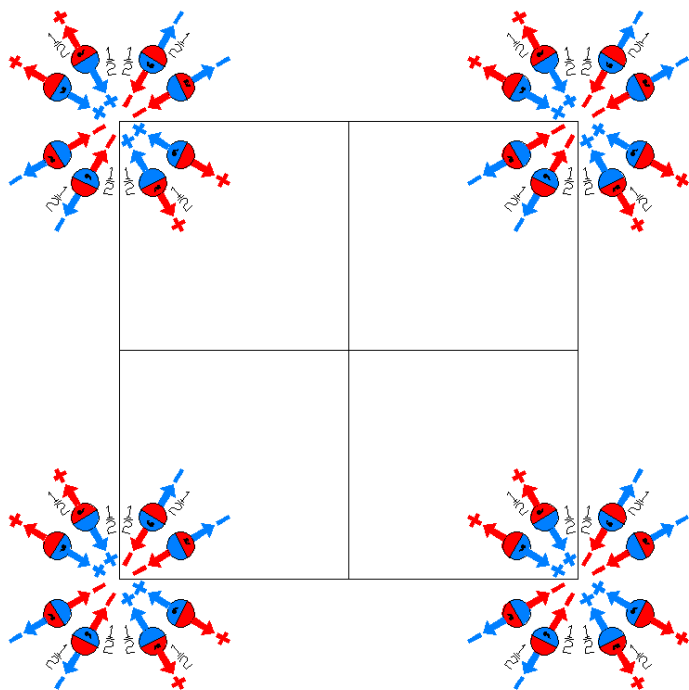
$P4_2'/mmc'$

131.5.1101

$4'/mmm'$

$P4_2'/m2/m2'/c'$

Tetragonal



Origin at center ( mmm ) at  $4_2'/m2/mc'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

**Symmetry Operations**

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                    | (8) 2' x,x̄,1/4<br>(2 <sub>xȳ</sub>  0,0,1/2)'                                |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)              | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (11) 4 <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub>  0,0,1/2)' | (12) 4 <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (15) c' (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)'          | (16) c' (0,0,1/2) x,x,z<br>(m <sub>xȳ</sub>  0,0,1/2)'                        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	r	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ]
			(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $v,u,w$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(10) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]
			(13) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x,z+1/2$ [ $v,u,w$ ]
8	q	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,1/2$ [0,0, $\bar{w}$ ]	$y,\bar{x},1/2$ [0,0, $\bar{w}$ ]
			$\bar{x},y,0$ [0,0, $\bar{w}$ ]	$x,\bar{y},0$ [0,0, $\bar{w}$ ]	$y,x,1/2$ [0,0,w]	$\bar{y},\bar{x},1/2$ [0,0,w]
8	p	.m.	1/2,y,z [u,0,0]	1/2, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},1/2,z+1/2$ [0, $\bar{u},0$ ]	$y,1/2,z+1/2$ [0,u,0]
			1/2, $y,\bar{z}$ [ $\bar{u},0,0$ ]	1/2, $\bar{y},\bar{z}$ [u,0,0]	$y,1/2,\bar{z}+1/2$ [0, $\bar{u},0$ ]	$\bar{y},1/2,\bar{z}+1/2$ [0,u,0]
8	o	.m.	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},0,z+1/2$ [0, $\bar{u},0$ ]	$y,0,z+1/2$ [0,u,0]
			0, $y,\bar{z}$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]	$y,0,\bar{z}+1/2$ [0, $\bar{u},0$ ]	$\bar{y},0,\bar{z}+1/2$ [0,u,0]
8	n	..2'	x,x,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [ $u,\bar{u},w$ ]	$\bar{x},x,3/4$ [ $u,u,\bar{w}$ ]	$x,\bar{x},3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x},\bar{x},3/4$ [ $\bar{u},u,w$ ]	$x,x,3/4$ [ $u,\bar{u},w$ ]	$x,\bar{x},1/4$ [ $u,u,\bar{w}$ ]	$\bar{x},x,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
4	m	m2m.	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]	1/2,x,1/2 [0,0,0]	1/2, $\bar{x},1/2$ [0,0,0]
4	l	m2m.	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x},0$ [0,0,0]
4	k	m2m.	x,1/2,1/2 [0,0,0]	$\bar{x},1/2,1/2$ [0,0,0]	1/2,x,0 [0,0,0]	1/2, $\bar{x},0$ [0,0,0]
4	j	m2m.	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,1/2 [0,0,0]	0, $\bar{x},1/2$ [0,0,0]
4	i	2mm.	0,1/2,z [0,0,0]	1/2,0,z+1/2 [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]
4	h	2mm.	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]
4	g	2mm.	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]
2	f	$\bar{4}'m2'$	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	e	$\bar{4}'m2'$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	d	mmm.	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]		
2	c	mmm.	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	b	mmm.	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

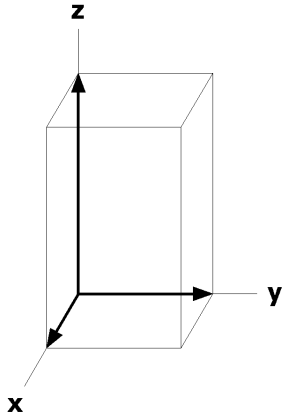
2      a    mmm.    0,0,0 [0,0,0]                      0,0,1/2 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$     $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}$     $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$     $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



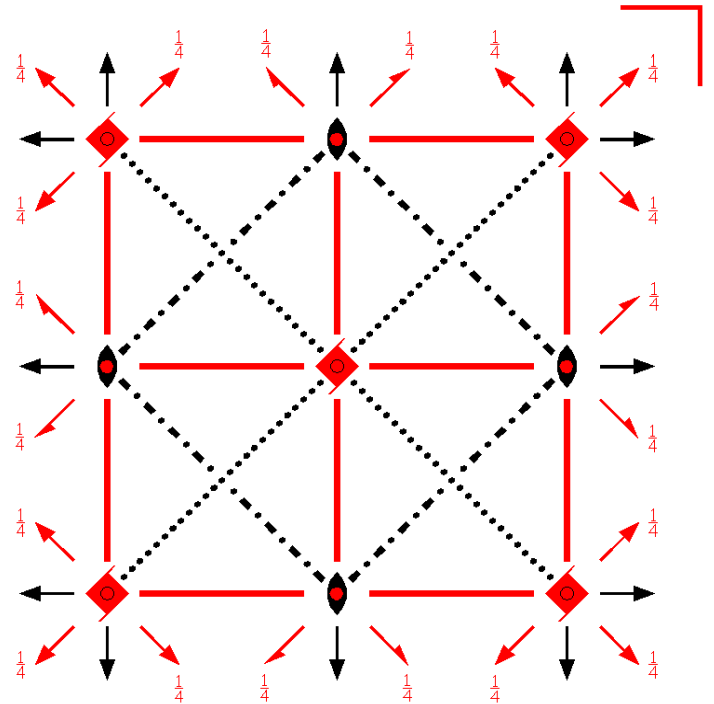
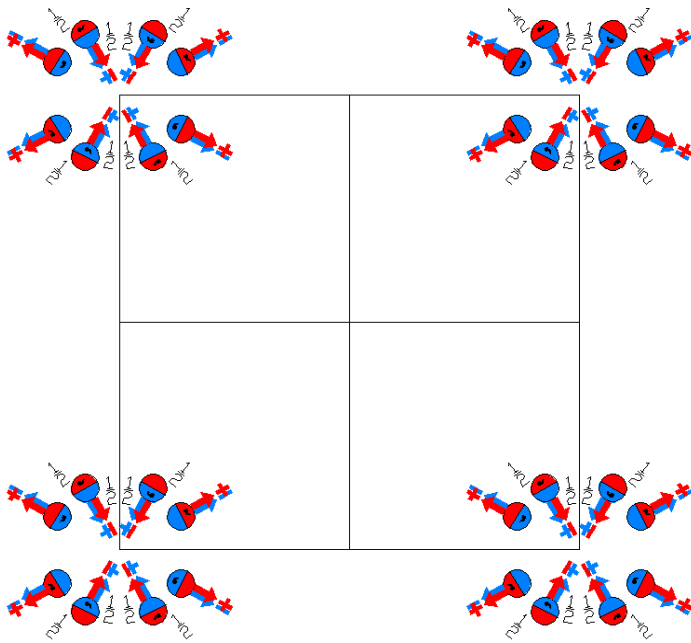
$P4_2/m'm'c$

131.6.1102

$4'/m'm'm$

$P4_2'/m'2/m'2'/c$

Tetragonal



Origin at center ( $m'm'm$ ) at  $4_2'/m'2/m'c$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)    | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)    | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                    | (8) 2' x,x̄,1/4<br>(2 <sub>xȳ</sub>  0,0,1/2)'                                |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'               | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) 4 <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub>  0,0,1/2)  | (12) 4 <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)  |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (15) c (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)            | (16) c (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)                           |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	r	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (13) x, $\bar{y}$ ,z [u, $\bar{v}$ ,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ] (10) x,y, $\bar{z}$ [u,v, $\bar{w}$ ] (14) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ] (7) y,x, $\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ] (11) y, $\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ] (15) $\bar{y},\bar{x},z+1/2$ [v,u, $\bar{w}$ ]	(4) y, $\bar{x},z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ] (8) $\bar{y},\bar{x},\bar{z}+1/2$ [v,u,w] (12) $\bar{y},x,\bar{z}+1/2$ [v, $\bar{u},w$ ] (16) y,x,z+1/2 [ $\bar{v},\bar{u},\bar{w}$ ]
8	q	m'..	x,y,0 [u,v,0] $\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ] x, $\bar{y},0$ [u, $\bar{v},0$ ]	$\bar{y},x,1/2$ [v, $\bar{u},0$ ] y,x,1/2 [ $\bar{v},\bar{u},0$ ]	y, $\bar{x},1/2$ [ $\bar{v},\bar{u},0$ ] $\bar{y},\bar{x},1/2$ [v,u,0]
8	p	.m'.	1/2,y,z [0,v,w] 1/2,y, $\bar{z}$ [0,v, $\bar{w}$ ]	1/2, $\bar{y},z$ [0, $\bar{v},w$ ] 1/2, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]	$\bar{y},1/2,z+1/2$ [v,0, $\bar{w}$ ] y,1/2, $\bar{z}+1/2$ [ $\bar{v},0,w$ ]	y,1/2,z+1/2 [ $\bar{v},0,\bar{w}$ ] $\bar{y},1/2,\bar{z}+1/2$ [v,0,w]
8	o	.m'.	0,y,z [0,v,w] 0,y, $\bar{z}$ [0,v, $\bar{w}$ ]	0, $\bar{y},z$ [0, $\bar{v},w$ ] 0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]	$\bar{y},0,z+1/2$ [v,0, $\bar{w}$ ] y,0, $\bar{z}+1/2$ [ $\bar{v},0,w$ ]	y,0,z+1/2 [ $\bar{v},0,\bar{w}$ ] $\bar{y},0,\bar{z}+1/2$ [v,0,w]
8	n	..2'	x,x,1/4 [ $\bar{u},u,w$ ] $\bar{x},\bar{x},3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	$\bar{x},\bar{x},1/4$ [u, $\bar{u},w$ ] x,x,3/4 [ $\bar{u},\bar{u},\bar{w}$ ]	$\bar{x},x,3/4$ [u,u, $\bar{w}$ ] x, $\bar{x},1/4$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},3/4$ [ $\bar{u},\bar{u},\bar{w}$ ] $\bar{x},x,1/4$ [u,u,w]
4	m	m'2m'.	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	1/2,x,1/2 [0, $\bar{u},0$ ]	1/2, $\bar{x},1/2$ [0,u,0]
4	l	m'2m'.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,0 [0, $\bar{u},0$ ]	0, $\bar{x},0$ [0,u,0]
4	k	m'2m'.	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	1/2,x,0 [0, $\bar{u},0$ ]	1/2, $\bar{x},0$ [0,u,0]
4	j	m'2m'.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,1/2 [0, $\bar{u},0$ ]	0, $\bar{x},1/2$ [0,u,0]
4	i	2m'm'.	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0,w]
4	h	2m'm'.	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]
4	g	2m'm'.	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0,w]
2	f	$\bar{4}m'2'$	1/2,1/2,1/4 [0,0,w]	1/2,1/2,3/4 [0,0, $\bar{w}$ ]		
2	e	$\bar{4}m'2'$	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		
2	d	m'm'm'.	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]		
2	c	m'm'm'.	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	b	m'm'm'.	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

2 a m'm'm'. 0,0,0 [0,0,0]

0,0,1/2 [0,0,0]

**Symmetry of Special Projections**Along [0,0,1]  $p4'm'm'$  $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$ 

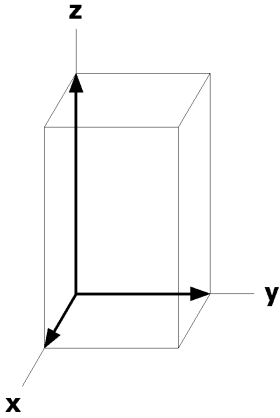
Origin at 0,0,z

Along [1,0,0]  $p2m'm'$  $\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}$ 

Origin at x,0,0

Along [1,1,0]  $p_{2a'} 2m'm'$  $\mathbf{a}^* = -\mathbf{c}/2 \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$ 

Origin at x,x,0



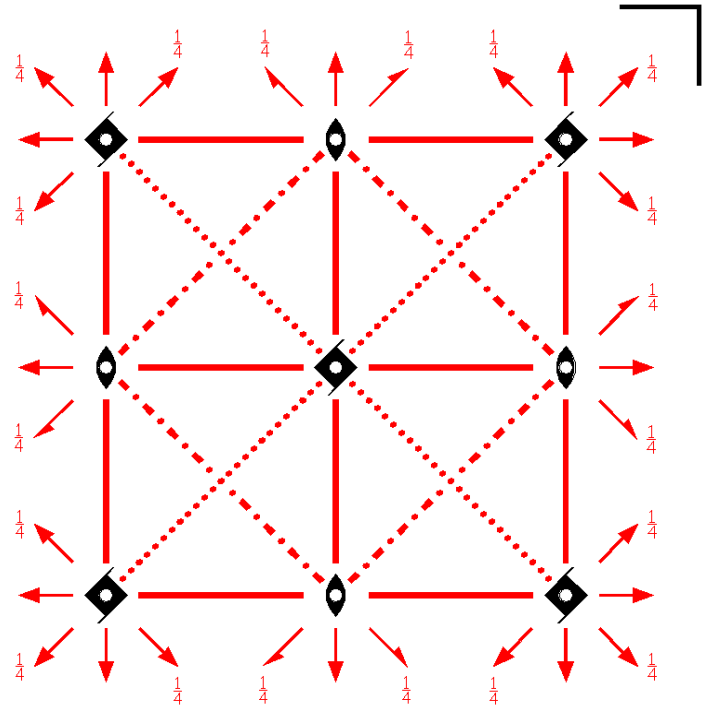
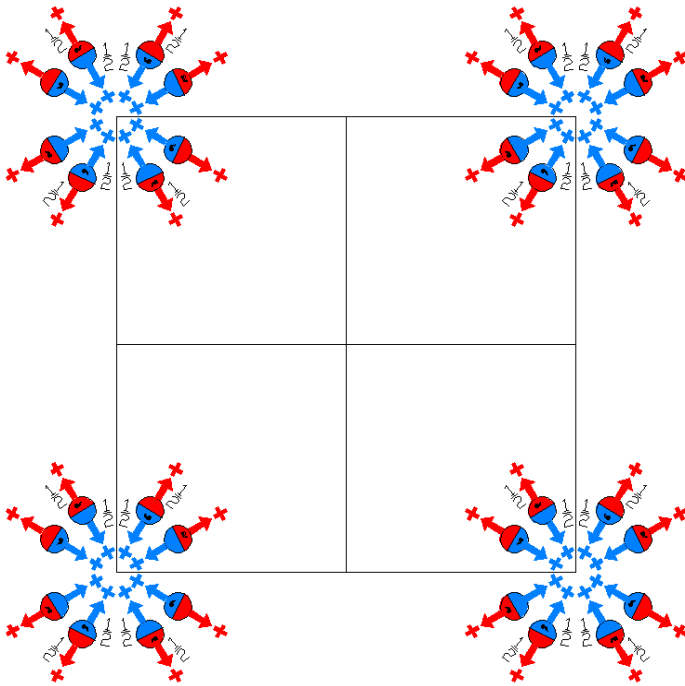
$P4_2/mm'c'$

131.7.1103

$4/mm'm'$

$P4_2/m2'/m'2'/c'$

Tetragonal



Origin at center ( $m'm'm'$ ) at  $4_2/m2'/m'c'$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

### Symmetry Operations

- |  |   |  |   |
|--|---|--|---|
| (1) $1$<br>$(1 0,0,0)$                         | (2) $2 \quad 0,0,z$<br>$(2_z 0,0,0)$    | (3) $4^+ (0,0,1/2) \quad 0,0,z$<br>$(4_z 0,0,1/2)$                   | (4) $4^- (0,0,1/2) \quad 0,0,z$<br>$(4_z^{-1} 0,0,1/2)$                   |
| (5) $2' \quad 0,y,0$<br>$(2_y 0,0,0)'$         | (6) $2' \quad x,0,0$<br>$(2_x 0,0,0)'$  | (7) $2' \quad x,x,1/4$<br>$(2_{xy} 0,0,1/2)'$                        | (8) $2' \quad x,\bar{x},1/4$<br>$(2_{\bar{xy}} 0,0,1/2)'$                 |
| (9) $\bar{1} \quad 0,0,0$<br>$(\bar{1} 0,0,0)$ | (10) $m \quad x,y,0$<br>$(m_z 0,0,0)$   | (11) $\bar{4}^+ \quad 0,0,z; \quad 0,0,1/4$<br>$(\bar{4}_z 0,0,1/2)$ | (12) $\bar{4}^- \quad 0,0,z; \quad 0,0,1/4$<br>$(\bar{4}_z^{-1} 0,0,1/2)$ |
| (13) $m' \quad x,0,z$<br>$(m_y 0,0,0)'$        | (14) $m' \quad 0,y,z$<br>$(m_x 0,0,0)'$ | (15) $c' (0,0,1/2) \quad x,\bar{x},z$<br>$(m_{xy} 0,0,1/2)'$         | (16) $c' (0,0,1/2) \quad x,x,z$<br>$(m_{\bar{xy}} 0,0,1/2)'$              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	r	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [u, $\bar{v}$ ,w] (9) $\bar{x},\bar{y},\bar{z}$ [u,v,w] (13) x, $\bar{y},z$ [u, $\bar{v}$ ,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v}$ ,w] (6) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ] (10) x,y, $\bar{z}$ [ $\bar{u},\bar{v}$ ,w] (14) $\bar{x},\bar{y},z$ [ $\bar{u},v,w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ] (7) y,x, $\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ] (11) y, $\bar{x},\bar{z}+1/2$ [ $\bar{v},u,w$ ] (15) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(4) y, $\bar{x},z+1/2$ [v, $\bar{u},w$ ] (8) $\bar{y},\bar{x},\bar{z}+1/2$ [v,u,w] (12) $\bar{y},x,\bar{z}+1/2$ [v, $\bar{u},w$ ] (16) y,x,z+1/2 [v,u,w]
8	q	m..	x,y,0 [0,0,w] $\bar{x},y,0$ [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w] x, $\bar{y},0$ [0,0,w]	$\bar{y},x,1/2$ [0,0,w] y,x,1/2 [0,0,w]	y, $\bar{x},1/2$ [0,0,w] $\bar{y},\bar{x},1/2$ [0,0,w]
8	p	.m'.	1/2,y,z [0,v,w] 1/2,y, $\bar{z}$ [0, $\bar{v}$ ,w]	1/2, $\bar{y},z$ [0, $\bar{v}$ ,w] 1/2, $\bar{y},\bar{z}$ [0,v,w]	$\bar{y},1/2,z+1/2$ [ $\bar{v},0,w$ ] y,1/2, $\bar{z}+1/2$ [ $\bar{v},0,w$ ]	y,1/2,z+1/2 [v,0,w] $\bar{y},1/2,\bar{z}+1/2$ [v,0,w]
8	o	.m'.	0,y,z [0,v,w] 0,y, $\bar{z}$ [0, $\bar{v}$ ,w]	0, $\bar{y},z$ [0, $\bar{v}$ ,w] 0, $\bar{y},\bar{z}$ [0,v,w]	$\bar{y},0,z+1/2$ [ $\bar{v},0,w$ ] y,0, $\bar{z}+1/2$ [ $\bar{v},0,w$ ]	y,0,z+1/2 [v,0,w] $\bar{y},0,\bar{z}+1/2$ [v,0,w]
8	n	..2'	x,x,1/4 [ $\bar{u},u,w$ ] $\bar{x},\bar{x},3/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [u, $\bar{u},w$ ] x,x,3/4 [u, $\bar{u},w$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},w$ ] x, $\bar{x},1/4$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},3/4$ [u,u,w] $\bar{x},x,1/4$ [u,u,w]
4	m	m2'm'.	x,1/2,0 [0,0,w]	$\bar{x},1/2,0$ [0,0,w]	1/2,x,1/2 [0,0,w]	1/2, $\bar{x},1/2$ [0,0,w]
4	l	m2'm'.	x,0,1/2 [0,0,w]	$\bar{x},0,1/2$ [0,0,w]	0,x,0 [0,0,w]	0, $\bar{x},0$ [0,0,w]
4	k	m2'm'.	x,1/2,1/2 [0,0,w]	$\bar{x},1/2,1/2$ [0,0,w]	1/2,x,0 [0,0,w]	1/2, $\bar{x},0$ [0,0,w]
4	j	m2'm'.	x,0,0 [0,0,w]	$\bar{x},0,0$ [0,0,w]	0,x,1/2 [0,0,w]	0, $\bar{x},1/2$ [0,0,w]
4	i	2m'm'.	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]
4	h	2m'm'.	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]
4	g	2m'm'.	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]
2	f	$\bar{4}m'2'$	1/2,1/2,1/4 [0,0,w]	1/2,1/2,3/4 [0,0,w]		
2	e	$\bar{4}m'2'$	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		
2	d	mm'm'.	0,1/2,1/2 [0,0,w]	1/2,0,0 [0,0,w]		
2	c	mm'm'.	0,1/2,0 [0,0,w]	1/2,0,1/2 [0,0,w]		
2	b	mm'm'.	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]		

2 a mm'm'. 0,0,0 [0,0,w]

0,0,1/2 [0,0,w]

**Symmetry of Special Projections**Along [0,0,1]  $p4mm1'$  $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$ 

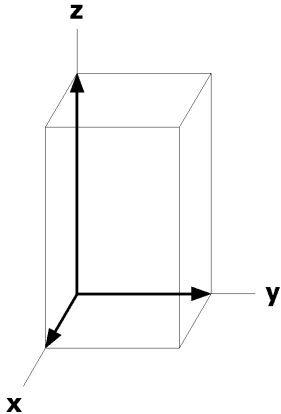
Origin at 0,0,z

Along [1,0,0]  $p2'mm'$  $\mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b}$ 

Origin at x,0,0

Along [1,1,0]  $p2'mm'$  $\mathbf{a}^* = -\mathbf{c}/2 \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$ 

Origin at x,x,0



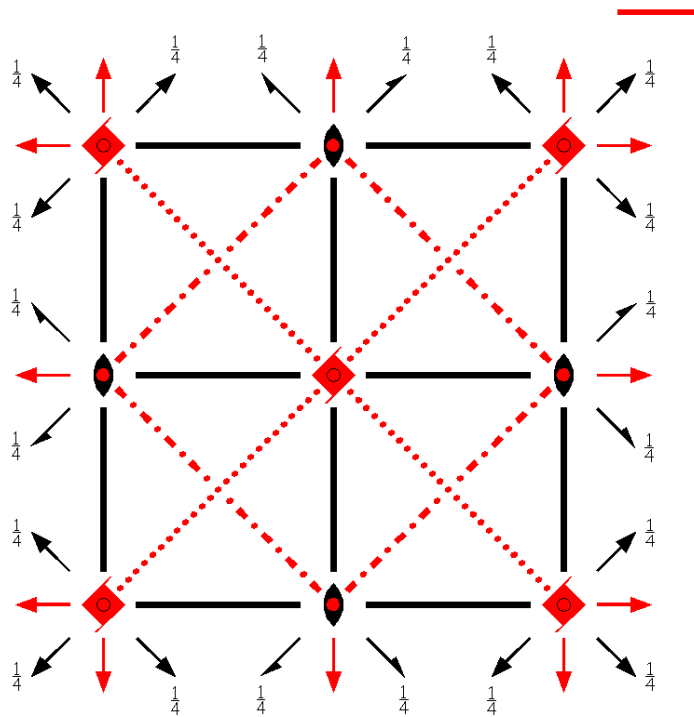
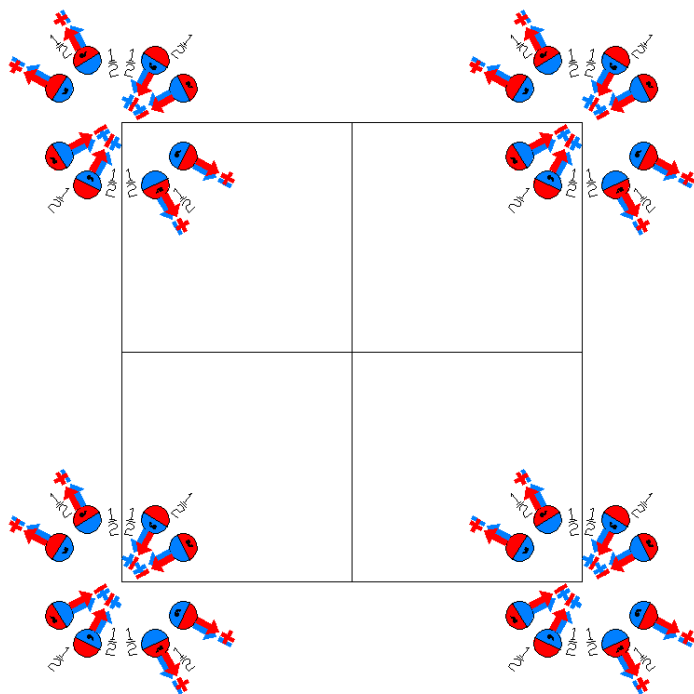
$P4_2/m'mc'$

131.8.1104

$4'/m'mm'$

$P4_2'/m'2'/m2/c'$

Tetragonal



Origin at center ( $mmm'$ ) at  $4_2'/m'2'/mc'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

**Symmetry Operations**

- |  |   |  |  |
|--|---|--|--|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)'             | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'  | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                                  | (8) 2 x,x̄,1/4<br>(2 <sub>xȳ</sub>  0,0,1/2)                                  |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'              | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) 4 <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>+</sup>  0,0,1/2) | (12) 4 <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)  |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)  | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   | (15) c' (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)'                      | (16) c' (0,0,1/2) x,x,z<br>(m <sub>xȳ</sub>  0,0,1/2)'                        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	r	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(13) $x,\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x},y,z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(16) $y,x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	q	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},\bar{u},0$ ]	$y,\bar{x},1/2$ [ $\bar{v},\bar{u},0$ ]
			$\bar{x},y,0$ [ $\bar{u},\bar{v},0$ ]	$x,\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$y,x,1/2$ [ $\bar{v},\bar{u},0$ ]	$\bar{y},\bar{x},1/2$ [ $\bar{v},\bar{u},0$ ]
8	p	.m.	1/2,y,z [u,0,0]	1/2, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},1/2,z+1/2$ [0, $\bar{u},0$ ]	$y,1/2,z+1/2$ [0,u,0]
			1/2, $y,\bar{z}$ [u,0,0]	1/2, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]	$y,1/2,\bar{z}+1/2$ [0,u,0]	$\bar{y},1/2,\bar{z}+1/2$ [0, $\bar{u},0$ ]
8	o	.m.	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},0,z+1/2$ [0, $\bar{u},0$ ]	$y,0,z+1/2$ [0,u,0]
			0, $y,\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]	$y,0,\bar{z}+1/2$ [0,u,0]	$\bar{y},0,\bar{z}+1/2$ [0, $\bar{u},0$ ]
8	n	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,3/4$ [u, $\bar{u},0$ ]	$x,\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	$x,x,3/4$ [u,u,0]	$x,\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/4$ [u, $\bar{u},0$ ]
4	m	m'2'm.	x,1/2,0 [0,v,0]	$\bar{x},1/2,0$ [0, $\bar{v},0$ ]	1/2,x,1/2 [v,0,0]	1/2, $\bar{x},1/2$ [ $\bar{v},0,0$ ]
4	l	m'2'm.	x,0,1/2 [0,v,0]	$\bar{x},0,1/2$ [0, $\bar{v},0$ ]	0,x,0 [v,0,0]	0, $\bar{x},0$ [ $\bar{v},0,0$ ]
4	k	m'2'm.	x,1/2,1/2 [0,v,0]	$\bar{x},1/2,1/2$ [0, $\bar{v},0$ ]	1/2,x,0 [v,0,0]	1/2, $\bar{x},0$ [ $\bar{v},0,0$ ]
4	j	m'2'm.	x,0,0 [0,v,0]	$\bar{x},0,0$ [0, $\bar{v},0$ ]	0,x,1/2 [v,0,0]	0, $\bar{x},1/2$ [ $\bar{v},0,0$ ]
4	i	2mm.	0,1/2,z [0,0,0]	1/2,0,z+1/2 [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]
4	h	2mm.	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]
4	g	2mm.	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]
2	f	$\bar{4}m2$	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	e	$\bar{4}m2$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	d	m'mm.	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]		
2	c	m'mm.	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	b	m'mm.	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

2 a m'mm. 0,0,0 [0,0,0]

0,0,1/2 [0,0,0]

**Symmetry of Special Projections**Along [0,0,1]  $p4'mm'$  $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$ 

Origin at 0,0,z

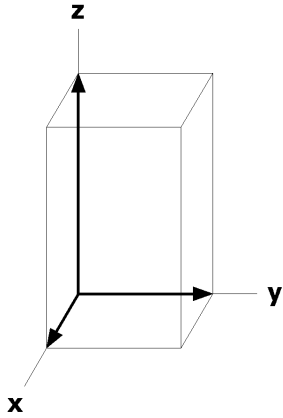
Along [1,0,0]  $p2mm1'$  $\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}$ 

Origin at x,0,0

Along [1,1,0]  $p2m'm'$  $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}/2$ 

Origin at x,x,0





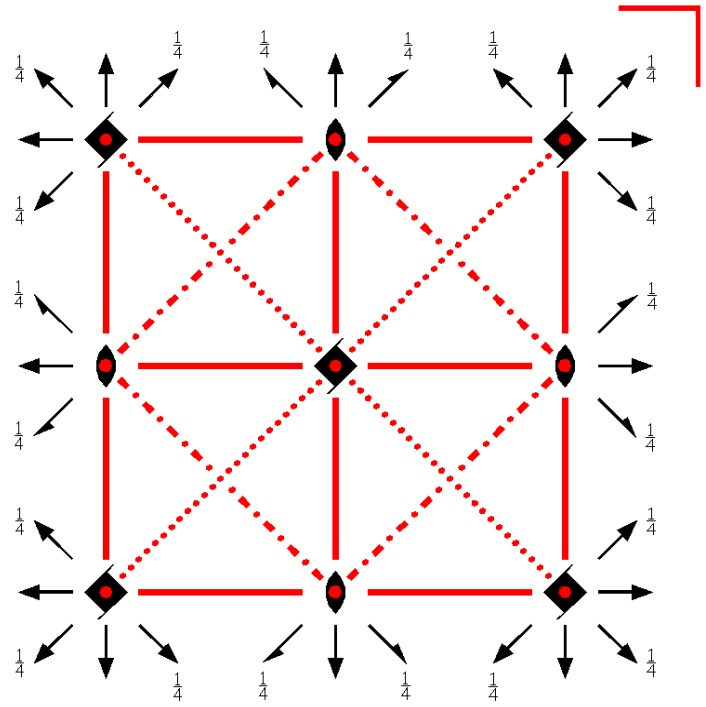
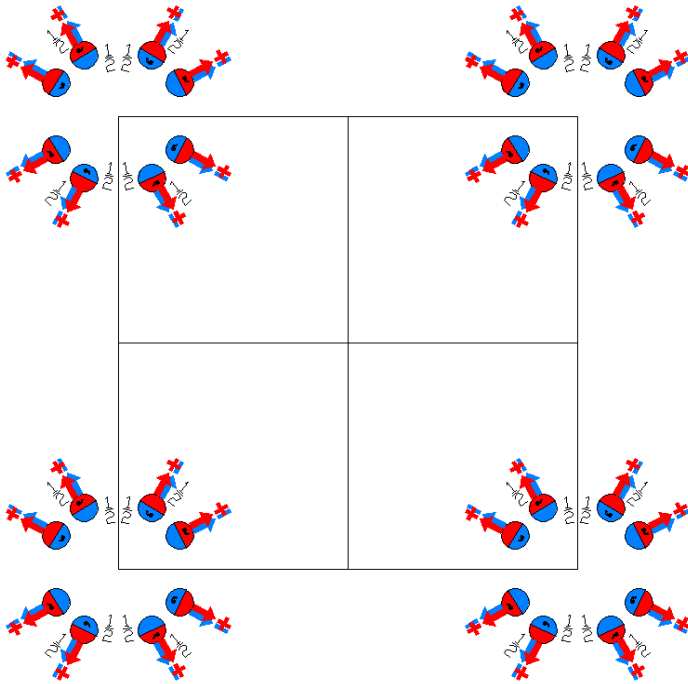
$P4_2/m'm'c'$

131.9.1105

$4/m'm'm'$

$P4_2/m'2/m'2/c'$

Tetragonal



Origin at center ( $m'm'm'$ ) at  $4_2/m'2/m'c'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                          | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)  | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)      | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)    | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                      | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)      |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)' | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) $\bar{4}^+$ 0,0,z; 0,0,1/4<br>( $\bar{4}_z^+$  0,0,1/2)'    | (12) $\bar{4}^-$ 0,0,z; 0,0,1/4<br>( $\bar{4}_z^-$  0,0,1/2)'                 |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)'   | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (15) c' (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2)' | (16) c' (0,0,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,1/2)'     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	r	1	(1) x,y,z [u,v,w] (5) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (13) $x,\bar{y},z$ [ $u,\bar{v},w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ] (10) $x,y,\bar{z}$ [ $u,v,\bar{w}$ ] (14) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ] (7) $y,x,\bar{z}+1/2$ [ $v,u,\bar{w}$ ] (11) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ] (15) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ] (8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ] (12) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ] (16) $y,x,z+1/2$ [ $v,u,w$ ]
8	q	m'..	x,y,0 [u,v,0] $\bar{x},y,0$ [ $\bar{u},v,0$ ]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ] x, $\bar{y},0$ [ $u,\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},u,0$ ] y,x,1/2 [v,u,0]	$y,\bar{x},1/2$ [ $v,\bar{u},0$ ] $\bar{y},\bar{x},1/2$ [ $\bar{v},\bar{u},0$ ]
8	p	.m'.	1/2,y,z [0,v,w] 1/2,y, $\bar{z}$ [0,v, $\bar{w}$ ]	1/2, $\bar{y},z$ [0, $\bar{v},w$ ] 1/2, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]	$\bar{y},1/2,z+1/2$ [ $\bar{v},0,w$ ] y,1/2, $\bar{z}+1/2$ [v,0, $\bar{w}$ ]	y,1/2,z+1/2 [v,0,w] $\bar{y},1/2,\bar{z}+1/2$ [ $\bar{v},0,\bar{w}$ ]
8	o	.m'.	0,y,z [0,v,w] 0,y, $\bar{z}$ [0,v, $\bar{w}$ ]	0, $\bar{y},z$ [0, $\bar{v},w$ ] 0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]	$\bar{y},0,z+1/2$ [ $\bar{v},0,w$ ] y,0, $\bar{z}+1/2$ [v,0, $\bar{w}$ ]	y,0,z+1/2 [v,0,w] $\bar{y},0,\bar{z}+1/2$ [ $\bar{v},0,\bar{w}$ ]
8	n	..2	x,x,1/4 [u,u,0] $\bar{x},\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ] x,x,3/4 [u,u,0]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ] x, $\bar{x},1/4$ [ $u,\bar{u},0$ ]	x, $\bar{x},3/4$ [ $u,\bar{u},0$ ] $\bar{x},x,1/4$ [ $\bar{u},u,0$ ]
4	m	m'2m'.	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	1/2,x,1/2 [0,u,0]	1/2, $\bar{x},1/2$ [0, $\bar{u},0$ ]
4	l	m'2m'.	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,0 [0,u,0]	0, $\bar{x},0$ [0, $\bar{u},0$ ]
4	k	m'2m'.	x,1/2,1/2 [u,0,0]	$\bar{x},1/2,1/2$ [ $\bar{u},0,0$ ]	1/2,x,0 [0,u,0]	1/2, $\bar{x},0$ [0, $\bar{u},0$ ]
4	j	m'2m'.	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,1/2 [0,u,0]	0, $\bar{x},1/2$ [0, $\bar{u},0$ ]
4	i	2m'm'.	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	h	2m'm'.	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	g	2m'm'.	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
2	f	$\bar{4}$ 'm'2	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	e	$\bar{4}$ 'm'2	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	d	m'm'm'.	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]		
2	c	m'm'm'.	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]		
2	b	m'm'm'.	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

2 a m'm'm'. 0,0,0 [0,0,0]

0,0,1/2 [0,0,0]

**Symmetry of Special Projections**Along [0,0,1]  $p4m'm'$  $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$ 

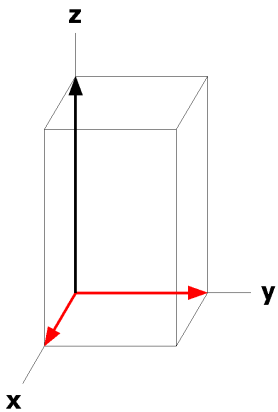
Origin at 0,0,z

Along [1,0,0]  $p2m'm'$  $\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}$ 

Origin at x,0,0

Along [1,1,0]  $p2m'm'$  $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}/2$ 

Origin at x,x,0



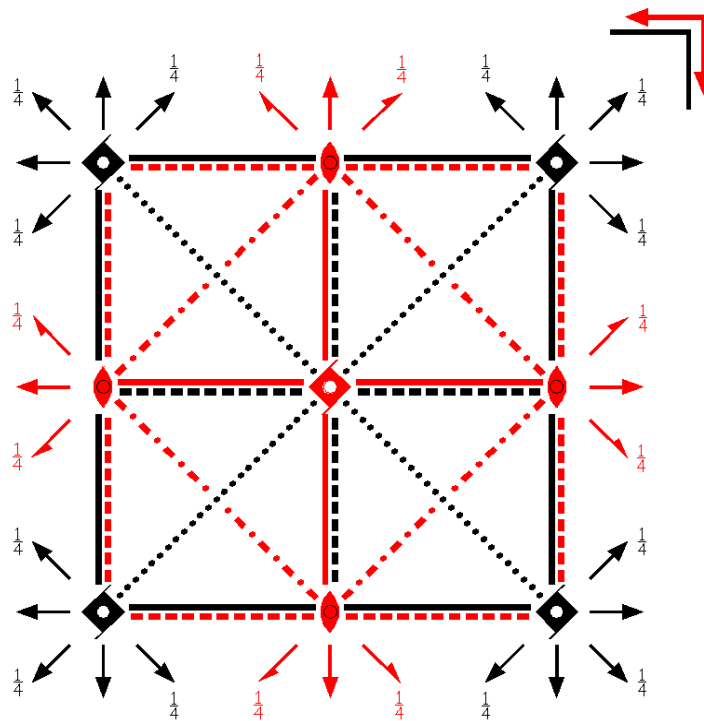
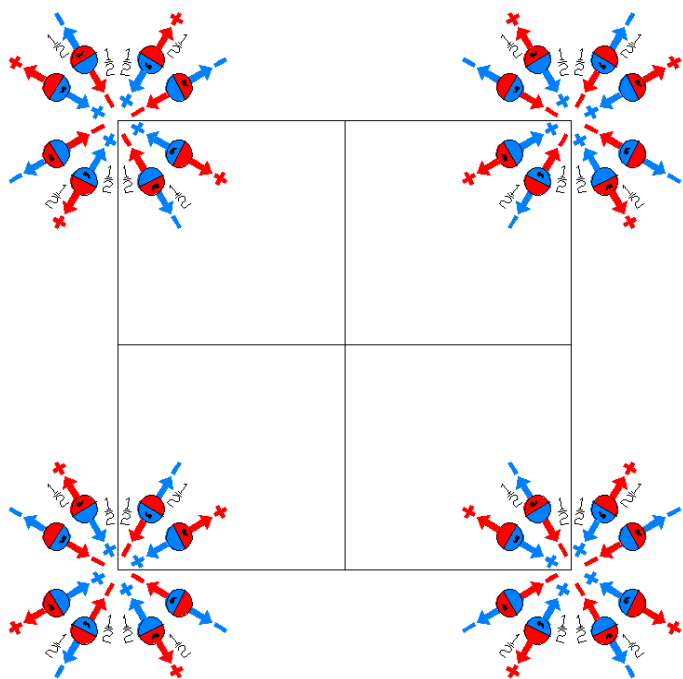
$P_P 4_2/mmc$

131.10.1106

$4/mmm1'$

$P_P 4_2/m2/m2/c$

Tetragonal



Origin at center ( mmm ) at  $4_2/m2/mc$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)              | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                                  | (8) 2 x,x̄,1/4<br>(2 <sub>xȳ</sub>  0,0,1/2)                                 |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)              | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (11) 4 <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>+</sup>  0,0,1/2) | (12) 4 <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (15) c (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)                        | (16) c (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)                          |

## For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> ' (0,0,1/2) 1/2,1/2,z (4 <sub>z</sub>  1,0,1/2)'	(4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,1/2)'
(5) 2' 1/2,y,0 (2 <sub>y</sub>  1,0,0)'	(6) 2' (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)'	(7) 2' (1/2,1/2,0) x+1/2,x,1/4 (2 <sub>xy</sub>  1,0,1/2)'	(8) 2' (1/2,-1/2,0) x+1/2,x̄,1/4 (2 <sub>xy</sub> <sup>-</sup>  1,0,1/2)'
(9) 1̄' 1/2,0,0 (1̄ 1,0,0)'	(10) a' (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)'	(11) 4 <sup>+</sup> ' 1/2,-1/2,z; 1/2,-1/2,1/4 (4 <sub>z</sub>  1,0,1/2)'	(12) 4 <sup>-</sup> ' 1/2,1/2,z; 1/2,1/2,1/4 (4 <sub>z</sub> <sup>-1</sup>  1,0,1/2)'
(13) a' (1,0,0) x,0,z (m <sub>y</sub>  1,0,0)'	(14) m' 1/2,y,z (m <sub>x</sub>  1,0,0)'	(15) n' (1/2,-1/2,1/2) x+1/2,x̄,z (m <sub>xy</sub>  1,0,1/2)'	(16) n' (1/2,1/2,1/2) x+1/2,x,z (m <sub>xy</sub> <sup>-</sup>  1,0,1/2)'

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1,0,0)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	r	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w]	(3) ȳ,x,z+1/2 [v̄,u,w]	(4) y,x̄,z+1/2 [v,ū,w]
			(5) x̄,y,z [ū,v,w]	(6) x,ȳ,z [u,v̄,w]	(7) y,x,z̄+1/2 [v,u,w̄]	(8) ȳ,x̄,z̄+1/2 [v̄,ū,w̄]
			(9) x̄,ȳ,z [u,v,w]	(10) x,y,z [ū,v̄,w]	(11) y,x̄,z̄+1/2 [v̄,u,w]	(12) ȳ,x,z̄+1/2 [v,ū,w]
			(13) x,y,z [ū,v,w]	(14) x̄,y,z [u,v̄,w]	(15) ȳ,x̄,z+1/2 [v,u,w̄]	(16) y,x,z+1/2 [v̄,ū,w̄]
16	q	m..	x,y,0 [0,0,w]	x̄,ȳ,0 [0,0,w]	ȳ,x,1/2 [0,0,w]	y,x̄,1/2 [0,0,w]
			x̄,y,0 [0,0,w̄]	x,ȳ,0 [0,0,w̄]	y,x,1/2 [0,0,w̄]	ȳ,x̄,1/2 [0,0,w̄]
16	p	.m'.	1/2,y,z [0,v,w]	1/2,ȳ,z [0,v̄,w]	ȳ,1/2,z+1/2 [v̄,0,w]	y,1/2,z+1/2 [v,0,w̄]
			1/2,y,z̄ [0,v̄,w]	1/2,ȳ,z̄ [0,v̄,w̄]	y,1/2,z̄+1/2 [v,0,w̄]	ȳ,1/2,z̄+1/2 [v̄,0,w]
16	o	.m.	0,y,z [u,0,0]	0,ȳ,z [ū,0,0]	ȳ,0,z+1/2 [0,u,0]	y,0,z+1/2 [0,ū,0]
			0,y,z̄ [ū,0,0]	0,ȳ,z̄ [u,0,0]	y,0,z̄+1/2 [0,u,0]	ȳ,0,z̄+1/2 [0,ū,0]
16	n	..2	x,x,1/4 [u,u,0]	x̄,x̄,1/4 [ū,ū,0]	x̄,x,3/4 [ū,u,0]	x,x̄,3/4 [u,ū,0]
			x̄,x̄,3/4 [u,u,0]	x,x,3/4 [ū,ū,0]	x,x̄,1/4 [ū,u,0]	x̄,x,1/4 [u,ū,0]
8	m	m2'm'.	x,1/2,0 [0,0,w]	x̄,1/2,0 [0,0,w̄]	1/2,x,1/2 [0,0,w̄]	1/2,x̄,1/2 [0,0,w]
8	l	m2m.	x,0,1/2 [0,0,0]	x̄,0,1/2 [0,0,0]	0,x,0 [0,0,0]	0,x̄,0 [0,0,0]
8	k	m2'm'.	x,1/2,1/2 [0,0,w]	x̄,1/2,1/2 [0,0,w̄]	1/2,x,0 [0,0,w̄]	1/2,x̄,0 [0,0,w]
8	j	m2m.	x,0,0 [0,0,0]	x̄,0,0 [0,0,0]	0,x,1/2 [0,0,0]	0,x̄,1/2 [0,0,0]
8	i	2'mm'.	0,1/2,z [u,0,0]	1/2,0,z+1/2 [0,ū,0]	0,1/2,z̄ [ū,0,0]	1/2,0,z̄+1/2 [0,u,0]

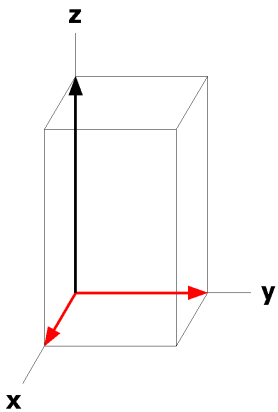
8	h	$2m'm'$	$1/2, 1/2, z [0,0,w]$	$1/2, 1/2, z+1/2 [0,0,\bar{w}]$	$1/2, 1/2, \bar{z} [0,0,w]$	$1/2, 1/2, \bar{z}+1/2 [0,0,\bar{w}]$
8	g	$2mm'$	$0,0,z [0,0,0]$	$0,0,z+1/2 [0,0,0]$	$0,0,\bar{z} [0,0,0]$	$0,0,\bar{z}+1/2 [0,0,0]$
4	f	$\bar{4}'m'2$	$1/2, 1/2, 1/4 [0,0,0]$	$1/2, 1/2, 3/4 [0,0,0]$		
4	e	$\bar{4}m'2$	$0,0,1/4 [0,0,0]$	$0,0,3/4 [0,0,0]$		
4	d	$mmm'$	$0,1/2,1/2 [0,0,0]$	$1/2,0,0 [0,0,0]$		
4	c	$mm'm'$	$0,1/2,0 [0,0,0]$	$1/2,0,1/2 [0,0,0]$		
4	b	$mm'm'$	$1/2,1/2,0 [0,0,w]$	$1/2,1/2,1/2 [0,0,\bar{w}]$		
4	a	$mmm'$	$0,0,0 [0,0,0]$	$0,0,1/2 [0,0,0]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p_2 2mm$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x-1/4, x+1/4, 0$



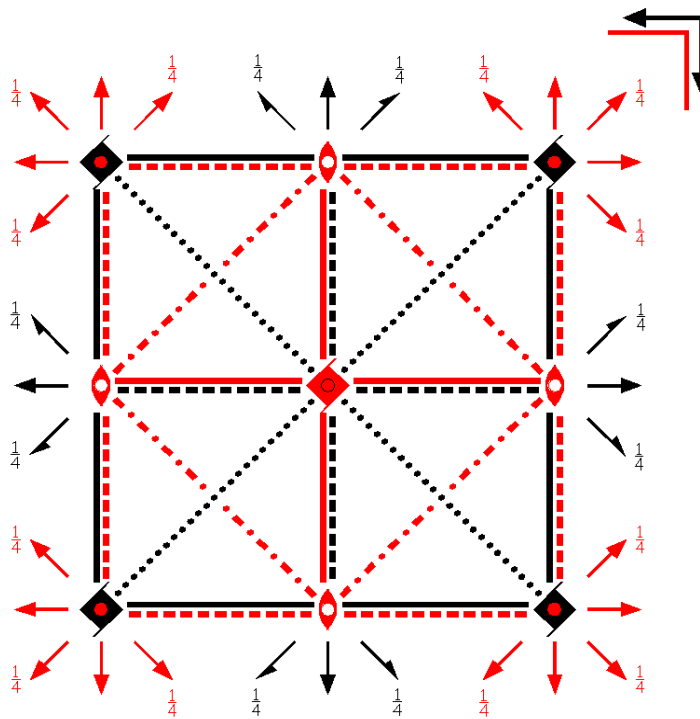
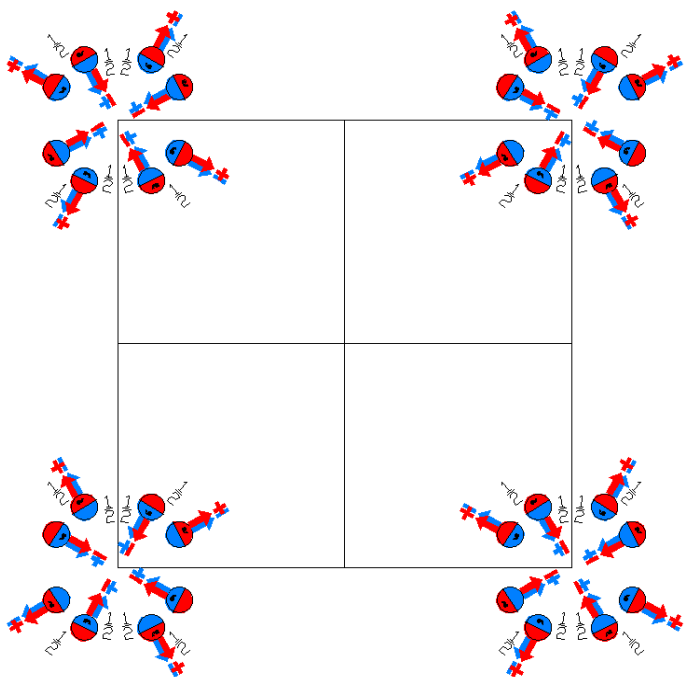
$P_P 4_2/m'mc$

131.11.1107

$4/mmm1'$

$P_P 4_2/m'2'/m2'/c$

Tetragonal



Origin at center ( $mmm'$ ) at  $4_2/m'2'/mc$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

For (0,0,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)                 | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)   |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'  | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                                   | (8) 2' x,x̄,1/4<br>(2 <sub>xȳ</sub>  0,0,1/2)'                                 |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'              | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) 4̄ <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' | (12) 4̄ <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)  | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   | (15) c (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)                           | (16) c (0,0,1/2) x,x,z<br>(m <sub>xȳ</sub>  0,0,1/2)                           |

## For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> (0,0,1/2) 1/2,1/2,z (4 <sub>z</sub>  1,0,1/2)'	(4) 4 <sup>-</sup> (0,0,1/2) 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,1/2)'
(5) 2 1/2,y,0 (2 <sub>y</sub>  1,0,0)	(6) 2 (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)	(7) 2 (1/2,1/2,0) x+1/2,x,1/4 (2 <sub>xy</sub>  1,0,1/2)	(8) 2 (1/2,-1/2,0) x+1/2,x̄,1/4 (2 <sub>xy</sub> <sup>-</sup>  1,0,1/2)
(9) 1̄ 1/2,0,0 (1̄ 1,0,0)	(10) a (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)	(11) 4 <sup>+</sup> 1/2,-1/2,z; 1/2,-1/2,1/4 (4 <sub>z</sub>  1,0,1/2)	(12) 4 <sup>-</sup> 1/2,1/2,z; 1/2,1/2,1/4 (4 <sub>z</sub> <sup>-1</sup>  1,0,1/2)
(13) a' (1,0,0) x,0,z (m <sub>y</sub>  1,0,0)'	(14) m' 1/2,y,z (m <sub>x</sub>  1,0,0)'	(15) n' (1/2,-1/2,1/2) x+1/2,x̄,z (m <sub>xy</sub>  1,0,1/2)'	(16) n' (1/2,1/2,1/2) x+1/2,x,z (m <sub>xy</sub> <sup>-</sup>  1,0,1/2)'

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1,0,0)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	r	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w]	(3) ȳ,x,z+1/2 [v̄,u,w]	(4) y,x̄,z+1/2 [v,ū,w]
			(5) x̄,y,z [ū,v̄,w]	(6) x,ȳ,z [u,v,w]	(7) y,x,z̄+1/2 [v̄,ū,w]	(8) ȳ,x̄,z̄+1/2 [v,u,w]
			(9) x̄,ȳ,z [ū,v̄,w̄]	(10) x,y,z̄ [u,v,w̄]	(11) y,x̄,z̄+1/2 [v̄,ū,w̄]	(12) ȳ,x,z̄+1/2 [v̄,u,w̄]
			(13) x,ȳ,z [ū,v,w̄]	(14) x̄,y,z [u,v̄,w̄]	(15) ȳ,x̄,z+1/2 [v,u,w̄]	(16) y,x,z+1/2 [v̄,ū,w̄]
16	q	m'..	x,y,0 [u,v,0]	x̄,ȳ,0 [ū,v̄,0]	ȳ,x,1/2 [v̄,u,0]	y,x̄,1/2 [v,ū,0]
			x̄,y,0 [ū,v̄,0]	x,ȳ,0 [u,v,0]	y,x,1/2 [v̄,ū,0]	ȳ,x̄,1/2 [v,u,0]
16	p	.m'.	1/2,y,z [0,v,w]	1/2,ȳ,z [0,v̄,w̄]	ȳ,1/2,z+1/2 [v̄,0,w]	y,1/2,z+1/2 [v̄,0,w̄]
			1/2,y,z̄ [0,v,w̄]	1/2,ȳ,z̄ [0,v̄,w̄]	y,1/2,z̄+1/2 [v̄,0,w]	ȳ,1/2,z̄+1/2 [v̄,0,w̄]
16	o	.m.	0,y,z [u,0,0]	0,ȳ,z [ū,0,0]	ȳ,0,z+1/2 [0,u,0]	y,0,z+1/2 [0,ū,0]
			0,y,z̄ [u,0,0]	0,ȳ,z̄ [ū,0,0]	y,0,z̄+1/2 [0,ū,0]	ȳ,0,z̄+1/2 [0,u,0]
16	n	..2'	x,x,1/4 [ū,u,w]	x̄,x̄,1/4 [ū,ū,w]	x̄,x,3/4 [ū,ū,w]	x,x̄,3/4 [u,u,w]
			x̄,x̄,3/4 [ū,ū,w̄]	x,x,3/4 [ū,u,w̄]	x,x̄,1/4 [u,u,w̄]	x̄,x,1/4 [ū,ū,w̄]
8	m	m'2m'.	x,1/2,0 [u,0,0]	x̄,1/2,0 [ū,0,0]	1/2,x,1/2 [0,ū,0]	1/2,x̄,1/2 [0,ū,0]
8	l	m'2'm.	x,0,1/2 [0,v,0]	x̄,0,1/2 [0,v̄,0]	0,x,0 [v̄,0,0]	0,x̄,0 [v,0,0]
8	k	m'2m'.	x,1/2,1/2 [u,0,0]	x̄,1/2,1/2 [ū,0,0]	1/2,x,0 [0,ū,0]	1/2,x̄,0 [0,ū,0]
8	j	m'2'm.	x,0,0 [0,v,0]	x̄,0,0 [0,v̄,0]	0,x,1/2 [v̄,0,0]	0,x̄,1/2 [v,0,0]
8	i	2'mm'.	0,1/2,z [u,0,0]	1/2,0,z+1/2 [0,ū,0]	0,1/2,z̄ [u,0,0]	1/2,0,z̄+1/2 [0,ū,0]



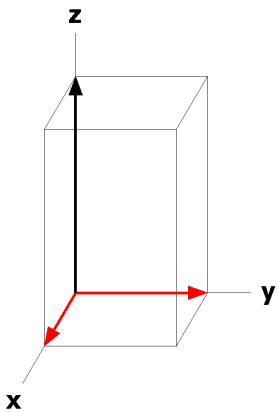
8	h	$2m'm'$	$1/2, 1/2, z [0, 0, w]$	$1/2, 1/2, z+1/2 [0, 0, \bar{w}]$	$1/2, 1/2, \bar{z} [0, 0, \bar{w}]$	$1/2, 1/2, \bar{z}+1/2 [0, 0, w]$
8	g	$2mm'$	$0, 0, z [0, 0, 0]$	$0, 0, z+1/2 [0, 0, 0]$	$0, 0, \bar{z} [0, 0, 0]$	$0, 0, \bar{z}+1/2 [0, 0, 0]$
4	f	$\bar{4}m'2'$	$1/2, 1/2, 1/4 [0, 0, w]$	$1/2, 1/2, 3/4 [0, 0, \bar{w}]$		
4	e	$\bar{4}'m'2'$	$0, 0, 1/4 [0, 0, 0]$	$0, 0, 3/4 [0, 0, 0]$		
4	d	$m'mm'$	$0, 1/2, 1/2 [u, 0, 0]$	$1/2, 0, 0 [0, \bar{u}, 0]$		
4	c	$m'mm'$	$0, 1/2, 0 [u, 0, 0]$	$1/2, 0, 1/2 [0, \bar{u}, 0]$		
4	b	$m'm'm'$	$1/2, 1/2, 0 [0, 0, 0]$	$1/2, 1/2, 1/2 [0, 0, 0]$		
4	a	$m'mm'$	$0, 0, 0 [0, 0, 0]$	$0, 0, 1/2 [0, 0, 0]$		

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p_4, 4mm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 0, 0$

Along  $[1, 1, 0]$   $p_4, 2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, x, 0$



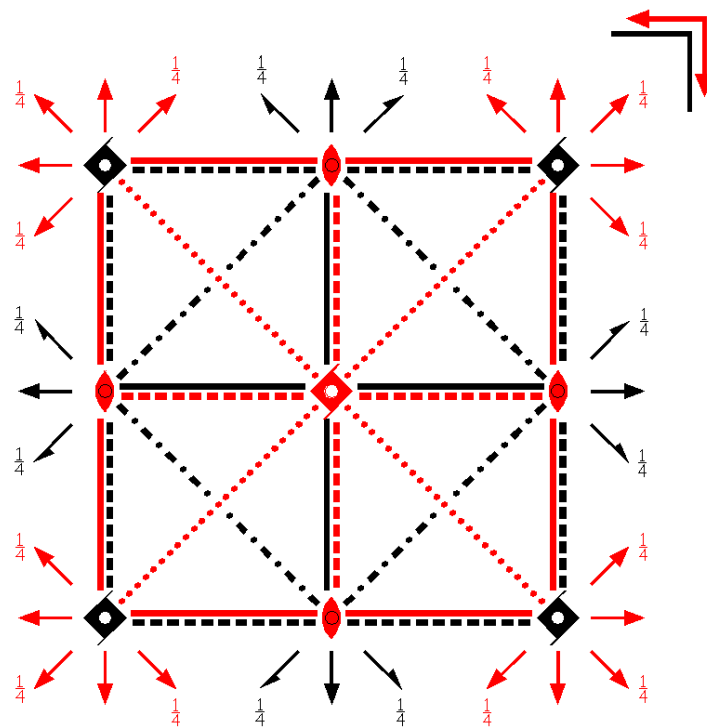
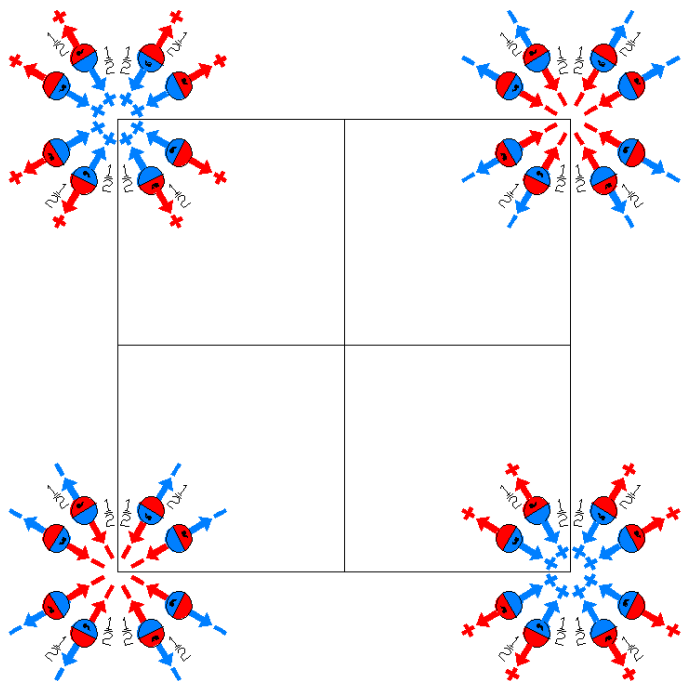
$P_P 4_2 / mm'c'$

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$4/mmm1'$

$P_P 4_2 / m2'/m'2'/c'$

Tetragonal



Origin at center ( $m'm'm$ ) at  $4_2 / m2'/m'c'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'  | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'  | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                   | (8) 2' x,x̄,1/4<br>(2 <sub>xȳ</sub>  0,0,1/2)'                               |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)                | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)   | (11) 4 <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub>  0,0,1/2) | (12) 4 <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (15) c' (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)'         | (16) c' (0,0,1/2) x,x,z<br>(m <sub>xȳ</sub>  0,0,1/2)'                       |

## For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> (0,0,1/2) 1/2,1/2,z (4 <sub>z</sub>  1,0,1/2)'	(4) 4 <sup>-</sup> (0,0,1/2) 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,1/2)'
(5) 2 1/2,y,0 (2 <sub>y</sub>  1,0,0)	(6) 2 (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)	(7) 2 (1/2,1/2,0) x+1/2,x,1/4 (2 <sub>xy</sub>  1,0,1/2)	(8) 2 (1/2,-1/2,0) x+1/2,x̄,1/4 (2 <sub>xy</sub> <sup>-</sup>  1,0,1/2)
(9) 1̄ 1/2,0,0 (1̄ 1,0,0)'	(10) a' (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)'	(11) 4 <sup>+</sup> 1/2,-1/2,z; 1/2,-1/2,1/4 (4 <sub>z</sub>  1,0,1/2)'	(12) 4 <sup>-</sup> 1/2,1/2,z; 1/2,1/2,1/4 (4 <sub>z</sub> <sup>-1</sup>  1,0,1/2)'
(13) a (1,0,0) x,0,z (m <sub>y</sub>  1,0,0)	(14) m 1/2,y,z (m <sub>x</sub>  1,0,0)	(15) n (1/2,-1/2,1/2) x+1/2,x̄,z (m <sub>xy</sub>  1,0,1/2)	(16) n (1/2,1/2,1/2) x+1/2,x,z (m <sub>xy</sub> <sup>-</sup>  1,0,1/2)

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1,0,0)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	r	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w]	(3) ȳ,x,z+1/2 [v̄,u,w]	(4) y,x̄,z+1/2 [v,ū,w]
			(5) x̄,y,z [ū,v̄,w]	(6) x,ȳ,z [u,v,w]	(7) y,x,z̄+1/2 [v̄,ū,w]	(8) ȳ,x̄,z̄+1/2 [v,u,w]
			(9) x̄,ȳ,z̄ [u,v,w]	(10) x,y,z̄ [ū,v̄,w]	(11) y,x̄,z̄+1/2 [v̄,u,w]	(12) ȳ,x,z̄+1/2 [v,ū,w]
			(13) x,ȳ,z [u,v̄,w]	(14) x̄,y,z [ū,v,w]	(15) ȳ,x̄,z+1/2 [v̄,ū,w]	(16) y,x,z+1/2 [v,u,w]
16	q	m..	x,y,0 [0,0,w]	x̄,ȳ,0 [0,0,w]	ȳ,x,1/2 [0,0,w]	y,x̄,1/2 [0,0,w]
			x̄,y,0 [0,0,w]	x,ȳ,0 [0,0,w]	y,x,1/2 [0,0,w]	ȳ,x̄,1/2 [0,0,w]
16	p	.m.	1/2,y,z [u,0,0]	1/2,ȳ,z [ū,0,0]	ȳ,1/2,z+1/2 [0,u,0]	y,1/2,z+1/2 [0,ū,0]
			1/2,y,z̄ [ū,0,0]	1/2,ȳ,z̄ [u,0,0]	y,1/2,z̄+1/2 [0,ū,0]	ȳ,1/2,z̄+1/2 [0,u,0]
16	o	.m'.	0,y,z [0,v,w]	0,ȳ,z [0,v̄,w]	ȳ,0,z+1/2 [v̄,0,w]	y,0,z+1/2 [v,0,w]
			0,y,z̄ [0,v̄,w]	0,ȳ,z̄ [0,v,w]	y,0,z̄+1/2 [v̄,0,w]	ȳ,0,z̄+1/2 [v,0,w]
16	n	..2'	x,x,1/4 [ū,u,w]	x̄,x̄,1/4 [u,ū,w]	x̄,x,3/4 [ū,ū,w]	x,x̄,3/4 [u,u,w]
			x̄,x̄,3/4 [ū,u,w]	x,x,3/4 [u,ū,w]	x,x̄,1/4 [ū,ū,w]	x̄,x,1/4 [u,u,w]
8	m	m2m.	x,1/2,0 [0,0,0]	x̄,1/2,0 [0,0,0]	1/2,x,1/2 [0,0,0]	1/2,x̄,1/2 [0,0,0]
8	l	m2'm'.	x,0,1/2 [0,0,w]	x̄,0,1/2 [0,0,w]	0,x,0 [0,0,w]	0,x̄,0 [0,0,w]
8	k	m2m.	x,1/2,1/2 [0,0,0]	x̄,1/2,1/2 [0,0,0]	1/2,x,0 [0,0,0]	1/2,x̄,0 [0,0,0]
8	j	m2'm'.	x,0,0 [0,0,w]	x̄,0,0 [0,0,w]	0,x,1/2 [0,0,w]	0,x̄,1/2 [0,0,w]
8	i	2'm'm.	0,1/2,z [0,v,0]	1/2,0,z+1/2 [v,0,0]	0,1/2,z̄ [0,v̄,0]	1/2,0,z̄+1/2 [v̄,0,0]

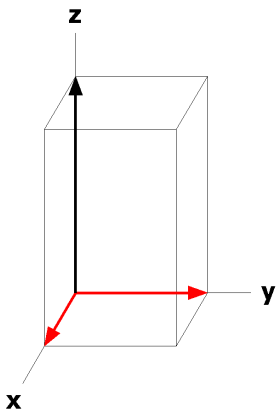
8	h	2mm.	$1/2, 1/2, z [0,0,0]$	$1/2, 1/2, z+1/2 [0,0,0]$	$1/2, 1/2, \bar{z} [0,0,0]$	$1/2, 1/2, \bar{z}+1/2 [0,0,0]$
8	g	2m'm'.	$0,0,z [0,0,w]$	$0,0,z+1/2 [0,0,w]$	$0,0,\bar{z} [0,0,w]$	$0,0,\bar{z}+1/2 [0,0,w]$
4	f	$\bar{4}'m2'$	$1/2, 1/2, 1/4 [0,0,0]$	$1/2, 1/2, 3/4 [0,0,0]$		
4	e	$\bar{4}'m2'$	$0,0,1/4 [0,0,w]$	$0,0,3/4 [0,0,w]$		
4	d	mm'm.	$0,1/2,1/2 [0,0,0]$	$1/2,0,0 [0,0,0]$		
4	c	mm'm.	$0,1/2,0 [0,0,0]$	$1/2,0,1/2 [0,0,0]$		
4	b	mmm.	$1/2,1/2,0 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$		
4	a	mm'm'.	$0,0,0 [0,0,w]$	$0,0,1/2 [0,0,w]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p_{2a} 2mm$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x-1/4, x+1/4, 0$



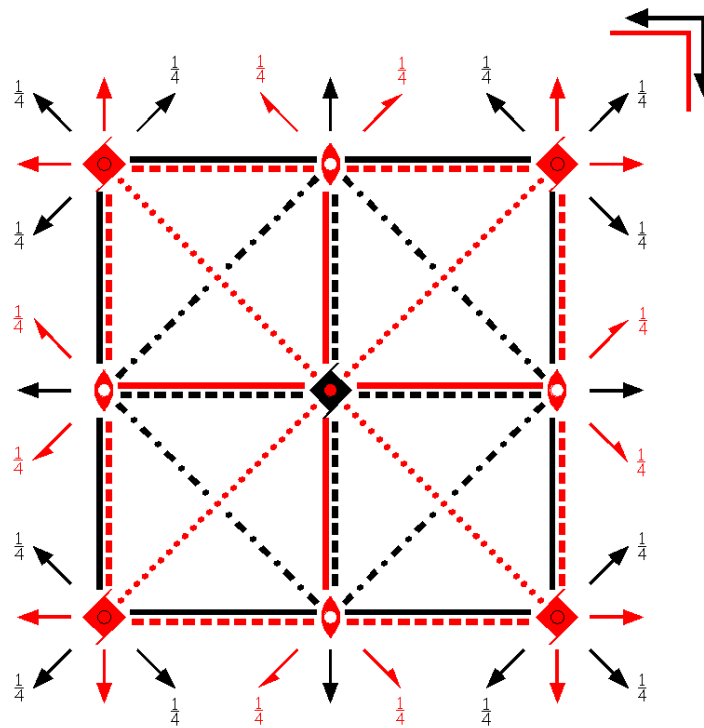
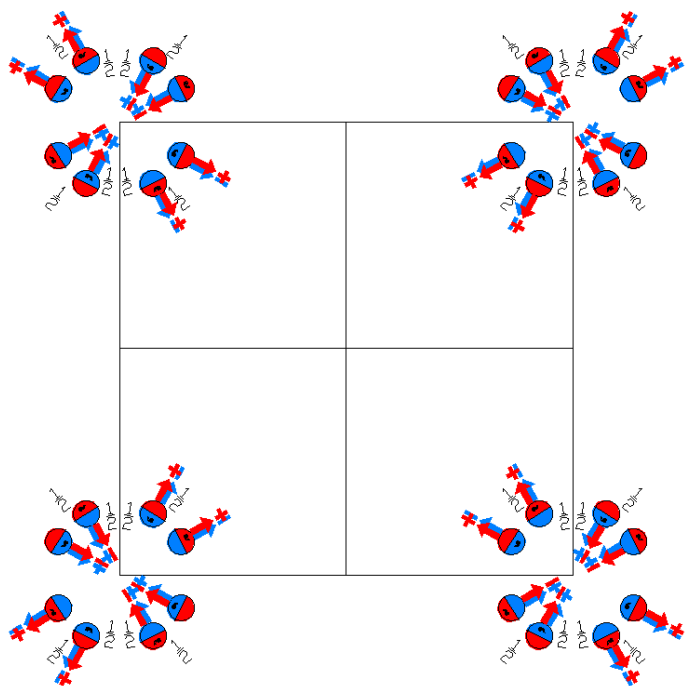
$P_P 4_2'/m'c'$

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$4/mmm1'$

$P_P 4_2'/m'2'/m2/c'$

Tetragonal



Origin at center ( $mmm'$ ) at  $4_2'/m'2'/mc'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

For (0,0,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,1/2)' |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'  | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                                   | (8) 2 x,x̄,1/4<br>(2 <sub>xȳ</sub>  0,0,1/2)                                 |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'              | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) 4 <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>+</sup>  0,0,1/2)  | (12) 4 <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-</sup>  0,0,1/2)  |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)  | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   | (15) c' (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)'                       | (16) c' (0,0,1/2) x,x,z<br>(m <sub>xȳ</sub>  0,0,1/2)'                       |

## For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> (0,0,1/2) 1/2,1/2,z (4 <sub>z</sub>  1,0,1/2)	(4) 4 <sup>-</sup> (0,0,1/2) 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,1/2)
(5) 2 1/2,y,0 (2 <sub>y</sub>  1,0,0)	(6) 2 (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)	(7) 2' (1/2,1/2,0) x+1/2,x,1/4 (2 <sub>xy</sub>  1,0,1/2)'	(8) 2' (1/2,-1/2,0) x+1/2,x̄,1/4 (2 <sub>xy</sub> <sup>-</sup>  1,0,1/2)'
(9) 1̄ 1/2,0,0 (1̄ 1,0,0)	(10) a (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)	(11) 4 <sup>+</sup> 1/2,-1/2,z; 1/2,-1/2,1/4 (4 <sub>z</sub>  1,0,1/2)'	(12) 4 <sup>-</sup> 1/2,1/2,z; 1/2,1/2,1/4 (4 <sub>z</sub> <sup>-1</sup>  1,0,1/2)'
(13) a' (1,0,0) x,0,z (m <sub>y</sub>  1,0,0)'	(14) m' 1/2,y,z (m <sub>x</sub>  1,0,0)'	(15) n (1/2,-1/2,1/2) x+1/2,x̄,z (m <sub>xy</sub>  1,0,1/2)	(16) n (1/2,1/2,1/2) x+1/2,x,z (m <sub>xy</sub> <sup>-</sup>  1,0,1/2)

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1,0,0)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	r	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w]	(3) ȳ,x,z+1/2 [v̄,ū,w̄]	(4) y,x̄,z+1/2 [v̄,ū,w̄]
			(5) x̄,y,z [ū,v̄,w]	(6) x,ȳ,z [u,v̄,w]	(7) y,x,z̄+1/2 [v̄,ū,w̄]	(8) ȳ,x̄,z̄+1/2 [v̄,ū,w̄]
			(9) x̄,ȳ,z [ū,v̄,w̄]	(10) x,y,z̄ [u,v̄,w̄]	(11) y,x̄,z̄+1/2 [v̄,ū,w̄]	(12) ȳ,x,z̄+1/2 [v̄,ū,w̄]
			(13) x,ȳ,z [ū,v̄,w̄]	(14) x̄,y,z [u,v̄,w̄]	(15) ȳ,x̄,z+1/2 [v̄,ū,w̄]	(16) y,x,z+1/2 [v̄,ū,w̄]
16	q	m'..	x,y,0 [u,v,0]	x̄,ȳ,0 [ū,v̄,0]	ȳ,x,1/2 [v̄,ū,0]	y,x̄,1/2 [v̄,ū,0]
			x̄,y,0 [ū,v̄,0]	x,ȳ,0 [u,v̄,0]	y,x,1/2 [v̄,ū,0]	ȳ,x̄,1/2 [v̄,ū,0]
16	p	.m'.	1/2,y,z [0,v,w]	1/2,ȳ,z [0,v̄,w̄]	ȳ,1/2,z+1/2 [v̄,0,w̄]	y,1/2,z+1/2 [v̄,0,w̄]
			1/2,y,z̄ [0,v̄,w̄]	1/2,ȳ,z̄ [0,v̄,w̄]	y,1/2,z̄+1/2 [v̄,0,w̄]	ȳ,1/2,z̄+1/2 [v̄,0,w̄]
16	o	.m.	0,y,z [u,0,0]	0,ȳ,z [ū,0,0]	ȳ,0,z+1/2 [0,ū,0]	y,0,z+1/2 [0,ū,0]
			0,y,z̄ [u,0,0]	0,ȳ,z̄ [ū,0,0]	y,0,z̄+1/2 [0,ū,0]	ȳ,0,z̄+1/2 [0,ū,0]
16	n	..2	x,x,1/4 [u,u,0]	x̄,x̄,1/4 [ū,ū,0]	x̄,x,3/4 [ū,ū,0]	x,x̄,3/4 [ū,ū,0]
			x̄,x̄,3/4 [ū,ū,0]	x,x,3/4 [u,u,0]	x,x̄,1/4 [ū,ū,0]	x̄,x,1/4 [u,ū,0]
8	m	m'2m'.	x,1/2,0 [u,0,0]	x̄,1/2,0 [ū,0,0]	1/2,x,1/2 [0,ū,0]	1/2,x̄,1/2 [0,ū,0]
8	l	m'2'm.	x,0,1/2 [0,v,0]	x̄,0,1/2 [0,v̄,0]	0,x,0 [v̄,0,0]	0,x̄,0 [v̄,0,0]
8	k	m'2m'.	x,1/2,1/2 [u,0,0]	x̄,1/2,1/2 [ū,0,0]	1/2,x,0 [0,ū,0]	1/2,x̄,0 [0,ū,0]
8	j	m'2'm.	x,0,0 [0,v,0]	x̄,0,0 [0,v̄,0]	0,x,1/2 [v̄,0,0]	0,x̄,1/2 [v̄,0,0]
8	i	2'mm'.	0,1/2,z [u,0,0]	1/2,0,z+1/2 [0,ū,0]	0,1/2,z̄ [u,0,0]	1/2,0,z̄+1/2 [0,ū,0]

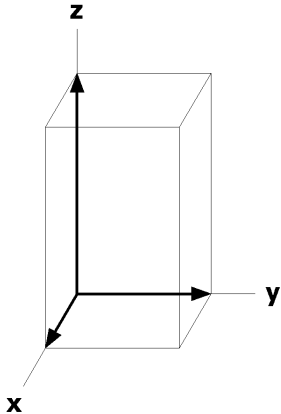
8	h	$2m'm'$	$1/2, 1/2, z [0, 0, w]$	$1/2, 1/2, z+1/2 [0, 0, \bar{w}]$	$1/2, 1/2, \bar{z} [0, 0, \bar{w}]$	$1/2, 1/2, \bar{z}+1/2 [0, 0, w]$
8	g	$2mm'$	$0, 0, z [0, 0, 0]$	$0, 0, z+1/2 [0, 0, 0]$	$0, 0, \bar{z} [0, 0, 0]$	$0, 0, \bar{z}+1/2 [0, 0, 0]$
4	f	$\bar{4}'m'2$	$1/2, 1/2, 1/4 [0, 0, 0]$	$1/2, 1/2, 3/4 [0, 0, 0]$		
4	e	$\bar{4}m'2$	$0, 0, 1/4 [0, 0, 0]$	$0, 0, 3/4 [0, 0, 0]$		
4	d	$m'mm'$	$0, 1/2, 1/2 [0, v, 0]$	$1/2, 0, 0 [v, 0, 0]$		
4	c	$m'mm'$	$0, 1/2, 0 [0, v, 0]$	$1/2, 0, 1/2 [v, 0, 0]$		
4	b	$m'm'm'$	$1/2, 1/2, 0 [0, 0, 0]$	$1/2, 1/2, 1/2 [0, 0, 0]$		
4	a	$m'mm'$	$0, 0, 0 [0, 0, 0]$	$0, 0, 1/2 [0, 0, 0]$		

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p_2$ ,  $4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $1/2, 1/2, z$

Along  $[1, 0, 0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 0, 0$

Along  $[1, 1, 0]$   $p_{2a}$ ,  $2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, x, 0$



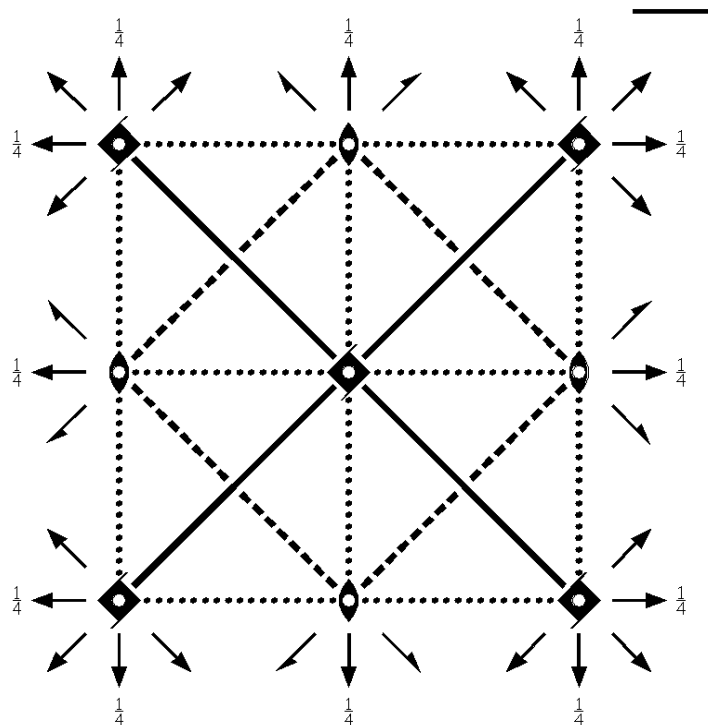
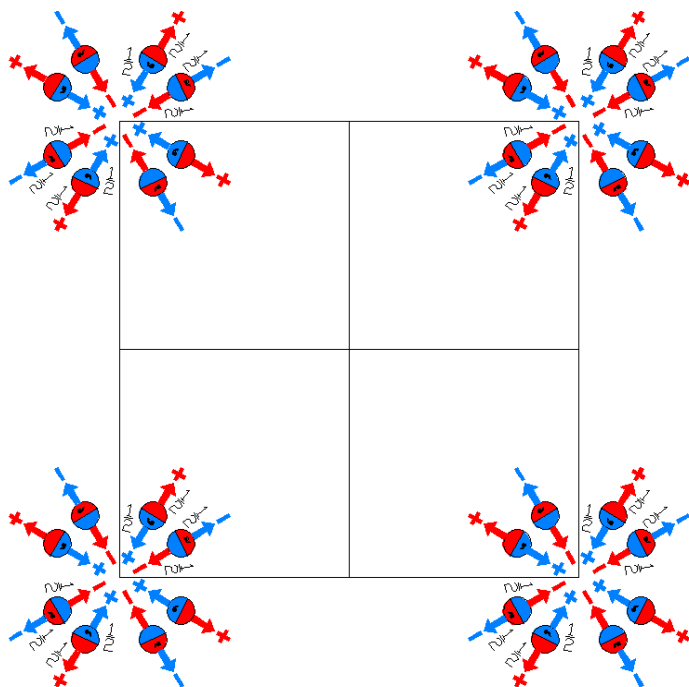
$P4_2/mcm$

132.1.1110

4/mmm

$P4_2/m2/c2/m$

Tetragonal



Origin at center ( mmm ) at  $4_2/mc2/m$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)              | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)          | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)          | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                         | (8) 2 x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)                                     |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)          | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)             | (11) $\bar{4}^+$ 0,0,z; 0,0,1/4<br>( $\bar{4}_z^+$  0,0,1/2)    | (12) $\bar{4}^-$ 0,0,z; 0,0,1/4<br>( $\bar{4}_z^-$  0,0,1/2)                  |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (15) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                       | (16) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                                      |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

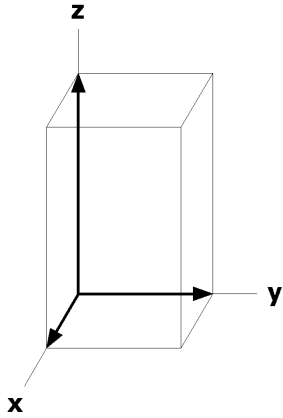
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	p	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(10) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $v,\bar{u},w$ ]
			(13) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(16) $y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	o	..m	$x,x,z$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]	$\bar{x},x,z+1/2$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},z+1/2$ [ $u,u,0$ ]
			$\bar{x},x,\bar{z}+1/2$ [ $u,u,0$ ]	$x,\bar{x},\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]	$x,x,\bar{z}$ [ $u,\bar{u},0$ ]	$\bar{x},\bar{x},\bar{z}$ [ $\bar{u},u,0$ ]
8	n	m..	$x,y,0$ [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,1/2$ [0,0,w]	$y,\bar{x},1/2$ [0,0,w]
			$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	$x,\bar{y},1/2$ [0,0, $\bar{w}$ ]	$y,x,0$ [0,0, $\bar{w}$ ]	$\bar{y},\bar{x},0$ [0,0, $\bar{w}$ ]
8	m	.2.	$x,1/2,1/4$ [u,0,0]	$\bar{x},1/2,1/4$ [ $\bar{u},0,0$ ]	$1/2,x,3/4$ [0,u,0]	$1/2,\bar{x},3/4$ [0, $\bar{u},0$ ]
			$\bar{x},1/2,3/4$ [u,0,0]	$x,1/2,3/4$ [ $\bar{u},0,0$ ]	$1/2,\bar{x},1/4$ [0,u,0]	$1/2,x,1/4$ [0, $\bar{u},0$ ]
8	l	.2.	$x,0,1/4$ [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	$0,x,3/4$ [0,u,0]	$0,\bar{x},3/4$ [0, $\bar{u},0$ ]
			$\bar{x},0,3/4$ [u,0,0]	$x,0,3/4$ [ $\bar{u},0,0$ ]	$0,\bar{x},1/4$ [0,u,0]	$0,x,1/4$ [0, $\bar{u},0$ ]
8	k	2..	$0,1/2,z$ [0,0,w]	$1/2,0,z+1/2$ [0,0,w]	$0,1/2,\bar{z}+1/2$ [0,0, $\bar{w}$ ]	$1/2,0,\bar{z}$ [0,0, $\bar{w}$ ]
			$0,1/2,\bar{z}$ [0,0,w]	$1/2,0,\bar{z}+1/2$ [0,0,w]	$0,1/2,z+1/2$ [0,0, $\bar{w}$ ]	$1/2,0,z$ [0,0, $\bar{w}$ ]
4	j	m.2m	$x,x,1/2$ [0,0,0]	$\bar{x},\bar{x},1/2$ [0,0,0]	$\bar{x},x,0$ [0,0,0]	$x,\bar{x},0$ [0,0,0]
4	i	m.2m	$x,x,0$ [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x},x,1/2$ [0,0,0]	$x,\bar{x},1/2$ [0,0,0]
4	h	2.mm	$1/2,1/2,z$ [0,0,0]	$1/2,1/2,z+1/2$ [0,0,0]	$1/2,1/2,\bar{z}+1/2$ [0,0,0]	$1/2,1/2,\bar{z}$ [0,0,0]
4	g	2.mm	$0,0,z$ [0,0,0]	$0,0,z+1/2$ [0,0,0]	$0,0,\bar{z}+1/2$ [0,0,0]	$0,0,\bar{z}$ [0,0,0]
4	f	2/m..	$0,1/2,0$ [0,0,w]	$1/2,0,1/2$ [0,0,w]	$0,1/2,1/2$ [0,0, $\bar{w}$ ]	$1/2,0,0$ [0,0, $\bar{w}$ ]
4	e	222.	$0,1/2,1/4$ [0,0,0]	$1/2,0,3/4$ [0,0,0]	$0,1/2,3/4$ [0,0,0]	$1/2,0,1/4$ [0,0,0]
2	d	$\bar{4}2m$	$1/2,1/2,1/4$ [0,0,0]	$1/2,1/2,3/4$ [0,0,0]		
2	c	m.mm	$1/2,1/2,0$ [0,0,0]	$1/2,1/2,1/2$ [0,0,0]		
2	b	$\bar{4}2m$	$0,0,1/4$ [0,0,0]	$0,0,3/4$ [0,0,0]		
2	a	m.mm	$0,0,0$ [0,0,0]	$0,0,1/2$ [0,0,0]		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a} 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $x,0,1/4$

Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,x,0$



$P4_2/mcm1'$

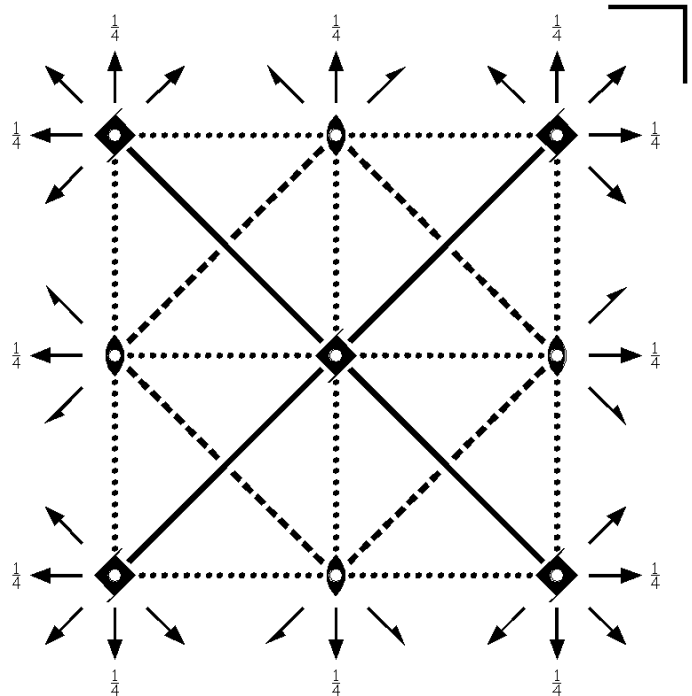
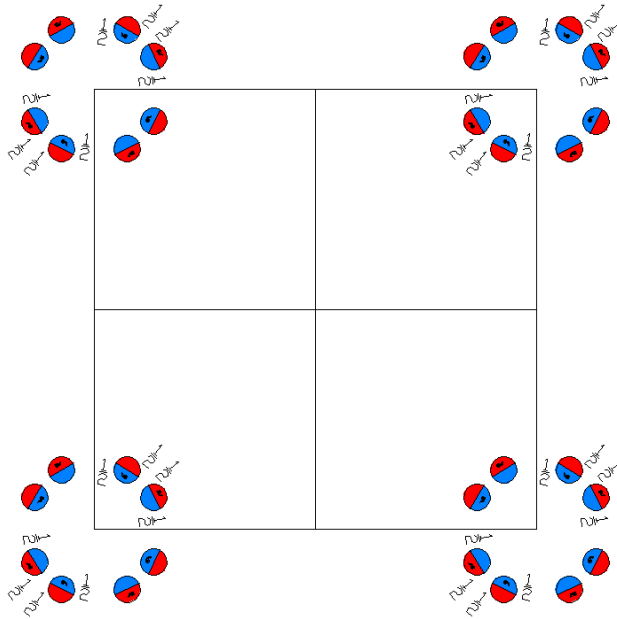
132.2.1111

$4/mmm1'$

$P4_2/m2/c2/m1'$

Tetragonal

1'



Origin at center ( $mmm1'$ ) at  $4_2/mc2/m1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

Symmetry Operations

For 1 + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)              | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)              | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)          | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)          | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                      | (8) 2 x,x̄,0<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,0)                        |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)                          | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)             | (11) 4 <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>+</sup>  0,0,1/2) | (12) 4 <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (15) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                                    | (16) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                                      |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> ' (0,0,1/2) 0,0,z (4 <sub>z</sub>  0,0,1/2)'	(4) 4 <sup>-</sup> ' (0,0,1/2) 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)'
(5) 2' 0,y,1/4 (2 <sub>y</sub>  0,0,1/2)'	(6) 2' x,0,1/4 (2 <sub>x</sub>  0,0,1/2)'	(7) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) 2' x,x̄,0 (2 <sub>xy</sub> <sup>-</sup>  0,0,0)'
(9) 1̄' 0,0,0 (1̄ 0,0,0)'	(10) m' x,y,0 (m <sub>z</sub>  0,0,0)'	(11) 4 <sup>+</sup> ' 0,0,z; 0,0,1/4 (4 <sub>z</sub> <sup>+</sup>  0,0,1/2)'	(12) 4 <sup>-</sup> ' 0,0,z; 0,0,1/4 (4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)'
(13) c' (0,0,1/2) x,0,z (m <sub>y</sub>  0,0,1/2)'	(14) c' (0,0,1/2) 0,y,z (m <sub>x</sub>  0,0,1/2)'	(15) m' x,x̄,z (m <sub>xy</sub>  0,0,0)'	(16) m' x,x,z (m <sub>xy</sub> <sup>-</sup>  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

**Positions**

			Coordinates			
			1 +		1' +	
Multiplicity, Wyckoff letter, Site Symmetry.						
16	p	11'	(1) x,y,z [0,0,0]	(2) x̄,ȳ,z [0,0,0]	(3) ȳ,x,z+1/2 [0,0,0]	(4) y,x̄,z+1/2 [0,0,0]
			(5) x̄,y,z̄+1/2 [0,0,0]	(6) x,ȳ,z̄+1/2 [0,0,0]	(7) y,x,z̄ [0,0,0]	(8) ȳ,x̄,z̄ [0,0,0]
			(9) x̄,ȳ,z̄ [0,0,0]	(10) x,y,z̄ [0,0,0]	(11) y,x̄,z̄+1/2 [0,0,0]	(12) ȳ,x,z̄+1/2 [0,0,0]
			(13) x,ȳ,z+1/2 [0,0,0]	(14) x̄,y,z+1/2 [0,0,0]	(15) ȳ,x̄,z [0,0,0]	(16) y,x,z [0,0,0]
8	o	..m1'	x,x,z [0,0,0]	x̄,x̄,z [0,0,0]	x̄,x,z+1/2 [0,0,0]	x,x̄,z+1/2 [0,0,0]
			x̄,x,z̄+1/2 [0,0,0]	x,x̄,z̄+1/2 [0,0,0]	x,x,z̄ [0,0,0]	x̄,x̄,z̄ [0,0,0]
8	n	m..1'	x,y,0 [0,0,0]	x̄,ȳ,0 [0,0,0]	ȳ,x,1/2 [0,0,0]	y,x̄,1/2 [0,0,0]
			x̄,y,1/2 [0,0,0]	x,ȳ,1/2 [0,0,0]	y,x,0 [0,0,0]	ȳ,x̄,0 [0,0,0]
8	m	.2.1'	x,1/2,1/4 [0,0,0]	x̄,1/2,1/4 [0,0,0]	1/2,x,3/4 [0,0,0]	1/2,x̄,3/4 [0,0,0]
			x̄,1/2,3/4 [0,0,0]	x,1/2,3/4 [0,0,0]	1/2,x̄,1/4 [0,0,0]	1/2,x,1/4 [0,0,0]
8	l	.2.1'	x,0,1/4 [0,0,0]	x̄,0,1/4 [0,0,0]	0,x,3/4 [0,0,0]	0,x̄,3/4 [0,0,0]
			x̄,0,3/4 [0,0,0]	x,0,3/4 [0,0,0]	0,x̄,1/4 [0,0,0]	0,x,1/4 [0,0,0]
8	k	2..1'	0,1/2,z [0,0,0]	1/2,0,z+1/2 [0,0,0]	0,1/2,z̄+1/2 [0,0,0]	1/2,0,z̄ [0,0,0]
			0,1/2,z̄ [0,0,0]	1/2,0,z̄+1/2 [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0,z [0,0,0]
4	j	m.2m1'	x,x,1/2 [0,0,0]	x̄,x̄,1/2 [0,0,0]	x̄,x,0 [0,0,0]	x,x̄,0 [0,0,0]
4	i	m.2m1'	x,x,0 [0,0,0]	x̄,x̄,0 [0,0,0]	x̄,x,1/2 [0,0,0]	x,x̄,1/2 [0,0,0]
4	h	2.mm1'	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2,z̄+1/2 [0,0,0]	1/2,1/2,z̄ [0,0,0]

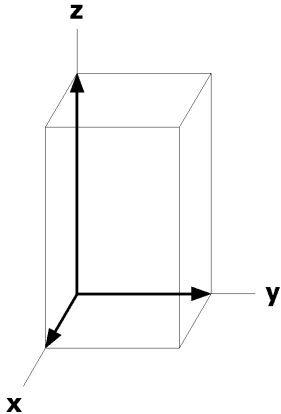
4	g	$2.mm1'$	$0,0,z [0,0,0]$	$0,0,z+1/2 [0,0,0]$	$0,0,\bar{z}+1/2 [0,0,0]$	$0,0,\bar{z} [0,0,0]$
4	f	$2/m..1'$	$0,1/2,0 [0,0,0]$	$1/2,0,1/2 [0,0,0]$	$0,1/2,1/2 [0,0,0]$	$1/2,0,0, [0,0,0]$
4	e	$222.1'$	$0,1/2,1/4 [0,0,0]$	$1/2,0,3/4 [0,0,0]$	$0,1/2,3/4 [0,0,0]$	$1/2,0,1/4 [0,0,0]$
2	d	$\bar{4}2m1'$	$1/2,1/2,1/4 [0,0,0]$	$1/2,1/2,3/4 [0,0,0]$		
2	c	$m.mm1'$	$1/2,1/2,0 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$		
2	b	$\bar{4}2m1'$	$0,0,1/4 [0,0,0]$	$0,0,3/4 [0,0,0]$		
2	a	$m.mm1'$	$0,0,0 [0,0,0]$	$0,0,1/2 [0,0,0]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$



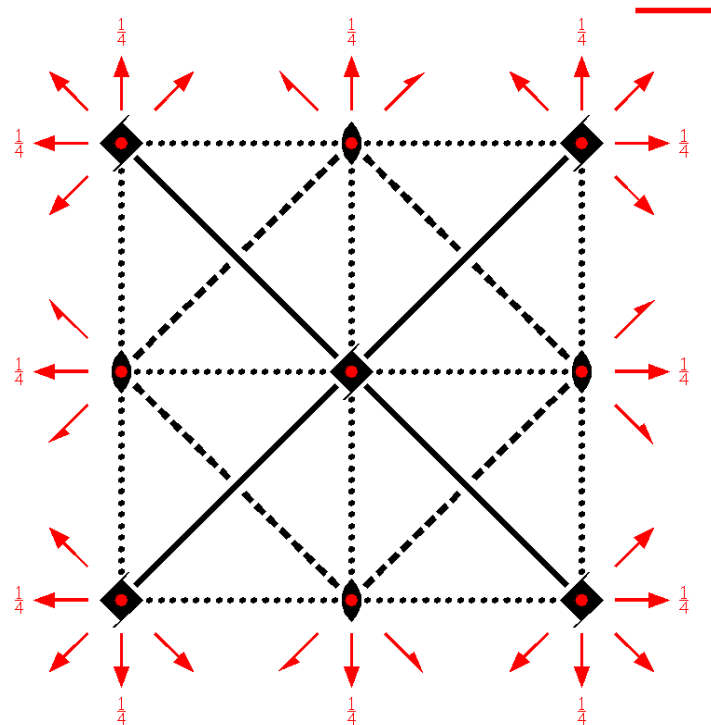
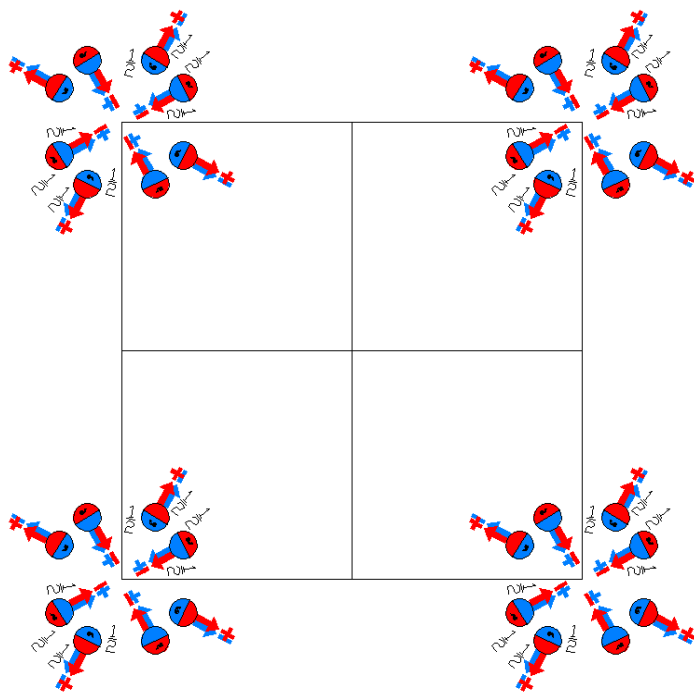
$P4_2/m'cm$

132.3.1112

$4/m'mm$

$P4_2/m'2'/c2'/m$

Tetragonal



Origin at center ( $mmm'$ ) at  $4_2/m'c2'/m$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

### Symmetry Operations

- |   |   |   |  |
|---|---|---|--|
| (1) $1$<br>( $1 0,0,0$ )                        | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )              | (3) $4^+$ $(0,0,1/2) 0,0,z$<br>( $4_z 0,0,1/2$ )              | (4) $4^-$ $(0,0,1/2) 0,0,z$<br>( $4_z^{-1} 0,0,1/2$ )              |
| (5) $2'$ $0,y,1/4$<br>( $2_y 0,0,1/2$ )'        | (6) $2'$ $x,0,1/4$<br>( $2_x 0,0,1/2$ )'        | (7) $2'$ $x,x,0$<br>( $2_{xy} 0,0,0$ )'                       | (8) $2'$ $x,\bar{x},0$<br>( $2_{\bar{xy}} 0,0,0$ )'                |
| (9) $\bar{1}'$ $0,0,0$<br>( $\bar{1} 0,0,0$ )'  | (10) $m'$ $x,y,0$<br>( $m_z 0,0,0$ )'           | (11) $\bar{4}^+$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z 0,0,1/2$ )' | (12) $\bar{4}^-$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z^{-1} 0,0,1/2$ )' |
| (13) $c$ $(0,0,1/2) x,0,z$<br>( $m_y 0,0,1/2$ ) | (14) $c$ $(0,0,1/2) 0,y,z$<br>( $m_x 0,0,1/2$ ) | (15) $m$ $x,\bar{x},z$<br>( $m_{xy} 0,0,0$ )                  | (16) $m$ $x,x,z$<br>( $m_{\bar{xy}} 0,0,0$ )                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
16	p	1	(1) x,y,z [u,v,w] (5) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v}$ ,w] (9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (13) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (6) $x,\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ] (10) $x,y,\bar{z}$ [u,v, $\bar{w}$ ] (14) $\bar{x},y,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ] (7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ] (11) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ] (15) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [v, $\bar{u},w$ ] (8) $\bar{y},\bar{x},\bar{z}$ [v,u,w] (12) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ] (16) $y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	o	..m	x,x,z [ $\bar{u},u,0$ ] $\bar{x},x,\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},\bar{x},z$ [u, $\bar{u},0$ ] $x,\bar{x},\bar{z}+1/2$ [u,u,0]	$\bar{x},x,z+1/2$ [ $\bar{u},\bar{u},0$ ] $x,x,\bar{z}$ [ $\bar{u},u,0$ ]	$x,\bar{x},z+1/2$ [u,u,0] $\bar{x},\bar{x},\bar{z}$ [u, $\bar{u},0$ ]
8	n	m'..	x,y,0 [u,v,0] $\bar{x},y,1/2$ [u, $\bar{v},0$ ]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ] $x,\bar{y},1/2$ [ $\bar{u},v,0$ ]	$\bar{y},x,1/2$ [ $\bar{v},u,0$ ] $y,x,0$ [ $\bar{v},\bar{u},0$ ]	$y,\bar{x},1/2$ [v, $\bar{u},0$ ] $\bar{y},\bar{x},0$ [v,u,0]
8	m	.2'.	x,1/2,1/4 [0,v,w] $\bar{x},1/2,3/4$ [0, $\bar{v},w$ ]	$\bar{x},1/2,1/4$ [0, $\bar{v},w$ ] $x,1/2,3/4$ [0,v,w]	1/2,x,3/4 [ $\bar{v},0,w$ ] 1/2, $\bar{x},1/4$ [ $\bar{v},0,w$ ]	1/2, $\bar{x},3/4$ [v,0,w] 1/2,x,1/4 [v,0,w]
8	l	.2'.	x,0,1/4 [0,v,w] $\bar{x},0,3/4$ [0, $\bar{v},w$ ]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ] $x,0,3/4$ [0,v,w]	0,x,3/4 [ $\bar{v},0,w$ ] 0, $\bar{x},1/4$ [ $\bar{v},0,w$ ]	0, $\bar{x},3/4$ [v,0,w] 0,x,1/4 [v,0,w]
8	k	2..	0,1/2,z [0,0,w] 0,1/2, $\bar{z}$ [0,0,w]	1/2,0,z+1/2 [0,0,w] 1/2,0, $\bar{z}+1/2$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w] 0,1/2,z+1/2 [0,0,w]	1/2,0, $\bar{z}$ [0,0,w] 1/2,0,z [0,0,w]
4	j	m'.2'm	x,x,1/2 [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},1/2$ [u, $\bar{u},0$ ]	$\bar{x},x,0$ [u, $\bar{u},0$ ]	$x,\bar{x},0$ [u,u,0]
4	i	m'.2'm	x,x,0 [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},0$ [u, $\bar{u},0$ ]	$\bar{x},x,1/2$ [u, $\bar{u},0$ ]	$x,\bar{x},1/2$ [u,u,0]
4	h	2.mm	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]
4	g	2.mm	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	f	2/m'..	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]
4	e	22'2'.	0,1/2,1/4 [0,0,w]	1/2,0,3/4 [0,0,w]	0,1/2,3/4 [0,0,w]	1/2,0,1/4 [0,0,w]
2	d	$\bar{4}$ '2'm	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	c	m'.mm	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	b	$\bar{4}$ '2'm	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	a	m'.mm	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

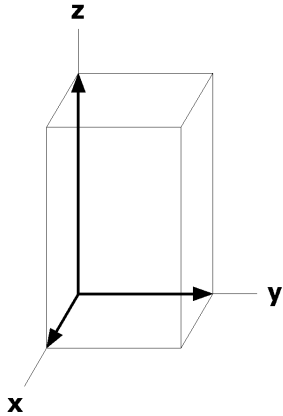
**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a'} 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$





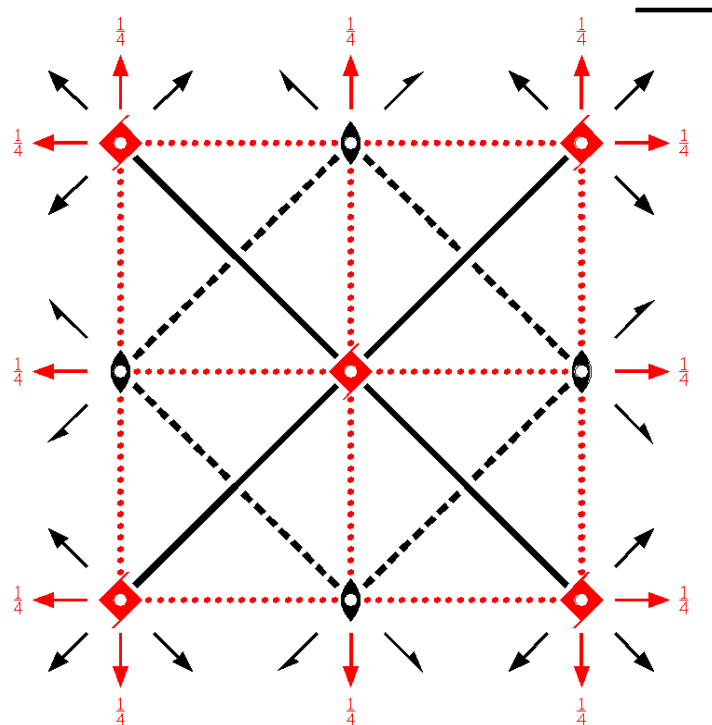
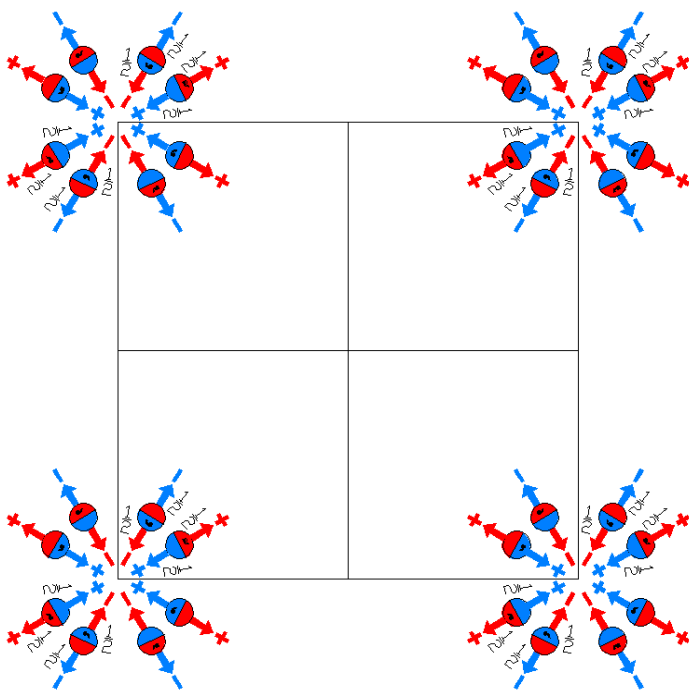
$P4_2'/mc'm$

132.4.1113

$4'/mm'm$

$P4_2'/m2'/c'2/m$

Tetragonal



Origin at center ( mmm ) at  $4_2'/mc'2/m$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                    | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'          | (6) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'          | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                          | (8) 2 x,x̄,0<br>(2 <sub>xy</sub>  0,0,0)                                       |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)                            | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)               | (11) 4 <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub>  0,0,1/2)' | (12) 4 <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (13) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (14) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' | (15) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                        | (16) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

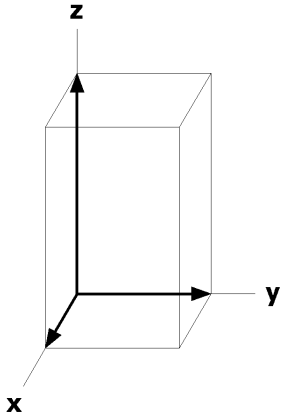
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
16	p	1	(1) x,y,z [u,v,w] (5) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v}$ ,w] (9) $\bar{x},\bar{y},\bar{z}$ [u,v,w] (13) x, $\bar{y},z+1/2$ [u, $\bar{v}$ ,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v}$ ,w] (6) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},v$ ,w] (10) x,y, $\bar{z}$ [ $\bar{u},\bar{v}$ ,w] (14) $\bar{x},y,z+1/2$ [ $\bar{u},v$ ,w]	(3) $\bar{y},x,z+1/2$ [v, $\bar{u},\bar{w}$ ] (7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ] (11) y, $\bar{x},\bar{z}+1/2$ [v, $\bar{u},\bar{w}$ ] (15) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ]	(4) y, $\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ] (8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ] (12) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ] (16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
8	o	..m	x,x,z [ $\bar{u},u,0$ ] $\bar{x},x,\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},\bar{x},z$ [u, $\bar{u},0$ ] x, $\bar{x},\bar{z}+1/2$ [u,u,0]	$\bar{x},x,z+1/2$ [u,u,0] x,x, $\bar{z}$ [u, $\bar{u},0$ ]	x, $\bar{x},z+1/2$ [ $\bar{u},\bar{u},0$ ] $\bar{x},\bar{x},\bar{z}$ [ $\bar{u},u,0$ ]
8	n	m..	x,y,0 [0,0,w] $\bar{x},y,1/2$ [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w] x, $\bar{y},1/2$ [0,0,w]	$\bar{y},x,1/2$ [0,0, $\bar{w}$ ] y,x,0 [0,0, $\bar{w}$ ]	y, $\bar{x},1/2$ [0,0, $\bar{w}$ ] $\bar{y},\bar{x},0$ [0,0, $\bar{w}$ ]
8	m	.2'	x,1/2,1/4 [0,v,w] $\bar{x},1/2,3/4$ [0, $\bar{v}$ ,w]	$\bar{x},1/2,1/4$ [0, $\bar{v}$ ,w] x,1/2,3/4 [0,v,w]	1/2,x,3/4 [v,0, $\bar{w}$ ] 1/2, $\bar{x},1/4$ [v,0, $\bar{w}$ ]	1/2, $\bar{x},3/4$ [ $\bar{v},0,\bar{w}$ ] 1/2,x,1/4 [ $\bar{v},0,\bar{w}$ ]
8	l	.2'	x,0,1/4 [0,v,w] $\bar{x},0,3/4$ [0, $\bar{v}$ ,w]	$\bar{x},0,1/4$ [0, $\bar{v}$ ,w] x,0,3/4 [0,v,w]	0,x,3/4 [v,0, $\bar{w}$ ] 0, $\bar{x},1/4$ [v,0, $\bar{w}$ ]	0, $\bar{x},3/4$ [ $\bar{v},0,\bar{w}$ ] 0,x,1/4 [ $\bar{v},0,\bar{w}$ ]
8	k	2..	0,1/2,z [0,0,w] 0,1/2, $\bar{z}$ [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ] 1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0,w] 0,1/2,z+1/2 [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ] 1/2,0,z [0,0, $\bar{w}$ ]
4	j	m.2m	x,x,1/2 [0,0,0]	$\bar{x},\bar{x},1/2$ [0,0,0]	$\bar{x},x,0$ [0,0,0]	x, $\bar{x},0$ [0,0,0]
4	i	m.2m	x,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x},x,1/2$ [0,0,0]	x, $\bar{x},1/2$ [0,0,0]
4	h	2.mm	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]
4	g	2.mm	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	f	2/m..	0,1/2,0 [0,0,w]	1/2,0,1/2 [0,0, $\bar{w}$ ]	0,1/2,1/2 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]
4	e	22'2'	0,1/2,1/4 [0,0,w]	1/2,0,3/4 [0,0, $\bar{w}$ ]	0,1/2,3/4 [0,0,w]	1/2,0,1/4 [0,0, $\bar{w}$ ]
2	d	$\bar{4}'2'm$	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	c	m.mm	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	b	$\bar{4}'2'm$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	a	m.mm	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $x,0,0$

Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,x,0$



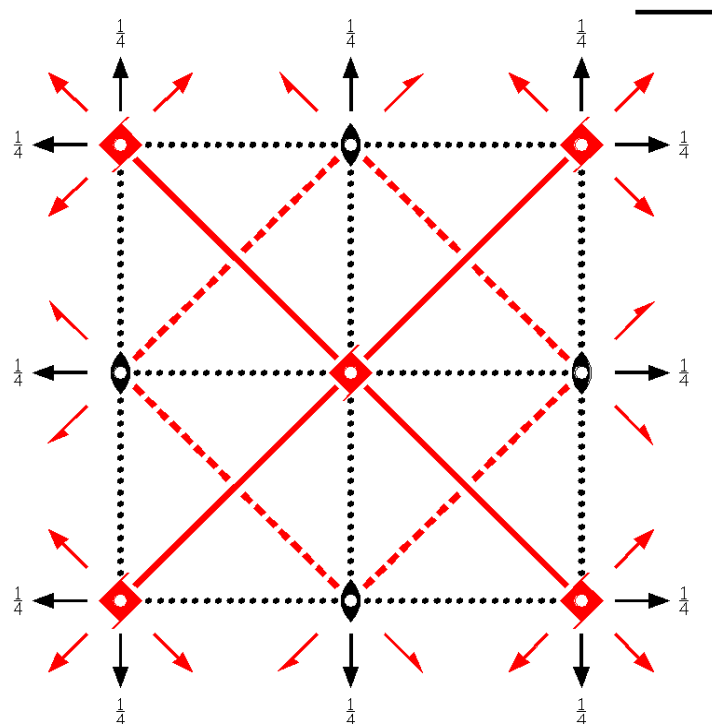
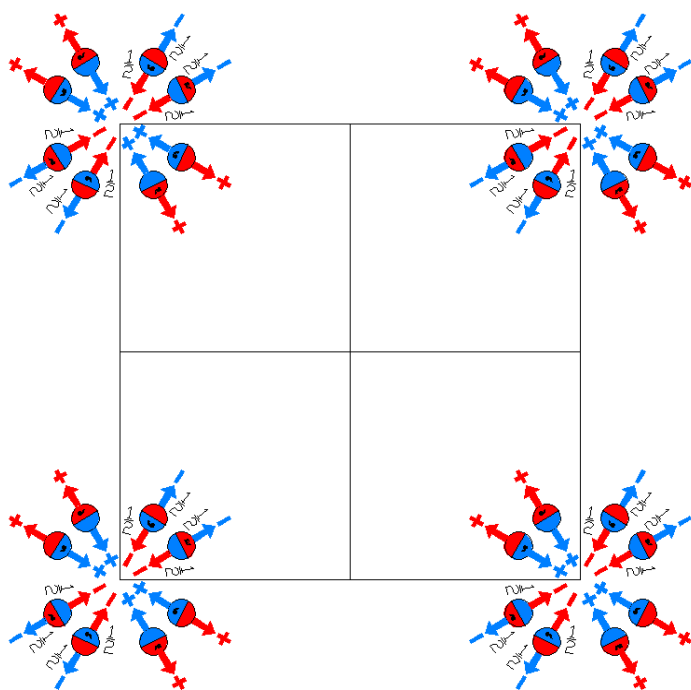
$P4_2'/mcm'$

132.5.1114

$4'/mmm'$

$P4_2'/m2/c2'/m'$

Tetragonal



Origin at center ( $m'm'm$ ) at  $4_2'/mc2'/m'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)              | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)          | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)          | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                        | (8) 2' x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)'                                    |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)                          | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)             | (11) 4 <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub>  0,0,1/2)' | (12) 4 <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (15) m' x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'                      | (16) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

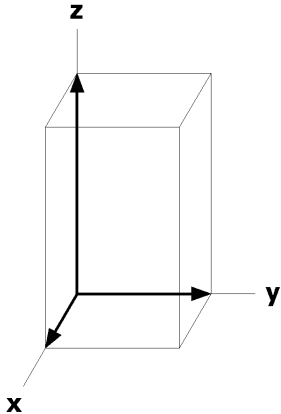
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	p	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},w$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(10) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(13) $x,\bar{y},z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x,z$ [ $\bar{v},\bar{u},w$ ]
8	o	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,z+1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]	$x,\bar{x},z+1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x},x,\bar{z}+1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]	$x,\bar{x},\bar{z}+1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]	$x,x,\bar{z}$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},\bar{z}$ [ $\bar{u},\bar{u},w$ ]
8	n	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,1/2$ [0,0, $\bar{w}$ ]	$y,\bar{x},1/2$ [0,0, $\bar{w}$ ]
			$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	$x,\bar{y},1/2$ [0,0, $\bar{w}$ ]	y,x,0 [0,0,w]	$\bar{y},\bar{x},0$ [0,0,w]
8	m	.2.	x,1/2,1/4 [u,0,0]	$\bar{x},1/2,1/4$ [ $\bar{u},0,0$ ]	1/2,x,3/4 [0, $\bar{u},0$ ]	1/2, $\bar{x},3/4$ [0,u,0]
			$\bar{x},1/2,3/4$ [ $\bar{u},0,0$ ]	x,1/2,3/4 [u,0,0]	1/2, $\bar{x},1/4$ [0, $\bar{u},0$ ]	1/2,x,1/4 [0,u,0]
8	l	.2.	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	0,x,3/4 [0, $\bar{u},0$ ]	0, $\bar{x},3/4$ [0,u,0]
			$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [u,0,0]	0, $\bar{x},1/4$ [0, $\bar{u},0$ ]	0,x,1/4 [0,u,0]
8	k	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]
			0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0,z [0,0,w]
4	j	m.2'm'	x,x,1/2 [0,0,w]	$\bar{x},\bar{x},1/2$ [0,0,w]	$\bar{x},x,0$ [0,0, $\bar{w}$ ]	$x,\bar{x},0$ [0,0, $\bar{w}$ ]
4	i	m.2'm'	x,x,0 [0,0,w]	$\bar{x},\bar{x},0$ [0,0,w]	$\bar{x},x,1/2$ [0,0, $\bar{w}$ ]	$x,\bar{x},1/2$ [0,0, $\bar{w}$ ]
4	h	2.m'm'	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0,w]
4	g	2.m'm'	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]
4	f	2/m..	0,1/2,0 [0,0,w]	1/2,0,1/2 [0,0, $\bar{w}$ ]	0,1/2,1/2 [0,0, $\bar{w}$ ]	1/2,0,0, [0,0,w]
4	e	222.	0,1/2,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]
2	d	$\bar{4}$ '2m'	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
2	c	m.m'm'	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]		
2	b	$\bar{4}$ '2m'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	a	m.m'm'	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a} 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $x,0,1/4$

Along  $[1,1,0]$   $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,0$



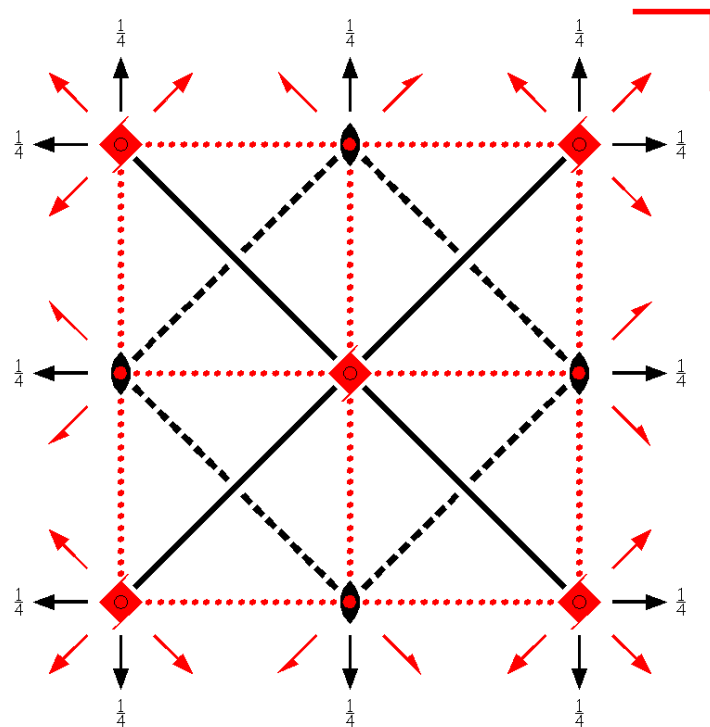
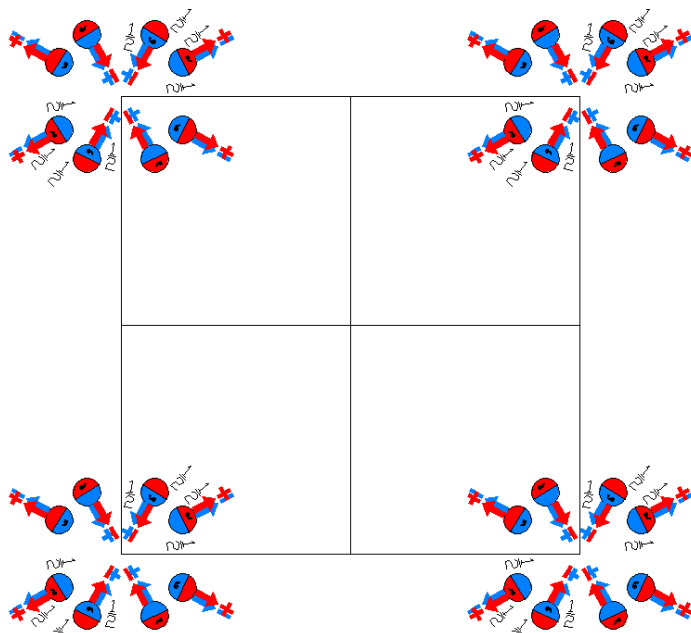
$P4_2/m'c'm$

132.6.1115

$4'/m'm'm$

$P4_2'/m'2/c'2'/m$

Tetragonal



Origin at center ( $mmm'$ ) at  $4_2'/m'c'2'/m$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                    | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)'             | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)            | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)            | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                                    | (8) 2' x,x̄,0<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,0)'                       |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'                           | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'             | (11) 4 <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>+</sup>  0,0,1/2) | (12) 4 <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)  |
| (13) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (14) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' | (15) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                                    | (16) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	p	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},w$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(13) $x,\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},\bar{v},w$ ]	(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(16) $y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	o	..m	$x,x,z$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]	$\bar{x},x,z+1/2$ [ $u,u,0$ ]	$x,\bar{x},z+1/2$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},x,\bar{z}+1/2$ [ $u,u,0$ ]	$x,\bar{x},\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]	$x,x,\bar{z}$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},\bar{z}$ [ $u,\bar{u},0$ ]
8	n	m'..	$x,y,0$ [ $u,v,0$ ]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},\bar{u},0$ ]	$y,\bar{x},1/2$ [ $\bar{v},\bar{u},0$ ]
			$\bar{x},y,1/2$ [ $\bar{u},\bar{v},0$ ]	$x,\bar{y},1/2$ [ $u,\bar{v},0$ ]	$y,x,0$ [ $\bar{v},\bar{u},0$ ]	$\bar{y},\bar{x},0$ [ $\bar{v},\bar{u},0$ ]
8	m	.2.	$x,1/2,1/4$ [ $u,0,0$ ]	$\bar{x},1/2,1/4$ [ $\bar{u},0,0$ ]	$1/2,x,3/4$ [ $0,\bar{u},0$ ]	$1/2,\bar{x},3/4$ [ $0,u,0$ ]
			$\bar{x},1/2,3/4$ [ $\bar{u},0,0$ ]	$x,1/2,3/4$ [ $u,0,0$ ]	$1/2,\bar{x},1/4$ [ $0,\bar{u},0$ ]	$1/2,x,1/4$ [ $0,u,0$ ]
8	l	.2.	$x,0,1/4$ [ $u,0,0$ ]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	$0,x,3/4$ [ $0,\bar{u},0$ ]	$0,\bar{x},3/4$ [ $0,u,0$ ]
			$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	$x,0,3/4$ [ $u,0,0$ ]	$0,\bar{x},1/4$ [ $0,\bar{u},0$ ]	$0,x,1/4$ [ $0,u,0$ ]
8	k	2..	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,z+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}$ [ $0,0,w$ ]
			$0,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}+1/2$ [ $0,0,w$ ]	$0,1/2,z+1/2$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,\bar{w}$ ]
4	j	m'.2'm	$x,x,1/2$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},1/2$ [ $u,\bar{u},0$ ]	$\bar{x},x,0$ [ $u,u,0$ ]	$x,\bar{x},0$ [ $\bar{u},\bar{u},0$ ]
4	i	m'.2'm	$x,x,0$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},0$ [ $u,\bar{u},0$ ]	$\bar{x},x,1/2$ [ $u,u,0$ ]	$x,\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]
4	h	2.mm	$1/2,1/2,z$ [ $0,0,0$ ]	$1/2,1/2,z+1/2$ [ $0,0,0$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,0$ ]	$1/2,1/2,\bar{z}$ [ $0,0,0$ ]
4	g	2.mm	$0,0,z$ [ $0,0,0$ ]	$0,0,z+1/2$ [ $0,0,0$ ]	$0,0,\bar{z}+1/2$ [ $0,0,0$ ]	$0,0,\bar{z}$ [ $0,0,0$ ]
4	f	2/m'..	$0,1/2,0$ [ $0,0,0$ ]	$1/2,0,1/2$ [ $0,0,0$ ]	$0,1/2,1/2$ [ $0,0,0$ ]	$1/2,0,0$ [ $0,0,0$ ]
4	e	222.	$0,1/2,1/4$ [ $0,0,0$ ]	$1/2,0,3/4$ [ $0,0,0$ ]	$0,1/2,3/4$ [ $0,0,0$ ]	$1/2,0,1/4$ [ $0,0,0$ ]
2	d	$\bar{4}2m$	$1/2,1/2,1/4$ [ $0,0,0$ ]	$1/2,1/2,3/4$ [ $0,0,0$ ]		
2	c	m'.mm	$1/2,1/2,0$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]		
2	b	$\bar{4}2m$	$0,0,1/4$ [ $0,0,0$ ]	$0,0,3/4$ [ $0,0,0$ ]		
2	a	m'.mm	$0,0,0$ [ $0,0,0$ ]	$0,0,1/2$ [ $0,0,0$ ]		

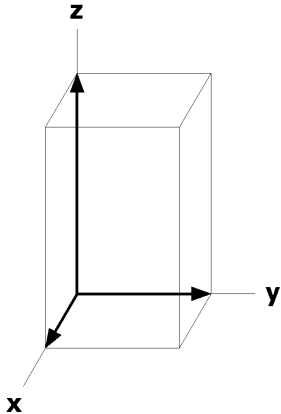


**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4'm'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at  $x,0,1/4$

Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,x,0$



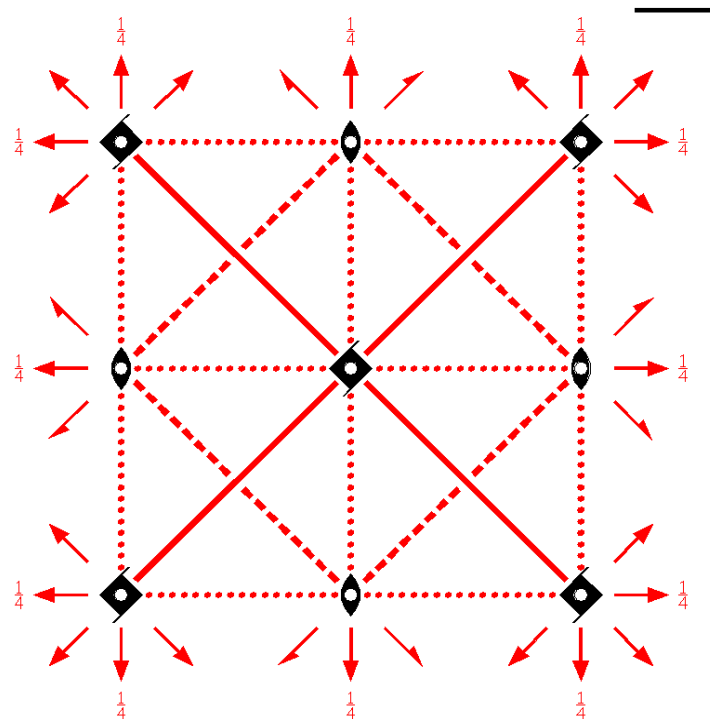
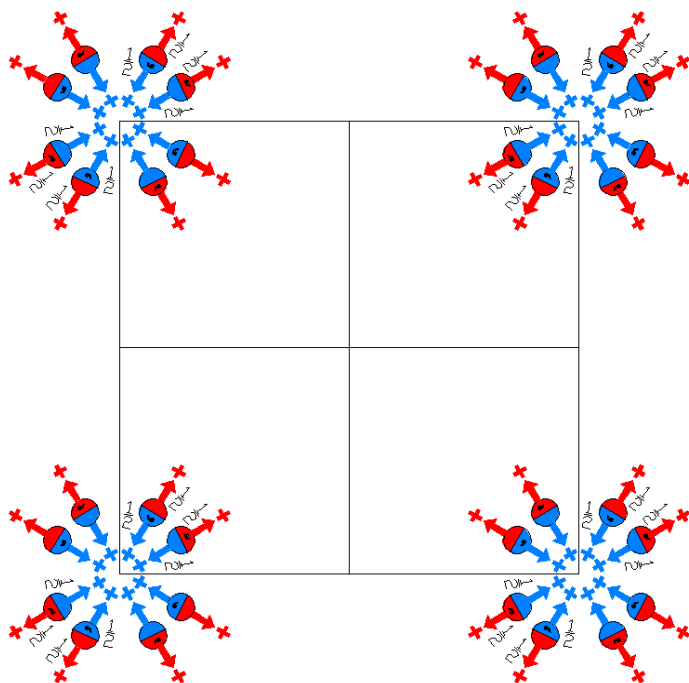
$P4_2/mc'm'$

132.7.1116

$4/mm'm'$

$P4_2/m2'/c'2'/m'$

Tetragonal



Origin at center ( $m'm'm'$ ) at  $4_2/mc'2'/m'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)       | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (5) 2' <sub>y</sub> 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)' | (6) 2' <sub>x</sub> x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)' | (7) 2' <sub>xy</sub> x,x,0<br>(2 <sub>xy</sub>  0,0,0)'         | (8) 2' <sub>xy</sub> x,x̄,0<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,0)'        |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)                | (10) m <sub>z</sub> x,y,0<br>(m <sub>z</sub>  0,0,0)      | (11) $\bar{4}^+$ 0,0,z; 0,0,1/4<br>( $\bar{4}_z^+$  0,0,1/2)    | (12) $\bar{4}^-$ 0,0,z; 0,0,1/4<br>( $\bar{4}_z^-$ <sup>-1</sup>  0,0,1/2)    |
| (13) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)'     | (14) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)'     | (15) m' <sub>xy</sub> x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'       | (16) m' <sub>xy</sub> x,x,z<br>(m <sub>xy</sub> <sup>-1</sup>  0,0,0)'        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

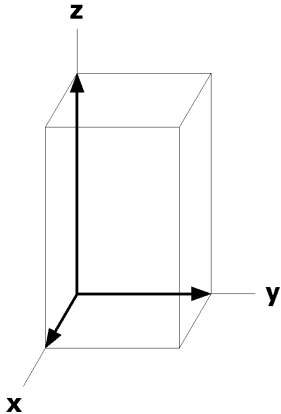
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	p	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(10) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $v,\bar{u},w$ ]
			(13) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]	(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x,z$ [ $v,u,w$ ]
8	o	..m'	$x,x,z$ [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,z+1/2$ [ $\bar{u},u,w$ ]	$x,\bar{x},z+1/2$ [ $u,\bar{u},w$ ]
			$\bar{x},x,\bar{z}+1/2$ [ $u,\bar{u},w$ ]	$x,\bar{x},\bar{z}+1/2$ [ $\bar{u},u,w$ ]	$x,x,\bar{z}$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},\bar{z}$ [ $u,u,w$ ]
8	n	m..	$x,y,0$ [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,1/2$ [0,0,w]	$y,\bar{x},1/2$ [0,0,w]
			$\bar{x},y,1/2$ [0,0,w]	$x,\bar{y},1/2$ [0,0,w]	$y,x,0$ [0,0,w]	$\bar{y},\bar{x},0$ [0,0,w]
8	m	.2'	$x,1/2,1/4$ [0,v,w]	$\bar{x},1/2,1/4$ [0, $\bar{v},w$ ]	$1/2,x,3/4$ [ $\bar{v},0,w$ ]	$1/2,\bar{x},3/4$ [ $v,0,w$ ]
			$\bar{x},1/2,3/4$ [0, $\bar{v},w$ ]	$x,1/2,3/4$ [0,v,w]	$1/2,\bar{x},1/4$ [ $\bar{v},0,w$ ]	$1/2,x,1/4$ [ $v,0,w$ ]
8	l	.2'	$x,0,1/4$ [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	$0,x,3/4$ [ $\bar{v},0,w$ ]	$0,\bar{x},3/4$ [ $v,0,w$ ]
			$\bar{x},0,3/4$ [0, $\bar{v},w$ ]	$x,0,3/4$ [0,v,w]	$0,\bar{x},1/4$ [ $\bar{v},0,w$ ]	$0,x,1/4$ [ $v,0,w$ ]
8	k	2..	$0,1/2,z$ [0,0,w]	$1/2,0,z+1/2$ [0,0,w]	$0,1/2,\bar{z}+1/2$ [0,0,w]	$1/2,0,\bar{z}$ [0,0,w]
			$0,1/2,\bar{z}$ [0,0,w]	$1/2,0,\bar{z}+1/2$ [0,0,w]	$0,1/2,z+1/2$ [0,0,w]	$1/2,0,z$ [0,0,w]
4	j	m.2'm'	$x,x,1/2$ [0,0,w]	$\bar{x},\bar{x},1/2$ [0,0,w]	$\bar{x},x,0$ [0,0,w]	$x,\bar{x},0$ [0,0,w]
4	i	m.2'm'	$x,x,0$ [0,0,w]	$\bar{x},\bar{x},0$ [0,0,w]	$\bar{x},x,1/2$ [0,0,w]	$x,\bar{x},1/2$ [0,0,w]
4	h	2.m'm'	$1/2,1/2,z$ [0,0,w]	$1/2,1/2,z+1/2$ [0,0,w]	$1/2,1/2,\bar{z}+1/2$ [0,0,w]	$1/2,1/2,\bar{z}$ [0,0,w]
4	g	2.m'm'	$0,0,z$ [0,0,w]	$0,0,z+1/2$ [0,0,w]	$0,0,\bar{z}+1/2$ [0,0,w]	$0,0,\bar{z}$ [0,0,w]
4	f	2/m..	$0,1/2,0$ [0,0,w]	$1/2,0,1/2$ [0,0,w]	$0,1/2,1/2$ [0,0,w]	$1/2,0,0$ [0,0,w]
4	e	22'2'.	$0,1/2,1/4$ [0,0,w]	$1/2,0,3/4$ [0,0,w]	$0,1/2,3/4$ [0,0,w]	$1/2,0,1/4$ [0,0,w]
2	d	$\bar{4}2'm'$	$1/2,1/2,1/4$ [0,0,w]	$1/2,1/2,3/4$ [0,0,w]		
2	c	m.m'm'	$1/2,1/2,0$ [0,0,w]	$1/2,1/2,1/2$ [0,0,w]		
2	b	$\bar{4}2'm'$	$0,0,1/4$ [0,0,w]	$0,0,3/4$ [0,0,w]		
2	a	m.m'm'	$0,0,0$ [0,0,w]	$0,0,1/2$ [0,0,w]		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $x,0,0$

Along  $[1,1,0]$   $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at  $x,x,0$



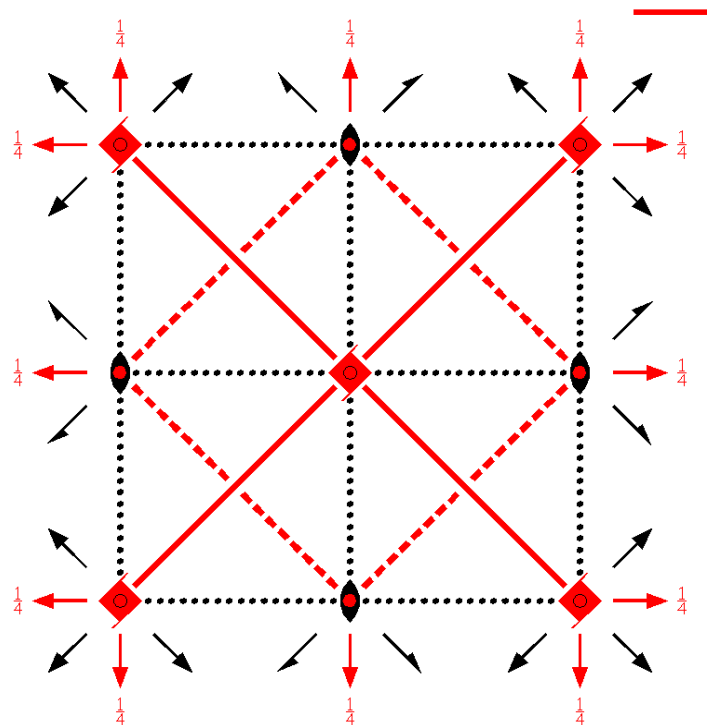
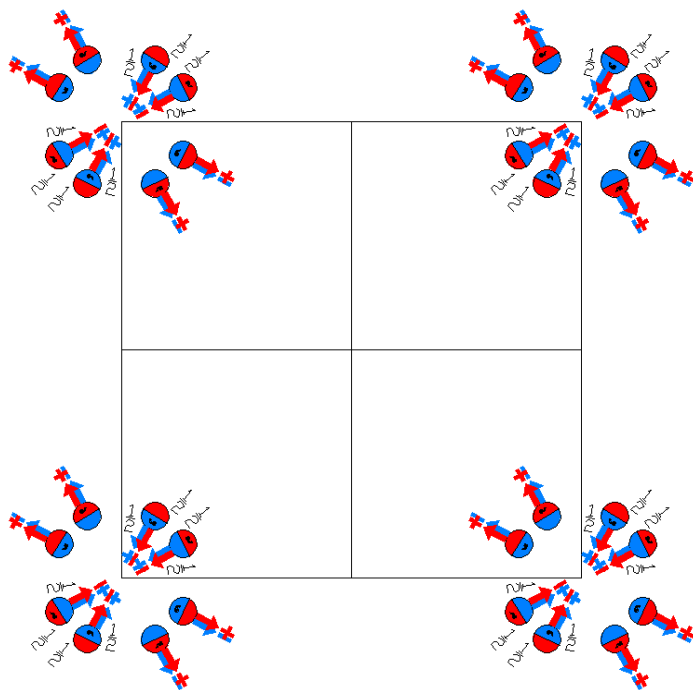
$P4_2/m'cm'$

132.8.1117

$4'/m'mm'$

$P4_2'/m'2'/c2/m'$

Tetragonal



Origin at center (  $m'm'm'$  ) at  $4_2'/m'c2/m'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

**Symmetry Operations**

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)              | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'        | (6) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'        | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                          | (8) 2 x,x̄,0<br>(2 <sub>xy</sub>  0,0,0)                                       |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'                         | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'           | (11) 4 <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub>  0,0,1/2)  | (12) 4 <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)  |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (15) m' x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'                      | (16) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

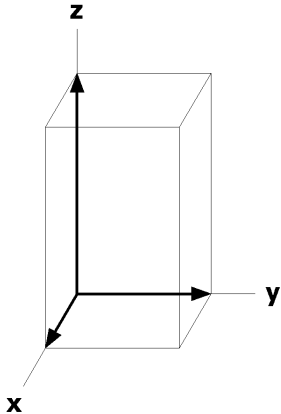
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	p	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(13) $x,\bar{y},z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(16) $y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	o	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,z+1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]	$x,\bar{x},z+1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x},x,\bar{z}+1/2$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x},\bar{z}+1/2$ [ $\bar{u},\bar{u},w$ ]	$x,x,\bar{z}$ [ $\bar{u},\bar{u},\bar{w}$ ]	$\bar{x},\bar{x},\bar{z}$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	n	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},\bar{u},0$ ]	$y,\bar{x},1/2$ [ $\bar{v},\bar{u},0$ ]
			$\bar{x},y,1/2$ [ $\bar{u},\bar{v},0$ ]	$x,\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	y,x,0 [v,u,0]	$\bar{y},\bar{x},0$ [ $\bar{v},\bar{u},0$ ]
8	m	.2'	x,1/2,1/4 [0,v,w]	$\bar{x},1/2,1/4$ [ $0,\bar{v},w$ ]	1/2,x,3/4 [v,0, $\bar{w}$ ]	1/2, $\bar{x},3/4$ [ $\bar{v},0,\bar{w}$ ]
			$\bar{x},1/2,3/4$ [ $0,\bar{v},w$ ]	x,1/2,3/4 [0,v,w]	1/2, $\bar{x},1/4$ [v,0, $\bar{w}$ ]	1/2,x,1/4 [ $\bar{v},0,\bar{w}$ ]
8	l	.2'	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [ $0,\bar{v},w$ ]	0,x,3/4 [v,0, $\bar{w}$ ]	0, $\bar{x},3/4$ [ $\bar{v},0,\bar{w}$ ]
			$\bar{x},0,3/4$ [ $0,\bar{v},w$ ]	x,0,3/4 [0,v,w]	0, $\bar{x},1/4$ [v,0, $\bar{w}$ ]	0,x,1/4 [ $\bar{v},0,\bar{w}$ ]
8	k	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
			0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0,z [0,0,w]
4	j	m'.2m'	x,x,1/2 [u,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [u, $\bar{u},0$ ]	$x,\bar{x},0$ [ $\bar{u},\bar{u},0$ ]
4	i	m'.2m'	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/2$ [u, $\bar{u},0$ ]	$x,\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]
4	h	2.m'm'	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]
4	g	2.m'm'	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4	f	2/m'..	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,0 [0,0,0]
4	e	22'2'	0,1/2,1/4 [0,0,w]	1/2,0,3/4 [0,0, $\bar{w}$ ]	0,1/2,3/4 [0,0, $\bar{w}$ ]	1/2,0,1/4 [0,0,w]
2	d	$\bar{4}2$ 'm'	1/2,1/2,1/4 [0,0,w]	1/2,1/2,3/4 [0,0, $\bar{w}$ ]		
2	c	m'.m'm'	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
2	b	$\bar{4}2$ 'm'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		
2	a	m'.m'm'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>' 2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



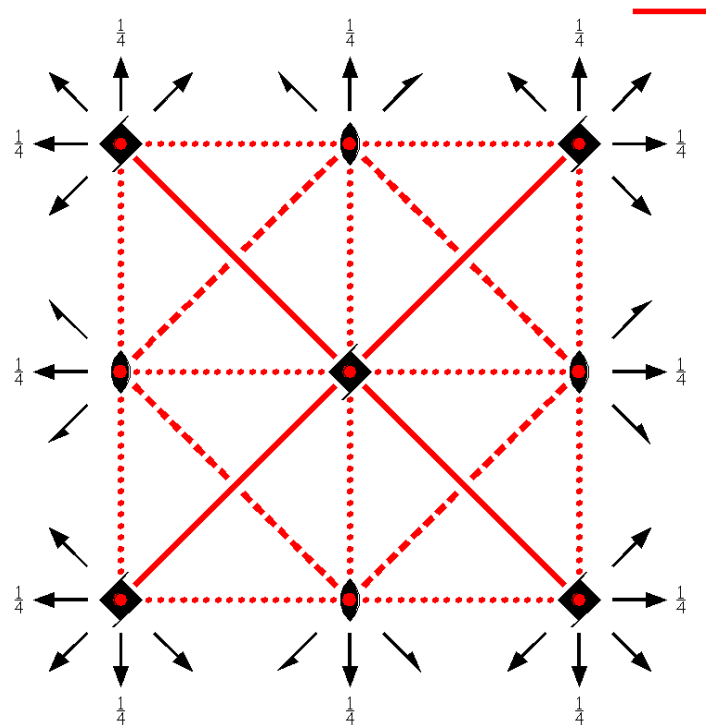
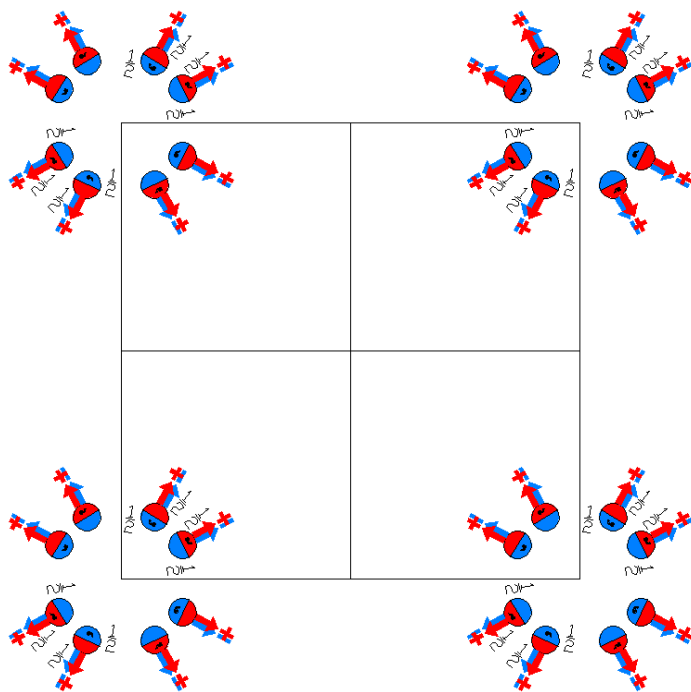
$P4_2/m'c'm'$

132.9.1118

$4/m'm'm'$

$P4_2/m'2/c'2/m'$

Tetragonal



Origin at center (  $m'm'm'$  ) at  $4_2/m'c'2/m'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

### Symmetry Operations

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                                | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                  | (3) $4^+$ (0,0,1/2) $0,0,z$<br>( $4_z$  0,0,1/2)              | (4) $4^-$ (0,0,1/2) $0,0,z$<br>( $4_z^{-1}$  0,0,1/2)              |
| (5) 2 $0,y,1/4$<br>( $2_y$  0,0,1/2)              | (6) 2 $x,0,1/4$<br>( $2_x$  0,0,1/2)              | (7) 2 $x,x,0$<br>( $2_{xy}$  0,0,0)                           | (8) 2 $x,\bar{x},0$<br>( $2_{\bar{xy}}$  0,0,0)                    |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)'     | (10) $m'$ $x,y,0$<br>( $m_z$  0,0,0)'             | (11) $\bar{4}^+$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z$  0,0,1/2)' | (12) $\bar{4}^-$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z^{-1}$  0,0,1/2)' |
| (13) $c'$ (0,0,1/2) $x,0,z$<br>( $m_y$  0,0,1/2)' | (14) $c'$ (0,0,1/2) $0,y,z$<br>( $m_x$  0,0,1/2)' | (15) $m'$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,0)'                | (16) $m'$ $x,x,z$<br>( $m_{\bar{xy}}$  0,0,0)'                     |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

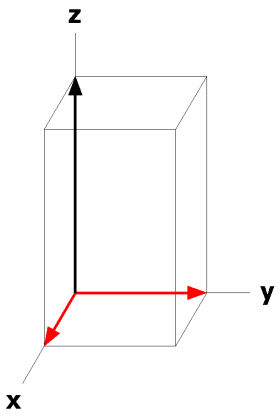
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
16	p	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]
			(13) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]	(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x,z$ [ $v,u,w$ ]
8	o	..m'	$x,x,z$ [ $u,u,w$ ]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,z+1/2$ [ $\bar{u},u,w$ ]	$x,\bar{x},z+1/2$ [ $u,\bar{u},w$ ]
			$\bar{x},x,\bar{z}+1/2$ [ $\bar{u},u,\bar{w}$ ]	$x,\bar{x},\bar{z}+1/2$ [ $u,\bar{u},\bar{w}$ ]	$x,x,\bar{z}$ [ $u,u,\bar{w}$ ]	$\bar{x},\bar{x},\bar{z}$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	n	m'..	$x,y,0$ [ $u,v,0$ ]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},u,0$ ]	$y,\bar{x},1/2$ [ $v,\bar{u},0$ ]
			$\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	$x,\bar{y},1/2$ [ $u,\bar{v},0$ ]	$y,x,0$ [ $v,u,0$ ]	$\bar{y},\bar{x},0$ [ $\bar{v},\bar{u},0$ ]
8	m	.2.	$x,1/2,1/4$ [ $u,0,0$ ]	$\bar{x},1/2,1/4$ [ $\bar{u},0,0$ ]	$1/2,x,3/4$ [ $0,u,0$ ]	$1/2,\bar{x},3/4$ [ $0,\bar{u},0$ ]
			$\bar{x},1/2,3/4$ [ $\bar{u},0,0$ ]	$x,1/2,3/4$ [ $u,0,0$ ]	$1/2,\bar{x},1/4$ [ $0,u,0$ ]	$1/2,x,1/4$ [ $0,\bar{u},0$ ]
8	l	.2.	$x,0,1/4$ [ $u,0,0$ ]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	$0,x,3/4$ [ $0,u,0$ ]	$0,\bar{x},3/4$ [ $0,\bar{u},0$ ]
			$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	$x,0,3/4$ [ $u,0,0$ ]	$0,\bar{x},1/4$ [ $0,u,0$ ]	$0,x,1/4$ [ $0,\bar{u},0$ ]
8	k	2..	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,z+1/2$ [ $0,0,w$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}$ [ $0,0,\bar{w}$ ]
			$0,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,z+1/2$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,w$ ]
4	j	m'.2m'	$x,x,1/2$ [ $u,u,0$ ]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]	$x,\bar{x},0$ [ $u,\bar{u},0$ ]
4	i	m'.2m'	$x,x,0$ [ $u,u,0$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/2$ [ $\bar{u},u,0$ ]	$x,\bar{x},1/2$ [ $u,\bar{u},0$ ]
4	h	2.m'm'	$1/2,1/2,z$ [ $0,0,w$ ]	$1/2,1/2,z+1/2$ [ $0,0,w$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$1/2,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]
4	g	2.m'm'	$0,0,z$ [ $0,0,w$ ]	$0,0,z+1/2$ [ $0,0,w$ ]	$0,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,0,\bar{z}$ [ $0,0,\bar{w}$ ]
4	f	2/m'..	$0,1/2,0$ [ $0,0,0$ ]	$1/2,0,1/2$ [ $0,0,0$ ]	$0,1/2,1/2$ [ $0,0,0$ ]	$1/2,0,0$ [ $0,0,0$ ]
4	e	222.	$0,1/2,1/4$ [ $0,0,0$ ]	$1/2,0,3/4$ [ $0,0,0$ ]	$0,1/2,3/4$ [ $0,0,0$ ]	$1/2,0,1/4$ [ $0,0,0$ ]
2	d	$\bar{4}'2m'$	$1/2,1/2,1/4$ [ $0,0,0$ ]	$1/2,1/2,3/4$ [ $0,0,0$ ]		
2	c	m'.m'm'	$1/2,1/2,0$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]		
2	b	$\bar{4}'2m'$	$0,0,1/4$ [ $0,0,0$ ]	$0,0,3/4$ [ $0,0,0$ ]		
2	a	m'.m'm'	$0,0,0$ [ $0,0,0$ ]	$0,0,1/2$ [ $0,0,0$ ]		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at  $x,0,0$

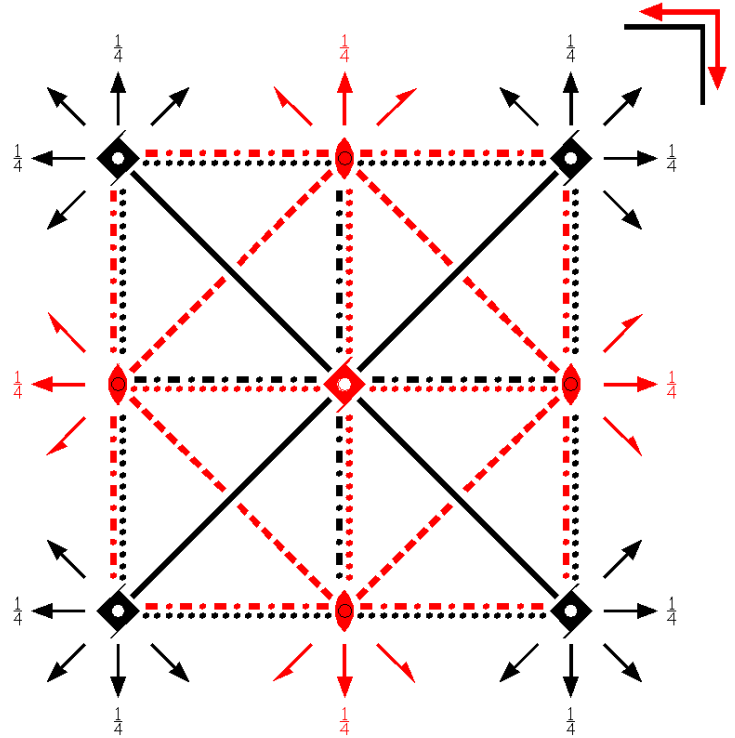
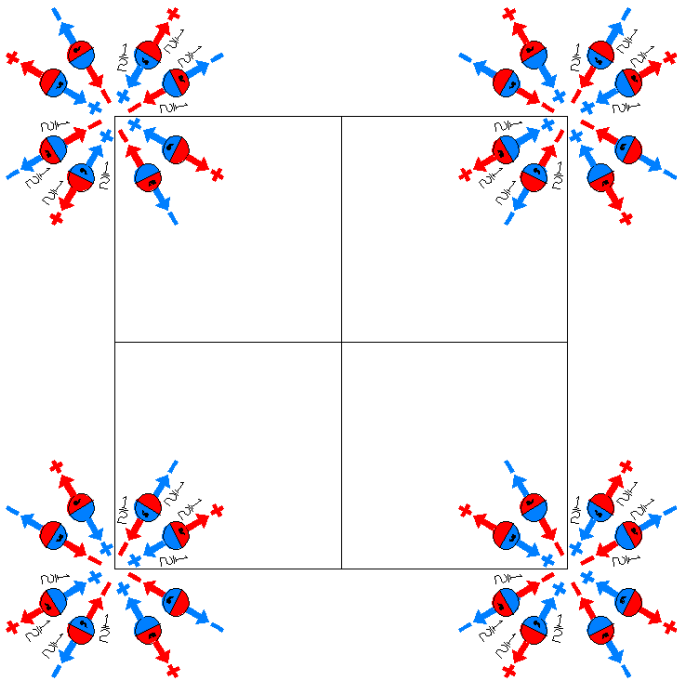
Along  $[1,1,0]$   $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,x,0$



$P_P 4_2/mcm$   
132.10.1119

$4/mmm1'$   
 $P_P 4_2/m2/c2/m$

Tetragonal



Origin at center ( mmm ) at  $4_2/mc2/m$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)              | (3) $4^+$ $(0,0,1/2) 0,0,z$<br>( $4_z$  0,0,1/2)             | (4) $4^-$ $(0,0,1/2) 0,0,z$<br>( $4_z^{-1}$  0,0,1/2)             |
| (5) 2 $0,y,1/4$<br>( $2_y$  0,0,1/2)          | (6) 2 $x,0,1/4$<br>( $2_x$  0,0,1/2)          | (7) 2 $x,x,0$<br>( $2_{xy}$  0,0,0)                          | (8) 2 $x,\bar{x},0$<br>( $2_{\bar{xy}}$  0,0,0)                   |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)  | (10) m $x,y,0$<br>( $m_z$  0,0,0)             | (11) $\bar{4}^+$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z$  0,0,1/2) | (12) $\bar{4}^-$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z^{-1}$  0,0,1/2) |
| (13) c $(0,0,1/2) x,0,z$<br>( $m_y$  0,0,1/2) | (14) c $(0,0,1/2) 0,y,z$<br>( $m_x$  0,0,1/2) | (15) m $x,\bar{x},z$<br>( $m_{xy}$  0,0,0)                   | (16) m $x,x,z$<br>( $m_{\bar{xy}}$  0,0,0)                        |

For (1,0,0)<sup>+</sup> + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> (0,0,1/2) 1/2,1/2,z (4 <sub>z</sub>  1,0,1/2)'	(4) 4' (0,0,1/2) 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,1/2)'
(5) 2' 1/2,y,1/4 (2 <sub>y</sub>  1,0,1/2)'	(6) 2' (1,0,0) x,0,1/4 (2 <sub>x</sub>  1,0,1/2)'	(7) 2' (1/2,1/2,0) x+1/2,x,0 (2 <sub>xy</sub>  1,0,0)'	(8) 2' (1/2,-1/2,0) x+1/2,x̄,0 (2 <sub>xy</sub> <sup>-</sup>  1,0,0)'
(9) 1̄' 1/2,0,0 (1̄ 1,0,0)'	(10) a' (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)'	(11) 4 <sup>+</sup> 1/2,-1/2,z; 1/2,-1/2,1/4 (4 <sub>z</sub>  1,0,1/2)'	(12) 4' 1/2,1/2,z; 1/2,1/2,1/4 (4 <sub>z</sub> <sup>-1</sup>  1,0,1/2)'
(13) n' (1,0,1/2) x,0,z (m <sub>y</sub>  1,0,1/2)'	(14) c' (0,0,1/2) 1/2,y,z (m <sub>x</sub>  1,0,1/2)'	(15) g' (1/2,-1/2,0) x+1/2,x̄,z (m <sub>xy</sub>  1,0,0)'	(16) g' (1/2,1/2,0) x+1/2,x,z (m <sub>xy</sub> <sup>-</sup>  1,0,0)'

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1,0,0) <sup>+</sup> +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	p	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w]	(3) ȳ,x,z+1/2 [v̄,u,w]	(4) y,x̄,z+1/2 [v,ū,w]
			(5) x̄,ȳ,z+1/2 [ū,v̄,w̄]	(6) x,ȳ,z+1/2 [u,v̄,w̄]	(7) y,x,z̄ [v,u,w̄]	(8) ȳ,x̄,z̄ [v̄,ū,w̄]
			(9) x̄,ȳ,z̄ [u,v,w]	(10) x,y,z̄ [ū,v̄,w]	(11) y,x̄,z̄+1/2 [v̄,u,w]	(12) ȳ,x,z̄+1/2 [v,ū,w]
			(13) x,ȳ,z+1/2 [ū,v̄,w̄]	(14) x̄,y,z+1/2 [u,v̄,w̄]	(15) ȳ,x̄,z [v,u,w̄]	(16) y,x,z [v̄,ū,w̄]
16	o	..m	x,x,z [ū,u,0]	x̄,x̄,z [u,ū,0]	x̄,x,z+1/2 [ū,ū,0]	x,x̄,z+1/2 [u,u,0]
			x̄,x,z̄+1/2 [u,u,0]	x,x̄,z̄+1/2 [ū,ū,0]	x,x,z̄ [u,ū,0]	x̄,x̄,z̄ [ū,ū,0]
16	n	m..	x,y,0 [0,0,w]	x̄,ȳ,0 [0,0,w]	ȳ,x,1/2 [0,0,w]	y,x̄,1/2 [0,0,w]
			x̄,y,1/2 [0,0,w̄]	x,ȳ,1/2 [0,0,w̄]	y,x,0 [0,0,w̄]	ȳ,x̄,0 [0,0,w̄]
16	m	.2'	x,1/2,1/4 [0,v,w]	x̄,1/2,1/4 [0,v,w̄]	1/2,x,3/4 [v,0,w̄]	1/2,x̄,3/4 [v,0,w]
			x̄,1/2,3/4 [0,v̄,w̄]	x,1/2,3/4 [0,v̄,w]	1/2,x̄,1/4 [v̄,0,w]	1/2,x,1/4 [v̄,0,w̄]
16	l	.2.	x,0,1/4 [u,0,0]	x̄,0,1/4 [ū,0,0]	0,x,3/4 [0,u,0]	0,x̄,3/4 [0,ū,0]
			x̄,0,3/4 [u,0,0]	x,0,3/4 [ū,0,0]	0,x̄,1/4 [0,u,0]	0,x,1/4 [0,ū,0]
16	k	2'..	0,1/2,z [u,v,0]	1/2,0,z+1/2 [v,ū,0]	0,1/2,z̄+1/2 [ū,v,0]	1/2,0,z̄ [v,u,0]
			0,1/2,z̄ [ū,v̄,0]	1/2,0,z̄+1/2 [v̄,u,0]	0,1/2,z+1/2 [u,v̄,0]	1/2,0,z [v̄,ū,0]
8	j	m.2m	x,x,1/2 [0,0,0]	x̄,x̄,1/2 [0,0,0]	x̄,x,0 [0,0,0]	x,x̄,0 [0,0,0]
8	i	m.2m	x,x,0 [0,0,0]	x̄,x̄,0 [0,0,0]	x̄,x,1/2 [0,0,0]	x,x̄,1/2 [0,0,0]
8	h	2.mm	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2,z̄+1/2 [0,0,0]	1/2,1/2,z̄ [0,0,0]

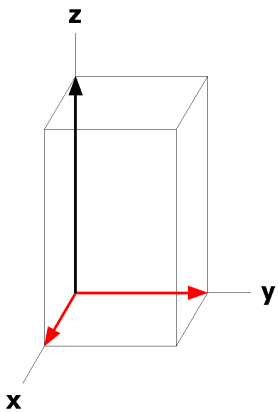
8	g	2.mm	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}$ +1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]
8	f	2'/m..	0,1/2,0 [u,v,0]	1/2,0,1/2 [v, $\bar{u}$ ,0]	0,1/2,1/2 [u, $\bar{v}$ ,0]	1/2,0,0, [ $\bar{v}$ , $\bar{u}$ ,0]
8	e	2'2'2.	0,1/2,1/4 [0,v,0]	1/2,0,3/4 [v,0,0]	0,1/2,3/4 [0, $\bar{v}$ ,0]	1/2,0,1/4 [ $\bar{v}$ ,0,0]
4	d	$\bar{4}$ '2'm	1/2,1/2,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]		
4	c	m.mm	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
4	b	$\bar{4}$ 2m	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
4	a	m.mm	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



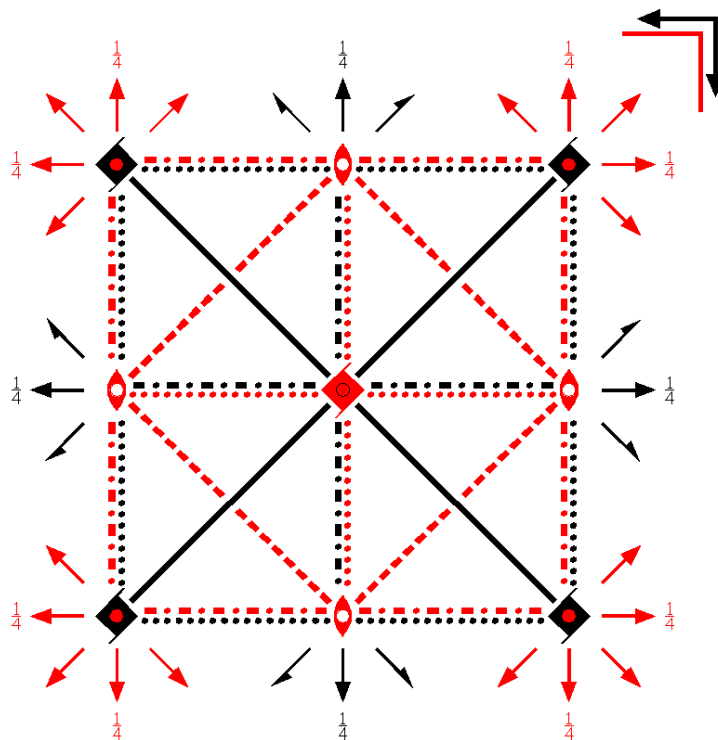
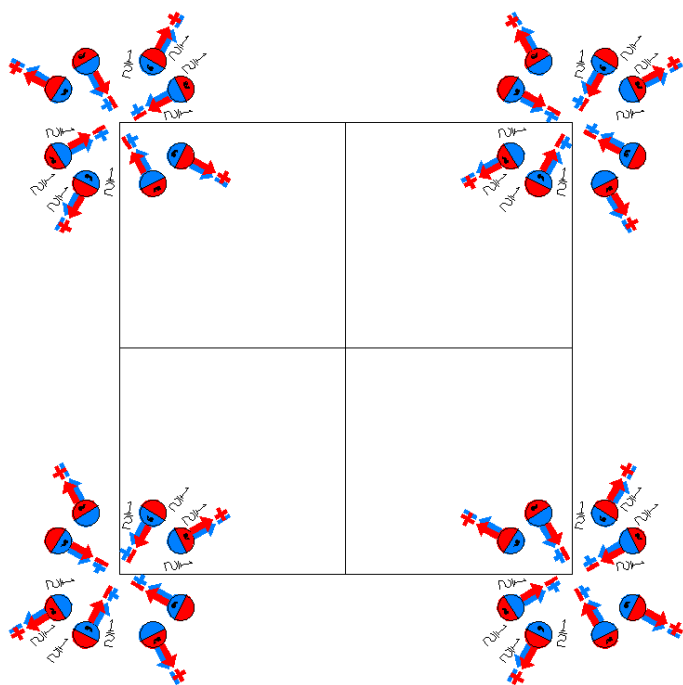
$P_P 4_2/m'cm$

132.11.1120

$4/mmm1'$

$P_P 4_2/m'2'/c'2/m$

Tetragonal



Origin at center ( $mmm'$ ) at  $4_2/m'c2'/m$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

### Symmetry Operations

For (0,0,0) + set

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                              | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                | (3) $4^+$ $(0,0,1/2) 0,0,z$<br>( $4_z$  0,0,1/2)              | (4) $4^-$ $(0,0,1/2) 0,0,z$<br>( $4_z^{-1}$  0,0,1/2)              |
| (5) $2'$ $0,y,1/4$<br>( $2_y$  0,0,1/2)'        | (6) $2'$ $x,0,1/4$<br>( $2_x$  0,0,1/2)'        | (7) $2'$ $x,x,0$<br>( $2_{xy}$  0,0,0)'                       | (8) $2'$ $x,\bar{x},0$<br>( $2_{\bar{xy}}$  0,0,0)'                |
| (9) $\bar{1}'$ $0,0,0$<br>( $\bar{1}$  0,0,0)'  | (10) $m'$ $x,y,0$<br>( $m_z$  0,0,0)'           | (11) $\bar{4}^+$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z$  0,0,1/2)' | (12) $\bar{4}^-$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z^{-1}$  0,0,1/2)' |
| (13) $c$ $(0,0,1/2) x,0,z$<br>( $m_y$  0,0,1/2) | (14) $c$ $(0,0,1/2) 0,y,z$<br>( $m_x$  0,0,1/2) | (15) $m$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,0)                  | (16) $m$ $x,x,z$<br>( $m_{\bar{xy}}$  0,0,0)                       |

## For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> ' (0,0,1/2) 1/2,1/2,z (4 <sub>z</sub>  1,0,1/2)'	(4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,1/2)'
(5) 2 1/2,y,1/4 (2 <sub>y</sub>  1,0,1/2)	(6) 2 (1,0,0) x,0,1/4 (2 <sub>x</sub>  1,0,1/2)	(7) 2 (1/2,1/2,0) x+1/2,x,0 (2 <sub>xy</sub>  1,0,0)	(8) 2 (1/2,-1/2,0) x+1/2,x,0 (2 <sub>-xy</sub>  1,0,0)
(9) $\bar{1}$ 1/2,0,0 ( $\bar{1}$  1,0,0)	(10) a (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)	(11) $\bar{4}^+$ 1/2,-1/2,z; 1/2,-1/2,1/4 ( $\bar{4}_z$  1,0,1/2)	(12) $\bar{4}^-$ 1/2,1/2,z; 1/2,1/2,1/4 ( $\bar{4}_z^{-1}$  1,0,1/2)
(13) n' (1,0,1/2) x,0,z (m <sub>y</sub>  1,0,1/2)'	(14) c' (0,0,1/2) 1/2,y,z (m <sub>x</sub>  1,0,1/2)'	(15) g' (1/2,-1/2,0) x+1/2,x,z (m <sub>xy</sub>  1,0,0)'	(16) g' (1/2,1/2,0) x+1/2,x,z (m <sub>-xy</sub>  1,0,0)'

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1,0,0)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	p	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]
			(13) $x,\bar{y},z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(16) $y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]
16	o	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]	$\bar{x},x,z+1/2$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},z+1/2$ [ $u,u,0$ ]
			$\bar{x},x,\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},\bar{z}+1/2$ [ $u,u,0$ ]	$x,x,\bar{z}$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},\bar{z}$ [ $u,\bar{u},0$ ]
16	n	m'..	x,y,0 [ $u,v,0$ ]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},u,0$ ]	$y,\bar{x},1/2$ [ $v,\bar{u},0$ ]
			$\bar{x},y,1/2$ [ $u,\bar{v},0$ ]	$x,\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$y,x,0$ [ $\bar{v},\bar{u},0$ ]	$\bar{y},\bar{x},0$ [ $v,u,0$ ]
16	m	.2.	x,1/2,1/4 [ $u,0,0$ ]	$\bar{x},1/2,1/4$ [ $u,0,0$ ]	1/2,x,3/4 [ $0,\bar{u},0$ ]	1/2, $\bar{x},3/4$ [ $0,\bar{u},0$ ]
			$\bar{x},1/2,3/4$ [ $u,0,0$ ]	$x,1/2,3/4$ [ $u,0,0$ ]	1/2, $\bar{x},1/4$ [ $0,\bar{u},0$ ]	1/2,x,1/4 [ $0,\bar{u},0$ ]
16	l	.2'.	x,0,1/4 [ $0,v,w$ ]	$\bar{x},0,1/4$ [ $0,\bar{v},w$ ]	0,x,3/4 [ $\bar{v},0,w$ ]	0, $\bar{x},3/4$ [ $v,0,w$ ]
			$\bar{x},0,3/4$ [ $0,\bar{v},w$ ]	$x,0,3/4$ [ $0,v,w$ ]	0, $\bar{x},1/4$ [ $\bar{v},0,w$ ]	0,x,1/4 [ $v,0,w$ ]
16	k	2'..	0,1/2,z [ $u,v,0$ ]	1/2,0,z+1/2 [ $v,\bar{u},0$ ]	0,1/2, $\bar{z}+1/2$ [ $u,\bar{v},0$ ]	1/2,0, $\bar{z}$ [ $\bar{v},\bar{u},0$ ]
			0,1/2, $\bar{z}$ [ $u,v,0$ ]	1/2,0, $\bar{z}+1/2$ [ $v,\bar{u},0$ ]	0,1/2,z+1/2 [ $u,\bar{v},0$ ]	1/2,0,z [ $\bar{v},\bar{u},0$ ]
8	j	m'.2'm	x,x,1/2 [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},1/2$ [ $u,\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},0$ [ $u,u,0$ ]
8	i	m'.2'm	x,x,0 [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},0$ [ $u,\bar{u},0$ ]	$\bar{x},x,1/2$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},1/2$ [ $u,u,0$ ]

8	h	2.mm	$1/2, 1/2, z [0,0,0]$	$1/2, 1/2, z+1/2 [0,0,0]$	$1/2, 1/2, \bar{z}+1/2 [0,0,0]$	$1/2, 1/2, \bar{z} [0,0,0]$
8	g	2.mm	$0,0,z [0,0,0]$	$0,0,z+1/2 [0,0,0]$	$0,0,\bar{z}+1/2 [0,0,0]$	$0,0,\bar{z} [0,0,0]$
8	f	$2'/m'..$	$0,1/2,0 [u,v,0]$	$1/2,0,1/2 [v,\bar{u},0]$	$0,1/2,1/2 [u,\bar{v},0]$	$1/2,0,0, [\bar{v},\bar{u},0]$
8	e	$2'22'.$	$0,1/2,1/4 [u,0,0]$	$1/2,0,3/4 [0,\bar{u},0]$	$0,1/2,3/4 [u,0,0]$	$1/2,0,1/4 [0,\bar{u},0]$
4	d	$\bar{4}2m$	$1/2,1/2,1/4 [0,0,0]$	$1/2,1/2,3/4 [0,0,0]$		
4	c	$m'.mm$	$1/2,1/2,0 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$		
4	b	$\bar{4}'2'm$	$0,0,1/4 [0,0,0]$	$0,0,3/4 [0,0,0]$		
4	a	$m'.mm$	$0,0,0 [0,0,0]$	$0,0,1/2 [0,0,0]$		

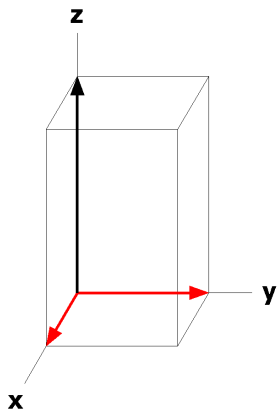
**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_4 \cdot 4mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$





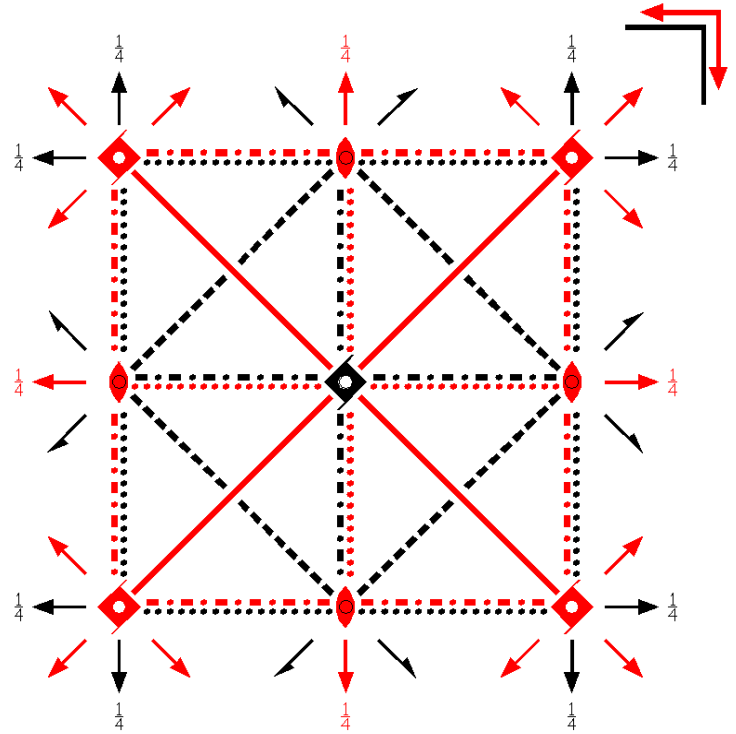
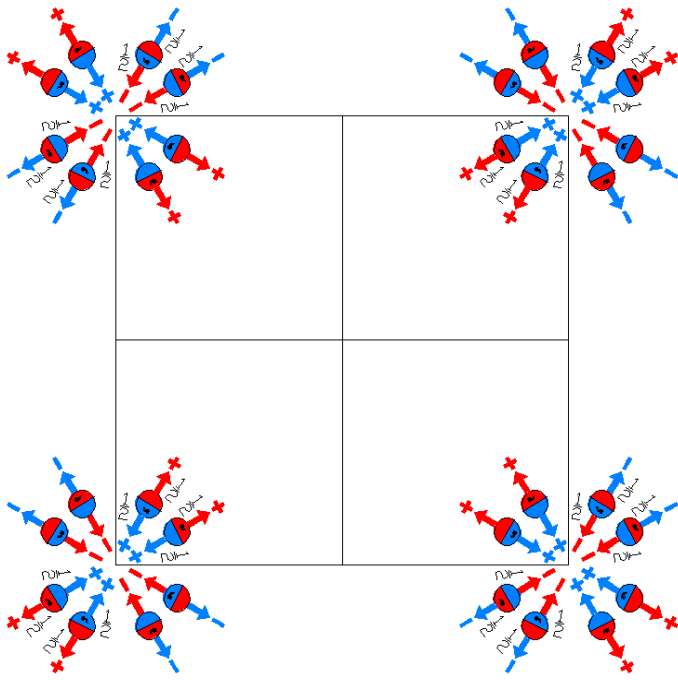
$P_P 4_2'/mcm'$

132.12.1121

$4/mmm1'$

$P_P 4_2'/m2/c2'/m'$

Tetragonal



Origin at center ( $m'm'm$ ) at  $4_2'/mc2'/m'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

### Symmetry Operations

For (0,0,0) + set

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                              | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                | (3) $4^+$ $(0,0,1/2) 0,0,z$<br>( $4_z$  0,0,1/2)'             | (4) $4^-$ $(0,0,1/2) 0,0,z$<br>( $4_z^{-1}$  0,0,1/2)'             |
| (5) 2 $0,y,1/4$<br>( $2_y$  0,0,1/2)            | (6) 2 $x,0,1/4$<br>( $2_x$  0,0,1/2)            | (7) $2'$ $x,x,0$<br>( $2_{xy}$  0,0,0)'                       | (8) $2'$ $x,\bar{x},0$<br>( $2_{\bar{xy}}$  0,0,0)'                |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)    | (10) $m$ $x,y,0$<br>( $m_z$  0,0,0)             | (11) $\bar{4}^+$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z$  0,0,1/2)' | (12) $\bar{4}^-$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z^{-1}$  0,0,1/2)' |
| (13) $c$ $(0,0,1/2) x,0,z$<br>( $m_y$  0,0,1/2) | (14) $c$ $(0,0,1/2) 0,y,z$<br>( $m_x$  0,0,1/2) | (15) $m'$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,0)'                | (16) $m'$ $x,x,z$<br>( $m_{\bar{xy}}$  0,0,0)'                     |

## For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> (0,0,1/2) 1/2,1/2,z (4 <sub>z</sub>  1,0,1/2)	(4) 4 <sup>-</sup> (0,0,1/2) 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,1/2)
(5) 2' 1/2,y,1/4 (2 <sub>y</sub>  1,0,1/2)'	(6) 2' (1,0,0) x,0,1/4 (2 <sub>x</sub>  1,0,1/2)'	(7) 2 (1/2,1/2,0) x+1/2,x,0 (2 <sub>xy</sub>  1,0,0)	(8) 2 (1/2,-1/2,0) x+1/2,x̄,0 (2 <sub>xy</sub> <sup>-</sup>  1,0,0)
(9) 1̄' 1/2,0,0 (1̄ 1,0,0)'	(10) a' (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)'	(11) 4 <sup>+</sup> 1/2,-1/2,z; 1/2,-1/2,1/4 (4 <sub>z</sub>  1,0,1/2)	(12) 4 <sup>-</sup> 1/2,1/2,z; 1/2,1/2,1/4 (4 <sub>z</sub> <sup>-1</sup>  1,0,1/2)
(13) n' (1,0,1/2) x,0,z (m <sub>y</sub>  1,0,1/2)'	(14) c' (0,0,1/2) 1/2,y,z (m <sub>x</sub>  1,0,1/2)'	(15) g (1/2,-1/2,0) x+1/2,x̄,z (m <sub>xy</sub>  1,0,0)	(16) g (1/2,1/2,0) x+1/2,x,z (m <sub>xy</sub> <sup>-</sup>  1,0,0)

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1,0,0)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	p	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w]	(3) ȳ,x,z+1/2 [v̄,ū,w̄]	(4) y,x̄,z+1/2 [v̄,ū,w̄]
			(5) x̄,ȳ,z+1/2 [ū,v̄,w̄]	(6) x,ȳ,z+1/2 [ū,v̄,w̄]	(7) y,x,z [v̄,ū,w]	(8) ȳ,x̄,z [v̄,ū,w]
			(9) x̄,ȳ,z [u,v,w]	(10) x,y,z [ū,v̄,w]	(11) y,x̄,z+1/2 [v̄,ū,w̄]	(12) ȳ,x,z+1/2 [v̄,ū,w̄]
			(13) x,ȳ,z+1/2 [ū,v̄,w̄]	(14) x̄,y,z+1/2 [ū,v̄,w̄]	(15) ȳ,x̄,z [v̄,ū,w]	(16) y,x,z [v̄,ū,w]
16	o	..m'	x,x,z [u,u,w]	x̄,x̄,z [ū,ū,w]	x̄,x,z+1/2 [u,ū,w̄]	x,x̄,z+1/2 [ū,ū,w̄]
			x̄,x,z+1/2 [ū,ū,w̄]	x,x̄,z+1/2 [u,ū,w̄]	x,x,z [ū,ū,w]	x̄,x̄,z [u,ū,w]
16	n	m..	x,y,0 [0,0,w]	x̄,ȳ,0 [0,0,w]	ȳ,x,1/2 [0,0,w̄]	y,x̄,1/2 [0,0,w̄]
			x̄,y,1/2 [0,0,w̄]	x,ȳ,1/2 [0,0,w̄]	y,x,0 [0,0,w]	ȳ,x̄,0 [0,0,w]
16	m	.2'	x,1/2,1/4 [0,v,w]	x̄,1/2,1/4 [0,v̄,w̄]	1/2,x,3/4 [v̄,0,w]	1/2,x̄,3/4 [v̄,0,w̄]
			x̄,1/2,3/4 [0,v̄,w̄]	x,1/2,3/4 [0,v̄,w̄]	1/2,x̄,1/4 [v,0,w̄]	1/2,x,1/4 [v,0,w]
16	l	.2.	x,0,1/4 [u,0,0]	x̄,0,1/4 [ū,0,0]	0,x,3/4 [0,ū,0]	0,x̄,3/4 [0,ū,0]
			x̄,0,3/4 [ū,0,0]	x,0,3/4 [u,0,0]	0,x̄,1/4 [0,ū,0]	0,x,1/4 [0,ū,0]
16	k	2'..	0,1/2,z [u,v,0]	1/2,0,z+1/2 [v̄,ū,0]	0,1/2,z+1/2 [ū,v,0]	1/2,0,z [v̄,ū,0]
			0,1/2,z̄ [ū,v̄,0]	1/2,0,z̄+1/2 [v̄,ū,0]	0,1/2,z+1/2 [u,v̄,0]	1/2,0,z [v,ū,0]
8	j	m.2'm'	x,x,1/2 [0,0,w]	x̄,x̄,1/2 [0,0,w]	x̄,x,0 [0,0,w̄]	x,x̄,0 [0,0,w̄]
8	i	m.2'm'	x,x,0 [0,0,w]	x̄,x̄,0 [0,0,w]	x̄,x,1/2 [0,0,w̄]	x,x̄,1/2 [0,0,w̄]
8	h	2.m'm'	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2,z̄+1/2 [0,0,w]	1/2,1/2,z̄ [0,0,w]

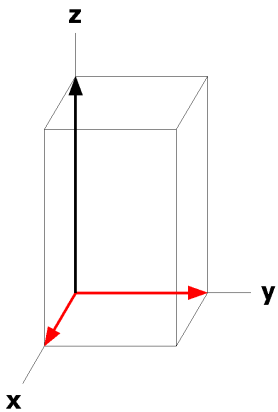
8	g	$2.m'm'$	$0,0,z [0,0,w]$	$0,0,z+1/2 [0,0,\bar{w}]$	$0,0,\bar{z}+1/2 [0,0,\bar{w}]$	$0,0,\bar{z} [0,0,w]$
8	f	$2'/m..$	$0,1/2,0 [0,0,0]$	$1/2,0,1/2 [0,0,0]$	$0,1/2,1/2 [0,0,0]$	$1/2,0,0, [0,0,0]$
8	e	$2'2'2.$	$0,1/2,1/4 [0,v,0]$	$1/2,0,3/4 [\bar{v},0,0]$	$0,1/2,3/4 [0,\bar{v},0]$	$1/2,0,1/4 [0,v,0]$
4	d	$\bar{4}2'm'$	$1/2,1/2,1/4 [0,0,w]$	$1/2,1/2,3/4 [0,0,w]$		
4	c	$m.mm$	$1/2,1/2,0 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$		
4	b	$\bar{4}'2m'$	$0,0,1/4 [0,0,0]$	$0,0,3/4 [0,0,0]$		
4	a	$m.m'm'$	$0,0,0 [0,0,w]$	$0,0,1/2 [0,0,\bar{w}]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p_{2a^*} 2mm$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x-1/4, x+1/4, 0$



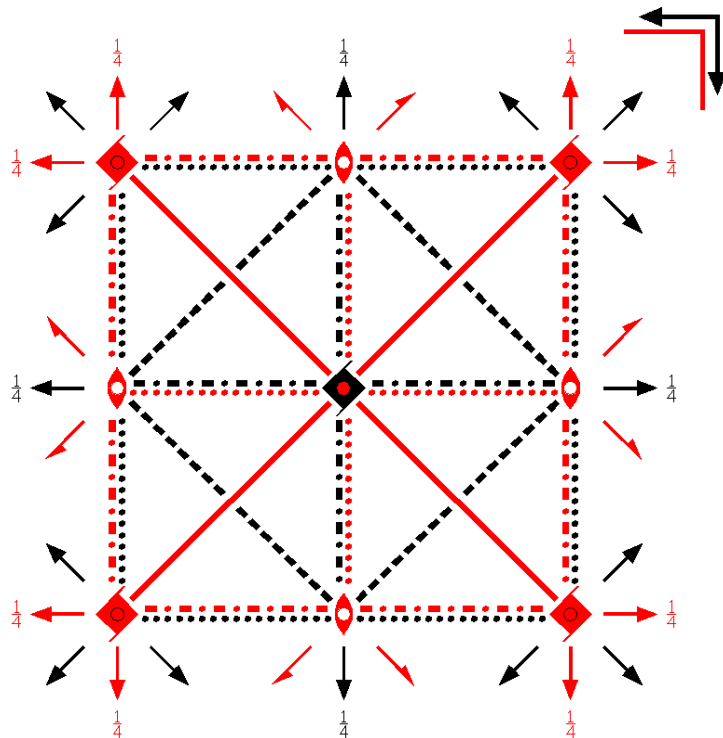
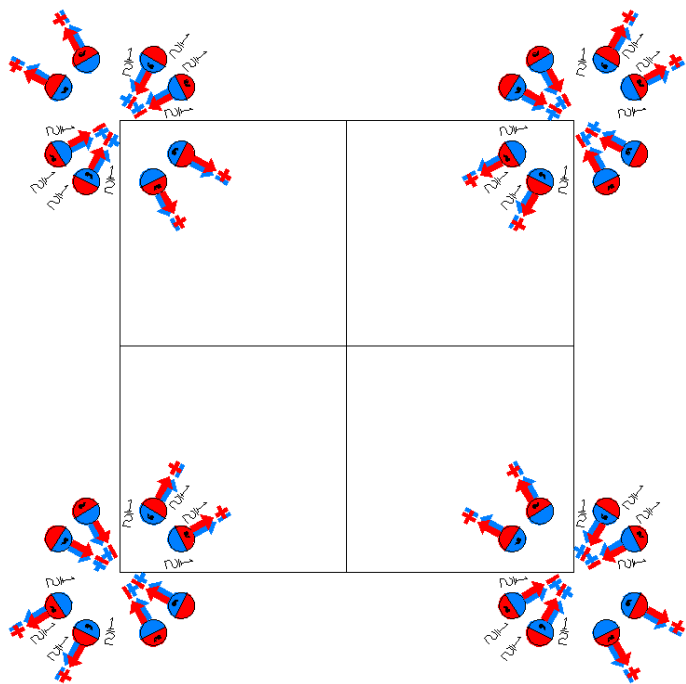
$P_P 4_2'/m'cm'$

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$4/mmm1'$

$P_P 4_2'/m'2'/c2/m'$

Tetragonal



Origin at center ( $m'm'm'$ ) at  $4_2'/m'c2/m'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)              | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)'             | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'        | (6) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'        | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                      | (8) 2 x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)                                      |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'                         | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'           | (11) 4 <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>+</sup>  0,0,1/2) | (12) 4 <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)  |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (15) m' x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'                                  | (16) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                                     |

## For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 4 <sup>+</sup> (0,0,1/2) 1/2,1/2,z (4 <sub>z</sub>  1,0,1/2)'	(4) 4 <sup>-</sup> (0,0,1/2) 1/2,-1/2,z (4 <sub>z</sub> <sup>-1</sup>  1,0,1/2)
(5) 2 1/2,y,1/4 (2 <sub>y</sub>  1,0,1/2)	(6) 2 (1,0,0) x,0,1/4 (2 <sub>x</sub>  1,0,1/2)	(7) 2' (1/2,1/2,0) x+1/2,x,0 (2 <sub>xy</sub>  1,0,0)'	(8) 2' (1/2,-1/2,0) x+1/2,x̄,0 (2 <sub>xy</sub> <sup>-</sup>  1,0,0)'
(9) 1̄ 1/2,0,0 (1̄ 1,0,0)	(10) a (1,0,0) x,y,0 (m <sub>z</sub>  1,0,0)	(11) 4 <sup>+</sup> 1/2,-1/2,z; 1/2,-1/2,1/4 (4 <sub>z</sub>  1,0,1/2)'	(12) 4 <sup>-</sup> 1/2,1/2,z; 1/2,1/2,1/4 (4 <sub>z</sub> <sup>-1</sup>  1,0,1/2)'
(13) n' (1,0,1/2) x,0,z (m <sub>y</sub>  1,0,1/2)'	(14) c' (0,0,1/2) 1/2,y,z (m <sub>x</sub>  1,0,1/2)'	(15) g (1/2,-1/2,0) x+1/2,x̄,z (m <sub>xy</sub>  1,0,0)	(16) g (1/2,1/2,0) x+1/2,x,z (m <sub>xy</sub> <sup>-</sup>  1,0,0)

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1,0,0)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	p	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w]	(3) ȳ,x,z+1/2 [v̄,ū,w̄]	(4) y,x̄,z+1/2 [v̄,ū,w̄]
			(5) x̄,ȳ,z̄+1/2 [ū,v̄,w]	(6) x,ȳ,z̄+1/2 [ū,v,w]	(7) y,x,z̄ [v̄,ū,w̄]	(8) ȳ,x̄,z̄ [v̄,ū,w̄]
			(9) x̄,ȳ,z̄ [ū,v̄,w̄]	(10) x,y,z̄ [ū,v,w̄]	(11) y,x̄,z̄+1/2 [v̄,ū,w]	(12) ȳ,x̄,z̄+1/2 [v̄,ū,w]
			(13) x,ȳ,z+1/2 [ū,v,w̄]	(14) x̄,y,z+1/2 [ū,v̄,w̄]	(15) ȳ,x̄,z [v̄,ū,w]	(16) y,x,z [v̄,ū,w]
16	o	..m'	x,x,z [u,u,w]	x̄,x̄,z [ū,ū,w]	x̄,x,z+1/2 [u,ū,w̄]	x,x̄,z+1/2 [ū,ū,w̄]
			x̄,x,z̄+1/2 [u,ū,w]	x,x̄,z̄+1/2 [ū,ū,w]	x,x,z̄ [u,ū,w̄]	x̄,x̄,z̄ [ū,ū,w̄]
16	n	m'..	x,y,0 [u,v,0]	x̄,ȳ,0 [ū,v̄,0]	ȳ,x,1/2 [v̄,ū,0]	y,x̄,1/2 [v̄,ū,0]
			x̄,y,1/2 [u,v̄,0]	x,ȳ,1/2 [ū,v,0]	y,x,0 [v̄,ū,0]	ȳ,x̄,0 [v̄,ū,0]
16	m	.2.	x,1/2,1/4 [u,0,0]	x̄,1/2,1/4 [ū,0,0]	1/2,x,3/4 [0,ū,0]	1/2,x̄,3/4 [0,ū,0]
			x̄,1/2,3/4 [u,0,0]	x,1/2,3/4 [ū,0,0]	1/2,x̄,1/4 [0,ū,0]	1/2,x,1/4 [0,ū,0]
16	l	.2'.	x,0,1/4 [0,v,w]	x̄,0,1/4 [0,v̄,w]	0,x,3/4 [v,0,w̄]	0,x̄,3/4 [v̄,0,w̄]
			x̄,0,3/4 [0,v̄,w]	x,0,3/4 [0,v,w]	0,x̄,1/4 [v,0,w̄]	0,x,1/4 [v̄,0,w̄]
16	k	2'..	0,1/2,z [u,v,0]	1/2,0,z+1/2 [v̄,ū,0]	0,1/2,z̄+1/2 [u,v̄,0]	1/2,0,z̄ [v̄,ū,0]
			0,1/2,z̄ [u,v,0]	1/2,0,z̄+1/2 [v̄,ū,0]	0,1/2,z+1/2 [u,v̄,0]	1/2,0,z [v̄,ū,0]
8	j	m'.2m'	x,x,1/2 [u,u,0]	x̄,x̄,1/2 [ū,ū,0]	x̄,x,0 [u,ū,0]	x,x̄,0 [ū,ū,0]
8	i	m'.2m'	x,x,0 [u,u,0]	x̄,x̄,0 [ū,ū,0]	x̄,x,1/2 [u,ū,0]	x,x̄,1/2 [ū,ū,0]
8	h	2.mm	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2,z̄+1/2 [0,0,0]	1/2,1/2,z̄ [0,0,0]

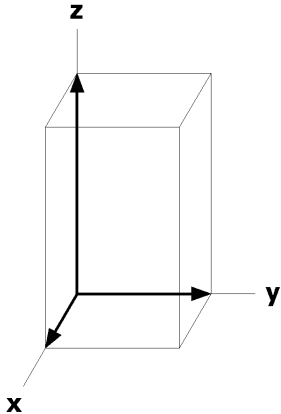
8	g	$2.m'm'$	$0,0,z [0,0,w]$	$0,0,z+1/2 [0,0,\bar{w}]$	$0,0,\bar{z}+1/2 [0,0,w]$	$0,0,\bar{z} [0,0,\bar{w}]$
8	f	$2'/m'..$	$0,1/2,0 [u,v,0]$	$1/2,0,1/2 [\bar{v},u,0]$	$0,1/2,1/2 [u,\bar{v},0]$	$1/2,0,0, [v,u,0]$
8	e	$2'22'.$	$0,1/2,1/4 [u,0,0]$	$1/2,0,3/4 [0,u,0]$	$0,1/2,3/4 [u,0,0]$	$1/2,0,1/4 [0,u,0]$
4	d	$\bar{4}'2m'$	$1/2,1/2,1/4 [0,0,0]$	$1/2,1/2,3/4 [0,0,0]$		
4	c	$m'.m'm'$	$1/2,1/2,0 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$		
4	b	$\bar{4}2'm'$	$0,0,1/4 [0,0,w]$	$0,0,3/4 [0,0,\bar{w}]$		
4	a	$m'.m'm'$	$0,0,0 [0,0,0]$	$0,0,1/2 [0,0,0]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_p 4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $1/2,1/2,z$

Along  $[1,0,0]$   $p_{2mm}1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,0,0$

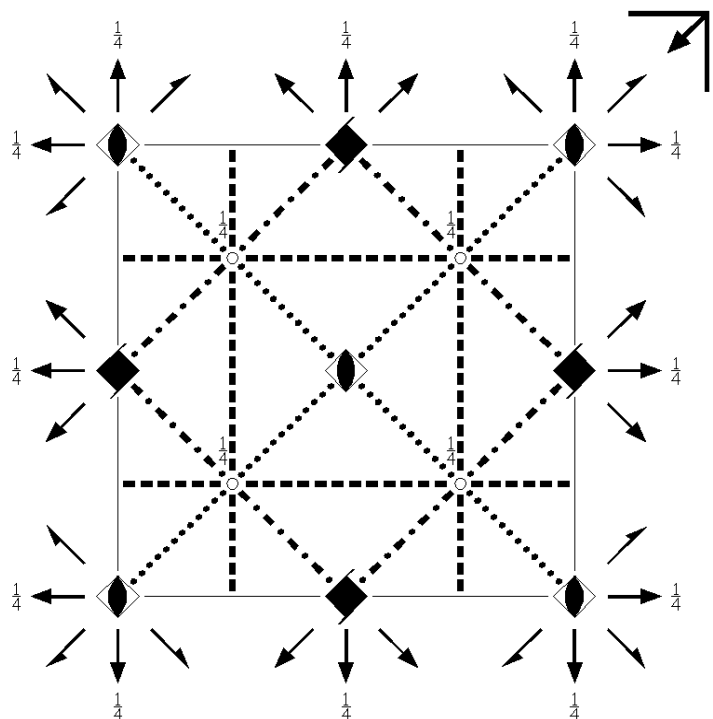
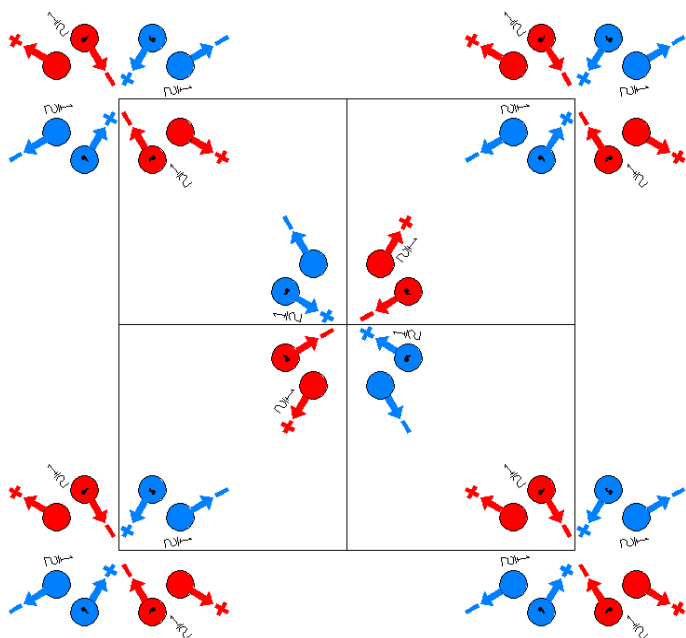
Along  $[1,1,0]$   $p_{2a'} 2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$



$P4_2/nbc$   
133.1.1123

$4/mmm$   
 $P4_2/n2/b2/c$

Tetragonal



Origin at  $\bar{4}12_1/c$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)              | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)                  | (7) 2 (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>  1/2,1/2,0)               | (8) 2 x, $\bar{x}+1/2,0$<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)         |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)  | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)              | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                            |
| (13) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (14) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)     | (15) c (0,0,1/2) x, $\bar{x},z$<br>(m <sub>xy</sub>  0,0,1/2)         | (16) c (0,0,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,1/2)             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y+1/2,x+1/2,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]		
			(13) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y},\bar{x},z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y,x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	j	.2	$x,x+1/2,0$ [ $u,u,0$ ]	$\bar{x},\bar{x}+1/2,0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,1/2$ [ $\bar{u},u,0$ ]	$x,\bar{x}+1/2,1/2$ [ $u,\bar{u},0$ ]
			$\bar{x}+1/2,\bar{x},1/2$ [ $u,u,0$ ]	$x+1/2,x,1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},0$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,x,0$ [ $u,\bar{u},0$ ]
8	i	.2.	$x,0,3/4$ [ $u,0,0$ ]	$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	$1/2,x+1/2,1/4$ [ $0,u,0$ ]	$1/2,\bar{x}+1/2,1/4$ [ $0,\bar{u},0$ ]
			$\bar{x}+1/2,1/2,3/4$ [ $u,0,0$ ]	$x+1/2,1/2,3/4$ [ $\bar{u},0,0$ ]	$0,\bar{x},1/4$ [ $0,u,0$ ]	$0,x,1/4$ [ $0,\bar{u},0$ ]
8	h	.2.	$x,0,1/4$ [ $u,0,0$ ]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	$1/2,x+1/2,3/4$ [ $0,u,0$ ]	$1/2,\bar{x}+1/2,3/4$ [ $0,\bar{u},0$ ]
			$\bar{x}+1/2,1/2,1/4$ [ $u,0,0$ ]	$x+1/2,1/2,1/4$ [ $\bar{u},0,0$ ]	$0,\bar{x},3/4$ [ $0,u,0$ ]	$0,x,3/4$ [ $0,\bar{u},0$ ]
8	g	2..	$0,0,z$ [ $0,0,w$ ]	$1/2,1/2,z+1/2$ [ $0,0,w$ ]	$0,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$1/2,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]
			$1/2,1/2,\bar{z}+1/2$ [ $0,0,w$ ]	$0,0,\bar{z}$ [ $0,0,w$ ]	$1/2,1/2,z$ [ $0,0,\bar{w}$ ]	$0,0,z+1/2$ [ $0,0,\bar{w}$ ]
8	f	2..	$0,1/2,z$ [ $0,0,w$ ]	$0,1/2,z+1/2$ [ $0,0,w$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]
			$1/2,0,\bar{z}+1/2$ [ $0,0,w$ ]	$1/2,0,\bar{z}$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,\bar{w}$ ]	$1/2,0,z+1/2$ [ $0,0,\bar{w}$ ]
8	e	$\bar{1}$	$1/4,1/4,1/4$ [ $u,v,w$ ]	$3/4,3/4,1/4$ [ $\bar{u},\bar{v},w$ ]	$1/4,3/4,3/4$ [ $\bar{v},u,w$ ]	$3/4,1/4,3/4$ [ $v,\bar{u},w$ ]
			$3/4,1/4,1/4$ [ $\bar{u},v,\bar{w}$ ]	$1/4,3/4,1/4$ [ $u,\bar{v},\bar{w}$ ]	$3/4,3/4,3/4$ [ $v,u,\bar{w}$ ]	$1/4,1/4,3/4$ [ $\bar{v},\bar{u},\bar{w}$ ]
4	d	$\bar{4}$	$0,0,0$ [ $0,0,w$ ]	$1/2,1/2,1/2$ [ $0,0,w$ ]	$0,0,1/2$ [ $0,0,\bar{w}$ ]	$1/2,1/2,0$ [ $0,0,\bar{w}$ ]
4	c	2.22	$0,1/2,0$ [ $0,0,0$ ]	$0,1/2,1/2$ [ $0,0,0$ ]	$1/2,0,1/2$ [ $0,0,0$ ]	$1/2,0,0$ [ $0,0,0$ ]
4	b	222.	$0,0,1/4$ [ $0,0,0$ ]	$1/2,1/2,3/4$ [ $0,0,0$ ]	$1/2,1/2,1/4$ [ $0,0,0$ ]	$0,0,3/4$ [ $0,0,0$ ]
4	a	222.	$0,1/2,1/4$ [ $0,0,0$ ]	$0,1/2,3/4$ [ $0,0,0$ ]	$1/2,0,1/4$ [ $0,0,0$ ]	$1/2,0,3/4$ [ $0,0,0$ ]

Continued

133.1.1123

P4<sub>2</sub>/nbc

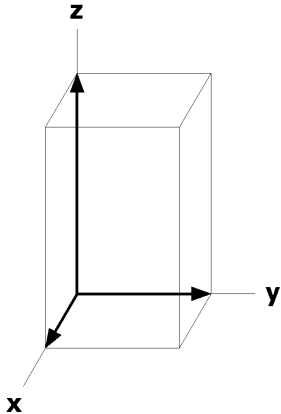


## Symmetry of Special Projections

Along  $[0,0,1]$   $p_{2a^*} 4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $1/2, 0, z$

Along  $[1,0,0]$   $p_{2a^*} 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x, 0, 1/4$

Along  $[1,1,0]$   $p_{2a^*} 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at  $x, x, 0$



$P4_2/nbc1'$

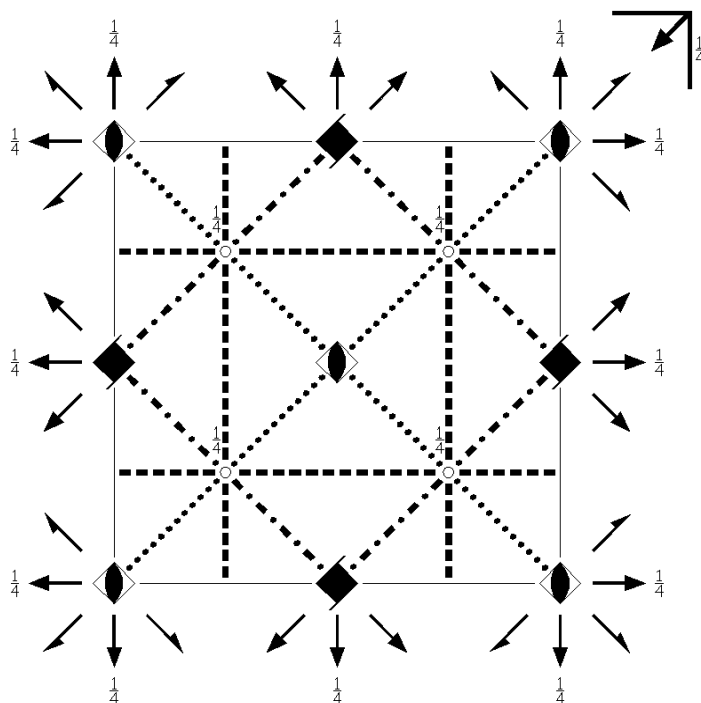
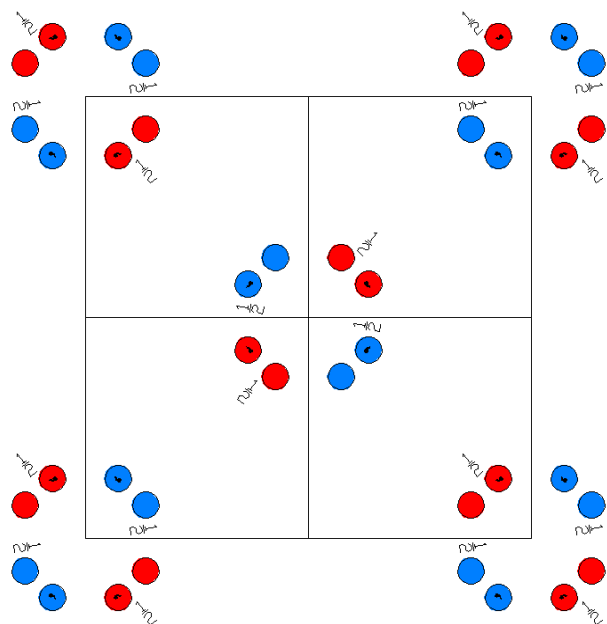
133.2.1124

$4/mmm1'$

$P4_2/n2/b2/c1'$

Tetragonal

$1'$



Origin at  $\bar{4}12_1/c1'$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

For  $1 +$  set

- |  |   |  |   |
|--|---|--|---|
| (1) $1$<br>( $1   0,0,0$ )                                 | (2) $2$ $0,0,z$<br>( $2_z   0,0,0$ )                      | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>( $4_z   1/2,1/2,1/2$ )   | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1}   1/2,1/2,1/2$ )   |
| (5) $2$ $0,y,1/4$<br>( $2_y   0,0,1/2$ )                   | (6) $2$ $x,0,1/4$<br>( $2_x   0,0,1/2$ )                  | (7) $2$ $(1/2,1/2,0) x,x,0$<br>( $2_{xy}   1/2,1/2,0$ )    | (8) $2$ $x,\bar{x}+1/2,0$<br>( $2_{\bar{xy}}   1/2,1/2,0$ )     |
| (9) $\bar{1}$ $1/4,1/4,1/4$<br>( $\bar{1}   1/2,1/2,1/2$ ) | (10) $n$ $(1/2,1/2,0) x,y,1/4$<br>( $m_z   1/2,1/2,1/2$ ) | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z   0,0,0$ ) | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1}   0,0,0$ ) |
| (13) $a$ $(1/2,0,0) x,1/4,z$<br>( $m_y   1/2,1/2,0$ )      | (14) $b$ $(0,1/2,0) 1/4,y,z$<br>( $m_x   1/2,1/2,0$ )     | (15) $c$ $(0,0,1/2) x,\bar{x},z$<br>( $m_{xy}   0,0,1/2$ ) | (16) $c$ $(0,0,1/2) x,x,z$<br>( $m_{\bar{xy}}   0,0,1/2$ )      |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)'	(4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'
(5) 2' 0,y,1/4 (2 <sub>y</sub>  0,0,1/2)'	(6) 2' x,0,1/4 (2 <sub>x</sub>  0,0,1/2)'	(7) 2' (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>  1/2,1/2,0)'	(8) 2' x, $\bar{x}$ +1/2,0 (2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)'
(9) $\bar{1}$ ' 1/4,1/4,1/4 ( $\bar{1}$  1/2,1/2,1/2)'	(10) n' (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>  1/2,1/2,1/2)'	(11) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z^+$  0,0,0)'	(12) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z^-$  0,0,0)'
(13) a' (1/2,0,0) x,1/4,z (m <sub>y</sub>  1/2,1/2,0)'	(14) b' (0,1/2,0) 1/4,y,z (m <sub>x</sub>  1/2,1/2,0)'	(15) c' (0,0,1/2) x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,1/2)'	(16) c' (0,0,1/2) x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			1 +		1' +	
16	k	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [0,0,0]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [0,0,0]		
			(5) $\bar{x},y,\bar{z}+1/2$ [0,0,0]	(6) $x,\bar{y},\bar{z}+1/2$ [0,0,0]		
			(7) $y+1/2,x+1/2,\bar{z}$ [0,0,0]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}$ [0,0,0]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [0,0,0]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [0,0,0]		
			(11) $y,\bar{x},\bar{z}$ [0,0,0]	(12) $\bar{y},x,\bar{z}$ [0,0,0]		
			(13) $x+1/2,\bar{y}+1/2,z$ [0,0,0]	(14) $\bar{x}+1/2,y+1/2,z$ [0,0,0]		
			(15) $\bar{y},\bar{x},z+1/2$ [0,0,0]	(16) $y,x,z+1/2$ [0,0,0]		
8	j	..21'	x,x+1/2,0 [0,0,0]	$\bar{x},\bar{x}+1/2,0$ [0,0,0]	$\bar{x},x+1/2,1/2$ [0,0,0]	$x,\bar{x}+1/2,1/2$ [0,0,0]
			$\bar{x}+1/2,\bar{x},1/2$ [0,0,0]	$x+1/2,x,1/2$ [0,0,0]	$x+1/2,\bar{x},0$ [0,0,0]	$\bar{x}+1/2,x,0$ [0,0,0]
8	i	..2.1'	x,0,3/4 [0,0,0]	$\bar{x},0,3/4$ [0,0,0]	1/2,x+1/2,1/4 [0,0,0]	1/2, $\bar{x}+1/2,1/4$ [0,0,0]
			$\bar{x}+1/2,1/2,3/4$ [0,0,0]	$x+1/2,1/2,3/4$ [0,0,0]	0, $\bar{x},1/4$ [0,0,0]	0,x,1/4 [0,0,0]
8	h	..2.1'	x,0,1/4 [0,0,0]	$\bar{x},0,1/4$ [0,0,0]	1/2,x+1/2,3/4 [0,0,0]	1/2, $\bar{x}+1/2,3/4$ [0,0,0]
			$\bar{x}+1/2,1/2,1/4$ [0,0,0]	$x+1/2,1/2,1/4$ [0,0,0]	0, $\bar{x},3/4$ [0,0,0]	0,x,3/4 [0,0,0]
8	g	2..1'	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]
			1/2,1/2, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2,z [0,0,0]	0,0,z+1/2 [0,0,0]

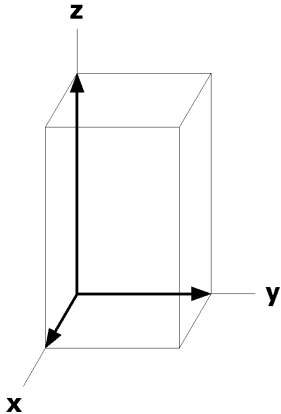
8	f	2..1'	0,1/2,z [0,0,0]	0,1/2,z+1/2 [0,0,0]	0,1/2, $\bar{z}$ +1/2 [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]
			1/2,0, $\bar{z}$ +1/2 [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	1/2,0,z [0,0,0]	1/2,0,z+1/2 [0,0,0]
8	e	$\bar{1}1'$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]
			3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]
4	d	$\bar{4}1'$	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
4	c	2.221'	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]
4	b	222.1'	0,0,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]	1/2,1/2,1/4 [0,0,0]	0,0,3/4 [0,0,0]
4	a	222.1'	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,1/4

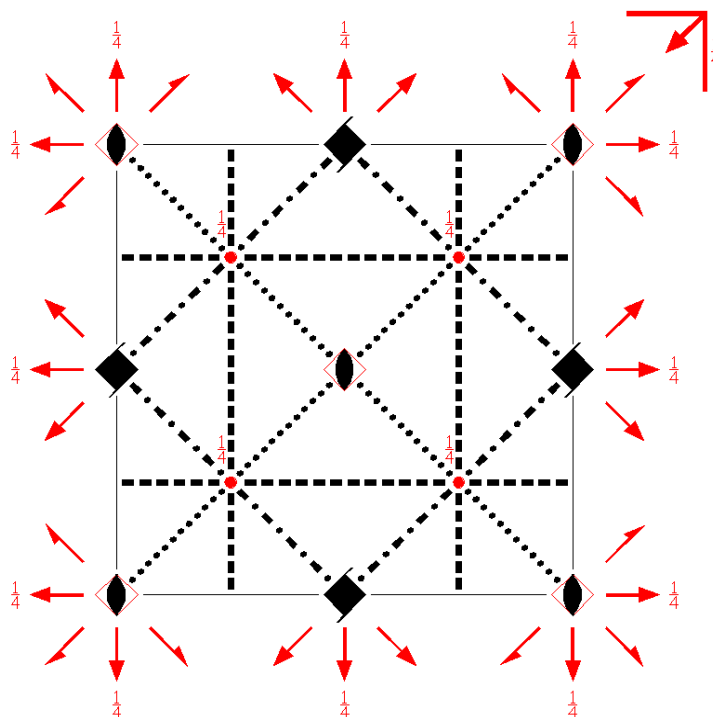
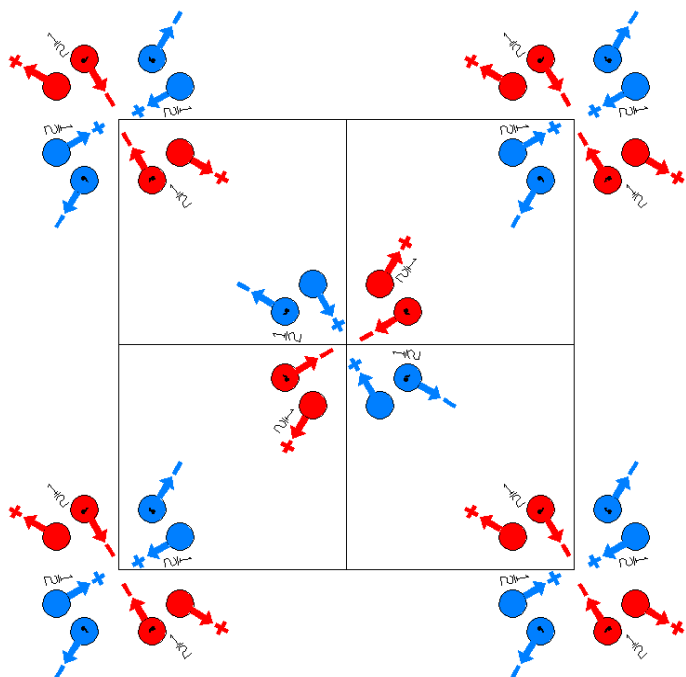
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P4_2/n'bc$   
133.3.1125

$4/m'mm$   
 $P4_2/n'2'/b2'/c$

Tetragonal



Origin at  $\bar{4}'12_1'/c$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |  |   |   |  |
|--|---|---|--|
| (1) $1$<br>( $1 0,0,0$ )                                   | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                        | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>( $4_z 1/2,1/2,1/2$ )    | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,1/2$ )    |
| (5) $2'$ $0,y,1/4$<br>( $2_y 0,0,1/2$ )'                   | (6) $2'$ $x,0,1/4$<br>( $2_x 0,0,1/2$ )'                  | (7) $2'$ $(1/2,1/2,0) x,x,0$<br>( $2_{xy} 1/2,1/2,0$ )'   | (8) $2'$ $x,\bar{x}+1/2,0$<br>( $2_{\bar{xy}} 1/2,1/2,0$ )'    |
| (9) $\bar{1}'$ $1/4,1/4,1/4$<br>( $\bar{1} 1/2,1/2,1/2$ )' | (10) $n'$ $(1/2,1/2,0) x,y,1/4$<br>( $m_z 1/2,1/2,1/2$ )' | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )' | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ )' |
| (13) $a$ $(1/2,0,0) x,1/4,z$<br>( $m_y 1/2,1/2,0$ )        | (14) $b$ $(0,1/2,0) 1/4,y,z$<br>( $m_x 1/2,1/2,0$ )       | (15) $c$ $(0,0,1/2) x,\bar{x},z$<br>( $m_{xy} 0,0,1/2$ )  | (16) $c$ $(0,0,1/2) x,x,z$<br>( $m_{\bar{xy}} 0,0,1/2$ )       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

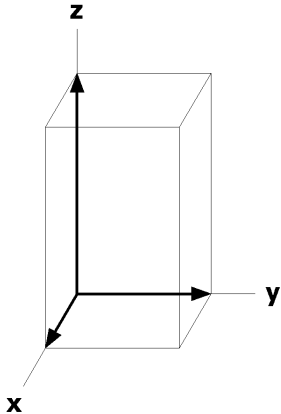
			Coordinates															
Multiplicity, Wyckoff letter, Site Symmetry.																		
16	k	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]	(5) $\bar{x},y,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(7) $y+1/2,x+1/2,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}$ [ $v,u,w$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(13) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y,x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	j	.2'	$x,x+1/2,0$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,0$ [ $u,\bar{u},w$ ]	$\bar{x},x+1/2,1/2$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x}+1/2,1/2$ [ $u,u,w$ ]	$\bar{x}+1/2,\bar{x},1/2$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x,1/2$ [ $\bar{u},u,\bar{w}$ ]	$x+1/2,\bar{x},0$ [ $u,u,\bar{w}$ ]	$\bar{x}+1/2,x,0$ [ $\bar{u},\bar{u},\bar{w}$ ]								
8	i	.2'	$x,0,3/4$ [0,v,w]	$\bar{x},0,3/4$ [0, $\bar{v},w$ ]	$1/2,x+1/2,1/4$ [ $\bar{v},0,w$ ]	$1/2,\bar{x}+1/2,1/4$ [ $v,0,w$ ]	$\bar{x}+1/2,1/2,3/4$ [0, $\bar{v},\bar{w}$ ]	$x+1/2,1/2,3/4$ [0,v, $\bar{w}$ ]	$0,\bar{x},1/4$ [ $v,0,\bar{w}$ ]	$0,x,1/4$ [ $\bar{v},0,\bar{w}$ ]								
8	h	.2'	$x,0,1/4$ [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	$1/2,x+1/2,3/4$ [ $\bar{v},0,w$ ]	$1/2,\bar{x}+1/2,3/4$ [ $v,0,w$ ]	$\bar{x}+1/2,1/2,1/4$ [0, $\bar{v},\bar{w}$ ]	$x+1/2,1/2,1/4$ [0,v, $\bar{w}$ ]	$0,\bar{x},3/4$ [ $v,0,\bar{w}$ ]	$0,x,3/4$ [ $\bar{v},0,\bar{w}$ ]								
8	g	2..	$0,0,z$ [0,0,w]	$1/2,1/2,z+1/2$ [0,0,w]	$0,0,\bar{z}+1/2$ [0,0,w]	$1/2,1/2,\bar{z}$ [0,0,w]	$1/2,1/2,\bar{z}+1/2$ [0,0, $\bar{w}$ ]	$0,0,\bar{z}$ [0,0, $\bar{w}$ ]	$1/2,1/2,z$ [0,0, $\bar{w}$ ]	$0,0,z+1/2$ [0,0, $\bar{w}$ ]								
8	f	2..	$0,1/2,z$ [0,0,w]	$0,1/2,z+1/2$ [0,0,w]	$0,1/2,\bar{z}+1/2$ [0,0,w]	$0,1/2,\bar{z}$ [0,0,w]	$1/2,0,\bar{z}+1/2$ [0,0, $\bar{w}$ ]	$1/2,0,\bar{z}$ [0,0, $\bar{w}$ ]	$1/2,0,z$ [0,0, $\bar{w}$ ]	$1/2,0,z+1/2$ [0,0, $\bar{w}$ ]								
8	e	$\bar{1}'$	$1/4,1/4,1/4$ [0,0,0]	$3/4,3/4,1/4$ [0,0,0]	$1/4,3/4,3/4$ [0,0,0]	$3/4,1/4,3/4$ [0,0,0]	$3/4,1/4,1/4$ [0,0,0]	$1/4,3/4,1/4$ [0,0,0]	$3/4,3/4,3/4$ [0,0,0]	$1/4,1/4,3/4$ [0,0,0]								
4	d	$\bar{4}'$	$0,0,0$ [0,0,0]	$1/2,1/2,1/2$ [0,0,0]	$0,0,1/2$ [0,0,0]	$1/2,1/2,0$ [0,0,0]												
4	c	2.2'2'	$0,1/2,0$ [0,0,w]	$0,1/2,1/2$ [0,0,w]	$1/2,0,1/2$ [0,0, $\bar{w}$ ]	$1/2,0,0$ [0,0, $\bar{w}$ ]												
4	b	22'2'	$0,0,1/4$ [0,0,w]	$1/2,1/2,3/4$ [0,0,w]	$1/2,1/2,1/4$ [0,0, $\bar{w}$ ]	$0,0,3/4$ [0,0, $\bar{w}$ ]												
4	a	22'2'	$0,1/2,1/4$ [0,0,w]	$0,1/2,3/4$ [0,0,w]	$1/2,0,1/4$ [0,0, $\bar{w}$ ]	$1/2,0,3/4$ [0,0, $\bar{w}$ ]												

**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,1/4,1/4

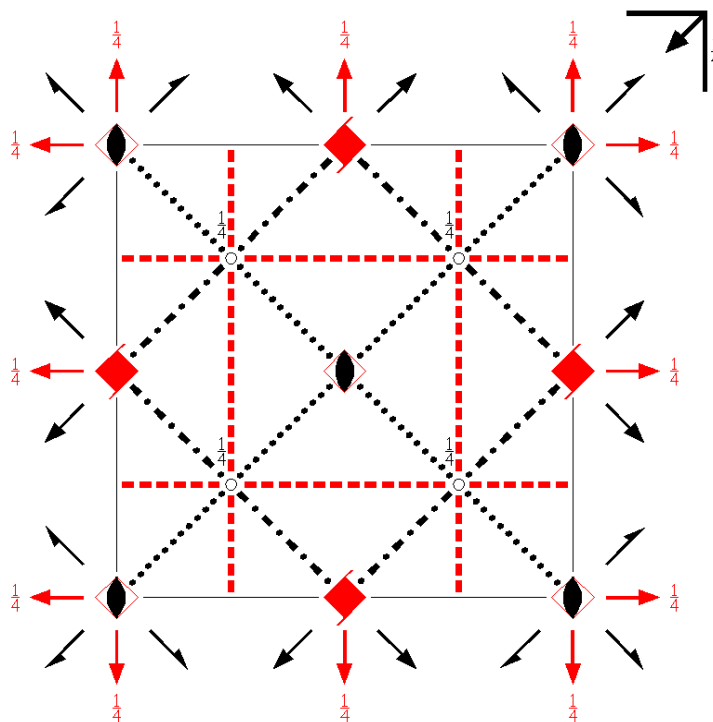
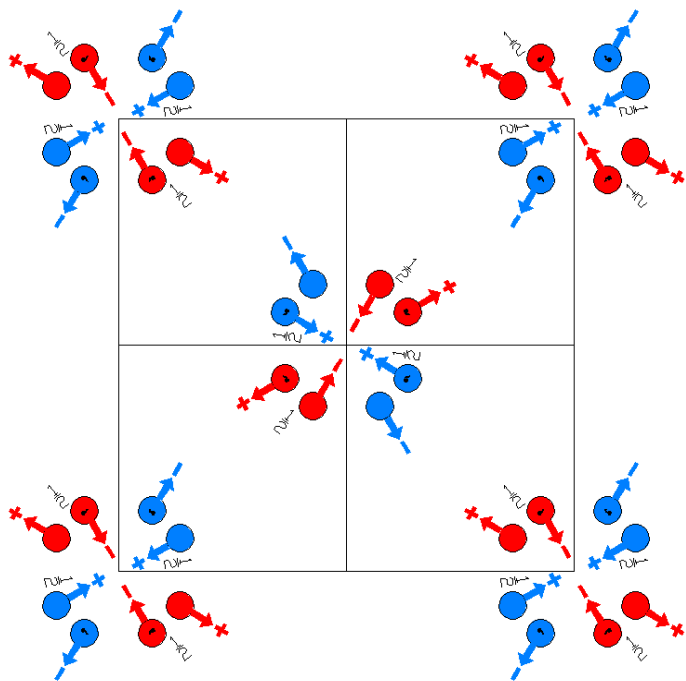
Along [1,1,0] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at x,x,1/4



$P4_2'/nb'c$   
133.4.1126

$4'/mm'm$   
 $P4_2'/n2'/b'2'/c$

Tetragonal



Origin at  $\bar{4}'12_1/c$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |  |   |   |  |
|--|---|---|--|
| (1) $1$<br>$(1 0,0,0)$                                 | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                      | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>$(4_z 1/2,1/2,1/2)'$   | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>$(4_z^{-1} 1/2,1/2,1/2)'$   |
| (5) $2'$ $0,y,1/4$<br>$(2_y 0,0,1/2)'$                 | (6) $2'$ $x,0,1/4$<br>$(2_x 0,0,1/2)'$                | (7) $2$ $(1/2,1/2,0) x,x,0$<br>$(2_{xy} 1/2,1/2,0)$     | (8) $2$ $x,\bar{x}+1/2,0$<br>$(2_{\bar{xy}} 1/2,1/2,0)$      |
| (9) $\bar{1}$ $1/4,1/4,1/4$<br>$(\bar{1} 1/2,1/2,1/2)$ | (10) $n$ $(1/2,1/2,0) x,y,1/4$<br>$(m_z 1/2,1/2,1/2)$ | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z 0,0,0)'$ | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1} 0,0,0)'$ |
| (13) $a'$ $(1/2,0,0) x,1/4,z$<br>$(m_y 1/2,1/2,0)'$    | (14) $b'$ $(0,1/2,0) 1/4,y,z$<br>$(m_x 1/2,1/2,0)'$   | (15) $c$ $(0,0,1/2) x,\bar{x},z$<br>$(m_{xy} 0,0,1/2)$  | (16) $c$ $(0,0,1/2) x,x,z$<br>$(m_{\bar{xy}} 0,0,1/2)$       |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

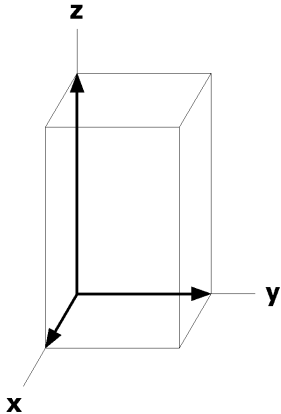
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	k	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [v, $\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x},y,\bar{z}+1/2$ [u, $\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ]		
			(7) $y+1/2,x+1/2,\bar{z}$ [v,u, $\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [u,v,w]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y,\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x+1/2,\bar{y}+1/2,z$ [u, $\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y},\bar{x},z+1/2$ [v,u, $\bar{w}$ ]	(16) $y,x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	j	..2	$x,x+1/2,0$ [u,u,0]	$\bar{x},\bar{x}+1/2,0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,1/2$ [u, $\bar{u},0$ ]	$x,\bar{x}+1/2,1/2$ [ $\bar{u},u,0$ ]
			$\bar{x}+1/2,\bar{x},1/2$ [u,u,0]	$x+1/2,x,1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},0$ [u, $\bar{u},0$ ]	$\bar{x}+1/2,x,0$ [ $\bar{u},u,0$ ]
8	i	.2'	$x,0,3/4$ [0,v,w]	$\bar{x},0,3/4$ [0, $\bar{v},w$ ]	$1/2,x+1/2,1/4$ [v,0, $\bar{w}$ ]	$1/2,\bar{x}+1/2,1/4$ [ $\bar{v},0,\bar{w}$ ]
			$\bar{x}+1/2,1/2,3/4$ [0,v,w]	$x+1/2,1/2,3/4$ [0, $\bar{v},w$ ]	$0,\bar{x},1/4$ [v,0, $\bar{w}$ ]	$0,x,1/4$ [ $\bar{v},0,\bar{w}$ ]
8	h	.2'	$x,0,1/4$ [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	$1/2,x+1/2,3/4$ [v,0, $\bar{w}$ ]	$1/2,\bar{x}+1/2,3/4$ [ $\bar{v},0,\bar{w}$ ]
			$\bar{x}+1/2,1/2,1/4$ [0,v,w]	$x+1/2,1/2,1/4$ [0, $\bar{v},w$ ]	$0,\bar{x},3/4$ [v,0, $\bar{w}$ ]	$0,x,3/4$ [ $\bar{v},0,\bar{w}$ ]
8	g	2..	$0,0,z$ [0,0,w]	$1/2,1/2,z+1/2$ [0,0, $\bar{w}$ ]	$0,0,\bar{z}+1/2$ [0,0,w]	$1/2,1/2,\bar{z}$ [0,0, $\bar{w}$ ]
			$1/2,1/2,\bar{z}+1/2$ [0,0,w]	$0,0,\bar{z}$ [0,0, $\bar{w}$ ]	$1/2,1/2,z$ [0,0,w]	$0,0,z+1/2$ [0,0, $\bar{w}$ ]
8	f	2..	$0,1/2,z$ [0,0,w]	$0,1/2,z+1/2$ [0,0, $\bar{w}$ ]	$0,1/2,\bar{z}+1/2$ [0,0,w]	$0,1/2,\bar{z}$ [0,0, $\bar{w}$ ]
			$1/2,0,\bar{z}+1/2$ [0,0,w]	$1/2,0,\bar{z}$ [0,0, $\bar{w}$ ]	$1/2,0,z$ [0,0,w]	$1/2,0,z+1/2$ [0,0, $\bar{w}$ ]
8	e	$\bar{1}$	$1/4,1/4,1/4$ [u,v,w]	$3/4,3/4,1/4$ [ $\bar{u},\bar{v},w$ ]	$1/4,3/4,3/4$ [v, $\bar{u},\bar{w}$ ]	$3/4,1/4,3/4$ [ $\bar{v},u,\bar{w}$ ]
			$3/4,1/4,1/4$ [u, $\bar{v},w$ ]	$1/4,3/4,1/4$ [ $\bar{u},v,w$ ]	$3/4,3/4,3/4$ [v,u, $\bar{w}$ ]	$1/4,1/4,3/4$ [ $\bar{v},\bar{u},\bar{w}$ ]
4	d	$\bar{4}'$	$0,0,0$ [0,0,0]	$1/2,1/2,1/2$ [0,0,0]	$0,0,1/2$ [0,0,0]	$1/2,1/2,0$ [0,0,0]
4	c	2.22	$0,1/2,0$ [0,0,0]	$0,1/2,1/2$ [0,0,0]	$1/2,0,1/2$ [0,0,0]	$1/2,0,0$ [0,0,0]
4	b	22'2'	$0,0,1/4$ [0,0,w]	$1/2,1/2,3/4$ [0,0, $\bar{w}$ ]	$1/2,1/2,1/4$ [0,0,w]	$0,0,3/4$ [0,0, $\bar{w}$ ]
4	a	22'2'	$0,1/2,1/4$ [0,0,w]	$0,1/2,3/4$ [0,0, $\bar{w}$ ]	$1/2,0,1/4$ [0,0,w]	$1/2,0,3/4$ [0,0, $\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p<sub>4</sub> 4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,0,1/4

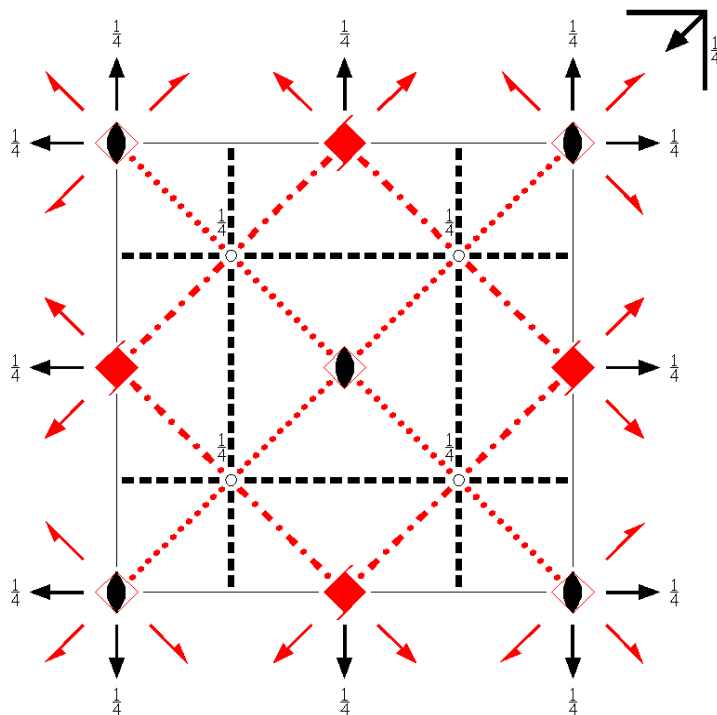
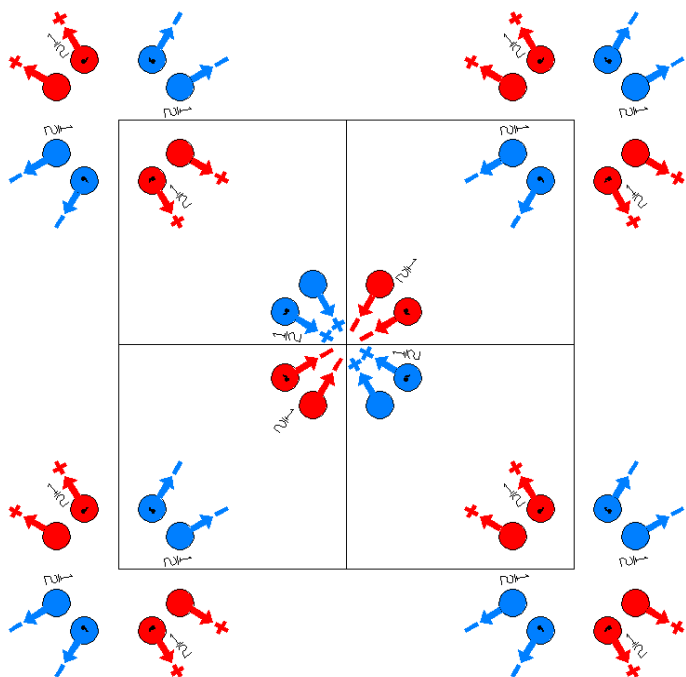
Along [1,1,0] p<sub>2a</sub> 2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at x,x,0



$P4_2'/nbc'$   
133.5.1127

$4'/mmm'$   
 $P4_2'/n2/b2'/c'$

Tetragonal



Origin at  $\bar{4}'12_1'/c'$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |  |   |  |  |
|--|---|--|--|
| (1) $1$<br>( $1 0,0,0$ )                                 | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                      | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>( $4_z 1/2,1/2,1/2$ )'    | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,1/2$ )'   |
| (5) $2$ $0,y,1/4$<br>( $2_y 0,0,1/2$ )                   | (6) $2$ $x,0,1/4$<br>( $2_x 0,0,1/2$ )                  | (7) $2'$ $(1/2,1/2,0) x,x,0$<br>( $2_{xy} 1/2,1/2,0$ )'    | (8) $2'$ $x,\bar{x}+1/2,0$<br>( $2_{\bar{xy}} 1/2,1/2,0$ )'    |
| (9) $\bar{1}$ $1/4,1/4,1/4$<br>( $\bar{1} 1/2,1/2,1/2$ ) | (10) $n$ $(1/2,1/2,0) x,y,1/4$<br>( $m_z 1/2,1/2,1/2$ ) | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )'  | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ )' |
| (13) $a$ $(1/2,0,0) x,1/4,z$<br>( $m_y 1/2,1/2,0$ )      | (14) $b$ $(0,1/2,0) 1/4,y,z$<br>( $m_x 1/2,1/2,0$ )     | (15) $c'$ $(0,0,1/2) x,\bar{x},z$<br>( $m_{xy} 0,0,1/2$ )' | (16) $c'$ $(0,0,1/2) x,x,z$<br>( $m_{\bar{xy}} 0,0,1/2$ )'     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

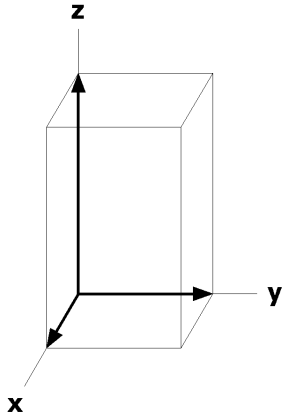
16	k	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}+1/2, x+1/2, z+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(4) $y+1/2, \bar{x}+1/2, z+1/2$ [ $\bar{v}, u, \bar{w}$ ]		
			(5) $\bar{x}, y, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(6) $x, \bar{y}, \bar{z}+1/2$ [ $u, \bar{v}, \bar{w}$ ]		
			(7) $y+1/2, x+1/2, \bar{z}$ [ $\bar{v}, \bar{u}, w$ ]	(8) $\bar{y}+1/2, \bar{x}+1/2, \bar{z}$ [ $v, u, w$ ]		
			(9) $\bar{x}+1/2, \bar{y}+1/2, \bar{z}+1/2$ [u,v,w]	(10) $x+1/2, y+1/2, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]		
			(11) $y, \bar{x}, \bar{z}$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(12) $\bar{y}, x, \bar{z}$ [ $\bar{v}, u, \bar{w}$ ]		
			(13) $x+1/2, \bar{y}+1/2, z$ [ $\bar{u}, v, \bar{w}$ ]	(14) $\bar{x}+1/2, y+1/2, z$ [ $u, \bar{v}, \bar{w}$ ]		
			(15) $\bar{y}, \bar{x}, z+1/2$ [ $\bar{v}, \bar{u}, w$ ]	(16) $y, x, z+1/2$ [ $v, u, w$ ]		
8	j	.2'	$x, x+1/2, 0$ [ $\bar{u}, u, w$ ]	$\bar{x}, \bar{x}+1/2, 0$ [ $u, \bar{u}, w$ ]	$\bar{x}, x+1/2, 1/2$ [ $u, u, \bar{w}$ ]	$x, \bar{x}+1/2, 1/2$ [ $\bar{u}, \bar{u}, \bar{w}$ ]
			$\bar{x}+1/2, \bar{x}, 1/2$ [ $\bar{u}, u, w$ ]	$x+1/2, x, 1/2$ [ $u, \bar{u}, w$ ]	$x+1/2, \bar{x}, 0$ [ $u, u, \bar{w}$ ]	$\bar{x}+1/2, x, 0$ [ $\bar{u}, \bar{u}, \bar{w}$ ]
8	i	.2.	$x, 0, 3/4$ [u,0,0]	$\bar{x}, 0, 3/4$ [ $\bar{u}, 0, 0$ ]	$1/2, x+1/2, 1/4$ [0, $\bar{u}, 0$ ]	$1/2, \bar{x}+1/2, 1/4$ [0,u,0]
			$\bar{x}+1/2, 1/2, 3/4$ [u,0,0]	$x+1/2, 1/2, 3/4$ [ $\bar{u}, 0, 0$ ]	$0, \bar{x}, 1/4$ [0, $\bar{u}, 0$ ]	$0, x, 1/4$ [0,u,0]
8	h	.2.	$x, 0, 1/4$ [u,0,0]	$\bar{x}, 0, 1/4$ [ $\bar{u}, 0, 0$ ]	$1/2, x+1/2, 3/4$ [0, $\bar{u}, 0$ ]	$1/2, \bar{x}+1/2, 3/4$ [0,u,0]
			$\bar{x}+1/2, 1/2, 1/4$ [u,0,0]	$x+1/2, 1/2, 1/4$ [ $\bar{u}, 0, 0$ ]	$0, \bar{x}, 3/4$ [0, $\bar{u}, 0$ ]	$0, x, 3/4$ [0,u,0]
8	g	2..	$0, 0, z$ [0,0,w]	$1/2, 1/2, z+1/2$ [0,0, $\bar{w}$ ]	$0, 0, \bar{z}+1/2$ [0,0,w]	$1/2, 1/2, \bar{z}$ [0,0, $\bar{w}$ ]
			$1/2, 1/2, \bar{z}+1/2$ [0,0,w]	$0, 0, \bar{z}$ [0,0, $\bar{w}$ ]	$1/2, 1/2, z$ [0,0,w]	$0, 0, z+1/2$ [0,0, $\bar{w}$ ]
8	f	2..	$0, 1/2, z$ [0,0,w]	$0, 1/2, z+1/2$ [0,0, $\bar{w}$ ]	$0, 1/2, \bar{z}+1/2$ [0,0,w]	$0, 1/2, \bar{z}$ [0,0, $\bar{w}$ ]
			$1/2, 0, \bar{z}+1/2$ [0,0,w]	$1/2, 0, \bar{z}$ [0,0, $\bar{w}$ ]	$1/2, 0, z$ [0,0,w]	$1/2, 0, z+1/2$ [0,0, $\bar{w}$ ]
8	e	$\bar{1}$	$1/4, 1/4, 1/4$ [u,v,w]	$3/4, 3/4, 1/4$ [ $\bar{u}, \bar{v}, w$ ]	$1/4, 3/4, 3/4$ [ $v, \bar{u}, \bar{w}$ ]	$3/4, 1/4, 3/4$ [ $\bar{v}, u, \bar{w}$ ]
			$3/4, 1/4, 1/4$ [ $\bar{u}, v, \bar{w}$ ]	$1/4, 3/4, 1/4$ [ $u, \bar{v}, \bar{w}$ ]	$3/4, 3/4, 3/4$ [ $\bar{v}, \bar{u}, w$ ]	$1/4, 1/4, 3/4$ [ $v, u, w$ ]
4	d	$\bar{4}'$	$0, 0, 0$ [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]	$0, 0, 1/2$ [0,0,0]	$1/2, 1/2, 0$ [0,0,0]
4	c	2.2'2'	$0, 1/2, 0$ [0,0,w]	$0, 1/2, 1/2$ [0,0, $\bar{w}$ ]	$1/2, 0, 1/2$ [0,0,w]	$1/2, 0, 0$ [0,0, $\bar{w}$ ]
4	b	222.	$0, 0, 1/4$ [0,0,0]	$1/2, 1/2, 3/4$ [0,0,0]	$1/2, 1/2, 1/4$ [0,0,0]	$0, 0, 3/4$ [0,0,0]
4	a	222.	$0, 1/2, 1/4$ [0,0,0]	$0, 1/2, 3/4$ [0,0,0]	$1/2, 0, 1/4$ [0,0,0]	$1/2, 0, 3/4$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub>-4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/2,0,z

Along [1,0,0] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,1/4

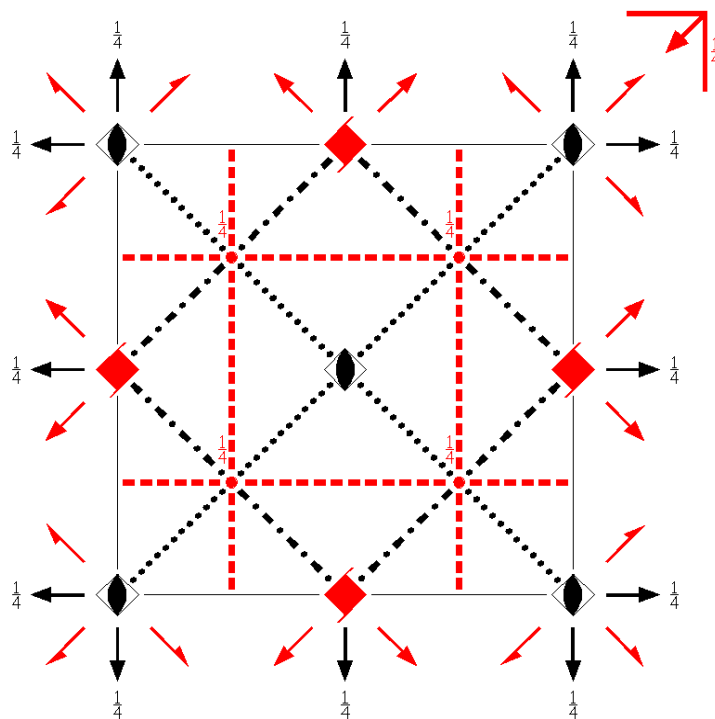
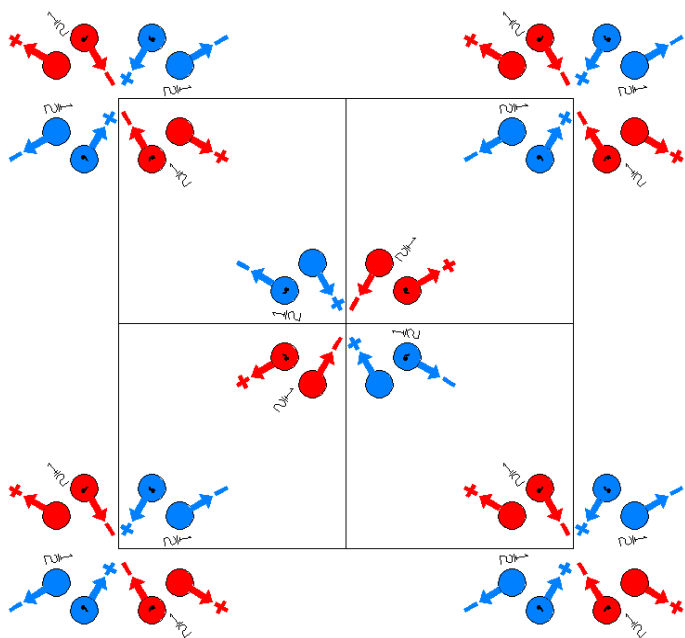
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P4_2'/n'b'c$   
133.6.1128

$4'/m'm'm$   
 $P4_2'/n'2/b'2'/c$

Tetragonal



Origin at  $\bar{4}12_1'/c$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |   |
|---|---|--|---|
| (1) $1$<br>$(1 0,0,0)$                                    | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                        | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>$(4_z 1/2,1/2,1/2)'$  | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>$(4_z^{-1} 1/2,1/2,1/2)'$  |
| (5) $2$ $0,y,1/4$<br>$(2_y 0,0,1/2)$                      | (6) $2$ $x,0,1/4$<br>$(2_x 0,0,1/2)$                    | (7) $2'$ $(1/2,1/2,0) x,x,0$<br>$(2_{xy} 1/2,1/2,0)'$  | (8) $2'$ $x,\bar{x}+1/2,0$<br>$(2_{\bar{xy}} 1/2,1/2,0)'$   |
| (9) $\bar{1}'$ $1/4,1/4,1/4$<br>$(\bar{1}' 1/2,1/2,1/2)'$ | (10) $n'$ $(1/2,1/2,0) x,y,1/4$<br>$(m_z 1/2,1/2,1/2)'$ | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z 0,0,0)$ | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1} 0,0,0)$ |
| (13) $a'$ $(1/2,0,0) x,1/4,z$<br>$(m_y 1/2,1/2,0)'$       | (14) $b'$ $(0,1/2,0) 1/4,y,z$<br>$(m_x 1/2,1/2,0)'$     | (15) $c$ $(0,0,1/2) x,\bar{x},z$<br>$(m_{xy} 0,0,1/2)$ | (16) $c$ $(0,0,1/2) x,x,z$<br>$(m_{\bar{xy}} 0,0,1/2)$      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y+1/2,x+1/2,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}$ [ $v,u,w$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]		
			(13) $x+1/2,\bar{y}+1/2,z$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y},\bar{x},z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y,x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	j	.2'	$x,x+1/2,0$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,0$ [ $u,\bar{u},w$ ]	$\bar{x},x+1/2,1/2$ [ $u,u,\bar{w}$ ]	$x,\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x}+1/2,\bar{x},1/2$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x,1/2$ [ $\bar{u},u,\bar{w}$ ]	$x+1/2,\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,0$ [ $u,u,w$ ]
8	i	.2.	$x,0,3/4$ [ $u,0,0$ ]	$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	$1/2,x+1/2,1/4$ [ $0,\bar{u},0$ ]	$1/2,\bar{x}+1/2,1/4$ [ $0,u,0$ ]
			$\bar{x}+1/2,1/2,3/4$ [ $\bar{u},0,0$ ]	$x+1/2,1/2,3/4$ [ $u,0,0$ ]	$0,\bar{x},1/4$ [ $0,u,0$ ]	$0,x,1/4$ [ $0,\bar{u},0$ ]
8	h	.2.	$x,0,1/4$ [ $u,0,0$ ]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	$1/2,x+1/2,3/4$ [ $0,\bar{u},0$ ]	$1/2,\bar{x}+1/2,3/4$ [ $0,u,0$ ]
			$\bar{x}+1/2,1/2,1/4$ [ $\bar{u},0,0$ ]	$x+1/2,1/2,1/4$ [ $u,0,0$ ]	$0,\bar{x},3/4$ [ $0,u,0$ ]	$0,x,3/4$ [ $0,\bar{u},0$ ]
8	g	2..	$0,0,z$ [ $0,0,w$ ]	$1/2,1/2,z+1/2$ [ $0,0,\bar{w}$ ]	$0,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$1/2,1/2,\bar{z}$ [ $0,0,w$ ]
			$1/2,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,0,\bar{z}$ [ $0,0,w$ ]	$1/2,1/2,z$ [ $0,0,w$ ]	$0,0,z+1/2$ [ $0,0,\bar{w}$ ]
8	f	2..	$0,1/2,z$ [ $0,0,w$ ]	$0,1/2,z+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}$ [ $0,0,w$ ]
			$1/2,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,w$ ]	$1/2,0,z+1/2$ [ $0,0,\bar{w}$ ]
8	e	$\bar{1}$ '	$1/4,1/4,1/4$ [ $0,0,0$ ]	$3/4,3/4,1/4$ [ $0,0,0$ ]	$1/4,3/4,3/4$ [ $0,0,0$ ]	$3/4,1/4,3/4$ [ $0,0,0$ ]
			$3/4,1/4,1/4$ [ $0,0,0$ ]	$1/4,3/4,1/4$ [ $0,0,0$ ]	$3/4,3/4,3/4$ [ $0,0,0$ ]	$1/4,1/4,3/4$ [ $0,0,0$ ]
4	d	$\bar{4}$	$0,0,0$ [ $0,0,w$ ]	$1/2,1/2,1/2$ [ $0,0,\bar{w}$ ]	$0,0,1/2$ [ $0,0,\bar{w}$ ]	$1/2,1/2,0$ [ $0,0,w$ ]
4	c	2.2'2'	$0,1/2,0$ [ $0,0,w$ ]	$0,1/2,1/2$ [ $0,0,\bar{w}$ ]	$1/2,0,1/2$ [ $0,0,\bar{w}$ ]	$1/2,0,0$ [ $0,0,w$ ]
4	b	222.	$0,0,1/4$ [ $0,0,0$ ]	$1/2,1/2,3/4$ [ $0,0,0$ ]	$1/2,1/2,1/4$ [ $0,0,0$ ]	$0,0,3/4$ [ $0,0,0$ ]
4	a	222.	$0,1/2,1/4$ [ $0,0,0$ ]	$0,1/2,3/4$ [ $0,0,0$ ]	$1/2,0,1/4$ [ $0,0,0$ ]	$1/2,0,3/4$ [ $0,0,0$ ]

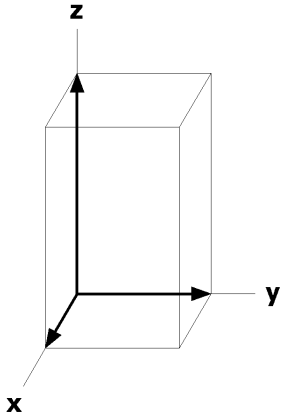
**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4'mm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,0,1/4$

Along  $[1,1,0]$   $p_{2a} 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at  $x,x,0$

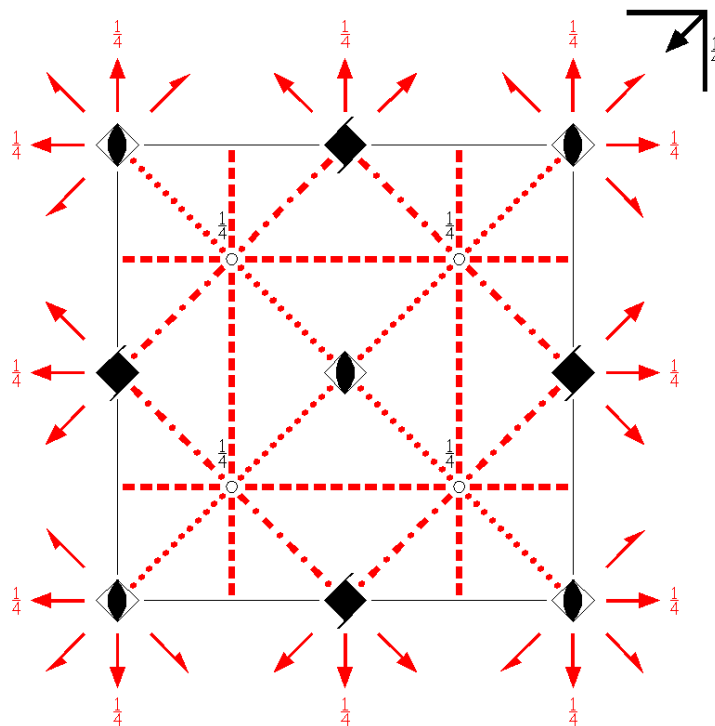
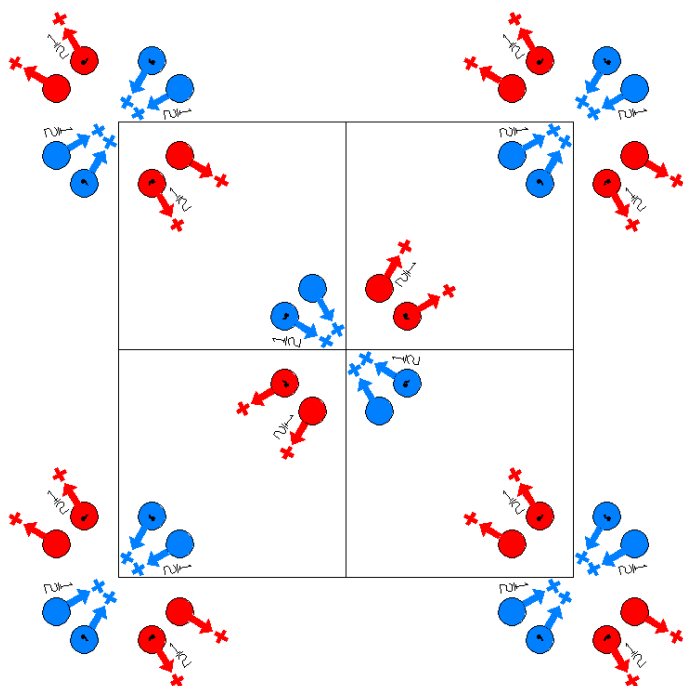




$P4_2/nb'c'$   
133.7.1129

$4/mm'm'$   
 $P4_2/n2'/b'2'/c'$

Tetragonal



Origin at  $\bar{4}12_1/c'$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |  |   |  |   |
|--|---|--|---|
| (1) $1$<br>( $1 0,0,0$ )                                 | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                      | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>( $4_z 1/2,1/2,1/2$ )     | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,1/2$ )   |
| (5) $2'$ $0,y,1/4$<br>( $2_y 0,0,1/2$ )'                 | (6) $2'$ $x,0,1/4$<br>( $2_x 0,0,1/2$ )'                | (7) $2'$ $(1/2,1/2,0) x,x,0$<br>( $2_{xy} 1/2,1/2,0$ )'    | (8) $2'$ $x,\bar{x}+1/2,0$<br>( $2_{\bar{xy}} 1/2,1/2,0$ )'   |
| (9) $\bar{1}$ $1/4,1/4,1/4$<br>( $\bar{1} 1/2,1/2,1/2$ ) | (10) $n$ $(1/2,1/2,0) x,y,1/4$<br>( $m_z 1/2,1/2,1/2$ ) | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )   | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ ) |
| (13) $a'$ $(1/2,0,0) x,1/4,z$<br>( $m_y 1/2,1/2,0$ )'    | (14) $b'$ $(0,1/2,0) 1/4,y,z$<br>( $m_x 1/2,1/2,0$ )'   | (15) $c'$ $(0,0,1/2) x,\bar{x},z$<br>( $m_{xy} 0,0,1/2$ )' | (16) $c'$ $(0,0,1/2) x,x,z$<br>( $m_{\bar{xy}} 0,0,1/2$ )'    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

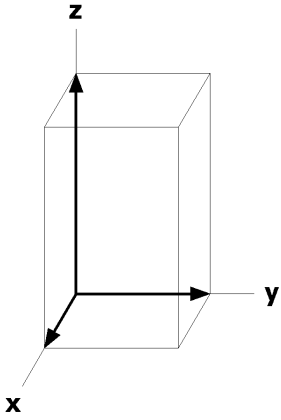
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ]		
			(7) $y+1/2,x+1/2,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}$ [ $v,u,w$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]		
			(13) $x+1/2,\bar{y}+1/2,z$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x,z+1/2$ [ $v,u,w$ ]		
8	j	.2'	$x,x+1/2,0$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,0$ [ $u,\bar{u},w$ ]	$\bar{x},x+1/2,1/2$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x}+1/2,1/2$ [ $u,u,w$ ]
			$\bar{x}+1/2,\bar{x},1/2$ [ $\bar{u},u,w$ ]	$x+1/2,x,1/2$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,0$ [ $u,u,w$ ]
8	i	.2'	$x,0,3/4$ [ $0,v,w$ ]	$\bar{x},0,3/4$ [ $0,\bar{v},w$ ]	$1/2,x+1/2,1/4$ [ $\bar{v},0,w$ ]	$1/2,\bar{x}+1/2,1/4$ [ $v,0,w$ ]
			$\bar{x}+1/2,1/2,3/4$ [ $0,v,w$ ]	$x+1/2,1/2,3/4$ [ $0,\bar{v},w$ ]	$0,\bar{x},1/4$ [ $\bar{v},0,w$ ]	$0,x,1/4$ [ $v,0,w$ ]
8	h	.2'	$x,0,1/4$ [ $0,v,w$ ]	$\bar{x},0,1/4$ [ $0,\bar{v},w$ ]	$1/2,x+1/2,3/4$ [ $\bar{v},0,w$ ]	$1/2,\bar{x}+1/2,3/4$ [ $v,0,w$ ]
			$\bar{x}+1/2,1/2,1/4$ [ $0,v,w$ ]	$x+1/2,1/2,1/4$ [ $0,\bar{v},w$ ]	$0,\bar{x},3/4$ [ $\bar{v},0,w$ ]	$0,x,3/4$ [ $v,0,w$ ]
8	g	2..	$0,0,z$ [ $0,0,w$ ]	$1/2,1/2,z+1/2$ [ $0,0,w$ ]	$0,0,\bar{z}+1/2$ [ $0,0,w$ ]	$1/2,1/2,\bar{z}$ [ $0,0,w$ ]
			$1/2,1/2,\bar{z}+1/2$ [ $0,0,w$ ]	$0,0,\bar{z}$ [ $0,0,w$ ]	$1/2,1/2,z$ [ $0,0,w$ ]	$0,0,z+1/2$ [ $0,0,w$ ]
8	f	2..	$0,1/2,z$ [ $0,0,w$ ]	$0,1/2,z+1/2$ [ $0,0,w$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,w$ ]	$0,1/2,\bar{z}$ [ $0,0,w$ ]
			$1/2,0,\bar{z}+1/2$ [ $0,0,w$ ]	$1/2,0,\bar{z}$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,w$ ]	$1/2,0,z+1/2$ [ $0,0,w$ ]
8	e	$\bar{1}$	$1/4,1/4,1/4$ [ $u,v,w$ ]	$3/4,3/4,1/4$ [ $\bar{u},\bar{v},w$ ]	$1/4,3/4,3/4$ [ $\bar{v},u,w$ ]	$3/4,1/4,3/4$ [ $v,\bar{u},w$ ]
			$3/4,1/4,1/4$ [ $u,\bar{v},w$ ]	$1/4,3/4,1/4$ [ $\bar{u},v,w$ ]	$3/4,3/4,3/4$ [ $\bar{v},\bar{u},w$ ]	$1/4,1/4,3/4$ [ $v,u,w$ ]
4	d	$\bar{4}$	$0,0,0$ [ $0,0,w$ ]	$1/2,1/2,1/2$ [ $0,0,w$ ]	$0,0,1/2$ [ $0,0,w$ ]	$1/2,1/2,0$ [ $0,0,w$ ]
4	c	2.2'2'	$0,1/2,0$ [ $0,0,w$ ]	$0,1/2,1/2$ [ $0,0,w$ ]	$1/2,0,1/2$ [ $0,0,w$ ]	$1/2,0,0$ [ $0,0,w$ ]
4	b	22'2'.	$0,0,1/4$ [ $0,0,w$ ]	$1/2,1/2,3/4$ [ $0,0,w$ ]	$1/2,1/2,1/4$ [ $0,0,w$ ]	$0,0,3/4$ [ $0,0,w$ ]
4	a	22'2'.	$0,1/2,1/4$ [ $0,0,w$ ]	$0,1/2,3/4$ [ $0,0,w$ ]	$1/2,0,1/4$ [ $0,0,w$ ]	$1/2,0,3/4$ [ $0,0,w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p<sub>g</sub> 4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 1/2,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,0,1/4

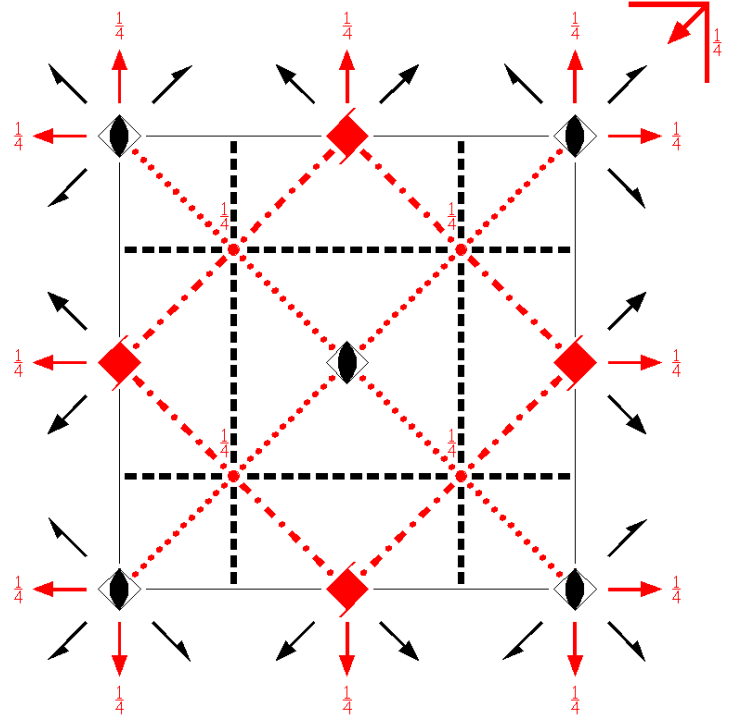
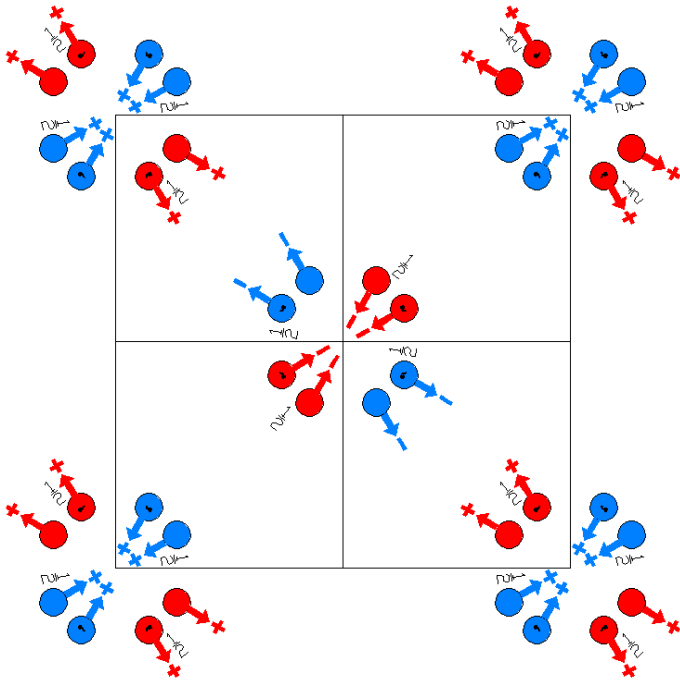
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at x,x,0



$P4_2'n'bc'$   
133.8.1130

$4'/m'mm'$   
 $P4_2'n'2'/b2/c'$

Tetragonal



Origin at  $\bar{4}12_1/c'$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |   |
|---|---|--|---|
| (1) $1$<br>( $1 0,0,0$ )                                    | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                        | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>( $4_z 1/2,1/2,1/2$ )'    | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,1/2$ )'  |
| (5) $2'$ $0,y,1/4$<br>( $2_y 0,0,1/2$ )'                    | (6) $2'$ $x,0,1/4$<br>( $2_x 0,0,1/2$ )'                  | (7) $2$ $(1/2,1/2,0) x,x,0$<br>( $2_{xy} 1/2,1/2,0$ )      | (8) $2$ $x,\bar{x}+1/2,0$<br>( $2_{\bar{xy}} 1/2,1/2,0$ )     |
| (9) $\bar{1}'$ $1/4,1/4,1/4$<br>( $\bar{1}' 1/2,1/2,1/2$ )' | (10) $n'$ $(1/2,1/2,0) x,y,1/4$<br>( $m_z 1/2,1/2,1/2$ )' | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )   | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ ) |
| (13) $a$ $(1/2,0,0) x,1/4,z$<br>( $m_y 1/2,1/2,0$ )         | (14) $b$ $(0,1/2,0) 1/4,y,z$<br>( $m_x 1/2,1/2,0$ )       | (15) $c'$ $(0,0,1/2) x,\bar{x},z$<br>( $m_{xy} 0,0,1/2$ )' | (16) $c'$ $(0,0,1/2) x,x,z$<br>( $m_{\bar{xy}} 0,0,1/2$ )'    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

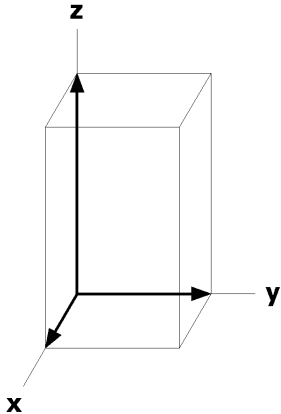
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
16	k	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]		
			(3) $\bar{y}+1/2, x+1/2, z+1/2$ [v, $\bar{u}, \bar{w}$ ]	(4) $y+1/2, \bar{x}+1/2, z+1/2$ [ $\bar{v}, u, \bar{w}$ ]		
			(5) $\bar{x}, y, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(6) $x, \bar{y}, \bar{z}+1/2$ [ $\bar{u}, v, w$ ]		
			(7) $y+1/2, x+1/2, \bar{z}$ [v,u, $\bar{w}$ ]	(8) $\bar{y}+1/2, \bar{x}+1/2, \bar{z}$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
			(9) $\bar{x}+1/2, \bar{y}+1/2, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(10) $x+1/2, y+1/2, \bar{z}+1/2$ [u,v, $\bar{w}$ ]		
			(11) $y, \bar{x}, \bar{z}$ [ $\bar{v}, u, w$ ]	(12) $\bar{y}, x, \bar{z}$ [v, $\bar{u}, w$ ]		
			(13) $x+1/2, \bar{y}+1/2, z$ [ $\bar{u}, v, \bar{w}$ ]	(14) $\bar{x}+1/2, y+1/2, z$ [u, $\bar{v}, \bar{w}$ ]		
			(15) $\bar{y}, \bar{x}, z+1/2$ [ $\bar{v}, \bar{u}, w$ ]	(16) $y, x, z+1/2$ [v,u,w]		
8	j	..2	$x, x+1/2, 0$ [u,u,0]	$\bar{x}, \bar{x}+1/2, 0$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}, x+1/2, 1/2$ [u, $\bar{u}, 0$ ]	$x, \bar{x}+1/2, 1/2$ [ $\bar{u}, u, 0$ ]
			$\bar{x}+1/2, \bar{x}, 1/2$ [ $\bar{u}, \bar{u}, 0$ ]	$x+1/2, x, 1/2$ [u,u,0]	$x+1/2, \bar{x}, 0$ [ $\bar{u}, u, 0$ ]	$\bar{x}+1/2, x, 0$ [u, $\bar{u}, 0$ ]
8	i	.2'	$x, 0, 3/4$ [0,v,w]	$\bar{x}, 0, 3/4$ [0, $\bar{v}, w$ ]	$1/2, x+1/2, 1/4$ [v,0, $\bar{w}$ ]	$1/2, \bar{x}+1/2, 1/4$ [ $\bar{v}, 0, \bar{w}$ ]
			$\bar{x}+1/2, 1/2, 3/4$ [0, $\bar{v}, \bar{w}$ ]	$x+1/2, 1/2, 3/4$ [0,v, $\bar{w}$ ]	$0, \bar{x}, 1/4$ [ $\bar{v}, 0, w$ ]	$0, x, 1/4$ [v,0,w]
8	h	.2'	$x, 0, 1/4$ [0,v,w]	$\bar{x}, 0, 1/4$ [0, $\bar{v}, w$ ]	$1/2, x+1/2, 3/4$ [v,0, $\bar{w}$ ]	$1/2, \bar{x}+1/2, 3/4$ [ $\bar{v}, 0, \bar{w}$ ]
			$\bar{x}+1/2, 1/2, 1/4$ [0, $\bar{v}, \bar{w}$ ]	$x+1/2, 1/2, 1/4$ [0,v, $\bar{w}$ ]	$0, \bar{x}, 3/4$ [ $\bar{v}, 0, w$ ]	$0, x, 3/4$ [v,0,w]
8	g	2..	$0, 0, z$ [0,0,w]	$1/2, 1/2, z+1/2$ [0,0, $\bar{w}$ ]	$0, 0, \bar{z}+1/2$ [0,0,w]	$1/2, 1/2, \bar{z}$ [0,0, $\bar{w}$ ]
			$1/2, 1/2, \bar{z}+1/2$ [0,0, $\bar{w}$ ]	$0, 0, \bar{z}$ [0,0,w]	$1/2, 1/2, z$ [0,0, $\bar{w}$ ]	$0, 0, z+1/2$ [0,0,w]
8	f	2..	$0, 1/2, z$ [0,0,w]	$0, 1/2, z+1/2$ [0,0, $\bar{w}$ ]	$0, 1/2, \bar{z}+1/2$ [0,0,w]	$0, 1/2, \bar{z}$ [0,0, $\bar{w}$ ]
			$1/2, 0, \bar{z}+1/2$ [0,0, $\bar{w}$ ]	$1/2, 0, \bar{z}$ [0,0,w]	$1/2, 0, z$ [0,0, $\bar{w}$ ]	$1/2, 0, z+1/2$ [0,0,w]
8	e	$\bar{1}'$	$1/4, 1/4, 1/4$ [0,0,0]	$3/4, 3/4, 1/4$ [0,0,0]	$1/4, 3/4, 3/4$ [0,0,0]	$3/4, 1/4, 3/4$ [0,0,0]
			$3/4, 1/4, 1/4$ [0,0,0]	$1/4, 3/4, 1/4$ [0,0,0]	$3/4, 3/4, 3/4$ [0,0,0]	$1/4, 1/4, 3/4$ [0,0,0]
4	d	$\bar{4}$	$0, 0, 0$ [0,0,w]	$1/2, 1/2, 1/2$ [0,0, $\bar{w}$ ]	$0, 0, 1/2$ [0,0,w]	$1/2, 1/2, 0$ [0,0, $\bar{w}$ ]
4	c	2.22	$0, 1/2, 0$ [0,0,0]	$0, 1/2, 1/2$ [0,0,0]	$1/2, 0, 1/2$ [0,0,0]	$1/2, 0, 0$ [0,0,0]
4	b	22'2'	$0, 0, 1/4$ [0,0,w]	$1/2, 1/2, 3/4$ [0,0, $\bar{w}$ ]	$1/2, 1/2, 1/4$ [0,0, $\bar{w}$ ]	$0, 0, 3/4$ [0,0,w]
4	a	22'2'	$0, 1/2, 1/4$ [0,0,w]	$0, 1/2, 3/4$ [0,0, $\bar{w}$ ]	$1/2, 0, 1/4$ [0,0, $\bar{w}$ ]	$1/2, 0, 3/4$ [0,0,w]

**Symmetry of Special Projections**

Along [0,0,1] p4'm'm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'-2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

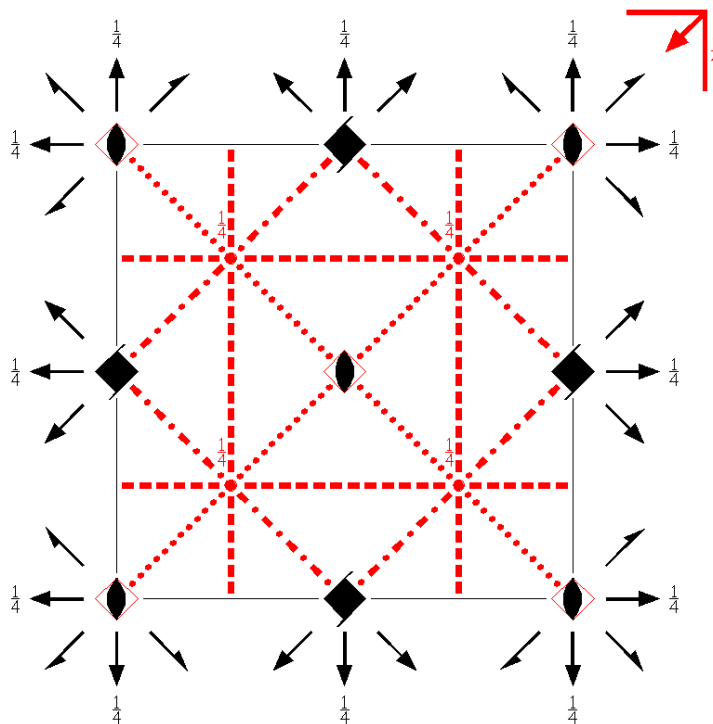
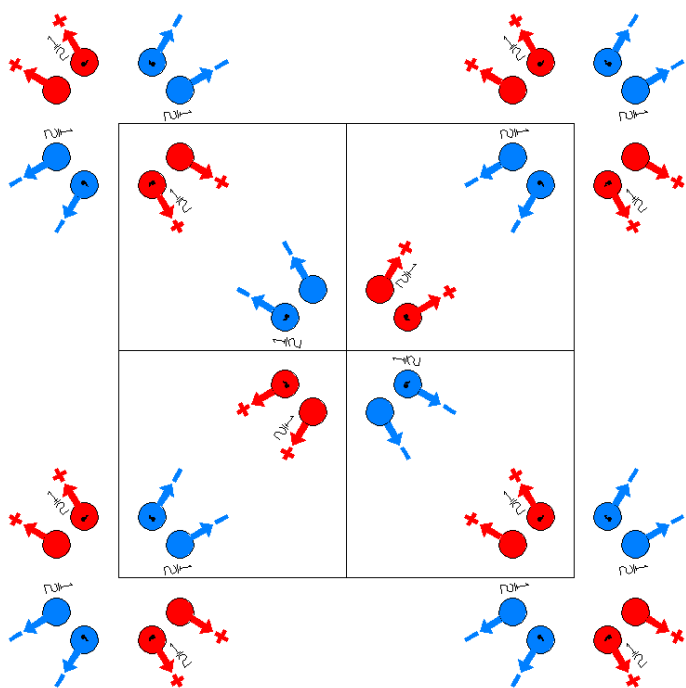
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P4_2/n'b'c'$   
133.9.1131

$4/m'm'm'$   
 $P4_2/n'2/b'2/c'$

Tetragonal



Origin at  $\bar{4}'12_1/c'$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |   |   |
|--|--|---|---|
| (1) $1$<br>( $1 0,0,0$ )                                   | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                       | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>( $4_z 1/2,1/2,1/2$ )    | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,1/2$ )   |
| (5) $2$ $0,y,1/4$<br>( $2_y 0,0,1/2$ )                     | (6) $2$ $x,0,1/4$<br>( $2_x 0,0,1/2$ )                   | (7) $2$ $(1/2,1/2,0) x,x,0$<br>( $2_{xy} 1/2,1/2,0$ )     | (8) $2$ $x,\bar{x}+1/2,0$<br>( $2_{\bar{xy}} 1/2,1/2,0$ )     |
| (9) $\bar{1}'$ $1/4,1/4,1/4$<br>( $\bar{1}' 1/2,1/2,1/2$ ) | (10) $n'$ $(1/2,1/2,0) x,y,1/4$<br>( $m_z 1/2,1/2,1/2$ ) | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )  | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ ) |
| (13) $a'$ $(1/2,0,0) x,1/4,z$<br>( $m_y 1/2,1/2,0$ )       | (14) $b'$ $(0,1/2,0) 1/4,y,z$<br>( $m_x 1/2,1/2,0$ )     | (15) $c'$ $(0,0,1/2) x,\bar{x},z$<br>( $m_{xy} 0,0,1/2$ ) | (16) $c'$ $(0,0,1/2) x,x,z$<br>( $m_{\bar{xy}} 0,0,1/2$ )     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y+1/2,x+1/2,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x+1/2,\bar{y}+1/2,z$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x,z+1/2$ [ $v,u,w$ ]		
8	j	.2	$x,x+1/2,0$ [ $u,u,0$ ]	$\bar{x},\bar{x}+1/2,0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,1/2$ [ $\bar{u},u,0$ ]	$x,\bar{x}+1/2,1/2$ [ $u,\bar{u},0$ ]
			$\bar{x}+1/2,\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x,1/2$ [ $u,u,0$ ]	$x+1/2,\bar{x},0$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x,0$ [ $\bar{u},u,0$ ]
8	i	.2.	$x,0,3/4$ [ $u,0,0$ ]	$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	$1/2,x+1/2,1/4$ [ $0,u,0$ ]	$1/2,\bar{x}+1/2,1/4$ [ $0,\bar{u},0$ ]
			$\bar{x}+1/2,1/2,3/4$ [ $\bar{u},0,0$ ]	$x+1/2,1/2,3/4$ [ $u,0,0$ ]	$0,\bar{x},1/4$ [ $0,\bar{u},0$ ]	$0,x,1/4$ [ $0,u,0$ ]
8	h	.2.	$x,0,1/4$ [ $u,0,0$ ]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	$1/2,x+1/2,3/4$ [ $0,u,0$ ]	$1/2,\bar{x}+1/2,3/4$ [ $0,\bar{u},0$ ]
			$\bar{x}+1/2,1/2,1/4$ [ $\bar{u},0,0$ ]	$x+1/2,1/2,1/4$ [ $u,0,0$ ]	$0,\bar{x},3/4$ [ $0,\bar{u},0$ ]	$0,x,3/4$ [ $0,u,0$ ]
8	g	2..	$0,0,z$ [ $0,0,w$ ]	$1/2,1/2,z+1/2$ [ $0,0,w$ ]	$0,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$1/2,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]
			$1/2,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,1/2,z$ [ $0,0,w$ ]	$0,0,z+1/2$ [ $0,0,w$ ]
8	f	2..	$0,1/2,z$ [ $0,0,w$ ]	$0,1/2,z+1/2$ [ $0,0,w$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]
			$1/2,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,0,z$ [ $0,0,w$ ]	$1/2,0,z+1/2$ [ $0,0,w$ ]
8	e	$\bar{1}'$	$1/4,1/4,1/4$ [ $0,0,0$ ]	$3/4,3/4,1/4$ [ $0,0,0$ ]	$1/4,3/4,3/4$ [ $0,0,0$ ]	$3/4,1/4,3/4$ [ $0,0,0$ ]
			$3/4,1/4,1/4$ [ $0,0,0$ ]	$1/4,3/4,1/4$ [ $0,0,0$ ]	$3/4,3/4,3/4$ [ $0,0,0$ ]	$1/4,1/4,3/4$ [ $0,0,0$ ]
4	d	$\bar{4}'$	$0,0,0$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]	$0,0,1/2$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]
4	c	2.22	$0,1/2,0$ [ $0,0,0$ ]	$0,1/2,1/2$ [ $0,0,0$ ]	$1/2,0,1/2$ [ $0,0,0$ ]	$1/2,0,0$ [ $0,0,0$ ]
4	b	222.	$0,0,1/4$ [ $0,0,0$ ]	$1/2,1/2,3/4$ [ $0,0,0$ ]	$1/2,1/2,1/4$ [ $0,0,0$ ]	$0,0,3/4$ [ $0,0,0$ ]
4	a	222.	$0,1/2,1/4$ [ $0,0,0$ ]	$0,1/2,3/4$ [ $0,0,0$ ]	$1/2,0,1/4$ [ $0,0,0$ ]	$1/2,0,3/4$ [ $0,0,0$ ]

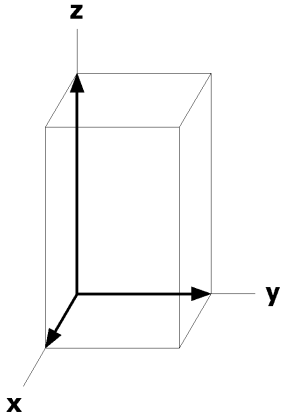


**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,0,1/4$

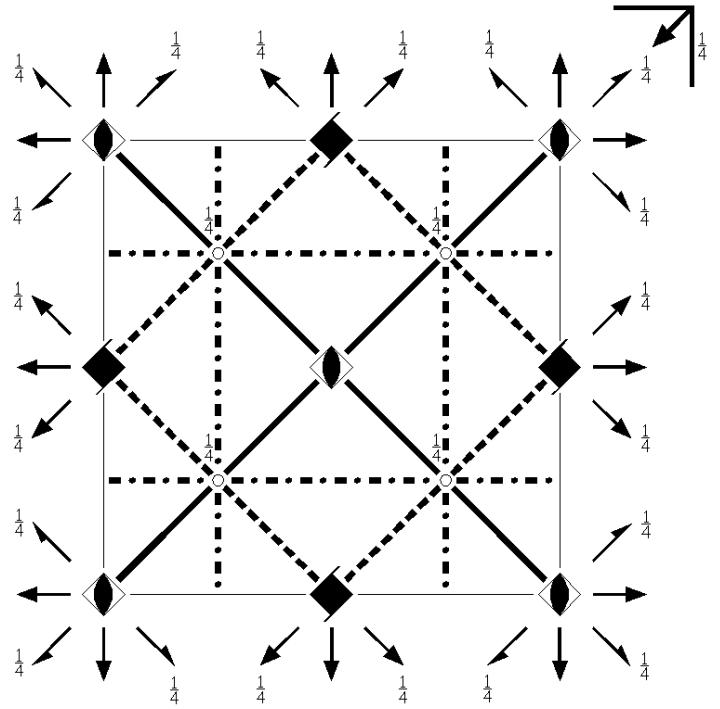
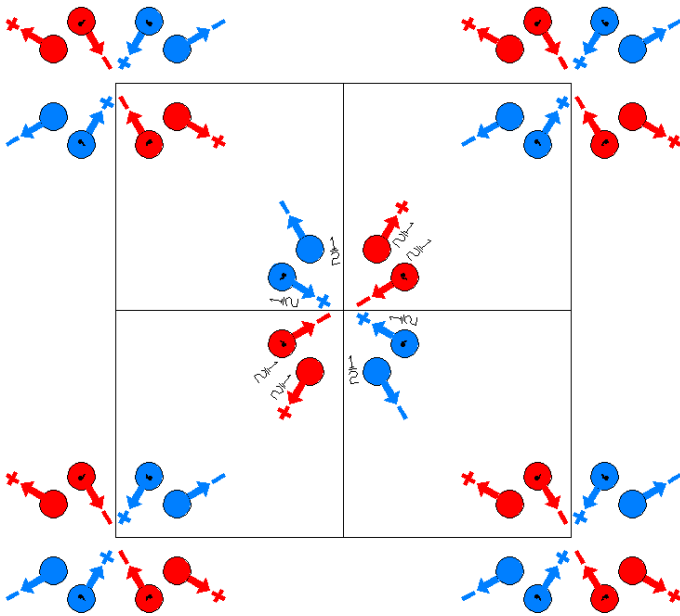
Along  $[1,1,0]$   $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at  $x,x,0$



$P4_2/nm$   
134.1.1132

$4/mmm$   
 $P4_2/n2/n2/m$

Tetragonal



Origin at  $\bar{4}2m$  at  $-1/4, 1/4, -1/4$  from center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$ ;  $x \leq y$ ;  $y \leq 1-x$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                      | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                      | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)           | (8) 2 x, $\bar{x}+1/2,1/4$<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)     |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)      | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)              | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                            |
| (13) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (14) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (15) m x, $\bar{x},z$<br>(m <sub>xy</sub>  0,0,0)                     | (16) m x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,0)                         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	n	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(16) $y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	m	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,z+1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,z+1/2$ [ $u,u,0$ ]
			$\bar{x},x,\bar{z}$ [ $u,u,0$ ]	$x,\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x+1/2,\bar{z}+1/2$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]
8	l	..2	x,x+1/2,3/4 [u,u,0]	$\bar{x},\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,1/4$ [ $\bar{u},u,0$ ]	$x,\bar{x}+1/2,1/4$ [ $u,\bar{u},0$ ]
			$\bar{x}+1/2,\bar{x},3/4$ [u,u,0]	$x+1/2,x,3/4$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},1/4$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,x,1/4$ [ $u,\bar{u},0$ ]
8	k	..2	x,x+1/2,1/4 [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,3/4$ [ $\bar{u},u,0$ ]	$x,\bar{x}+1/2,3/4$ [ $u,\bar{u},0$ ]
			$\bar{x}+1/2,\bar{x},1/4$ [u,u,0]	$x+1/2,x,1/4$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},3/4$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,x,3/4$ [ $u,\bar{u},0$ ]
8	j	..2	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	1/2,x+1/2,0 [0,u,0]	1/2, $\bar{x}+1/2,0$ [0, $\bar{u},0$ ]
			$\bar{x}+1/2,1/2,0$ [u,0,0]	$x+1/2,1/2,0$ [ $\bar{u},0,0$ ]	0, $\bar{x},1/2$ [0,u,0]	0,x,1/2 [0, $\bar{u},0$ ]
8	i	..2	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	1/2,x+1/2,1/2 [0,u,0]	1/2, $\bar{x}+1/2,1/2$ [0, $\bar{u},0$ ]
			$\bar{x}+1/2,1/2,1/2$ [u,0,0]	$x+1/2,1/2,1/2$ [ $\bar{u},0,0$ ]	0, $\bar{x},0$ [0,u,0]	0,x,0 [0, $\bar{u},0$ ]
8	h	2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
			1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	1/2,0,z [0,0, $\bar{w}$ ]
4	g	2.mm	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]
4	f	..2/m	3/4,3/4,3/4 [ $\bar{u},u,0$ ]	1/4,1/4,3/4 [ $u,\bar{u},0$ ]	3/4,1/4,1/4 [ $\bar{u},\bar{u},0$ ]	1/4,3/4,1/4 [ $u,u,0$ ]
4	e	..2/m	1/4,1/4,1/4 [ $\bar{u},u,0$ ]	3/4,3/4,1/4 [ $u,\bar{u},0$ ]	1/4,3/4,3/4 [ $\bar{u},\bar{u},0$ ]	3/4,1/4,3/4 [ $u,u,0$ ]
4	d	2.22	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]

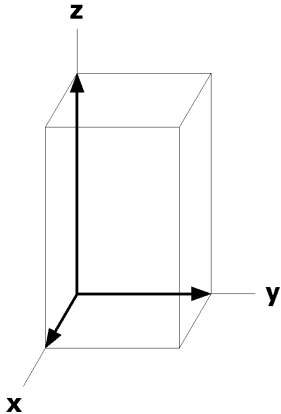
4	c	222.	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]
2	b	$\overline{4}2m$	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a	$\overline{4}2m$	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>g</sub>-4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/2,0,z

Along [1,0,0] c<sub>g</sub>-2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



$P4_2/nm1'$

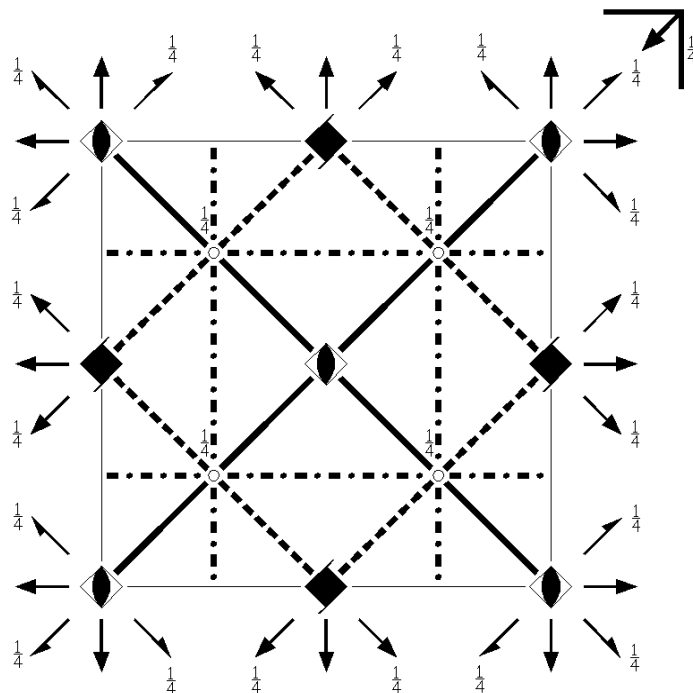
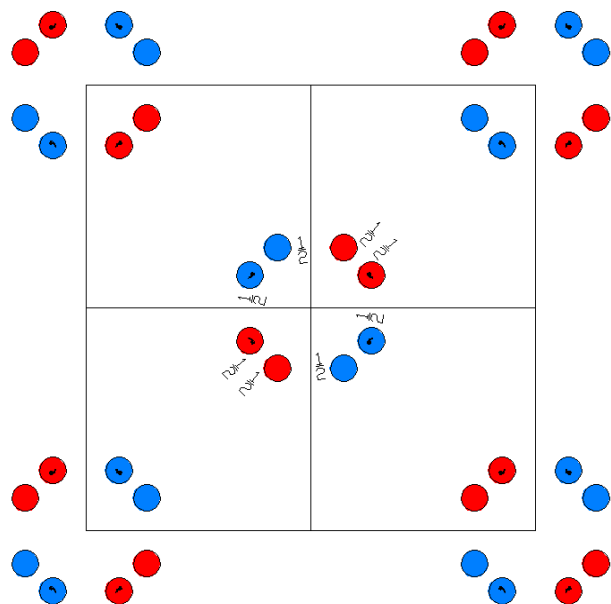
134.2.1133

$4/mmm1'$

$P4_2/n2/n2/m1'$

Tetragonal

$1'$



Origin at  $\bar{4}2m1'$  at  $-1/4, 1/4, -1/4$  from center ( $2/m1'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4; x \leq y; y \leq 1-x$

### Symmetry Operations

For 1 + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub> <sup>+</sup>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-</sup>  1/2,1/2,1/2) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                      | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                      | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)                        | (8) 2 x, $\bar{x}+1/2,1/4$<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)    |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)      | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)                           | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                           |
| (13) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (14) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (15) m x, $\bar{x},z$<br>(m <sub>xy</sub>  0,0,0)                                  | (16) m x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,0)                        |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)'	(4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'
(5) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(6) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'	(7) 2' (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(8) 2' x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)'
(9) $\bar{1}$ ' 1/4,1/4,1/4 ( $\bar{1}$  1/2,1/2,1/2)'	(10) n' (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>  1/2,1/2,1/2)'	(11) $\bar{4}^+$ ' 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'	(12) $\bar{4}^-$ ' 0,0,z; 0,0,0 ( $\bar{4}_z^{-1}$  0,0,0)'
(13) n' (1/2,0,1/2) x,1/4,z (m <sub>y</sub>  1/2,1/2,1/2)'	(14) n' (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1/2)'	(15) m' x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)'	(16) m' x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	n	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [0,0,0]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [0,0,0]		
			(5) $\bar{x},y,\bar{z}$ [0,0,0]	(6) $x,\bar{y},\bar{z}$ [0,0,0]		
			(7) $y+1/2,x+1/2,\bar{z}+1/2$ [0,0,0]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [0,0,0]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [0,0,0]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [0,0,0]		
			(11) $y,\bar{x},\bar{z}$ [0,0,0]	(12) $\bar{y},x,\bar{z}$ [0,0,0]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [0,0,0]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [0,0,0]		
			(15) $\bar{y},\bar{x},z$ [0,0,0]	(16) $y,x,z$ [0,0,0]		
8	m	..m1'	x,x,z [0,0,0]	$\bar{x},\bar{x},z$ [0,0,0]	$\bar{x}+1/2,x+1/2,z+1/2$ [0,0,0]	$x+1/2,\bar{x}+1/2,z+1/2$ [0,0,0]
			$\bar{x},x,\bar{z}$ [0,0,0]	$x,\bar{x},\bar{z}$ [0,0,0]	$x+1/2,x+1/2,\bar{z}+1/2$ [0,0,0]	$\bar{x}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [0,0,0]
8	l	..21'	x,x+1/2,3/4 [0,0,0]	$\bar{x},\bar{x}+1/2,3/4$ [0,0,0]	$\bar{x},x+1/2,1/4$ [0,0,0]	$x,\bar{x}+1/2,1/4$ [0,0,0]
			$\bar{x}+1/2,\bar{x},3/4$ [0,0,0]	$x+1/2,x,3/4$ [0,0,0]	$x+1/2,\bar{x},1/4$ [0,0,0]	$\bar{x}+1/2,x,1/4$ [0,0,0]
8	k	..21'	x,x+1/2,1/4 [0,0,0]	$\bar{x},\bar{x}+1/2,1/4$ [0,0,0]	$\bar{x},x+1/2,3/4$ [0,0,0]	$x,\bar{x}+1/2,3/4$ [0,0,0]
			$\bar{x}+1/2,\bar{x},1/4$ [0,0,0]	$x+1/2,x,1/4$ [0,0,0]	$x+1/2,\bar{x},3/4$ [0,0,0]	$\bar{x}+1/2,x,3/4$ [0,0,0]
8	j	..2.1'	x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]	1/2,x+1/2,0 [0,0,0]	1/2, $\bar{x}+1/2,0$ [0,0,0]
			$\bar{x}+1/2,1/2,0$ [0,0,0]	$x+1/2,1/2,0$ [0,0,0]	0, $\bar{x},1/2$ [0,0,0]	0,x,1/2 [0,0,0]

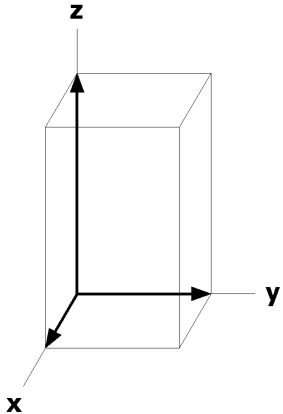
8	i	.2.1'	x,0,0 [0,0,0] $\bar{x}+1/2,1/2,1/2$ [0,0,0]	$\bar{x},0,0$ [0,0,0] x+1/2,1/2,1/2 [0,0,0]	1/2,x+1/2,1/2 [0,0,0] 0, $\bar{x},0$ [0,0,0]	1/2, $\bar{x}+1/2,1/2$ [0,0,0] 0,x,0 [0,0,0]
8	h	2..1'	0,1/2,z [0,0,0] 1/2,0, $\bar{z}+1/2$ [0,0,0]	0,1/2,z+1/2 [0,0,0] 1/2,0, $\bar{z}$ [0,0,0]	0,1/2, $\bar{z}$ [0,0,0] 1/2,0,z+1/2 [0,0,0]	0,1/2, $\bar{z}+1/2$ [0,0,0] 1/2,0,z [0,0,0]
4	g	2.mm1'	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]
4	f	..2/m1'	3/4,3/4,3/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]
4	e	..2/m1'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]
4	d	2.221'	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]
4	c	222.1'	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]
2	b	$\bar{4}2m1'$	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a	$\bar{4}2m1'$	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

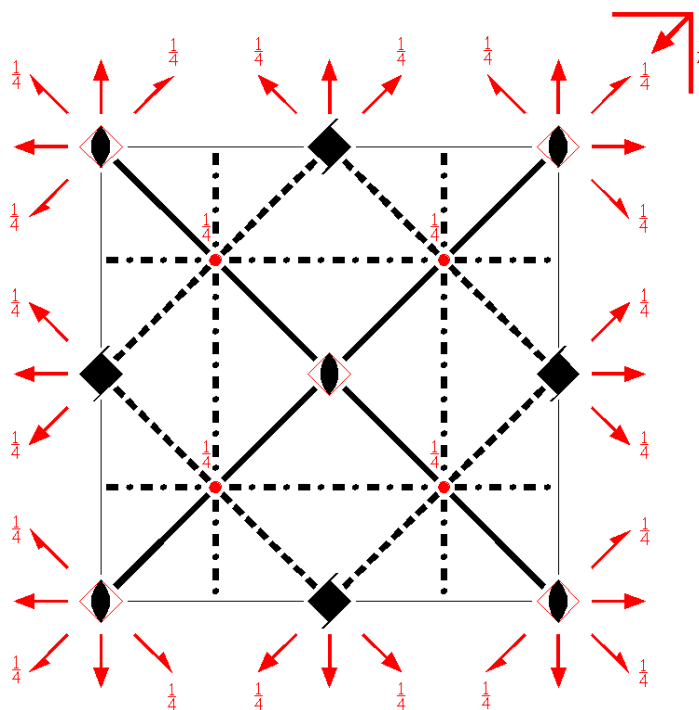
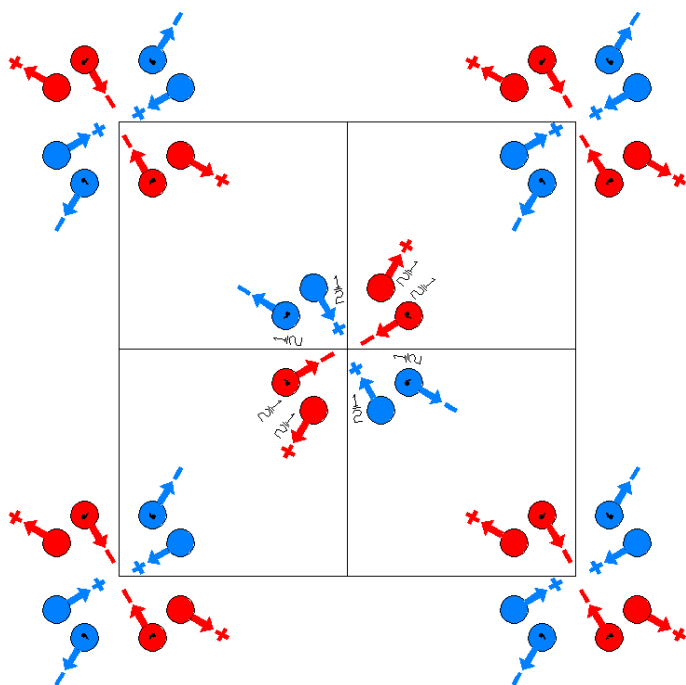
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



$P4_2/n'm$   
134.3.1134

$4/m'mm$   
 $P4_2/n'2'/n2'/m$

Tetragonal



Origin at  $\bar{4}'2'm$  at  $-1/4, 1/4, -1/4$  from center ( $2'/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4; x \leq y; y \leq 1-x$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) $1$<br>( $1 0,0,0$ )                                    | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                          | (3) $4^+$ $(0,0,1/2)$ $0,1/2,z$<br>( $4_z 1/2,1/2,1/2$ )      | (4) $4^-$ $(0,0,1/2)$ $1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,1/2$ )   |
| (5) $2'$ $0,y,0$<br>( $2_y 0,0,0$ )'                        | (6) $2'$ $x,0,0$<br>( $2_x 0,0,0$ )'                        | (7) $2'$ $(1/2,1/2,0)$ $x,x,1/4$<br>( $2_{xy} 1/2,1/2,1/2$ )' | (8) $2'$ $x,\bar{x}+1/2,1/4$<br>( $2_{\bar{xy}} 1/2,1/2,1/2$ )' |
| (9) $\bar{1}'$ $1/4,1/4,1/4$<br>( $\bar{1}' 1/2,1/2,1/2$ )' | (10) $n'$ $(1/2,1/2,0)$ $x,y,1/4$<br>( $m_z 1/2,1/2,1/2$ )' | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )'     | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ )'  |
| (13) $n$ $(1/2,0,1/2)$ $x,1/4,z$<br>( $m_y 1/2,1/2,1/2$ )   | (14) $n$ $(0,1/2,1/2)$ $1/4,y,z$<br>( $m_x 1/2,1/2,1/2$ )   | (15) $m$ $x,\bar{x},z$<br>( $m_{xy} 0,0,0$ )                  | (16) $m$ $x,x,z$<br>( $m_{\bar{xy}} 0,0,0$ )                    |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	n	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},z$ [ $\bar{u},v,w$ ]		
			(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $v,u,w$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,z$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(16) $y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	m	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,z+1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,z+1/2$ [ $u,u,0$ ]
			$\bar{x},x,\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},z$ [ $u,u,0$ ]	$x+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $u,\bar{u},0$ ]
8	l	..2'	x,x+1/2,3/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,3/4$ [ $u,\bar{u},w$ ]	$\bar{x},x+1/2,1/4$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x}+1/2,1/4$ [ $u,u,w$ ]
			$\bar{x}+1/2,\bar{x},3/4$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x,3/4$ [ $\bar{u},u,\bar{w}$ ]	$x+1/2,\bar{x},1/4$ [ $u,u,\bar{w}$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	k	..2'	x,x+1/2,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $u,\bar{u},w$ ]	$\bar{x},x+1/2,3/4$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x}+1/2,3/4$ [ $u,u,w$ ]
			$\bar{x}+1/2,\bar{x},1/4$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x,1/4$ [ $\bar{u},u,\bar{w}$ ]	$x+1/2,\bar{x},3/4$ [ $u,u,\bar{w}$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	j	..2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	1/2,x+1/2,0 [ $\bar{v},0,w$ ]	1/2, $\bar{x}+1/2,0$ [ $v,0,w$ ]
			$\bar{x}+1/2,1/2,0$ [0, $\bar{v},\bar{w}$ ]	$x+1/2,1/2,0$ [0,v, $\bar{w}$ ]	0, $\bar{x},1/2$ [ $v,0,\bar{w}$ ]	0,x,1/2 [ $\bar{v},0,\bar{w}$ ]
8	i	..2'	x,0,0 [0,v,w]	$\bar{x},0,0$ [0, $\bar{v},w$ ]	1/2,x+1/2,1/2 [ $\bar{v},0,w$ ]	1/2, $\bar{x}+1/2,1/2$ [ $v,0,w$ ]
			$\bar{x}+1/2,1/2,1/2$ [0, $\bar{v},\bar{w}$ ]	$x+1/2,1/2,1/2$ [0,v, $\bar{w}$ ]	0, $\bar{x},0$ [ $v,0,\bar{w}$ ]	0,x,0 [ $\bar{v},0,\bar{w}$ ]
8	h	2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]
			1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	1/2,0,z [0,0, $\bar{w}$ ]
4	g	2.mm	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]
4	f	..2'/m	3/4,3/4,3/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]
4	e	..2'/m	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]
4	d	2.2'2'	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0,w]	1/2,0,1/4 [0,0, $\bar{w}$ ]	1/2,0,3/4 [0,0, $\bar{w}$ ]

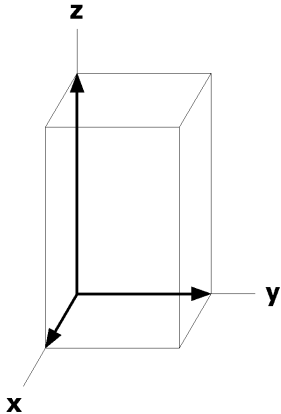
4	c	22'2'.	0,1/2,0 [0,0,w]	0,1/2,1/2 [0,0,w]	1/2,0,1/2 [0,0, $\bar{w}$ ]	1/2,0,0 [0,0, $\bar{w}$ ]
2	b	$\bar{4}$ '2'm	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a	$\bar{4}$ '2'm	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c<sub>2v</sub>' 2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

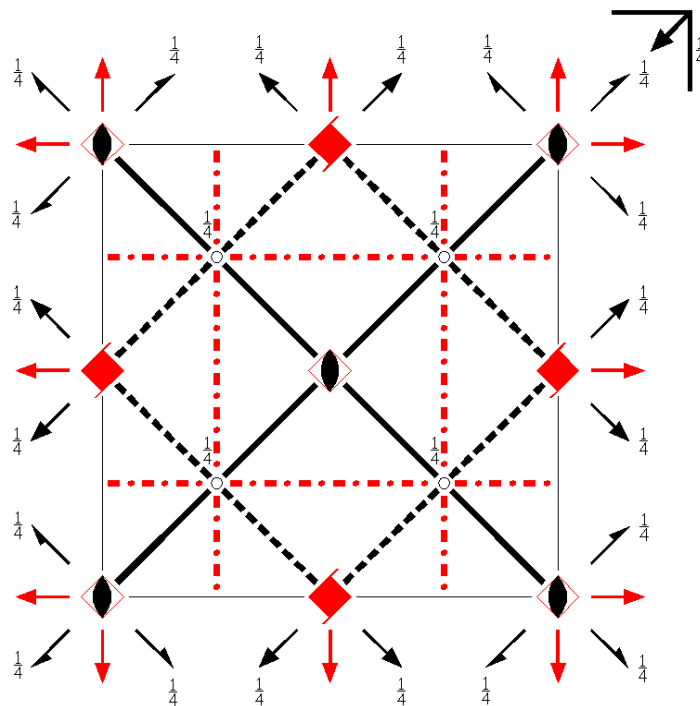
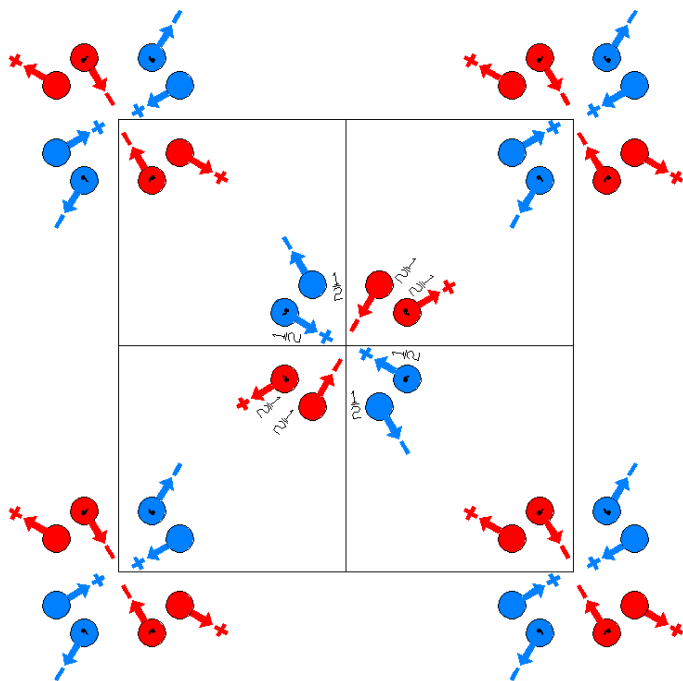
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



$P4_2'/nn'm$   
134.4.1135

$4'/mm'm$   
 $P4_2'/n2'/n'2'/m$

Tetragonal



Origin at  $\bar{4}'2'm$  at  $-1/4, 1/4, -1/4$  from center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4; x \leq y; y \leq 1-x$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                        | (3) $4^+ 1$ (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub> <sup>+</sup>  1/2,1/2,1/2)' | (4) $4^- 1$ (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-</sup>  1/2,1/2,1/2)'     |
| (5) 2' 0,y,0<br>(2 <sub>y</sub> ' 0,0,0)'                     | (6) 2' x,0,0<br>(2 <sub>x</sub> ' 0,0,0)'                     | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)                  | (8) 2 $x, \bar{x}+1/2, 1/4$<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2) |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)        | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)   | (11) $\bar{4}^+ 1$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'                  | (12) $\bar{4}^- 1$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                      |
| (13) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (14) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (15) m $x, \bar{x}, z$<br>(m <sub>xy</sub>  0,0,0)                           | (16) m x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,0)                      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	n	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]		
			(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y},\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]	(16) $y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	m	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,z+1/2$ [ $u,u,0$ ]	$x+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},x,\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},\bar{z}$ [ $u,u,0$ ]	$x+1/2,x+1/2,\bar{z}+1/2$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{u},u,0$ ]
8	l	..2	x,x+1/2,3/4 [ $u,u,0$ ]	$\bar{x},\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,1/4$ [ $u,\bar{u},0$ ]	$x,\bar{x}+1/2,1/4$ [ $\bar{u},u,0$ ]
			$\bar{x}+1/2,\bar{x},3/4$ [ $u,u,0$ ]	$x+1/2,x,3/4$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},1/4$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},u,0$ ]
8	k	..2	x,x+1/2,1/4 [ $u,u,0$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,3/4$ [ $u,\bar{u},0$ ]	$x,\bar{x}+1/2,3/4$ [ $\bar{u},u,0$ ]
			$\bar{x}+1/2,\bar{x},1/4$ [ $u,u,0$ ]	$x+1/2,x,1/4$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},3/4$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},u,0$ ]
8	j	..2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	1/2,x+1/2,0 [v,0, $\bar{w}$ ]	1/2, $\bar{x}+1/2,0$ [ $\bar{v},0,\bar{w}$ ]
			$\bar{x}+1/2,1/2,0$ [0,v,w]	$x+1/2,1/2,0$ [0, $\bar{v},w$ ]	0, $\bar{x},1/2$ [v,0, $\bar{w}$ ]	0,x,1/2 [ $\bar{v},0,\bar{w}$ ]
8	i	..2'	x,0,0 [0,v,w]	$\bar{x},0,0$ [0, $\bar{v},w$ ]	1/2,x+1/2,1/2 [v,0, $\bar{w}$ ]	1/2, $\bar{x}+1/2,1/2$ [ $\bar{v},0,\bar{w}$ ]
			$\bar{x}+1/2,1/2,1/2$ [0,v,w]	$x+1/2,1/2,1/2$ [0, $\bar{v},w$ ]	0, $\bar{x},0$ [v,0, $\bar{w}$ ]	0,x,0 [ $\bar{v},0,\bar{w}$ ]
8	h	2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
			1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]
4	g	2.mm	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]
4	f	..2/m	3/4,3/4,3/4 [ $\bar{u},u,0$ ]	1/4,1/4,3/4 [ $u,\bar{u},0$ ]	3/4,1/4,1/4 [ $u,u,0$ ]	1/4,3/4,1/4 [ $\bar{u},\bar{u},0$ ]
4	e	..2/m	1/4,1/4,1/4 [ $\bar{u},u,0$ ]	3/4,3/4,1/4 [ $u,\bar{u},0$ ]	1/4,3/4,3/4 [ $u,u,0$ ]	3/4,1/4,3/4 [ $\bar{u},\bar{u},0$ ]
4	d	2.22	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]

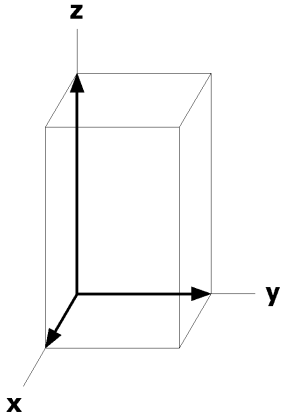
4	c	22'2'.	0,1/2,0 [0,0,w]	0,1/2,1/2 [0,0, $\bar{w}$ ]	1/2,0,1/2 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]
2	b	$\bar{4}$ '2'm	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a	$\bar{4}$ '2'm	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p<sub>g</sub>' 4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

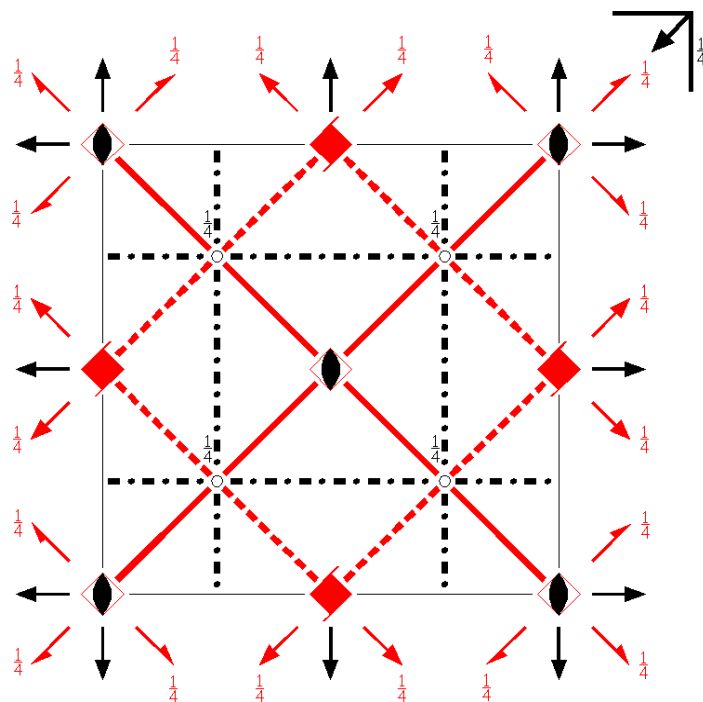
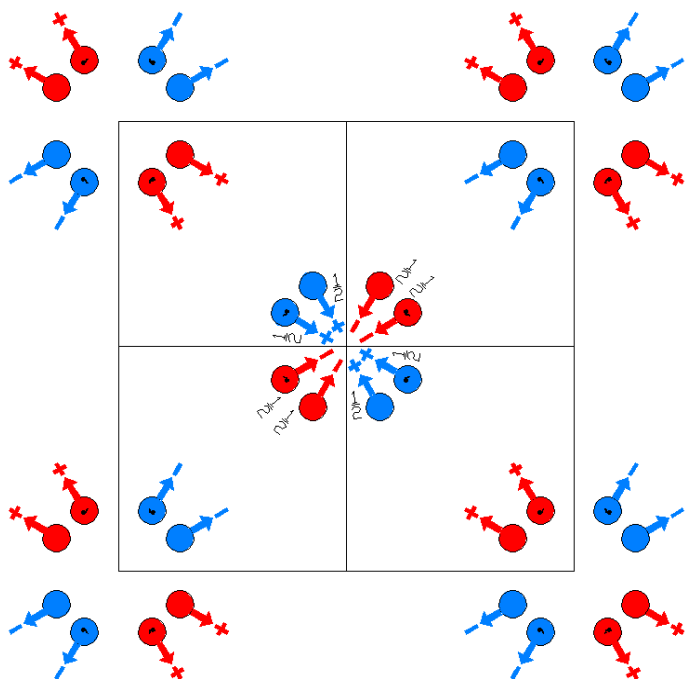
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



$P4_2'/nm'$   
134.5.1136

$4'/mmm'$   
 $P4_2'/n2/n2'/m'$

Tetragonal



Origin at  $\bar{4}'2m'$  at  $-1/4, 1/4, -1/4$  from center ( $2'/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$ ;  $x \leq y$ ;  $y \leq 1-x$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)'        | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'        |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                      | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                      | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'                 | (8) 2' x, $\bar{x}+1/2,1/4$<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)'           |
| (9) $\bar{4}$ 1/4,1/4,1/4<br>( $\bar{4}$  1/2,1/2,1/2)      | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (11) $\bar{4}$ <sup>+</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub>  0,0,0)' | (12) $\bar{4}$ <sup>-</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (13) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (14) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (15) m' x, $\bar{x},z$<br>(m <sub>xy</sub>  0,0,0)'                           | (16) m' x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,0)'                               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			Multiplicity, Wyckoff letter, Site Symmetry.			
16	n	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $v,u,w$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x,z$ [ $v,u,w$ ]		
8	m	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,z+1/2$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{u},u,\bar{w}$ ]
			$\bar{x},x,\bar{z}$ [ $\bar{u},u,\bar{w}$ ]	$x,\bar{x},\bar{z}$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $u,u,w$ ]
8	l	..2'	$x,x+1/2,3/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,3/4$ [ $u,\bar{u},w$ ]	$\bar{x},x+1/2,1/4$ [ $u,u,\bar{w}$ ]	$x,\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x}+1/2,\bar{x},3/4$ [ $\bar{u},u,w$ ]	$x+1/2,x,3/4$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x},1/4$ [ $u,u,\bar{w}$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	k	..2'	$x,x+1/2,1/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $u,\bar{u},w$ ]	$\bar{x},x+1/2,3/4$ [ $u,u,\bar{w}$ ]	$x,\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x}+1/2,\bar{x},1/4$ [ $\bar{u},u,w$ ]	$x+1/2,x,1/4$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x},3/4$ [ $u,u,\bar{w}$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	j	..2.	$x,0,1/2$ [ $u,0,0$ ]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	$1/2,x+1/2,0$ [ $0,\bar{u},0$ ]	$1/2,\bar{x}+1/2,0$ [ $0,u,0$ ]
			$\bar{x}+1/2,1/2,0$ [ $u,0,0$ ]	$x+1/2,1/2,0$ [ $\bar{u},0,0$ ]	$0,\bar{x},1/2$ [ $0,\bar{u},0$ ]	$0,x,1/2$ [ $0,u,0$ ]
8	i	..2.	$x,0,0$ [ $u,0,0$ ]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	$1/2,x+1/2,1/2$ [ $0,\bar{u},0$ ]	$1/2,\bar{x}+1/2,1/2$ [ $0,u,0$ ]
			$\bar{x}+1/2,1/2,1/2$ [ $u,0,0$ ]	$x+1/2,1/2,1/2$ [ $\bar{u},0,0$ ]	$0,\bar{x},0$ [ $0,\bar{u},0$ ]	$0,x,0$ [ $0,u,0$ ]
8	h	2..	$0,1/2,z$ [ $0,0,w$ ]	$0,1/2,z+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,w$ ]
			$1/2,0,\bar{z}+1/2$ [ $0,0,w$ ]	$1/2,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,0,z+1/2$ [ $0,0,\bar{w}$ ]	$1/2,0,z$ [ $0,0,w$ ]
4	g	2.m'm'	$0,0,z$ [ $0,0,w$ ]	$1/2,1/2,z+1/2$ [ $0,0,\bar{w}$ ]	$0,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,w$ ]
4	f	..2'/m'	$3/4,3/4,3/4$ [ $u,u,w$ ]	$1/4,1/4,3/4$ [ $\bar{u},\bar{u},w$ ]	$3/4,1/4,1/4$ [ $u,\bar{u},\bar{w}$ ]	$1/4,3/4,1/4$ [ $\bar{u},u,\bar{w}$ ]
4	e	..2'/m'	$1/4,1/4,1/4$ [ $u,u,w$ ]	$3/4,3/4,1/4$ [ $\bar{u},\bar{u},w$ ]	$1/4,3/4,3/4$ [ $u,\bar{u},\bar{w}$ ]	$3/4,1/4,3/4$ [ $\bar{u},u,\bar{w}$ ]
4	d	2.2'2'	$0,1/2,1/4$ [ $0,0,w$ ]	$0,1/2,3/4$ [ $0,0,\bar{w}$ ]	$1/2,0,1/4$ [ $0,0,w$ ]	$1/2,0,3/4$ [ $0,0,\bar{w}$ ]

4	c	222.	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]
2	b	$\bar{4}$ '2m'	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a	$\bar{4}$ '2m'	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

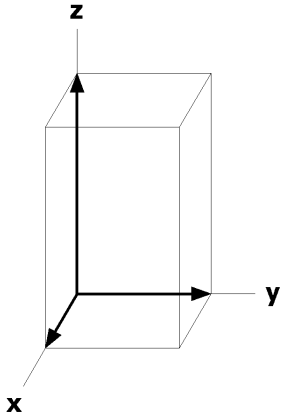
**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub>' 4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c<sub>p</sub>' 2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4





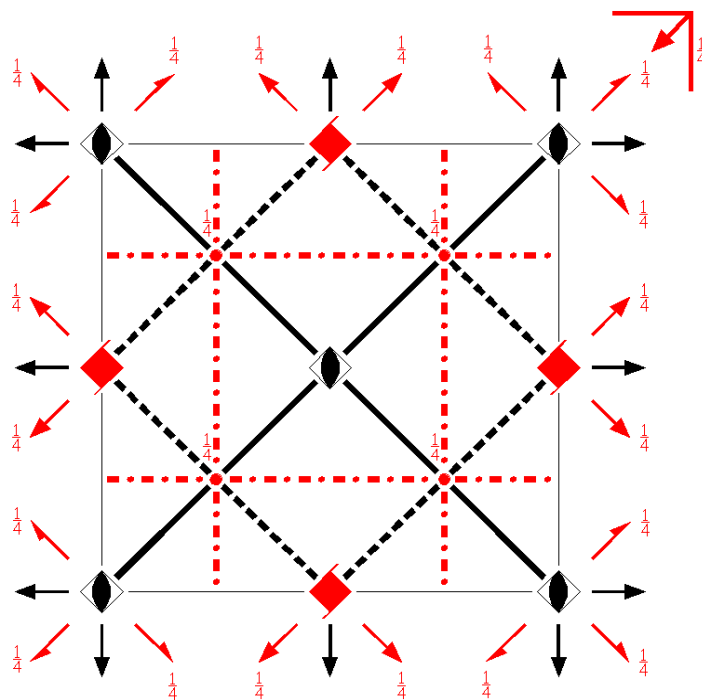
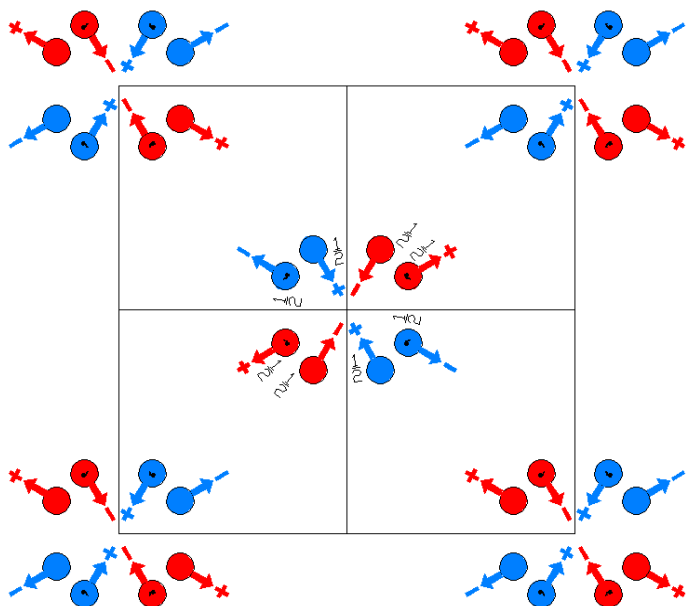
$P4_2/n'n'm$

134.6.1137

$4'/m'm'm$

$P4_2'/n'2/n'2'/m$

Tetragonal



Origin at  $\bar{4}2m$  at  $-1/4, 1/4, -1/4$  from center ( $2'/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4; x \leq y; y \leq 1-x$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) $1$<br>( $1 0,0,0$ )                                  | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                        | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>( $4_z 1/2,1/2,1/2$ )'     | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,1/2$ )'    |
| (5) $2$ $0,y,0$<br>( $2_y 0,0,0$ )                        | (6) $2$ $x,0,0$<br>( $2_x 0,0,0$ )                        | (7) $2'$ $(1/2,1/2,0) x,x,1/4$<br>( $2_{xy} 1/2,1/2,1/2$ )' | (8) $2'$ $x,\bar{x}+1/2,1/4$<br>( $2_{\bar{xy}} 1/2,1/2,1/2$ )' |
| (9) $\bar{1}$ $1/4,1/4,1/4$<br>( $\bar{1} 1/2,1/2,1/2$ )' | (10) $n'$ $(1/2,1/2,0) x,y,1/4$<br>( $m_z 1/2,1/2,1/2$ )' | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )    | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ )   |
| (13) $n'$ $(1/2,0,1/2) x,1/4,z$<br>( $m_y 1/2,1/2,1/2$ )' | (14) $n'$ $(0,1/2,1/2) 1/4,y,z$<br>( $m_x 1/2,1/2,1/2$ )' | (15) $m$ $x,\bar{x},z$<br>( $m_{xy} 0,0,0$ )                | (16) $m$ $x,x,z$<br>( $m_{\bar{xy}} 0,0,0$ )                    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			Multiplicity, Wyckoff letter, Site Symmetry.			
16	n	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $v,u,w$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(16) $y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	m	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,z+1/2$ [ $u,u,0$ ]	$x+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},x,\bar{z}$ [ $u,u,0$ ]	$x,\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $u,\bar{u},0$ ]
8	l	..2'	$x,x+1/2,3/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,3/4$ [ $u,\bar{u},w$ ]	$\bar{x},x+1/2,1/4$ [ $u,u,\bar{w}$ ]	$x,\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x}+1/2,\bar{x},3/4$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x,3/4$ [ $\bar{u},u,\bar{w}$ ]	$x+1/2,\bar{x},1/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,1/4$ [ $u,u,w$ ]
8	k	..2'	$x,x+1/2,1/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $u,\bar{u},w$ ]	$\bar{x},x+1/2,3/4$ [ $u,u,\bar{w}$ ]	$x,\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x}+1/2,\bar{x},1/4$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x,1/4$ [ $\bar{u},u,\bar{w}$ ]	$x+1/2,\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,3/4$ [ $u,u,w$ ]
8	j	..2.	$x,0,1/2$ [ $u,0,0$ ]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	$1/2,x+1/2,0$ [ $0,\bar{u},0$ ]	$1/2,\bar{x}+1/2,0$ [ $0,u,0$ ]
			$\bar{x}+1/2,1/2,0$ [ $\bar{u},0,0$ ]	$x+1/2,1/2,0$ [ $u,0,0$ ]	$0,\bar{x},1/2$ [ $0,u,0$ ]	$0,x,1/2$ [ $0,\bar{u},0$ ]
8	i	..2.	$x,0,0$ [ $u,0,0$ ]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	$1/2,x+1/2,1/2$ [ $0,\bar{u},0$ ]	$1/2,\bar{x}+1/2,1/2$ [ $0,u,0$ ]
			$\bar{x}+1/2,1/2,1/2$ [ $\bar{u},0,0$ ]	$x+1/2,1/2,1/2$ [ $u,0,0$ ]	$0,\bar{x},0$ [ $0,u,0$ ]	$0,x,0$ [ $0,\bar{u},0$ ]
8	h	2..	$0,1/2,z$ [ $0,0,w$ ]	$0,1/2,z+1/2$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,w$ ]
			$1/2,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}$ [ $0,0,w$ ]	$1/2,0,z+1/2$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,\bar{w}$ ]
4	g	2.mm	$0,0,z$ [ $0,0,0$ ]	$1/2,1/2,z+1/2$ [ $0,0,0$ ]	$0,0,\bar{z}$ [ $0,0,0$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,0$ ]
4	f	..2'/m	$3/4,3/4,3/4$ [ $0,0,0$ ]	$1/4,1/4,3/4$ [ $0,0,0$ ]	$3/4,1/4,1/4$ [ $0,0,0$ ]	$1/4,3/4,1/4$ [ $0,0,0$ ]
4	e	..2'/m	$1/4,1/4,1/4$ [ $0,0,0$ ]	$3/4,3/4,1/4$ [ $0,0,0$ ]	$1/4,3/4,3/4$ [ $0,0,0$ ]	$3/4,1/4,3/4$ [ $0,0,0$ ]
4	d	2.2'2'	$0,1/2,1/4$ [ $0,0,w$ ]	$0,1/2,3/4$ [ $0,0,\bar{w}$ ]	$1/2,0,1/4$ [ $0,0,\bar{w}$ ]	$1/2,0,3/4$ [ $0,0,w$ ]

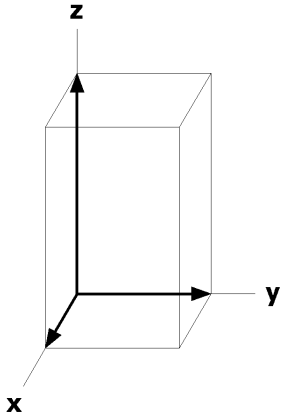
4	c	222.	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]
2	b	$\bar{4}2m$	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a	$\bar{4}2m$	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



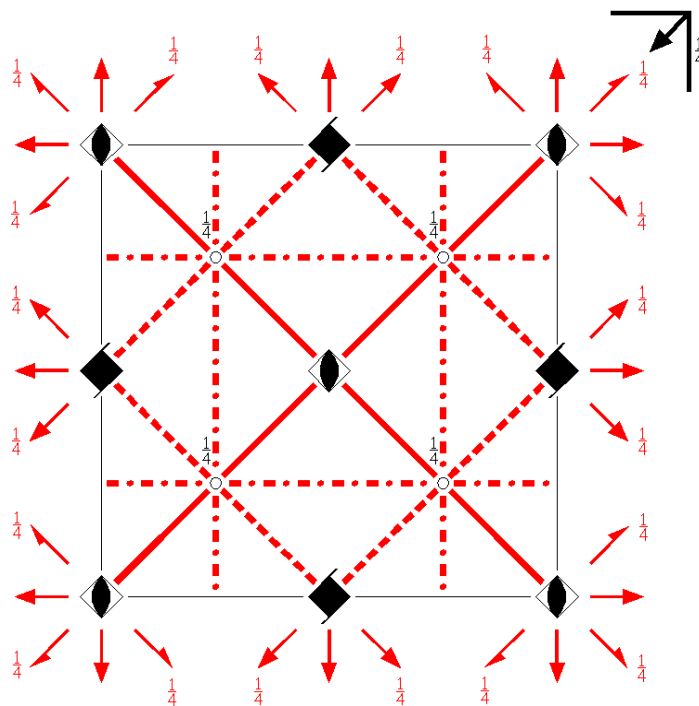
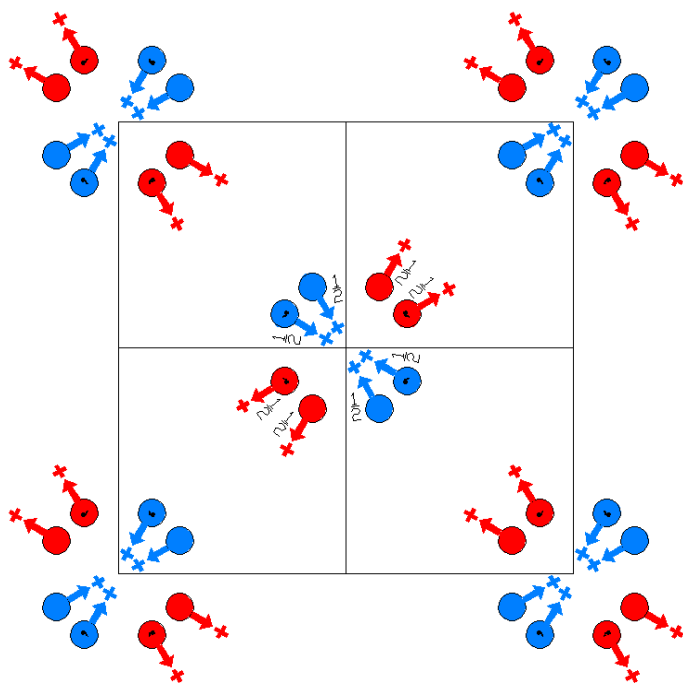
$P4_2/nm'$

134.7.1138

$4/m\bar{m}'m'$

$P4_2/n2'/n2'/m'$

Tetragonal



Origin at  $\bar{4}2'm'$  at  $-1/4, 1/4, -1/4$  from center ( $2'/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4; x \leq y; y \leq 1-x$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                        | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                      | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                      | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'         | (8) 2' x, $\bar{x}+1/2,1/4$<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)'   |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)        | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)   | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)                | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)                         |
| (13) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (14) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (15) m' x, $\bar{x},z$<br>(m <sub>xy</sub>  0,0,0)'                   | (16) m' x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,0)'                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	n	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]		
			(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $v,u,w$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x,z$ [ $v,u,w$ ]		
8	m	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,z+1/2$ [ $\bar{u},u,w$ ]	$x+1/2,\bar{x}+1/2,z+1/2$ [ $u,\bar{u},w$ ]
			$\bar{x},x,\bar{z}$ [ $u,\bar{u},w$ ]	$x,\bar{x},\bar{z}$ [ $\bar{u},u,w$ ]	$x+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $u,u,w$ ]
8	l	..2'	$x,x+1/2,3/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,3/4$ [ $u,\bar{u},w$ ]	$\bar{x},x+1/2,1/4$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x}+1/2,1/4$ [ $u,u,w$ ]
			$\bar{x}+1/2,\bar{x},3/4$ [ $\bar{u},u,w$ ]	$x+1/2,x,3/4$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x},1/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,1/4$ [ $u,u,w$ ]
8	k	..2'	$x,x+1/2,1/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $u,\bar{u},w$ ]	$\bar{x},x+1/2,3/4$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x}+1/2,3/4$ [ $u,u,w$ ]
			$\bar{x}+1/2,\bar{x},1/4$ [ $\bar{u},u,w$ ]	$x+1/2,x,1/4$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,3/4$ [ $u,u,w$ ]
8	j	..2'	$x,0,1/2$ [ $0,v,w$ ]	$\bar{x},0,1/2$ [ $0,\bar{v},w$ ]	$1/2,x+1/2,0$ [ $\bar{v},0,w$ ]	$1/2,\bar{x}+1/2,0$ [ $v,0,w$ ]
			$\bar{x}+1/2,1/2,0$ [ $0,v,w$ ]	$x+1/2,1/2,0$ [ $0,\bar{v},w$ ]	$0,\bar{x},1/2$ [ $\bar{v},0,w$ ]	$0,x,1/2$ [ $v,0,w$ ]
8	i	..2'	$x,0,0$ [ $0,v,w$ ]	$\bar{x},0,0$ [ $0,\bar{v},w$ ]	$1/2,x+1/2,1/2$ [ $\bar{v},0,w$ ]	$1/2,\bar{x}+1/2,1/2$ [ $v,0,w$ ]
			$\bar{x}+1/2,1/2,1/2$ [ $0,v,w$ ]	$x+1/2,1/2,1/2$ [ $0,\bar{v},w$ ]	$0,\bar{x},0$ [ $\bar{v},0,w$ ]	$0,x,0$ [ $v,0,w$ ]
8	h	2..	$0,1/2,z$ [ $0,0,w$ ]	$0,1/2,z+1/2$ [ $0,0,w$ ]	$0,1/2,\bar{z}$ [ $0,0,w$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,w$ ]
			$1/2,0,\bar{z}+1/2$ [ $0,0,w$ ]	$1/2,0,\bar{z}$ [ $0,0,w$ ]	$1/2,0,z+1/2$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,w$ ]
4	g	2.m'm'	$0,0,z$ [ $0,0,w$ ]	$1/2,1/2,z+1/2$ [ $0,0,w$ ]	$0,0,\bar{z}$ [ $0,0,w$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,w$ ]
4	f	..2'/m'	$3/4,3/4,3/4$ [ $u,u,w$ ]	$1/4,1/4,3/4$ [ $\bar{u},\bar{u},w$ ]	$3/4,1/4,1/4$ [ $\bar{u},u,w$ ]	$1/4,3/4,1/4$ [ $u,\bar{u},w$ ]
4	e	..2'/m'	$1/4,1/4,1/4$ [ $u,u,w$ ]	$3/4,3/4,1/4$ [ $\bar{u},\bar{u},w$ ]	$1/4,3/4,3/4$ [ $\bar{u},u,w$ ]	$3/4,1/4,3/4$ [ $u,\bar{u},w$ ]
4	d	2.2'2'	$0,1/2,1/4$ [ $0,0,w$ ]	$0,1/2,3/4$ [ $0,0,w$ ]	$1/2,0,1/4$ [ $0,0,w$ ]	$1/2,0,3/4$ [ $0,0,w$ ]

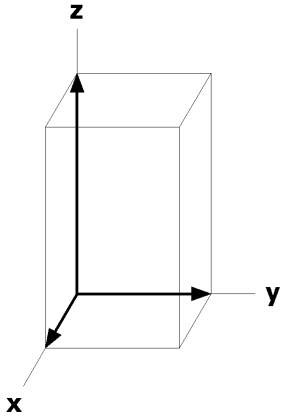
4	c	22'2'. $\overline{4}2'm'$	0,1/2,0 [0,0,w]	0,1/2,1/2 [0,0,w]	1/2,0,1/2 [0,0,w]	1/2,0,0 [0,0,w]
2	b	$\overline{4}2'm'$	0,0,1/2 [0,0,w]	1/2,1/2,0 [0,0,w]		
2	a	$\overline{4}2'm'$	0,0,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p<sub>g</sub>-4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/2,0,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



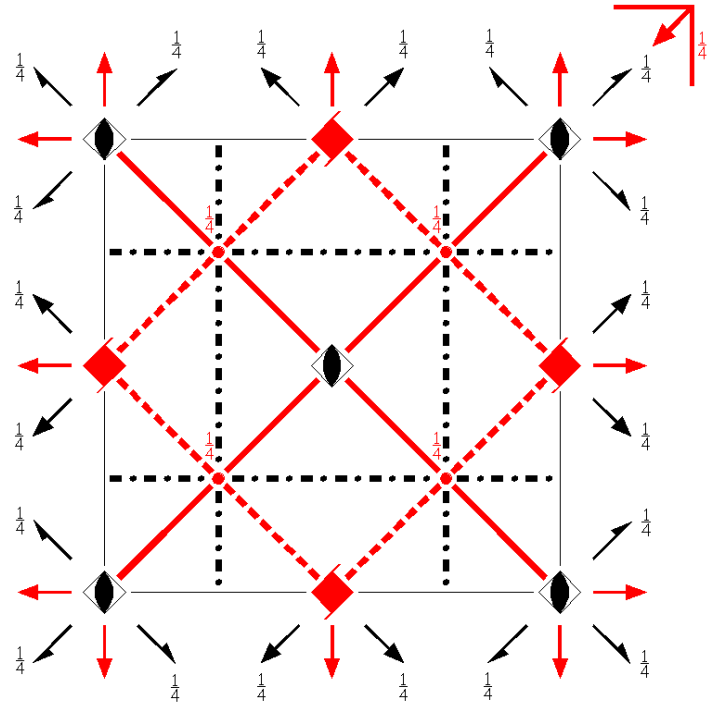
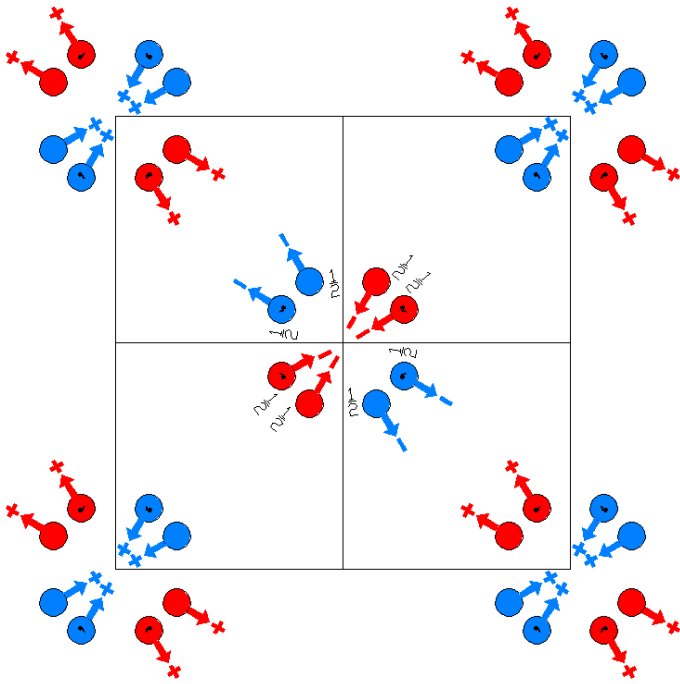
$P4_2'n'm'$

134.8.1139

$4'/m'mm'$

$P4_2'n'2'/n2/m'$

Tetragonal



Origin at  $\bar{4}2'm'$  at  $-1/4, 1/4, -1/4$  from center ( $2/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4; x \leq y; y \leq 1-x$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) $1$<br>( $1 0,0,0$ )                                  | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                        | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>( $4_z 1/2,1/2,1/2$ )'   | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,1/2$ )'  |
| (5) $2'$ $0,y,0$<br>( $2_y 0,0,0$ )'                      | (6) $2'$ $x,0,0$<br>( $2_x 0,0,0$ )'                      | (7) $2$ $(1/2,1/2,0) x,x,1/4$<br>( $2_{xy} 1/2,1/2,1/2$ ) | (8) $2$ $x,\bar{x}+1/2,1/4$<br>( $2_{\bar{xy}} 1/2,1/2,1/2$ ) |
| (9) $\bar{1}$ $1/4,1/4,1/4$<br>( $\bar{1} 1/2,1/2,1/2$ )' | (10) $n'$ $(1/2,1/2,0) x,y,1/4$<br>( $m_z 1/2,1/2,1/2$ )' | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )  | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ ) |
| (13) $n$ $(1/2,0,1/2) x,1/4,z$<br>( $m_y 1/2,1/2,1/2$ )   | (14) $n$ $(0,1/2,1/2) 1/4,y,z$<br>( $m_x 1/2,1/2,1/2$ )   | (15) $m'$ $x,\bar{x},z$<br>( $m_{xy} 0,0,0$ )'            | (16) $m'$ $x,x,z$<br>( $m_{\bar{xy}} 0,0,0$ )'                |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	n	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]		
			(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x,z$ [ $v,u,w$ ]		
8	m	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,z+1/2$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{u},u,\bar{w}$ ]
			$\bar{x},x,\bar{z}$ [ $u,\bar{u},w$ ]	$x,\bar{x},\bar{z}$ [ $\bar{u},u,w$ ]	$x+1/2,x+1/2,\bar{z}+1/2$ [ $u,\bar{u},\bar{w}$ ]	$\bar{x}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	l	..2	x,x+1/2,3/4 [u,u,0]	$\bar{x},\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,1/4$ [ $u,\bar{u},0$ ]	$x,\bar{x}+1/2,1/4$ [ $\bar{u},u,0$ ]
			$\bar{x}+1/2,\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x,3/4$ [ $u,u,0$ ]	$x+1/2,\bar{x},1/4$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,x,1/4$ [ $u,\bar{u},0$ ]
8	k	..2	x,x+1/2,1/4 [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,3/4$ [ $u,\bar{u},0$ ]	$x,\bar{x}+1/2,3/4$ [ $\bar{u},u,0$ ]
			$\bar{x}+1/2,\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x,1/4$ [ $u,u,0$ ]	$x+1/2,\bar{x},3/4$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,x,3/4$ [ $u,\bar{u},0$ ]
8	j	..2'	x,0,1/2 [0,v,w]	$\bar{x},0,1/2$ [0, $\bar{v},w$ ]	1/2,x+1/2,0 [ $\bar{v},0,\bar{w}$ ]	1/2, $\bar{x}+1/2,0$ [ $\bar{v},0,\bar{w}$ ]
			$\bar{x}+1/2,1/2,0$ [0, $\bar{v},\bar{w}$ ]	$x+1/2,1/2,0$ [0,v, $\bar{w}$ ]	0, $\bar{x},1/2$ [ $\bar{v},0,w$ ]	0,x,1/2 [ $\bar{v},0,w$ ]
8	i	..2'	x,0,0 [0,v,w]	$\bar{x},0,0$ [0, $\bar{v},w$ ]	1/2,x+1/2,1/2 [ $\bar{v},0,\bar{w}$ ]	1/2, $\bar{x}+1/2,1/2$ [ $\bar{v},0,\bar{w}$ ]
			$\bar{x}+1/2,1/2,1/2$ [0, $\bar{v},\bar{w}$ ]	$x+1/2,1/2,1/2$ [0,v, $\bar{w}$ ]	0, $\bar{x},0$ [ $\bar{v},0,w$ ]	0,x,0 [ $\bar{v},0,w$ ]
8	h	2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
			1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	1/2,0,z [0,0,w]
4	g	2.m'm'	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	f	..2/m'	3/4,3/4,3/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]
4	e	..2/m'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]
4	d	2.22	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]



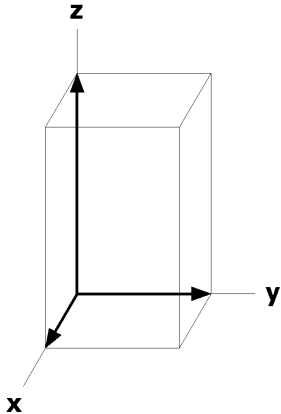
4	c	$22'2'$	$0,1/2,0 [0,0,w]$	$0,1/2,1/2 [0,0,\bar{w}]$	$1/2,0,1/2 [0,0,\bar{w}]$	$1/2,0,0 [0,0,w]$
2	b	$\bar{4}2'm'$	$0,0,1/2 [0,0,w]$	$1/2,1/2,0 [0,0,\bar{w}]$		
2	a	$\bar{4}2'm'$	$0,0,0 [0,0,w]$	$1/2,1/2,1/2 [0,0,\bar{w}]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4'm'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,1/4$



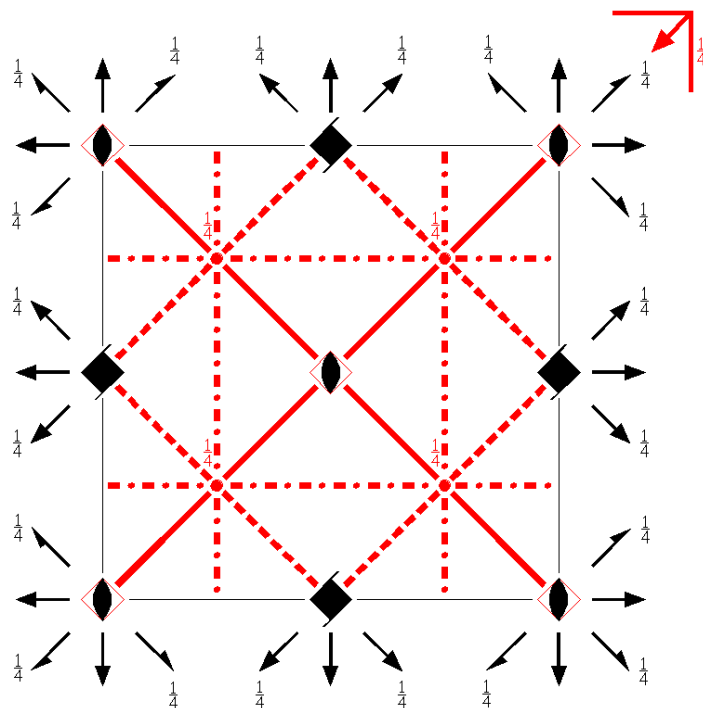
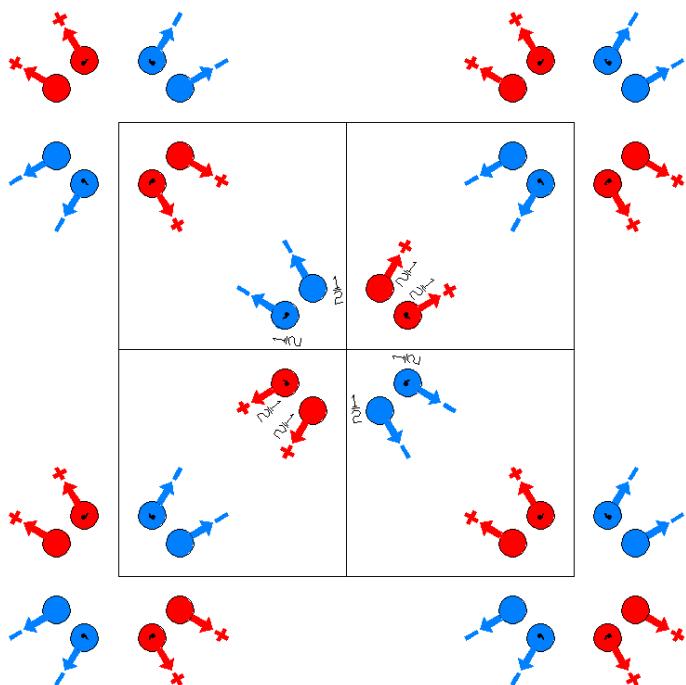
$P4_2/n'n'm'$

134.9.1140

$4/m'm'm'$

$P4_2/n'2/n'2/m'$

Tetragonal



Origin at  $\bar{4}'2m'$  at  $-1/4, 1/4, -1/4$  from center ( $2/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1/4; x \leq y; y \leq 1-x$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                        | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                        | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                        | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)           | (8) 2 x, $\bar{x}+1/2,1/4$<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)     |
| (9) $\bar{1}'$ 1/4,1/4,1/4<br>( $\bar{1}'$  1/2,1/2,1/2)'     | (10) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (11) $\bar{4}^{+}$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{+}$  0,0,0)'         | (12) $\bar{4}^{-}$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)'                      |
| (13) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (14) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (15) m' x, $\bar{x},z$<br>(m <sub>xy</sub>  0,0,0)'                   | (16) m' x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,0)'                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
			Multiplicity, Wyckoff letter, Site Symmetry.			
16	n	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x,z$ [ $v,u,w$ ]		
8	m	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,z+1/2$ [ $\bar{u},u,w$ ]	$x+1/2,\bar{x}+1/2,z+1/2$ [ $u,\bar{u},w$ ]
			$\bar{x},x,\bar{z}$ [ $\bar{u},u,\bar{w}$ ]	$x,\bar{x},\bar{z}$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x+1/2,\bar{z}+1/2$ [ $u,u,\bar{w}$ ]	$\bar{x}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	l	..2	x,x+1/2,3/4 [u,u,0]	$\bar{x},\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,1/4$ [ $\bar{u},u,0$ ]	$x,\bar{x}+1/2,1/4$ [ $u,\bar{u},0$ ]
			$\bar{x}+1/2,\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x,3/4$ [ $u,u,0$ ]	$x+1/2,\bar{x},1/4$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},u,0$ ]
8	k	..2	x,x+1/2,1/4 [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,3/4$ [ $\bar{u},u,0$ ]	$x,\bar{x}+1/2,3/4$ [ $u,\bar{u},0$ ]
			$\bar{x}+1/2,\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x,1/4$ [ $u,u,0$ ]	$x+1/2,\bar{x},3/4$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},u,0$ ]
8	j	..2	x,0,1/2 [u,0,0]	$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	1/2,x+1/2,0 [0,u,0]	1/2, $\bar{x}+1/2,0$ [0, $\bar{u},0$ ]
			$\bar{x}+1/2,1/2,0$ [ $\bar{u},0,0$ ]	$x+1/2,1/2,0$ [ $u,0,0$ ]	0, $\bar{x},1/2$ [0, $\bar{u},0$ ]	0,x,1/2 [0,u,0]
8	i	..2	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	1/2,x+1/2,1/2 [0,u,0]	1/2, $\bar{x}+1/2,1/2$ [0, $\bar{u},0$ ]
			$\bar{x}+1/2,1/2,1/2$ [ $\bar{u},0,0$ ]	$x+1/2,1/2,1/2$ [ $u,0,0$ ]	0, $\bar{x},0$ [0, $\bar{u},0$ ]	0,x,0 [0,u,0]
8	h	2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
			1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0,w]	1/2,0,z [0,0,w]
4	g	2.m'm'	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	f	..2/m'	3/4,3/4,3/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]
4	e	..2/m'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]
4	d	2.22	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]

Continued

134.9.1140

 $P4_2/n'n'm'$ 

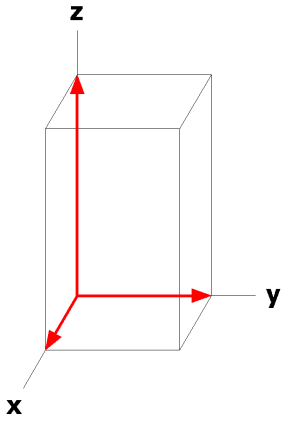
4	c	222.	$0,1/2,0 [0,0,0]$	$0,1/2,1/2 [0,0,0]$	$1/2,0,1/2 [0,0,0]$	$1/2,0,0 [0,0,0]$
2	b	$\bar{4}'2m'$	$0,0,1/2 [0,0,0]$	$1/2,1/2,0 [0,0,0]$		
2	a	$\bar{4}'2m'$	$0,0,0 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

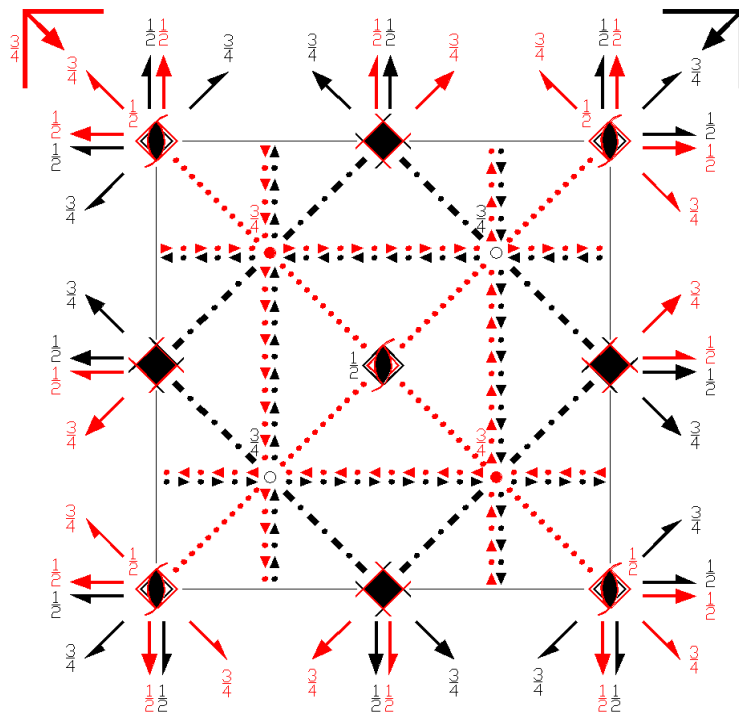
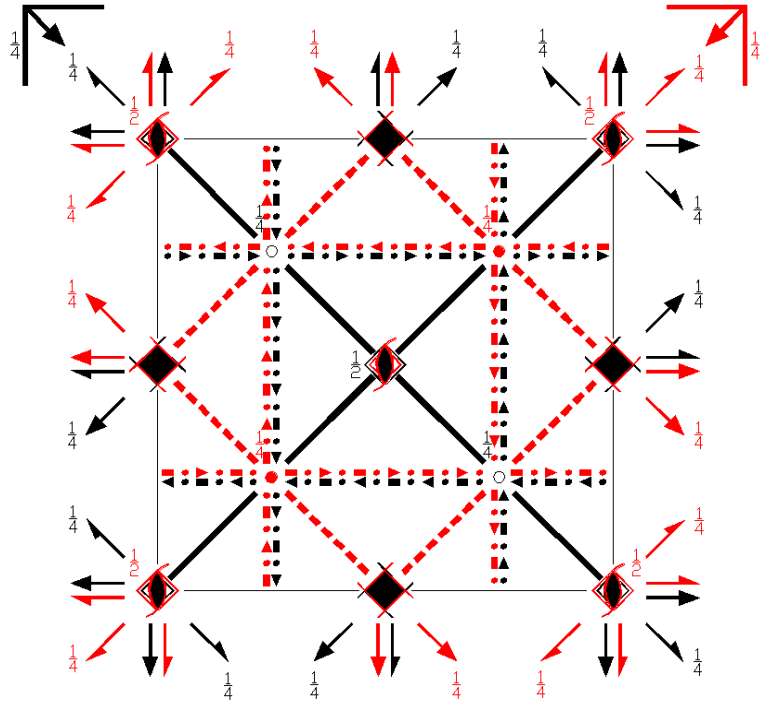
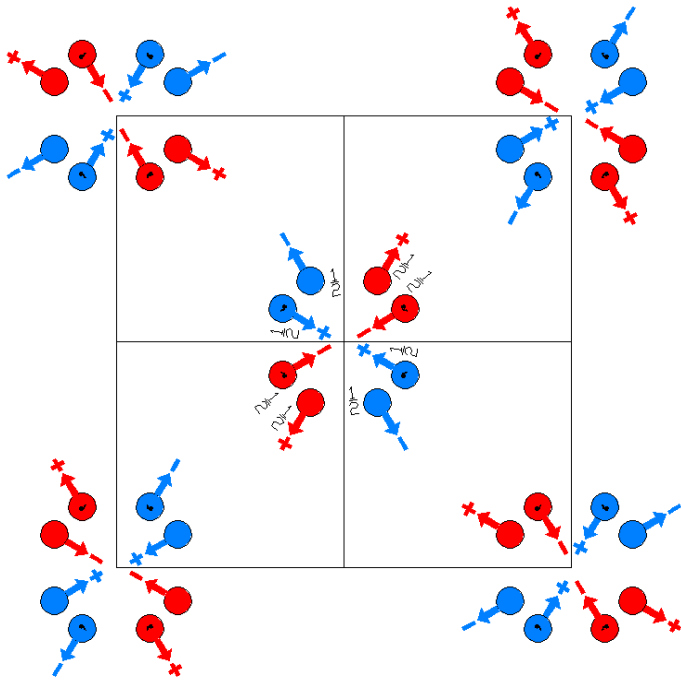
Along  $[1,1,0]$   $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,1/4$



$P_14_2/nm$   
134.10.1141

$4/mmm1'$   
 $P_14_2/n2/n2/m$

Tetragonal



**Origin** at  $\bar{4}2m$  at  $-1/4, 1/4, -1/4$  from center ( $2/m$ )

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$ ;  $x \leq y$ ;  $y \leq 1-x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                      | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                      | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)           | (8) 2 x, $\bar{x}+1/2,1/4$<br>(2 <sub>xy</sub> <sup>-1</sup>  1/2,1/2,1/2)          |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)      | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)                | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z$ <sup>-1</sup>  0,0,0)                |
| (13) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (14) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (15) m x, $\bar{x},z$<br>(m <sub>xy</sub>  0,0,0)                     | (16) m x,x,z<br>(m <sub>xy</sub> <sup>-1</sup>  0,0,0)                              |

For (1,0,0)<sup>'</sup> + set

- |   |   |   |   |
|---|---|---|---|
| (1) t' (1,0,0)<br>(1 1,0,0)'                                  | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'                    | (3) 4 <sup>+</sup> ' (0,0,1/2) -1/2,0,z<br>(4 <sub>z</sub>  3/2,1/2,1/2)' | (4) 4 <sup>-</sup> ' (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub> <sup>-1</sup>  3/2,1/2,1/2)'        |
| (5) 2' 1/2,y,0<br>(2 <sub>y</sub>  1,0,0)'                    | (6) 2' (1,0,0) x,0,0<br>(2 <sub>x</sub>  1,0,0)'              | (7) 2' x-1/2,x,1/4<br>(2 <sub>xy</sub>  3/2,1/2,1/2)'                     | (8) 2' (1/2,-1/2,0) x+1/2, $\bar{x}+1/2,1/4$<br>(2 <sub>xy</sub> <sup>-1</sup>  3/2,1/2,1/2)' |
| (9) $\bar{1}$ ' 3/4,1/4,1/4<br>( $\bar{1}$  3/2,1/2,1/2)'     | (10) n' (3/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  3/2,1/2,1/2)' | (11) $\bar{4}^+$ ' 1/2,-1/2,z; 1/2,-1/2,0<br>( $\bar{4}_z$  1,0,0)'       | (12) $\bar{4}^-$ ' 1/2,1/2,z; 1/2,1/2,0<br>( $\bar{4}_z$ <sup>-1</sup>  1,0,0)'               |
| (13) n' (3/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  3/2,1/2,1/2)' | (14) n' (0,1/2,1/2) 3/4,y,z<br>(m <sub>x</sub>  3/2,1/2,1/2)' | (15) g' (1/2,-1/2,0) x+1/2, $\bar{x},z$<br>(m <sub>xy</sub>  1,0,0)'      | (16) g' (1/2,1/2,0) x+1/2,x,z<br>(m <sub>xy</sub> <sup>-1</sup>  1,0,0)'                      |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5); (9).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

- |    |   |   |   |   |
|----|---|---|---|---|
| 32 | n | 1 | (1) x,y,z [u,v,w]   | (2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]                         |
|    |   |   | (3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]                         | (4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]                         |
|    |   |   | (5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]                         | (6) $x,\bar{y},z$ [ $u,\bar{v},\bar{w}$ ]                               |
|    |   |   | (7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]                         | (8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ] |
|    |   |   | (9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ] | (10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]                  |
|    |   |   | (11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]                              | (12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]                              |
|    |   |   | (13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]                  | (14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]                  |

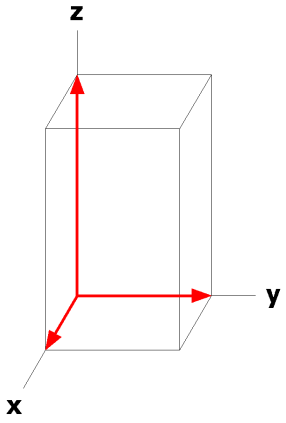
			(15) $\bar{y}, \bar{x}, z$ [v,u, $\bar{w}$ ]	(16) $y, x, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]		
16	m	..m	$x, x, z$ [ $\bar{u}, u, 0$ ]	$\bar{x}, \bar{x}, z$ [ $u, \bar{u}, 0$ ]	$\bar{x}+1/2, x+1/2, z+1/2$ [ $\bar{u}, \bar{u}, 0$ ]	$x+1/2, \bar{x}+1/2, z+1/2$ [ $u, u, 0$ ]
			$\bar{x}, x, \bar{z}$ [ $u, u, 0$ ]	$x, \bar{x}, \bar{z}$ [ $\bar{u}, \bar{u}, 0$ ]	$x+1/2, x+1/2, \bar{z}+1/2$ [ $u, \bar{u}, 0$ ]	$\bar{x}+1/2, \bar{x}+1/2, \bar{z}+1/2$ [ $\bar{u}, \bar{u}, 0$ ]
16	l	..2	$x, x+1/2, 3/4$ [ $u, u, 0$ ]	$\bar{x}, \bar{x}+1/2, 3/4$ [ $u, u, 0$ ]	$\bar{x}, x+1/2, 1/4$ [ $u, \bar{u}, 0$ ]	$x, \bar{x}+1/2, 1/4$ [ $u, \bar{u}, 0$ ]
			$\bar{x}+1/2, \bar{x}, 3/4$ [ $\bar{u}, \bar{u}, 0$ ]	$x+1/2, x, 3/4$ [ $\bar{u}, \bar{u}, 0$ ]	$x+1/2, \bar{x}, 1/4$ [ $u, \bar{u}, 0$ ]	$\bar{x}+1/2, x, 1/4$ [ $u, \bar{u}, 0$ ]
16	k	..2'	$x, x+1/2, 1/4$ [ $\bar{u}, u, w$ ]	$\bar{x}, \bar{x}+1/2, 1/4$ [ $\bar{u}, u, \bar{w}$ ]	$\bar{x}, x+1/2, 3/4$ [ $\bar{u}, \bar{u}, w$ ]	$x, \bar{x}+1/2, 3/4$ [ $\bar{u}, \bar{u}, \bar{w}$ ]
			$\bar{x}+1/2, \bar{x}, 1/4$ [ $\bar{u}, u, w$ ]	$x+1/2, x, 1/4$ [ $\bar{u}, u, \bar{w}$ ]	$x+1/2, \bar{x}, 3/4$ [ $u, u, \bar{w}$ ]	$\bar{x}+1/2, x, 3/4$ [ $u, u, w$ ]
16	j	..2'	$x, 0, 1/2$ [ $0, v, w$ ]	$\bar{x}, 0, 1/2$ [ $0, \bar{v}, w$ ]	$1/2, x+1/2, 0$ [ $v, 0, \bar{w}$ ]	$1/2, \bar{x}+1/2, 0$ [ $\bar{v}, 0, \bar{w}$ ]
			$\bar{x}+1/2, 1/2, 0$ [ $0, v, w$ ]	$x+1/2, 1/2, 0$ [ $0, \bar{v}, w$ ]	$0, \bar{x}, 1/2$ [ $v, 0, \bar{w}$ ]	$0, x, 1/2$ [ $\bar{v}, 0, \bar{w}$ ]
16	i	..2	$x, 0, 0$ [ $u, 0, 0$ ]	$\bar{x}, 0, 0$ [ $\bar{u}, 0, 0$ ]	$1/2, x+1/2, 1/2$ [ $0, u, 0$ ]	$1/2, \bar{x}+1/2, 1/2$ [ $0, \bar{u}, 0$ ]
			$\bar{x}+1/2, 1/2, 1/2$ [ $u, 0, 0$ ]	$x+1/2, 1/2, 1/2$ [ $\bar{u}, 0, 0$ ]	$0, \bar{x}, 0$ [ $0, u, 0$ ]	$0, x, 0$ [ $0, \bar{u}, 0$ ]
16	h	2'	$0, 1/2, z$ [ $u, v, 0$ ]	$0, 1/2, z+1/2$ [ $\bar{v}, u, 0$ ]	$0, 1/2, \bar{z}$ [ $\bar{u}, v, 0$ ]	$0, 1/2, \bar{z}+1/2$ [ $\bar{v}, \bar{u}, 0$ ]
			$1/2, 0, \bar{z}+1/2$ [ $u, v, 0$ ]	$1/2, 0, \bar{z}$ [ $\bar{v}, u, 0$ ]	$1/2, 0, z+1/2$ [ $\bar{u}, v, 0$ ]	$1/2, 0, z$ [ $\bar{v}, \bar{u}, 0$ ]
8	g	2.mm	$0, 0, z$ [ $0, 0, 0$ ]	$1/2, 1/2, z+1/2$ [ $0, 0, 0$ ]	$0, 0, \bar{z}$ [ $0, 0, 0$ ]	$1/2, 1/2, \bar{z}+1/2$ [ $0, 0, 0$ ]
8	f	..2'/m	$3/4, 3/4, 3/4$ [ $0, 0, 0$ ]	$1/4, 1/4, 3/4$ [ $0, 0, 0$ ]	$3/4, 1/4, 1/4$ [ $0, 0, 0$ ]	$1/4, 3/4, 1/4$ [ $0, 0, 0$ ]
8	e	..2/m	$1/4, 1/4, 1/4$ [ $\bar{u}, u, 0$ ]	$3/4, 3/4, 1/4$ [ $u, \bar{u}, 0$ ]	$1/4, 3/4, 3/4$ [ $\bar{u}, \bar{u}, 0$ ]	$3/4, 1/4, 3/4$ [ $u, u, 0$ ]
8	d	2'.2'2	$0, 1/2, 1/4$ [ $\bar{u}, u, 0$ ]	$0, 1/2, 3/4$ [ $\bar{u}, \bar{u}, 0$ ]	$1/2, 0, 1/4$ [ $\bar{u}, u, 0$ ]	$1/2, 0, 3/4$ [ $u, u, 0$ ]
8	c	2'2'2.	$0, 1/2, 0$ [ $0, v, 0$ ]	$0, 1/2, 1/2$ [ $\bar{v}, 0, 0$ ]	$1/2, 0, 1/2$ [ $0, v, 0$ ]	$1/2, 0, 0$ [ $\bar{v}, 0, 0$ ]
4	b	$\bar{4}$ '2'm	$0, 0, 1/2$ [ $0, 0, 0$ ]	$1/2, 1/2, 0$ [ $0, 0, 0$ ]		
4	a	$\bar{4}$ 2m	$0, 0, 0$ [ $0, 0, 0$ ]	$1/2, 1/2, 1/2$ [ $0, 0, 0$ ]		

### Symmetry of Special Projections

Along  $[0, 0, 1]$  p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$  c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 0, 0$

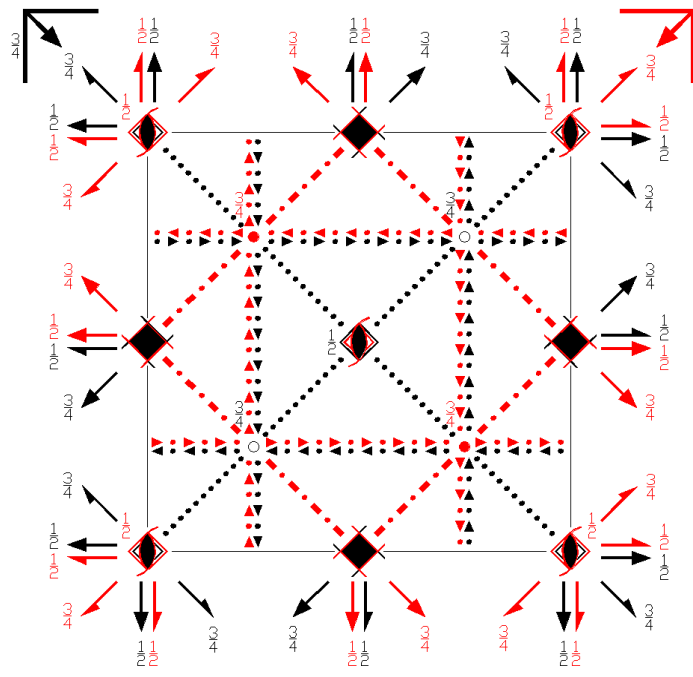
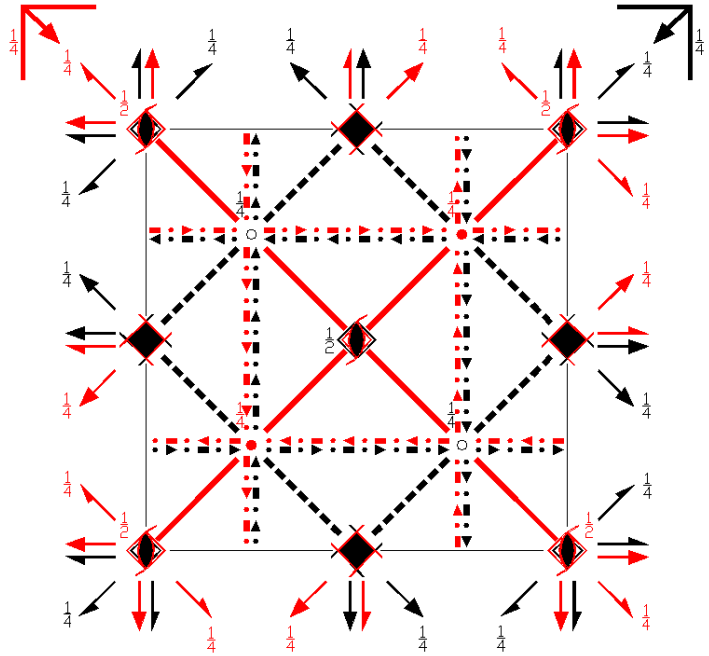
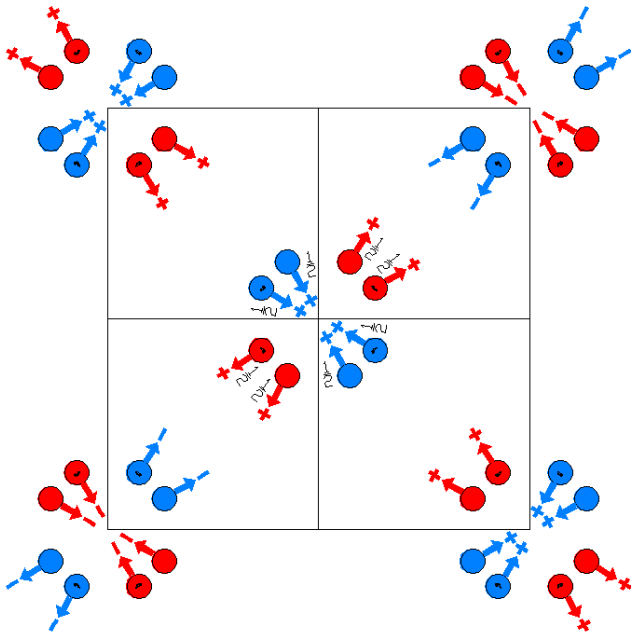
Along  $[1, 1, 0]$  p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 1/4$



$P_14_2 / nn'm'$   
134.11.1142

$4/mmm1'$   
 $P_14_2 / n2'/n'2'/m'$

Tetragonal





**Origin** at  $\bar{4}2$ 'm' at -1/4,1/4,-1/4 from center ( 2'/m' )

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/4$ ;  $x \leq y$ ;  $y \leq 1-x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                        | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                      | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                      | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'         | (8) 2' x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)'  |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)        | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)   | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)                | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z$ <sup>-1</sup>  0,0,0)                |
| (13) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (14) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (15) m' x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)'                  | (16) m' x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,0)'                       |

For (1,0,0)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) t' (1,0,0)<br>(1 1,0,0)'                                | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'                    | (3) 4 <sup>+</sup> ' (0,0,1/2) -1/2,0,z<br>(4 <sub>z</sub>  3/2,1/2,1/2)' | (4) 4 <sup>-</sup> ' (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub> <sup>-1</sup>  3/2,1/2,1/2)'            |
| (5) 2 1/2,y,0<br>(2 <sub>y</sub>  1,0,0)                    | (6) 2 (1,0,0) x,0,0<br>(2 <sub>x</sub>  1,0,0)                | (7) 2 x-1/2,x,1/4<br>(2 <sub>xy</sub>  3/2,1/2,1/2)                       | (8) 2 (1/2,-1/2,0) x+1/2, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  3/2,1/2,1/2) |
| (9) $\bar{1}$ ' 3/4,1/4,1/4<br>( $\bar{1}$  3/2,1/2,1/2)'   | (10) n' (3/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  3/2,1/2,1/2)' | (11) $\bar{4}^+$ ' 1/2,-1/2,z; 1/2,-1/2,0<br>( $\bar{4}_z$  1,0,0)'       | (12) $\bar{4}^-$ ' 1/2,1/2,z; 1/2,1/2,0<br>( $\bar{4}_z$ <sup>-1</sup>  1,0,0)'                   |
| (13) n (3/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  3/2,1/2,1/2) | (14) n (0,1/2,1/2) 3/4,y,z<br>(m <sub>x</sub>  3/2,1/2,1/2)   | (15) g (1/2,-1/2,0) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1,0,0)       | (16) g (1/2,1/2,0) x+1/2,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1,0,0)                       |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5); (9).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

- |    |   |   |  |            |
|----|---|---|--|------------|
| 32 | n | 1   | (0,0,0) +  | (1,0,0)' + |
|    |   | (1) x,y,z [u,v,w]                                     | (2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]        |            |
|    |   | (3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]       | (4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]        |            |
|    |   | (5) $\bar{x},y,\bar{z}$ [ $u,\bar{v},w$ ]             | (6) $x,\bar{y},z$ [ $\bar{u},v,w$ ]                    |            |
|    |   | (7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ] | (8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $v,u,w$ ]  |            |
|    |   | (9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,v,w$ ] | (10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ] |            |
|    |   | (11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]            | (12) $\bar{y},x,z$ [ $v,\bar{u},w$ ]                   |            |
|    |   | (13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]      | (14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]       |            |

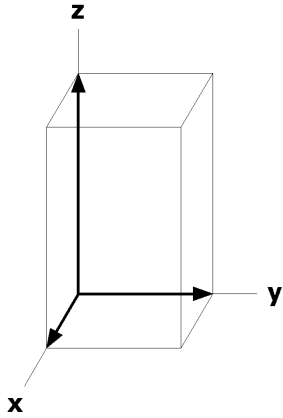
			(15) $\bar{y}, \bar{x}, z [\bar{v}, \bar{u}, w]$	(16) $y, x, z [v, u, w]$	
16	m	..m'	$x, x, z [u, u, w]$ $\bar{x}, x, \bar{z} [u, \bar{u}, w]$	$\bar{x}, \bar{x}, z [\bar{u}, \bar{u}, w]$ $x, \bar{x}, \bar{z} [\bar{u}, u, w]$	$\bar{x}+1/2, x+1/2, z+1/2 [\bar{u}, u, w]$ $x+1/2, \bar{x}+1/2, z+1/2 [u, \bar{u}, w]$ $x+1/2, x+1/2, \bar{z}+1/2 [\bar{u}, \bar{u}, w]$ $\bar{x}+1/2, \bar{x}+1/2, \bar{z}+1/2 [u, u, w]$
16	l	..2'	$x, x+1/2, 3/4 [\bar{u}, u, w]$ $\bar{x}+1/2, \bar{x}, 3/4 [u, \bar{u}, \bar{w}]$	$\bar{x}, \bar{x}+1/2, 3/4 [\bar{u}, u, \bar{w}]$ $x+1/2, x, 3/4 [u, \bar{u}, w]$	$\bar{x}, x+1/2, 1/4 [u, u, \bar{w}]$ $x+1/2, \bar{x}, 1/4 [u, u, \bar{w}]$ $x, \bar{x}+1/2, 1/4 [u, u, w]$ $\bar{x}+1/2, x, 1/4 [u, u, w]$
16	k	..2	$x, x+1/2, 1/4 [u, u, 0]$ $\bar{x}+1/2, \bar{x}, 1/4 [u, u, 0]$	$\bar{x}, \bar{x}+1/2, 1/4 [u, u, 0]$ $x+1/2, x, 1/4 [u, u, 0]$	$\bar{x}, x+1/2, 3/4 [\bar{u}, u, 0]$ $x+1/2, \bar{x}, 3/4 [u, \bar{u}, 0]$ $x, \bar{x}+1/2, 3/4 [\bar{u}, u, 0]$ $\bar{x}+1/2, x, 3/4 [u, \bar{u}, 0]$
16	j	..2.	$x, 0, 1/2 [u, 0, 0]$ $\bar{x}+1/2, 1/2, 0 [u, 0, 0]$	$\bar{x}, 0, 1/2 [\bar{u}, 0, 0]$ $x+1/2, 1/2, 0 [\bar{u}, 0, 0]$	$1/2, x+1/2, 0 [0, \bar{u}, 0]$ $0, \bar{x}, 1/2 [0, \bar{u}, 0]$ $1/2, \bar{x}+1/2, 0 [0, u, 0]$ $0, x, 1/2 [0, u, 0]$
16	i	..2'.	$x, 0, 0 [0, v, w]$ $\bar{x}+1/2, 1/2, 1/2 [0, v, w]$	$\bar{x}, 0, 0 [0, \bar{v}, w]$ $x+1/2, 1/2, 1/2 [0, \bar{v}, w]$	$1/2, x+1/2, 1/2 [\bar{v}, 0, w]$ $0, \bar{x}, 0 [\bar{v}, 0, w]$ $1/2, \bar{x}+1/2, 1/2 [v, 0, w]$ $0, x, 0 [v, 0, w]$
16	h	2'..	$0, 1/2, z [u, v, 0]$ $1/2, 0, \bar{z}+1/2 [u, v, 0]$	$0, 1/2, z+1/2 [\bar{v}, u, 0]$ $1/2, 0, \bar{z} [\bar{v}, u, 0]$	$0, 1/2, \bar{z} [u, \bar{v}, 0]$ $1/2, 0, z+1/2 [u, \bar{v}, 0]$ $0, 1/2, \bar{z}+1/2 [v, u, 0]$ $1/2, 0, z [v, u, 0]$
8	g	2.m'm'	$0, 0, z [0, 0, w]$	$1/2, 1/2, z+1/2 [0, 0, w]$	$0, 0, \bar{z} [0, 0, w]$ $1/2, 1/2, \bar{z}+1/2 [0, 0, w]$
8	f	..2/m'	$3/4, 3/4, 3/4 [0, 0, 0]$	$1/4, 1/4, 3/4 [0, 0, 0]$	$3/4, 1/4, 1/4 [0, 0, 0]$ $1/4, 3/4, 1/4 [0, 0, 0]$
8	e	..2'/m'	$1/4, 1/4, 1/4 [u, u, w]$	$3/4, 3/4, 1/4 [\bar{u}, \bar{u}, w]$	$1/4, 3/4, 3/4 [\bar{u}, u, w]$ $3/4, 1/4, 3/4 [u, \bar{u}, w]$
8	d	2'.22'	$0, 1/2, 1/4 [\bar{u}, u, 0]$	$0, 1/2, 3/4 [u, u, 0]$	$1/2, 0, 1/4 [\bar{u}, u, 0]$ $1/2, 0, 3/4 [u, \bar{u}, 0]$
8	c	2'22'.	$0, 1/2, 0 [u, 0, 0]$	$0, 1/2, 1/2 [0, u, 0]$	$1/2, 0, 1/2 [u, 0, 0]$ $1/2, 0, 0 [0, u, 0]$
4	b	$\bar{4}$ '2m'	$0, 0, 1/2 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$	
4	a	$\bar{4}$ '2m'	$0, 0, 0 [0, 0, w]$	$1/2, 1/2, 1/2 [0, 0, w]$	

### Symmetry of Special Projections

Along  $[0, 0, 1]$  p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$  c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 0, 0$

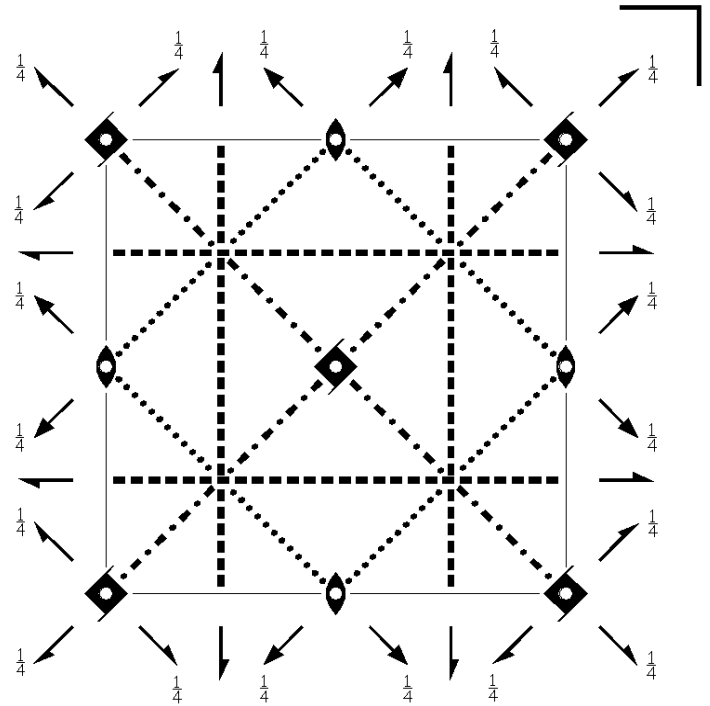
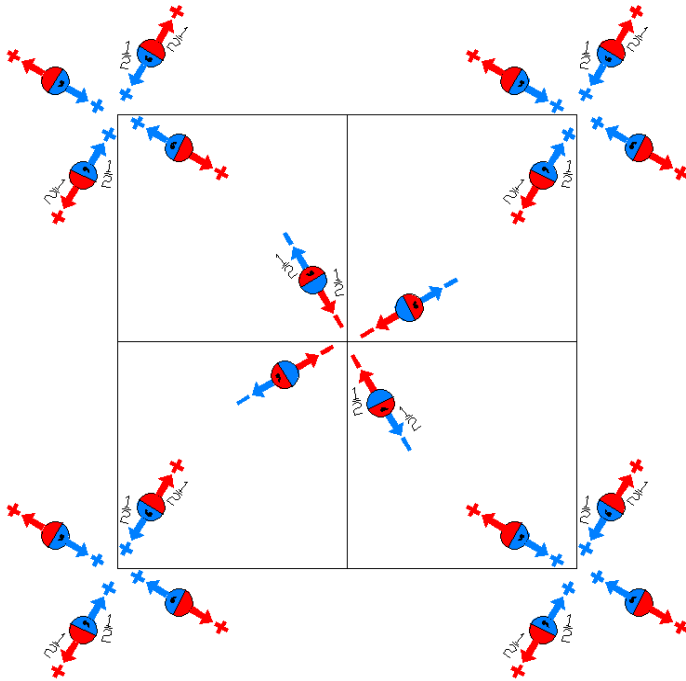
Along  $[1, 1, 0]$  p<sub>c</sub>-2mm  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x-1/4, x+1/4, 1/4$



$P4_2/mbc$   
135.1.1143

4/mmm  
 $P4_2/m2_1/b2/c$

Tetragonal



Origin at center ( $2/m$ ) at  $4_2/m1n$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 $0,0,z$<br>(2 <sub>z</sub>  0,0,0)                  | (3) 4 <sup>+</sup> $(0,0,1/2) 0,0,z$<br>(4 <sub>z</sub>  0,0,1/2)    | (4) 4 <sup>-</sup> $(0,0,1/2) 0,0,z$<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2) |
| (5) 2 $(0,1/2,0) 1/4,y,0$<br>(2 <sub>y</sub>  1/2,1/2,0)  | (6) 2 $(1/2,0,0) x,1/4,0$<br>(2 <sub>x</sub>  1/2,1/2,0)  | (7) 2 $(1/2,1/2,0) x,x,1/4$<br>(2 <sub>xy</sub>  1/2,1/2,1/2)        | (8) 2 $x,\bar{x}+1/2,1/4$<br>(2 <sub>xy</sub> <sup>-</sup>  1/2,1/2,1/2)        |
| (9) $\bar{1} 0,0,0$<br>( $\bar{1}$  0,0,0)                | (10) m $x,y,0$<br>(m <sub>z</sub>  0,0,0)                 | (11) $\bar{4}^+$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z^+$  0,0,1/2)       | (12) $\bar{4}^- 0,0,z; 0,0,1/4$<br>( $\bar{4}_z^-$  0,0,1/2)                    |
| (13) a $(1/2,0,0) x,1/4,z$<br>(m <sub>y</sub>  1/2,1/2,0) | (14) b $(0,1/2,0) 1/4,y,z$<br>(m <sub>x</sub>  1/2,1/2,0) | (15) c $(0,0,1/2) x+1/2,\bar{x},z$<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (16) n $(1/2,1/2,1/2) x,x,z$<br>(m <sub>xy</sub> <sup>-</sup>  1/2,1/2,1/2)     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

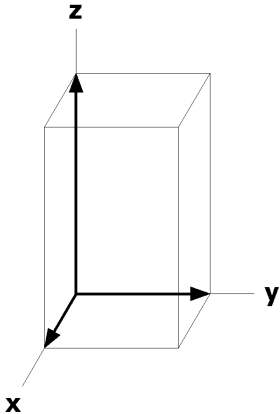
			Coordinates															
Multiplicity, Wyckoff letter, Site Symmetry.																		
16	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $v,\bar{u},w$ ]	(13) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	h	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,1/2$ [0,0,w]	$y,\bar{x},1/2$ [0,0,w]	$\bar{x}+1/2,y+1/2,0$ [0,0, $\bar{w}$ ]	$x+1/2,\bar{y}+1/2,0$ [0,0, $\bar{w}$ ]	$y+1/2,x+1/2,1/2$ [0,0, $\bar{w}$ ]	$\bar{y}+1/2,\bar{x}+1/2,1/2$ [0,0, $\bar{w}$ ]								
8	g	..2	x,x+1/2,1/4 [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},u,0$ ]	$x+1/2,\bar{x},3/4$ [ $u,\bar{u},0$ ]	$\bar{x},\bar{x}+1/2,3/4$ [u,u,0]	$x,x+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},1/4$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,x,1/4$ [ $u,\bar{u},0$ ]								
8	f	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]								
8	e	2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	1/2,1/2,z [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]								
4	d	2.22	0,1/2,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]												
4	c	2/m..	0,1/2,0 [0,0,w]	1/2,0,1/2 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]	0,1/2,1/2 [0,0, $\bar{w}$ ]												
4	b	$\bar{4}$ ..	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]	1/2,1/2,3/4 [0,0, $\bar{w}$ ]	1/2,1/2,1/4 [0,0, $\bar{w}$ ]												
4	a	2/m..	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]	1/2,1/2,0 [0,0, $\bar{w}$ ]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]												

**Symmetry of Special Projections**

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>· 2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,0

Along [1,1,0] p<sub>2a</sub>· 2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



$P4_2/mbc1'$

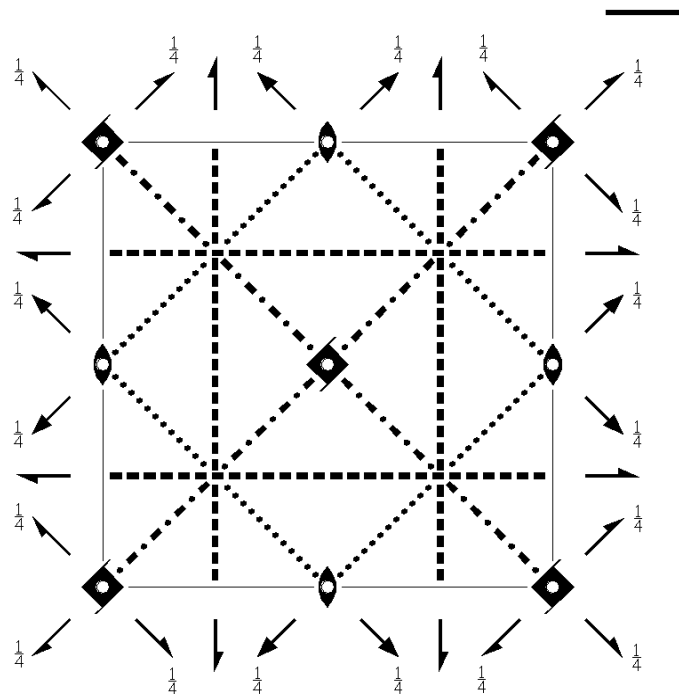
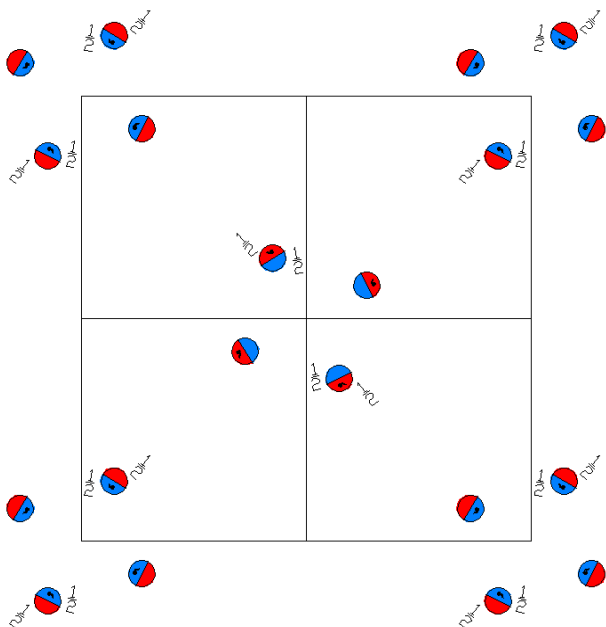
135.2.1144

$4/mmm1'$

$P4_2/m2_1/b2/c1'$

Tetragonal

1'



Origin at center ( $2/m1'$ ) at  $4_2/m1n1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

Symmetry Operations

For 1 + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                  | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)        | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)    |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)  | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)  | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)            | (8) 2 $x, \bar{x}+1/2, 1/4$<br>(2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2) |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)              | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)                 | (11) $\bar{4}^+$ 0,0,z; 0,0,1/4<br>( $\bar{4}_z^+$  0,0,1/2)           | (12) $\bar{4}^-$ 0,0,z; 0,0,1/4<br>( $\bar{4}_z^-$  0,0,1/2)                     |
| (13) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0) | (14) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0) | (15) c (0,0,1/2) $x+1/2, \bar{x}, z$<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (16) n (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)  |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> ' (0,0,1/2) 0,0,z (4 <sub>z</sub>  0,0,1/2)'	(4) 4 <sup>-</sup> ' (0,0,1/2) 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)'
(5) 2' (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>  1/2,1/2,0)'	(6) 2' (1/2,0,0) x,1/4,0 (2 <sub>x</sub>  1/2,1/2,0)'	(7) 2' (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(8) 2' x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub> <sup>-</sup>  1/2,1/2,1/2)'
(9) $\bar{1}$ ' 0,0,0 ( $\bar{1}$  0,0,0)'	(10) m' x,y,0 (m <sub>z</sub>  0,0,0)'	(11) $\bar{4}^+$ ' 0,0,z; 0,0,1/4 ( $\bar{4}_z$  0,0,1/2)'	(12) $\bar{4}^-$ ' 0,0,z; 0,0,1/4 ( $\bar{4}_z^{-1}$  0,0,1/2)'
(13) a' (1/2,0,0) x,1/4,z (m <sub>y</sub>  1/2,1/2,0)'	(14) b' (0,1/2,0) 1/4,y,z (m <sub>x</sub>  1/2,1/2,0)'	(15) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,1/2)'	(16) n' (1/2,1/2,1/2) x,x,z (m <sub>xy</sub> <sup>-</sup>  1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

**Positions**

			Coordinates															
Multiplicity, Wyckoff letter, Site Symmetry.			1 +	1' +														
16	i	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y},x,z+1/2$ [0,0,0]	(4) y, $\bar{x},z+1/2$ [0,0,0]	(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [0,0,0]	(6) x+1/2, $\bar{y}+1/2,\bar{z}$ [0,0,0]	(7) y+1/2,x+1/2, $\bar{z}+1/2$ [0,0,0]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [0,0,0]	(9) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(10) x,y, $\bar{z}$ [0,0,0]	(11) y, $\bar{x},\bar{z}+1/2$ [0,0,0]	(12) $\bar{y},x,\bar{z}+1/2$ [0,0,0]	(13) x+1/2, $\bar{y}+1/2,z$ [0,0,0]	(14) $\bar{x}+1/2,y+1/2,z$ [0,0,0]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [0,0,0]	(16) y+1/2,x+1/2,z+1/2 [0,0,0]
8	h	m..1'	x,y,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0]	$\bar{y},x,1/2$ [0,0,0]	y, $\bar{x},1/2$ [0,0,0]	$\bar{x}+1/2,y+1/2,0$ [0,0,0]	x+1/2, $\bar{y}+1/2,0$ [0,0,0]	y+1/2,x+1/2,1/2 [0,0,0]	$\bar{y}+1/2,\bar{x}+1/2,1/2$ [0,0,0]								
8	g	..21'	x,x+1/2,1/4 [0,0,0]	$\bar{x},\bar{x}+1/2,1/4$ [0,0,0]	$\bar{x}+1/2,x,3/4$ [0,0,0]	x+1/2, $\bar{x},3/4$ [0,0,0]	$\bar{x},\bar{x}+1/2,3/4$ [0,0,0]	x,x+1/2,3/4 [0,0,0]	x+1/2, $\bar{x},1/4$ [0,0,0]	$\bar{x}+1/2,x,1/4$ [0,0,0]								
8	f	2..1'	0,1/2,z [0,0,0]	1/2,0,z+1/2 [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	0,1/2, $\bar{z}+1/2$ [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	1/2,0,z [0,0,0]	0,1/2,z+1/2 [0,0,0]								
8	e	2..1'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	1/2,1/2,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]								
4	d	2.221'	0,1/2,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]												

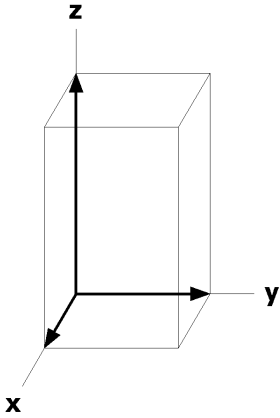
4	c	2/m..1'	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]
4	b	$\bar{4}$ ..1'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]	1/2,1/2,1/4 [0,0,0]
4	a	2/m..1'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

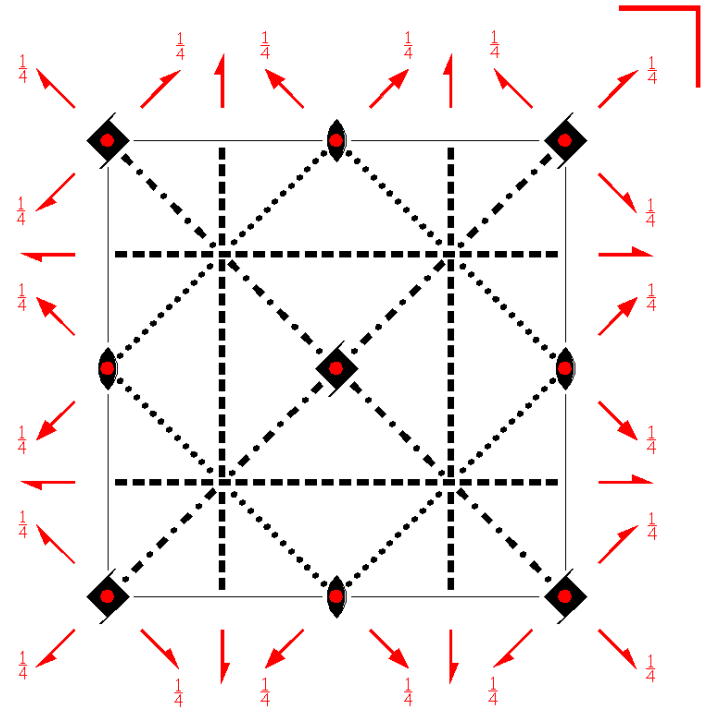
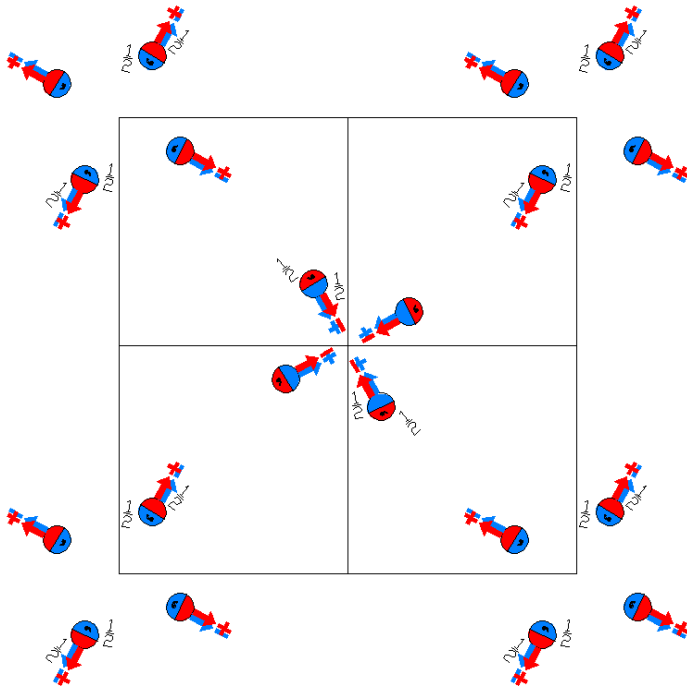
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,1/4



$P4_2/m'bc$   
135.3.1145

$4/m'mm$   
 $P4_2/m'2_1'/b2'/c$

Tetragonal



Origin at center ( $2/m'$ ) at  $4_2/m'1n$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) $1$<br>( $1 0,0,0$ )                               | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                     | (3) $4^+$ $(0,0,1/2)$ $0,0,z$<br>( $4_z 0,0,1/2$ )                 | (4) $4^-$ $(0,0,1/2)$ $0,0,z$<br>( $4_z^{-1} 0,0,1/2$ )            |
| (5) $2'$ $(0,1/2,0)$ $1/4,y,0$<br>( $2_y 1/2,1/2,0$ )' | (6) $2'$ $(1/2,0,0)$ $x,1/4,0$<br>( $2_x 1/2,1/2,0$ )' | (7) $2'$ $(1/2,1/2,0)$ $x,x,1/4$<br>( $2_{xy} 1/2,1/2,1/2$ )'      | (8) $2'$ $x,\bar{x}+1/2,1/4$<br>( $2_{\bar{xy}} 1/2,1/2,1/2$ )'    |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1} 0,0,0$ )'          | (10) $m'$ $x,y,0$<br>( $m_z 0,0,0$ )'                  | (11) $\bar{4}^+$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z 0,0,1/2$ )'      | (12) $\bar{4}^-$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z^{-1} 0,0,1/2$ )' |
| (13) $a$ $(1/2,0,0)$ $x,1/4,z$<br>( $m_y 1/2,1/2,0$ )  | (14) $b$ $(0,1/2,0)$ $1/4,y,z$<br>( $m_x 1/2,1/2,0$ )  | (15) $c$ $(0,0,1/2)$ $x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,1/2$ ) | (16) $n$ $(1/2,1/2,1/2)$ $x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,1/2$ ) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

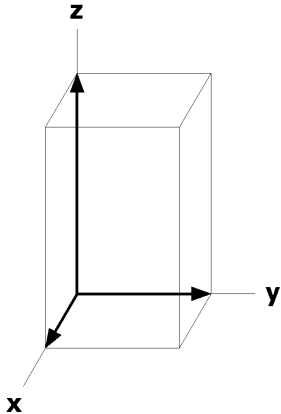
			Coordinates															
Multiplicity,	Wyckoff letter,	Site Symmetry.																
16	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]	(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $v,u,w$ ]	(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]	(13) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	h	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},u,0$ ]	$y,\bar{x},1/2$ [ $v,\bar{u},0$ ]	$\bar{x}+1/2,y+1/2,0$ [ $\bar{u},\bar{v},0$ ]	$x+1/2,\bar{y}+1/2,0$ [ $\bar{u},v,0$ ]	$y+1/2,x+1/2,1/2$ [ $\bar{v},\bar{u},0$ ]	$\bar{y}+1/2,\bar{x}+1/2,1/2$ [ $v,u,0$ ]								
8	g	..2'	$x,x+1/2,1/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},\bar{u},w$ ]	$x+1/2,\bar{x},3/4$ [ $u,u,w$ ]	$\bar{x},\bar{x}+1/2,3/4$ [ $u,\bar{u},\bar{w}$ ]	$x,x+1/2,3/4$ [ $\bar{u},u,\bar{w}$ ]	$x+1/2,\bar{x},1/4$ [ $u,u,\bar{w}$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]								
8	f	2'..	0,1/2,z [u,v,0]	1/2,0,z+1/2 [ $\bar{v},u,0$ ]	1/2,0, $\bar{z}$ [ $u,\bar{v},0$ ]	0,1/2, $\bar{z}+1/2$ [ $\bar{v},\bar{u},0$ ]	0,1/2, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	1/2,0, $\bar{z}+1/2$ [ $v,\bar{u},0$ ]	1/2,0,z [ $\bar{u},v,0$ ]	0,1/2,z+1/2 [ $v,u,0$ ]								
8	e	2'..	0,0,z [u,v,0]	0,0,z+1/2 [ $\bar{v},u,0$ ]	1/2,1/2, $\bar{z}$ [ $u,\bar{v},0$ ]	1/2,1/2, $\bar{z}+1/2$ [ $\bar{v},\bar{u},0$ ]	0,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	0,0, $\bar{z}+1/2$ [ $v,\bar{u},0$ ]	1/2,1/2,z [ $\bar{u},v,0$ ]	1/2,1/2,z+1/2 [ $v,u,0$ ]								
4	d	2.2'2'	0,1/2,1/4 [0,0,w]	1/2,0,3/4 [0,0,w]	0,1/2,3/4 [0,0, $\bar{w}$ ]	1/2,0,1/4 [0,0, $\bar{w}$ ]												
4	c	2/m'..	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]												
4	b	$\bar{4}'$ ..	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]	1/2,1/2,1/4 [0,0,0]												
4	a	2/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]												

**Symmetry of Special Projections**

Along [0,0,1] p4gm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>' 2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

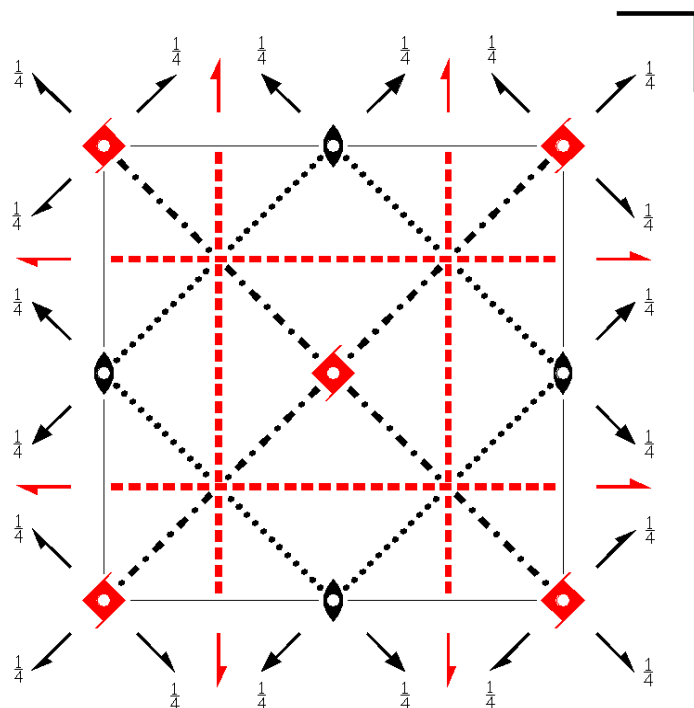
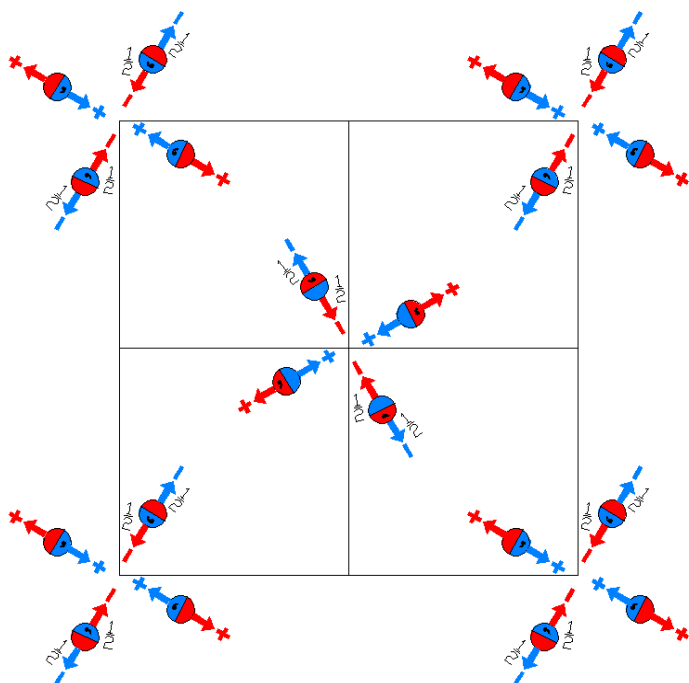
Along [1,1,0] p<sub>2a</sub>' 2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$P4_2'/mb'c$   
135.4.1146

$4'/mm'm$   
 $P4_2'/m2_1'/b'2/c$

Tetragonal



Origin at center ( $2/m$ ) at  $4_2'/m1n$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) $1$<br>( $1 0,0,0$ )                              | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                    | (3) $4^+$ $(0,0,1/2) 0,0,z$<br>( $4_z 0,0,1/2$ )'                | (4) $4^-$ $(0,0,1/2) 0,0,z$<br>( $4_z^{-1} 0,0,1/2$ )'             |
| (5) $2'$ $(0,1/2,0) 1/4,y,0$<br>( $2_y 1/2,1/2,0$ )'  | (6) $2'$ $(1/2,0,0) x,1/4,0$<br>( $2_x 1/2,1/2,0$ )'  | (7) $2$ $(1/2,1/2,0) x,x,1/4$<br>( $2_{xy} 1/2,1/2,1/2$ )        | (8) $2$ $x,\bar{x}+1/2,1/4$<br>( $2_{\bar{xy}} 1/2,1/2,1/2$ )      |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1} 0,0,0$ )          | (10) $m$ $x,y,0$<br>( $m_z 0,0,0$ )                   | (11) $\bar{4}^+$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z 0,0,1/2$ )'    | (12) $\bar{4}^-$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z^{-1} 0,0,1/2$ )' |
| (13) $a'$ $(1/2,0,0) x,1/4,z$<br>( $m_y 1/2,1/2,0$ )' | (14) $b'$ $(0,1/2,0) 1/4,y,z$<br>( $m_x 1/2,1/2,0$ )' | (15) $c$ $(0,0,1/2) x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,1/2$ ) | (16) $n$ $(1/2,1/2,1/2) x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,1/2$ )   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

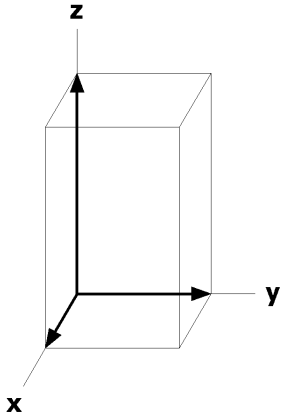
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(10) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(13) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},\bar{v},w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	h	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,1/2$ [0,0, $\bar{w}$ ]	$y,\bar{x},1/2$ [0,0, $\bar{w}$ ]	$\bar{x}+1/2,y+1/2,0$ [0,0,w]	$x+1/2,\bar{y}+1/2,0$ [0,0,w]	$y+1/2,x+1/2,1/2$ [0,0, $\bar{w}$ ]	$\bar{y}+1/2,\bar{x}+1/2,1/2$ [0,0, $\bar{w}$ ]								
8	g	..2	x,x+1/2,1/4 [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,3/4$ [u, $\bar{u},0$ ]	$x+1/2,\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},\bar{x}+1/2,3/4$ [u,u,0]	$x,x+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},1/4$ [u, $\bar{u},0$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},\bar{u},0$ ]								
8	f	2'..	0,1/2,z [u,v,0]	1/2,0,z+1/2 [ $\bar{v},\bar{u},0$ ]	1/2,0, $\bar{z}$ [u, $\bar{v},0$ ]	0,1/2, $\bar{z}+1/2$ [ $\bar{v},\bar{u},0$ ]	0,1/2, $\bar{z}$ [u,v,0]	1/2,0, $\bar{z}+1/2$ [ $\bar{v},\bar{u},0$ ]	1/2,0,z [u, $\bar{v},0$ ]	0,1/2,z+1/2 [ $\bar{v},\bar{u},0$ ]								
8	e	2'..	0,0,z [u,v,0]	0,0,z+1/2 [ $\bar{v},\bar{u},0$ ]	1/2,1/2, $\bar{z}$ [u, $\bar{v},0$ ]	1/2,1/2, $\bar{z}+1/2$ [ $\bar{v},\bar{u},0$ ]	0,0, $\bar{z}$ [u,v,0]	0,0, $\bar{z}+1/2$ [ $\bar{v},\bar{u},0$ ]	1/2,1/2,z [u, $\bar{v},0$ ]	1/2,1/2,z+1/2 [ $\bar{v},\bar{u},0$ ]								
4	d	2.22	0,1/2,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]												
4	c	2/m..	0,1/2,0 [0,0,w]	1/2,0,1/2 [0,0, $\bar{w}$ ]	1/2,0,0 [0,0,w]	0,1/2,1/2 [0,0, $\bar{w}$ ]												
4	b	$\bar{4}'$ ..	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]	1/2,1/2,1/4 [0,0,0]												
4	a	2/m..	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]												

### Symmetry of Special Projections

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

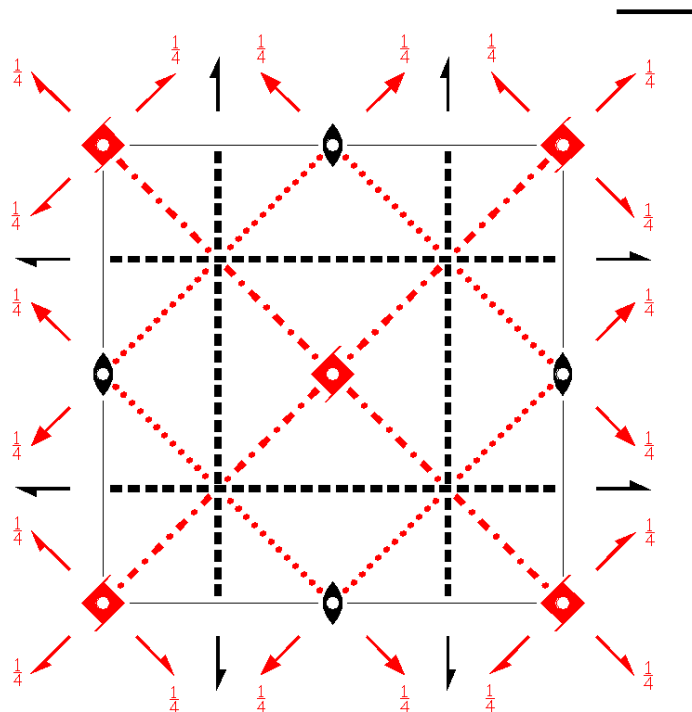
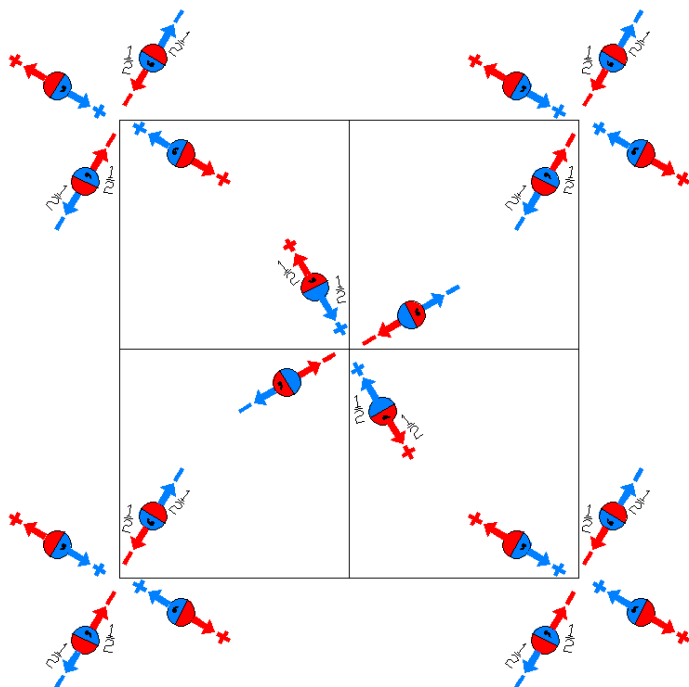
Along [1,1,0] p<sub>2a</sub>' 2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



$P4_2'/mbc'$   
135.5.1147

$4'/mmm'$   
 $P4_2'/m2_1/b2'/c'$

Tetragonal



Origin at center ( $2/m$ ) at  $4_2'/m1n'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) $1$<br>$(1 0,0,0)$                              | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                    | (3) $4^+$ $(0,0,1/2)$ $0,0,z$<br>$(4_z 0,0,1/2)'$                  | (4) $4^-$ $(0,0,1/2)$ $0,0,z$<br>$(4_z^{-1} 0,0,1/2)'$             |
| (5) $2$ $(0,1/2,0)$ $1/4,y,0$<br>$(2_y 1/2,1/2,0)$  | (6) $2$ $(1/2,0,0)$ $x,1/4,0$<br>$(2_x 1/2,1/2,0)$  | (7) $2'$ $(1/2,1/2,0)$ $x,x,1/4$<br>$(2_{xy} 1/2,1/2,1/2)'$        | (8) $2'$ $x,\bar{x}+1/2,1/4$<br>$(2_{\bar{xy}} 1/2,1/2,1/2)'$      |
| (9) $\bar{1}$ $0,0,0$<br>$(\bar{1} 0,0,0)$          | (10) $m$ $x,y,0$<br>$(m_z x,y,0)$                   | (11) $\bar{4}^+$ $0,0,z; 0,0,1/4$<br>$(\bar{4}_z 0,0,1/2)'$        | (12) $\bar{4}^-$ $0,0,z; 0,0,1/4$<br>$(\bar{4}_z^{-1} 0,0,1/2)'$   |
| (13) $a$ $(1/2,0,0)$ $x,1/4,z$<br>$(m_y 1/2,1/2,0)$ | (14) $b$ $(0,1/2,0)$ $1/4,y,z$<br>$(m_x 1/2,1/2,0)$ | (15) $c'$ $(0,0,1/2)$ $x+1/2,\bar{x},z$<br>$(m_{xy} 1/2,1/2,1/2)'$ | (16) $n'$ $(1/2,1/2,1/2)$ $x,x,z$<br>$(m_{\bar{xy}} 1/2,1/2,1/2)'$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

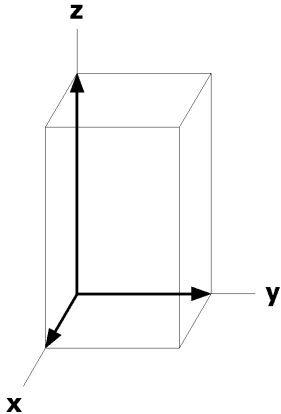
			Coordinates															
Multiplicity,	Wyckoff letter,	Site Symmetry.																
16	i	1	(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(4) $y, \bar{x}, z+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(5) $\bar{x}+1/2, y+1/2, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]	(7) $y+1/2, x+1/2, \bar{z}+1/2$ [ $\bar{v}, \bar{u}, w$ ]	(8) $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2$ [ $v, u, w$ ]	(9) $\bar{x}, \bar{y}, \bar{z}$ [ $u, v, w$ ]	(10) $x, y, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(11) $y, \bar{x}, \bar{z}+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(12) $\bar{y}, x, \bar{z}+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(13) $x+1/2, \bar{y}+1/2, z$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(14) $\bar{x}+1/2, y+1/2, z$ [ $u, \bar{v}, \bar{w}$ ]	(15) $\bar{y}+1/2, \bar{x}+1/2, z+1/2$ [ $\bar{v}, \bar{u}, w$ ]	(16) $y+1/2, x+1/2, z+1/2$ [ $v, u, w$ ]
8	h	m..	$x, y, 0$ [ $0, 0, w$ ]	$\bar{x}, \bar{y}, 0$ [ $0, 0, w$ ]	$\bar{y}, x, 1/2$ [ $0, 0, \bar{w}$ ]	$y, \bar{x}, 1/2$ [ $0, 0, \bar{w}$ ]	$\bar{x}+1/2, y+1/2, 0$ [ $0, 0, \bar{w}$ ]	$x+1/2, \bar{y}+1/2, 0$ [ $0, 0, \bar{w}$ ]	$y+1/2, x+1/2, 1/2$ [ $0, 0, w$ ]	$\bar{y}+1/2, \bar{x}+1/2, 1/2$ [ $0, 0, w$ ]								
8	g	..2'	$x, x+1/2, 1/4$ [ $\bar{u}, u, w$ ]	$\bar{x}, \bar{x}+1/2, 1/4$ [ $u, \bar{u}, w$ ]	$\bar{x}+1/2, x, 3/4$ [ $u, u, \bar{w}$ ]	$x+1/2, \bar{x}, 3/4$ [ $\bar{u}, \bar{u}, \bar{w}$ ]	$\bar{x}, \bar{x}+1/2, 3/4$ [ $\bar{u}, u, w$ ]	$x, x+1/2, 3/4$ [ $u, \bar{u}, w$ ]	$x+1/2, \bar{x}, 1/4$ [ $u, u, \bar{w}$ ]	$\bar{x}+1/2, x, 1/4$ [ $\bar{u}, \bar{u}, \bar{w}$ ]								
8	f	2..	$0, 1/2, z$ [ $0, 0, w$ ]	$1/2, 0, z+1/2$ [ $0, 0, \bar{w}$ ]	$1/2, 0, \bar{z}$ [ $0, 0, \bar{w}$ ]	$0, 1/2, \bar{z}+1/2$ [ $0, 0, w$ ]	$0, 1/2, \bar{z}$ [ $0, 0, w$ ]	$1/2, 0, \bar{z}+1/2$ [ $0, 0, \bar{w}$ ]	$1/2, 0, z$ [ $0, 0, \bar{w}$ ]	$0, 1/2, z+1/2$ [ $0, 0, w$ ]								
8	e	2..	$0, 0, z$ [ $0, 0, w$ ]	$0, 0, z+1/2$ [ $0, 0, \bar{w}$ ]	$1/2, 1/2, \bar{z}$ [ $0, 0, \bar{w}$ ]	$1/2, 1/2, \bar{z}+1/2$ [ $0, 0, w$ ]	$0, 0, \bar{z}$ [ $0, 0, w$ ]	$0, 0, \bar{z}+1/2$ [ $0, 0, \bar{w}$ ]	$1/2, 1/2, z$ [ $0, 0, \bar{w}$ ]	$1/2, 1/2, z+1/2$ [ $0, 0, w$ ]								
4	d	2.2'2'	$0, 1/2, 1/4$ [ $0, 0, w$ ]	$1/2, 0, 3/4$ [ $0, 0, \bar{w}$ ]	$0, 1/2, 3/4$ [ $0, 0, w$ ]	$1/2, 0, 1/4$ [ $0, 0, \bar{w}$ ]												
4	c	2/m..	$0, 1/2, 0$ [ $0, 0, w$ ]	$1/2, 0, 1/2$ [ $0, 0, \bar{w}$ ]	$1/2, 0, 0$ [ $0, 0, \bar{w}$ ]	$0, 1/2, 1/2$ [ $0, 0, w$ ]												
4	b	$\bar{4}'$ ..	$0, 0, 1/4$ [ $0, 0, 0$ ]	$0, 0, 3/4$ [ $0, 0, 0$ ]	$1/2, 1/2, 3/4$ [ $0, 0, 0$ ]	$1/2, 1/2, 1/4$ [ $0, 0, 0$ ]												
4	a	2/m..	$0, 0, 0$ [ $0, 0, w$ ]	$0, 0, 1/2$ [ $0, 0, \bar{w}$ ]	$1/2, 1/2, 0$ [ $0, 0, \bar{w}$ ]	$1/2, 1/2, 1/2$ [ $0, 0, w$ ]												

### Symmetry of Special Projections

Along  $[0, 0, 1]$  p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$  p<sub>2a</sub>·2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, 1/4, 0$

Along  $[1, 1, 0]$  p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, x, 1/4$



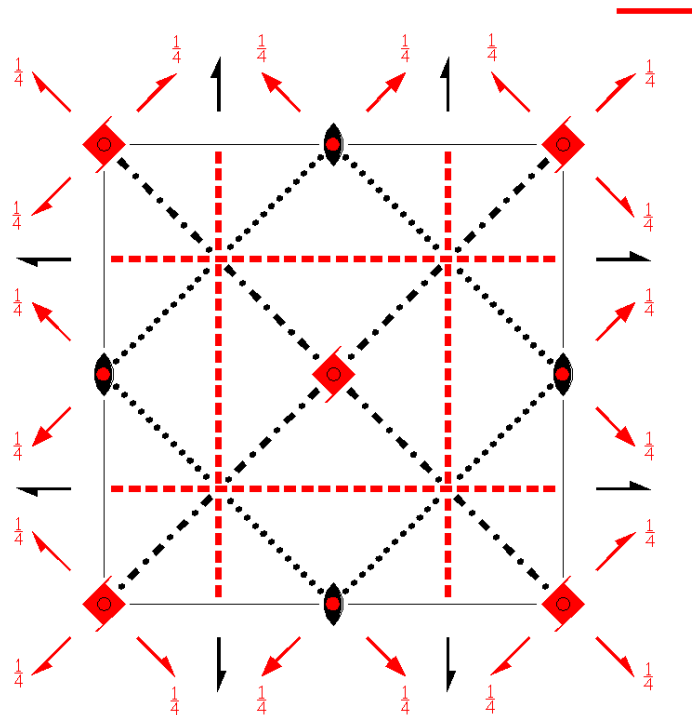
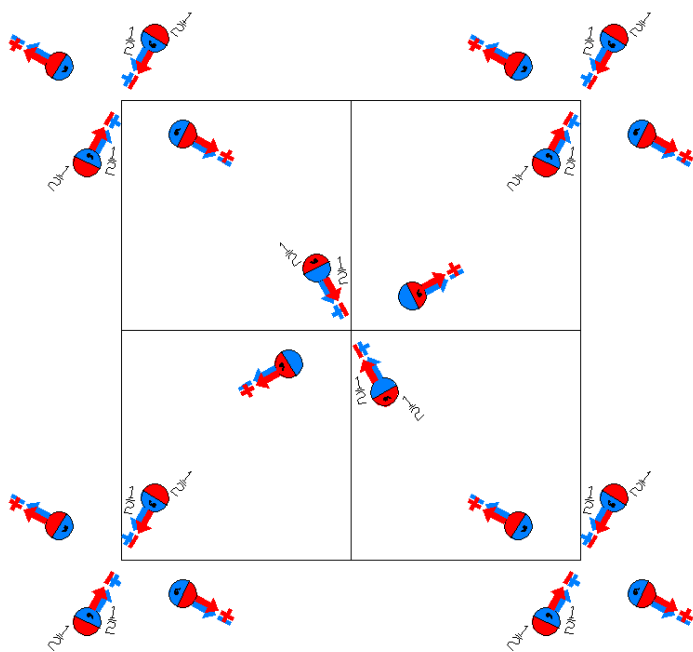
$P4_2/m'b'c$

135.6.1148

$4'/m'm'm$

$P4_2'/m'2_1/b'2'/c$

Tetragonal



Origin at center ( $2/m'$ ) at  $4_2'/m'1n$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                    | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)'             | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)    | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)    | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'                | (8) 2' x,x̄+1/2,1/4<br>(2 <sub>xy</sub> <sup>-</sup>  1/2,1/2,1/2)'            |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'                               | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'                 | (11) 4 <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>+</sup>  0,0,1/2) | (12) 4 <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)  |
| (13) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)' | (14) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)' | (15) c (0,0,1/2) x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)                | (16) n (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub> <sup>-</sup>  1/2,1/2,1/2)      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

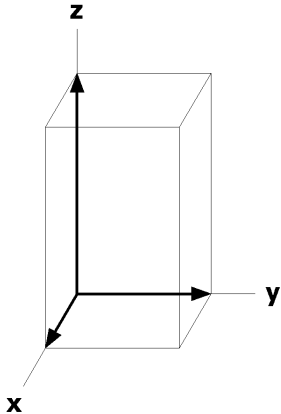
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	i	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x},z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $v,u,w$ ]	(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $v,\bar{u},w$ ]	(13) $x+1/2,\bar{y}+1/2,z$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	h	m'..	$x,y,0$ [ $u,v,0$ ]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $v,\bar{u},0$ ]	$y,\bar{x},1/2$ [ $\bar{v},u,0$ ]	$\bar{x}+1/2,y+1/2,0$ [ $\bar{u},v,0$ ]	$x+1/2,\bar{y}+1/2,0$ [ $u,\bar{v},0$ ]	$y+1/2,x+1/2,1/2$ [ $\bar{v},\bar{u},0$ ]	$\bar{y}+1/2,\bar{x}+1/2,1/2$ [ $v,u,0$ ]								
8	g	..2'	$x,x+1/2,1/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x,3/4$ [ $u,u,\bar{w}$ ]	$x+1/2,\bar{x},3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	$\bar{x},\bar{x}+1/2,3/4$ [ $u,\bar{u},\bar{w}$ ]	$x,x+1/2,3/4$ [ $\bar{u},u,\bar{w}$ ]	$x+1/2,\bar{x},1/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,1/4$ [ $u,u,w$ ]								
8	f	2..	$0,1/2,z$ [ $0,0,w$ ]	$1/2,0,z+1/2$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$0,1/2,\bar{z}+1/2$ [ $0,0,w$ ]	$0,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}+1/2$ [ $0,0,w$ ]	$1/2,0,z$ [ $0,0,w$ ]	$0,1/2,z+1/2$ [ $0,0,\bar{w}$ ]								
8	e	2..	$0,0,z$ [ $0,0,w$ ]	$0,0,z+1/2$ [ $0,0,\bar{w}$ ]	$1/2,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,w$ ]	$0,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$0,0,\bar{z}+1/2$ [ $0,0,w$ ]	$1/2,1/2,z$ [ $0,0,w$ ]	$1/2,1/2,z+1/2$ [ $0,0,\bar{w}$ ]								
4	d	2.2'2'	$0,1/2,1/4$ [ $0,0,w$ ]	$1/2,0,3/4$ [ $0,0,\bar{w}$ ]	$0,1/2,3/4$ [ $0,0,\bar{w}$ ]	$1/2,0,1/4$ [ $0,0,w$ ]												
4	c	2/m'..	$0,1/2,0$ [ $0,0,0$ ]	$1/2,0,1/2$ [ $0,0,0$ ]	$1/2,0,0$ [ $0,0,0$ ]	$0,1/2,1/2$ [ $0,0,0$ ]												
4	b	$\bar{4}$ ..	$0,0,1/4$ [ $0,0,w$ ]	$0,0,3/4$ [ $0,0,\bar{w}$ ]	$1/2,1/2,3/4$ [ $0,0,\bar{w}$ ]	$1/2,1/2,1/4$ [ $0,0,w$ ]												
4	a	2/m'..	$0,0,0$ [ $0,0,0$ ]	$0,0,1/2$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]												

### Symmetry of Special Projections

Along  $[0,0,1]$  p4'g'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

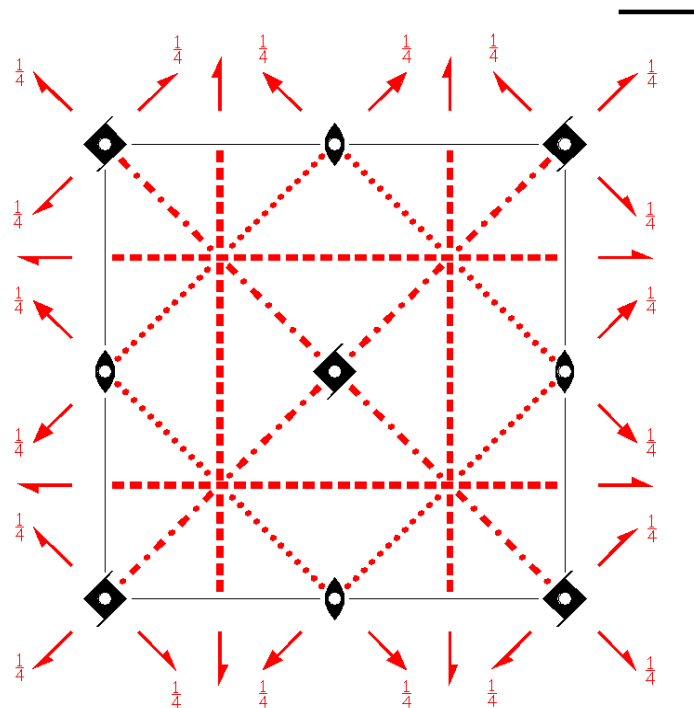
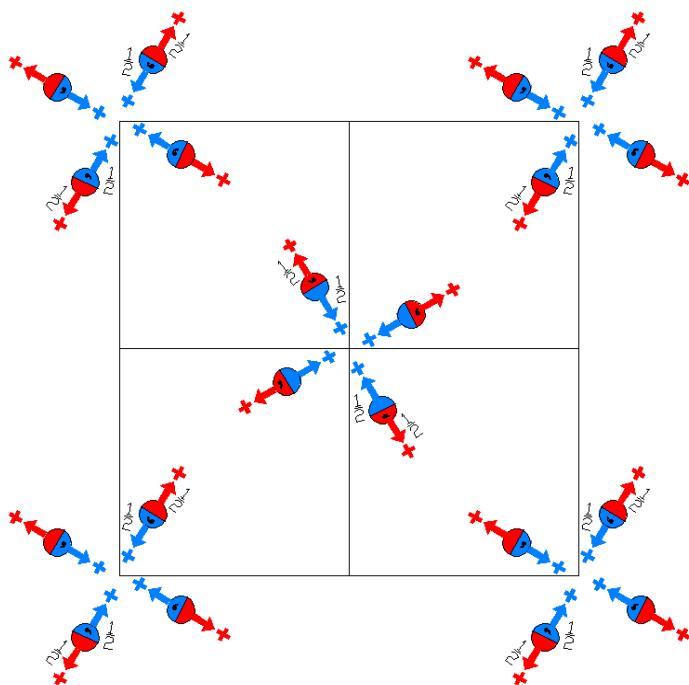
Along  $[1,1,0]$  p<sub>2a</sub>' 2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,0$



$P4_2/m'b'c'$   
135.7.1149

$4/mm'm'$   
 $P4_2/m2_1'b'2'/c'$

Tetragonal



Origin at center ( $2/m$ ) at  $4_2/m1n'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) $1$<br>$(1 0,0,0)$                              | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                    | (3) $4^+$ $(0,0,1/2) 0,0,z$<br>$(4_z 0,0,1/2)$                   | (4) $4^-$ $(0,0,1/2) 0,0,z$<br>$(4_z^{-1} 0,0,1/2)$              |
| (5) $2'$ $(0,1/2,0) 1/4,y,0$<br>$(2_y 1/2,1/2,0)'$  | (6) $2'$ $(1/2,0,0) x,1/4,0$<br>$(2_x 1/2,1/2,0)'$  | (7) $2'$ $(1/2,1/2,0) x,x,1/4$<br>$(2_{xy} 1/2,1/2,1/2)'$        | (8) $2'$ $x,\bar{x}+1/2,1/4$<br>$(2_{\bar{xy}} 1/2,1/2,1/2)'$    |
| (9) $\bar{1}$ $0,0,0$<br>$(\bar{1} 0,0,0)$          | (10) $m$ $x,y,0$<br>$(m_z 0,0,0)$                   | (11) $\bar{4}^+$ $0,0,z; 0,0,1/4$<br>$(\bar{4}_z 0,0,1/2)$       | (12) $\bar{4}^-$ $0,0,z; 0,0,1/4$<br>$(\bar{4}_z^{-1} 0,0,1/2)$  |
| (13) $a'$ $(1/2,0,0) x,1/4,z$<br>$(m_y 1/2,1/2,0)'$ | (14) $b'$ $(0,1/2,0) 1/4,y,z$<br>$(m_x 1/2,1/2,0)'$ | (15) $c'$ $(0,0,1/2) x+1/2,\bar{x},z$<br>$(m_{xy} 1/2,1/2,1/2)'$ | (16) $n'$ $(1/2,1/2,1/2) x,x,z$<br>$(m_{\bar{xy}} 1/2,1/2,1/2)'$ |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

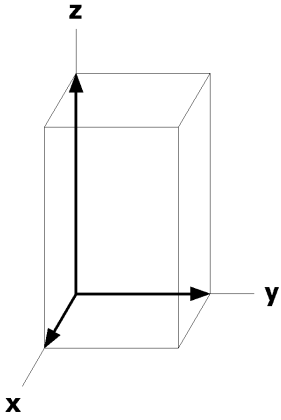
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $\bar{u},v,w$ ]	(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $v,u,w$ ]	(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(10) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $v,\bar{u},w$ ]	(13) $x+1/2,\bar{y}+1/2,z$ [ $\bar{u},\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $v,u,w$ ]
8	h	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,1/2$ [0,0,w]	$y,\bar{x},1/2$ [0,0,w]	$\bar{x}+1/2,y+1/2,0$ [0,0,w]	$x+1/2,\bar{y}+1/2,0$ [0,0,w]	$y+1/2,x+1/2,1/2$ [0,0,w]	$\bar{y}+1/2,\bar{x}+1/2,1/2$ [0,0,w]								
8	g	..2'	$x,x+1/2,1/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},\bar{u},w$ ]	$x+1/2,\bar{x},3/4$ [ $u,u,w$ ]	$\bar{x},\bar{x}+1/2,3/4$ [ $\bar{u},u,w$ ]	$x,x+1/2,3/4$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x},1/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,1/4$ [ $u,u,w$ ]								
8	f	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0,z [0,0,w]	0,1/2,z+1/2 [0,0,w]								
8	e	2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]								
4	d	2.2'2'	0,1/2,1/4 [0,0,w]	1/2,0,3/4 [0,0,w]	0,1/2,3/4 [0,0,w]	1/2,0,1/4 [0,0,w]												
4	c	2/m..	0,1/2,0 [0,0,w]	1/2,0,1/2 [0,0,w]	1/2,0,0 [0,0,w]	0,1/2,1/2 [0,0,w]												
4	b	$\bar{4}$ ..	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]	1/2,1/2,3/4 [0,0,w]	1/2,1/2,1/4 [0,0,w]												
4	a	2/m..	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]	1/2,1/2,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]												

### Symmetry of Special Projections

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,1/4



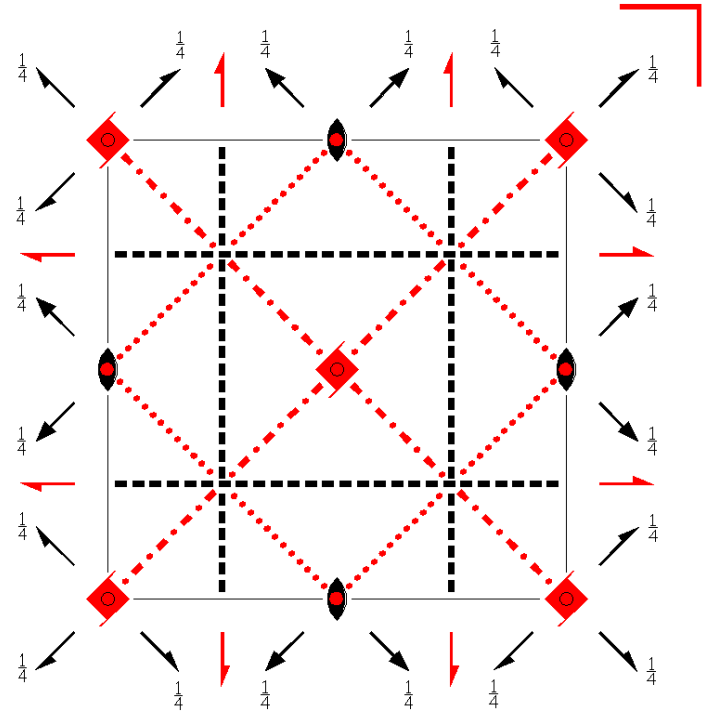
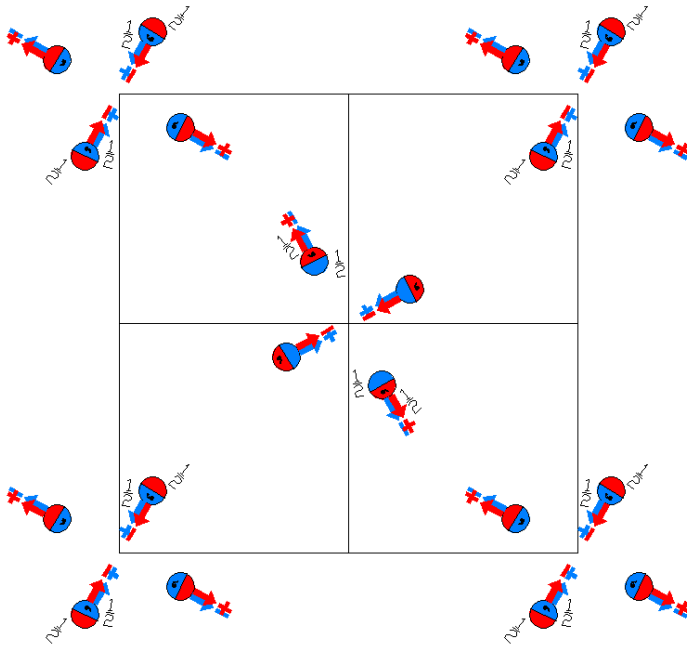
$P4_2'/m'bc'$

135.8.1150

$4'/m'mm'$

$P4_2'/m'2_1'/b2/c'$

Tetragonal



Origin at center ( $2/m'$ ) at  $4_2'/m'1n'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                   | (3) 4 <sup>+</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>  0,0,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' |
| (5) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (6) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)' | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)      | (8) 2 x,x̄+1/2,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)                           |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'                              | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'                | (11) 4 <sup>+</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub>  0,0,1/2)  | (12) 4 <sup>-</sup> 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,1/2)  |
| (13) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,0)  | (14) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)  | (15) c' (0,0,1/2) x+1/2,x̄,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)'  | (16) n' (1/2,1/2,1/2) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,1/2)'                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

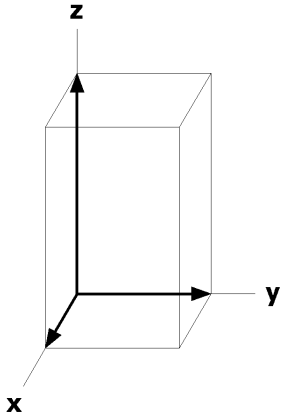
			Coordinates															
Multiplicity,	Wyckoff letter,	Site Symmetry.																
16	i	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{y}, x, z+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(4) $y, \bar{x}, z+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(5) $\bar{x}+1/2, y+1/2, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(6) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(7) $y+1/2, x+1/2, \bar{z}+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(8) $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(9) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(10) $x, y, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(11) $y, \bar{x}, \bar{z}+1/2$ [ $\bar{v}, \bar{u}, w$ ]	(12) $\bar{y}, x, \bar{z}+1/2$ [ $\bar{v}, \bar{u}, w$ ]	(13) $x+1/2, \bar{y}+1/2, z$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(14) $\bar{x}+1/2, y+1/2, z$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(15) $\bar{y}+1/2, \bar{x}+1/2, z+1/2$ [ $\bar{v}, \bar{u}, w$ ]	(16) $y+1/2, x+1/2, z+1/2$ [ $\bar{v}, \bar{u}, w$ ]
8	h	m'..	$x, y, 0$ [u,v,0]	$\bar{x}, \bar{y}, 0$ [ $\bar{u}, \bar{v}, 0$ ]	$\bar{y}, x, 1/2$ [ $\bar{v}, \bar{u}, 0$ ]	$y, \bar{x}, 1/2$ [ $\bar{v}, \bar{u}, 0$ ]	$\bar{x}+1/2, y+1/2, 0$ [ $\bar{u}, \bar{v}, 0$ ]	$x+1/2, \bar{y}+1/2, 0$ [ $\bar{u}, \bar{v}, 0$ ]	$y+1/2, x+1/2, 1/2$ [ $\bar{v}, \bar{u}, 0$ ]	$\bar{y}+1/2, \bar{x}+1/2, 1/2$ [ $\bar{v}, \bar{u}, 0$ ]								
8	g	..2	$x, x+1/2, 1/4$ [u,u,0]	$\bar{x}, \bar{x}+1/2, 1/4$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}+1/2, x, 3/4$ [u, $\bar{u}$ ,0]	$x+1/2, \bar{x}, 3/4$ [u, $\bar{u}$ ,0]	$\bar{x}, \bar{x}+1/2, 3/4$ [ $\bar{u}, \bar{u}, 0$ ]	$x, x+1/2, 3/4$ [u,u,0]	$x+1/2, \bar{x}, 1/4$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}+1/2, x, 1/4$ [u, $\bar{u}$ ,0]								
8	f	2..	$0, 1/2, z$ [0,0,w]	$1/2, 0, z+1/2$ [0,0, $\bar{w}$ ]	$1/2, 0, \bar{z}$ [0,0,w]	$0, 1/2, \bar{z}+1/2$ [0,0, $\bar{w}$ ]	$0, 1/2, \bar{z}$ [0,0, $\bar{w}$ ]	$1/2, 0, \bar{z}+1/2$ [0,0,w]	$1/2, 0, z$ [0,0, $\bar{w}$ ]	$0, 1/2, z+1/2$ [0,0,w]								
8	e	2..	$0, 0, z$ [0,0,w]	$0, 0, z+1/2$ [0,0, $\bar{w}$ ]	$1/2, 1/2, \bar{z}$ [0,0,w]	$1/2, 1/2, \bar{z}+1/2$ [0,0, $\bar{w}$ ]	$0, 0, \bar{z}$ [0,0, $\bar{w}$ ]	$0, 0, \bar{z}+1/2$ [0,0,w]	$1/2, 1/2, z$ [0,0, $\bar{w}$ ]	$1/2, 1/2, z+1/2$ [0,0,w]								
4	d	2.22	$0, 1/2, 1/4$ [0,0,0]	$1/2, 0, 3/4$ [0,0,0]	$0, 1/2, 3/4$ [0,0,0]	$1/2, 0, 1/4$ [0,0,0]												
4	c	2/m'..	$0, 1/2, 0$ [0,0,0]	$1/2, 0, 1/2$ [0,0,0]	$1/2, 0, 0$ [0,0,0]	$0, 1/2, 1/2$ [0,0,0]												
4	b	$\bar{4}$ ..	$0, 0, 1/4$ [0,0,w]	$0, 0, 3/4$ [0,0, $\bar{w}$ ]	$1/2, 1/2, 3/4$ [0,0,w]	$1/2, 1/2, 1/4$ [0,0, $\bar{w}$ ]												
4	a	2/m'..	$0, 0, 0$ [0,0,0]	$0, 0, 1/2$ [0,0,0]	$1/2, 1/2, 0$ [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]												

**Symmetry of Special Projections**

Along [0,0,1] p4'gm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>' 2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

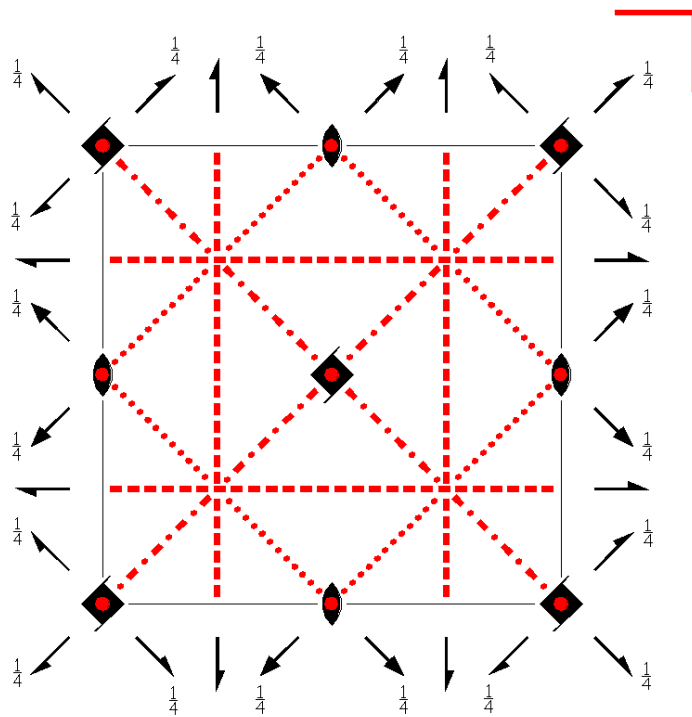
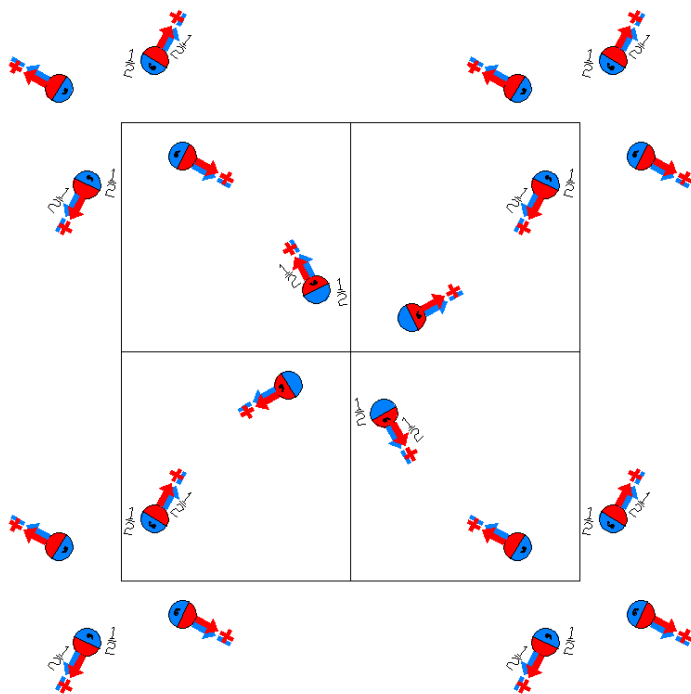
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P4_2/m'b'c'$   
135.9.1151

$4/m'm'm'$   
 $P4_2/m'2_1/b'2/c'$

Tetragonal



Origin at center ( $2/m'$ ) at  $4_2/m'1n'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) $1$<br>( $1 0,0,0$ )                                | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                      | (3) $4^+$ $(0,0,1/2)$ $0,0,z$<br>( $4_z 0,0,1/2$ )                   | (4) $4^-$ $(0,0,1/2)$ $0,0,z$<br>( $4_z^{-1} 0,0,1/2$ )              |
| (5) $2$ $(0,1/2,0)$ $1/4,y,0$<br>( $2_y 1/2,1/2,0$ )    | (6) $2$ $(1/2,0,0)$ $x,1/4,0$<br>( $2_x 1/2,1/2,0$ )    | (7) $2$ $(1/2,1/2,0)$ $x,x,1/4$<br>( $2_{xy} 1/2,1/2,1/2$ )          | (8) $2$ $x,\bar{x}+1/2,1/4$<br>( $2_{\bar{xy}} 1/2,1/2,1/2$ )        |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1} 0,0,0$ )'           | (10) $m'$ $x,y,0$<br>( $m_z 0,0,0$ )'                   | (11) $\bar{4}^+$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z 0,0,1/2$ )'        | (12) $\bar{4}^-$ $0,0,z; 0,0,1/4$<br>( $\bar{4}_z^{-1} 0,0,1/2$ )'   |
| (13) $a'$ $(1/2,0,0)$ $x,1/4,z$<br>( $m_y 1/2,1/2,0$ )' | (14) $b'$ $(0,1/2,0)$ $1/4,y,z$<br>( $m_x 1/2,1/2,0$ )' | (15) $c'$ $(0,0,1/2)$ $x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,1/2$ )' | (16) $n'$ $(1/2,1/2,1/2)$ $x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,1/2$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

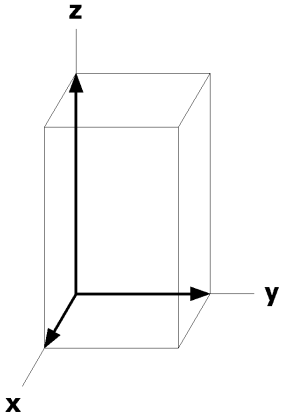
			Coordinates															
Multiplicity, Wyckoff letter, Site Symmetry.																		
16	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x},z+1/2$ [ $v,\bar{u},w$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) $y+1/2,x+1/2,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y,\bar{z}$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}+1/2$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]	(13) $x+1/2,\bar{y}+1/2,z$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $v,u,w$ ]
8	h	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,1/2$ [ $\bar{v},u,0$ ]	$y,\bar{x},1/2$ [ $v,\bar{u},0$ ]	$\bar{x}+1/2,y+1/2,0$ [ $\bar{u},v,0$ ]	$x+1/2,\bar{y}+1/2,0$ [ $u,\bar{v},0$ ]	$y+1/2,x+1/2,1/2$ [ $v,u,0$ ]	$\bar{y}+1/2,\bar{x}+1/2,1/2$ [ $\bar{v},\bar{u},0$ ]								
8	g	..2	x,x+1/2,1/4 [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},u,0$ ]	$x+1/2,\bar{x},3/4$ [ $u,\bar{u},0$ ]	$\bar{x},\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$x,x+1/2,3/4$ [ $u,u,0$ ]	$x+1/2,\bar{x},1/4$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},u,0$ ]								
8	f	2..	0,1/2,z [0,0,w]	1/2,0,z+1/2 [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0,z [0,0,w]	0,1/2,z+1/2 [0,0,w]								
8	e	2..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,1/2,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]								
4	d	2.22	0,1/2,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]												
4	c	2/m'..	0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]	0,1/2,1/2 [0,0,0]												
4	b	$\bar{4}'$ ..	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]	1/2,1/2,1/4 [0,0,0]												
4	a	2/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]												

### Symmetry of Special Projections

Along [0,0,1] p4g'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p 2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

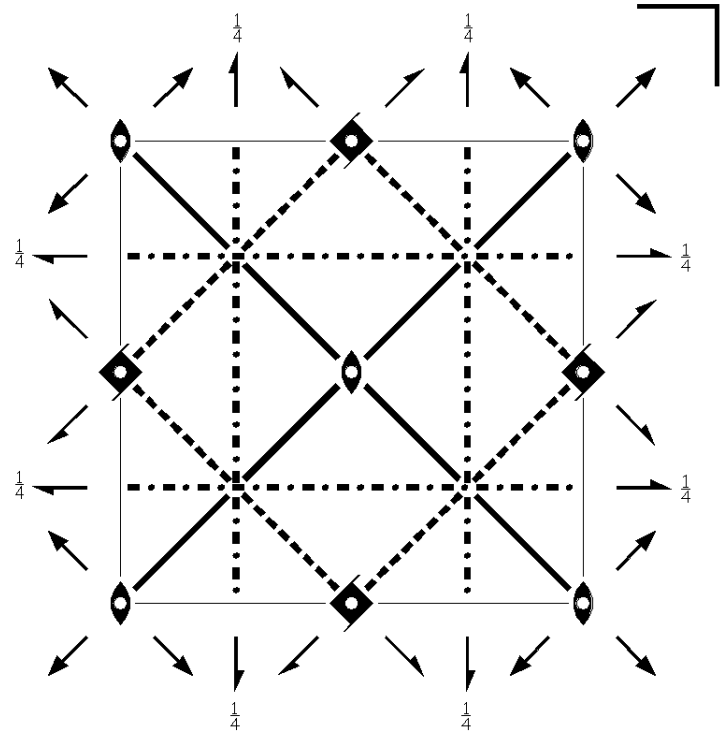
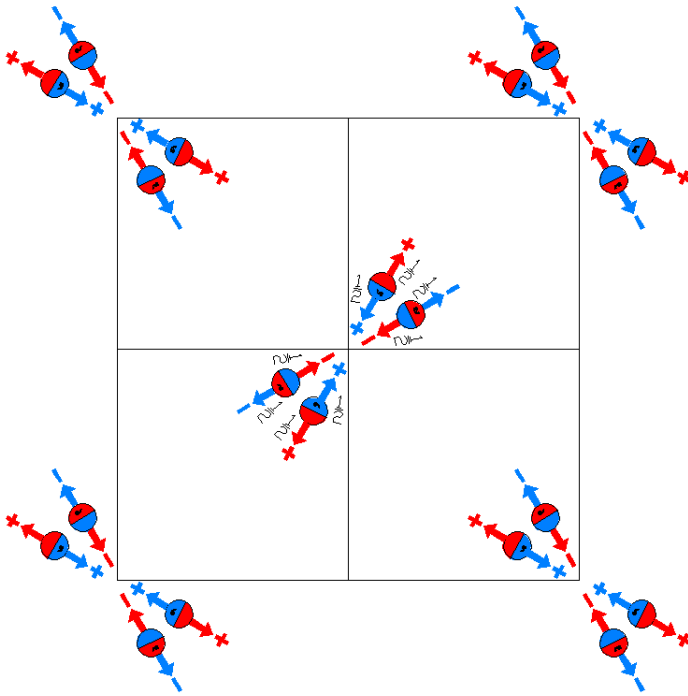
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P4_2/mnm$   
136.1.1152

$4/mmm$   
 $P4_2/m2_1/n2/m$

Tetragonal



Origin at center ( mmm ) at  $2/m12/m$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)  | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                               | (8) 2 x,x̄,0<br>(2 <sub>xy</sub>  0,0,0)  |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)                  | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)                     | (11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2)  | (12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2)                |
| (13) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (14) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (15) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                             | (16) m x,x,z<br>(m <sub>xy</sub>  0,0,0)  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},u,w$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [ $v,\bar{u},w$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]		
8	j	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]		
			$\bar{x}+1/2,x+1/2,z+1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,z+1/2$ [ $u,u,0$ ]		
			$\bar{x}+1/2,x+1/2,\bar{z}+1/2$ [ $u,u,0$ ]	$x+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]		
			x,x, $\bar{z}$ [ $u,\bar{u},0$ ]	$\bar{x},\bar{x},\bar{z}$ [ $\bar{u},u,0$ ]		
8	i	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]		
			$\bar{y}+1/2,x+1/2,1/2$ [0,0,w]	$y+1/2,\bar{x}+1/2,1/2$ [0,0,w]		
			$\bar{x}+1/2,y+1/2,1/2$ [0,0, $\bar{w}$ ]	$x+1/2,\bar{y}+1/2,1/2$ [0,0, $\bar{w}$ ]		
			y,x,0 [0,0, $\bar{w}$ ]	$\bar{y},\bar{x},0$ [0,0, $\bar{w}$ ]		
8	h	2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
			0,1/2, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2,z [0,0, $\bar{w}$ ]
4	g	m.2m	x, $\bar{x},0$ [0,0,0]	$\bar{x},x,0$ [0,0,0]	$x+1/2,x+1/2,1/2$ [0,0,0]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [0,0,0]
4	f	m.2m	x,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x}+1/2,x+1/2,1/2$ [0,0,0]	$x+1/2,\bar{x}+1/2,1/2$ [0,0,0]
4	e	2.mm	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	d	$\bar{4}$ ..	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0,w]	1/2,0,1/4 [0,0, $\bar{w}$ ]	1/2,0,3/4 [0,0, $\bar{w}$ ]
4	c	2/m..	0,1/2,0 [0,0,w]	0,1/2,1/2 [0,0,w]	1/2,0,1/2 [0,0, $\bar{w}$ ]	1/2,0,0 [0,0, $\bar{w}$ ]
2	b	m.mm	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		

2 a m.mm 0,0,0 [0,0,0]

1/2,1/2,1/2 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4gm1'

$\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$

Origin at 0,1/2,z

Along [1,0,0] c<sub>p</sub> 2'mm'

$\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$

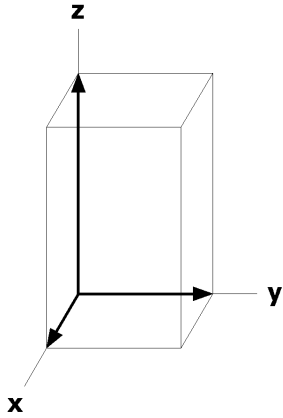
Origin at x,0,0

Along [1,1,0] p2mm1'

$\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$

Origin at x,x,0





$P4_2/mnm1'$

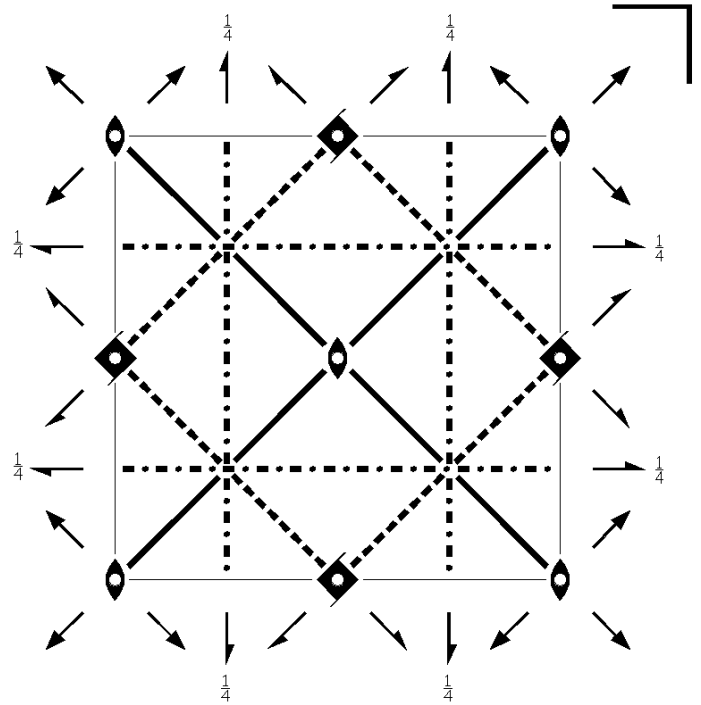
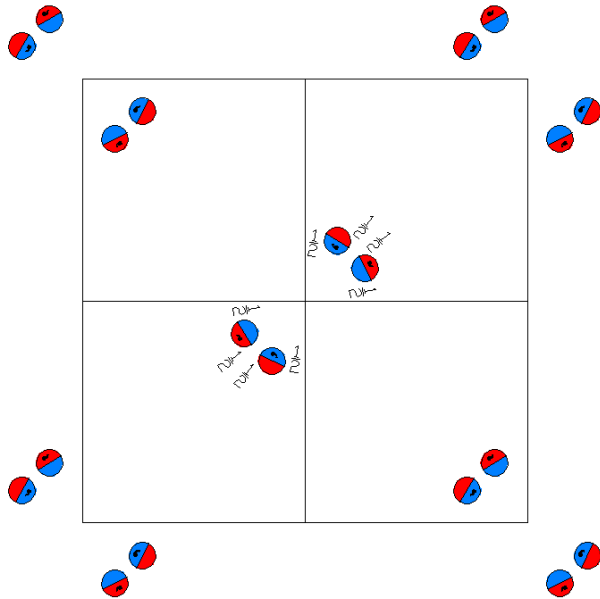
136.2.1153

$4/mmm1'$

$P4_2/m2_1/n2/m1'$

Tetragonal

1'



Origin at center ( $mmm1'$ ) at  $2/m12/m1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

Symmetry Operations

1 + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)  | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                               | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)                |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)                  | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)                     | (11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$  1/2,1/2,1/2)  | (12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$  1/2,1/2,1/2)                |
| (13) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2) | (14) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2) | (15) m x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)                    | (16) m x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,0)                         |

## 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)'	(4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'
(5) 2' (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>  1/2,1/2,1/2)'	(6) 2' (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>  1/2,1/2,1/2)'	(7) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) 2' x, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  0,0,0)'
(9) $\bar{1}$ ' 0,0,0 ( $\bar{1}$  0,0,0)'	(10) m' x,y,0 (m <sub>z</sub>  0,0,0)'	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$  1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$  1/2,1/2,1/2)'
(13) n' (1/2,0,1/2) x,1/4,z (m <sub>y</sub>  1/2,1/2,1/2)'	(14) n' (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1/2)'	(15) m' x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)'	(16) m' x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

**Positions**

			Coordinates	
Multiplicity, Wyckoff letter, Site Symmetry.			1 +	1' +
16	k	11'	(1) x,y,z [0,0,0] (3) $\bar{y}+1/2,x+1/2,z+1/2$ [0,0,0] (5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [0,0,0] (7) y,x, $\bar{z}$ [0,0,0] (9) $\bar{x},\bar{y},\bar{z}$ [0,0,0] (11) y+1/2, $\bar{x}+1/2,\bar{z}+1/2$ [0,0,0] (13) x+1/2, $\bar{y}+1/2,z+1/2$ [0,0,0] (15) $\bar{y},\bar{x},z$ [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0] (4) y+1/2, $\bar{x}+1/2,z+1/2$ [0,0,0] (6) x+1/2, $\bar{y}+1/2,\bar{z}+1/2$ [0,0,0] (8) $\bar{y},\bar{x},\bar{z}$ [0,0,0] (10) x,y, $\bar{z}$ [0,0,0] (12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [0,0,0] (14) $\bar{x}+1/2,y+1/2,z+1/2$ [0,0,0] (16) y,x,z [0,0,0]
8	j	..m1'	x,x,z [0,0,0] $\bar{x}+1/2,x+1/2,z+1/2$ [0,0,0] $\bar{x}+1/2,x+1/2,\bar{z}+1/2$ [0,0,0] x,x, $\bar{z}$ [0,0,0]	$\bar{x},\bar{x},z$ [0,0,0] x+1/2, $\bar{x}+1/2,z+1/2$ [0,0,0] x+1/2, $\bar{x}+1/2,\bar{z}+1/2$ [0,0,0] $\bar{x},\bar{x},\bar{z}$ [0,0,0]
8	i	m..1'	x,y,0 [0,0,0] $\bar{y}+1/2,x+1/2,1/2$ [0,0,0] $\bar{x}+1/2,y+1/2,1/2$ [0,0,0] y,x,0 [0,0,0]	$\bar{x},\bar{y},0$ [0,0,0] y+1/2, $\bar{x}+1/2,1/2$ [0,0,0] x+1/2, $\bar{y}+1/2,1/2$ [0,0,0] $\bar{y},\bar{x},0$ [0,0,0]

Continued

136.2.1153

 $P4_2/mnm1'$ 

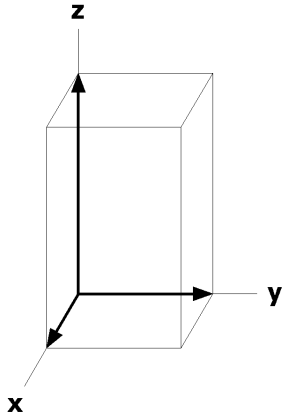
8	h	2..1'	0,1/2,z [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0, $\bar{z}$ +1/2 [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]
			0,1/2, $\bar{z}$ [0,0,0]	0,1/2, $\bar{z}$ +1/2 [0,0,0]	1/2,0,z+1/2 [0,0,0]	0,1/2,z [0,0,0]
4	g	m.2m1'	x, $\bar{x}$ ,0 [0,0,0]	$\bar{x}$ ,x,0 [0,0,0]	x+1/2,x+1/2,1/2 [0,0,0]	$\bar{x}$ +1/2, $\bar{x}$ +1/2,1/2 [0,0,0]
4	f	m.2m1'	x,x,0 [0,0,0]	$\bar{x}$ , $\bar{x}$ ,0 [0,0,0]	$\bar{x}$ +1/2,x+1/2,1/2 [0,0,0]	x+1/2, $\bar{x}$ +1/2,1/2 [0,0,0]
4	e	2.mm1'	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}$ +1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	d	$\bar{4}$ ..1'	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]
4	c	2/m..1'	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]
2	b	m.mm1'	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		
2	a	m.mm1'	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4gm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,0,0]  $c2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



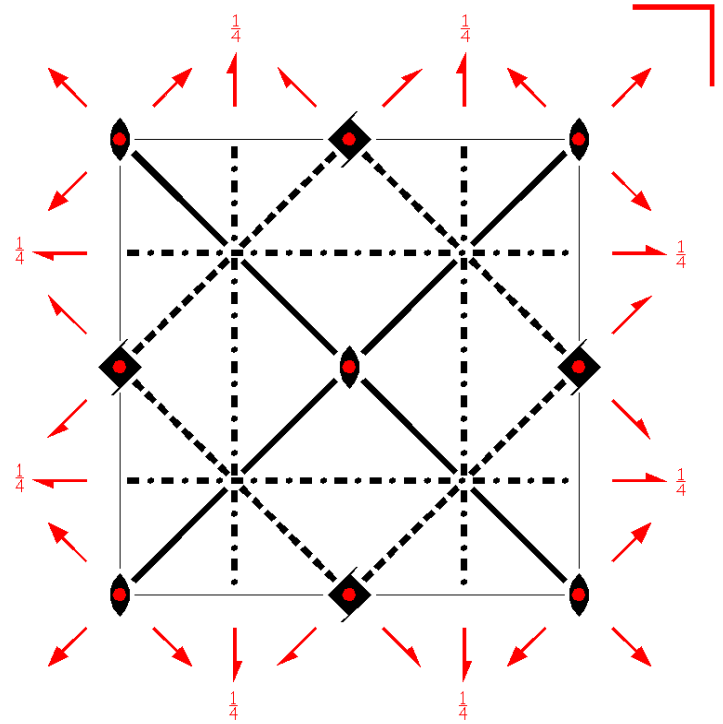
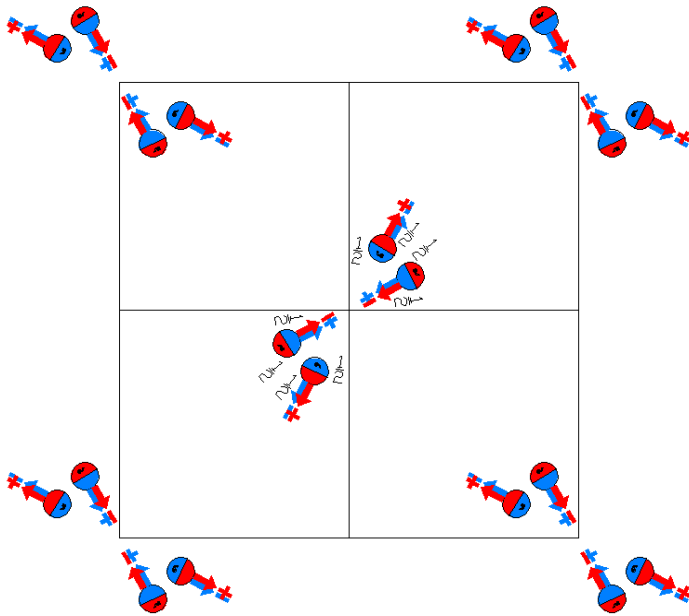
$P4_2/m'n'm$

136.3.1154

$4/m'mm$

$P4_2/m'2_1'n2'/m$

Tetragonal



Origin at center (  $mmm'$  ) at  $2/m'12'/m$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y$

### Symmetry Operations

- |  |  |   |  |
|--|--|---|--|
| (1) $1$<br>( $1 0,0,0$ )                                     | (2) $2 \quad 0,0,z$<br>( $2_z 0,0,0$ )                       | (3) $4^+ (0,0,1/2) \quad 0,1/2,z$<br>( $4_z 1/2,1/2,1/2$ )                      | (4) $4^- (0,0,1/2) \quad 1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,1/2$ )                      |
| (5) $2' (0,1/2,0) \quad 1/4,y,1/4$<br>( $2_y 1/2,1/2,1/2$ )' | (6) $2' (1/2,0,0) \quad x,1/4,1/4$<br>( $2_x 1/2,1/2,1/2$ )' | (7) $2' \quad x,x,0$<br>( $2_{xy} 0,0,0$ )'                                     | (8) $2' \quad x,\bar{x},0$<br>( $2_{\bar{xy}} 0,0,0$ )'                              |
| (9) $\bar{1}' \quad 0,0,0$<br>( $\bar{1}' 0,0,0$ )'          | (10) $m' \quad x,y,0$<br>( $m_z 0,0,0$ )'                    | (11) $\bar{4}^+ \quad 1/2,0,z; \quad 1/2,0,1/4$<br>( $\bar{4}_z 1/2,1/2,1/2$ )' | (12) $\bar{4}^- \quad 0,1/2,z; \quad 0,1/2,1/4$<br>( $\bar{4}_z^{-1} 1/2,1/2,1/2$ )' |
| (13) $n (1/2,0,1/2) \quad x,1/4,z$<br>( $m_y 1/2,1/2,1/2$ )  | (14) $n (0,1/2,1/2) \quad 1/4,y,z$<br>( $m_x 1/2,1/2,1/2$ )  | (15) $m \quad x,\bar{x},z$<br>( $m_{xy} 0,0,0$ )                                | (16) $m \quad x,x,z$<br>( $m_{\bar{xy}} 0,0,0$ )                                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]		
			(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]		
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x,y, $\bar{z}$ [ $u,v,\bar{w}$ ]		
			(11) $y+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]		
8	j	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]		
			$\bar{x}+1/2,x+1/2,z+1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,z+1/2$ [ $u,u,0$ ]		
			$\bar{x}+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $u,u,0$ ]		
			x,x, $\bar{z}$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},\bar{z}$ [ $u,\bar{u},0$ ]		
8	i	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]		
			$\bar{y}+1/2,x+1/2,1/2$ [ $\bar{v},u,0$ ]	$y+1/2,\bar{x}+1/2,1/2$ [ $v,\bar{u},0$ ]		
			$\bar{x}+1/2,y+1/2,1/2$ [ $u,\bar{v},0$ ]	$x+1/2,\bar{y}+1/2,1/2$ [ $\bar{u},v,0$ ]		
			y,x,0 [ $\bar{v},\bar{u},0$ ]	$\bar{y},\bar{x},0$ [ $v,u,0$ ]		
8	h	2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]
			0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2,z [0,0, $\bar{w}$ ]
4	g	m'.2'm	x, $\bar{x},0$ [u,u,0]	$\bar{x},x,0$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x+1/2,1/2$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $u,\bar{u},0$ ]
4	f	m'.2'm	x,x,0 [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},0$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $u,u,0$ ]
4	e	2.mm	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	d	$\bar{4}'..$	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]
4	c	2/m'..	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]
2	b	m.mm	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		

2 a m.mm 0,0,0 [0,0,0]

$1/2, 1/2, 1/2$  [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p4gm$

$\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$

Origin at  $0, 1/2, z$

Along [1,0,0]  $c_p, 2m'm'$

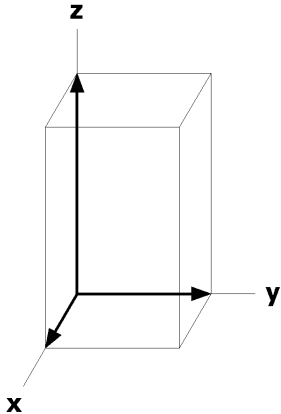
$\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$

Origin at  $x, 0, 0$

Along [1,1,0]  $p2mm1'$

$\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$

Origin at  $x, x, 0$



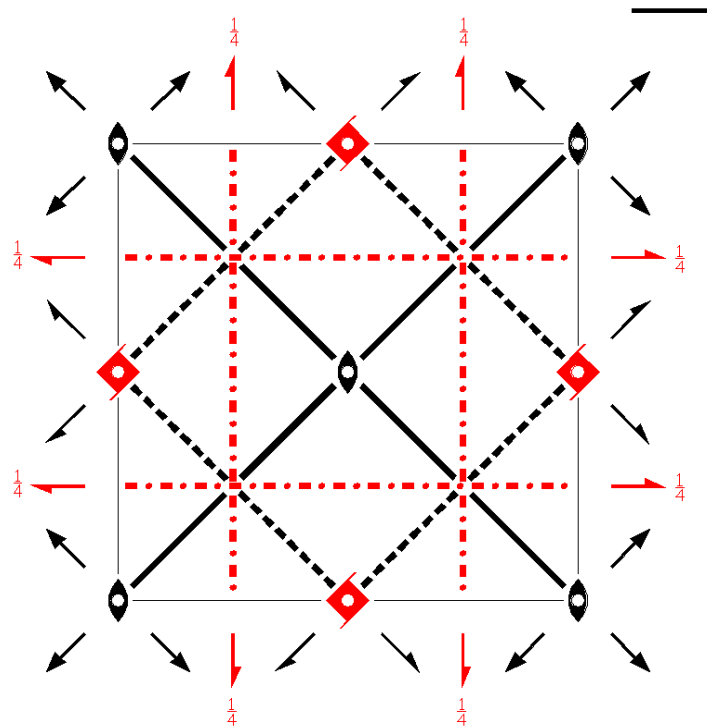
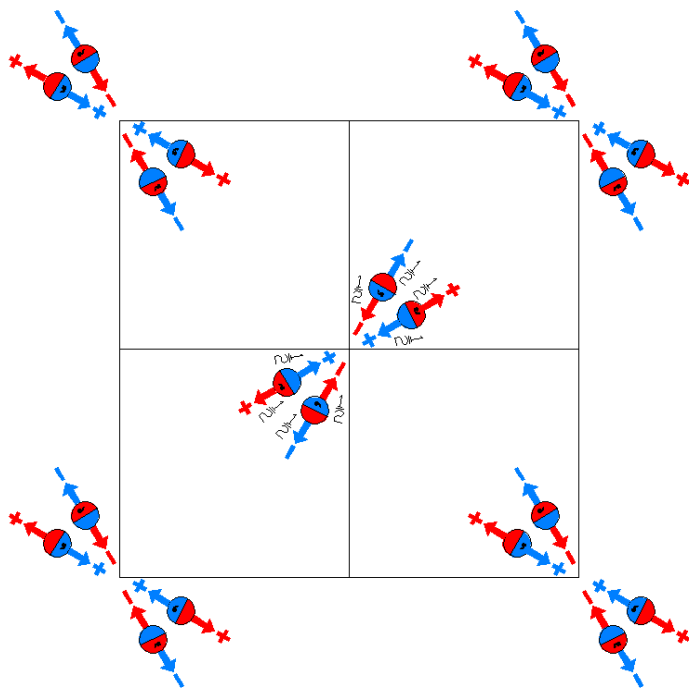
$P4_2'/mn'm$

136.4.1155

$4'/mm'm$

$P4_2'/m2_1/n'2/m$

Tetragonal



Origin at center ( mmm ) at 2/m12/m

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                        | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)'   | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'   |
| (5) 2' (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2)'  | (6) 2' (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)'  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                  | (8) 2 x,x̄,0<br>(2 <sub>xy</sub>  0,0,0)   |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)                                    | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)                       | (11) 4 <sup>+</sup> 1/2,0,z; 1/2,0,1/4<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (12) 4 <sup>-</sup> 0,1/2,z; 0,1/2,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (13) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)' | (14) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)' | (15) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                                | (16) m x,x,z<br>(m <sub>xy</sub>  0,0,0)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]		
			(7) y,x, $\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y},\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]	(16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]		
8	j	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]		
			$\bar{x}+1/2,x+1/2,z+1/2$ [ $u,u,0$ ]	$x+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{u},\bar{u},0$ ]		
			$\bar{x}+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $u,u,0$ ]		
			x,x, $\bar{z}$ [ $u,\bar{u},0$ ]	$\bar{x},\bar{x},\bar{z}$ [ $\bar{u},u,0$ ]		
8	i	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]		
			$\bar{y}+1/2,x+1/2,1/2$ [0,0, $\bar{w}$ ]	$y+1/2,\bar{x}+1/2,1/2$ [0,0, $\bar{w}$ ]		
			$\bar{x}+1/2,y+1/2,1/2$ [0,0,w]	$x+1/2,\bar{y}+1/2,1/2$ [0,0,w]		
			y,x,0 [0,0, $\bar{w}$ ]	$\bar{y},\bar{x},0$ [0,0, $\bar{w}$ ]		
8	h	2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
			0,1/2, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0,w]	0,1/2,z [0,0, $\bar{w}$ ]
4	g	m.2m	x, $\bar{x}$ ,0 [0,0,0]	$\bar{x},x,0$ [0,0,0]	$x+1/2,x+1/2,1/2$ [0,0,0]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [0,0,0]
4	f	m.2m	x,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x}+1/2,x+1/2,1/2$ [0,0,0]	$x+1/2,\bar{x}+1/2,1/2$ [0,0,0]
4	e	2.mm	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	d	$\bar{4}'..$	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]
4	c	2/m..	0,1/2,0 [0,0,w]	0,1/2,1/2 [0,0, $\bar{w}$ ]	1/2,0,1/2 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]
2	b	m.mm	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		



2 a m.mm 0,0,0 [0,0,0]

$1/2, 1/2, 1/2$  [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p4gm1'$

$\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$

Origin at  $0, 1/2, z$

Along [1,0,0]  $c2'mm'$

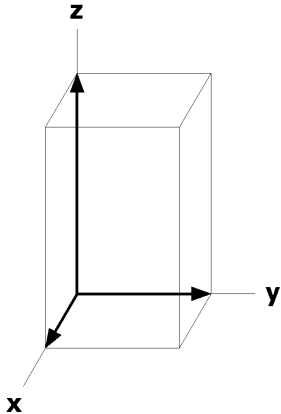
$\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$

Origin at  $x, 0, 0$

Along [1,1,0]  $p2mm1'$

$\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$

Origin at  $x, x, 0$



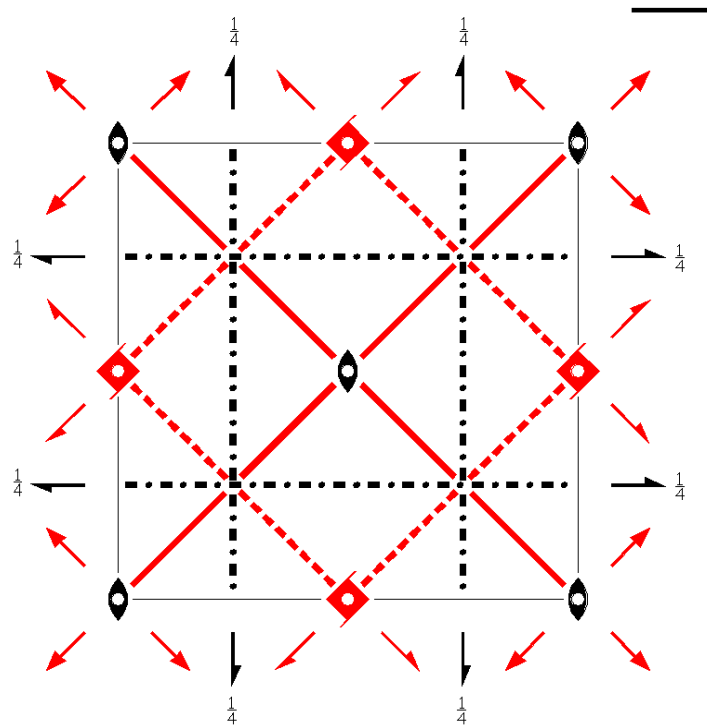
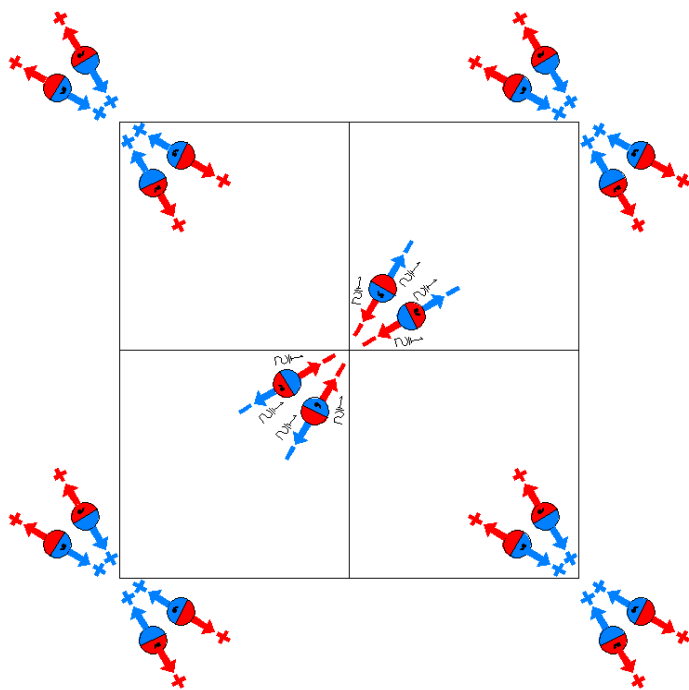
$P4_2'/mnm'$

136.5.1156

$4'/mmm'$

$P4_2'/m2_1/n2'/m'$

Tetragonal



Origin at center ( $m'm'm$ ) at  $2/m12'/m'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

### Symmetry Operations

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                          | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>( $4_z$   $1/2,1/2,1/2$ )'               | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1}$   $1/2,1/2,1/2$ )'               |
| (5) 2 $(0,1/2,0) 1/4,y,1/4$<br>( $2_y$   $1/2,1/2,1/2$ )  | (6) 2 $(1/2,0,0) x,1/4,1/4$<br>( $2_x$   $1/2,1/2,1/2$ )  | (7) $2'$ $x,x,0$<br>( $2_{xy}$  0,0,0)'                                   | (8) $2'$ $x,\bar{x},0$<br>( $2_{\bar{xy}}$  0,0,0)'                            |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)              | (10) m $x,y,0$<br>( $m_z$  0,0,0)                         | (11) $\bar{4}^+$ $1/2,0,z; 1/2,0,1/4$<br>( $\bar{4}_z$   $1/2,1/2,1/2$ )' | (12) $\bar{4}^-$ $0,1/2,z; 0,1/2,1/4$<br>( $\bar{4}_z^{-1}$   $1/2,1/2,1/2$ )' |
| (13) n $(1/2,0,1/2) x,1/4,z$<br>( $m_y$   $1/2,1/2,1/2$ ) | (14) n $(0,1/2,1/2) 1/4,y,z$<br>( $m_x$   $1/2,1/2,1/2$ ) | (15) $m'$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,0)'                            | (16) $m'$ $x,x,z$<br>( $m_{\bar{xy}}$  0,0,0)'                                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]		
			(9) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(16) y,x,z [ $v,u,w$ ]		
8	j	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]		
			$\bar{x}+1/2,x+1/2,z+1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]	$x+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{u},u,\bar{w}$ ]		
			$\bar{x}+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{u},u,\bar{w}$ ]	$x+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $u,\bar{u},\bar{w}$ ]		
			x,x, $\bar{z}$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},\bar{z}$ [ $u,u,w$ ]		
8	i	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]		
			$\bar{y}+1/2,x+1/2,1/2$ [0,0, $\bar{w}$ ]	$y+1/2,\bar{x}+1/2,1/2$ [0,0, $\bar{w}$ ]		
			$\bar{x}+1/2,y+1/2,1/2$ [0,0, $\bar{w}$ ]	$x+1/2,\bar{y}+1/2,1/2$ [0,0, $\bar{w}$ ]		
			y,x,0 [0,0,w]	$\bar{y},\bar{x},0$ [0,0,w]		
8	h	2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]
			0,1/2, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2,z [0,0,w]
4	g	m.2'm'	x, $\bar{x}$ ,0 [0,0,w]	$\bar{x},x,0$ [0,0, $\bar{w}$ ]	$x+1/2,x+1/2,1/2$ [0,0, $\bar{w}$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [0,0,w]
4	f	m.2'm'	x,x,0 [0,0,w]	$\bar{x},\bar{x},0$ [0,0, $\bar{w}$ ]	$\bar{x}+1/2,x+1/2,1/2$ [0,0, $\bar{w}$ ]	$x+1/2,\bar{x}+1/2,1/2$ [0,0,w]
4	e	2.m'm'	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]
4	d	$\bar{4}'..$	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]
4	c	2/m..	0,1/2,0 [0,0,w]	0,1/2,1/2 [0,0, $\bar{w}$ ]	1/2,0,1/2 [0,0, $\bar{w}$ ]	1/2,0,0 [0,0,w]
2	b	m.m'm'	0,0,1/2 [0,0,w]	1/2,1/2,0 [0,0, $\bar{w}$ ]		

2 a m.m'm' 0,0,0 [0,0,w]

$1/2, 1/2, 1/2 [0,0,\bar{w}]$

### Symmetry of Special Projections

Along [0,0,1]  $p4gm1'$

$\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$

Origin at 0,1/2,z

Along [1,0,0]  $c 2'mm'$

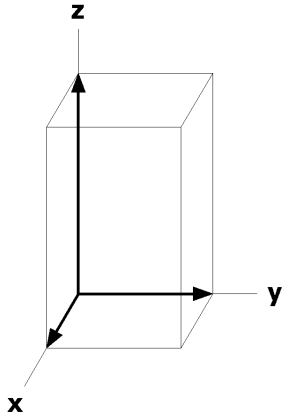
$\mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b}$

Origin at x,0,0

Along [1,1,0]  $p2'mm'$

$\mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$

Origin at x,x,0



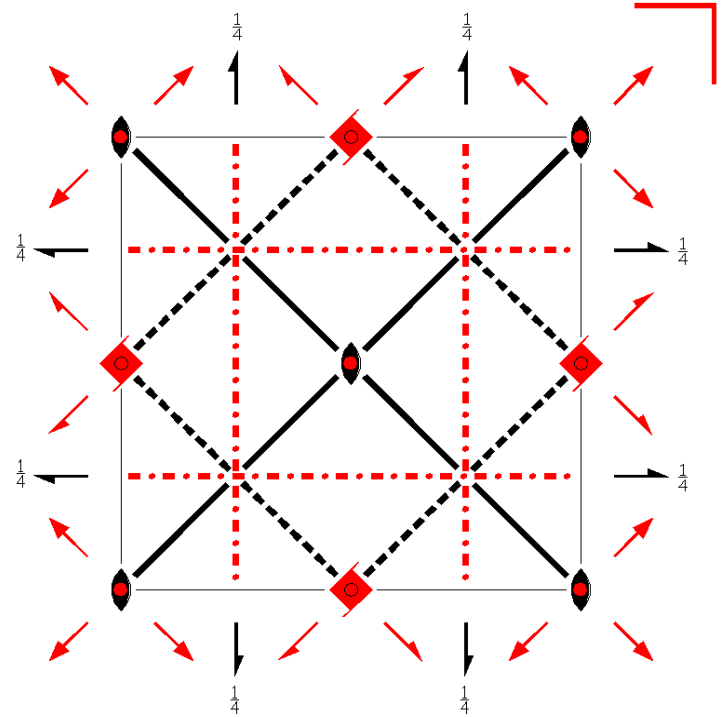
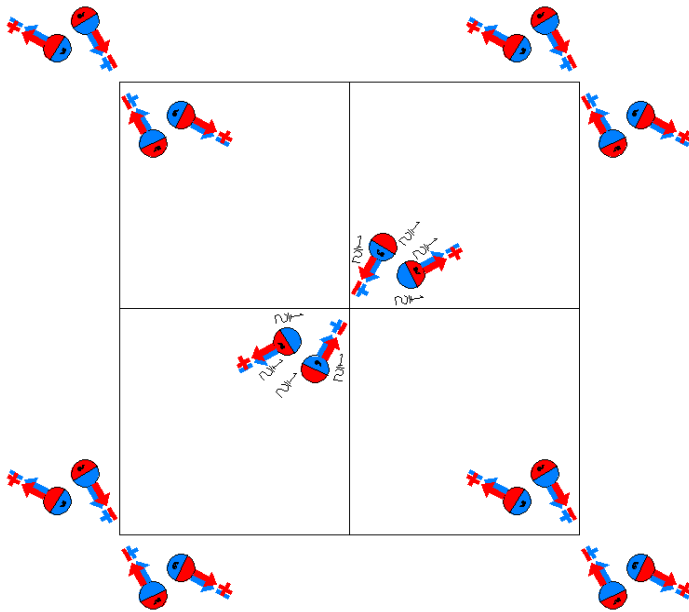
$P4_2'/m'n'm$

136.6.1157

$4'/m'm'm$

$P4_2'/m'2_1/n'2'/m$

Tetragonal



Origin at center ( $mmm'$ ) at  $2/m'12'/m$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

### Symmetry Operations

- |   |   |  |   |
|---|---|--|---|
| (1) $1$<br>( $1 0,0,0$ )                                  | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                        | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>( $4_z 1/2,1/2,1/2$ )'              | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,1/2$ )'              |
| (5) $2$ $(0,1/2,0) 1/4,y,1/4$<br>( $2_y 1/2,1/2,1/2$ )    | (6) $2$ $(1/2,0,0) x,1/4,1/4$<br>( $2_x 1/2,1/2,1/2$ )    | (7) $2'$ $x,x,0$<br>( $2_{xy} 0,0,0$ )'                              | (8) $2'$ $x,\bar{x},0$<br>( $2_{\bar{xy}} 0,0,0$ )'                       |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1} 0,0,0$ )'             | (10) $m'$ $x,y,0$<br>( $m_z 0,0,0$ )'                     | (11) $\bar{4}^+$ $1/2,0,z; 1/2,0,1/4$<br>( $\bar{4}_z 1/2,1/2,1/2$ ) | (12) $\bar{4}^-$ $0,1/2,z; 0,1/2,1/4$<br>( $\bar{4}_z^{-1} 1/2,1/2,1/2$ ) |
| (13) $n'$ $(1/2,0,1/2) x,1/4,z$<br>( $m_y 1/2,1/2,1/2$ )' | (14) $n'$ $(0,1/2,1/2) 1/4,y,z$<br>( $m_x 1/2,1/2,1/2$ )' | (15) $m$ $x,\bar{x},z$<br>( $m_{xy} 0,0,0$ )                         | (16) $m$ $x,x,z$<br>( $m_{\bar{xy}} 0,0,0$ )                              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]		
			(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},w$ ]		
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]		
			(11) $y+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},\bar{v},w$ ]		
			(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]		
8	j	..m	x,x,z [ $\bar{u},\bar{u},0$ ]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},0$ ]		
			$\bar{x}+1/2,x+1/2,z+1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{u},\bar{u},0$ ]		
			$\bar{x}+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]		
			x,x, $\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]		
8	i	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]		
			$\bar{y}+1/2,x+1/2,1/2$ [ $\bar{v},\bar{u},0$ ]	$y+1/2,\bar{x}+1/2,1/2$ [ $\bar{v},\bar{u},0$ ]		
			$\bar{x}+1/2,y+1/2,1/2$ [ $\bar{u},\bar{v},0$ ]	$x+1/2,\bar{y}+1/2,1/2$ [ $\bar{u},\bar{v},0$ ]		
			y,x,0 [ $\bar{v},\bar{u},0$ ]	$\bar{y},\bar{x},0$ [ $\bar{v},\bar{u},0$ ]		
8	h	2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]
			0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,0,z+1/2 [0,0,w]	0,1/2,z [0,0, $\bar{w}$ ]
4	g	m'.2'm	x, $\bar{x}$ ,0 [u,u,0]	$\bar{x},x,0$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]
4	f	m'.2'm	x,x,0 [ $\bar{u},\bar{u},0$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]
4	e	2.mm	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	d	$\bar{4}$ ..	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0, $\bar{w}$ ]	1/2,0,1/4 [0,0, $\bar{w}$ ]	1/2,0,3/4 [0,0,w]
4	c	2/m'..	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]
2	b	m'.mm	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		

2 a m'.mm 0,0,0 [0,0,0]

1/2,1/2,1/2 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p4'g'm$

$\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$

Origin at 0,1/2,z

Along [1,0,0]  $c 2m'm'$

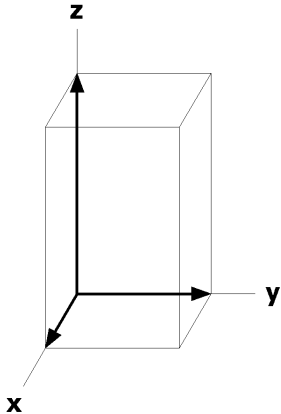
$\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$

Origin at x,0,0

Along [1,1,0]  $p2mm1'$

$\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$

Origin at x,x,0



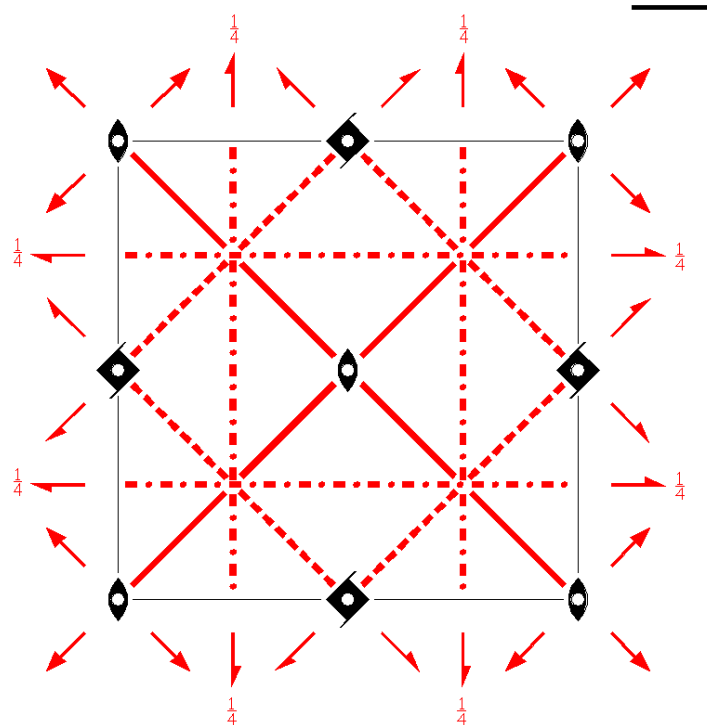
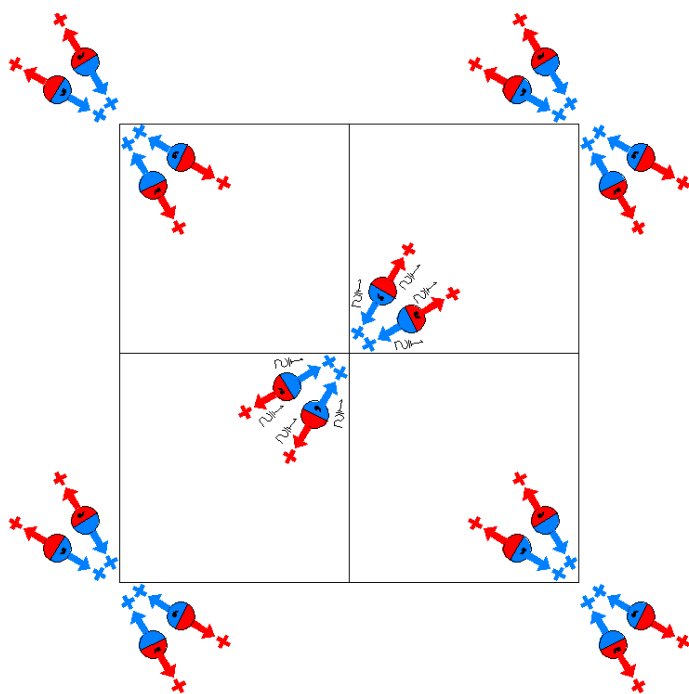
$P4_2/mn'm'$

136.7.1158

$4/mm'm'$

$P4_2/m2_1'n'2'/m'$

Tetragonal



Origin at center (  $m'm'm'$  ) at  $2/m12'/m'$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y$

### Symmetry Operations

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                | (3) $4^+$ $(0,0,1/2) \ 0,1/2,z$<br>( $4_z$   $1/2,1/2,1/2$ )               | (4) $4^-$ $(0,0,1/2) \ 1/2,0,z$<br>( $4_z^{-1}$   $1/2,1/2,1/2$ )               |
| (5) $2'$ $(0,1/2,0) \ 1/4,y,1/4$<br>( $2_y$   $1/2,1/2,1/2$ )'  | (6) $2'$ $(1/2,0,0) \ x,1/4,1/4$<br>( $2_x$   $1/2,1/2,1/2$ )'  | (7) $2'$ $x,x,0$<br>( $2_{xy}$  0,0,0)'                                    | (8) $2'$ $x,\bar{x},0$<br>( $2_{\bar{xy}}$  0,0,0)'                             |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)                    | (10) m $x,y,0$<br>( $m_z$  0,0,0)                               | (11) $\bar{4}^+$ $1/2,0,z; \ 1/2,0,1/4$<br>( $\bar{4}_z$   $1/2,1/2,1/2$ ) | (12) $\bar{4}^-$ $0,1/2,z; \ 0,1/2,1/4$<br>( $\bar{4}_z^{-1}$   $1/2,1/2,1/2$ ) |
| (13) $n'$ $(1/2,0,1/2) \ x,1/4,z$<br>( $m_y$   $1/2,1/2,1/2$ )' | (14) $n'$ $(0,1/2,1/2) \ 1/4,y,z$<br>( $m_x$   $1/2,1/2,1/2$ )' | (15) $m'$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,0)'                             | (16) $m'$ $x,x,z$<br>( $m_{\bar{xy}}$  0,0,0)'                                  |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]		
			(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]		
			(9) $\bar{x},\bar{y},\bar{z}$ [ $u,v,w$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},u,w$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [ $v,\bar{u},w$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(16) y,x,z [ $v,u,w$ ]		
8	j	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]		
			$\bar{x}+1/2,x+1/2,z+1/2$ [ $\bar{u},u,w$ ]	$x+1/2,\bar{x}+1/2,z+1/2$ [ $u,\bar{u},w$ ]		
			$\bar{x}+1/2,x+1/2,\bar{z}+1/2$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{u},u,w$ ]		
			x,x, $\bar{z}$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},\bar{z}$ [ $u,u,w$ ]		
8	i	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]		
			$\bar{y}+1/2,x+1/2,1/2$ [0,0,w]	$y+1/2,\bar{x}+1/2,1/2$ [0,0,w]		
			$\bar{x}+1/2,y+1/2,1/2$ [0,0,w]	$x+1/2,\bar{y}+1/2,1/2$ [0,0,w]		
			y,x,0 [0,0,w]	$\bar{y},\bar{x},0$ [0,0,w]		
8	h	2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]
			0,1/2, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,0,z+1/2 [0,0,w]	0,1/2,z [0,0,w]
4	g	m.2'm'	x, $\bar{x}$ ,0 [0,0,w]	$\bar{x},x,0$ [0,0,w]	$x+1/2,x+1/2,1/2$ [0,0,w]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [0,0,w]
4	f	m.2'm'	x,x,0 [0,0,w]	$\bar{x},\bar{x},0$ [0,0,w]	$\bar{x}+1/2,x+1/2,1/2$ [0,0,w]	$x+1/2,\bar{x}+1/2,1/2$ [0,0,w]
4	e	2.m'm'	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]
4	d	$\bar{4}$ ..	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0,w]	1/2,0,1/4 [0,0,w]	1/2,0,3/4 [0,0,w]
4	c	2/m..	0,1/2,0 [0,0,w]	0,1/2,1/2 [0,0,w]	1/2,0,1/2 [0,0,w]	1/2,0,0 [0,0,w]
2	b	m.m'm'	0,0,1/2 [0,0,w]	1/2,1/2,0 [0,0,w]		

2 a m.m'm' 0,0,0 [0,0,w]

1/2,1/2,1/2 [0,0,w]

### Symmetry of Special Projections

Along [0,0,1]  $p4gm1'$

$\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$

Origin at 0,1/2,z

Along [1,0,0]  $c2mm$

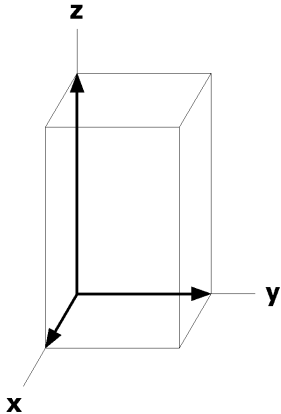
$\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$

Origin at x,0,0

Along [1,1,0]  $p2'mm'$

$\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$

Origin at x,x,0



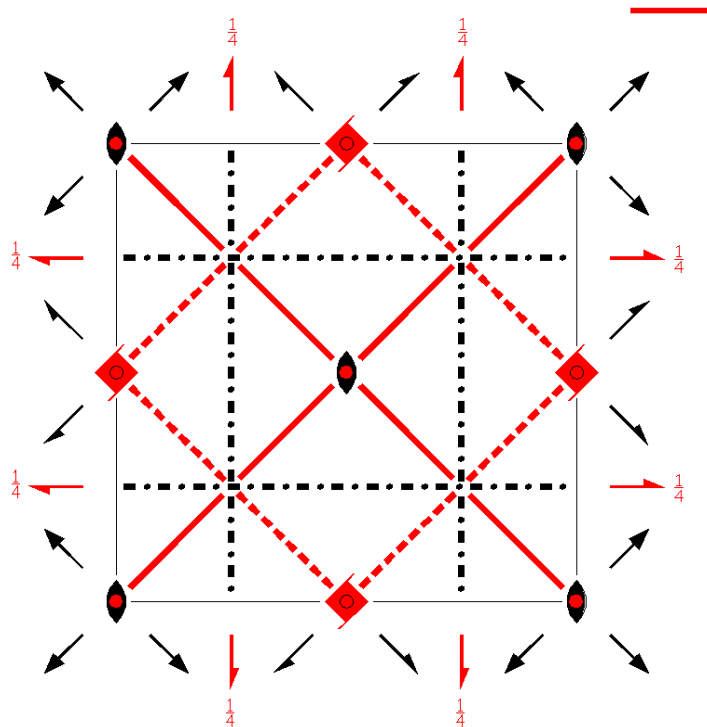
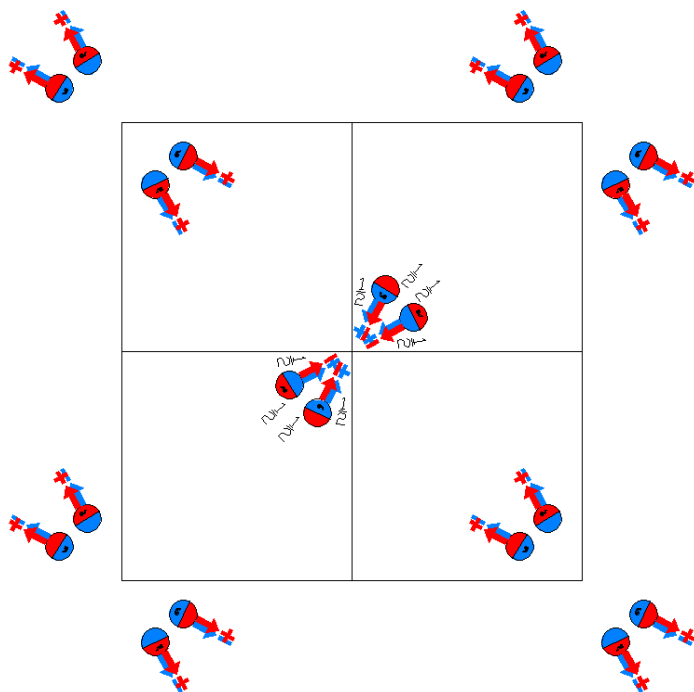
$P4_2'/m'nm'$

136.8.1159

$4'/m'mm'$

$P4_2'/m'2_1'n2/m'$

Tetragonal



Origin at center ( $m'm'm'$ ) at  $2/m'12/m'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; x \leq y$

### Symmetry Operations

- |  |  |  |   |
|--|--|--|---|
| (1) $1$<br>( $1 0,0,0$ )                                 | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                       | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>( $4_z 1/2,1/2,1/2$ )'              | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,1/2$ )'              |
| (5) $2'$ $(0,1/2,0) 1/4,y,1/4$<br>( $2_y 1/2,1/2,1/2$ )' | (6) $2'$ $(1/2,0,0) x,1/4,1/4$<br>( $2_x 1/2,1/2,1/2$ )' | (7) $2$ $x,x,0$<br>( $2_{xy} 0,0,0$ )                                | (8) $2$ $x,\bar{x},0$<br>( $2_{\bar{xy}} 0,0,0$ )                         |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1} 0,0,0$ )'            | (10) $m'$ $x,y,0$<br>( $m_z 0,0,0$ )'                    | (11) $\bar{4}^+$ $1/2,0,z; 1/2,0,1/4$<br>( $\bar{4}_z 1/2,1/2,1/2$ ) | (12) $\bar{4}^-$ $0,1/2,z; 0,1/2,1/4$<br>( $\bar{4}_z^{-1} 1/2,1/2,1/2$ ) |
| (13) $n$ $(1/2,0,1/2) x,1/4,z$<br>( $m_y 1/2,1/2,1/2$ )  | (14) $n$ $(0,1/2,1/2) 1/4,y,z$<br>( $m_x 1/2,1/2,1/2$ )  | (15) $m'$ $x,\bar{x},z$<br>( $m_{xy} 0,0,0$ )'                       | (16) $m'$ $x,x,z$<br>( $m_{\bar{xy}} 0,0,0$ )'                            |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]		
			(7) y,x, $\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x,y, $\bar{z}$ [ $u,v,\bar{w}$ ]		
			(11) $y+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{v},u,w$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(16) y,x,z [v,u,w]		
8	j	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]		
			$\bar{x}+1/2,x+1/2,z+1/2$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{u},u,\bar{w}$ ]		
			$\bar{x}+1/2,x+1/2,\bar{z}+1/2$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{u},u,w$ ]		
			x,x, $\bar{z}$ [ $u,u,\bar{w}$ ]	$\bar{x},\bar{x},\bar{z}$ [ $\bar{u},\bar{u},\bar{w}$ ]		
8	i	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]		
			$\bar{y}+1/2,x+1/2,1/2$ [ $\bar{v},\bar{u},0$ ]	$y+1/2,\bar{x}+1/2,1/2$ [ $\bar{v},u,0$ ]		
			$\bar{x}+1/2,y+1/2,1/2$ [ $u,\bar{v},0$ ]	$x+1/2,\bar{y}+1/2,1/2$ [ $\bar{u},v,0$ ]		
			y,x,0 [v,u,0]	$\bar{y},\bar{x},0$ [ $\bar{v},\bar{u},0$ ]		
8	h	2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
			0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2,z [0,0,w]
4	g	m'.2m'	x, $\bar{x}$ ,0 [ $\bar{u},u,0$ ]	$\bar{x},x,0$ [ $u,\bar{u},0$ ]	$x+1/2,x+1/2,1/2$ [ $u,u,0$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]
4	f	m'.2m'	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $u,\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},u,0$ ]
4	e	2.m'm'	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4	d	$\bar{4}$ ..	0,1/2,1/4 [0,0,w]	0,1/2,3/4 [0,0, $\bar{w}$ ]	1/2,0,1/4 [0,0,w]	1/2,0,3/4 [0,0, $\bar{w}$ ]
4	c	2/m'..	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]
2	b	m'.m'm'	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		

2 a m'.m'm' 0,0,0 [0,0,0]

1/2,1/2,1/2 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p4'gm'$

$\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$

Origin at 0,1/2,z

Along [1,0,0]  $c_p 2m'm'$

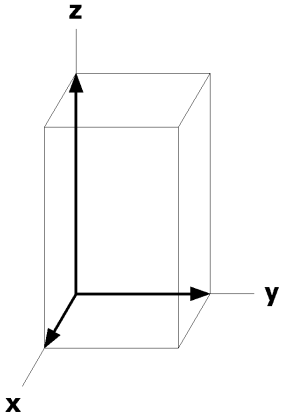
$\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$

Origin at x,0,0

Along [1,1,0]  $p2m'm'$

$\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$

Origin at x,x,0



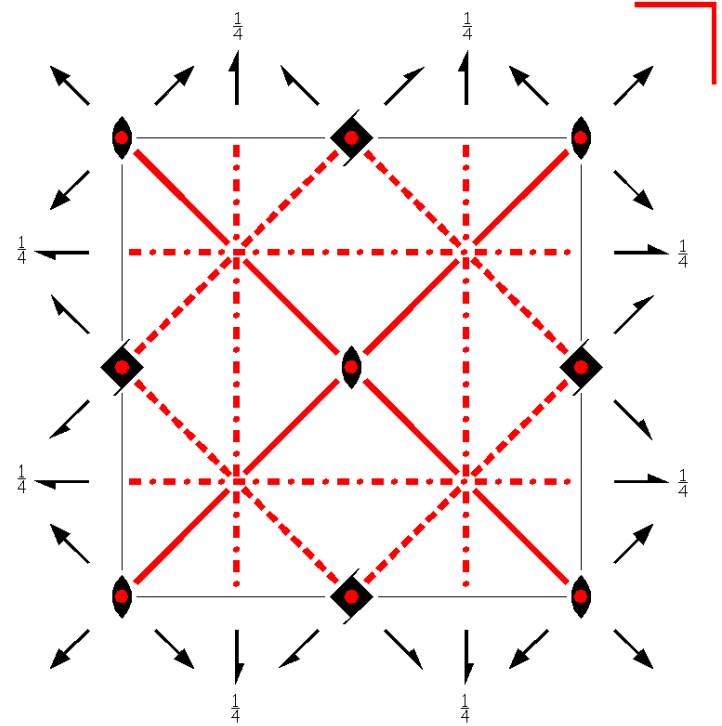
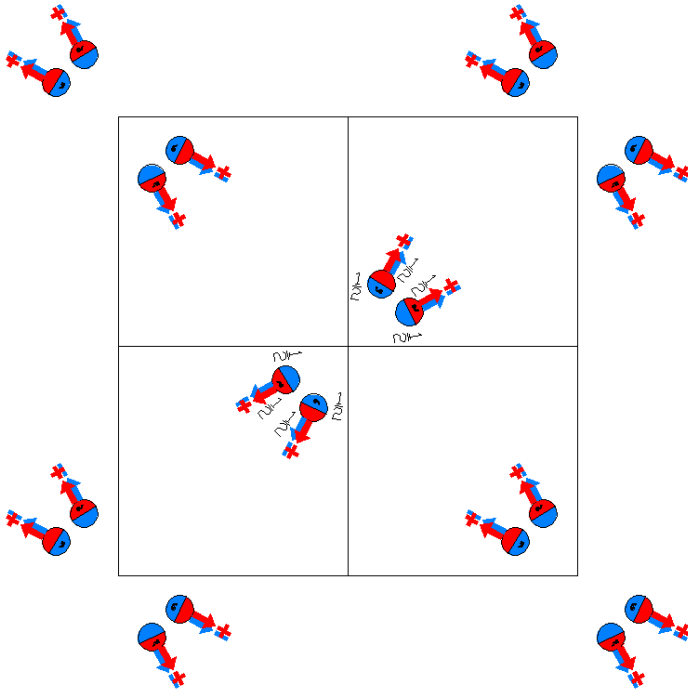
$P4_2/m'n'm'$

136.9.1160

$4/m'm'm'$

$P4_2/m'2_1/n'2/m'$

Tetragonal



Origin at center (  $m'm'm'$  ) at  $2/m'12/m'$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y$

### Symmetry Operations

- |  |  |  |   |
|--|--|--|---|
| (1) $1$<br>( $1 0,0,0$ )                                     | (2) $2 \quad 0,0,z$<br>( $2_z 0,0,0$ )                       | (3) $4^+ (0,0,1/2) \quad 0,1/2,z$<br>( $4_z 1/2,1/2,1/2$ )                     | (4) $4^- (0,0,1/2) \quad 1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,1/2$ )                     |
| (5) $2 (0,1/2,0) \quad 1/4,y,1/4$<br>( $2_y 1/2,1/2,1/2$ )   | (6) $2 (1/2,0,0) \quad x,1/4,1/4$<br>( $2_x 1/2,1/2,1/2$ )   | (7) $2 \quad x,x,0$<br>( $2_{xy} 0,0,0$ )                                      | (8) $2 \quad x,\bar{x},0$<br>( $2_{\bar{xy}} 0,0,0$ )                               |
| (9) $\bar{1} \quad 0,0,0$<br>( $\bar{1} 0,0,0$ )             | (10) $m' \quad x,y,0$<br>( $m_z 0,0,0$ )                     | (11) $\bar{4}^+ \quad 1/2,0,z; \quad 1/2,0,1/4$<br>( $\bar{4}_z 1/2,1/2,1/2$ ) | (12) $\bar{4}^- \quad 0,1/2,z; \quad 0,1/2,1/4$<br>( $\bar{4}_z^{-1} 1/2,1/2,1/2$ ) |
| (13) $n' (1/2,0,1/2) \quad x,1/4,z$<br>( $m_y 1/2,1/2,1/2$ ) | (14) $n' (0,1/2,1/2) \quad 1/4,y,z$<br>( $m_x 1/2,1/2,1/2$ ) | (15) $m' \quad x,\bar{x},z$<br>( $m_{xy} 0,0,0$ )                              | (16) $m' \quad x,x,z$<br>( $m_{\bar{xy}} 0,0,0$ )                                   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

16	k	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(7) y,x, $\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x,y, $\bar{z}$ [ $u,v,\bar{w}$ ]		
			(11) $y+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x+1/2,\bar{y}+1/2,z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x}+1/2,y+1/2,z+1/2$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(16) y,x,z [v,u,w]		
8	j	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]		
			$\bar{x}+1/2,x+1/2,z+1/2$ [ $\bar{u},u,w$ ]	$x+1/2,\bar{x}+1/2,z+1/2$ [ $u,\bar{u},w$ ]		
			$\bar{x}+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{u},u,\bar{w}$ ]	$x+1/2,\bar{x}+1/2,\bar{z}+1/2$ [ $u,\bar{u},\bar{w}$ ]		
			x,x, $\bar{z}$ [ $u,u,\bar{w}$ ]	$\bar{x},\bar{x},\bar{z}$ [ $\bar{u},\bar{u},\bar{w}$ ]		
8	i	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]		
			$\bar{y}+1/2,x+1/2,1/2$ [ $\bar{v},u,0$ ]	$y+1/2,\bar{x}+1/2,1/2$ [ $v,\bar{u},0$ ]		
			$\bar{x}+1/2,y+1/2,1/2$ [ $\bar{u},v,0$ ]	$x+1/2,\bar{y}+1/2,1/2$ [ $u,\bar{v},0$ ]		
			y,x,0 [v,u,0]	$\bar{y},\bar{x},0$ [ $\bar{v},\bar{u},0$ ]		
8	h	2..	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
			0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0,w]	0,1/2,z [0,0,w]
4	g	m'.2m'	x, $\bar{x}$ ,0 [ $\bar{u},u,0$ ]	$\bar{x},x,0$ [ $u,\bar{u},0$ ]	$x+1/2,x+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $u,u,0$ ]
4	f	m'.2m'	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $\bar{u},u,0$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $u,\bar{u},0$ ]
4	e	2.m'm'	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4	d	$\bar{4}$ '..	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]
4	c	2/m'..	0,1/2,0 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,0,0 [0,0,0]
2	b	m'.m'm'	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		

2 a m'.m'm' 0,0,0 [0,0,0]

1/2,1/2,1/2 [0,0,0]

**Symmetry of Special Projections**Along [0,0,1]  $p4g'm'$  $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$ 

Origin at 0,1/2,z

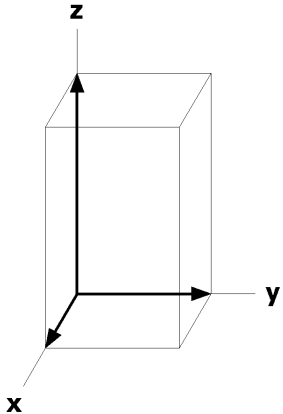
Along [1,0,0]  $c2m'm'$  $\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}$ 

Origin at x,0,0

Along [1,1,0]  $p2m'm'$  $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}$ 

Origin at x,x,0

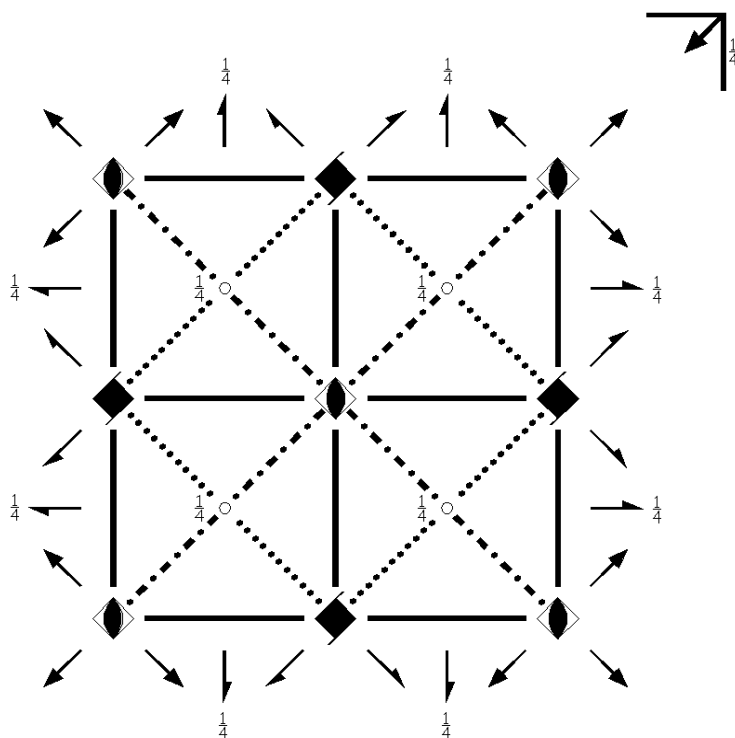
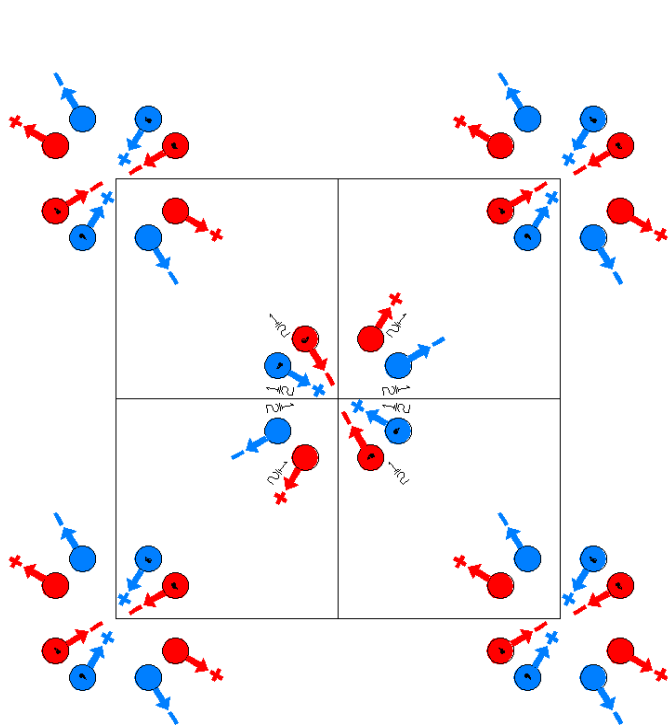




$P4_2/nmc$   
137.1.1161

$4/mmm$   
 $P4_2/n2_1/m2/c$

Tetragonal



Origin at  $\bar{4}m2/n$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |  |   |  |  |
|--|---|--|--|
| (1) $1$<br>$(1 0,0,0)$                                 | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                      | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>$(4_z 1/2,1/2,1/2)$           | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>$(4_z^{-1} 1/2,1/2,1/2)$      |
| (5) $2$ $(0,1/2,0) 1/4,y,1/4$<br>$(2_y 1/2,1/2,1/2)$   | (6) $2$ $(1/2,0,0) x,1/4,1/4$<br>$(2_x 1/2,1/2,1/2)$  | (7) $2$ $x,x,0$<br>$(2_{xy} 0,0,0)$                            | (8) $2$ $x,\bar{x},0$<br>$(2_{\bar{xy}} 0,0,0)$                |
| (9) $\bar{1}$ $1/4,1/4,1/4$<br>$(\bar{1} 1/2,1/2,1/2)$ | (10) $n$ $(1/2,1/2,0) x,y,1/4$<br>$(m_z 1/2,1/2,1/2)$ | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z 0,0,0)$         | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1} 0,0,0)$    |
| (13) $m$ $x,0,z$<br>$(m_y 0,0,0)$                      | (14) $m$ $0,y,z$<br>$(m_x 0,0,0)$                     | (15) $c$ $(0,0,1/2) x+1/2,\bar{x},z$<br>$(m_{xy} 1/2,1/2,1/2)$ | (16) $n$ $(1/2,1/2,1/2) x,x,z$<br>$(m_{\bar{xy}} 1/2,1/2,1/2)$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

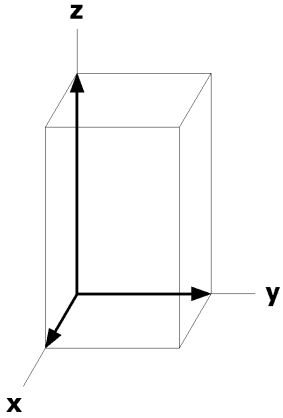
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	h	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},z$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]	(13) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	g	.m.	0,y,z [u,0,0]	0, $\bar{y}$ ,z [ $\bar{u},0,0$ ]	$\bar{y}+1/2,1/2,z+1/2$ [0,u,0]	$y+1/2,1/2,z+1/2$ [0, $\bar{u},0$ ]	$1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},0,0$ ]	$1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,0,0$ ]	$y,0,\bar{z}$ [0,u,0]	$\bar{y},0,\bar{z}$ [0, $\bar{u},0$ ]								
8	f	.2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $\bar{u},u,0$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $u,u,0$ ]	$x+1/2,x+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},0$ [ $\bar{u},u,0$ ]	$\bar{x},x,0$ [ $u,\bar{u},0$ ]								
8	e	$\bar{1}$	1/4,1/4,1/4 [u,v,w]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,3/4 [ $\bar{v},u,w$ ]	3/4,1/4,3/4 [ $v,\bar{u},w$ ]	1/4,3/4,1/4 [ $\bar{u},v,\bar{w}$ ]	3/4,1/4,1/4 [ $u,\bar{v},\bar{w}$ ]	1/4,1/4,3/4 [ $v,u,\bar{w}$ ]	3/4,3/4,3/4 [ $\bar{v},\bar{u},\bar{w}$ ]								
4	d	2mm.	0,1/2,z [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]												
4	c	2mm.	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]												
2	b	$\bar{4}m2$	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]														
2	a	$\bar{4}m2$	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]														

### Symmetry of Special Projections

Along [0,0,1] p<sub>p</sub>-4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [1,1,0] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$P4_2/nmc1'$

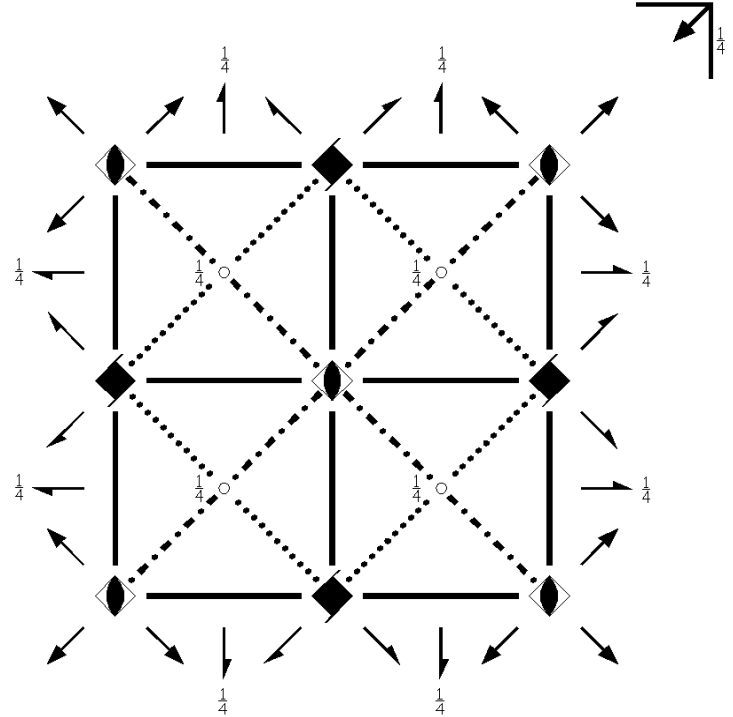
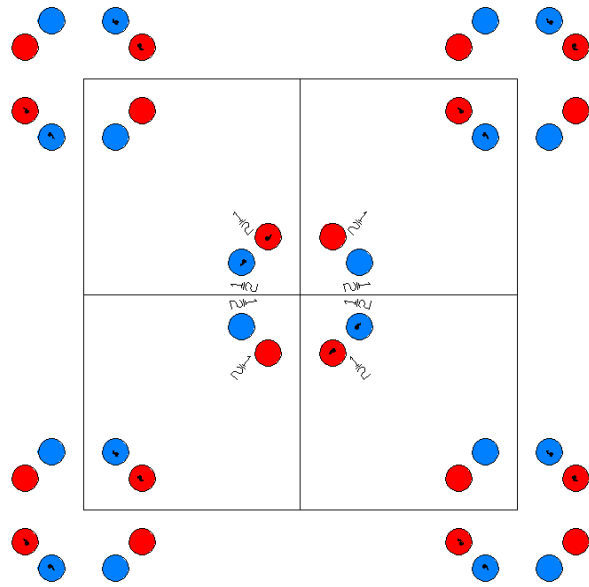
137.2.1162

$4/mmm1'$

$P4_2/n2_1/m2/c1'$

Tetragonal

1'



Origin at  $\bar{4}m2/n1'$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

For 1 + set

- |  |   |  |   |
|--|---|--|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)  | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) 2 (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,1/2,1/2) | (6) 2 (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>  1/2,1/2,1/2)  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)                |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)     | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)               | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                            |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)                    | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)                     | (15) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,1/2) | (16) n (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)     |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)'	(4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'
(5) 2' (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>  1/2,1/2,1/2)'	(6) 2' (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>  1/2,1/2,1/2)'	(7) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) 2' x, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  0,0,0)'
(9) $\bar{1}$ ' 1/4,1/4,1/4 ( $\bar{1}$  1/2,1/2,1/2)'	(10) n' (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>  1/2,1/2,1/2)'	(11) $\bar{4}^+$ ' 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'	(12) $\bar{4}^-$ ' 0,0,z; 0,0,0 ( $\bar{4}_z^{-1}$  0,0,0)'
(13) m' x,0,z (m <sub>y</sub>  0,0,0)'	(14) m' 0,y,z (m <sub>x</sub>  0,0,0)'	(15) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,1/2)'	(16) n' (1/2,1/2,1/2) x,x,z (m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

16	h	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [0,0,0]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [0,0,0]		
			(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [0,0,0]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [0,0,0]		
			(7) y,x, $\bar{z}$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}$ [0,0,0]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [0,0,0]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [0,0,0]		
			(11) y, $\bar{x},\bar{z}$ [0,0,0]	(12) $\bar{y},x,\bar{z}$ [0,0,0]		
			(13) x, $\bar{y},z$ [0,0,0]	(14) $\bar{x},y,z$ [0,0,0]		
			(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [0,0,0]	(16) $y+1/2,x+1/2,z+1/2$ [0,0,0]		
8	g	.m.1'	0,y,z [0,0,0]	0, $\bar{y},z$ [0,0,0]	$\bar{y}+1/2,1/2,z+1/2$ [0,0,0]	$y+1/2,1/2,z+1/2$ [0,0,0]
			1/2, $y+1/2,\bar{z}+1/2$ [0,0,0]	1/2, $\bar{y}+1/2,\bar{z}+1/2$ [0,0,0]	y,0, $\bar{z}$ [0,0,0]	$\bar{y},0,\bar{z}$ [0,0,0]
8	f	..21'	x,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x}+1/2,x+1/2,1/2$ [0,0,0]	$x+1/2,\bar{x}+1/2,1/2$ [0,0,0]
			$\bar{x}+1/2,\bar{x}+1/2,1/2$ [0,0,0]	$x+1/2,x+1/2,1/2$ [0,0,0]	x, $\bar{x},0$ [0,0,0]	$\bar{x},x,0$ [0,0,0]
8	e	$\bar{1}$ 1'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]
			1/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]
4	d	2mm.1'	0,1/2,z [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]
4	c	2mm.1'	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]
2	b	$\bar{4}$ m21'	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]		

2 a  $\bar{4}m21'$  0,0,0 [0,0,0]

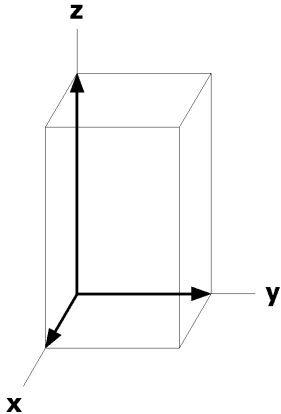
1/2,1/2,1/2 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

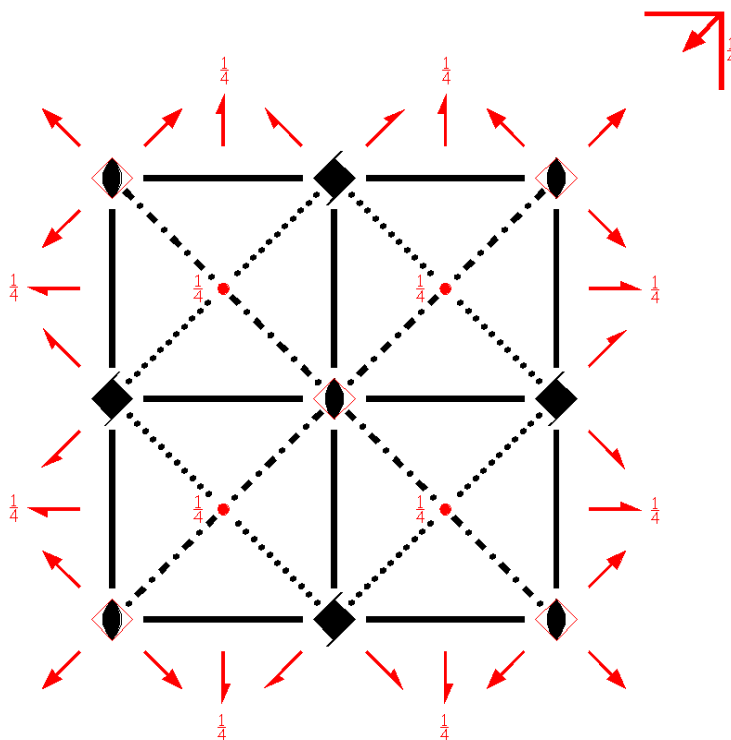
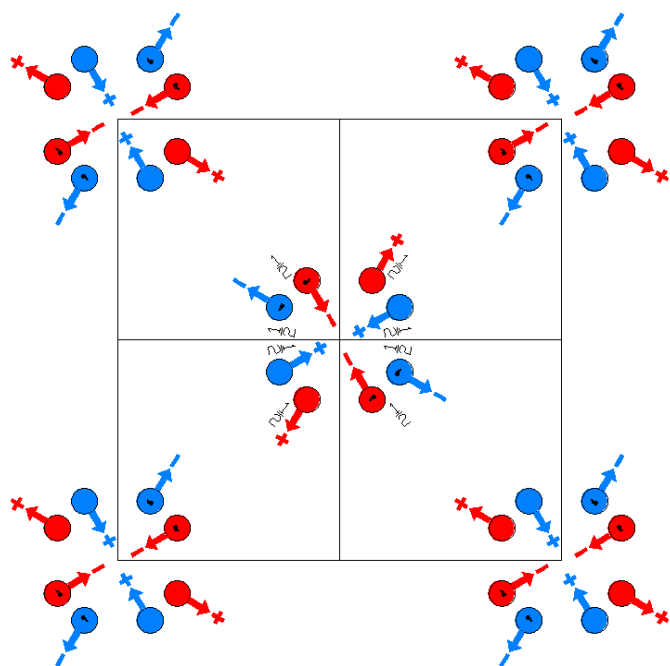
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P4_2/n'mc$   
137.3.1163

$4/m'mm$   
 $P4_2/n'2_1'/m2'/c$

Tetragonal



Origin at  $\bar{4}'m2'/n$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) $1$<br>( $1 0,0,0$ )                                    | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                        | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>( $4_z 1/2,1/2,1/2$ )           | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,1/2$ )      |
| (5) $2'$ $(0,1/2,0) 1/4,y,1/4$<br>( $2_y 1/2,1/2,1/2$ )'    | (6) $2'$ $(1/2,0,0) x,1/4,1/4$<br>( $2_x 1/2,1/2,1/2$ )'  | (7) $2'$ $x,x,0$<br>( $2_{xy} 0,0,0$ )'                          | (8) $2'$ $x,\bar{x},0$<br>( $2_{\bar{xy}} 0,0,0$ )'              |
| (9) $\bar{1}'$ $1/4,1/4,1/4$<br>( $\bar{1}' 1/2,1/2,1/2$ )' | (10) $n'$ $(1/2,1/2,0) x,y,1/4$<br>( $m_z 1/2,1/2,1/2$ )' | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )'        | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ )'   |
| (13) $m$ $x,0,z$<br>( $m_y 0,0,0$ )                         | (14) $m$ $0,y,z$<br>( $m_x 0,0,0$ )                       | (15) $c$ $(0,0,1/2) x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,1/2$ ) | (16) $n$ $(1/2,1/2,1/2) x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,1/2$ ) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

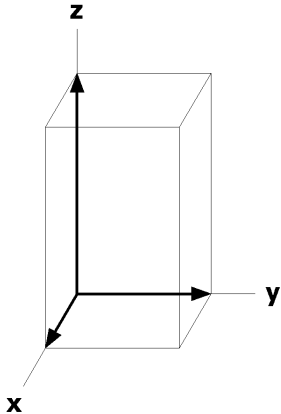
			Coordinates															
			Multiplicity, Wyckoff letter, Site Symmetry.															
16	h	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(13) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	g	.m.	0,y,z [u,0,0]	0, $\bar{y}$ ,z [ $\bar{u},0,0$ ]	$\bar{y}+1/2,1/2,z+1/2$ [0,u,0]	$y+1/2,1/2,z+1/2$ [0, $\bar{u},0$ ]	$1/2,y+1/2,\bar{z}+1/2$ [u,0,0]	$1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},0,0$ ]	$y,0,\bar{z}$ [0, $\bar{u},0$ ]	$\bar{y},0,\bar{z}$ [0,u,0]								
8	f	..2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $\bar{u},\bar{u},w$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $u,u,w$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x+1/2,1/2$ [ $\bar{u},u,\bar{w}$ ]	$x,\bar{x},0$ [ $u,u,\bar{w}$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},\bar{w}$ ]								
8	e	$\bar{1}$ '	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]								
4	d	2mm.	0,1/2,z [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]												
4	c	2mm.	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]												
2	b	$\bar{4}$ 'm2'	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]														
2	a	$\bar{4}$ 'm2'	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]														

**Symmetry of Special Projections**

Along [0,0,1] p4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

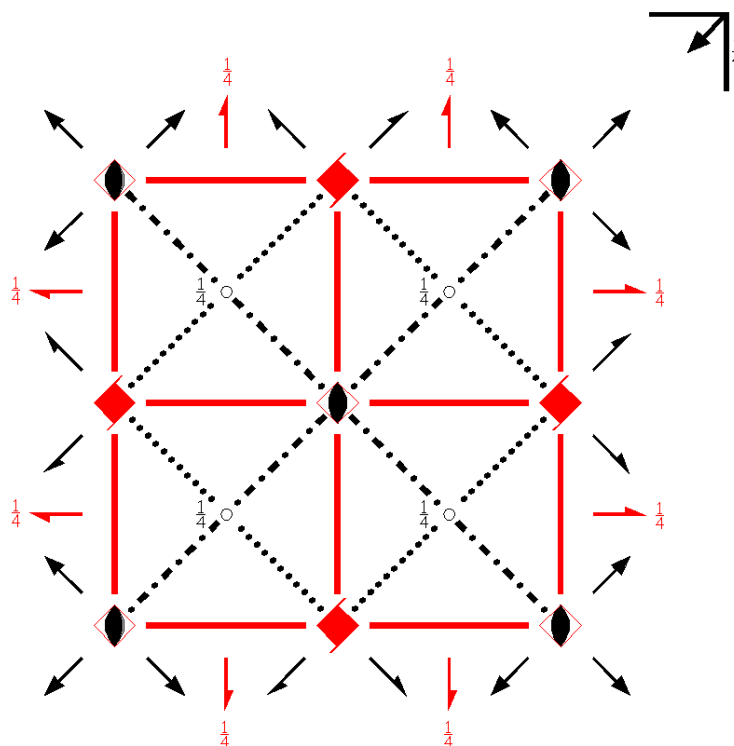
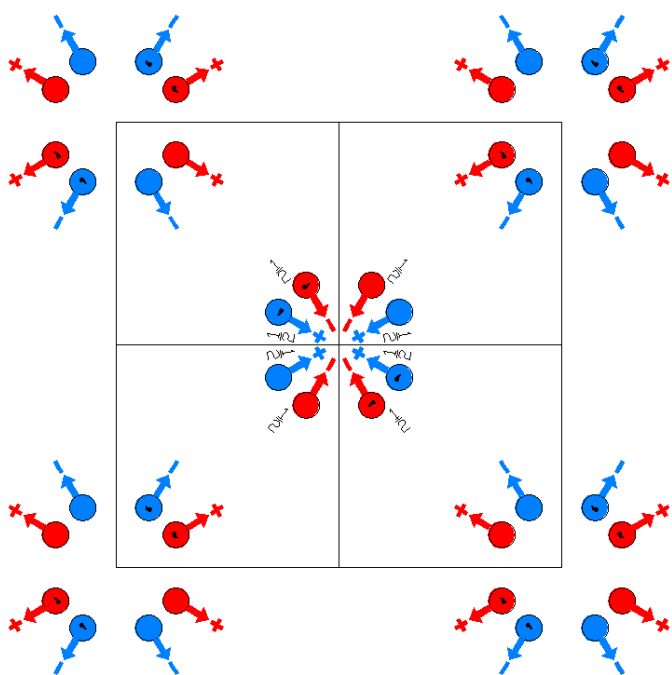
Along [1,1,0] p<sub>2a</sub>' 2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$P4_2'/nm'c$   
137.4.1164

$4'/mm'm$   
 $P4_2'/n2_1'/m'2/c$

Tetragonal



Origin at  $\bar{4}'m'2/n$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) $1$<br>( $1 0,0,0$ )   | (2) $2 \quad 0,0,z$<br>( $2_z 0,0,0$ )                             | (3) $4^+ \quad (0,0,1/2) \quad 0,1/2,z$<br>( $4_z^+ 1/2,1/2,1/2$ )'        | (4) $4^- \quad (0,0,1/2) \quad 1/2,0,z$<br>( $4_z^- 1/2,1/2,1/2$ )'        |
| (5) $2' \quad (0,1/2,0) \quad 1/4,y,1/4$<br>( $2_y 1/2,1/2,1/2$ )' | (6) $2' \quad (1/2,0,0) \quad x,1/4,1/4$<br>( $2_x 1/2,1/2,1/2$ )' | (7) $2 \quad x,x,0$<br>( $2_{xy} 0,0,0$ )                                  | (8) $2 \quad x,\bar{x},0$<br>( $2_{\bar{xy}} 0,0,0$ )                      |
| (9) $\bar{1} \quad 1/4,1/4,1/4$<br>( $\bar{1} 1/2,1/2,1/2$ )       | (10) $n \quad (1/2,1/2,0) \quad x,y,1/4$<br>( $m_z 1/2,1/2,1/2$ )  | (11) $\bar{4}^+ \quad 0,0,z; \quad 0,0,0$<br>( $\bar{4}_z^+ 0,0,0$ )'      | (12) $\bar{4}^- \quad 0,0,z; \quad 0,0,0$<br>( $\bar{4}_z^- 0,0,0$ )'      |
| (13) $m' \quad x,0,z$<br>( $m_y 0,0,0$ )'                          | (14) $m' \quad 0,y,z$<br>( $m_x 0,0,0$ )'                          | (15) $c \quad (0,0,1/2) \quad x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,1/2$ ) | (16) $n \quad (1/2,1/2,1/2) \quad x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,1/2$ ) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

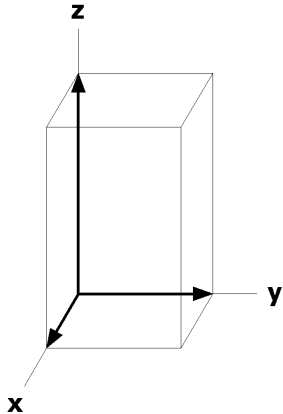
			Coordinates															
			Multiplicity, Wyckoff letter, Site Symmetry.															
16	h	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(13) $x,\bar{y},z$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	g	.m'	0,y,z [0,v,w]	0, $\bar{y}$ ,z [0, $\bar{v}$ ,w]	$\bar{y}+1/2,1/2,z+1/2$ [ $\bar{v},0,\bar{w}$ ]	$y+1/2,1/2,z+1/2$ [ $\bar{v},0,\bar{w}$ ]	$1/2,y+1/2,\bar{z}+1/2$ [0, $\bar{v}$ ,w]	$1/2,\bar{y}+1/2,\bar{z}+1/2$ [0,v,w]	$y,0,\bar{z}$ [ $\bar{v},0,\bar{w}$ ]	$\bar{y},0,\bar{z}$ [ $\bar{v},0,\bar{w}$ ]								
8	f	.2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $u,\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $u,u,0$ ]	$x+1/2,x+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},0$ [ $u,\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]								
8	e	$\bar{1}$	1/4,1/4,1/4 [u,v,w]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,3/4 [ $\bar{v},\bar{u},\bar{w}$ ]	3/4,1/4,3/4 [ $\bar{v},u,\bar{w}$ ]	1/4,3/4,1/4 [ $u,\bar{v},w$ ]	3/4,1/4,1/4 [ $\bar{u},v,w$ ]	1/4,1/4,3/4 [ $\bar{v},u,\bar{w}$ ]	3/4,3/4,3/4 [ $\bar{v},\bar{u},\bar{w}$ ]								
4	d	2m'm'	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]												
4	c	2m'm'	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]												
2	b	$\bar{4}$ 'm'2	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]														
2	a	$\bar{4}$ 'm'2	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]														

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub>' 4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'m'g  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

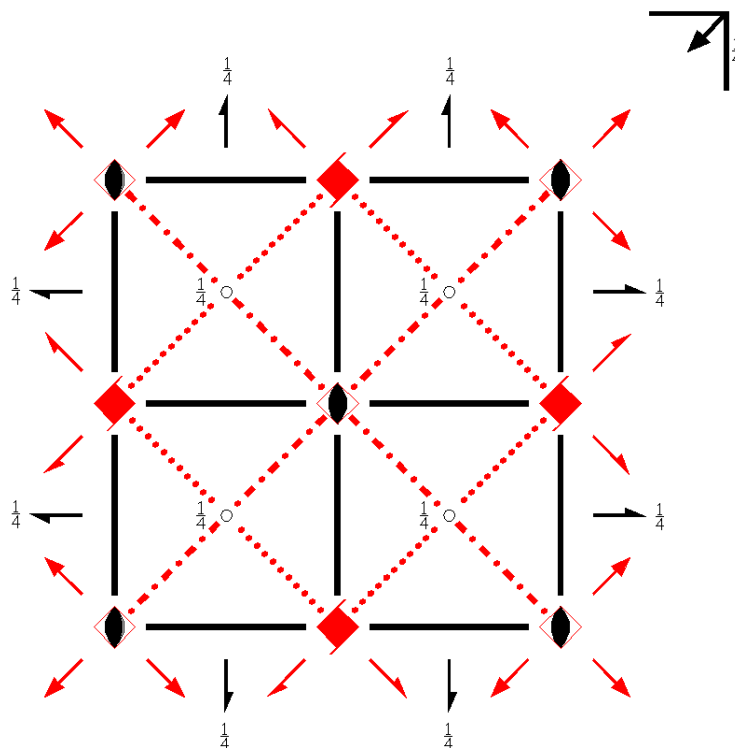
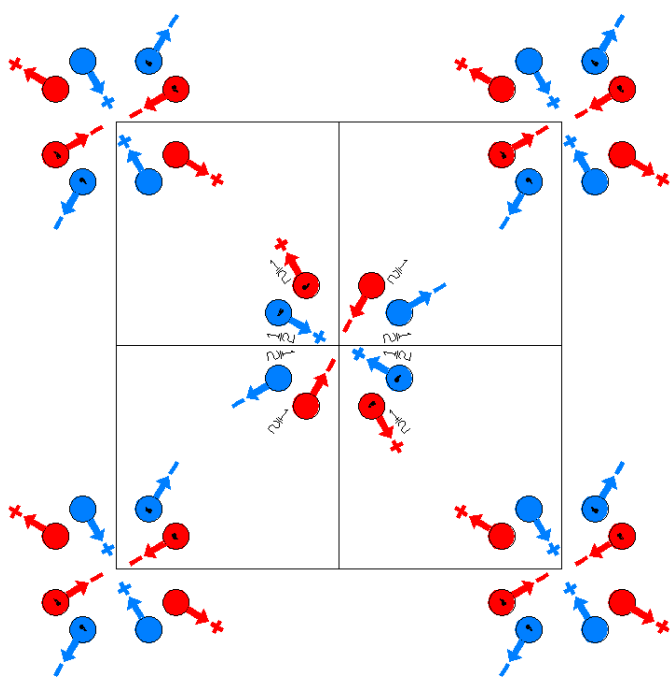
Along [1,1,0] p<sub>2a</sub>' 2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$P4_2'/nmc'$   
137.5.1165

$4'/mmm'$   
 $P4_2'/n2_1/m2'/c'$

Tetragonal



Origin at  $\bar{4}'m2'/n'$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |  |   |  |  |
|--|---|--|--|
| (1) $1$<br>$(1 0,0,0)$                                 | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                      | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>$(4_z 1/2,1/2,1/2)'$            | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>$(4_z^{-1} 1/2,1/2,1/2)'$       |
| (5) $2$ $(0,1/2,0) 1/4,y,1/4$<br>$(2_y 1/2,1/2,1/2)$   | (6) $2$ $(1/2,0,0) x,1/4,1/4$<br>$(2_x 1/2,1/2,1/2)$  | (7) $2'$ $x,x,0$<br>$(2_{xy} 0,0,0)'$                            | (8) $2'$ $x,\bar{x},0$<br>$(2_{\bar{xy}} 0,0,0)'$                |
| (9) $\bar{1}$ $1/4,1/4,1/4$<br>$(\bar{1} 1/2,1/2,1/2)$ | (10) $n$ $(1/2,1/2,0) x,y,1/4$<br>$(m_z 1/2,1/2,1/2)$ | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z 0,0,0)'$          | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1} 0,0,0)'$     |
| (13) $m$ $x,0,z$<br>$(m_y 0,0,0)$                      | (14) $m$ $0,y,z$<br>$(m_x 0,0,0)$                     | (15) $c'$ $(0,0,1/2) x+1/2,\bar{x},z$<br>$(m_{xy} 1/2,1/2,1/2)'$ | (16) $n'$ $(1/2,1/2,1/2) x,x,z$<br>$(m_{\bar{xy}} 1/2,1/2,1/2)'$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

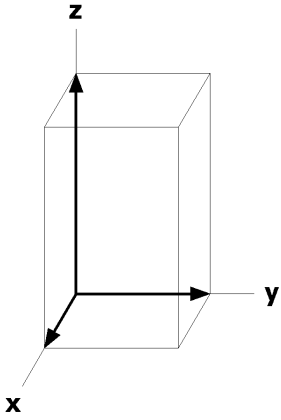
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	h	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(13) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $v,u,w$ ]
8	g	.m.	0,y,z [u,0,0]	0, $\bar{y}$ ,z [ $\bar{u},0,0$ ]	$\bar{y}+1/2,1/2,z+1/2$ [ $0,\bar{u},0$ ]	$y+1/2,1/2,z+1/2$ [0,u,0]	$1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},0,0$ ]	$1/2,\bar{y}+1/2,\bar{z}+1/2$ [u,0,0]	$y,0,\bar{z}$ [0, $\bar{u},0$ ]	$\bar{y},0,\bar{z}$ [0,u,0]								
8	f	..2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $u,u,\bar{w}$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},u,w$ ]	$x+1/2,x+1/2,1/2$ [ $u,\bar{u},w$ ]	$x,\bar{x},0$ [ $u,u,\bar{w}$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},\bar{w}$ ]								
8	e	$\bar{1}$	1/4,1/4,1/4 [u,v,w]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,3/4 [ $v,\bar{u},\bar{w}$ ]	3/4,1/4,3/4 [ $\bar{v},u,\bar{w}$ ]	1/4,3/4,1/4 [ $\bar{u},v,\bar{w}$ ]	3/4,1/4,1/4 [ $u,\bar{v},\bar{w}$ ]	1/4,1/4,3/4 [ $\bar{v},\bar{u},w$ ]	3/4,3/4,3/4 [ $v,u,w$ ]								
4	d	2mm.	0,1/2,z [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]												
4	c	2mm.	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]												
2	b	$\bar{4}'m2'$	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]														
2	a	$\bar{4}'m2'$	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]														

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub> 4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



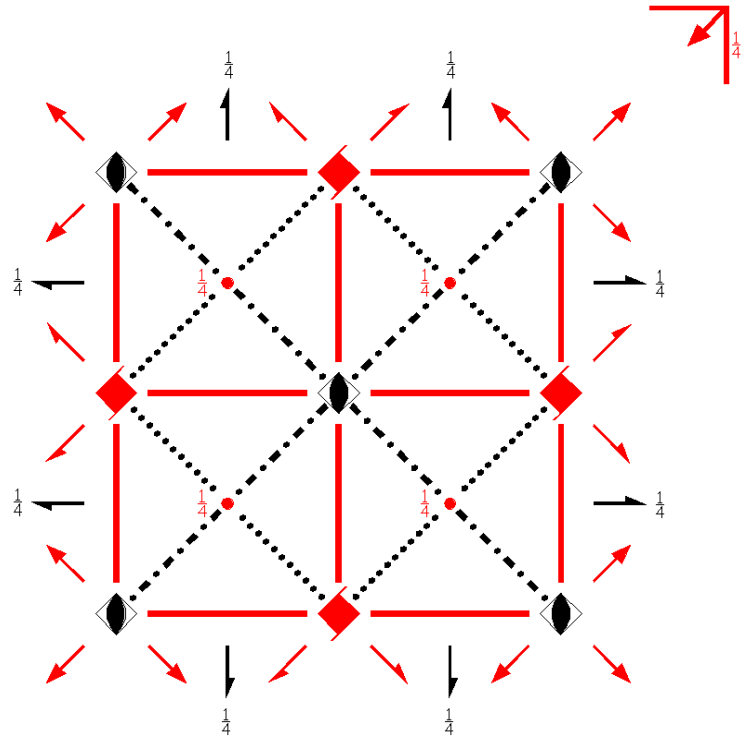
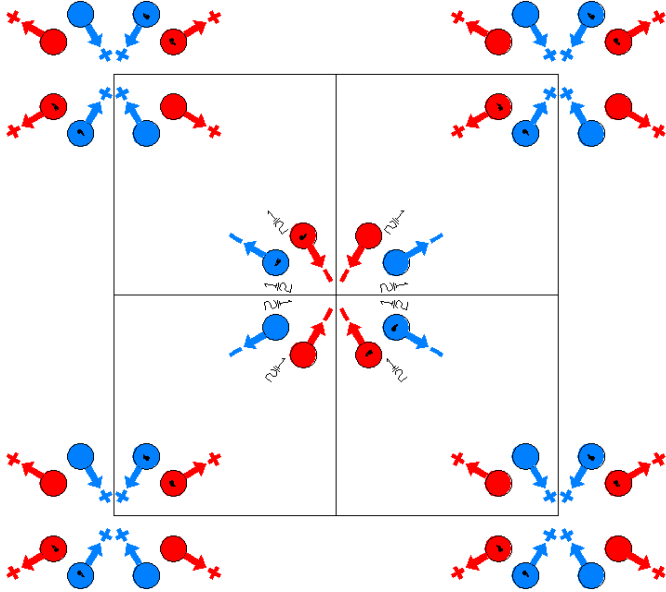
$P4_2/n'm'c$

137.6.1166

$4'/m'm'm$

$P4_2/n'2_1/m'2'/c$

Tetragonal



Origin at  $\bar{4}m'2'/n$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) $1$<br>( $1 0,0,0$ )                                    | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                        | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>( $4_z 1/2,1/2,1/2$ )'          | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,1/2$ )'     |
| (5) $2$ $(0,1/2,0) 1/4,y,1/4$<br>( $2_y 1/2,1/2,1/2$ )      | (6) $2$ $(1/2,0,0) x,1/4,1/4$<br>( $2_x 1/2,1/2,1/2$ )    | (7) $2'$ $x,x,0$<br>( $2_{xy} 0,0,0$ )'                          | (8) $2'$ $x,\bar{x},0$<br>( $2_{\bar{xy}} 0,0,0$ )'              |
| (9) $\bar{1}'$ $1/4,1/4,1/4$<br>( $\bar{1}' 1/2,1/2,1/2$ )' | (10) $n'$ $(1/2,1/2,0) x,y,1/4$<br>( $m_z 1/2,1/2,1/2$ )' | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )         | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ )    |
| (13) $m'$ $x,0,z$<br>( $m_y 0,0,0$ )'                       | (14) $m'$ $0,y,z$<br>( $m_x 0,0,0$ )'                     | (15) $c$ $(0,0,1/2) x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,1/2$ ) | (16) $n$ $(1/2,1/2,1/2) x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,1/2$ ) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

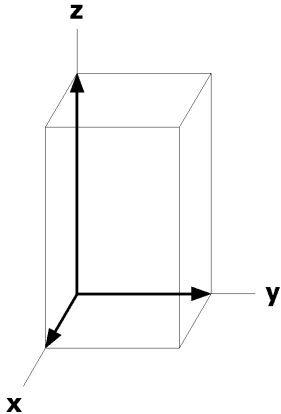
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	h	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]	(13) $x,\bar{y},z$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $v,u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	g	.m'	0,y,z [0,v,w]	0, $\bar{y}$ ,z [0, $\bar{v}$ ,w]	$\bar{y}+1/2,1/2,z+1/2$ [ $v,0,\bar{w}$ ]	$y+1/2,1/2,z+1/2$ [ $\bar{v},0,\bar{w}$ ]	1/2,y+1/2, $\bar{z}+1/2$ [0,v, $\bar{w}$ ]	1/2, $\bar{y}+1/2,\bar{z}+1/2$ [0, $\bar{v},\bar{w}$ ]	y,0, $\bar{z}$ [ $\bar{v},0,w$ ]	$\bar{y},0,\bar{z}$ [ $v,0,w$ ]								
8	f	..2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $u,u,\bar{w}$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x+1/2,1/2$ [ $\bar{u},u,\bar{w}$ ]	x, $\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,0$ [ $u,u,w$ ]								
8	e	$\bar{1}'$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]								
4	d	2m'm'	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]												
4	c	2m'm'	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]												
2	b	$\bar{4}m'2'$	0,0,1/2 [0,0,w]	1/2,1/2,0 [0,0, $\bar{w}$ ]														
2	a	$\bar{4}m'2'$	0,0,0 [0,0,w]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]														

**Symmetry of Special Projections**

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [1,1,0] p<sub>2a</sub>' 2m'm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



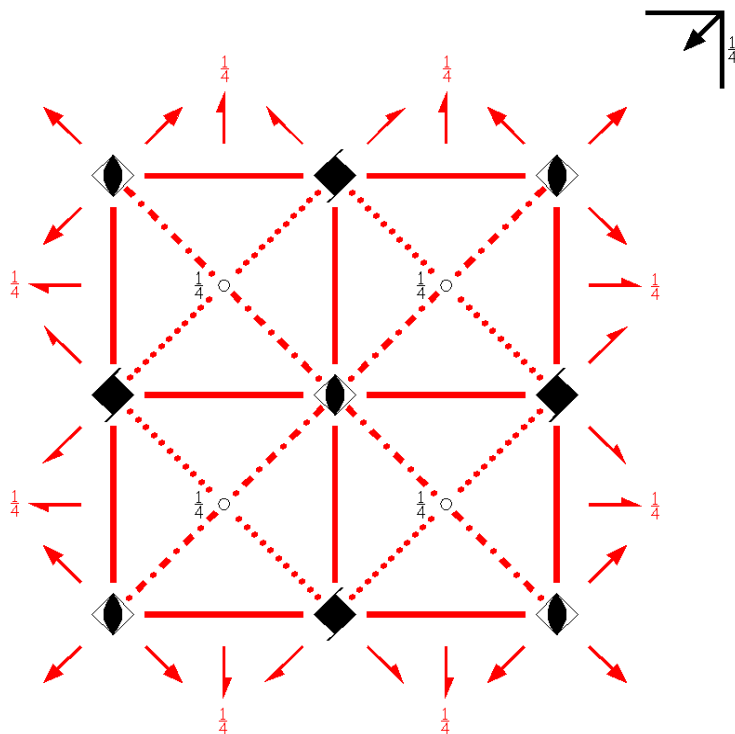
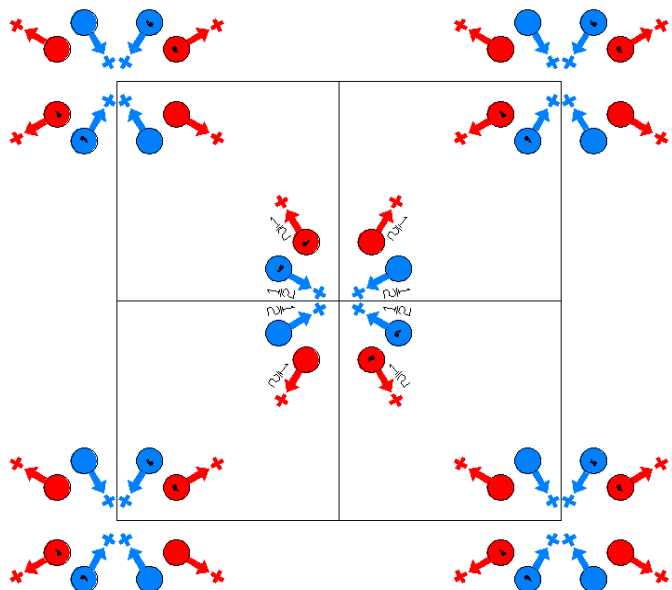
$P4_2/nm'c'$

137.7.1167

$4/m\bar{m}'m'$

$P4_2/n2_1'/m'2'/c'$

Tetragonal



Origin at  $\bar{4}m'2'/n'$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |  |  |  |  |
|--|--|--|--|
| (1) $1$<br>( $\bar{1}   0,0,0$ )                           | (2) $2$ $0,0,z$<br>( $2_z   0,0,0$ )                       | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>( $4_z   1/2,1/2,1/2$ )             | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1}   1/2,1/2,1/2$ )        |
| (5) $2'$ $(0,1/2,0) 1/4,y,1/4$<br>( $2_y   1/2,1/2,1/2$ )' | (6) $2'$ $(1/2,0,0) x,1/4,1/4$<br>( $2_x   1/2,1/2,1/2$ )' | (7) $2'$ $x,x,0$<br>( $2_{xy}   0,0,0$ )'                            | (8) $2'$ $x,\bar{x},0$<br>( $2_{\bar{xy}}   0,0,0$ )'                |
| (9) $\bar{1}$ $1/4,1/4,1/4$<br>( $\bar{1}   1/2,1/2,1/2$ ) | (10) $n$ $(1/2,1/2,0) x,y,1/4$<br>( $m_z   1/2,1/2,1/2$ )  | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z   0,0,0$ )           | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1}   0,0,0$ )      |
| (13) $m'$ $x,0,z$<br>( $m_y   0,0,0$ )'                    | (14) $m'$ $0,y,z$<br>( $m_x   0,0,0$ )'                    | (15) $c'$ $(0,0,1/2) x+1/2,\bar{x},z$<br>( $m_{xy}   1/2,1/2,1/2$ )' | (16) $n'$ $(1/2,1/2,1/2) x,x,z$<br>( $m_{\bar{xy}}   1/2,1/2,1/2$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

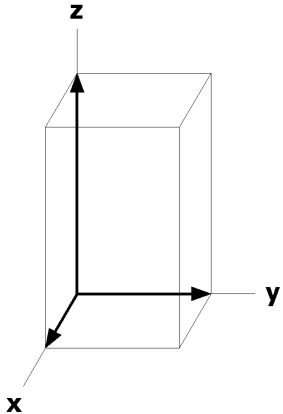
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	h	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]	(13) $x,\bar{y},z$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $v,u,w$ ]
8	g	.m'	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	$\bar{y}+1/2,1/2,z+1/2$ [ $\bar{v},0,w$ ]	$y+1/2,1/2,z+1/2$ [ $v,0,w$ ]	$1/2,y+1/2,\bar{z}+1/2$ [0, $\bar{v},w$ ]	$1/2,\bar{y}+1/2,\bar{z}+1/2$ [0,v,w]	$y,0,\bar{z}$ [ $\bar{v},0,w$ ]	$\bar{y},0,\bar{z}$ [ $v,0,w$ ]								
8	f	..2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $\bar{u},\bar{u},w$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $u,u,w$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},u,w$ ]	$x+1/2,x+1/2,1/2$ [ $u,\bar{u},w$ ]	$x,\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,0$ [ $u,u,w$ ]								
8	e	$\bar{1}$	1/4,1/4,1/4 [u,v,w]	3/4,3/4,1/4 [ $\bar{u},\bar{v},w$ ]	1/4,3/4,3/4 [ $\bar{v},u,w$ ]	3/4,1/4,3/4 [ $v,\bar{u},w$ ]	1/4,3/4,1/4 [u, $\bar{v},w$ ]	3/4,1/4,1/4 [ $\bar{u},v,w$ ]	1/4,1/4,3/4 [ $\bar{v},\bar{u},w$ ]	3/4,3/4,3/4 [ $v,u,w$ ]								
4	d	2m'm'	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]												
4	c	2m'm'	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]												
2	b	$\bar{4}m'2'$	0,0,1/2 [0,0,w]	1/2,1/2,0 [0,0,w]														
2	a	$\bar{4}m'2'$	0,0,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]														

### Symmetry of Special Projections

Along [0,0,1] p<sub>p</sub>' 4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,1/2,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



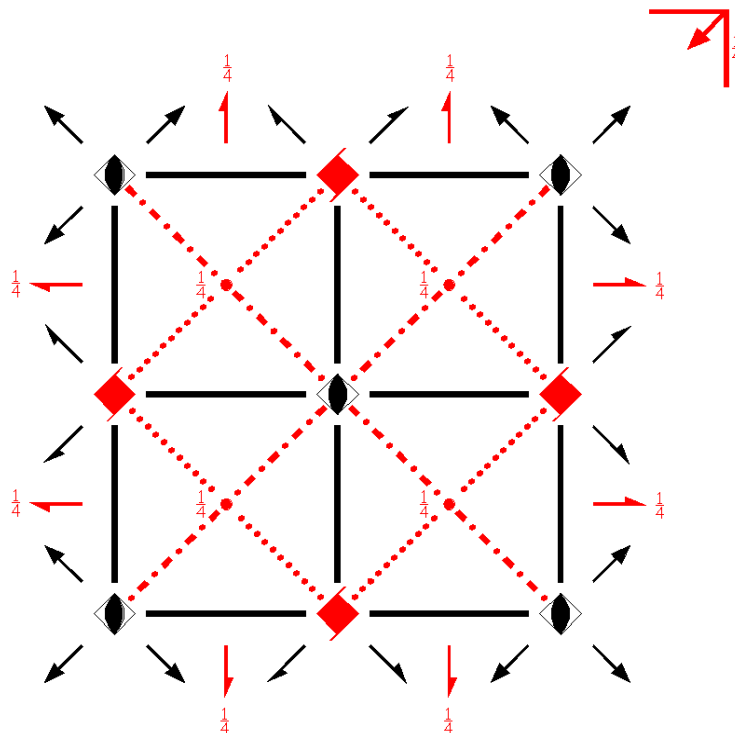
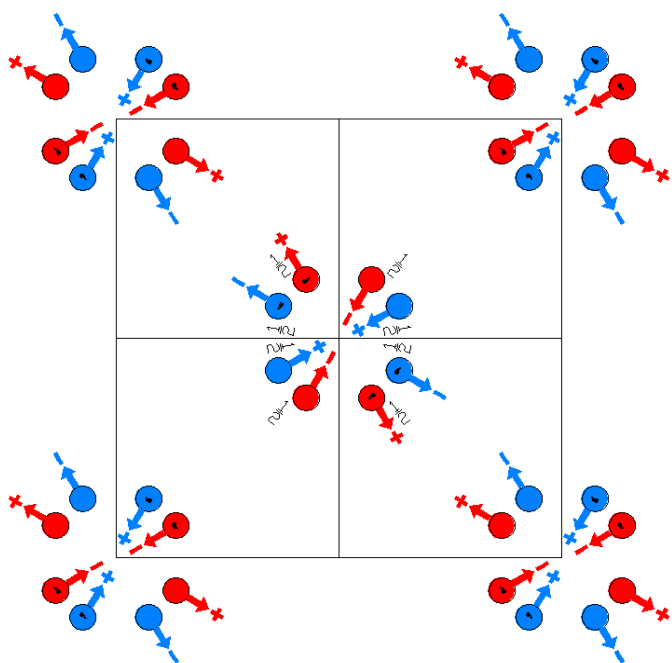
$P4_2/n'mc'$

137.8.1168

$4'/m'mm'$

$P4_2/n'2_1'/m2/c'$

Tetragonal



Origin at  $\bar{4}m2/n'$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |  |   |  |  |
|--|---|--|--|
| (1) $1$<br>( $1 0,0,0$ )                                   | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                        | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>( $4_z 1/2,1/2,1/2$ )'            | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,1/2$ )'       |
| (5) $2'$ $(0,1/2,0) 1/4,y,1/4$<br>( $2_y 1/2,1/2,1/2$ )'   | (6) $2'$ $(1/2,0,0) x,1/4,1/4$<br>( $2_x 1/2,1/2,1/2$ )'  | (7) $2$ $x,x,0$<br>( $2_{xy} 0,0,0$ )                              | (8) $2$ $x,\bar{x},0$<br>( $2_{\bar{xy}} 0,0,0$ )                  |
| (9) $\bar{1}'$ $1/4,1/4,1/4$<br>( $\bar{1} 1/2,1/2,1/2$ )' | (10) $n'$ $(1/2,1/2,0) x,y,1/4$<br>( $m_z 1/2,1/2,1/2$ )' | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )           | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ )      |
| (13) $m$ $x,0,z$<br>( $m_y 0,0,0$ )                        | (14) $m$ $0,y,z$<br>( $m_x 0,0,0$ )                       | (15) $c'$ $(0,0,1/2) x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,1/2$ )' | (16) $n'$ $(1/2,1/2,1/2) x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,1/2$ )' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

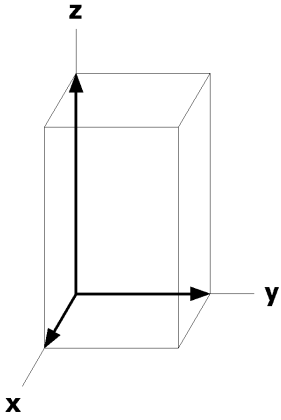
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	h	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $u,\bar{v},w$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(13) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $v,u,w$ ]
8	g	.m.	0,y,z [u,0,0]	0, $\bar{y}$ ,z [ $\bar{u},0,0$ ]	$\bar{y}+1/2,1/2,z+1/2$ [ $0,\bar{u},0$ ]	$y+1/2,1/2,z+1/2$ [ $0,u,0$ ]	$1/2,y+1/2,\bar{z}+1/2$ [ $u,0,0$ ]	$1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},0,0$ ]	$y,0,\bar{z}$ [ $0,u,0$ ]	$\bar{y},0,\bar{z}$ [ $0,\bar{u},0$ ]								
8	f	.2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $u,\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x+1/2,1/2$ [ $u,u,0$ ]	$x,\bar{x},0$ [ $\bar{u},u,0$ ]	$\bar{x},x,0$ [ $u,\bar{u},0$ ]								
8	e	$\bar{1}'$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]								
4	d	2mm.	0,1/2,z [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]												
4	c	2mm.	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]												
2	b	$\bar{4}m2$	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]														
2	a	$\bar{4}m2$	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]														

**Symmetry of Special Projections**

Along [0,0,1] p4'm'm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



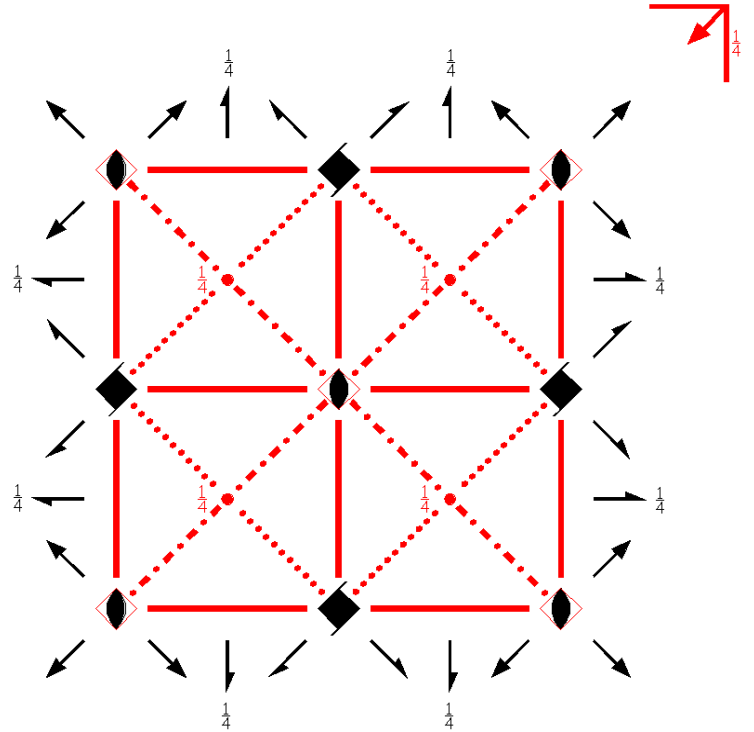
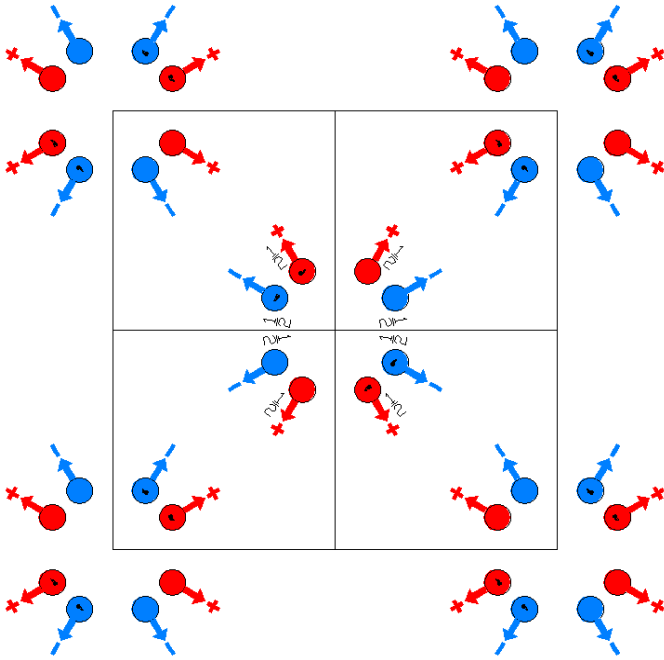
$P4_2/n'm'c'$

137.9.1169

$4/m'm'm'$

$P4_2/n'2_1/m'2/c'$

Tetragonal



Origin at  $\bar{4}'m'2/n'$ , at  $-1/4, 1/4, -1/4$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4$

### Symmetry Operations

- |   |   |  |  |
|---|---|--|--|
| (1) $1$<br>$(1 0,0,0)$                                    | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                          | (3) $4^+$ $(0,0,1/2)$ $0,1/2,z$<br>$(4_z 1/2,1/2,1/2)$             | (4) $4^-$ $(0,0,1/2)$ $1/2,0,z$<br>$(4_z^{-1} 1/2,1/2,1/2)$        |
| (5) $2$ $(0,1/2,0)$ $1/4,y,1/4$<br>$(2_y 1/2,1/2,1/2)$    | (6) $2$ $(1/2,0,0)$ $x,1/4,1/4$<br>$(2_x 1/2,1/2,1/2)$    | (7) $2$ $x,x,0$<br>$(2_{xy} 0,0,0)$                                | (8) $2$ $x,\bar{x},0$<br>$(2_{\bar{xy}} 0,0,0)$                    |
| (9) $\bar{1}'$ $1/4,1/4,1/4$<br>$(\bar{1}' 1/2,1/2,1/2)'$ | (10) $n'$ $(1/2,1/2,0)$ $x,y,1/4$<br>$(m_z 1/2,1/2,1/2)'$ | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z 0,0,0)'$            | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1} 0,0,0)'$       |
| (13) $m'$ $x,0,z$<br>$(m_y 0,0,0)'$                       | (14) $m'$ $0,y,z$<br>$(m_x 0,0,0)'$                       | (15) $c'$ $(0,0,1/2)$ $x+1/2,\bar{x},z$<br>$(m_{xy} 1/2,1/2,1/2)'$ | (16) $n'$ $(1/2,1/2,1/2)$ $x,x,z$<br>$(m_{\bar{xy}} 1/2,1/2,1/2)'$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

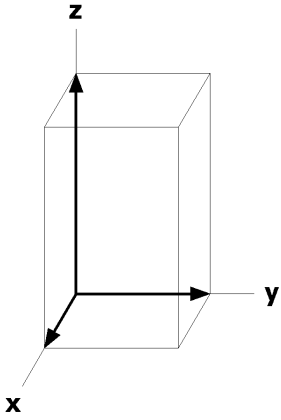
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	h	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,z$ [ $\bar{v},u,\bar{w}$ ]	(13) $x,\bar{y},z$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z+1/2$ [ $v,u,w$ ]
8	g	.m'	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	$\bar{y}+1/2,1/2,z+1/2$ [ $\bar{v},0,w$ ]	$y+1/2,1/2,z+1/2$ [ $v,0,w$ ]	$1/2,y+1/2,\bar{z}+1/2$ [0,v, $\bar{w}$ ]	$1/2,\bar{y}+1/2,\bar{z}+1/2$ [0, $\bar{v},\bar{w}$ ]	$y,0,\bar{z}$ [v,0, $\bar{w}$ ]	$\bar{y},0,\bar{z}$ [ $\bar{v},0,\bar{w}$ ]								
8	f	.2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/2$ [ $\bar{u},u,0$ ]	$x+1/2,\bar{x}+1/2,1/2$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x+1/2,1/2$ [ $u,u,0$ ]	$x,\bar{x},0$ [ $u,\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]								
8	e	$\bar{1}'$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]								
4	d	2m'm'	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]												
4	c	2m'm'	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]												
2	b	$\bar{4}'m'2$	0,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]														
2	a	$\bar{4}'m'2$	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]														

### Symmetry of Special Projections

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,1/4,1/4

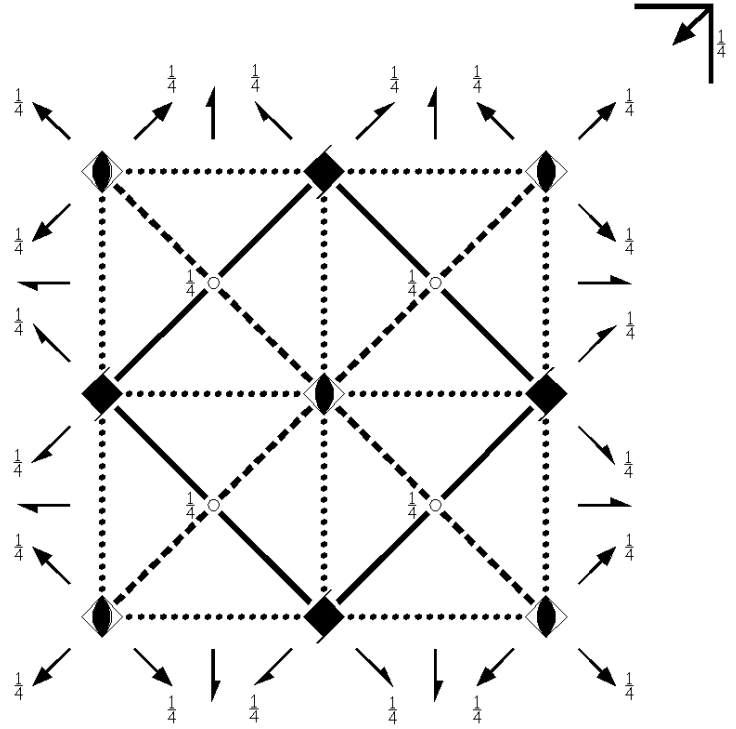
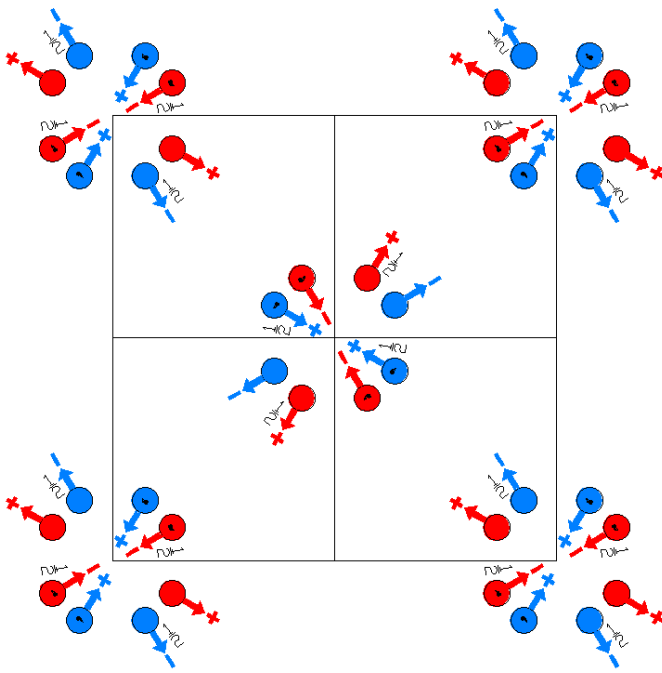
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P4_2/nm$   
138.1.1170

$4/mmm$   
 $P4_2/n2_1/c2/m$

Tetragonal



Origin at  $\bar{4}cg$ , at  $-1/4, 1/4, -1/4$  from center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$ ;  $x \leq y$ ;  $y \leq 1/2 - x$

### Symmetry Operations

- |  |   |  |   |
|--|---|--|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub> <sup>+</sup>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)      | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)  | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)            |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2) | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)                           | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)                         |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)    | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)         | (15) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0)                         | (16) g (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

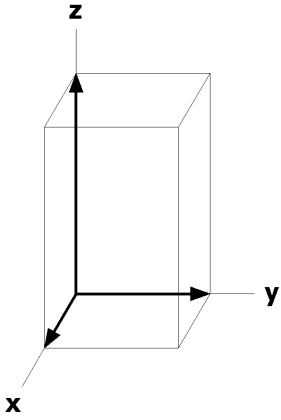
16	j	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,+1/2\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y,x,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]		
			(13) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $v,u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z$ [ $\bar{v},\bar{u},\bar{w}$ ]		
8	i	..m	$x,x+1/2,z$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}+1/2,z$ [ $u,\bar{u},0$ ]	$\bar{x},x+1/2,z+1/2$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x}+1/2,z+1/2$ [ $u,u,0$ ]
			$\bar{x}+1/2,x,\bar{z}$ [ $u,u,0$ ]	$x+1/2,\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x,\bar{z}+1/2$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,\bar{x},\bar{z}+1/2$ [ $\bar{u},u,0$ ]
8	h	..2	$x,x,3/4$ [ $u,u,0$ ]	$\bar{x},\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/4$ [ $\bar{u},u,0$ ]	$x+1/2,\bar{x}+1/2,1/4$ [ $u,\bar{u},0$ ]
			$\bar{x}+1/2,\bar{x}+1/2,3/4$ [ $u,u,0$ ]	$x+1/2,x+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},1/4$ [ $\bar{u},u,0$ ]	$\bar{x},x,1/4$ [ $u,\bar{u},0$ ]
8	g	..2	$x,x,1/4$ [ $u,u,0$ ]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,3/4$ [ $\bar{u},u,0$ ]	$x+1/2,\bar{x}+1/2,3/4$ [ $u,\bar{u},0$ ]
			$\bar{x}+1/2,\bar{x}+1/2,1/4$ [ $u,u,0$ ]	$x+1/2,x+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},3/4$ [ $\bar{u},u,0$ ]	$\bar{x},x,3/4$ [ $u,\bar{u},0$ ]
8	f	2..	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
			1/2,1/2, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2,z [0,0, $\bar{w}$ ]
4	e	2.mm	0,1/2,z [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]
4	d	..2/m	1/4,1/4,3/4 [u,u,0]	3/4,3/4,3/4 [ $\bar{u},\bar{u},0$ ]	1/4,3/4,1/4 [ $\bar{u},u,0$ ]	3/4,1/4,1/4 [ $u,\bar{u},0$ ]
4	c	..2/m	1/4,1/4,1/4 [u,u,0]	3/4,3/4,1/4 [ $\bar{u},\bar{u},0$ ]	1/4,3/4,3/4 [ $\bar{u},u,0$ ]	3/4,1/4,3/4 [ $u,\bar{u},0$ ]
4	b	$\bar{4}$ ..	0,0,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]	1/2,1/2,0 [0,0, $\bar{w}$ ]	0,0,1/2 [0,0, $\bar{w}$ ]
4	a	2.22	0,0,1/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]	1/2,1/2,1/4 [0,0,0]	0,0,3/4 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub> 4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub> 2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,1/4,0

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,x,1/4



$P4_2/nm1'$

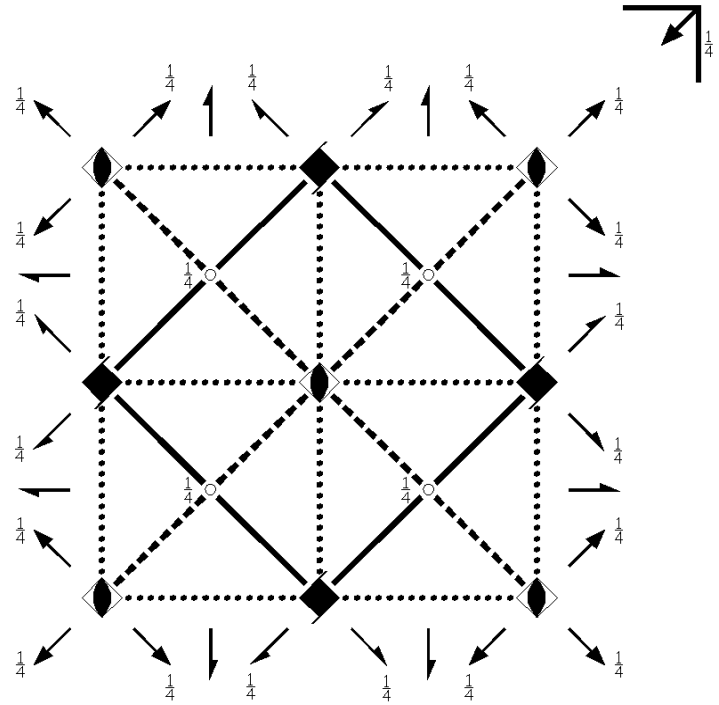
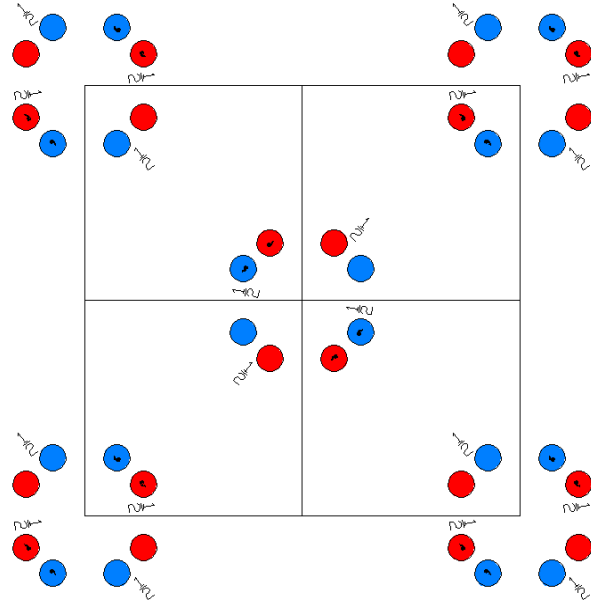
138.2.1171

$4/mmm1'$

$P4_2/n2_1/c2/m1'$

Tetragonal

1'



Origin at  $\bar{4}cg1'$ , at  $-1/4, 1/4, -1/4$  from center ( $2/m1'$ )

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y; y \leq 1/2 - x$

**Symmetry Operations**

For 1 + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)      | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                           | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)            |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2) | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)              | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                            |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)    | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)         | (15) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0)            | (16) g (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)         |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)'	(4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'
(5) 2' (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>  1/2,1/2,0)'	(6) 2' (1/2,0,0) x,1/4,0 (2 <sub>x</sub>  1/2,1/2,0)'	(7) 2' x,x,1/4 (2 <sub>xy</sub>  0,0,1/2)'	(8) 2' x, $\bar{x}$ ,1/4 (2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)'
(9) $\bar{1}$ ' 1/4,1/4,1/4 ( $\bar{1}$  1/2,1/2,1/2)'	(10) n' (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>  1/2,1/2,1/2)'	(11) $\bar{4}^+$ ' 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'	(12) $\bar{4}^-$ ' 0,0,z; 0,0,0 ( $\bar{4}_z^{-1}$  0,0,0)'
(13) c' (0,0,1/2) x,0,z (m <sub>y</sub>  0,0,1/2)'	(14) c' (0,0,1/2) 0,y,z (m <sub>x</sub>  0,0,1/2)'	(15) m' x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,0)'	(16) g' (1/2,1/2,0) x,x,z (m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

**Positions**

			Coordinates															
			1 +	1' +														
Multiplicity,	Wyckoff letter,	Site Symmetry.																
16	j	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{y}+1/2,x+1/2,z+1/2$ [0,0,0]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [0,0,0]	(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [0,0,0]	(6) $x+1/2,+1/2\bar{y},\bar{z}$ [0,0,0]	(7) $y,x,\bar{z}+1/2$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [0,0,0]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [0,0,0]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [0,0,0]	(11) $y,\bar{x},\bar{z}$ [0,0,0]	(12) $\bar{y},x,\bar{z}$ [0,0,0]	(13) $x,\bar{y},z+1/2$ [0,0,0]	(14) $\bar{x},y,z+1/2$ [0,0,0]	(15) $\bar{y}+1/2,\bar{x}+1/2,z$ [0,0,0]	(16) $y+1/2,x+1/2,z$ [0,0,0]
8	i	..m1'	x,x+1/2,z [0,0,0]	$\bar{x},\bar{x}+1/2,z$ [0,0,0]	$\bar{x},x+1/2,z+1/2$ [0,0,0]	$x,\bar{x}+1/2,z+1/2$ [0,0,0]	$\bar{x}+1/2,x,\bar{z}$ [0,0,0]	$x+1/2,\bar{x},\bar{z}$ [0,0,0]	$x+1/2,x,\bar{z}+1/2$ [0,0,0]	$\bar{x}+1/2,\bar{x},\bar{z}+1/2$ [0,0,0]								
8	h	..21'	x,x,3/4 [0,0,0]	$\bar{x},\bar{x},3/4$ [0,0,0]	$\bar{x}+1/2,x+1/2,1/4$ [0,0,0]	$x+1/2,\bar{x}+1/2,1/4$ [0,0,0]	$\bar{x}+1/2,\bar{x}+1/2,3/4$ [0,0,0]	$x+1/2,x+1/2,3/4$ [0,0,0]	$x,\bar{x},1/4$ [0,0,0]	$\bar{x},x,1/4$ [0,0,0]								
8	g	..21'	x,x,1/4 [0,0,0]	$\bar{x},\bar{x},1/4$ [0,0,0]	$\bar{x}+1/2,x+1/2,3/4$ [0,0,0]	$x+1/2,\bar{x}+1/2,3/4$ [0,0,0]	$\bar{x}+1/2,\bar{x}+1/2,1/4$ [0,0,0]	$x+1/2,x+1/2,1/4$ [0,0,0]	$x,\bar{x},3/4$ [0,0,0]	$\bar{x},x,3/4$ [0,0,0]								
8	f	2..1'	0,0,z [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	1/2,1/2, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0,z+1/2 [0,0,0]	1/2,1/2,z [0,0,0]								
4	e	2.mm1'	0,1/2,z [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]												



Continued

138.2.1171

 $P4_2/ncm1'$ 

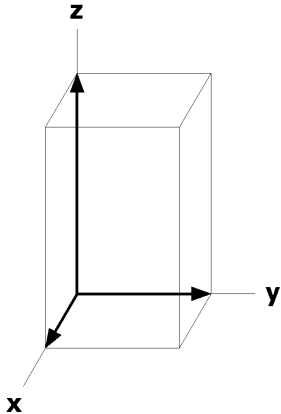
4	d	$\sqrt{2}/m1'$	$1/4, 1/4, 3/4 [0,0,0]$	$3/4, 3/4, 3/4 [0,0,0]$	$1/4, 3/4, 1/4 [0,0,0]$	$3/4, 1/4, 1/4 [0,0,0]$
4	c	$\sqrt{2}/m1'$	$1/4, 1/4, 1/4 [0,0,0]$	$3/4, 3/4, 1/4 [0,0,0]$	$1/4, 3/4, 3/4 [0,0,0]$	$3/4, 1/4, 3/4 [0,0,0]$
4	b	$\sqrt{4}..1'$	$0,0,0 [0,0,0]$	$1/2, 1/2, 1/2 [0,0,0]$	$1/2, 1/2, 0 [0,0,0]$	$0,0, 1/2 [0,0,0]$
4	a	$2.221'$	$0,0, 1/4 [0,0,0]$	$1/2, 1/2, 3/4 [0,0,0]$	$1/2, 1/2, 1/4 [0,0,0]$	$0,0, 3/4 [0,0,0]$

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mg1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, 1/4, 0$

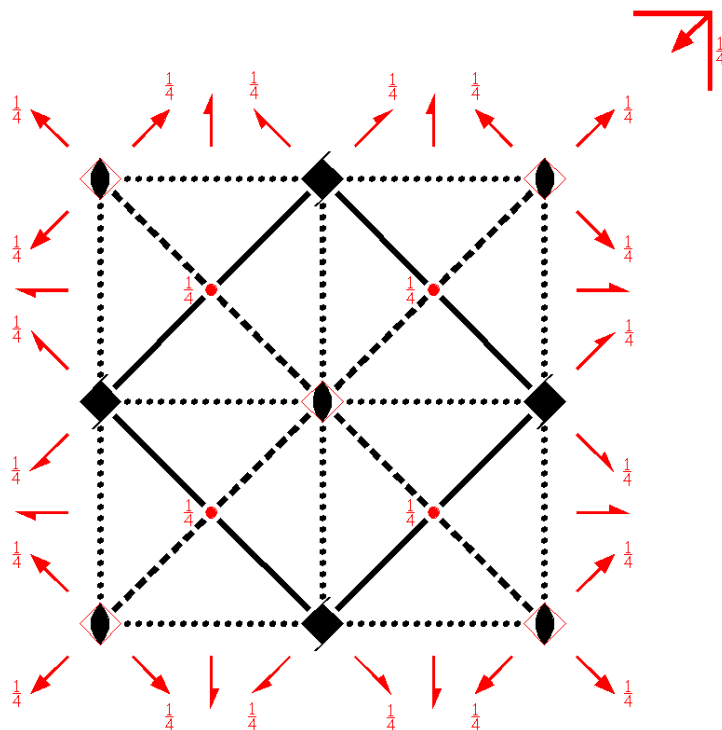
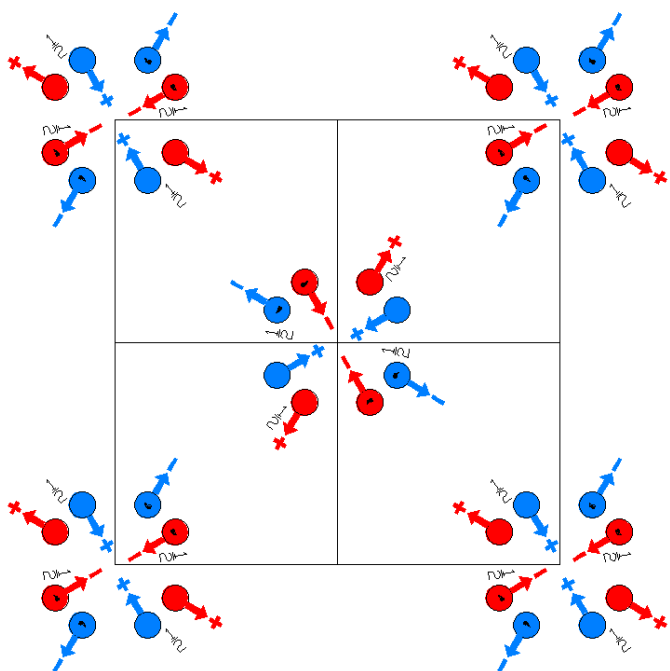
Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x, 1/4$



$P4_2/n'cm$   
138.3.1172

$4/m'mm$   
 $P4_2/n'2_1'/c2'/m$

Tetragonal



Origin at  $\bar{4}'cg$ , at  $-1/4, 1/4, -1/4$  from center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$ ;  $x \leq y$ ;  $y \leq 1/2 - x$

### Symmetry Operations

- |   |   |   |  |
|---|---|---|--|
| (1) $1$<br>( $1 0,0,0$ )                                    | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                        | (3) $4^+$ $(0,0,1/2) 0,1/2,z$<br>( $4_z 1/2,1/2,1/2$ )    | (4) $4^-$ $(0,0,1/2) 1/2,0,z$<br>( $4_z^{-1} 1/2,1/2,1/2$ )    |
| (5) $2'$ $(0,1/2,0) 1/4,y,0$<br>( $2_y 1/2,1/2,0$ )'        | (6) $2'$ $(1/2,0,0) x,1/4,0$<br>( $2_x 1/2,1/2,0$ )'      | (7) $2'$ $x,x,1/4$<br>( $2_{xy} 0,0,1/2$ )'               | (8) $2'$ $x,\bar{x},1/4$<br>( $2_{\bar{xy}} 0,0,1/2$ )'        |
| (9) $\bar{1}'$ $1/4,1/4,1/4$<br>( $\bar{1}' 1/2,1/2,1/2$ )' | (10) $n'$ $(1/2,1/2,0) x,y,1/4$<br>( $m_z 1/2,1/2,1/2$ )' | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )' | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ )' |
| (13) $c$ $(0,0,1/2) x,0,z$<br>( $m_y 0,0,1/2$ )             | (14) $c$ $(0,0,1/2) 0,y,z$<br>( $m_x 0,0,1/2$ )           | (15) $m$ $x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,0$ )      | (16) $g$ $(1/2,1/2,0) x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,0$ )   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

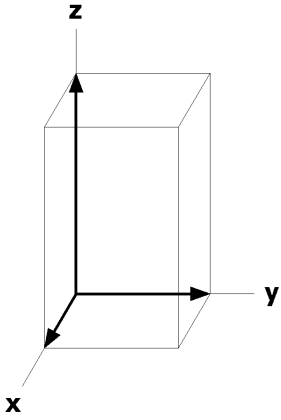
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	j	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},u,w$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $v,\bar{u},w$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $u,\bar{v},w$ ]	(6) $x+1/2,+1/2\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $v,u,w$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(13) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $v,u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	i	..m	$x,x+1/2,z$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}+1/2,z$ [ $u,\bar{u},0$ ]	$\bar{x},x+1/2,z+1/2$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x}+1/2,z+1/2$ [ $u,u,0$ ]	$\bar{x}+1/2,x,\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},\bar{z}$ [ $u,u,0$ ]	$x+1/2,x,\bar{z}+1/2$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,\bar{x},\bar{z}+1/2$ [ $u,\bar{u},0$ ]								
8	h	..2'	$x,x,3/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},3/4$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,1/4$ [ $\bar{u},\bar{u},w$ ]	$x+1/2,\bar{x}+1/2,1/4$ [ $u,u,w$ ]	$\bar{x}+1/2,\bar{x}+1/2,3/4$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x+1/2,3/4$ [ $\bar{u},u,\bar{w}$ ]	$x,\bar{x},1/4$ [ $u,u,\bar{w}$ ]	$\bar{x},x,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]								
8	g	..2'	$x,x,1/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,3/4$ [ $\bar{u},\bar{u},w$ ]	$x+1/2,\bar{x}+1/2,3/4$ [ $u,u,w$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/4$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x+1/2,1/4$ [ $\bar{u},u,\bar{w}$ ]	$x,\bar{x},3/4$ [ $u,u,\bar{w}$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]								
8	f	2..	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	1/2,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2,z [0,0, $\bar{w}$ ]								
4	e	2.mm	0,1/2,z [0,0,0]	0,1/2,z+1/2 [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]												
4	d	..2'/m	1/4,1/4,3/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]												
4	c	..2'/m	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]												
4	b	$\bar{4}'$ ..	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	0,0,1/2 [0,0,0]												
4	a	2.2'2'	0,0,1/4 [0,0,w]	1/2,1/2,3/4 [0,0,w]	1/2,1/2,1/4 [0,0, $\bar{w}$ ]	0,0,3/4 [0,0, $\bar{w}$ ]												

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2b} 2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at  $x, 1/4, 1/4$

Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,x,1/4$



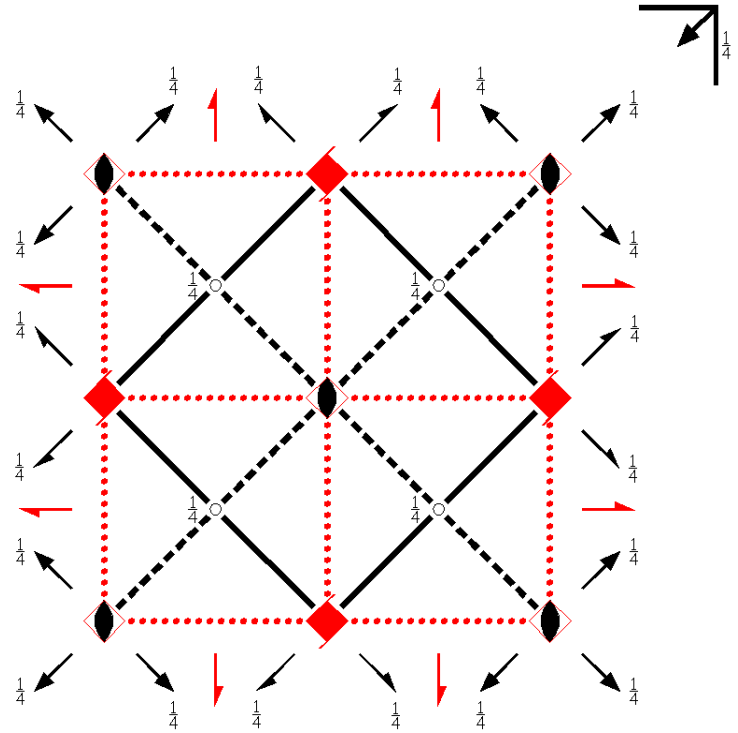
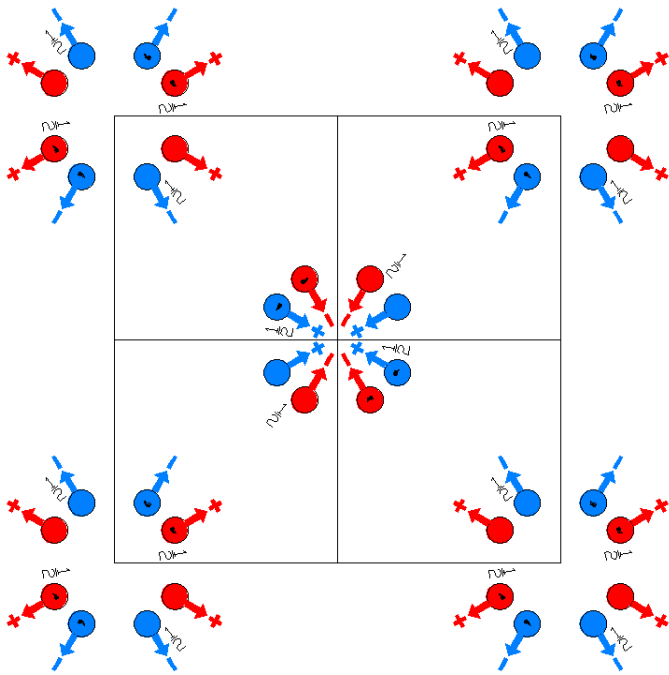
$P4_2'/nc'm$

138.4.1173

$4'/mm'm$

$P4_2'/n2_1'/c'2/m$

Tetragonal



Origin at  $\bar{4}'c'g$ , at  $-1/4, 1/4, -1/4$  from center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y; y \leq 1/2 - x$

**Symmetry Operations**

- |  |   |  |  |
|--|---|--|--|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (6) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)'    | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                            | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)             |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)   | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'              | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                            |
| (13) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)'    | (14) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)'       | (15) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0)             | (16) g (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

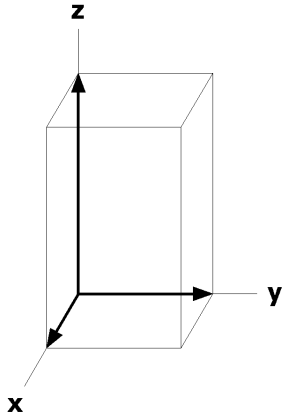
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	j	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) $x+1/2,+1/2\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(13) $x,\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $\bar{v},u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	i	..m	$x,x+1/2,z$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}+1/2,z$ [ $u,\bar{u},0$ ]	$\bar{x},x+1/2,z+1/2$ [ $u,u,0$ ]	$x,\bar{x}+1/2,z+1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,\bar{x},\bar{z}$ [ $u,u,0$ ]	$x+1/2,x,\bar{z}+1/2$ [ $u,\bar{u},0$ ]	$\bar{x}+1/2,\bar{x},\bar{z}+1/2$ [ $\bar{u},u,0$ ]								
8	h	..2	$x,x,3/4$ [ $u,u,0$ ]	$\bar{x},\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/4$ [ $u,\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,1/4$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,\bar{x}+1/2,3/4$ [ $u,u,0$ ]	$x+1/2,x+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},1/4$ [ $u,\bar{u},0$ ]	$\bar{x},x,1/4$ [ $\bar{u},u,0$ ]								
8	g	..2	$x,x,1/4$ [ $u,u,0$ ]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,3/4$ [ $u,\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,3/4$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/4$ [ $u,u,0$ ]	$x+1/2,x+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},3/4$ [ $u,\bar{u},0$ ]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]								
8	f	2..	$0,0,z$ [ $0,0,w$ ]	$1/2,1/2,z+1/2$ [ $0,0,\bar{w}$ ]	$1/2,1/2,\bar{z}$ [ $0,0,w$ ]	$0,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,w$ ]	$0,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$0,0,z+1/2$ [ $0,0,w$ ]	$1/2,1/2,z$ [ $0,0,\bar{w}$ ]								
4	e	2.mm	$0,1/2,z$ [ $0,0,0$ ]	$0,1/2,z+1/2$ [ $0,0,0$ ]	$1/2,0,\bar{z}$ [ $0,0,0$ ]	$1/2,0,\bar{z}+1/2$ [ $0,0,0$ ]												
4	d	..2/m	$1/4,1/4,3/4$ [ $u,u,0$ ]	$3/4,3/4,3/4$ [ $\bar{u},\bar{u},0$ ]	$1/4,3/4,1/4$ [ $u,\bar{u},0$ ]	$3/4,1/4,1/4$ [ $\bar{u},u,0$ ]												
4	c	..2/m	$1/4,1/4,1/4$ [ $u,u,0$ ]	$3/4,3/4,1/4$ [ $\bar{u},\bar{u},0$ ]	$1/4,3/4,3/4$ [ $u,\bar{u},0$ ]	$3/4,1/4,3/4$ [ $\bar{u},u,0$ ]												
4	b	$\bar{4}'$ ..	$0,0,0$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]	$0,0,1/2$ [ $0,0,0$ ]												
4	a	2.22	$0,0,1/4$ [ $0,0,0$ ]	$1/2,1/2,3/4$ [ $0,0,0$ ]	$1/2,1/2,1/4$ [ $0,0,0$ ]	$0,0,3/4$ [ $0,0,0$ ]												

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub> 4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 0,0,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,1/4,0

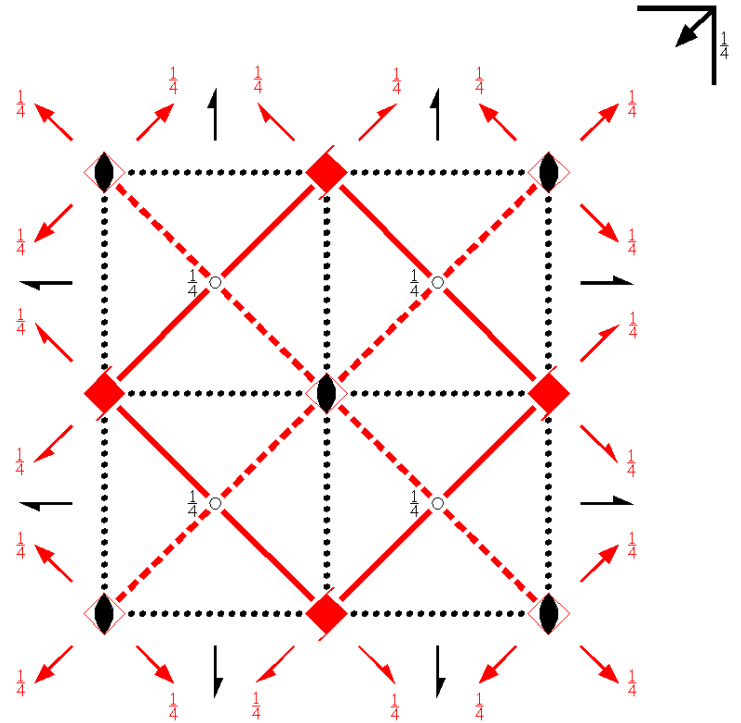
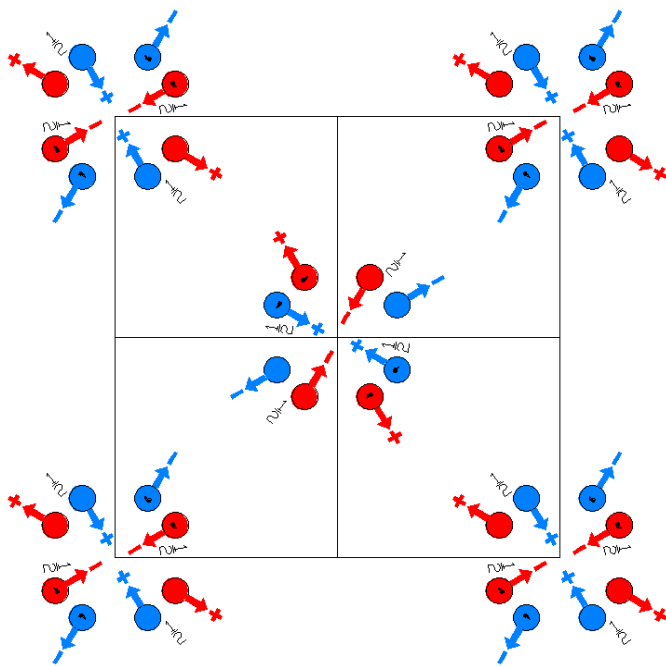
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,x,1/4



$P4_2'/ncm'$   
138.5.1174

$4'/mmm'$   
 $P4_2'/n2_1/c2'/m'$

Tetragonal



Origin at  $\bar{4}'c'$ , at  $-1/4, 1/4, -1/4$  from center ( $2'/m'$ )

Asymmetric unit  $0 \leq x \leq 1/4$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1$ ;  $x \leq y$ ;  $y \leq 1/2 - x$

### Symmetry Operations

- |  |   |  |  |
|--|---|--|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)' | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)' |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0) | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)      | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                          | (8) 2' x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)'           |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2) | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'              | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                            |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)    | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)         | (15) m' x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0)'           | (16) g' (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)'        |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

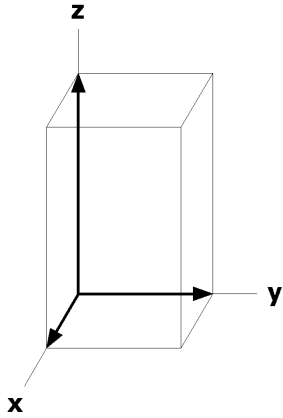
16	j	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,+1/2\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $v,u,w$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $u,v,w$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z$ [ $v,u,w$ ]		
8	i	..m'	$x,x+1/2,z$ [ $u,u,w$ ]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x+1/2,z+1/2$ [ $u,\bar{u},\bar{w}$ ]	$x,\bar{x}+1/2,z+1/2$ [ $\bar{u},u,\bar{w}$ ]
			$\bar{x}+1/2,x,\bar{z}$ [ $\bar{u},u,\bar{w}$ ]	$x+1/2,\bar{x},\bar{z}$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x,\bar{z}+1/2$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,\bar{x},\bar{z}+1/2$ [ $u,u,w$ ]
8	h	..2'	$x,x,3/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},3/4$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,1/4$ [ $u,u,\bar{w}$ ]	$x+1/2,\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x}+1/2,\bar{x}+1/2,3/4$ [ $\bar{u},u,w$ ]	$x+1/2,x+1/2,3/4$ [ $u,\bar{u},w$ ]	$x,\bar{x},1/4$ [ $u,u,\bar{w}$ ]	$\bar{x},x,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	g	..2'	$x,x,1/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,3/4$ [ $u,u,\bar{w}$ ]	$x+1/2,\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x}+1/2,\bar{x}+1/2,1/4$ [ $\bar{u},u,w$ ]	$x+1/2,x+1/2,1/4$ [ $u,\bar{u},w$ ]	$x,\bar{x},3/4$ [ $u,u,\bar{w}$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	f	2..	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0,w]
			1/2,1/2, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2,z [0,0,w]
4	e	2.m'm'	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0,w]
4	d	..2'/m'	1/4,1/4,3/4 [ $\bar{u},u,w$ ]	3/4,3/4,3/4 [ $u,\bar{u},w$ ]	1/4,3/4,1/4 [ $u,u,\bar{w}$ ]	3/4,1/4,1/4 [ $\bar{u},\bar{u},\bar{w}$ ]
4	c	..2'/m'	1/4,1/4,1/4 [ $\bar{u},u,w$ ]	3/4,3/4,1/4 [ $u,\bar{u},w$ ]	1/4,3/4,3/4 [ $u,u,\bar{w}$ ]	3/4,1/4,3/4 [ $\bar{u},\bar{u},\bar{w}$ ]
4	b	$\bar{4}'$ ..	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	0,0,1/2 [0,0,0]
4	a	2.2'2'	0,0,1/4 [0,0,w]	1/2,1/2,3/4 [0,0, $\bar{w}$ ]	1/2,1/2,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p<sub>p</sub>' 4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>' 2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,1/4,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at x,x,1/4



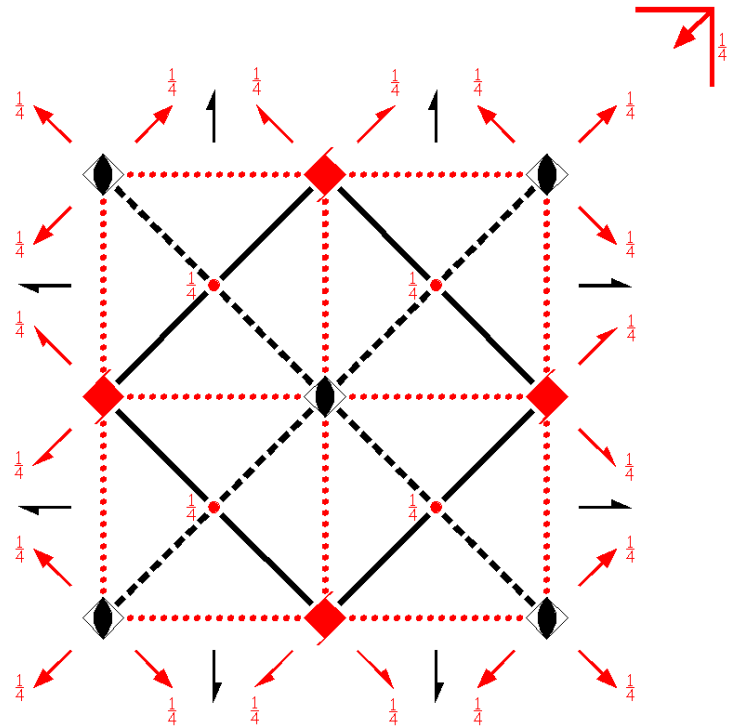
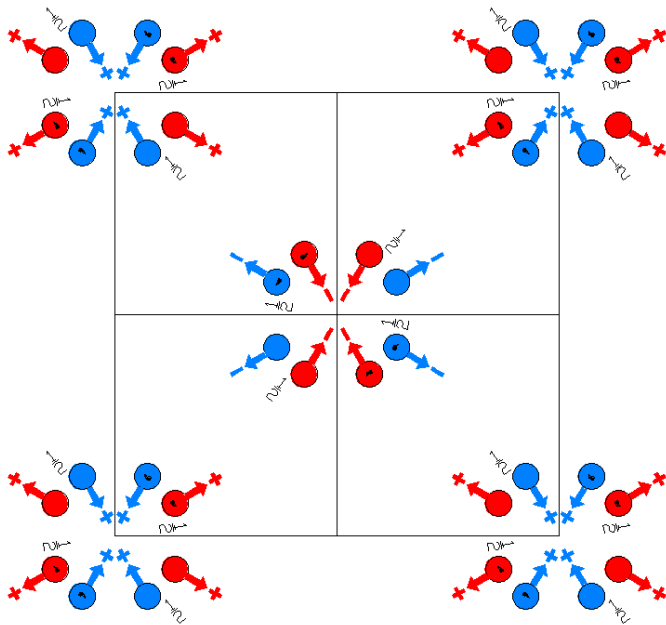
$P4_2/n'c'm$

138.6.1175

$4'/m'm'm$

$P4_2/n'2_1/c'2'/m$

Tetragonal



Origin at  $\bar{4}c'g$ , at  $-1/4, 1/4, -1/4$  from center ( $2'/m$ )

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y; y \leq 1/2 - x$

**Symmetry Operations**

- |  |   |   |  |
|--|---|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                        | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)'                    | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'       |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)     | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)        | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'   | (8) 2' x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)'                 |
| (9) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$ ' 1/2,1/2,1/2)' | (10) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (11) $\bar{4}$ <sup>+</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>+</sup>  0,0,0) | (12) $\bar{4}$ <sup>-</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)'      | (14) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)'         | (15) m x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0)                                | (16) g (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)                |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

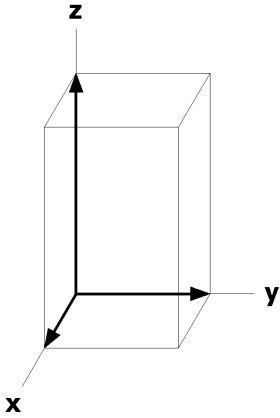
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates															
16	j	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]	(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) $x+1/2,+1/2\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $v,u,w$ ]	(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]	(13) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]	(15) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $v,u,\bar{w}$ ]	(16) $y+1/2,x+1/2,z$ [ $\bar{v},\bar{u},\bar{w}$ ]
8	i	..m	$x,x+1/2,z$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}+1/2,z$ [ $u,\bar{u},0$ ]	$\bar{x},x+1/2,z+1/2$ [ $u,u,0$ ]	$x,\bar{x}+1/2,z+1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,\bar{z}$ [ $u,u,0$ ]	$x+1/2,\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x,\bar{z}+1/2$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,\bar{x},\bar{z}+1/2$ [ $u,\bar{u},0$ ]								
8	h	..2'	$x,x,3/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},3/4$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,1/4$ [ $u,u,\bar{w}$ ]	$x+1/2,\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	$\bar{x}+1/2,\bar{x}+1/2,3/4$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x+1/2,3/4$ [ $\bar{u},u,\bar{w}$ ]	$x,\bar{x},1/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,1/4$ [ $u,u,w$ ]								
8	g	..2'	$x,x,1/4$ [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [ $u,\bar{u},w$ ]	$\bar{x}+1/2,x+1/2,3/4$ [ $u,u,\bar{w}$ ]	$x+1/2,\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	$\bar{x}+1/2,\bar{x}+1/2,1/4$ [ $u,\bar{u},\bar{w}$ ]	$x+1/2,x+1/2,1/4$ [ $\bar{u},u,\bar{w}$ ]	$x,\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,3/4$ [ $u,u,w$ ]								
8	f	2..	$0,0,z$ [ $0,0,w$ ]	$1/2,1/2,z+1/2$ [ $0,0,\bar{w}$ ]	$1/2,1/2,\bar{z}$ [ $0,0,\bar{w}$ ]	$0,0,\bar{z}+1/2$ [ $0,0,w$ ]	$1/2,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,0,\bar{z}$ [ $0,0,w$ ]	$0,0,z+1/2$ [ $0,0,w$ ]	$1/2,1/2,z$ [ $0,0,\bar{w}$ ]								
4	e	2.mm	$0,1/2,z$ [ $0,0,0$ ]	$0,1/2,z+1/2$ [ $0,0,0$ ]	$1/2,0,\bar{z}$ [ $0,0,0$ ]	$1/2,0,\bar{z}+1/2$ [ $0,0,0$ ]												
4	d	..2'/m	$1/4,1/4,3/4$ [ $0,0,0$ ]	$3/4,3/4,3/4$ [ $0,0,0$ ]	$1/4,3/4,1/4$ [ $0,0,0$ ]	$3/4,1/4,1/4$ [ $0,0,0$ ]												
4	c	..2'/m	$1/4,1/4,1/4$ [ $0,0,0$ ]	$3/4,3/4,1/4$ [ $0,0,0$ ]	$1/4,3/4,3/4$ [ $0,0,0$ ]	$3/4,1/4,3/4$ [ $0,0,0$ ]												
4	b	$\bar{4}$ ..	$0,0,0$ [ $0,0,w$ ]	$1/2,1/2,1/2$ [ $0,0,\bar{w}$ ]	$1/2,1/2,0$ [ $0,0,\bar{w}$ ]	$0,0,1/2$ [ $0,0,w$ ]												
4	a	2.2'2'	$0,0,1/4$ [ $0,0,w$ ]	$1/2,1/2,3/4$ [ $0,0,\bar{w}$ ]	$1/2,1/2,1/4$ [ $0,0,\bar{w}$ ]	$0,0,3/4$ [ $0,0,w$ ]												

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4'mm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at  $x,1/4,0$

Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,x,1/4$



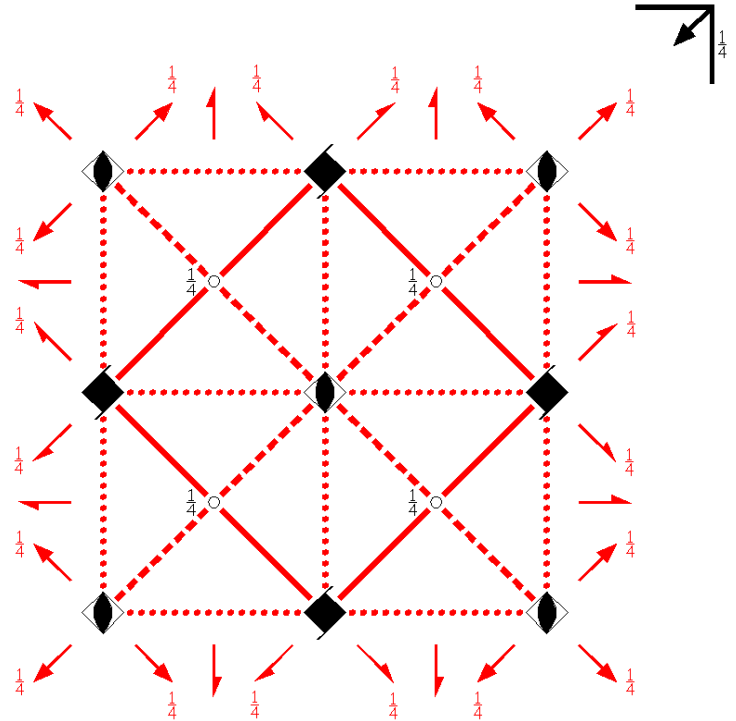
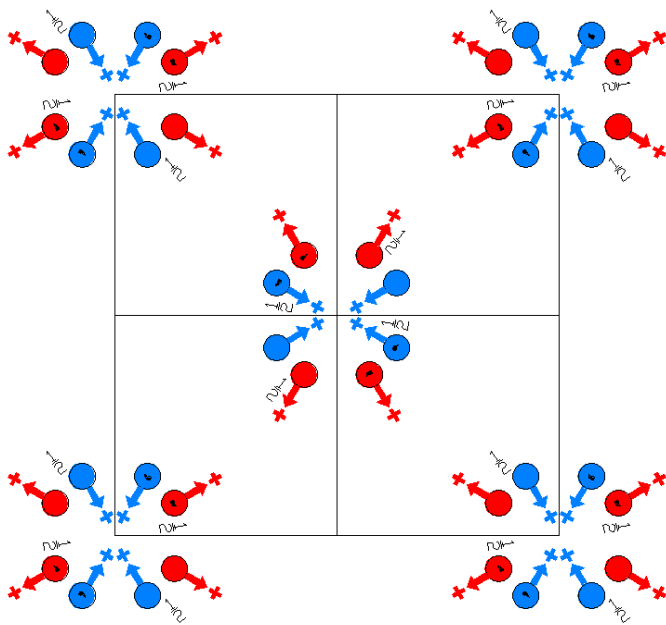
$P4_2/nc'm'$

138.7.1176

$4/mm'm'$

$P4_2/n2_1'/c'2'/m'$

Tetragonal



Origin at  $\bar{4}c'g'$ , at  $-1/4, 1/4, -1/4$  from center ( $2'/m'$ )

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y; y \leq 1/2 - x$

### Symmetry Operations

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                      | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)' | (6) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)'    | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                         | (8) 2' x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)'          |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)   | (10) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)                | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)                         |
| (13) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)'    | (14) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)'       | (15) m' x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0)'          | (16) g' (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)'       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

16	j	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$		
			(3) $\bar{y}+1/2,x+1/2,z+1/2 [\bar{v},u,w]$	(4) $y+1/2,\bar{x}+1/2,z+1/2 [v,\bar{u},w]$		
			(5) $\bar{x}+1/2,y+1/2,\bar{z} [u,\bar{v},w]$	(6) $x+1/2,+1/2 \bar{y},\bar{z} [\bar{u},v,w]$		
			(7) $y,x,\bar{z}+1/2 [\bar{v},\bar{u},w]$	(8) $\bar{y},\bar{x},\bar{z}+1/2 [v,u,w]$		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2 [u,v,w]$	(10) $x+1/2,y+1/2,\bar{z}+1/2 [\bar{u},\bar{v},w]$		
			(11) $y,\bar{x},\bar{z} [\bar{v},u,w]$	(12) $\bar{y},x,\bar{z} [v,\bar{u},w]$		
			(13) $x,\bar{y},z+1/2 [u,\bar{v},w]$	(14) $\bar{x},y,z+1/2 [\bar{u},v,w]$		
			(15) $\bar{y}+1/2,\bar{x}+1/2,z [\bar{v},\bar{u},w]$	(16) $y+1/2,x+1/2,z [v,u,w]$		
8	i	..m'	$x,x+1/2,z [u,u,w]$	$\bar{x},\bar{x}+1/2,z [\bar{u},\bar{u},w]$	$\bar{x},x+1/2,z+1/2 [\bar{u},u,w]$	$x,\bar{x}+1/2,z+1/2 [u,\bar{u},w]$
			$\bar{x}+1/2,x,\bar{z} [u,\bar{u},w]$	$x+1/2,\bar{x},\bar{z} [\bar{u},u,w]$	$x+1/2,x,\bar{z}+1/2 [\bar{u},\bar{u},w]$	$\bar{x}+1/2,\bar{x},\bar{z}+1/2 [u,u,w]$
8	h	..2'	$x,x,3/4 [\bar{u},u,w]$	$\bar{x},\bar{x},3/4 [u,\bar{u},w]$	$\bar{x}+1/2,x+1/2,1/4 [\bar{u},\bar{u},w]$	$x+1/2,\bar{x}+1/2,1/4 [u,u,w]$
			$\bar{x}+1/2,\bar{x}+1/2,3/4 [\bar{u},u,w]$	$x+1/2,x+1/2,3/4 [u,\bar{u},w]$	$x,\bar{x},1/4 [\bar{u},\bar{u},w]$	$\bar{x},x,1/4 [u,u,w]$
8	g	..2'	$x,x,1/4 [\bar{u},u,w]$	$\bar{x},\bar{x},1/4 [u,\bar{u},w]$	$\bar{x}+1/2,x+1/2,3/4 [\bar{u},\bar{u},w]$	$x+1/2,\bar{x}+1/2,3/4 [u,u,w]$
			$\bar{x}+1/2,\bar{x}+1/2,1/4 [\bar{u},u,w]$	$x+1/2,x+1/2,1/4 [u,\bar{u},w]$	$x,\bar{x},3/4 [\bar{u},\bar{u},w]$	$\bar{x},x,3/4 [u,u,w]$
8	f	2..	0,0,z [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]
			1/2,1/2, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0,w]	1/2,1/2,z [0,0,w]
4	e	2.m'm'	0,1/2,z [0,0,w]	0,1/2,z+1/2 [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]
4	d	..2'/m'	1/4,1/4,3/4 [ $\bar{u},u,w$ ]	3/4,3/4,3/4 [ $u,\bar{u},w$ ]	1/4,3/4,1/4 [ $\bar{u},\bar{u},w$ ]	3/4,1/4,1/4 [ $u,u,w$ ]
4	c	..2'/m'	1/4,1/4,1/4 [ $\bar{u},u,w$ ]	3/4,3/4,1/4 [ $u,\bar{u},w$ ]	1/4,3/4,3/4 [ $\bar{u},\bar{u},w$ ]	3/4,1/4,3/4 [ $u,u,w$ ]
4	b	$\bar{4}$ ..	0,0,0 [0,0,w]	1/2,1/2,1/2 [0,0,w]	1/2,1/2,0 [0,0,w]	0,0,1/2 [0,0,w]
4	a	2.2'2'	0,0,1/4 [0,0,w]	1/2,1/2,3/4 [0,0,w]	1/2,1/2,1/4 [0,0,w]	0,0,3/4 [0,0,w]

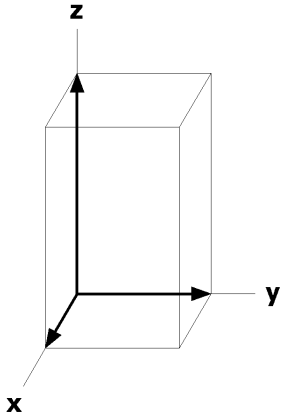
**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_4m'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mg$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at  $x,1/4,0$

Along  $[1,1,0]$   $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at  $x,x,1/4$





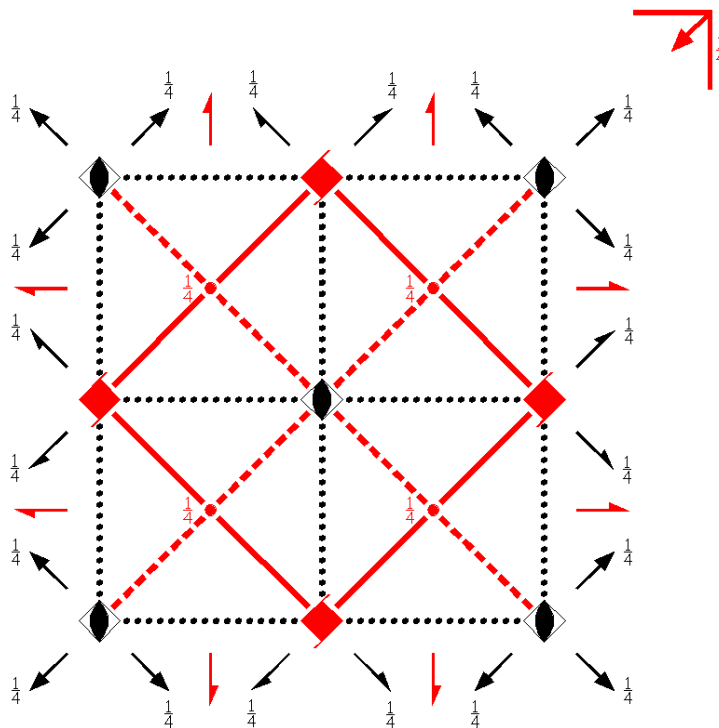
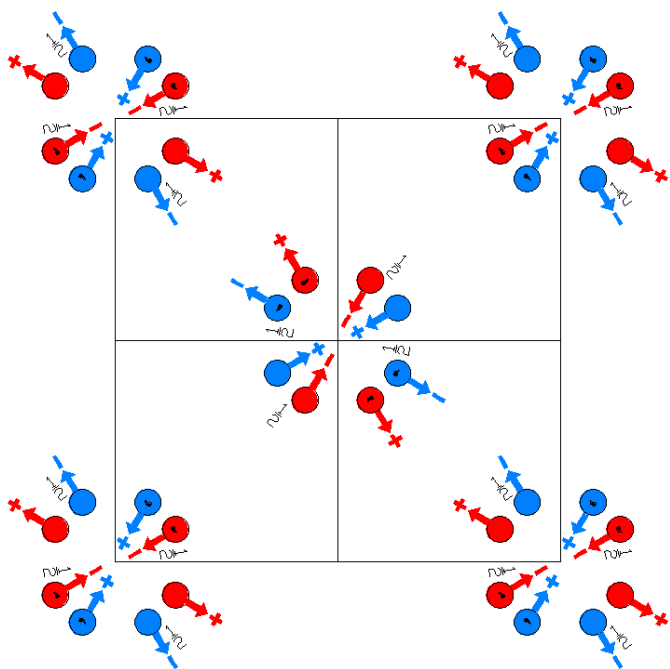
$P4_2'n'cm'$

138.8.1177

$4'/m'mm'$

$P4_2'n'2_1'/c2/m'$

Tetragonal



Origin at  $\bar{4}cg'$ , at  $-1/4, 1/4, -1/4$  from center ( $2/m'$ )

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y; y \leq 1/2 - x$

**Symmetry Operations**

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                        | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)'       | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'       |
| (5) 2' (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)'  | (6) 2' (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)'      | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                                  | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)                   |
| (9) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)' | (10) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (11) $\bar{4}$ <sup>+</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub>  0,0,0) | (12) $\bar{4}$ <sup>-</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)       | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)           | (15) m' x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0)'                 | (16) g' (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)'              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

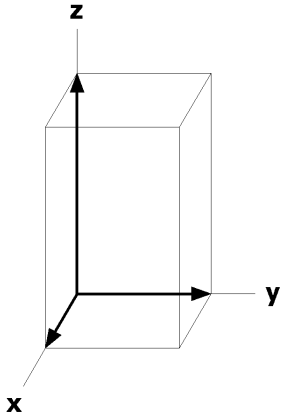
16	j	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y}+1/2,x+1/2,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x}+1/2,y+1/2,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) $x+1/2,+1/2\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]		
			(7) $y,x,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x+1/2,y+1/2,\bar{z}+1/2$ [ $u,v,\bar{w}$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]		
			(13) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y}+1/2,\bar{x}+1/2,z$ [ $\bar{v},\bar{u},w$ ]	(16) $y+1/2,x+1/2,z$ [ $v,u,w$ ]		
8	i	..m'	$x,x+1/2,z$ [ $u,u,w$ ]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x+1/2,z+1/2$ [ $u,\bar{u},\bar{w}$ ]	$x,\bar{x}+1/2,z+1/2$ [ $\bar{u},u,\bar{w}$ ]
			$\bar{x}+1/2,x,\bar{z}$ [ $u,\bar{u},w$ ]	$x+1/2,\bar{x},\bar{z}$ [ $\bar{u},u,w$ ]	$x+1/2,x,\bar{z}+1/2$ [ $u,\bar{u},\bar{w}$ ]	$\bar{x}+1/2,\bar{x},\bar{z}+1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	h	..2	$x,x,3/4$ [ $u,u,0$ ]	$\bar{x},\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,1/4$ [ $u,\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,1/4$ [ $\bar{u},u,0$ ]
			$\bar{x}+1/2,\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x+1/2,3/4$ [ $u,u,0$ ]	$x,\bar{x},1/4$ [ $\bar{u},u,0$ ]	$\bar{x},x,1/4$ [ $u,\bar{u},0$ ]
8	g	..2	$x,x,1/4$ [ $u,u,0$ ]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x+1/2,3/4$ [ $u,\bar{u},0$ ]	$x+1/2,\bar{x}+1/2,3/4$ [ $\bar{u},u,0$ ]
			$\bar{x}+1/2,\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$x+1/2,x+1/2,1/4$ [ $u,u,0$ ]	$x,\bar{x},3/4$ [ $\bar{u},u,0$ ]	$\bar{x},x,3/4$ [ $u,\bar{u},0$ ]
8	f	2..	$0,0,z$ [ $0,0,w$ ]	$1/2,1/2,z+1/2$ [ $0,0,\bar{w}$ ]	$1/2,1/2,\bar{z}$ [ $0,0,w$ ]	$0,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]
			$1/2,1/2,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,0,\bar{z}$ [ $0,0,w$ ]	$0,0,z+1/2$ [ $0,0,\bar{w}$ ]	$1/2,1/2,z$ [ $0,0,w$ ]
4	e	2.m'm'	$0,1/2,z$ [ $0,0,w$ ]	$0,1/2,z+1/2$ [ $0,0,\bar{w}$ ]	$1/2,0,\bar{z}$ [ $0,0,w$ ]	$1/2,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]
4	d	..2/m'	$1/4,1/4,3/4$ [ $0,0,0$ ]	$3/4,3/4,3/4$ [ $0,0,0$ ]	$1/4,3/4,1/4$ [ $0,0,0$ ]	$3/4,1/4,1/4$ [ $0,0,0$ ]
4	c	..2/m'	$1/4,1/4,1/4$ [ $0,0,0$ ]	$3/4,3/4,1/4$ [ $0,0,0$ ]	$1/4,3/4,3/4$ [ $0,0,0$ ]	$3/4,1/4,3/4$ [ $0,0,0$ ]
4	b	$\bar{4}$ ..	$0,0,0$ [ $0,0,w$ ]	$1/2,1/2,1/2$ [ $0,0,\bar{w}$ ]	$1/2,1/2,0$ [ $0,0,w$ ]	$0,0,1/2$ [ $0,0,\bar{w}$ ]
4	a	2.22	$0,0,1/4$ [ $0,0,0$ ]	$1/2,1/2,3/4$ [ $0,0,0$ ]	$1/2,1/2,1/4$ [ $0,0,0$ ]	$0,0,3/4$ [ $0,0,0$ ]

**Symmetry of Special Projections**

Along [0,0,1] p4'm'm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>' 2m'g'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,1/4

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



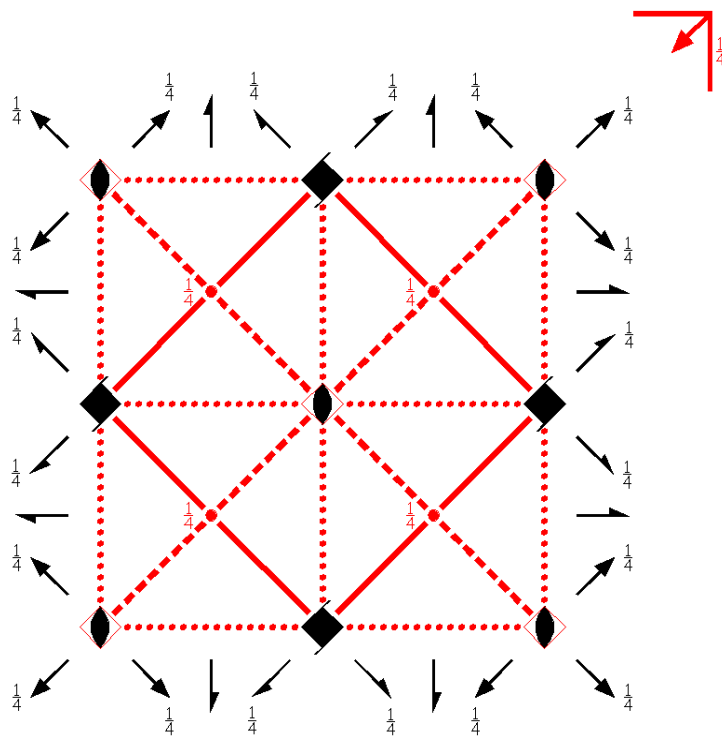
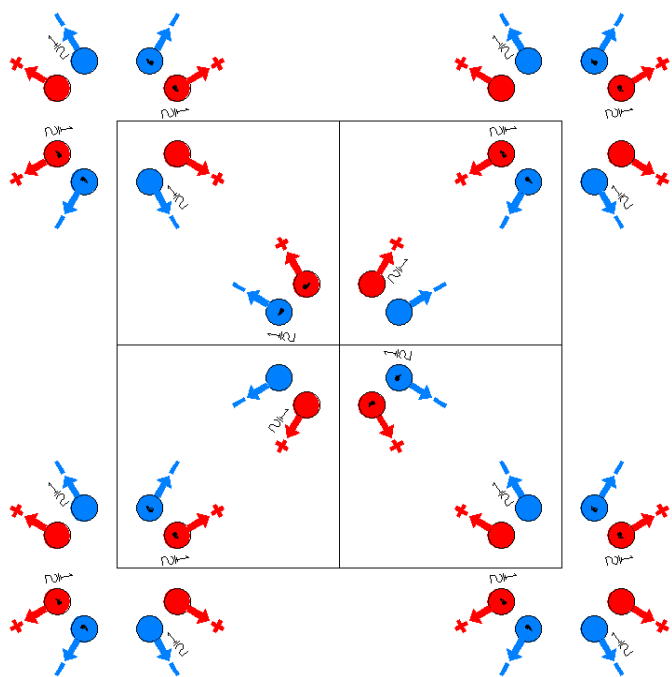
$P4_2/n'c'm'$

138.9.1178

$4/m'm'm'$

$P4_2/n'2_1/c'2/m'$

Tetragonal



Origin at  $\bar{4}'c'g'$ , at  $-1/4, 1/4, -1/4$  from center ( $2/m'$ )

Asymmetric unit  $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y; y \leq 1/2 - x$

### Symmetry Operations

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                        | (3) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2) | (4) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2) |
| (5) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)   | (6) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)        | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                           | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)            |
| (9) $\bar{1}'$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)' | (10) n' (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)' | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)'               | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)'                        |
| (13) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)'    | (14) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)'         | (15) m' x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0)'          | (16) g' (1/2,1/2,0) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  1/2,1/2,0)'       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

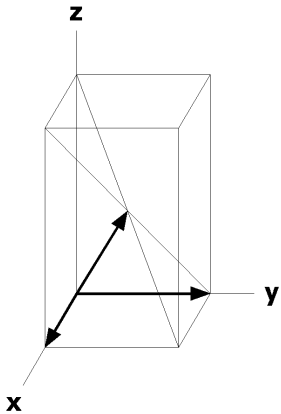
16	j	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$		
			(3) $\bar{y}+1/2,x+1/2,z+1/2 [\bar{v},u,w]$	(4) $y+1/2,\bar{x}+1/2,z+1/2 [v,\bar{u},w]$		
			(5) $\bar{x}+1/2,y+1/2,\bar{z} [\bar{u},v,\bar{w}]$	(6) $x+1/2,+1/2 \bar{y},\bar{z} [u,\bar{v},\bar{w}]$		
			(7) $y,x,\bar{z}+1/2 [v,u,\bar{w}]$	(8) $\bar{y},\bar{x},\bar{z}+1/2 [\bar{v},\bar{u},\bar{w}]$		
			(9) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2 [\bar{u},\bar{v},\bar{w}]$	(10) $x+1/2,y+1/2,\bar{z}+1/2 [u,v,\bar{w}]$		
			(11) $y,\bar{x},\bar{z} [v,\bar{u},\bar{w}]$	(12) $\bar{y},x,\bar{z} [\bar{v},u,\bar{w}]$		
			(13) $x,\bar{y},z+1/2 [u,\bar{v},w]$	(14) $\bar{x},y,z+1/2 [\bar{u},v,w]$		
			(15) $\bar{y}+1/2,\bar{x}+1/2,z [\bar{v},\bar{u},w]$	(16) $y+1/2,x+1/2,z [v,u,w]$		
8	i	..m'	$x,x+1/2,z [u,u,w]$	$\bar{x},\bar{x}+1/2,z [\bar{u},\bar{u},w]$	$\bar{x},x+1/2,z+1/2 [\bar{u},u,w]$	$x,\bar{x}+1/2,z+1/2 [u,\bar{u},w]$
			$\bar{x}+1/2,x,\bar{z} [\bar{u},u,\bar{w}]$	$x+1/2,\bar{x},\bar{z} [u,\bar{u},\bar{w}]$	$x+1/2,x,\bar{z}+1/2 [u,u,\bar{w}]$	$\bar{x}+1/2,\bar{x},\bar{z}+1/2 [\bar{u},\bar{u},\bar{w}]$
8	h	..2	$x,x,3/4 [u,u,0]$	$\bar{x},\bar{x},3/4 [\bar{u},\bar{u},0]$	$\bar{x}+1/2,x+1/2,1/4 [\bar{u},u,0]$	$x+1/2,\bar{x}+1/2,1/4 [u,\bar{u},0]$
			$\bar{x}+1/2,\bar{x}+1/2,3/4 [\bar{u},\bar{u},0]$	$x+1/2,x+1/2,3/4 [u,u,0]$	$x,\bar{x},1/4 [u,\bar{u},0]$	$\bar{x},x,1/4 [\bar{u},u,0]$
8	g	..2	$x,x,1/4 [u,u,0]$	$\bar{x},\bar{x},1/4 [\bar{u},\bar{u},0]$	$\bar{x}+1/2,x+1/2,3/4 [\bar{u},u,0]$	$x+1/2,\bar{x}+1/2,3/4 [u,\bar{u},0]$
			$\bar{x}+1/2,\bar{x}+1/2,1/4 [\bar{u},\bar{u},0]$	$x+1/2,x+1/2,1/4 [u,u,0]$	$x,\bar{x},3/4 [u,\bar{u},0]$	$\bar{x},x,3/4 [\bar{u},u,0]$
8	f	2..	$0,0,z [0,0,w]$	$1/2,1/2,z+1/2 [0,0,w]$	$1/2,1/2,\bar{z} [0,0,\bar{w}]$	$0,0,\bar{z}+1/2 [0,0,\bar{w}]$
			$1/2,1/2,\bar{z}+1/2 [0,0,\bar{w}]$	$0,0,\bar{z} [0,0,\bar{w}]$	$0,0,z+1/2 [0,0,w]$	$1/2,1/2,z [0,0,w]$
4	e	2.m'm'	$0,1/2,z [0,0,w]$	$0,1/2,z+1/2 [0,0,w]$	$1/2,0,\bar{z} [0,0,\bar{w}]$	$1/2,0,\bar{z}+1/2 [0,0,\bar{w}]$
4	d	..2/m'	$1/4,1/4,3/4 [0,0,0]$	$3/4,3/4,3/4 [0,0,0]$	$1/4,3/4,1/4 [0,0,0]$	$3/4,1/4,1/4 [0,0,0]$
4	c	..2/m'	$1/4,1/4,1/4 [0,0,0]$	$3/4,3/4,1/4 [0,0,0]$	$1/4,3/4,3/4 [0,0,0]$	$3/4,1/4,3/4 [0,0,0]$
4	b	$\bar{4}'..$	$0,0,0 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$	$1/2,1/2,0 [0,0,0]$	$0,0,1/2 [0,0,0]$
4	a	2.22	$0,0,1/4 [0,0,0]$	$1/2,1/2,3/4 [0,0,0]$	$1/2,1/2,1/4 [0,0,0]$	$0,0,3/4 [0,0,0]$

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'g'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at  $x,1/4,0$

Along  $[1,1,0]$   $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,x,1/4$



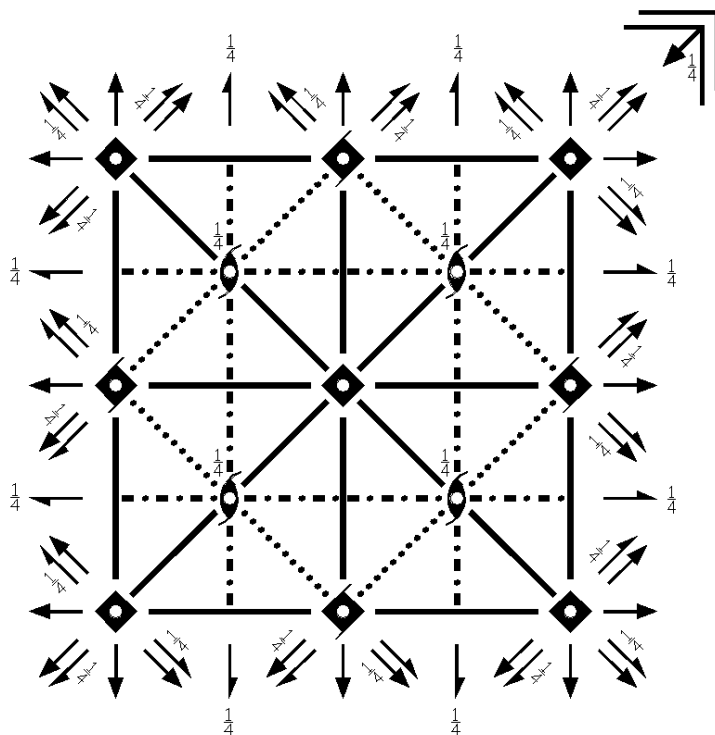
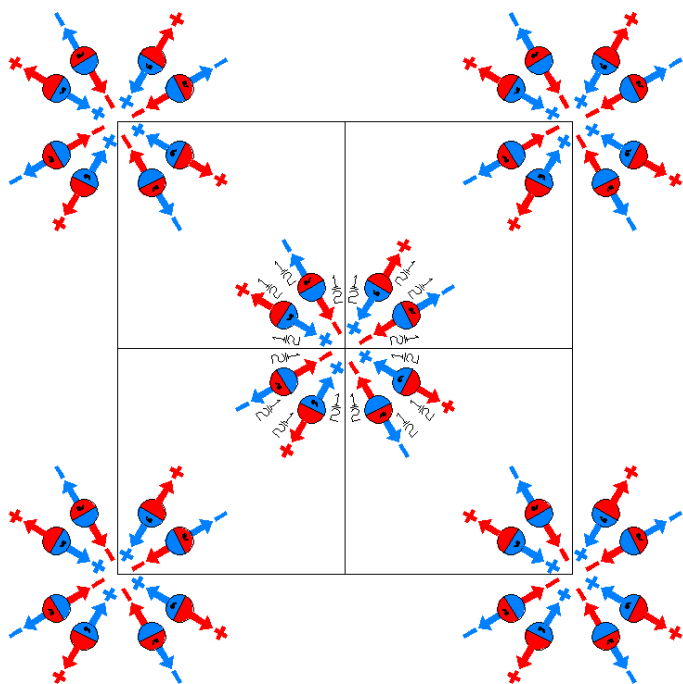
I4/mmm

139.1.1179

4/mmm

I4/m2/m2/m

Tetragonal



Origin at center ( 4/mmm )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; x \leq y$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                      | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)         |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                  | (8) 2 x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)                                 |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)              | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (15) m x,x̄,z<br>(m <sub>xȳ</sub>  0,0,0)                               | (16) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                                  |

## For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)	(4) $4^-$ (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)
(5) $2$ (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>   1/2,1/2,1/2)	(6) $2$ (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>   1/2,1/2,1/2)	(7) $2$ (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)	(8) $2$ x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)
(9) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)	(10) $n$ (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$   1/2,1/2,1/2)
(13) $n$ (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)	(14) $n$ (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)	(15) $c$ (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,1/2)	(16) $n$ (1/2,1/2,1/2) x,x,z (m <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1/2,1/2,1/2) +		
32	o	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [v, $\bar{u},w$ ]
			(13) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ]	(16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
16	n	.m.	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},0,z$ [0,u,0]	y,0,z [0, $\bar{u},0$ ]
			0,y, $\bar{z}$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]	y,0, $\bar{z}$ [0,u,0]	$\bar{y},0,\bar{z}$ [0, $\bar{u},0$ ]
16	m	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [u, $\bar{u},0$ ]	$\bar{x},x,z$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},z$ [u,u,0]
			$\bar{x},x,\bar{z}$ [u,u,0]	x, $\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]	x,x, $\bar{z}$ [u, $\bar{u},0$ ]	$\bar{x},\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]
16	l	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0,w]	y, $\bar{x},0$ [0,0,w]
			$\bar{x},y,0$ [0,0, $\bar{w}$ ]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]	y,x,0 [0,0, $\bar{w}$ ]	$\bar{y},\bar{x},0$ [0,0, $\bar{w}$ ]
16	k	..2	x,x+1/2,1/4 [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},u,0$ ]	x+1/2, $\bar{x},1/4$ [u, $\bar{u},0$ ]
			$\bar{x},\bar{x}+1/2,3/4$ [u,u,0]	x,x+1/2,3/4 [ $\bar{u},\bar{u},0$ ]	x+1/2, $\bar{x},3/4$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,x,3/4$ [u, $\bar{u},0$ ]
8	j	m2m.	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]	1/2,x,0 [0,0,0]	1/2, $\bar{x},0$ [0,0,0]
8	i	m2m.	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x},0$ [0,0,0]
8	h	m.2m	x,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x},x,0$ [0,0,0]	x, $\bar{x},0$ [0,0,0]
8	g	2mm.	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]
8	f	..2/m	1/4,1/4,1/4 [ $\bar{u},u,0$ ]	3/4,3/4,1/4 [u, $\bar{u},0$ ]	3/4,1/4,1/4 [ $\bar{u},\bar{u},0$ ]	1/4,3/4,1/4 [u,u,0]



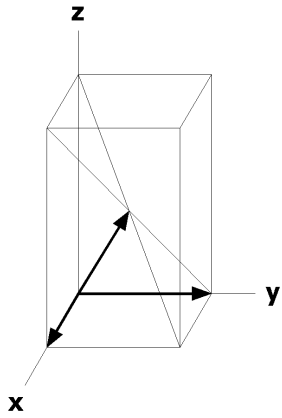
4	e	4mm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	d	$\bar{4}m2$	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	c	mmm.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]
2	b	4/mmm	0,0,1/2 [0,0,0]	
2	a	4/mmm	0,0,0 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



I4/mmm1'

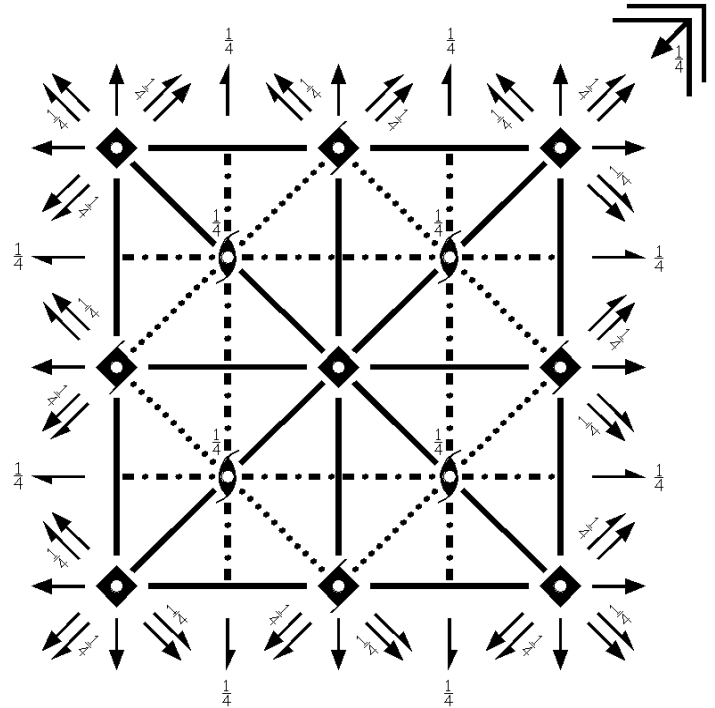
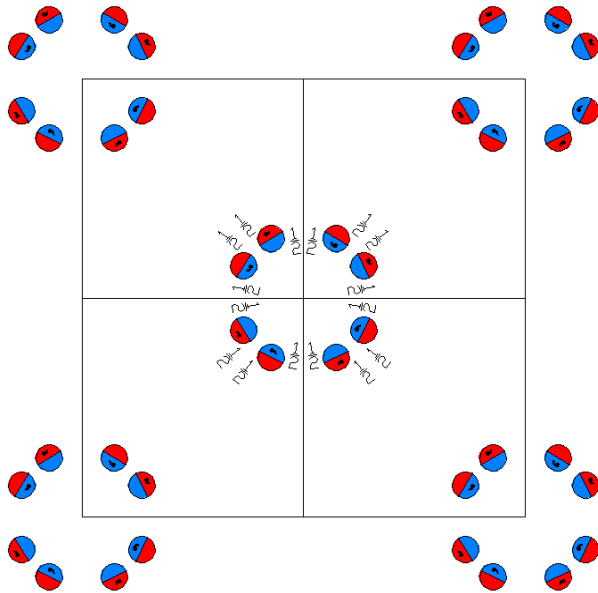
139.2.1180

4/mmm1'

I4/m2/m2/m1'

Tetragonal

1'



Origin at center ( 4/mmm1' )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad x \leq y$

Symmetry Operations

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                      | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)         |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                  | (8) 2 x,x̄,0<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,0)                    |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)              | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (15) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                                | (16) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                                  |

## For (1/2,1/2,1/2) + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t$ (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)                     | (2) $2$ (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2)  | (3) $4^+$ (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>   1/2,1/2,1/2)             | (4) $4^-$ (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)         |
| (5) $2$ (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,1/2,1/2)  | (6) $2$ (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>   1/2,1/2,1/2)  | (7) $2$ (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>   1/2,1/2,1/2)            | (8) $2$ x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2) |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$   1/2,1/2,1/2)        | (10) $n$ (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>   1/2,1/2,1/2) | (11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$   1/2,1/2,1/2)     | (12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$   1/2,1/2,1/2)               |
| (13) $n$ (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,1/2) | (14) $n$ (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,1/2) | (15) $c$ (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>   1/2,1/2,1/2) | (16) $n$ (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)  |

## For (0,0,0)' + set

- |   |  |   |   |
|---|--|---|---|
| (1) $1'$<br>(1   0,0,0)'                      | (2) $2'$ 0,0,z<br>(2 <sub>z</sub>   0,0,0)'  | (3) $4^{+'}$ 0,0,z<br>(4 <sub>z</sub>   0,0,0)'               | (4) $4^{-'}$ 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>   0,0,0)'             |
| (5) $2'$ 0,y,0<br>(2 <sub>y</sub>   0,0,0)'   | (6) $2'$ x,0,0<br>(2 <sub>x</sub>   0,0,0)'  | (7) $2'$ x,x,0<br>(2 <sub>xy</sub>   0,0,0)'                  | (8) $2'$ x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>   0,0,0)' |
| (9) $\bar{1}'$ 0,0,0<br>( $\bar{1}$   0,0,0)' | (10) $m'$ x,y,0<br>(m <sub>z</sub>   0,0,0)' | (11) $\bar{4}^{+'}$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$   0,0,0)' | (12) $\bar{4}^{-'}$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$   0,0,0)'             |
| (13) $m'$ x,0,z<br>(m <sub>y</sub>   0,0,0)'  | (14) $m'$ 0,y,z<br>(m <sub>x</sub>   0,0,0)' | (15) $m'$ x, $\bar{x}$ ,z<br>(m <sub>xy</sub>   0,0,0)'       | (16) $m'$ x,x,z<br>(m <sub><math>\bar{xy}</math></sub>   0,0,0)'          |

## For (1/2,1/2,1/2)' + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t'$ (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)'                     | (2) $2'$ (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2)'  | (3) $4^{+'}$ (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>   1/2,1/2,1/2)'           | (4) $4^{-'}$ (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)'       |
| (5) $2'$ (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,1/2,1/2)'  | (6) $2'$ (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>   1/2,1/2,1/2)'  | (7) $2'$ (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>   1/2,1/2,1/2)'            | (8) $2'$ x, $\bar{x}$ +1/2,1/4<br>(2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)' |
| (9) $\bar{1}'$ 1/4,1/4,1/4<br>( $\bar{1}$   1/2,1/2,1/2)'        | (10) $n'$ (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>   1/2,1/2,1/2)' | (11) $\bar{4}^{+'}$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z^+$   1/2,1/2,1/2)'   | (12) $\bar{4}^{-'}$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^-$   1/2,1/2,1/2)'             |
| (13) $n'$ (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,1/2)' | (14) $n'$ (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,1/2)' | (15) $c'$ (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>   1/2,1/2,1/2)' | (16) $n'$ (1/2,1/2,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)'  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

(0,0,0) + (1/2,1/2,1/2) +  
(0,0,0)' + (1/2,1/2,1/2)' +

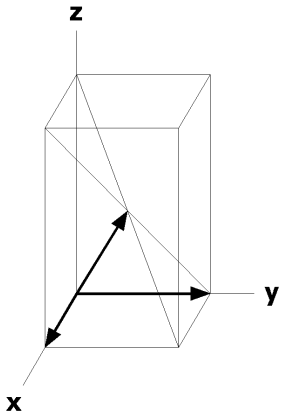
32	o	11'	(1) $x,y,z [0,0,0]$	(2) $\bar{x},\bar{y},z [0,0,0]$	(3) $\bar{y},x,z [0,0,0]$	(4) $y,\bar{x},z [0,0,0]$
			(5) $\bar{x},y,\bar{z} [0,0,0]$	(6) $x,\bar{y},\bar{z} [0,0,0]$	(7) $y,x,\bar{z} [0,0,0]$	(8) $\bar{y},\bar{x},\bar{z} [0,0,0]$
			(9) $\bar{x},\bar{y},\bar{z} [0,0,0]$	(10) $x,y,\bar{z} [0,0,0]$	(11) $y,\bar{x},\bar{z} [0,0,0]$	(12) $\bar{y},x,\bar{z} [0,0,0]$
			(13) $x,\bar{y},z [0,0,0]$	(14) $\bar{x},\bar{y},z [0,0,0]$	(15) $\bar{y},\bar{x},z [0,0,0]$	(16) $y,x,z [0,0,0]$
16	n	.m.1'	$0,y,z [0,0,0]$	$0,\bar{y},z [0,0,0]$	$\bar{y},0,z [0,0,0]$	$y,0,z [0,0,0]$
			$0,y,\bar{z} [0,0,0]$	$0,\bar{y},\bar{z} [0,0,0]$	$y,0,\bar{z} [0,0,0]$	$\bar{y},0,\bar{z} [0,0,0]$
16	m	..m1'	$x,x,z [0,0,0]$	$\bar{x},\bar{x},z [0,0,0]$	$\bar{x},x,z [0,0,0]$	$x,\bar{x},z [0,0,0]$
			$\bar{x},x,\bar{z} [0,0,0]$	$x,\bar{x},\bar{z} [0,0,0]$	$x,x,\bar{z} [0,0,0]$	$\bar{x},\bar{x},\bar{z} [0,0,0]$
16	l	m..1'	$x,y,0 [0,0,0]$	$\bar{x},\bar{y},0 [0,0,0]$	$\bar{y},x,0 [0,0,0]$	$y,\bar{x},0 [0,0,0]$
			$\bar{x},y,0 [0,0,0]$	$x,\bar{y},0 [0,0,0]$	$y,x,0 [0,0,0]$	$\bar{y},\bar{x},0 [0,0,0]$
16	k	..21'	$x,x+1/2,1/4 [0,0,0]$	$\bar{x},\bar{x}+1/2,1/4 [0,0,0]$	$\bar{x}+1/2,x,1/4 [0,0,0]$	$x+1/2,\bar{x},1/4 [0,0,0]$
			$\bar{x},\bar{x}+1/2,3/4 [0,0,0]$	$x,x+1/2,3/4 [0,0,0]$	$x+1/2,\bar{x},3/4 [0,0,0]$	$\bar{x}+1/2,x,3/4 [0,0,0]$
8	j	m2m.1'	$x,1/2,0 [0,0,0]$	$\bar{x},1/2,0 [0,0,0]$	$1/2,x,0 [0,0,0]$	$1/2,\bar{x},0 [0,0,0]$
8	i	m2m.1'	$x,0,0 [0,0,0]$	$\bar{x},0,0 [0,0,0]$	$0,x,0 [0,0,0]$	$0,\bar{x},0 [0,0,0]$
8	h	m.2m1'	$x,x,0 [0,0,0]$	$\bar{x},\bar{x},0 [0,0,0]$	$\bar{x},x,0 [0,0,0]$	$x,\bar{x},0 [0,0,0]$
8	g	2mm.1'	$0,1/2,z [0,0,0]$	$1/2,0,z [0,0,0]$	$0,1/2,\bar{z} [0,0,0]$	$1/2,0,\bar{z} [0,0,0]$
8	f	..2/m1'	$1/4,1/4,1/4 [0,0,0]$	$3/4,3/4,1/4 [0,0,0]$	$3/4,1/4,1/4 [0,0,0]$	$1/4,3/4,1/4 [0,0,0]$
4	e	4mm1'	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$		
4	d	$\bar{4}m21'$	$0,1/2,1/4 [0,0,0]$	$1/2,0,1/4 [0,0,0]$		
4	c	mmm.1'	$0,1/2,0 [0,0,0]$	$1/2,0,0 [0,0,0]$		
2	b	4/mmm1'	$0,0,1/2 [0,0,0]$			
2	a	4/mmm1'	$0,0,0 [0,0,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

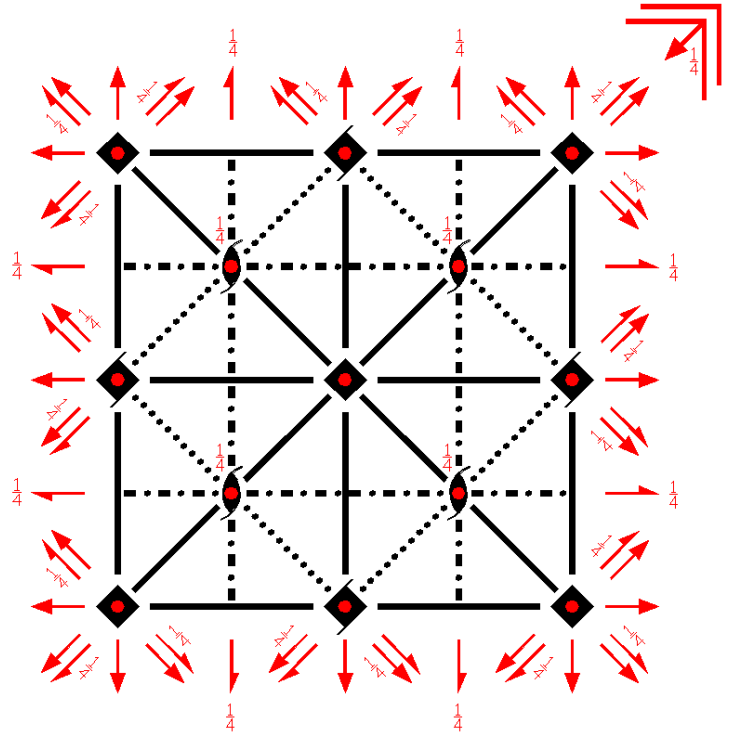
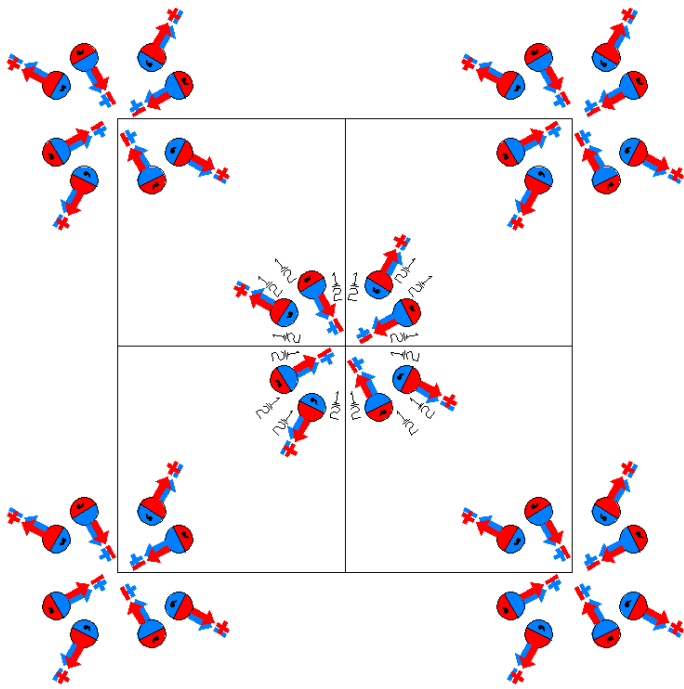
Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



I4/m'mm  
139.3.1181

4/m'mm  
I4/m'2'/m2'/m

Tetragonal



Origin at center ( 4/m'mm )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; x \leq y$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |  |
|--|---|---|--|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                       | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)          |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'  | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                                 | (8) 2' x,x̄,0<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,0)'                   |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'              | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)' | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)  | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   | (15) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                                 | (16) m x,x,z<br>(m <sub>xy</sub> <sup>-1</sup>  0,0,0)                     |

## For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)	(4) $4^-$ (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)
(5) $2'$ (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>   1/2,1/2,1/2)'	(6) $2'$ (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>   1/2,1/2,1/2)'	(7) $2'$ (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)'	(8) $2'$ x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)'
(9) $\bar{1}$ ' 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)'	(10) $n'$ (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)'	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$   1/2,1/2,1/2)'
(13) $n$ (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)	(14) $n$ (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)	(15) $c$ (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,1/2)	(16) $n$ (1/2,1/2,1/2) x,x,z (m <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	o	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [v,u,w]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(11) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
			(13) x, $\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ]	(16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
16	n	.m.	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},0,z$ [0,u,0]	y,0,z [0, $\bar{u},0$ ]
			0,y, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]	y,0, $\bar{z}$ [0, $\bar{u},0$ ]	$\bar{y},0,\bar{z}$ [0,u,0]
16	m	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [u, $\bar{u},0$ ]	$\bar{x},x,z$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},z$ [u,u,0]
			$\bar{x},x,\bar{z}$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},\bar{z}$ [u,u,0]	x,x, $\bar{z}$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},\bar{z}$ [u, $\bar{u},0$ ]
16	l	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},u,0$ ]	y, $\bar{x},0$ [v, $\bar{u},0$ ]
			$\bar{x},y,0$ [u, $\bar{v},0$ ]	x, $\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	y,x,0 [ $\bar{v},\bar{u},0$ ]	$\bar{y},\bar{x},0$ [v,u,0]
16	k	..2'	x,x+1/2,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [u, $\bar{u},w$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},\bar{u},w$ ]	x+1/2, $\bar{x},1/4$ [u,u,w]
			$\bar{x},\bar{x}+1/2,3/4$ [u, $\bar{u},\bar{w}$ ]	x,x+1/2,3/4 [ $\bar{u},u,\bar{w}$ ]	x+1/2, $\bar{x},3/4$ [u,u, $\bar{w}$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	j	m'2'm.	x,1/2,0 [0,v,0]	$\bar{x},1/2,0$ [0, $\bar{v},0$ ]	1/2,x,0 [ $\bar{v},0,0$ ]	1/2, $\bar{x},0$ [v,0,0]
8	i	m'2'm.	x,0,0 [0,v,0]	$\bar{x},0,0$ [0, $\bar{v},0$ ]	0,x,0 [ $\bar{v},0,0$ ]	0, $\bar{x},0$ [v,0,0]
8	h	m'.2'm	x,x,0 [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},0$ [u, $\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},0$ [u,u,0]
8	g	2mm.	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]
8	f	..2'/m	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]

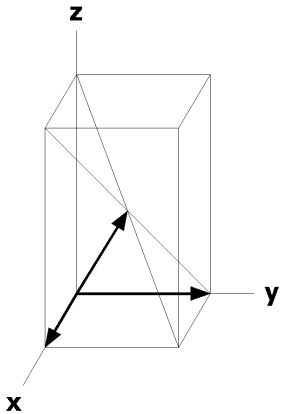
4	e	4mm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	d	$\bar{4}$ 'm2'	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	c	m'mm.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]
2	b	4/m'mm	0,0,1/2 [0,0,0]	
2	a	4/m'mm	0,0,0 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] p4mm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

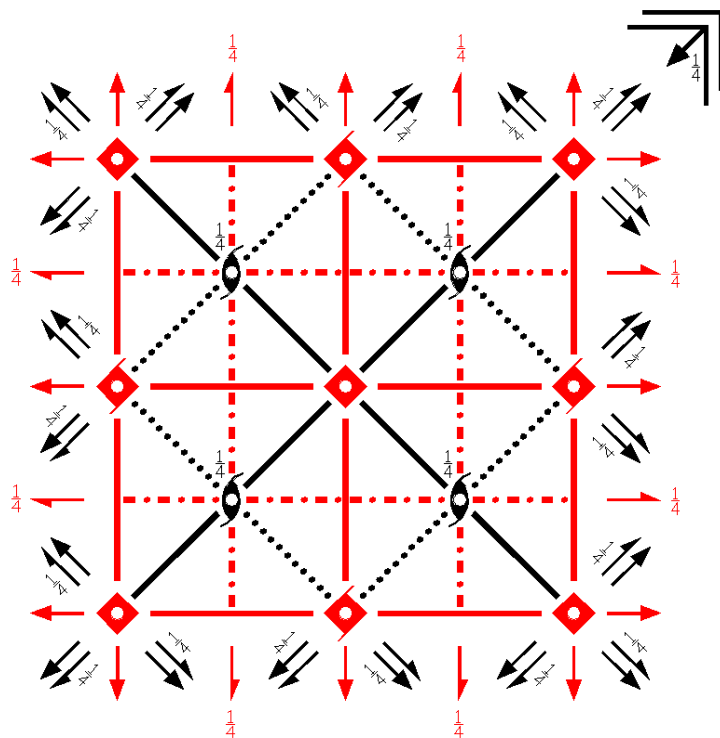
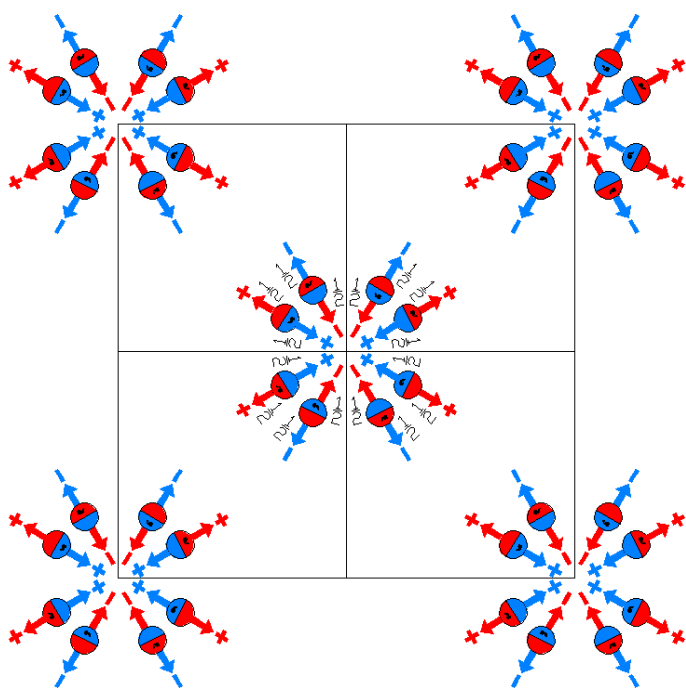
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I4'/mm'm$   
139.4.1182

$4'/mm'm$   
 $I4'/m2'/m'2'/m$

Tetragonal



Origin at center ( $4'/mm'm$ )

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $x \leq y$

### Symmetry Operations

For (0,0,0) + set

- |  |   |   |  |
|--|---|---|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)' | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'    |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'   | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                           | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0) |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)   | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'         | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'            |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)'  | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (15) m x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)                | (16) m x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,0)          |



For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)'	(4) $4^-$ ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)'
(5) $2'$ (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>   1/2,1/2,1/2)'	(6) $2'$ (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>   1/2,1/2,1/2)'	(7) $2$ (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)	(8) $2$ x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)
(9) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)	(10) $n$ (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)'
(13) $n'$ (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)'	(14) $n'$ (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)'	(15) $c$ (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,1/2)	(16) $n$ (1/2,1/2,1/2) x,x,z (m <sub>xy</sub>   1/2,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	o	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(5) $\bar{x},y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(13) x, $\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},\bar{v},w$ ]	(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
16	n	.m'	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	$\bar{y},0,z$ [v,0, $\bar{w}$ ]	y,0,z [ $\bar{v},0,\bar{w}$ ]
			0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]	y,0, $\bar{z}$ [v,0, $\bar{w}$ ]	$\bar{y},0,\bar{z}$ [ $\bar{v},0,\bar{w}$ ]
16	m	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,z$ [u,u,0]	x, $\bar{x},z$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},x,\bar{z}$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},\bar{z}$ [u,u,0]	x,x, $\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]
16	l	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0, $\bar{w}$ ]	y, $\bar{x},0$ [0,0, $\bar{w}$ ]
			$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0,w]	y,x,0 [0,0, $\bar{w}$ ]	$\bar{y},\bar{x},0$ [0,0, $\bar{w}$ ]
16	k	..2	x,x+1/2,1/4 [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,1/4$ [u, $\bar{u},0$ ]	x+1/2, $\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},\bar{x}+1/2,3/4$ [u,u,0]	x,x+1/2,3/4 [ $\bar{u},\bar{u},0$ ]	x+1/2, $\bar{x},3/4$ [u, $\bar{u},0$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},\bar{u},0$ ]
8	j	m2'm'	x,1/2,0 [0,0,w]	$\bar{x},1/2,0$ [0,0,w]	1/2,x,0 [0,0, $\bar{w}$ ]	1/2, $\bar{x},0$ [0,0, $\bar{w}$ ]
8	i	m2'm'	x,0,0 [0,0,w]	$\bar{x},0,0$ [0,0,w]	0,x,0 [0,0, $\bar{w}$ ]	0, $\bar{x},0$ [0,0, $\bar{w}$ ]
8	h	m.2m	x,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x},x,0$ [0,0,0]	x, $\bar{x},0$ [0,0,0]
8	g	2m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
8	f	..2/m	1/4,1/4,1/4 [ $\bar{u},u,0$ ]	3/4,3/4,1/4 [u, $\bar{u},0$ ]	3/4,1/4,1/4 [u,u,0]	1/4,3/4,1/4 [ $\bar{u},\bar{u},0$ ]

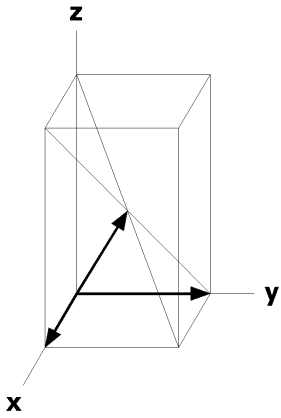
4	e	4'm'm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	d	$\bar{4}$ 'm'2	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	c	mm'm'.	0,1/2,0 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]
2	b	4'/mm'm	0,0,1/2 [0,0,0]	
2	a	4'/mm'm	0,0,0 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2'mm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

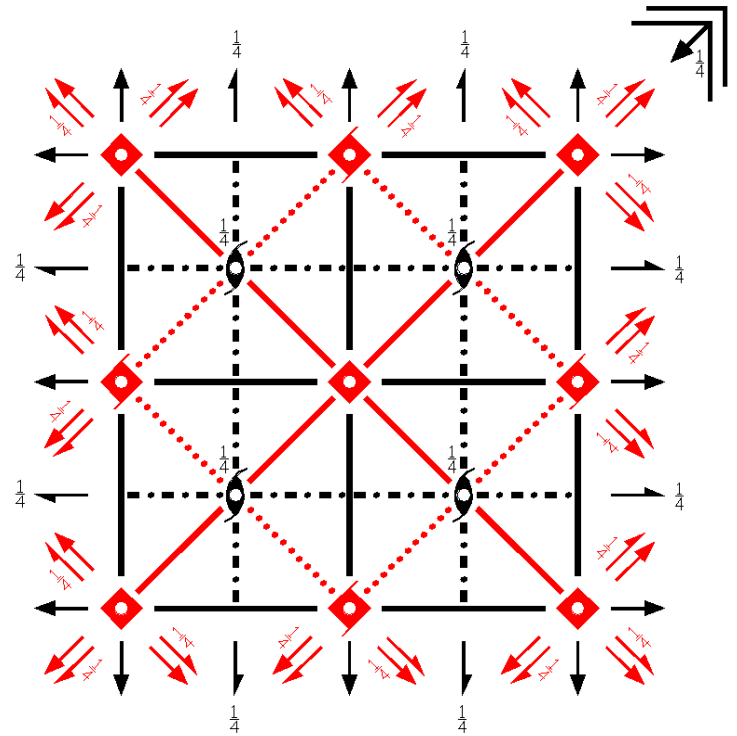
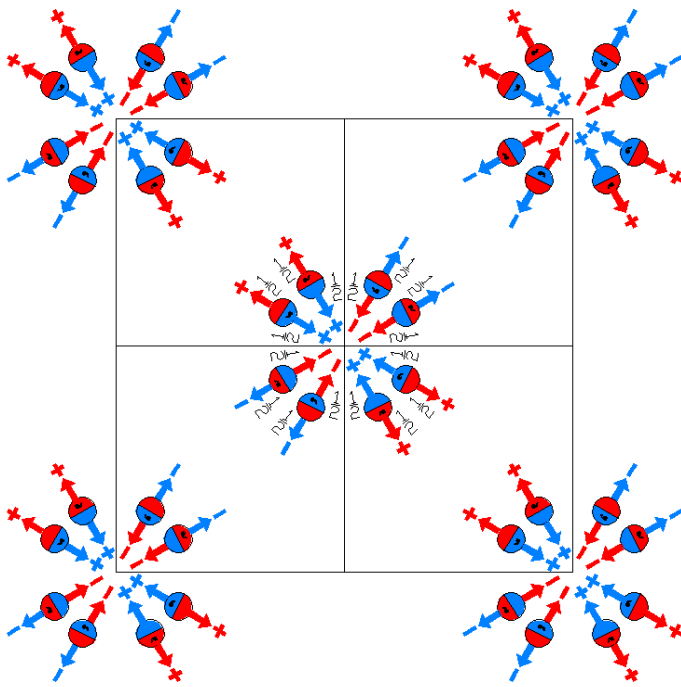
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I4'/mmm'$   
139.5.1183

$4'/mmm'$   
 $I4'/m2/m2'/m'$

Tetragonal



Origin at center ( $4'/mmm'$ )

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $x \leq y$

Symmetry Operations

For (0,0,0) + set

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'                      | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'         |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                                 | (8) 2' x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)'                                |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)              | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)' | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (15) m' x,x̄,z<br>(m <sub>xȳ</sub>  0,0,0)'                              | (16) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                                 |

## For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)'	(4) $4^-$ ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)'
(5) $2$ (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>   1/2,1/2,1/2)	(6) $2$ (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>   1/2,1/2,1/2)	(7) $2'$ (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)'	(8) $2'$ x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub> <sup>-1</sup>   1/2,1/2,1/2)'
(9) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)	(10) $n$ (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)'
(13) $n$ (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)	(14) $n$ (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)	(15) $c'$ (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,1/2)'	(16) $n'$ (1/2,1/2,1/2) x,x,z (m <sub>xy</sub> <sup>-1</sup>   1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates				
			(0,0,0) +	(1/2,1/2,1/2) +			
Multiplicity,	Wyckoff letter,	Site Symmetry.					
32	o	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ]	
			(5) $\bar{x},y,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	
			(9) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	
			(13) x, $\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x},y,z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(16) y,x,z [v,u,w]	
16	n	.m.	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},0,z$ [0, $\bar{u},0$ ]	y,0,z [0,u,0]	
			0,y, $\bar{z}$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]	y,0, $\bar{z}$ [0, $\bar{u},0$ ]	$\bar{y},0,\bar{z}$ [0,u,0]	
16	m	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,z$ [u, $\bar{u},\bar{w}$ ]	x, $\bar{x},z$ [ $\bar{u},\bar{u},\bar{w}$ ]	
			$\bar{x},x,\bar{z}$ [ $\bar{u},\bar{u},\bar{w}$ ]	x, $\bar{x},\bar{z}$ [u, $\bar{u},\bar{w}$ ]	x,x, $\bar{z}$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},\bar{z}$ [u,u,w]	
16	l	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0, $\bar{w}$ ]	y, $\bar{x},0$ [0,0, $\bar{w}$ ]	
			$\bar{x},y,0$ [0,0, $\bar{w}$ ]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]	y,x,0 [0,0,w]	$\bar{y},\bar{x},0$ [0,0,w]	
16	k	..2'	x,x+1/2,1/4 [ $\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [u, $\bar{u},w$ ]	$\bar{x}+1/2,x,1/4$ [u,u, $\bar{w}$ ]	x+1/2, $\bar{x},1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	
			$\bar{x},\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},w$ ]	x,x+1/2,3/4 [u, $\bar{u},w$ ]	x+1/2, $\bar{x},3/4$ [u,u, $\bar{w}$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	
8	j	m2m.	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]	1/2,x,0 [0,0,0]	1/2, $\bar{x},0$ [0,0,0]	
8	i	m2m.	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x},0$ [0,0,0]	
8	h	m.2'm'	x,x,0 [0,0,w]	$\bar{x},\bar{x},0$ [0,0,w]	$\bar{x},x,0$ [0,0, $\bar{w}$ ]	x, $\bar{x},0$ [0,0, $\bar{w}$ ]	
8	g	2mm.	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	
8	f	..2'/m'	1/4,1/4,1/4 [u,u,w]	3/4,3/4,1/4 [ $\bar{u},\bar{u},w$ ]	3/4,1/4,1/4 [u, $\bar{u},\bar{w}$ ]	1/4,3/4,1/4 [ $\bar{u},\bar{u},\bar{w}$ ]	

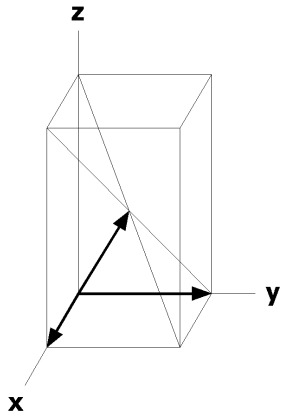
4	e	4'mm'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	d	$\bar{4}$ 'm2'	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	c	mmm.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]
2	b	4'/mmm'	0,0,1/2 [0,0,0]	
2	a	4'/mmm'	0,0,0 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

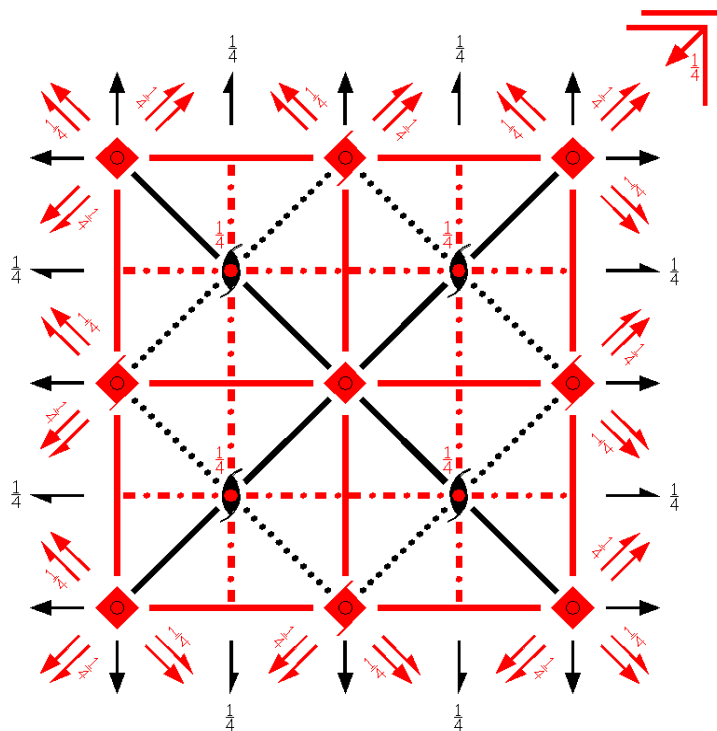
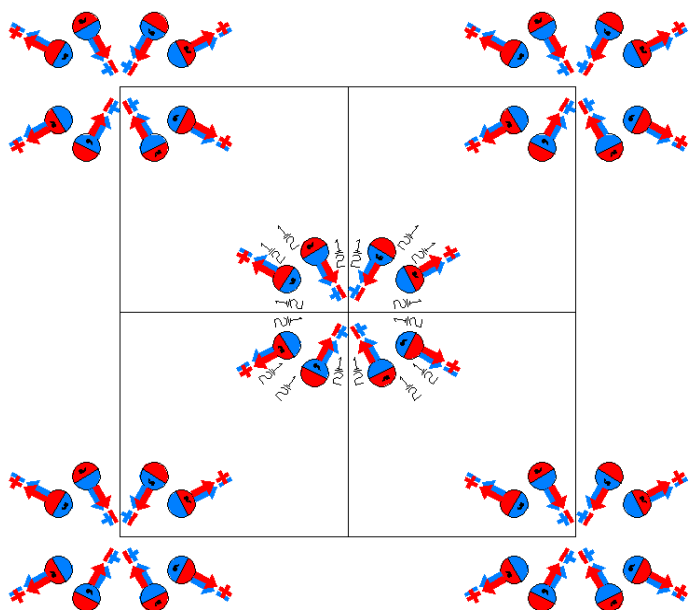
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$I4'/m'm'm$   
139.6.1184

$4'/m'm'm$   
 $I4'/m'2/m'2'/m$

Tetragonal



Origin at center ( $4'/m'm'm$ )

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $x \leq y$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'                     | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'        |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)    | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)    | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                                | (8) 2' x,x̄,0<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,0)'                  |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'               | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (15) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                                | (16) m x,x,z<br>(m <sub>xy</sub> <sup>-1</sup>  0,0,0)                    |

For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)'	(4) $4^-$ ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)'
(5) $2$ (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>   1/2,1/2,1/2)	(6) $2$ (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>   1/2,1/2,1/2)	(7) $2'$ (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)'	(8) $2'$ x, $\bar{x}+1/2,1/4$ (2 <sub>xy</sub>   1/2,1/2,1/2)'
(9) $\bar{1}$ ' 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)'	(10) $n'$ (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)'	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$   1/2,1/2,1/2)
(13) $n'$ (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)'	(14) $n'$ (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)'	(15) $c$ (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,1/2)	(16) $n$ (1/2,1/2,1/2) x,x,z (m <sub>xy</sub>   1/2,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	o	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(5) $\bar{x},y,\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(13) x, $\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},\bar{v},w$ ]	(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
16	n	.m'	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	$\bar{y},0,z$ [v,0, $\bar{w}$ ]	y,0,z [ $\bar{v},0,\bar{w}$ ]
			0,y, $\bar{z}$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]	y,0, $\bar{z}$ [ $\bar{v},0,w$ ]	$\bar{y},0,\bar{z}$ [v,0,w]
16	m	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,z$ [u,u,0]	x, $\bar{x},z$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},x,\bar{z}$ [u,u,0]	x, $\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]	x,x, $\bar{z}$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},\bar{z}$ [u, $\bar{u},0$ ]
16	l	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [v, $\bar{u},0$ ]	y, $\bar{x},0$ [ $\bar{v},\bar{u},0$ ]
			$\bar{x},y,0$ [ $\bar{u},\bar{v},0$ ]	x, $\bar{y},0$ [u, $\bar{v},0$ ]	y,x,0 [ $\bar{v},\bar{u},0$ ]	$\bar{y},\bar{x},0$ [v,u,0]
16	k	..2'	x,x+1/2,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,1/4$ [u,u, $\bar{w}$ ]	x+1/2, $\bar{x},1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x},\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	x,x+1/2,3/4 [ $\bar{u},u,\bar{w}$ ]	x+1/2, $\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,3/4$ [u,u,w]
8	j	m'2m'	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	1/2,x,0 [0, $\bar{u},0$ ]	1/2, $\bar{x},0$ [0,u,0]
8	i	m'2m'	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0, $\bar{u},0$ ]	0, $\bar{x},0$ [0,u,0]
8	h	m'.2'm	x,x,0 [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},0$ [u, $\bar{u},0$ ]	$\bar{x},x,0$ [u,u,0]	x, $\bar{x},0$ [ $\bar{u},\bar{u},0$ ]
8	g	2m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0,w]
8	f	..2'/m	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]

4	e	4'm'm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	d	$\bar{4}$ m'2'	0,1/2,1/4 [0,0,w]	1/2,0,1/4 [0,0, $\bar{w}$ ]
4	c	m'm'm'	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]
2	b	4'/m'm'm	0,0,1/2 [0,0,0]	
2	a	4'/m'm'm	0,0,0 [0,0,0]	

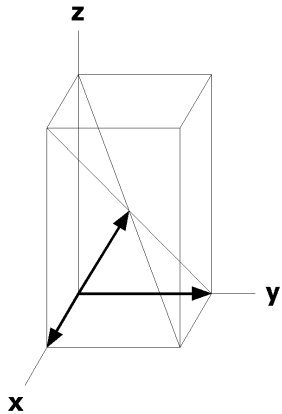
### Symmetry of Special Projections

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

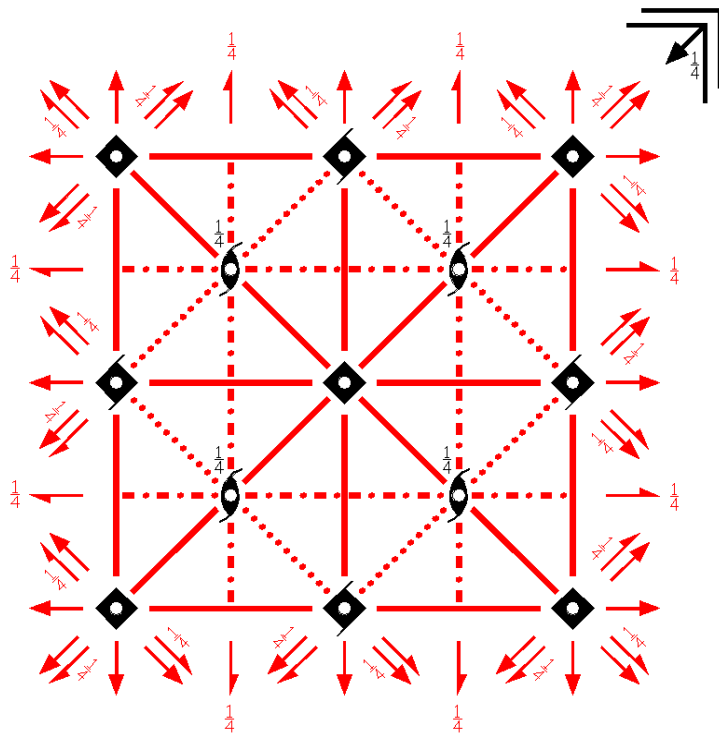
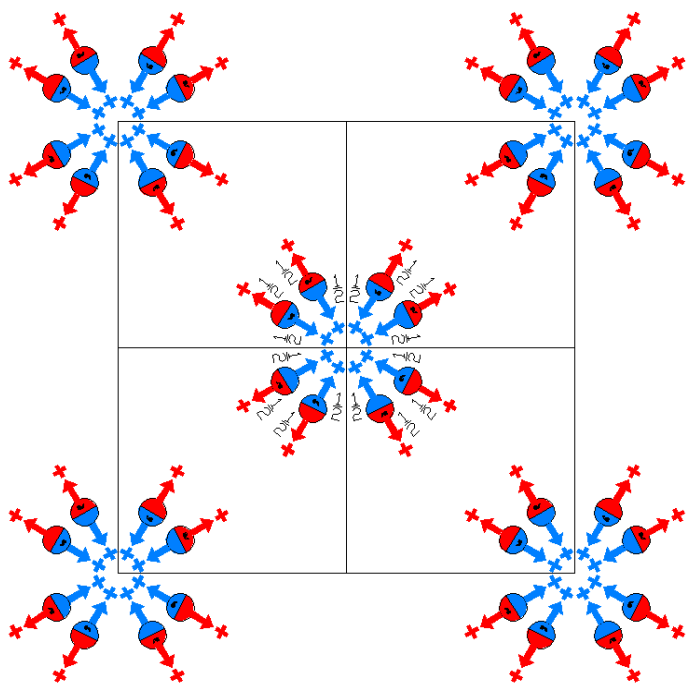




I4/mm'm'  
139.7.1185

4/mm'm'  
I4/m2'/m'2'/m'

Tetragonal



Origin at center ( 4/mm'm' )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; x \leq y$

### Symmetry Operations

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 <sub>z</sub> 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)         | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)         |
| (5) 2' <sub>y</sub> 0,y,0<br>(2 <sub>y</sub>  0,0,0)'  | (6) 2' <sub>x</sub> x,0,0<br>(2 <sub>x</sub>  0,0,0)'  | (7) 2' <sub>xy</sub> x,x,0<br>(2 <sub>xy</sub>  0,0,0)'     | (8) 2' <sub>xy</sub> x,x̄,0<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,0)'    |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)                             | (10) m <sub>z</sub> x,y,0<br>(m <sub>z</sub>  0,0,0)   | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub>  0,0,0) | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) m' <sub>y</sub> x,0,z<br>(m <sub>y</sub>  0,0,0)' | (14) m' <sub>x</sub> 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (15) m' <sub>xy</sub> x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'   | (16) m' <sub>xy</sub> x,x,z<br>(m <sub>xy</sub>  0,0,0)'                  |

For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)	(4) $4^-$ (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)
(5) $2'$ (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>   1/2,1/2,1/2)'	(6) $2'$ (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>   1/2,1/2,1/2)'	(7) $2'$ (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)'	(8) $2'$ x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub> <sup>-</sup>   1/2,1/2,1/2)'
(9) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)	(10) $n$ (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)
(13) $n'$ (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)'	(14) $n'$ (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)'	(15) $c'$ (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,1/2)'	(16) $n'$ (1/2,1/2,1/2) x,x,z (m <sub>xy</sub> <sup>-</sup>   1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	o	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [v,u,w]
			(9) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [v, $\bar{u},w$ ]
			(13) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},\bar{v},w$ ]	(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(16) y,x,z [v,u,w]
16	n	.m'	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	$\bar{y},0,z$ [ $\bar{v},0,w$ ]	y,0,z [v,0,w]
			0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]	y,0, $\bar{z}$ [ $\bar{v},0,w$ ]	$\bar{y},0,z$ [v,0,w]
16	m	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,z$ [ $\bar{u},u,w$ ]	x, $\bar{x},z$ [u, $\bar{u},w$ ]
			$\bar{x},x,\bar{z}$ [u, $\bar{u},w$ ]	x, $\bar{x},\bar{z}$ [ $\bar{u},\bar{u},w$ ]	x,x, $\bar{z}$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},\bar{z}$ [u,u,w]
16	l	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0,w]	y, $\bar{x},0$ [0,0,w]
			$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0,w]	y,x,0 [0,0,w]	$\bar{y},\bar{x},0$ [0,0,w]
16	k	..2'	x,x+1/2,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},\bar{u},w$ ]	x+1/2, $\bar{x},1/4$ [u,u,w]
			$\bar{x},\bar{x}+1/2,3/4$ [ $\bar{u},u,w$ ]	x,x+1/2,3/4 [u, $\bar{u},w$ ]	x+1/2, $\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,3/4$ [u,u,w]
8	j	m2'm'	x,1/2,0 [0,0,w]	$\bar{x},1/2,0$ [0,0,w]	1/2,x,0 [0,0,w]	1/2, $\bar{x},0$ [0,0,w]
8	i	m2'm'	x,0,0 [0,0,w]	$\bar{x},0,0$ [0,0,w]	0,x,0 [0,0,w]	0, $\bar{x},0$ [0,0,w]
8	h	m.2'm'	x,x,0 [0,0,w]	$\bar{x},\bar{x},0$ [0,0,w]	$\bar{x},x,0$ [0,0,w]	x, $\bar{x},0$ [0,0,w]
8	g	2m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]
8	f	..2'/m'	1/4,1/4,1/4 [ $\bar{u},u,w$ ]	3/4,3/4,1/4 [u, $\bar{u},w$ ]	3/4,1/4,1/4 [ $\bar{u},\bar{u},w$ ]	1/4,3/4,1/4 [u,u,w]

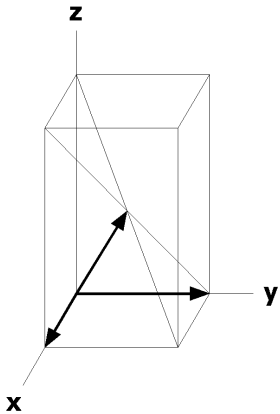
4	e	4m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]
4	d	$\bar{4}m'2'$	0,1/2,1/4 [0,0,w]	1/2,0,1/4 [0,0,w]
4	c	mm'm'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]
2	b	4/mmm'm'	0,0,1/2 [0,0,w]	
2	a	4/mmm'm'	0,0,0 [0,0,w]	

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



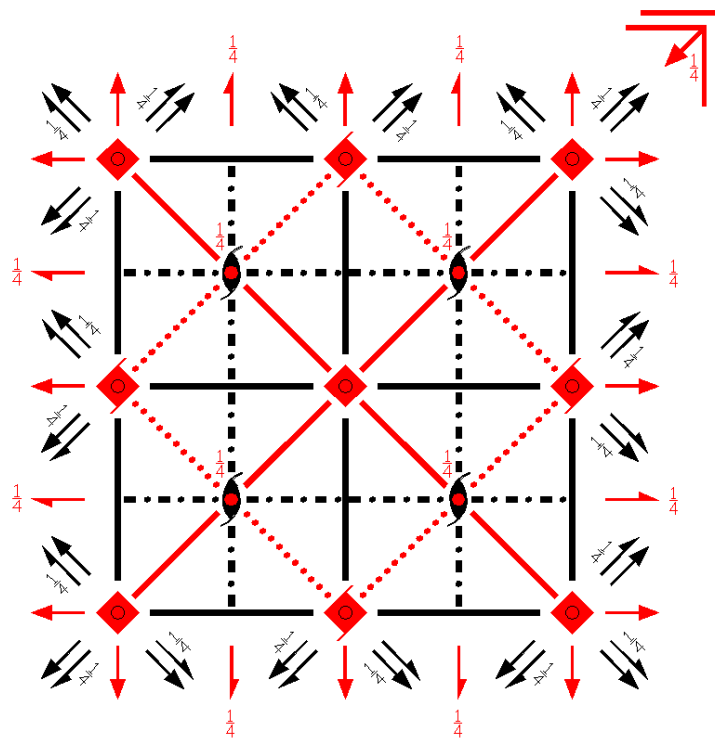
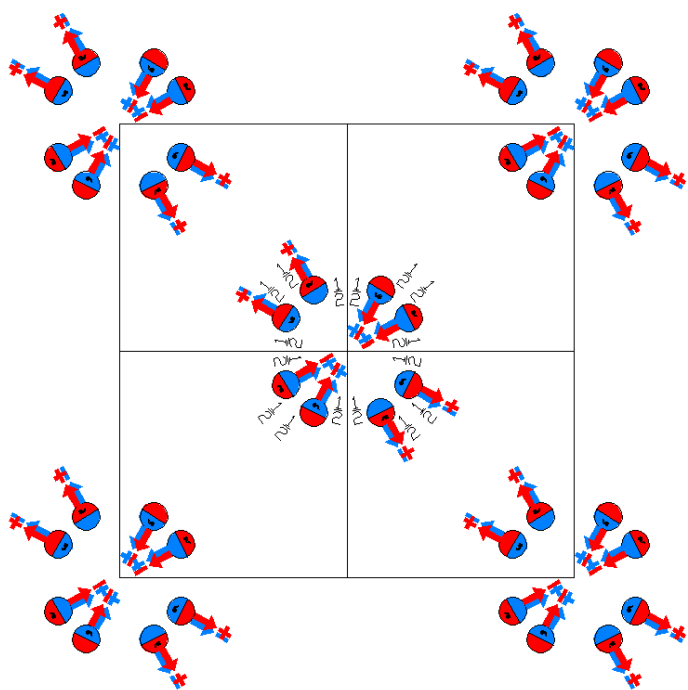
$I4'/m'mm'$

139.8.1186

$4'/m'mm'$

$I4'/m'2'/m2/m'$

Tetragonal



Origin at center ( $4'/m'mm'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; x \leq y$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |  |   |
|--|---|--|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'                     | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'        |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                  | (8) 2 x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)                                 |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'              | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)  | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   | (15) m' x,x̄,z<br>(m <sub>xȳ</sub>  0,0,0)'                             | (16) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                                |

## For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)'	(4) $4^-$ (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)'
(5) $2'$ (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>   1/2,1/2,1/2)'	(6) $2'$ (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>   1/2,1/2,1/2)'	(7) $2$ (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)	(8) $2$ x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)
(9) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)'	(10) $n'$ (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)'	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$   1/2,1/2,1/2)
(13) $n$ (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)	(14) $n$ (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)	(15) $c'$ (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,1/2)'	(16) $n'$ (1/2,1/2,1/2) x,x,z (m <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	o	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(5) $\bar{x},y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]
			(13) x, $\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x},y,z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(16) y,x,z [v,u,w]
16	n	.m.	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},0,z$ [0, $\bar{u},0$ ]	y,0,z [0,u,0]
			0,y, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]	y,0, $\bar{z}$ [0,u,0]	$\bar{y},0,\bar{z}$ [0, $\bar{u},0$ ]
16	m	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,z$ [u, $\bar{u},\bar{w}$ ]	x, $\bar{x},z$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x},x,\bar{z}$ [u, $\bar{u},w$ ]	x, $\bar{x},\bar{z}$ [ $\bar{u},\bar{u},w$ ]	x,x, $\bar{z}$ [u,u, $\bar{w}$ ]	$\bar{x},\bar{x},\bar{z}$ [ $\bar{u},\bar{u},\bar{w}$ ]
16	l	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [v, $\bar{u},0$ ]	y, $\bar{x},0$ [ $\bar{v},\bar{u},0$ ]
			$\bar{x},y,0$ [u, $\bar{v},0$ ]	x, $\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	y,x,0 [v,u,0]	$\bar{y},\bar{x},0$ [ $\bar{v},\bar{u},0$ ]
16	k	..2	x,x+1/2,1/4 [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,1/4$ [u, $\bar{u},0$ ]	x+1/2, $\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	x,x+1/2,3/4 [u,u,0]	x+1/2, $\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,3/4$ [u, $\bar{u},0$ ]
8	j	m'2'm.	x,1/2,0 [0,v,0]	$\bar{x},1/2,0$ [0, $\bar{v},0$ ]	1/2,x,0 [v,0,0]	1/2, $\bar{x},0$ [ $\bar{v},0,0$ ]
8	i	m'2'm.	x,0,0 [0,v,0]	$\bar{x},0,0$ [0, $\bar{v},0$ ]	0,x,0 [v,0,0]	0, $\bar{x},0$ [ $\bar{v},0,0$ ]
8	h	m'.2m'	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [u, $\bar{u},0$ ]	x, $\bar{x},0$ [ $\bar{u},\bar{u},0$ ]
8	g	2mm.	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]
8	f	..2/m'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]

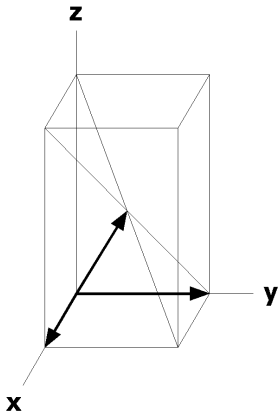
4	e	4'mm'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	d	$\bar{4}m2$	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	c	m'mm.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]
2	b	4'/m'mm'	0,0,1/2 [0,0,0]	
2	a	4'/m'mm'	0,0,0 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] p4'm'm  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

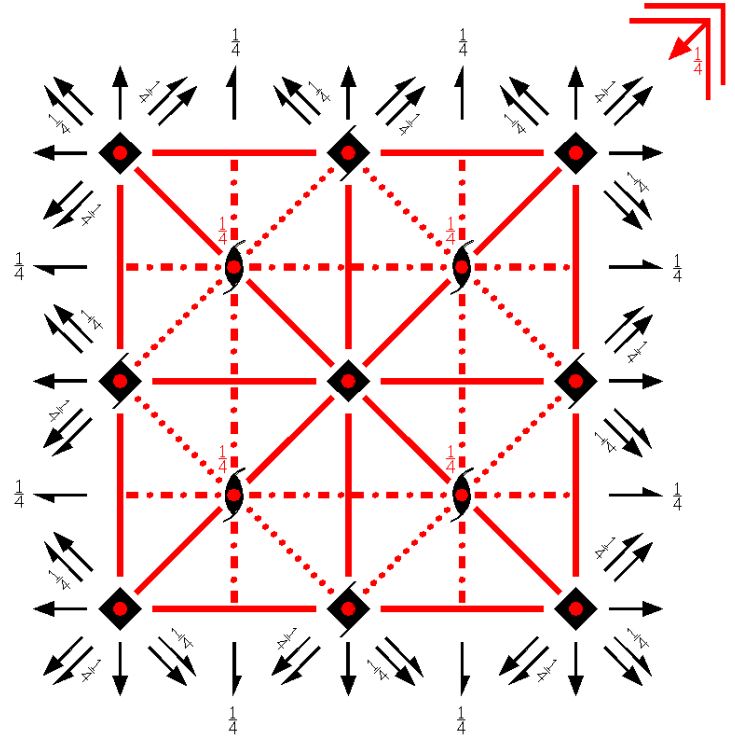
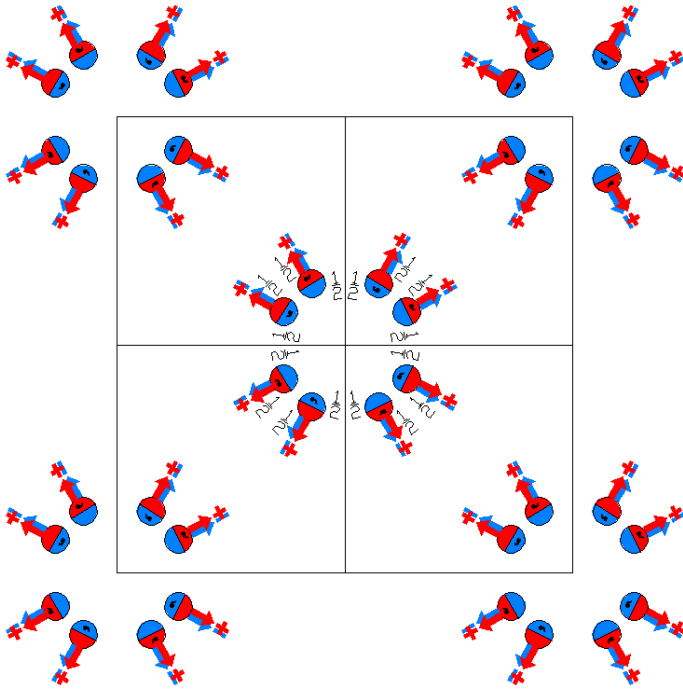
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



I4/m'm'm'  
139.9.1187

4/m'm'm'  
I4/m'2/m'2/m'

Tetragonal



Origin at center ( 4/m'm'm' )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad x \leq y$

### Symmetry Operations

For (0,0,0) + set

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                       | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)          |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)    | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)    | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                   | (8) 2 x, x̄, 0<br>(2 <sub>xȳ</sub>  0,0,0)                                |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'               | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)' | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (15) m' x, x̄, z<br>(m <sub>xȳ</sub>  0,0,0)'                            | (16) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                                 |

For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)	(4) $4^-$ (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)
(5) $2$ (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>   1/2,1/2,1/2)	(6) $2$ (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>   1/2,1/2,1/2)	(7) $2$ (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)	(8) $2$ x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)
(9) $\bar{1}$ ' 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)'	(10) $n'$ (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)'	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)'
(13) $n'$ (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)'	(14) $n'$ (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)'	(15) $c'$ (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,1/2)'	(16) $n'$ (1/2,1/2,1/2) x,x,z (m <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	o	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(11) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
			(13) x, $\bar{y},z$ [u, $\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(16) y,x,z [v,u,w]
16	n	.m'	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	$\bar{y},0,z$ [ $\bar{v},0,w$ ]	y,0,z [v,0,w]
			0,y, $\bar{z}$ [0,v, $\bar{w}$ ]	0, $\bar{y},\bar{z}$ [0, $\bar{v},\bar{w}$ ]	y,0, $\bar{z}$ [v,0, $\bar{w}$ ]	$\bar{y},0,\bar{z}$ [ $\bar{v},0,\bar{w}$ ]
16	m	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,z$ [ $\bar{u},u,w$ ]	x, $\bar{x},z$ [u, $\bar{u},w$ ]
			$\bar{x},x,\bar{z}$ [ $\bar{u},u,\bar{w}$ ]	x, $\bar{x},\bar{z}$ [u, $\bar{u},\bar{w}$ ]	x,x, $\bar{z}$ [u,u, $\bar{w}$ ]	$\bar{x},\bar{x},\bar{z}$ [ $\bar{u},\bar{u},\bar{w}$ ]
16	l	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [v,u,0]	y, $\bar{x},0$ [v, $\bar{u},0$ ]
			$\bar{x},y,0$ [ $\bar{u},v,0$ ]	x, $\bar{y},0$ [u, $\bar{v},0$ ]	y,x,0 [v,u,0]	$\bar{y},\bar{x},0$ [ $\bar{v},\bar{u},0$ ]
16	k	..2	x,x+1/2,1/4 [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},u,0$ ]	x+1/2, $\bar{x},1/4$ [u, $\bar{u},0$ ]
			$\bar{x},\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	x,x+1/2,3/4 [u,u,0]	x+1/2, $\bar{x},3/4$ [u, $\bar{u},0$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},u,0$ ]
8	j	m'2m'	x,1/2,0 [u,0,0]	$\bar{x},1/2,0$ [ $\bar{u},0,0$ ]	1/2,x,0 [0,u,0]	1/2, $\bar{x},0$ [0, $\bar{u},0$ ]
8	i	m'2m'	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0,u,0]	0, $\bar{x},0$ [0, $\bar{u},0$ ]
8	h	m'.2m'	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]	x, $\bar{x},0$ [u, $\bar{u},0$ ]
8	g	2m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]
8	f	..2/m'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]



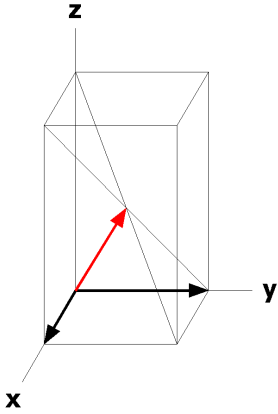
4	e	4m'm'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4	d	$\bar{4}$ 'm'2	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	c	m'm'm'.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]
2	b	4/m'm'm'	0,0,1/2 [0,0,0]	
2	a	4/m'm'm'	0,0,0 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

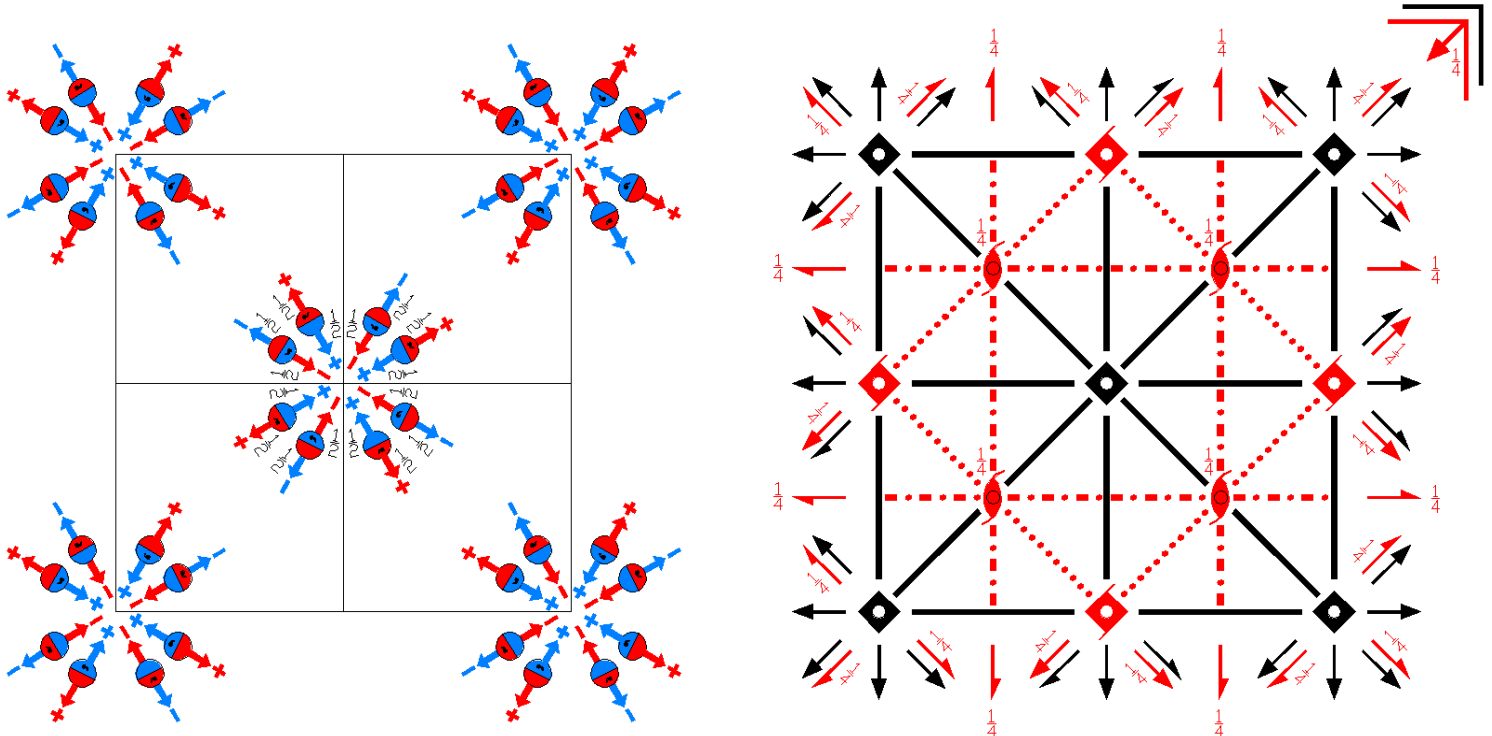
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I_p 4/mmm$   
139.10.1188

$4/mmm1'$   
 $I_p 4/m2/m2/m$

Tetragonal



Origin at center (  $4/mmm$  )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; x \leq y$

Symmetry Operations

For (0,0,0) + set

- |  |   |  |  |
|--|---|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)     |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)     | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                          | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0) |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)         | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)             |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)    | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (15) m x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)               | (16) m x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,0)          |

## For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (1   1/2,1/2,1/2)'	(2) 2' (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)'	(3) 4* ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)'	(4) 4' ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)'
(5) 2' (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>   1/2,1/2,1/2)'	(6) 2' (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>   1/2,1/2,1/2)'	(7) 2' (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)'	(8) 2' x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)'
(9) $\bar{1}$ ' 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)'	(10) n' (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)'	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}$ ' ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)'
(13) n' (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)'	(14) n' (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)'	(15) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,1/2)'	(16) n' (1/2,1/2,1/2) x,x,z (m <sub>xy</sub>   1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	o	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(6) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [v, $\bar{u},w$ ]
			(13) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z$ [u, $\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ]	(16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
16	n	.m.	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},0,z$ [0,u,0]	y,0,z [0, $\bar{u},0$ ]
			0,y, $\bar{z}$ [ $\bar{u},0,0$ ]	0, $\bar{y},\bar{z}$ [u,0,0]	y,0, $\bar{z}$ [0,u,0]	$\bar{y},0,\bar{z}$ [0, $\bar{u},0$ ]
16	m	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [u, $\bar{u},0$ ]	$\bar{x},x,z$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},z$ [u,u,0]
			$\bar{x},x,\bar{z}$ [u,u,0]	x, $\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]	x,x, $\bar{z}$ [u, $\bar{u},0$ ]	$\bar{x},\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]
16	l	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0,w]	y, $\bar{x},0$ [0,0,w]
			$\bar{x},y,0$ [0,0, $\bar{w}$ ]	x, $\bar{y},0$ [0,0, $\bar{w}$ ]	y,x,0 [0,0, $\bar{w}$ ]	$\bar{y},\bar{x},0$ [0,0, $\bar{w}$ ]
16	k	..2'	x,x+1/2,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x}+1/2,1/4$ [u, $\bar{u},w$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},\bar{u},w$ ]	x+1/2, $\bar{x},1/4$ [u,u,w]
			$\bar{x},\bar{x}+1/2,3/4$ [ $\bar{u},u,w$ ]	x,x+1/2,3/4 [u, $\bar{u},w$ ]	x+1/2, $\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,3/4$ [u,u,w]
8	j	m2m.	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]	1/2,x,0 [0,0,0]	1/2, $\bar{x},0$ [0,0,0]
8	i	m2m.	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x},0$ [0,0,0]
8	h	m.2m	x,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x},x,0$ [0,0,0]	x, $\bar{x},0$ [0,0,0]
8	g	2mm.	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]
8	f	..2'/m	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]

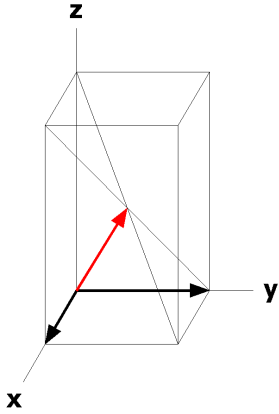
4	e	4mm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	d	$\bar{4}'m2'$	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	c	mmm.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]
2	b	4/mmm	0,0,1/2 [0,0,0]	
2	a	4/mmm	0,0,0 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

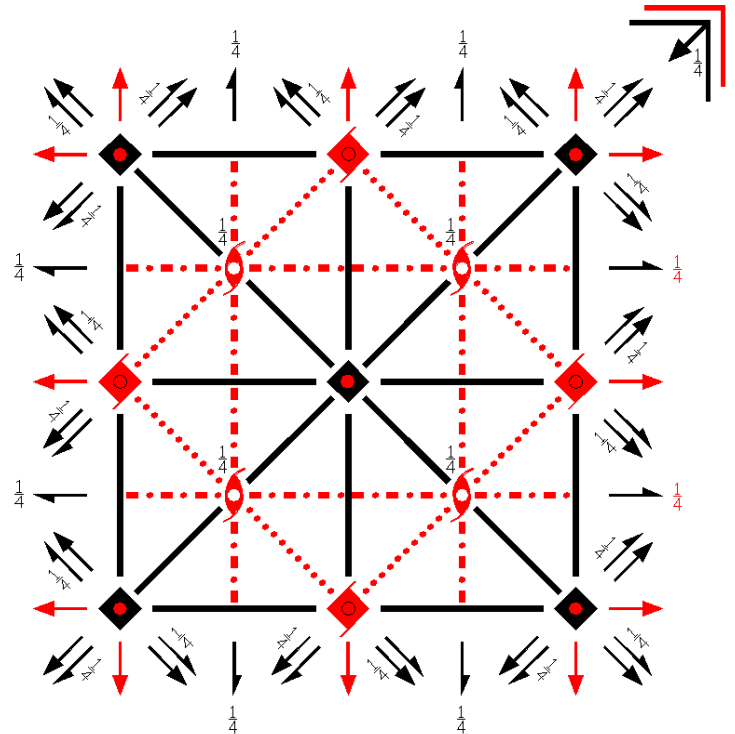
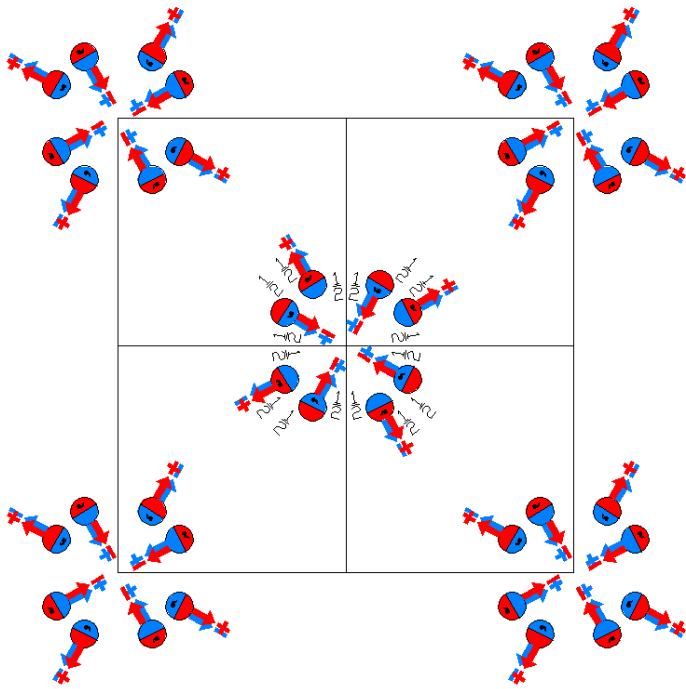
Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I_P 4/m'mm$   
139.11.1189

$4/mmm1'$   
 $I_P 4/m'2'/m2'/m$

Tetragonal



Origin at center ( $4/m'mm$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; x \leq y$

Symmetry Operations

For (0,0,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                         | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)           |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'  | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                                   | (8) 2' x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)'                                 |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'              | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) 4̄ <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (12) 4̄ <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)  | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   | (15) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                                   | (16) m x,x,z<br>(m <sub>xy</sub>  0,0,0)                                    |

## For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (1   1/2,1/2,1/2)'	(2) 2' (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)'	(3) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)'	(4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)'
(5) 2 (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>   1/2,1/2,1/2)	(6) 2 (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>   1/2,1/2,1/2)	(7) 2 (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)	(8) 2 x, $\bar{x}+1/2,1/4$ (2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)
(9) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)	(10) n (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$   1/2,1/2,1/2)
(13) n' (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)'	(14) n' (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)'	(15) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,1/2)'	(16) n' (1/2,1/2,1/2) x,x,z (m <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	o	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [ $v,\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) x, $\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
			(13) x, $\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]	(16) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]
16	n	.m.	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},0,z$ [0,u,0]	y,0,z [0, $\bar{u},0$ ]
			0,y, $\bar{z}$ [u,0,0]	0, $\bar{y},\bar{z}$ [ $\bar{u},0,0$ ]	y,0, $\bar{z}$ [0, $\bar{u},0$ ]	$\bar{y},0,\bar{z}$ [0,u,0]
16	m	..m	x,x,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,z$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},z$ [ $\bar{u},u,0$ ]
			$\bar{x},x,\bar{z}$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},\bar{z}$ [ $\bar{u},u,0$ ]	x,x, $\bar{z}$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]
16	l	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},u,0$ ]	y, $\bar{x},0$ [ $\bar{v},\bar{u},0$ ]
			$\bar{x},y,0$ [ $\bar{u},\bar{v},0$ ]	x, $\bar{y},0$ [ $\bar{u},v,0$ ]	y,x,0 [ $\bar{v},\bar{u},0$ ]	$\bar{y},\bar{x},0$ [ $\bar{v},u,0$ ]
16	k	..2	x,x+1/2,1/4 [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},u,0$ ]	x+1/2, $\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},\bar{x}+1/2,3/4$ [ $\bar{u},\bar{u},0$ ]	x,x+1/2,3/4 [u,u,0]	x+1/2, $\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,3/4$ [ $\bar{u},u,0$ ]
8	j	m'2'm.	x,1/2,0 [0,v,0]	$\bar{x},1/2,0$ [0, $\bar{v},0$ ]	1/2,x,0 [ $\bar{v},0,0$ ]	1/2, $\bar{x},0$ [ $\bar{v},0,0$ ]
8	i	m'2'm.	x,0,0 [0,v,0]	$\bar{x},0,0$ [0, $\bar{v},0$ ]	0,x,0 [ $\bar{v},0,0$ ]	0, $\bar{x},0$ [ $\bar{v},0,0$ ]
8	h	m'.2'm	x,x,0 [ $\bar{u},u,0$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},0$ [ $\bar{u},u,0$ ]
8	g	2mm.	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]
8	f	..2/m	1/4,1/4,1/4 [ $\bar{u},u,0$ ]	3/4,3/4,1/4 [ $\bar{u},\bar{u},0$ ]	3/4,1/4,1/4 [ $\bar{u},\bar{u},0$ ]	1/4,3/4,1/4 [ $\bar{u},u,0$ ]

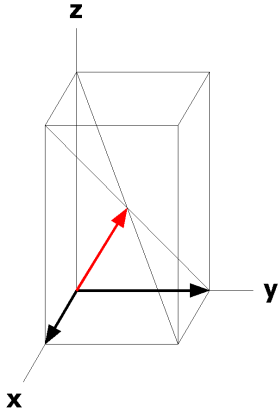
4	e	4mm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	d	$\bar{4}m2$	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	c	m'mm.	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]
2	b	4/m'mm	0,0,1/2 [0,0,0]	
2	a	4/m'mm	0,0,0 [0,0,0]	

**Symmetry of Special Projections**

Along [0,0,1]  $p_p 4mm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

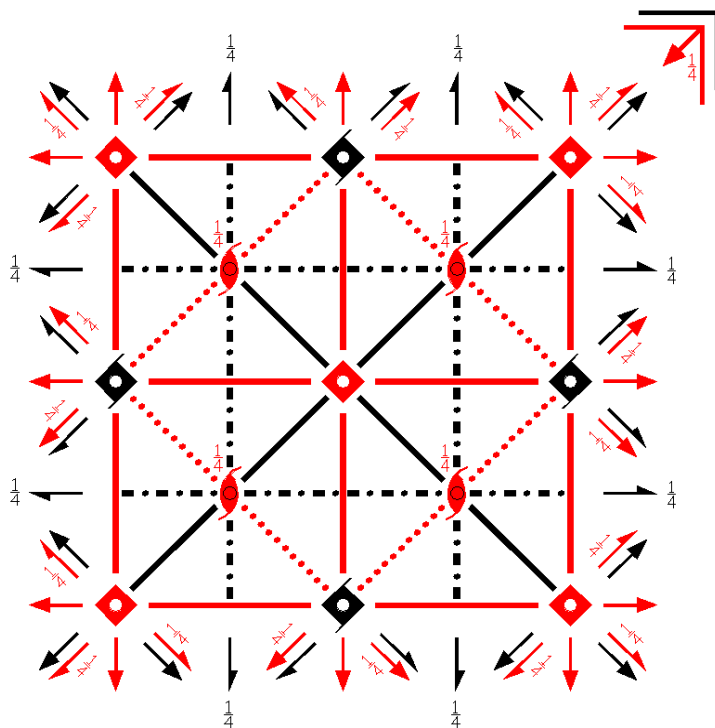
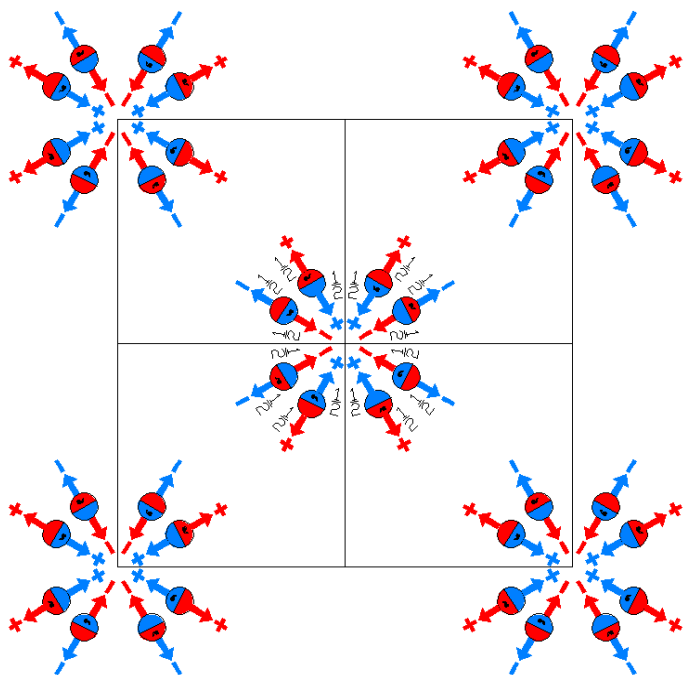
Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I_p 4'/mm'm$   
139.12.1190

$4/mmm1'$   
 $I_p 4'/m2'/m'2'/m$

Tetragonal



Origin at center ( $4'/mm'm$ )

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $x \leq y$

Symmetry Operations

For (0,0,0) + set

- |  |                                       |   |   |
|--|---------------------------------------|---|---|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)      | (3) $4^+$ $0,0,z$<br>( $4_z^+$  0,0,0)'                     | (4) $4^-$ $0,0,z$<br>( $4_z^-$  0,0,0)'                     |
| (5) $2'$ $0,y,0$<br>( $2_y$  0,0,0)'         | (6) $2'$ $x,0,0$<br>( $2_x$  0,0,0)'  | (7) 2 $x,x,0$<br>( $2_{xy}$  0,0,0)                         | (8) 2 $x,\bar{x},0$<br>( $2_{\bar{xy}}$  0,0,0)             |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0) | (10) m $x,y,0$<br>( $m_z$  0,0,0)     | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^+$  0,0,0)' | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^-$  0,0,0)' |
| (13) $m'$ $x,0,z$<br>( $m_y$  0,0,0)'        | (14) $m'$ $0,y,z$<br>( $m_x$  0,0,0)' | (15) m $x,\bar{x},z$<br>( $m_{xy}$  0,0,0)                  | (16) m $x,x,z$<br>( $m_{\bar{xy}}$  0,0,0)                  |



For  $(1/2, 1/2, 1/2)'$  + set

(1) $t' (1/2, 1/2, 1/2)$ $(1   1/2, 1/2, 1/2)'$	(2) $2' (0, 0, 1/2) \ 1/4, 1/4, z$ $(2_z   1/2, 1/2, 1/2)'$	(3) $4^+ (0, 0, 1/2) \ 0, 1/2, z$ $(4_z   1/2, 1/2, 1/2)$	(4) $4^- (0, 0, 1/2) \ 1/2, 0, z$ $(4_z^{-1}   1/2, 1/2, 1/2)$
(5) $2 (0, 1/2, 0) \ 1/4, y, 1/4$ $(2_y   1/2, 1/2, 1/2)$	(6) $2 (1/2, 0, 0) \ x, 1/4, 1/4$ $(2_x   1/2, 1/2, 1/2)$	(7) $2' (1/2, 1/2, 0) \ x, x, 1/4$ $(2_{xy}   1/2, 1/2, 1/2)'$	(8) $2' \ x, \bar{x} + 1/2, 1/4$ $(2_{\bar{xy}}   1/2, 1/2, 1/2)'$
(9) $\bar{1}' \ 1/4, 1/4, 1/4$ $(\bar{1}   1/2, 1/2, 1/2)'$	(10) $n' (1/2, 1/2, 0) \ x, y, 1/4$ $(m_z   1/2, 1/2, 1/2)'$	(11) $\bar{4}^+ \ 1/2, 0, z; \ 1/2, 0, 1/4$ $(\bar{4}_z   1/2, 1/2, 1/2)$	(12) $\bar{4}^- \ 0, 1/2, z; \ 0, 1/2, 1/4$ $(\bar{4}_z^{-1}   1/2, 1/2, 1/2)$
(13) $n (1/2, 0, 1/2) \ x, 1/4, z$ $(m_y   1/2, 1/2, 1/2)$	(14) $n (0, 1/2, 1/2) \ 1/4, y, z$ $(m_x   1/2, 1/2, 1/2)$	(15) $c' (0, 0, 1/2) \ x + 1/2, \bar{x}, z$ $(m_{xy}   1/2, 1/2, 1/2)'$	(16) $n' (1/2, 1/2, 1/2) \ x, x, z$ $(m_{\bar{xy}}   1/2, 1/2, 1/2)'$

**Generators selected** (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ;  $t'(1/2, 1/2, 1/2)$ ; (2); (3); (5); (9).**Positions**

			Coordinates				
			(0, 0, 0) +	(1/2, 1/2, 1/2)' +			
Multiplicity,	Wyckoff letter,	Site Symmetry.					
32	o	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{y}, x, z [v, \bar{u}, \bar{w}]$	(4) $y, \bar{x}, z [\bar{v}, u, \bar{w}]$	
			(5) $\bar{x}, y, \bar{z} [\bar{u}, \bar{v}, w]$	(6) $x, \bar{y}, \bar{z} [\bar{u}, v, w]$	(7) $y, x, \bar{z} [v, u, \bar{w}]$	(8) $\bar{y}, \bar{x}, \bar{z} [\bar{v}, \bar{u}, \bar{w}]$	
			(9) $\bar{x}, \bar{y}, \bar{z} [u, v, w]$	(10) $x, y, \bar{z} [\bar{u}, \bar{v}, w]$	(11) $y, \bar{x}, \bar{z} [v, \bar{u}, \bar{w}]$	(12) $\bar{y}, x, \bar{z} [\bar{v}, u, \bar{w}]$	
			(13) $x, \bar{y}, z [u, \bar{v}, w]$	(14) $\bar{x}, y, z [\bar{u}, v, w]$	(15) $\bar{y}, \bar{x}, z [v, u, \bar{w}]$	(16) $y, x, z [\bar{v}, \bar{u}, \bar{w}]$	
16	n	.m'	$0, y, z [0, v, w]$	$0, \bar{y}, z [0, \bar{v}, w]$	$\bar{y}, 0, z [v, 0, \bar{w}]$	$y, 0, z [\bar{v}, 0, \bar{w}]$	
			$0, y, \bar{z} [0, \bar{v}, w]$	$0, \bar{y}, \bar{z} [0, v, w]$	$y, 0, \bar{z} [v, 0, \bar{w}]$	$\bar{y}, 0, \bar{z} [\bar{v}, 0, \bar{w}]$	
16	m	..m	$x, x, z [\bar{u}, u, 0]$	$\bar{x}, \bar{x}, z [u, \bar{u}, 0]$	$\bar{x}, x, z [u, u, 0]$	$x, \bar{x}, z [\bar{u}, \bar{u}, 0]$	
			$\bar{x}, x, \bar{z} [\bar{u}, \bar{u}, 0]$	$x, \bar{x}, \bar{z} [u, u, 0]$	$x, x, \bar{z} [u, \bar{u}, 0]$	$\bar{x}, \bar{x}, \bar{z} [\bar{u}, \bar{u}, 0]$	
16	l	m..	$x, y, 0 [0, 0, w]$	$\bar{x}, \bar{y}, 0 [0, 0, w]$	$\bar{y}, x, 0 [0, 0, \bar{w}]$	$y, \bar{x}, 0 [0, 0, \bar{w}]$	
			$\bar{x}, y, 0 [0, 0, w]$	$x, \bar{y}, 0 [0, 0, w]$	$y, x, 0 [0, 0, \bar{w}]$	$\bar{y}, \bar{x}, 0 [0, 0, \bar{w}]$	
16	k	..2'	$x, x + 1/2, 1/4 [\bar{u}, u, w]$	$\bar{x}, \bar{x} + 1/2, 1/4 [u, \bar{u}, w]$	$\bar{x} + 1/2, x, 1/4 [u, u, \bar{w}]$	$x + 1/2, \bar{x}, 1/4 [\bar{u}, \bar{u}, \bar{w}]$	
			$\bar{x}, \bar{x} + 1/2, 3/4 [\bar{u}, u, w]$	$x, x + 1/2, 3/4 [u, \bar{u}, w]$	$x + 1/2, \bar{x}, 3/4 [u, u, \bar{w}]$	$\bar{x} + 1/2, x, 3/4 [\bar{u}, \bar{u}, \bar{w}]$	
8	j	m2'm'	$x, 1/2, 0 [0, 0, w]$	$\bar{x}, 1/2, 0 [0, 0, w]$	$1/2, x, 0 [0, 0, \bar{w}]$	$1/2, \bar{x}, 0 [0, 0, \bar{w}]$	
8	i	m2'm'	$x, 0, 0 [0, 0, w]$	$\bar{x}, 0, 0 [0, 0, w]$	$0, x, 0 [0, 0, \bar{w}]$	$0, \bar{x}, 0 [0, 0, \bar{w}]$	
8	h	m.2m	$x, x, 0 [0, 0, 0]$	$\bar{x}, \bar{x}, 0 [0, 0, 0]$	$\bar{x}, x, 0 [0, 0, 0]$	$x, \bar{x}, 0 [0, 0, 0]$	
8	g	2m'm'	$0, 1/2, z [0, 0, w]$	$1/2, 0, z [0, 0, \bar{w}]$	$0, 1/2, \bar{z} [0, 0, w]$	$1/2, 0, \bar{z} [0, 0, \bar{w}]$	
8	f	..2'/m	$1/4, 1/4, 1/4 [0, 0, 0]$	$3/4, 3/4, 1/4 [0, 0, 0]$	$3/4, 1/4, 1/4 [0, 0, 0]$	$1/4, 3/4, 1/4 [0, 0, 0]$	

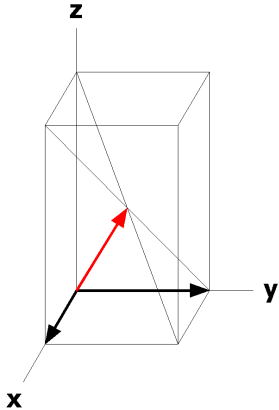
4	e	$4'm'm$	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$
4	d	$\bar{4}m'2'$	$0,1/2,1/4 [0,0,w]$	$1/2,0,1/4 [0,0,\bar{w}]$
4	c	$mm'm'$	$0,1/2,0 [0,0,w]$	$1/2,0,0 [0,0,\bar{w}]$
2	b	$4'/mm'm$	$0,0,1/2 [0,0,0]$	
2	a	$4'/mm'm$	$0,0,0 [0,0,0]$	

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c_p 2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $x,0,0$

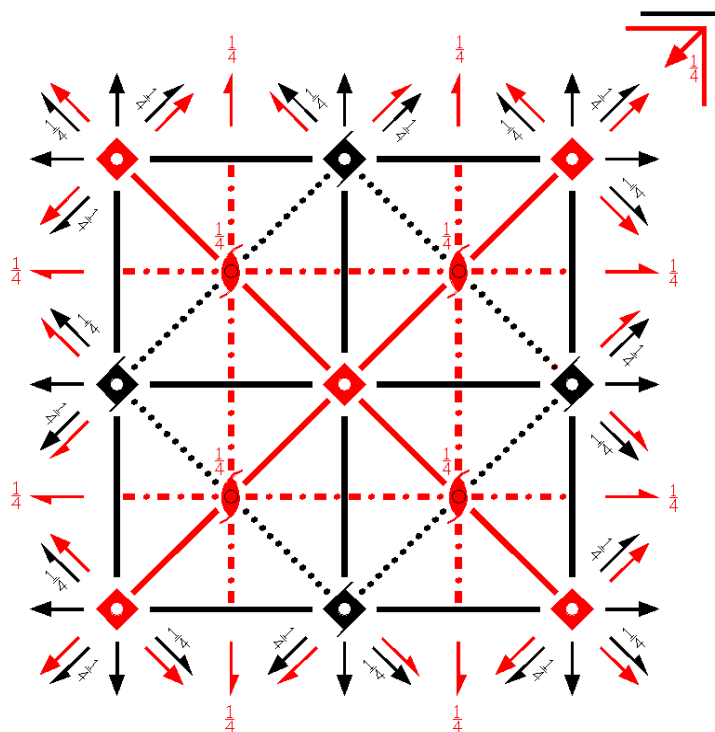
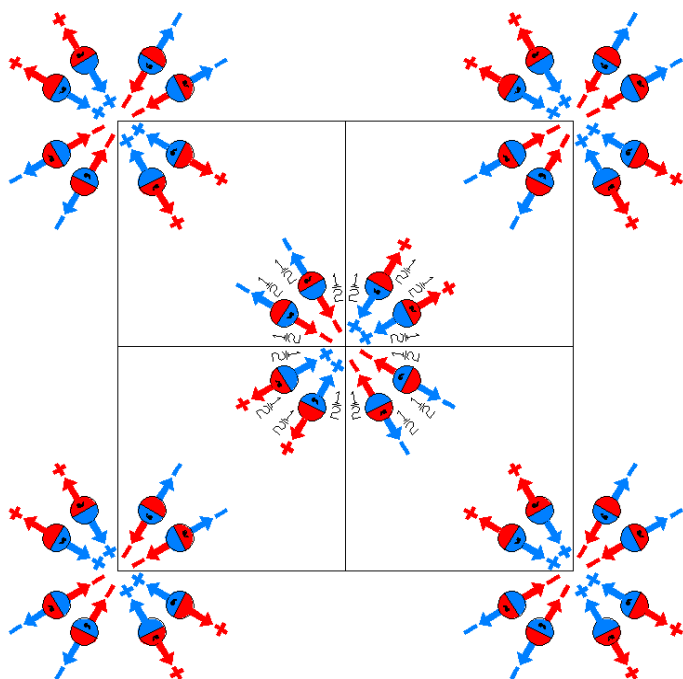
Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



$I_p 4'/mmm'$   
139.13.1191

$4/mmm1'$   
 $I_p 4'/m2/m2'/m'$

Tetragonal



Origin at center ( $4'/mmm'$ )

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $x \leq y$

Symmetry Operations

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                      | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'         | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'         |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                    | (8) 2' x,x̄,0<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,0)'                   |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)              | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub>  0,0,0)' | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0) | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (15) m' x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'                  | (16) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                                 |

For  $(1/2, 1/2, 1/2)'$  + set

(1) $t' (1/2, 1/2, 1/2)$ $(1   1/2, 1/2, 1/2)'$	(2) $2' (0, 0, 1/2) \ 1/4, 1/4, z$ $(2_z   1/2, 1/2, 1/2)'$	(3) $4^+ (0, 0, 1/2) \ 0, 1/2, z$ $(4_z   1/2, 1/2, 1/2)$	(4) $4^- (0, 0, 1/2) \ 1/2, 0, z$ $(4_z^{-1}   1/2, 1/2, 1/2)$
(5) $2' (0, 1/2, 0) \ 1/4, y, 1/4$ $(2_y   1/2, 1/2, 1/2)'$	(6) $2' (1/2, 0, 0) \ x, 1/4, 1/4$ $(2_x   1/2, 1/2, 1/2)'$	(7) $2 (1/2, 1/2, 0) \ x, x, 1/4$ $(2_{xy}   1/2, 1/2, 1/2)$	(8) $2 \ x, \bar{x} + 1/2, 1/4$ $(2_{\bar{xy}}   1/2, 1/2, 1/2)$
(9) $\bar{1}' \ 1/4, 1/4, 1/4$ $(\bar{1}   1/2, 1/2, 1/2)'$	(10) $n' (1/2, 1/2, 0) \ x, y, 1/4$ $(m_z   1/2, 1/2, 1/2)'$	(11) $\bar{4}^+ \ 1/2, 0, z; \ 1/2, 0, 1/4$ $(\bar{4}_z   1/2, 1/2, 1/2)$	(12) $\bar{4}^- \ 0, 1/2, z; \ 0, 1/2, 1/4$ $(\bar{4}_z^{-1}   1/2, 1/2, 1/2)$
(13) $n' (1/2, 0, 1/2) \ x, 1/4, z$ $(m_y   1/2, 1/2, 1/2)'$	(14) $n' (0, 1/2, 1/2) \ 1/4, y, z$ $(m_x   1/2, 1/2, 1/2)'$	(15) $c (0, 0, 1/2) \ x + 1/2, \bar{x}, z$ $(m_{xy}   1/2, 1/2, 1/2)$	(16) $n (1/2, 1/2, 1/2) \ x, x, z$ $(m_{\bar{xy}}   1/2, 1/2, 1/2)$

**Generators selected** (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ;  $t'(1/2, 1/2, 1/2)$ ; (2); (3); (5); (9).

**Positions**

			Coordinates			
			$(0, 0, 0) +$		$(1/2, 1/2, 1/2)'$ +	
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	o	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{y}, x, z [v, \bar{u}, \bar{w}]$	(4) $y, \bar{x}, z [\bar{v}, u, \bar{w}]$
			(5) $\bar{x}, y, z [\bar{u}, v, \bar{w}]$	(6) $x, \bar{y}, z [u, \bar{v}, \bar{w}]$	(7) $y, x, z [v, \bar{u}, w]$	(8) $\bar{y}, \bar{x}, z [v, u, w]$
			(9) $\bar{x}, \bar{y}, z [u, v, w]$	(10) $x, y, z [\bar{u}, \bar{v}, w]$	(11) $y, \bar{x}, z [v, \bar{u}, \bar{w}]$	(12) $\bar{y}, x, z [\bar{v}, u, \bar{w}]$
			(13) $x, \bar{y}, z [\bar{u}, v, \bar{w}]$	(14) $\bar{x}, y, z [u, \bar{v}, \bar{w}]$	(15) $\bar{y}, \bar{x}, z [v, \bar{u}, w]$	(16) $y, x, z [v, u, w]$
16	n	.m.	$0, y, z [u, 0, 0]$	$0, \bar{y}, z [\bar{u}, 0, 0]$	$\bar{y}, 0, z [0, \bar{u}, 0]$	$y, 0, z [0, u, 0]$
			$0, y, z [\bar{u}, 0, 0]$	$0, \bar{y}, z [u, 0, 0]$	$y, 0, z [0, \bar{u}, 0]$	$\bar{y}, 0, z [0, u, 0]$
16	m	..m'	$x, x, z [u, u, w]$	$\bar{x}, \bar{x}, z [\bar{u}, \bar{u}, w]$	$\bar{x}, x, z [u, \bar{u}, \bar{w}]$	$x, \bar{x}, z [\bar{u}, u, \bar{w}]$
			$\bar{x}, x, z [\bar{u}, u, \bar{w}]$	$x, \bar{x}, z [u, \bar{u}, w]$	$x, x, z [u, \bar{u}, w]$	$\bar{x}, \bar{x}, z [\bar{u}, u, w]$
16	l	m..	$x, y, 0 [0, 0, w]$	$\bar{x}, \bar{y}, 0 [0, 0, w]$	$\bar{y}, x, 0 [0, 0, \bar{w}]$	$y, \bar{x}, 0 [0, 0, \bar{w}]$
			$\bar{x}, y, 0 [0, 0, \bar{w}]$	$x, \bar{y}, 0 [0, 0, w]$	$y, x, 0 [0, 0, w]$	$\bar{y}, \bar{x}, 0 [0, 0, w]$
16	k	..2	$x, x + 1/2, 1/4 [u, u, 0]$	$\bar{x}, \bar{x} + 1/2, 1/4 [\bar{u}, \bar{u}, 0]$	$\bar{x} + 1/2, x, 1/4 [u, \bar{u}, 0]$	$x + 1/2, \bar{x}, 1/4 [\bar{u}, u, 0]$
			$\bar{x}, \bar{x} + 1/2, 3/4 [u, u, 0]$	$x, x + 1/2, 3/4 [\bar{u}, \bar{u}, 0]$	$x + 1/2, \bar{x}, 3/4 [u, \bar{u}, 0]$	$\bar{x} + 1/2, x, 3/4 [\bar{u}, u, 0]$
8	j	m2m.	$x, 1/2, 0 [0, 0, 0]$	$\bar{x}, 1/2, 0 [0, 0, 0]$	$1/2, x, 0 [0, 0, 0]$	$1/2, \bar{x}, 0 [0, 0, 0]$
8	i	m2m.	$x, 0, 0 [0, 0, 0]$	$\bar{x}, 0, 0 [0, 0, 0]$	$0, x, 0 [0, 0, 0]$	$0, \bar{x}, 0 [0, 0, 0]$
8	h	m.2'm'	$x, x, 0 [0, 0, w]$	$\bar{x}, \bar{x}, 0 [0, 0, w]$	$\bar{x}, x, 0 [0, 0, \bar{w}]$	$x, \bar{x}, 0 [0, 0, \bar{w}]$
8	g	2mm.	$0, 1/2, z [0, 0, 0]$	$1/2, 0, z [0, 0, 0]$	$0, 1/2, \bar{z} [0, 0, 0]$	$1/2, 0, \bar{z} [0, 0, 0]$
8	f	..2/m'	$1/4, 1/4, 1/4 [0, 0, 0]$	$3/4, 3/4, 1/4 [0, 0, 0]$	$3/4, 1/4, 1/4 [0, 0, 0]$	$1/4, 3/4, 1/4 [0, 0, 0]$

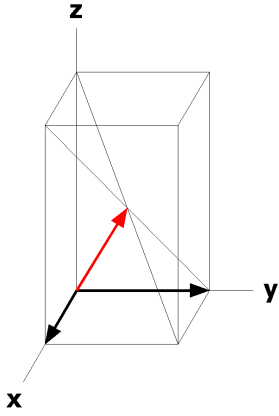
4	e	$4'mm'$	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$
4	d	$\bar{4}m2$	$0,1/2,1/4 [0,0,0]$	$1/2,0,1/4 [0,0,0]$
4	c	$mmm.$	$0,1/2,0 [0,0,0]$	$1/2,0,0 [0,0,0]$
2	b	$4'/mmm'$	$0,0,1/2 [0,0,0]$	
2	a	$4'/mmm'$	$0,0,0 [0,0,0]$	

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p_{2a} 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,1/4$



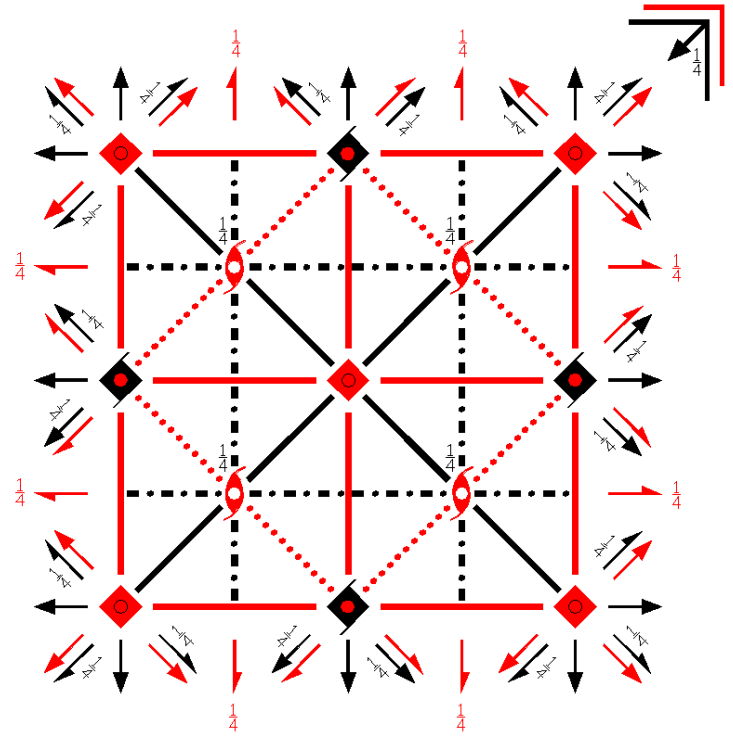
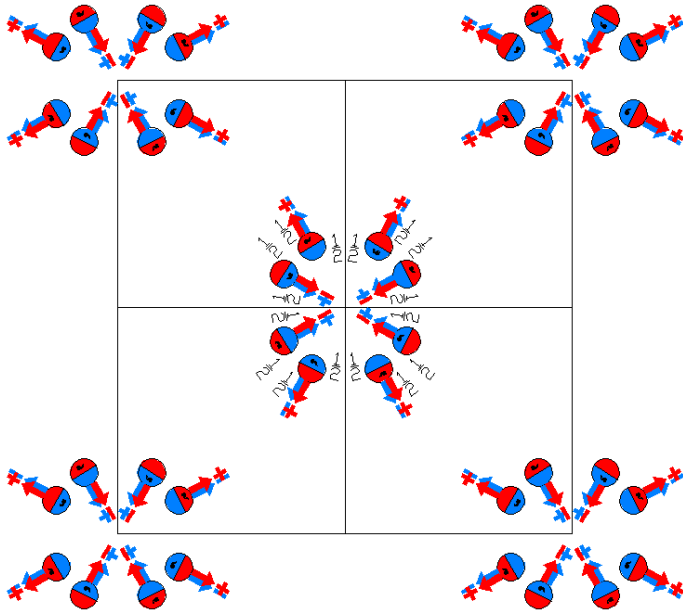
$I_p 4'/m'm'm$

139.14.1192

$4/mmm1'$

$I_p 4'/m'2'/m'2'/m$

Tetragonal



Origin at center ( $4'/m'm'm$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; x \leq y$

Symmetry Operations

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                        | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'                     | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'        |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)    | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)    | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                                | (8) 2' x,x̄,0<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,0)'                   |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'               | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)' | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (15) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                                | (16) m x,x,z<br>(m <sub>xy</sub> <sup>-</sup>  0,0,0)                     |

For  $(1/2, 1/2, 1/2)'$  + set

(1) $t' (1/2, 1/2, 1/2)$ $(1   1/2, 1/2, 1/2)'$	(2) $2' (0, 0, 1/2) \quad 1/4, 1/4, z$ $(2_z   1/2, 1/2, 1/2)'$	(3) $4^+ (0, 0, 1/2) \quad 0, 1/2, z$ $(4_z   1/2, 1/2, 1/2)$	(4) $4^- (0, 0, 1/2) \quad 1/2, 0, z$ $(4_z^{-1}   1/2, 1/2, 1/2)$
(5) $2' (0, 1/2, 0) \quad 1/4, y, 1/4$ $(2_y   1/2, 1/2, 1/2)'$	(6) $2' (1/2, 0, 0) \quad x, 1/4, 1/4$ $(2_x   1/2, 1/2, 1/2)'$	(7) $2 (1/2, 1/2, 0) \quad x, x, 1/4$ $(2_{xy}   1/2, 1/2, 1/2)$	(8) $2 \quad x, \bar{x} + 1/2, 1/4$ $(2_{\bar{xy}}   1/2, 1/2, 1/2)$
(9) $\bar{1} \quad 1/4, 1/4, 1/4$ $(\bar{1}   1/2, 1/2, 1/2)$	(10) $n (1/2, 1/2, 0) \quad x, y, 1/4$ $(m_z   1/2, 1/2, 1/2)$	(11) $\bar{4}^+ \quad 1/2, 0, z; \quad 1/2, 0, 1/4$ $(\bar{4}_z   1/2, 1/2, 1/2)'$	(12) $\bar{4}^- \quad 0, 1/2, z; \quad 0, 1/2, 1/4$ $(\bar{4}_z^{-1}   1/2, 1/2, 1/2)'$
(13) $n (1/2, 0, 1/2) \quad x, 1/4, z$ $(m_y   1/2, 1/2, 1/2)$	(14) $n (0, 1/2, 1/2) \quad 1/4, y, z$ $(m_x   1/2, 1/2, 1/2)$	(15) $c' (0, 0, 1/2) \quad x + 1/2, \bar{x}, z$ $(m_{xy}   1/2, 1/2, 1/2)'$	(16) $n' (1/2, 1/2, 1/2) \quad x, x, z$ $(m_{\bar{xy}}   1/2, 1/2, 1/2)'$

**Generators selected** (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ;  $t'(1/2, 1/2, 1/2)$ ; (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0, 0, 0) +	(1/2, 1/2, 1/2)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	o	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{y}, x, z [v, \bar{u}, \bar{w}]$	(4) $y, \bar{x}, z [\bar{v}, u, \bar{w}]$
			(5) $\bar{x}, y, z [\bar{u}, v, \bar{w}]$	(6) $x, \bar{y}, z [u, \bar{v}, \bar{w}]$	(7) $y, x, z [\bar{v}, \bar{u}, w]$	(8) $\bar{y}, \bar{x}, z [v, u, w]$
			(9) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, \bar{w}]$	(10) $x, y, z [u, v, \bar{w}]$	(11) $y, \bar{x}, z [\bar{v}, u, w]$	(12) $\bar{y}, x, z [v, \bar{u}, w]$
			(13) $x, \bar{y}, z [u, \bar{v}, w]$	(14) $\bar{x}, y, z [\bar{u}, v, w]$	(15) $\bar{y}, \bar{x}, z [v, u, \bar{w}]$	(16) $y, x, z [\bar{v}, \bar{u}, \bar{w}]$
16	n	.m'	$0, y, z [0, v, w]$	$0, \bar{y}, z [0, \bar{v}, w]$	$\bar{y}, 0, z [v, 0, \bar{w}]$	$y, 0, z [\bar{v}, 0, \bar{w}]$
			$0, y, z [0, v, \bar{w}]$	$0, \bar{y}, z [0, \bar{v}, \bar{w}]$	$y, 0, z [\bar{v}, 0, w]$	$\bar{y}, 0, z [v, 0, \bar{w}]$
16	m	..m	$x, x, z [\bar{u}, u, 0]$	$\bar{x}, \bar{x}, z [u, \bar{u}, 0]$	$\bar{x}, x, z [u, u, 0]$	$x, \bar{x}, z [\bar{u}, \bar{u}, 0]$
			$\bar{x}, x, z [u, u, 0]$	$x, \bar{x}, z [\bar{u}, \bar{u}, 0]$	$x, x, z [\bar{u}, u, 0]$	$\bar{x}, \bar{x}, z [u, \bar{u}, 0]$
16	l	m'..	$x, y, 0 [u, v, 0]$	$\bar{x}, \bar{y}, 0 [\bar{u}, \bar{v}, 0]$	$\bar{y}, x, 0 [v, \bar{u}, 0]$	$y, \bar{x}, 0 [\bar{v}, u, 0]$
			$\bar{x}, y, 0 [\bar{u}, v, 0]$	$x, \bar{y}, 0 [u, \bar{v}, 0]$	$y, x, 0 [v, \bar{u}, 0]$	$\bar{y}, \bar{x}, 0 [v, u, 0]$
16	k	..2	$x, x + 1/2, 1/4 [u, u, 0]$	$\bar{x}, \bar{x} + 1/2, 1/4 [\bar{u}, \bar{u}, 0]$	$\bar{x} + 1/2, x, 1/4 [u, \bar{u}, 0]$	$x + 1/2, \bar{x}, 1/4 [\bar{u}, u, 0]$
			$\bar{x}, \bar{x} + 1/2, 3/4 [\bar{u}, \bar{u}, 0]$	$x, x + 1/2, 3/4 [u, u, 0]$	$x + 1/2, \bar{x}, 3/4 [\bar{u}, u, 0]$	$\bar{x} + 1/2, x, 3/4 [u, \bar{u}, 0]$
8	j	m'2m'	$x, 1/2, 0 [u, 0, 0]$	$\bar{x}, 1/2, 0 [\bar{u}, 0, 0]$	$1/2, x, 0 [0, \bar{u}, 0]$	$1/2, \bar{x}, 0 [0, u, 0]$
8	i	m'2m'	$x, 0, 0 [u, 0, 0]$	$\bar{x}, 0, 0 [\bar{u}, 0, 0]$	$0, x, 0 [0, \bar{u}, 0]$	$0, \bar{x}, 0 [0, u, 0]$
8	h	m'.2'm	$x, x, 0 [\bar{u}, u, 0]$	$\bar{x}, \bar{x}, 0 [u, \bar{u}, 0]$	$\bar{x}, x, 0 [u, u, 0]$	$x, \bar{x}, 0 [\bar{u}, \bar{u}, 0]$
8	g	2m'm'	$0, 1/2, z [0, 0, w]$	$1/2, 0, z [0, 0, \bar{w}]$	$0, 1/2, z [0, 0, \bar{w}]$	$1/2, 0, z [0, 0, w]$
8	f	..2/m	$1/4, 1/4, 1/4 [\bar{u}, u, 0]$	$3/4, 3/4, 1/4 [u, \bar{u}, 0]$	$3/4, 1/4, 1/4 [u, u, 0]$	$1/4, 3/4, 1/4 [\bar{u}, \bar{u}, 0]$

4	e	$4'm'm$	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$
4	d	$\bar{4}'m'2$	$0,1/2,1/4 [0,0,0]$	$1/2,0,1/4 [0,0,0]$
4	c	$m'm'm'$	$0,1/2,0 [0,0,0]$	$1/2,0,0 [0,0,0]$
2	b	$4'/m'm'm$	$0,0,1/2 [0,0,0]$	
2	a	$4'/m'm'm$	$0,0,0 [0,0,0]$	

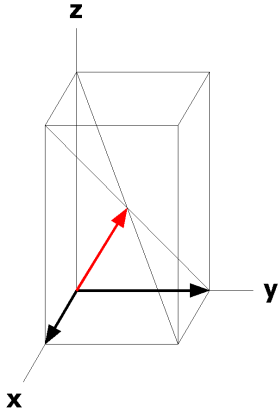
### Symmetry of Special Projections

Along  $[0,0,1]$   $p_p 4'mm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c_p 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$

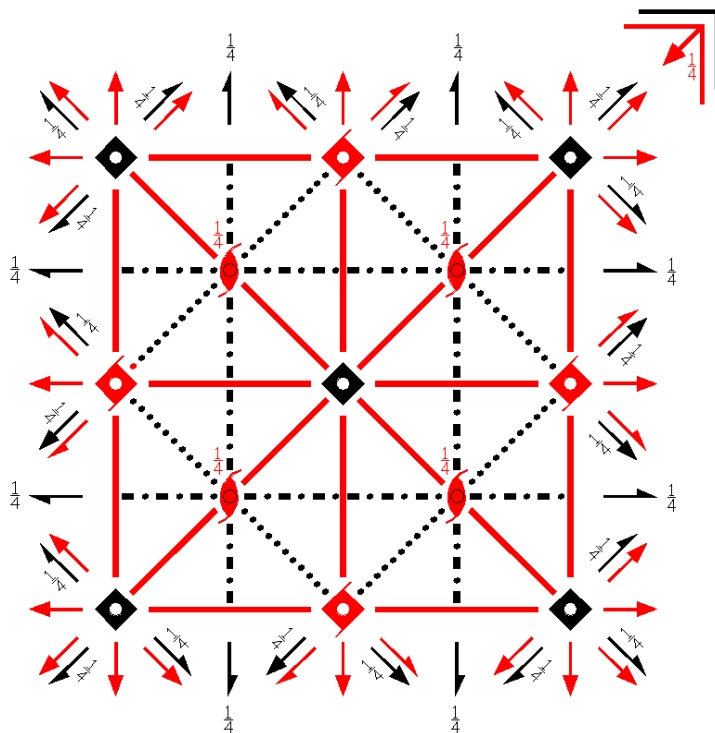
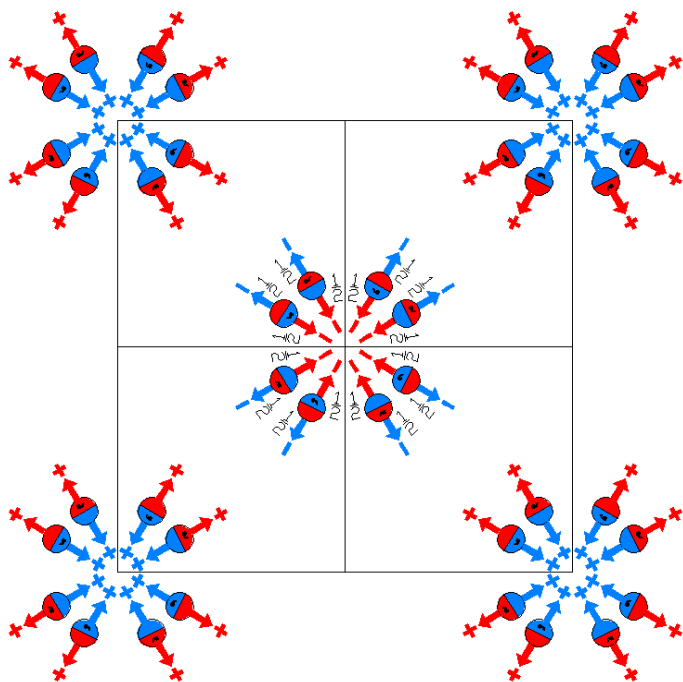




$I_P 4/m\bar{m}'m'$   
139.15.1193

$4/m\bar{m}m1'$   
 $I_P 4/m2'/m'2'/m'$

Tetragonal



Origin at center ( $4/m\bar{m}'m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; x \leq y$

Symmetry Operations

For (0,0,0) + set

- |  |   |  |  |
|--|---|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)      | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)      |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'   | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'  | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                | (8) 2' x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)' |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)   | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0) | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)               |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)'  | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)' | (15) m' x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)'     | (16) m' x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,0)'          |

## For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (1   1/2,1/2,1/2)'	(2) 2' (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)'	(3) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)'	(4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)'
(5) 2 (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>   1/2,1/2,1/2)	(6) 2 (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>   1/2,1/2,1/2)	(7) 2 (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)	(8) 2 x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub> <sup>-</sup>   1/2,1/2,1/2)
(9) $\bar{1}$ ' 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)'	(10) n' (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)'	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$   1/2,1/2,1/2)'
(13) n (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)	(14) n (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)	(15) c (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,1/2)	(16) n (1/2,1/2,1/2) x,x,z (m <sub>xy</sub> <sup>-</sup>   1/2,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	o	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(6) x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]
			(13) x, $\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},\bar{v},w$ ]	(15) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(16) y,x,z [v,u,w]
16	n	.m'	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	$\bar{y},0,z$ [ $\bar{v},0,w$ ]	y,0,z [v,0,w]
			0,y, $\bar{z}$ [0, $\bar{v},w$ ]	0, $\bar{y},\bar{z}$ [0,v,w]	y,0, $\bar{z}$ [ $\bar{v},0,w$ ]	$\bar{y},0,\bar{z}$ [v,0,w]
16	m	..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,z$ [ $\bar{u},u,w$ ]	x, $\bar{x},z$ [ $\bar{u},\bar{u},w$ ]
			$\bar{x},x,\bar{z}$ [u, $\bar{u},w$ ]	x, $\bar{x},\bar{z}$ [ $\bar{u},u,w$ ]	x,x, $\bar{z}$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},\bar{z}$ [u,u,w]
16	l	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0,w]	y, $\bar{x},0$ [0,0,w]
			$\bar{x},y,0$ [0,0,w]	x, $\bar{y},0$ [0,0,w]	y,x,0 [0,0,w]	$\bar{y},\bar{x},0$ [0,0,w]
16	k	..2	x,x+1/2,1/4 [u,u,0]	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,1/4$ [ $\bar{u},u,0$ ]	x+1/2, $\bar{x},1/4$ [u, $\bar{u},0$ ]
			$\bar{x},\bar{x}+1/2,3/4$ [u,u,0]	x,x+1/2,3/4 [ $\bar{u},\bar{u},0$ ]	x+1/2, $\bar{x},3/4$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,x,3/4$ [u, $\bar{u},0$ ]
8	j	m2'm'	x,1/2,0 [0,0,w]	$\bar{x},1/2,0$ [0,0,w]	1/2,x,0 [0,0,w]	1/2, $\bar{x},0$ [0,0,w]
8	i	m2'm'	x,0,0 [0,0,w]	$\bar{x},0,0$ [0,0,w]	0,x,0 [0,0,w]	0, $\bar{x},0$ [0,0,w]
8	h	m.2'm'	x,x,0 [0,0,w]	$\bar{x},\bar{x},0$ [0,0,w]	$\bar{x},x,0$ [0,0,w]	x, $\bar{x},0$ [0,0,w]
8	g	2m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]
8	f	..2/m'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]

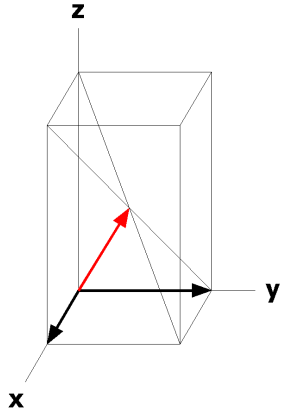
4	e	$4m'm'$	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,w]$
4	d	$\bar{4}'m'2$	$0,1/2,1/4 [0,0,0]$	$1/2,0,1/4 [0,0,0]$
4	c	$mm'm'$	$0,1/2,0 [0,0,w]$	$1/2,0,0 [0,0,w]$
2	b	$4/mm'm'$	$0,0,1/2 [0,0,w]$	
2	a	$4/mm'm'$	$0,0,0 [0,0,w]$	

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c_p \cdot 2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $x,0,0$

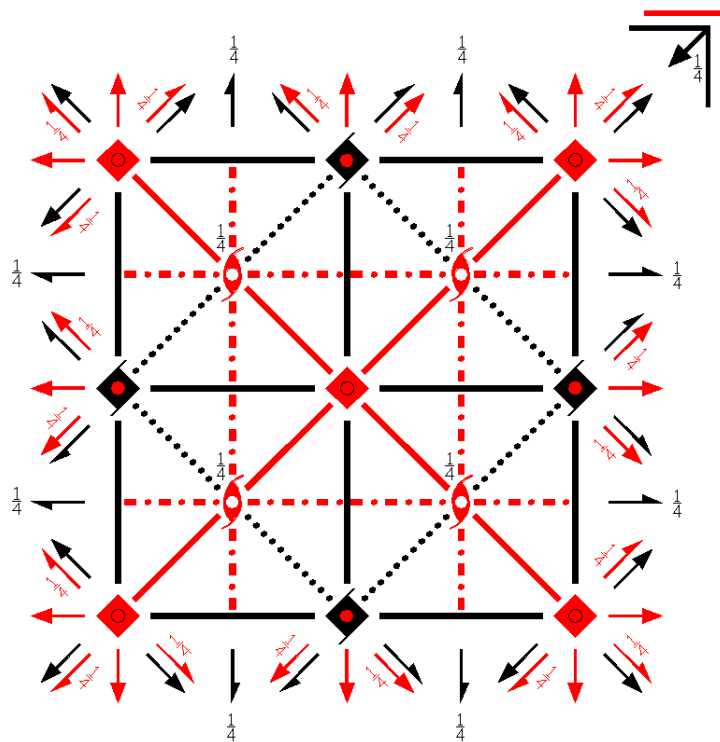
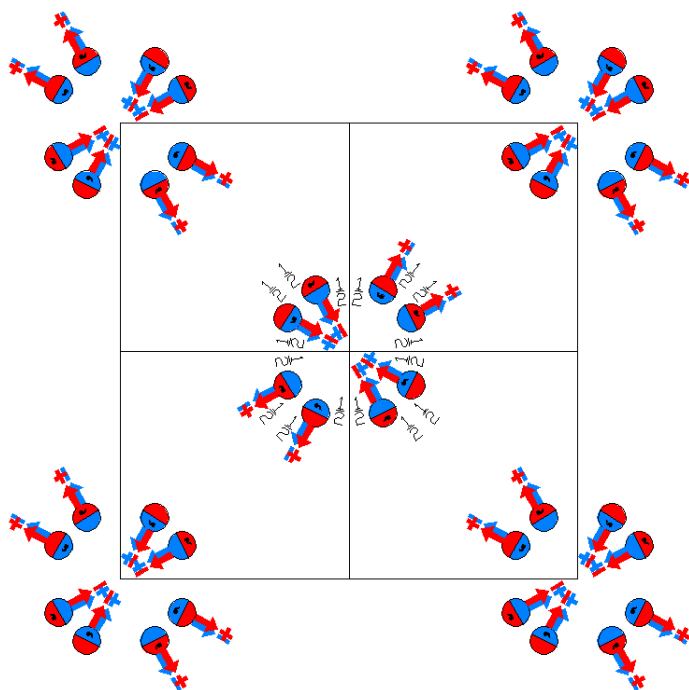
Along  $[1,1,0]$   $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,1/4$



$I_P 4'/m'mm'$   
139.16.1194

$4/mmm1'$   
 $I_P 4'/m'2'/m2/m'$

Tetragonal



Origin at center ( $4'/m'mm'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; x \leq y$

### Symmetry Operations

For (0,0,0) + set

- |  |   |  |  |
|--|---|--|--|
| (1) 1<br>(1 0,0,0)                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)    | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)'        | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'        |
| (5) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)' | (6) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                  | (8) 2 x,x̄,0<br>(2 <sub>xȳ</sub>  0,0,0)                                |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'              | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)' | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0) |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)  | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   | (15) m' x,x̄,z<br>(m <sub>xy</sub>  0,0,0)'                              | (16) m' x,x,z<br>(m <sub>xy</sub>  0,0,0)'                               |

For  $(1/2, 1/2, 1/2)'$  + set

(1) $t' (1/2, 1/2, 1/2)$ $(1   1/2, 1/2, 1/2)'$	(2) $2' (0, 0, 1/2) \ 1/4, 1/4, z$ $(2_z   1/2, 1/2, 1/2)'$	(3) $4^+ (0, 0, 1/2) \ 0, 1/2, z$ $(4_z   1/2, 1/2, 1/2)$	(4) $4^- (0, 0, 1/2) \ 1/2, 0, z$ $(4_z^{-1}   1/2, 1/2, 1/2)$
(5) $2 (0, 1/2, 0) \ 1/4, y, 1/4$ $(2_y   1/2, 1/2, 1/2)$	(6) $2 (1/2, 0, 0) \ x, 1/4, 1/4$ $(2_x   1/2, 1/2, 1/2)$	(7) $2' (1/2, 1/2, 0) \ x, x, 1/4$ $(2_{xy}   1/2, 1/2, 1/2)'$	(8) $2' \ x, \bar{x} + 1/2, 1/4$ $(2_{\bar{xy}}   1/2, 1/2, 1/2)'$
(9) $\bar{1} \ 1/4, 1/4, 1/4$ $(\bar{1}   1/2, 1/2, 1/2)$	(10) $n (1/2, 1/2, 0) \ x, y, 1/4$ $(m_z   1/2, 1/2, 1/2)$	(11) $\bar{4}^+ \ 1/2, 0, z; \ 1/2, 0, 1/4$ $(\bar{4}_z   1/2, 1/2, 1/2)'$	(12) $\bar{4}^- \ 0, 1/2, z; \ 0, 1/2, 1/4$ $(\bar{4}_z^{-1}   1/2, 1/2, 1/2)'$
(13) $n' (1/2, 0, 1/2) \ x, 1/4, z$ $(m_y   1/2, 1/2, 1/2)'$	(14) $n' (0, 1/2, 1/2) \ 1/4, y, z$ $(m_x   1/2, 1/2, 1/2)'$	(15) $c (0, 0, 1/2) \ x + 1/2, \bar{x}, z$ $(m_{xy}   1/2, 1/2, 1/2)$	(16) $n (1/2, 1/2, 1/2) \ x, x, z$ $(m_{\bar{xy}}   1/2, 1/2, 1/2)$

**Generators selected** (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ;  $t'(1/2, 1/2, 1/2)$ ; (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0, 0, 0) +	(1/2, 1/2, 1/2)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	o	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{y}, x, z [v, \bar{u}, \bar{w}]$	(4) $y, \bar{x}, z [\bar{v}, u, \bar{w}]$
			(5) $\bar{x}, y, \bar{z} [u, \bar{v}, w]$	(6) $x, \bar{y}, \bar{z} [\bar{u}, v, w]$	(7) $y, x, \bar{z} [v, u, \bar{w}]$	(8) $\bar{y}, \bar{x}, \bar{z} [\bar{v}, \bar{u}, \bar{w}]$
			(9) $\bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$	(10) $x, y, \bar{z} [u, v, \bar{w}]$	(11) $y, \bar{x}, \bar{z} [\bar{v}, u, w]$	(12) $\bar{y}, x, \bar{z} [v, \bar{u}, w]$
			(13) $x, \bar{y}, z [\bar{u}, v, \bar{w}]$	(14) $\bar{x}, y, z [u, \bar{v}, \bar{w}]$	(15) $\bar{y}, \bar{x}, z [\bar{v}, \bar{u}, w]$	(16) $y, x, z [v, u, w]$
16	n	.m.	$0, y, z [u, 0, 0]$	$0, \bar{y}, z [\bar{u}, 0, 0]$	$\bar{y}, 0, z [0, \bar{u}, 0]$	$y, 0, z [0, u, 0]$
			$0, y, \bar{z} [u, 0, 0]$	$0, \bar{y}, \bar{z} [\bar{u}, 0, 0]$	$y, 0, \bar{z} [0, u, 0]$	$\bar{y}, 0, \bar{z} [0, \bar{u}, 0]$
16	m	..m'	$x, x, z [u, u, w]$	$\bar{x}, \bar{x}, z [\bar{u}, \bar{u}, w]$	$\bar{x}, x, z [u, \bar{u}, \bar{w}]$	$x, \bar{x}, z [\bar{u}, u, \bar{w}]$
			$\bar{x}, x, \bar{z} [u, \bar{u}, w]$	$x, \bar{x}, \bar{z} [\bar{u}, u, w]$	$x, x, \bar{z} [u, u, \bar{w}]$	$\bar{x}, \bar{x}, \bar{z} [\bar{u}, \bar{u}, \bar{w}]$
16	l	m'..	$x, y, 0 [u, v, 0]$	$\bar{x}, \bar{y}, 0 [\bar{u}, \bar{v}, 0]$	$\bar{y}, x, 0 [v, \bar{u}, 0]$	$y, \bar{x}, 0 [\bar{v}, u, 0]$
			$\bar{x}, y, 0 [u, \bar{v}, 0]$	$x, \bar{y}, 0 [\bar{u}, v, 0]$	$y, x, 0 [v, u, 0]$	$\bar{y}, \bar{x}, 0 [\bar{v}, \bar{u}, 0]$
16	k	..2'	$x, x + 1/2, 1/4 [\bar{u}, u, w]$	$\bar{x}, \bar{x} + 1/2, 1/4 [u, \bar{u}, w]$	$\bar{x} + 1/2, x, 1/4 [u, u, \bar{w}]$	$x + 1/2, \bar{x}, 1/4 [\bar{u}, \bar{u}, \bar{w}]$
			$\bar{x}, \bar{x} + 1/2, 3/4 [u, \bar{u}, \bar{w}]$	$x, x + 1/2, 3/4 [\bar{u}, u, w]$	$x + 1/2, \bar{x}, 3/4 [\bar{u}, \bar{u}, w]$	$\bar{x} + 1/2, x, 3/4 [u, u, w]$
8	j	m'2'm.	$x, 1/2, 0 [0, v, 0]$	$\bar{x}, 1/2, 0 [0, \bar{v}, 0]$	$1/2, x, 0 [v, 0, 0]$	$1/2, \bar{x}, 0 [\bar{v}, 0, 0]$
8	i	m'2'm.	$x, 0, 0 [0, v, 0]$	$\bar{x}, 0, 0 [0, \bar{v}, 0]$	$0, x, 0 [v, 0, 0]$	$0, \bar{x}, 0 [\bar{v}, 0, 0]$
8	h	m'.2m'	$x, x, 0 [u, u, 0]$	$\bar{x}, \bar{x}, 0 [\bar{u}, \bar{u}, 0]$	$\bar{x}, x, 0 [u, \bar{u}, 0]$	$x, \bar{x}, 0 [\bar{u}, u, 0]$
8	g	2mm.	$0, 1/2, z [0, 0, 0]$	$1/2, 0, z [0, 0, 0]$	$0, 1/2, \bar{z} [0, 0, 0]$	$1/2, 0, \bar{z} [0, 0, 0]$
8	f	..2'/m'	$1/4, 1/4, 1/4 [\bar{u}, u, 0]$	$3/4, 3/4, 1/4 [u, \bar{u}, 0]$	$3/4, 1/4, 1/4 [u, u, 0]$	$1/4, 3/4, 1/4 [\bar{u}, \bar{u}, 0]$

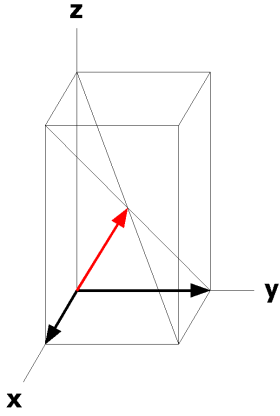
4	e	$4'mm'$	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$
4	d	$\bar{4}'m2'$	$0,1/2,1/4 [0,0,0]$	$1/2,0,1/4 [0,0,0]$
4	c	$m'mm.$	$0,1/2,0 [0,0,0]$	$1/2,0,0 [0,0,0]$
2	b	$4'/m'mm'$	$0,0,1/2 [0,0,0]$	
2	a	$4'/m'mm'$	$0,0,0 [0,0,0]$	

### Symmetry of Special Projections

Along  $[0,0,1]$   $p_p 4'm'm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p_{2a} 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,0$



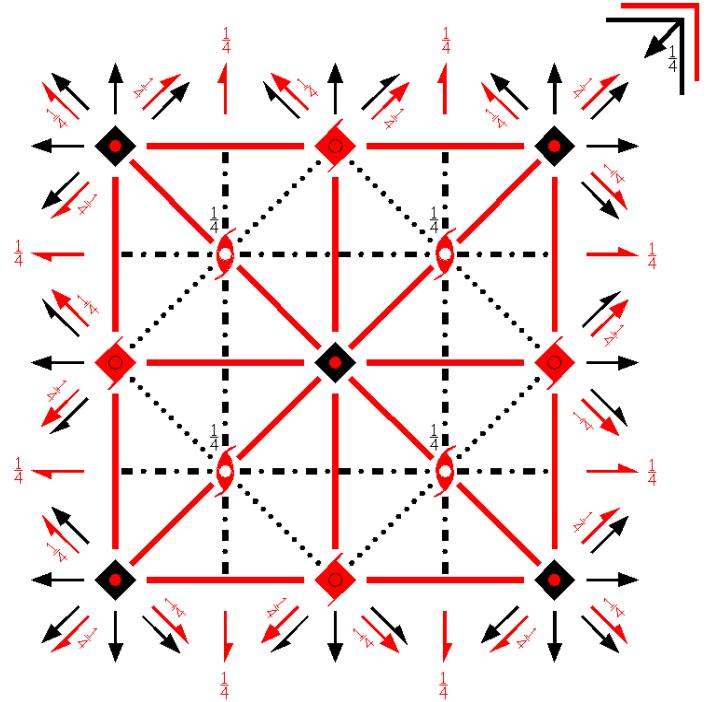
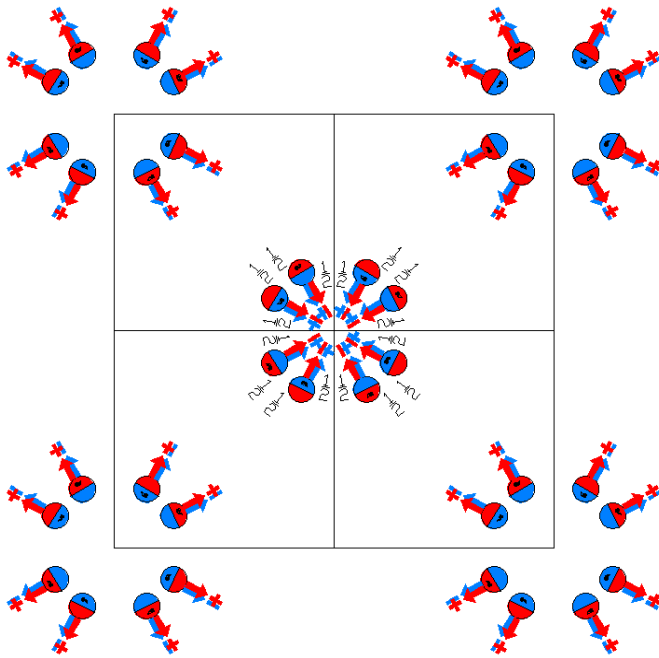
$I_P 4/m'm'm'$

139.17.1195

$4/mmm1'$

$I_P 4/m'2/m'2/m'$

Tetragonal



Origin at center ( $4/m'm'm'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; x \leq y$

Symmetry Operations

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                             | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)     | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)   | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)                             |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)         | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)     | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)   | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)                          |
| (9) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$ ' 0,0,0)' | (10) m' x,y,0<br>(m' <sub>z</sub>  0,0,0)' | (11) $\bar{4}$ <sup>+</sup> ' 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>+</sup> ' 0,0,0)' | (12) $\bar{4}$ <sup>-</sup> ' 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>-</sup> ' 0,0,0)' |
| (13) m' x,0,z<br>(m' <sub>y</sub>  0,0,0)'     | (14) m' 0,y,z<br>(m' <sub>x</sub>  0,0,0)' | (15) m' x, $\bar{x}$ ,z<br>(m' <sub>xy</sub>  0,0,0)'   | (16) m' x,x,z<br>(m' <sub><math>\bar{xy}</math></sub>  0,0,0)'                                |

For  $(1/2, 1/2, 1/2)'$  + set

(1) $t' (1/2, 1/2, 1/2)$ $(1   1/2, 1/2, 1/2)'$	(2) $2' (0, 0, 1/2) \quad 1/4, 1/4, z$ $(2_z   1/2, 1/2, 1/2)'$	(3) $4^{*+} (0, 0, 1/2) \quad 0, 1/2, z$ $(4_z   1/2, 1/2, 1/2)'$	(4) $4' (0, 0, 1/2) \quad 1/2, 0, z$ $(4_z^{-1}   1/2, 1/2, 1/2)'$
(5) $2' (0, 1/2, 0) \quad 1/4, y, 1/4$ $(2_y   1/2, 1/2, 1/2)'$	(6) $2' (1/2, 0, 0) \quad x, 1/4, 1/4$ $(2_x   1/2, 1/2, 1/2)'$	(7) $2' (1/2, 1/2, 0) \quad x, x, 1/4$ $(2_{xy}   1/2, 1/2, 1/2)'$	(8) $2' \quad x, \bar{x} + 1/2, 1/4$ $(2_{\bar{xy}}   1/2, 1/2, 1/2)'$
(9) $\bar{1}' \quad 1/4, 1/4, 1/4$ $(\bar{1}   1/2, 1/2, 1/2)'$	(10) $n' (1/2, 1/2, 0) \quad x, y, 1/4$ $(m_z   1/2, 1/2, 1/2)'$	(11) $\bar{4}^{+} (1/2, 0, z; 1/2, 0, 1/4)$ $(\bar{4}_z   1/2, 1/2, 1/2)'$	(12) $\bar{4}' (0, 1/2, z; 0, 1/2, 1/4)$ $(\bar{4}_z^{-1}   1/2, 1/2, 1/2)'$
(13) $n (1/2, 0, 1/2) \quad x, 1/4, z$ $(m_y   1/2, 1/2, 1/2)$	(14) $n (0, 1/2, 1/2) \quad 1/4, y, z$ $(m_x   1/2, 1/2, 1/2)$	(15) $c (0, 0, 1/2) \quad x + 1/2, \bar{x}, z$ $(m_{xy}   1/2, 1/2, 1/2)$	(16) $n (1/2, 1/2, 1/2) \quad x, x, z$ $(m_{\bar{xy}}   1/2, 1/2, 1/2)$

**Generators selected** (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ;  $t(1/2, 1/2, 1/2)$ ; (2); (3); (5); (9).**Positions**

			Coordinates			
			(0, 0, 0) +	$(1/2, 1/2, 1/2)'$ +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	o	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{y}, x, z [\bar{v}, u, w]$	(4) $y, \bar{x}, z [v, \bar{u}, w]$
			(5) $\bar{x}, y, \bar{z} [\bar{u}, v, \bar{w}]$	(6) $x, \bar{y}, \bar{z} [u, \bar{v}, \bar{w}]$	(7) $y, x, \bar{z} [v, u, \bar{w}]$	(8) $\bar{y}, \bar{x}, \bar{z} [\bar{v}, \bar{u}, \bar{w}]$
			(9) $\bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$	(10) $x, y, \bar{z} [u, v, \bar{w}]$	(11) $y, \bar{x}, \bar{z} [v, \bar{u}, \bar{w}]$	(12) $\bar{y}, x, \bar{z} [\bar{v}, u, \bar{w}]$
			(13) $x, \bar{y}, z [u, \bar{v}, w]$	(14) $\bar{x}, y, z [\bar{u}, v, w]$	(15) $\bar{y}, \bar{x}, z [\bar{v}, \bar{u}, w]$	(16) $y, x, z [v, u, w]$
16	n	.m'	$0, y, z [0, v, w]$	$0, \bar{y}, z [0, \bar{v}, w]$	$\bar{y}, 0, z [\bar{v}, 0, w]$	$y, 0, z [v, 0, w]$
			$0, y, \bar{z} [0, v, \bar{w}]$	$0, \bar{y}, \bar{z} [0, \bar{v}, \bar{w}]$	$y, 0, \bar{z} [v, 0, \bar{w}]$	$\bar{y}, 0, \bar{z} [\bar{v}, 0, \bar{w}]$
16	m	..m'	$x, x, z [u, u, w]$	$\bar{x}, \bar{x}, z [\bar{u}, \bar{u}, w]$	$\bar{x}, x, z [\bar{u}, u, w]$	$x, \bar{x}, z [u, \bar{u}, w]$
			$\bar{x}, x, \bar{z} [\bar{u}, u, \bar{w}]$	$x, \bar{x}, \bar{z} [u, \bar{u}, \bar{w}]$	$x, x, \bar{z} [u, u, \bar{w}]$	$\bar{x}, \bar{x}, \bar{z} [\bar{u}, \bar{u}, \bar{w}]$
16	l	m'..	$x, y, 0 [u, v, 0]$	$\bar{x}, \bar{y}, 0 [\bar{u}, \bar{v}, 0]$	$\bar{y}, x, 0 [\bar{v}, u, 0]$	$y, \bar{x}, 0 [v, \bar{u}, 0]$
			$\bar{x}, y, 0 [\bar{u}, v, 0]$	$x, \bar{y}, 0 [u, \bar{v}, 0]$	$y, x, 0 [v, u, 0]$	$\bar{y}, \bar{x}, 0 [\bar{v}, \bar{u}, 0]$
16	k	..2'	$x, x + 1/2, 1/4 [\bar{u}, u, w]$	$\bar{x}, \bar{x} + 1/2, 1/4 [u, \bar{u}, w]$	$\bar{x} + 1/2, x, 1/4 [\bar{u}, \bar{u}, w]$	$x + 1/2, \bar{x}, 1/4 [u, u, w]$
			$\bar{x}, \bar{x} + 1/2, 3/4 [u, \bar{u}, \bar{w}]$	$x, x + 1/2, 3/4 [\bar{u}, u, \bar{w}]$	$x + 1/2, \bar{x}, 3/4 [u, u, \bar{w}]$	$\bar{x} + 1/2, x, 3/4 [\bar{u}, \bar{u}, \bar{w}]$
8	j	m'2m'	$x, 1/2, 0 [u, 0, 0]$	$\bar{x}, 1/2, 0 [\bar{u}, 0, 0]$	$1/2, x, 0 [0, u, 0]$	$1/2, \bar{x}, 0 [0, \bar{u}, 0]$
8	i	m'2m'	$x, 0, 0 [u, 0, 0]$	$\bar{x}, 0, 0 [\bar{u}, 0, 0]$	$0, x, 0 [0, u, 0]$	$0, \bar{x}, 0 [0, \bar{u}, 0]$
8	h	m'.2m'	$x, x, 0 [u, u, 0]$	$\bar{x}, \bar{x}, 0 [\bar{u}, \bar{u}, 0]$	$\bar{x}, x, 0 [\bar{u}, u, 0]$	$x, \bar{x}, 0 [u, \bar{u}, 0]$
8	g	2m'm'	$0, 1/2, z [0, 0, w]$	$1/2, 0, z [0, 0, w]$	$0, 1/2, \bar{z} [0, 0, \bar{w}]$	$1/2, 0, \bar{z} [0, 0, \bar{w}]$
8	f	..2'/m'	$1/4, 1/4, 1/4 [\bar{u}, u, 0]$	$3/4, 3/4, 1/4 [u, \bar{u}, 0]$	$3/4, 1/4, 1/4 [\bar{u}, \bar{u}, 0]$	$1/4, 3/4, 1/4 [u, u, 0]$



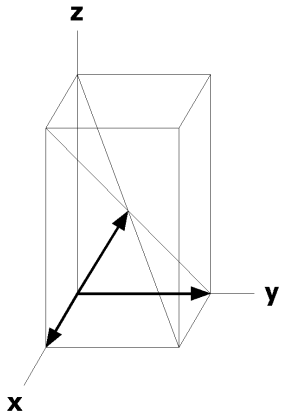
4	e	$4m'm'$	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,\bar{w}]$
4	d	$\bar{4}m'2'$	$0,1/2,1/4 [0,0,w]$	$1/2,0,1/4 [0,0,w]$
4	c	$m'm'm'$	$0,1/2,0 [0,0,0]$	$1/2,0,0 [0,0,0]$
2	b	$4/m'm'm'$	$0,0,1/2 [0,0,0]$	
2	a	$4/m'm'm'$	$0,0,0 [0,0,0]$	

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $c_p \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,0$



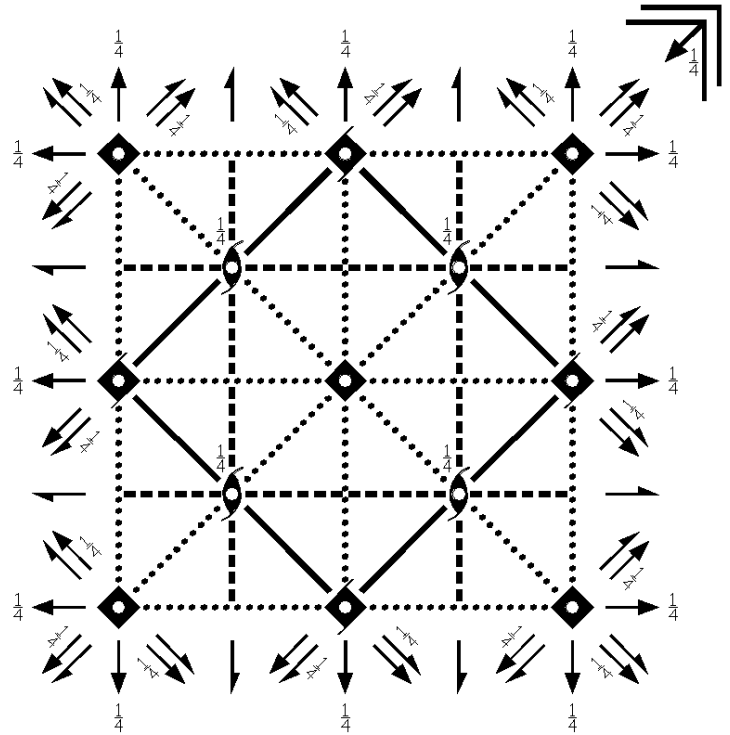
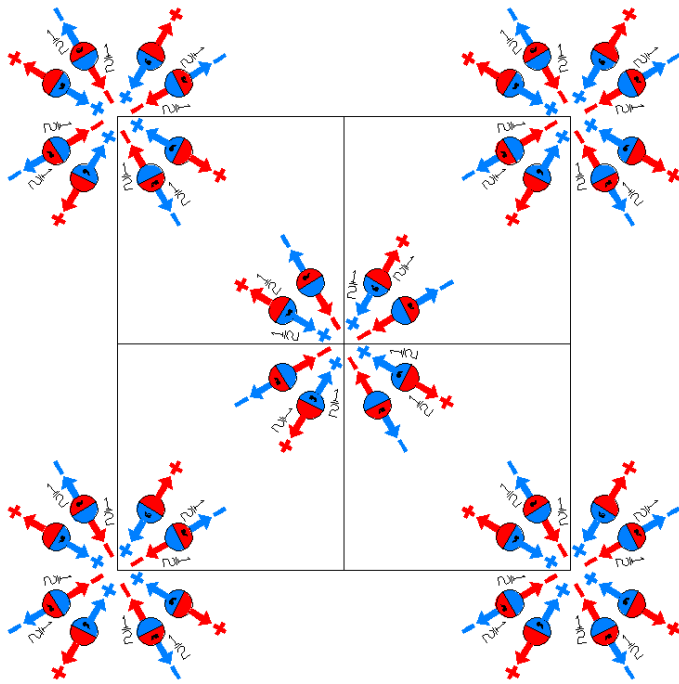
I4/mcm

140.1.1196

4/mmm

I4/m2/c2/m

Tetragonal



Origin at center ( 4/m ) at 4/mc2<sub>1</sub>/c

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)              | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)            | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)        |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)          | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)          | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                    | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2) |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)          | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)             | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)       | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                 |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (15) c (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2) | (16) c (0,0,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,1/2)  |

## For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)	(4) $4^-$ (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)
(5) $2$ (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)	(6) $2$ (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)	(7) $2$ (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)	(8) $2$ x, $\bar{x}$ +1/2,0 (2 <sub>xy</sub> <sup>-</sup>   1/2,1/2,0)
(9) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)	(10) $n$ (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)
(13) $a$ (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)	(14) $b$ (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)	(15) $m$ x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,0)	(16) $g$ (1/2,1/2,0) x,x,z (m <sub>xy</sub> <sup>-</sup>   1/2,1/2,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	m	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]
			(13) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ]	(16) y,x,z+1/2 [ $\bar{v},\bar{u},\bar{w}$ ]
16	l	..m	x,x+1/2,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,z$ [ $\bar{u},\bar{u},0$ ]	x+1/2, $\bar{x},z$ [ $\bar{u},u,0$ ]
			$\bar{x},x+1/2,\bar{z}+1/2$ [u,u,0]	x, $\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]	x+1/2,x, $\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,\bar{x},\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]
16	k	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0,w]	y, $\bar{x},0$ [0,0,w]
			$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]	y,x,1/2 [0,0, $\bar{w}$ ]	$\bar{y},\bar{x},1/2$ [0,0, $\bar{w}$ ]
16	j	.2.	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	0,x,1/4 [0,u,0]	0, $\bar{x},1/4$ [0, $\bar{u},0$ ]
			$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [u,0,0]	0, $\bar{x},3/4$ [0,u,0]	0,x,3/4 [0, $\bar{u},0$ ]
16	i	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/4$ [ $\bar{u},u,0$ ]	x, $\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},\bar{x},3/4$ [u,u,0]	x,x,3/4 [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},3/4$ [ $\bar{u},u,0$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},0$ ]
8	h	m.2m	x,x+1/2,0 [0,0,0]	$\bar{x},\bar{x}+1/2,0$ [0,0,0]	$\bar{x}+1/2,x,0$ [0,0,0]	x+1/2, $\bar{x},0$ [0,0,0]
8	g	2.mm	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]
8	f	4..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]
8	e	..2/m	1/4,1/4,1/4 [u,u,0]	3/4,3/4,1/4 [ $\bar{u},\bar{u},0$ ]	3/4,1/4,1/4 [ $\bar{u},u,0$ ]	1/4,3/4,1/4 [ $\bar{u},\bar{u},0$ ]
4	d	m.mm	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		

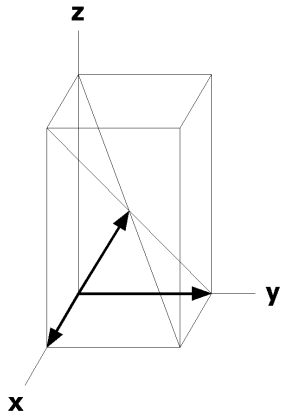
4	c	4/m..	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]
4	b	$\bar{4}2m$	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	a	422	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_c2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,0

Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

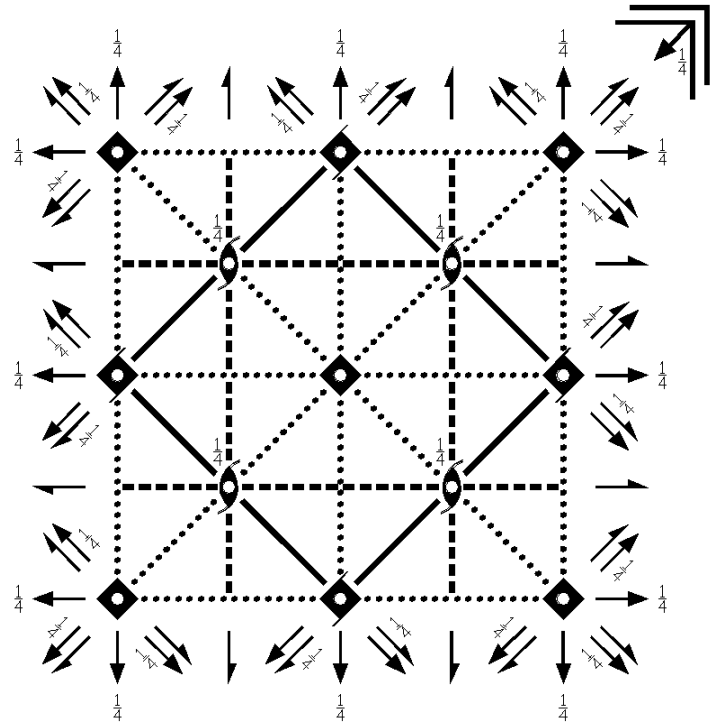
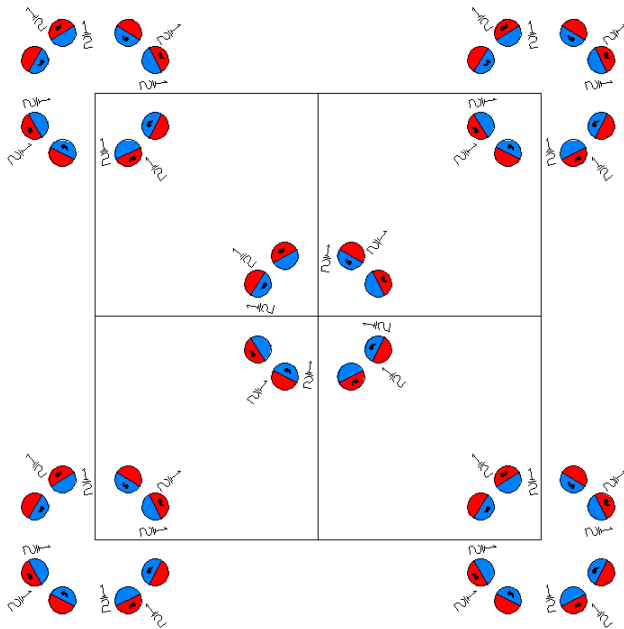


I4/mcm1'  
140.2.1197

4/mmm1'  
I4/m2/c2/m1'

Tetragonal

1'



Origin at center ( $4/m1'$ ) at  $4/mc2_1/c1'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)              | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)            | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)        |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)          | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)          | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                    | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2) |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)          | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)             | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)       | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)                 |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (15) c (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2) | (16) c (0,0,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,1/2)  |

## For (1/2,1/2,1/2) + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t$ (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)                 | (2) $2$ (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2)  | (3) $4^+$ (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>   1/2,1/2,1/2)       | (4) $4^-$ (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)       |
| (5) $2$ (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)  | (6) $2$ (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)      | (7) $2$ (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>   1/2,1/2,0)          | (8) $2$ x, $\bar{x}$ +1/2,0<br>(2 <sub>xy</sub>   1/2,1/2,0)                      |
| (9) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$   1/2,1/2,1/2)    | (10) $n$ (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>   1/2,1/2,1/2) | (11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$   1/2,1/2,1/2) | (12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2) |
| (13) $a$ (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0) | (14) $b$ (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)     | (15) $m$ x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>   1/2,1/2,0)       | (16) $g$ (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>   1/2,1/2,0)                       |

## For (0,0,0)' + set

- |  |  |   |   |
|--|--|---|---|
| (1) $1'$<br>(1   0,0,0)'                                 | (2) $2'$ 0,0,z<br>(2 <sub>z</sub>   0,0,0)'              | (3) $4^{+'}$ 0,0,z<br>(4 <sub>z</sub>   0,0,0)'                     | (4) $4^{-'}$ 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>   0,0,0)'             |
| (5) $2'$ 0,y,1/4<br>(2 <sub>y</sub>   0,0,1/2)'          | (6) $2'$ x,0,1/4<br>(2 <sub>x</sub>   0,0,1/2)'          | (7) $2'$ x,x,1/4<br>(2 <sub>xy</sub>   0,0,1/2)'                    | (8) $2'$ x, $\bar{x}$ ,1/4<br>(2 <sub>xy</sub>   0,0,1/2)'                |
| (9) $\bar{1}'$ 0,0,0<br>( $\bar{1}$   0,0,0)'            | (10) $m'$ x,y,0<br>(m <sub>z</sub>   0,0,0)'             | (11) $\bar{4}^{+'}$ 0,0,z; 0,0,0<br>( $\bar{4}_z$   0,0,0)'         | (12) $\bar{4}^{-'}$ 0,0,z; 0,0,0<br>( $\bar{4}_z$ <sup>-1</sup>   0,0,0)' |
| (13) $c'$ (0,0,1/2) x,0,z<br>(m <sub>y</sub>   0,0,1/2)' | (14) $c'$ (0,0,1/2) 0,y,z<br>(m <sub>x</sub>   0,0,1/2)' | (15) $c'$ (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>   0,0,1/2)' | (16) $c'$ (0,0,1/2) x,x,z<br>(m <sub>xy</sub>   0,0,1/2)'                 |

## For (1/2,1/2,1/2)' + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t'$ (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)'                 | (2) $2'$ (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2)'  | (3) $4^{+'}$ (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>   1/2,1/2,1/2)'       | (4) $4^{-'}$ (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)'       |
| (5) $2'$ (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)'  | (6) $2'$ (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)'      | (7) $2'$ (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>   1/2,1/2,0)'            | (8) $2'$ x, $\bar{x}$ +1/2,0<br>(2 <sub>xy</sub>   1/2,1/2,0)'                        |
| (9) $\bar{1}'$ 1/4,1/4,1/4<br>( $\bar{1}$   1/2,1/2,1/2)'    | (10) $n'$ (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>   1/2,1/2,1/2)' | (11) $\bar{4}^{+'}$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$   1/2,1/2,1/2)' | (12) $\bar{4}^{-'}$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)' |
| (13) $a'$ (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0)' | (14) $b'$ (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)'     | (15) $m'$ x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>   1/2,1/2,0)'         | (16) $g'$ (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>   1/2,1/2,0)'                         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9); 1'

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

(0,0,0) + (1/2,1/2,1/2) +  
(0,0,0)' + (1/2,1/2,1/2)'

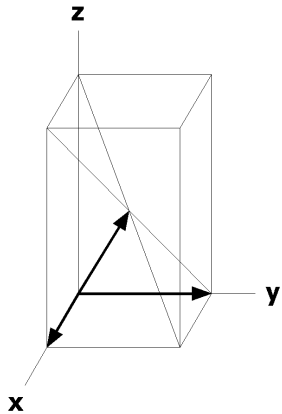
32	m	11'	(1) $x,y,z [0,0,0]$	(2) $\bar{x},\bar{y},z [0,0,0]$	(3) $\bar{y},x,z [0,0,0]$	(4) $y,\bar{x},z [0,0,0]$
			(5) $\bar{x},y,\bar{z}+1/2 [0,0,0]$	(6) $x,\bar{y},\bar{z}+1/2 [0,0,0]$	(7) $y,x,\bar{z}+1/2 [0,0,0]$	(8) $\bar{y},\bar{x},\bar{z}+1/2 [0,0,0]$
			(9) $\bar{x},\bar{y},\bar{z} [0,0,0]$	(10) $x,y,\bar{z} [0,0,0]$	(11) $y,\bar{x},\bar{z} [0,0,0]$	(12) $\bar{y},x,\bar{z} [0,0,0]$
			(13) $x,\bar{y},z+1/2 [0,0,0]$	(14) $\bar{x},\bar{y},z+1/2 [0,0,0]$	(15) $\bar{y},\bar{x},z+1/2 [0,0,0]$	(16) $y,x,z+1/2 [0,0,0]$
16	l	..m1'	$x,x+1/2,z [0,0,0]$	$\bar{x},\bar{x}+1/2,z [0,0,0]$	$\bar{x}+1/2,x,z [0,0,0]$	$x+1/2,\bar{x},z [0,0,0]$
			$\bar{x},x+1/2,\bar{z}+1/2 [0,0,0]$	$x,\bar{x}+1/2,\bar{z}+1/2 [0,0,0]$	$x+1/2,x,\bar{z}+1/2 [0,0,0]$	$\bar{x}+1/2,\bar{x},\bar{z}+1/2 [0,0,0]$
16	k	m..1'	$x,y,0 [0,0,0]$	$\bar{x},\bar{y},0 [0,0,0]$	$\bar{y},x,0 [0,0,0]$	$y,\bar{x},0 [0,0,0]$
			$\bar{x},y,1/2 [0,0,0]$	$x,\bar{y},1/2 [0,0,0]$	$y,x,1/2 [0,0,0]$	$\bar{y},\bar{x},1/2 [0,0,0]$
16	j	.2.1'	$x,0,1/4 [0,0,0]$	$\bar{x},0,1/4 [0,0,0]$	$0,x,1/4 [0,0,0]$	$0,\bar{x},1/4 [0,0,0]$
			$\bar{x},0,3/4 [0,0,0]$	$x,0,3/4 [0,0,0]$	$0,\bar{x},3/4 [0,0,0]$	$0,x,3/4 [0,0,0]$
16	i	..21'	$x,x,1/4 [0,0,0]$	$\bar{x},\bar{x},1/4 [0,0,0]$	$\bar{x},x,1/4 [0,0,0]$	$x,\bar{x},1/4 [0,0,0]$
			$\bar{x},\bar{x},3/4 [0,0,0]$	$x,x,3/4 [0,0,0]$	$x,\bar{x},3/4 [0,0,0]$	$\bar{x},x,3/4 [0,0,0]$
8	h	m.2m1'	$x,x+1/2,0 [0,0,0]$	$\bar{x},\bar{x}+1/2,0 [0,0,0]$	$\bar{x}+1/2,x,0 [0,0,0]$	$x+1/2,\bar{x},0 [0,0,0]$
8	g	2.mm1'	$0,1/2,z [0,0,0]$	$1/2,0,z [0,0,0]$	$0,1/2,\bar{z}+1/2 [0,0,0]$	$1/2,0,\bar{z}+1/2 [0,0,0]$
8	f	4..1'	$0,0,z [0,0,0]$	$0,0,\bar{z}+1/2 [0,0,0]$	$0,0,\bar{z} [0,0,0]$	$0,0,z+1/2 [0,0,0]$
8	e	..2/m1'	$1/4,1/4,1/4 [0,0,0]$	$3/4,3/4,1/4 [0,0,0]$	$3/4,1/4,1/4 [0,0,0]$	$1/4,3/4,1/4 [0,0,0]$
4	d	m.mm1'	$0,1/2,0 [0,0,0]$	$1/2,0,0 [0,0,0]$		
4	c	4/m..1'	$0,0,0 [0,0,0]$	$0,0,1/2 [0,0,0]$		
4	b	$\bar{4}2m1'$	$0,1/2,1/4 [0,0,0]$	$1/2,0,1/4 [0,0,0]$		
4	a	4221'	$0,0,1/4 [0,0,0]$	$0,0,3/4 [0,0,0]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



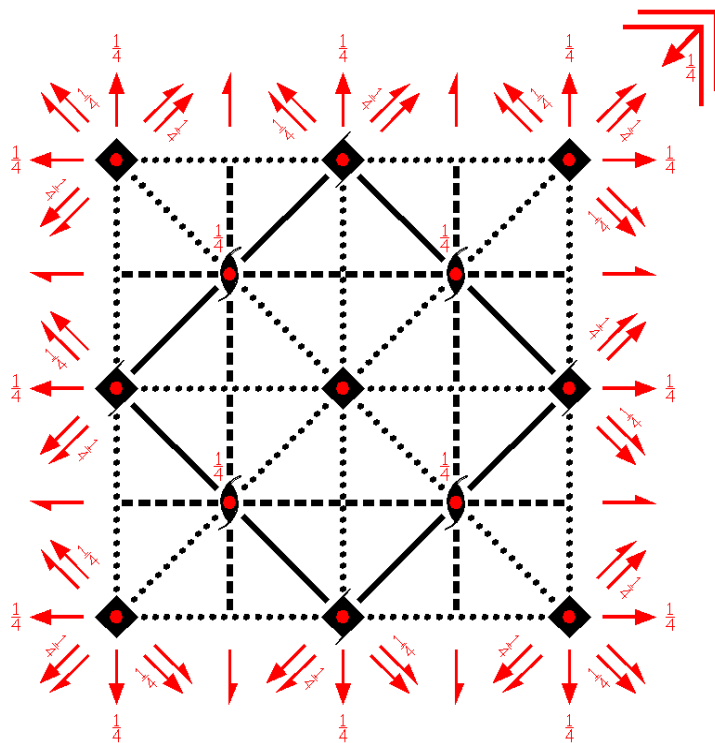
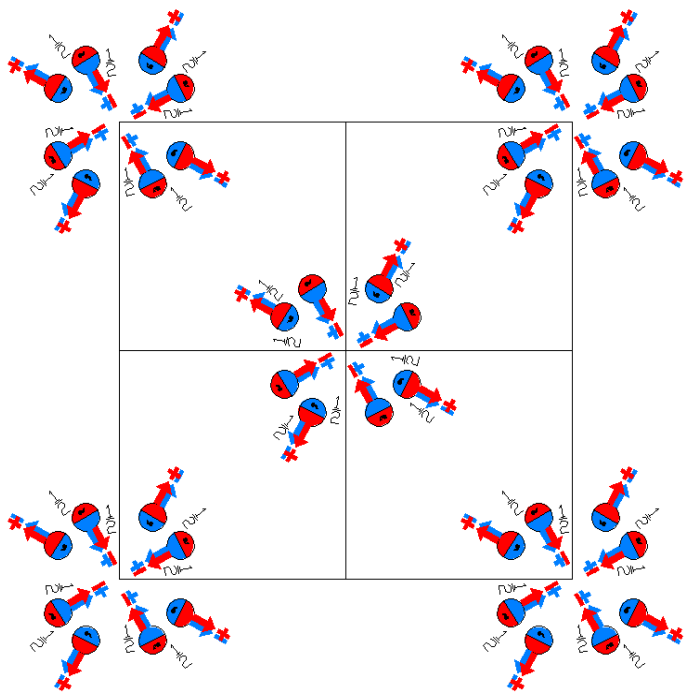
I4/m'cm

140.3.1198

4/m'mm

I4/m'2'/c2'/m

Tetragonal



Origin at center ( 4/m' ) at 4/m'c2',1/c

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)              | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)            | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)            |
| (5) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'        | (6) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'        | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                  | (8) 2' x,x̄,1/4<br>(2 <sub>xȳ</sub>  0,0,1/2)'                              |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'                         | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'           | (11) 4̄ <sup>+</sup> 0,0,z; 0,0,0<br>(4̄ <sub>z</sub>  0,0,0)' | (12) 4̄ <sup>-</sup> 0,0,z; 0,0,0<br>(4̄ <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (15) c (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)          | (16) c (0,0,1/2) x,x,z<br>(m <sub>xȳ</sub>  0,0,1/2)                        |



## For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)	(4) $4^-$ (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)
(5) $2'$ (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)'	(6) $2'$ (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)'	(7) $2'$ (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)'	(8) $2'$ x, $\bar{x}$ +1/2,0 (2 <sub>xy</sub> <sup>-</sup>   1/2,1/2,0)'
(9) $\bar{1}$ ' 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)'	(10) $n'$ (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)'	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)'
(13) $a$ (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)	(14) $b$ (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)	(15) $m$ x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,0)	(16) $g$ (1/2,1/2,0) x,x,z (m <sub>xy</sub> <sup>-</sup>   1/2,1/2,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	m	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(6) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},v,w$ ]	(7) y,x, $\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [v,u,w]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(11) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
			(13) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z+1/2$ [v,u, $\bar{w}$ ]	(16) y,x,z+1/2 [ $\bar{v},\bar{u},\bar{w}$ ]
16	l	..m	x,x+1/2,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}+1/2,z$ [u, $\bar{u},0$ ]	$\bar{x}+1/2,x,z$ [ $\bar{u},\bar{u},0$ ]	x+1/2, $\bar{x},z$ [u,u,0]
			$\bar{x},x+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x}+1/2,\bar{z}+1/2$ [u,u,0]	x+1/2,x, $\bar{z}+1/2$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,\bar{x},\bar{z}+1/2$ [u, $\bar{u},0$ ]
16	k	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [v,u,0]	y, $\bar{x},0$ [v, $\bar{u},0$ ]
			$\bar{x},y,1/2$ [u, $\bar{v},0$ ]	x, $\bar{y},1/2$ [ $\bar{u},v,0$ ]	y,x,1/2 [v, $\bar{u},0$ ]	$\bar{y},\bar{x},1/2$ [v,u,0]
16	j	.2'	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	0,x,1/4 [v,0,w]	0, $\bar{x},1/4$ [v,0,w]
			$\bar{x},0,3/4$ [0, $\bar{v},w$ ]	x,0,3/4 [0,v,w]	0, $\bar{x},3/4$ [v,0,w]	0,x,3/4 [v,0,w]
16	i	..2'	x,x,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [u, $\bar{u},w$ ]	$\bar{x},x,1/4$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},1/4$ [u,u,w]
			$\bar{x},\bar{x},3/4$ [u, $\bar{u},\bar{w}$ ]	x,x,3/4 [ $\bar{u},u,\bar{w}$ ]	x, $\bar{x},3/4$ [u,u, $\bar{w}$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	h	m'.2'm	x,x+1/2,0 [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}+1/2,0$ [u, $\bar{u},0$ ]	$\bar{x}+1/2,x,0$ [ $\bar{u},\bar{u},0$ ]	x+1/2, $\bar{x},0$ [u,u,0]
8	g	2.mm	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]
8	f	4..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]
8	e	..2'/m	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]
4	d	m.mm	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		

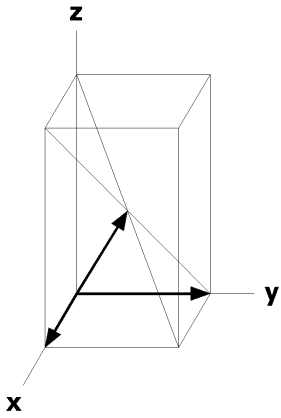
4	c	4/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]
4	b	$\bar{4}$ '2'm	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	a	42'2'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]

### Symmetry of Special Projections

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_c2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,1/4

Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



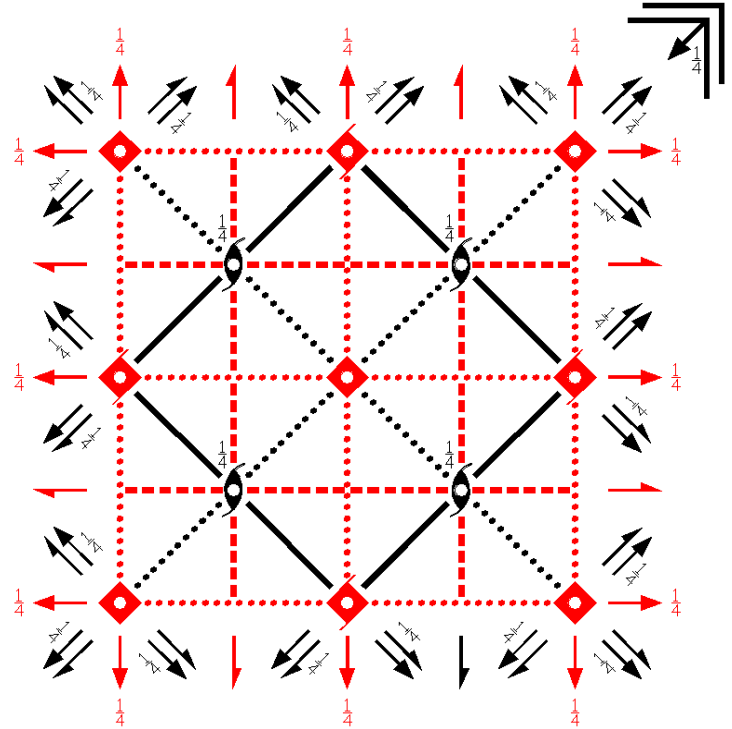
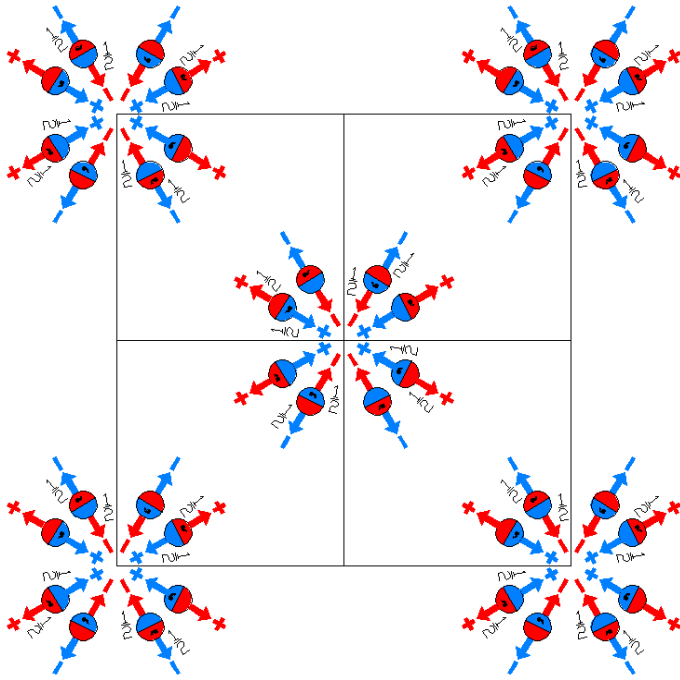
$I4'/mc'm$

140.4.1199

$4'/mm'm$

$I4'/m2'/c'2/m$

Tetragonal



Origin at center ( $4'/m$ ) at  $4'/mc'2_1/c$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                    | (3) $4^+$ $0,0,z$<br>( $4_z^+$  0,0,0)'                     | (4) $4^-$ $0,0,z$<br>( $4_z^-$  0,0,0)'                     |
| (5) $2'$ $0,y,1/4$<br>( $2_y$  0,0,1/2)'            | (6) $2'$ $x,0,1/4$<br>( $2_x$  0,0,1/2)'            | (7) 2 $x,x,1/4$<br>( $2_{xy}$  0,0,1/2)                     | (8) 2 $x,\bar{x},1/4$<br>( $2_{\bar{xy}}$  0,0,1/2)         |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)        | (10) m $x,y,0$<br>( $m_z$  0,0,0)                   | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^+$  0,0,0)' | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^-$  0,0,0)' |
| (13) $c'$ $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2)' | (14) $c'$ $(0,0,1/2)$ $0,y,z$<br>( $m_x$  0,0,1/2)' | (15) $c$ $(0,0,1/2)$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2)  | (16) $c$ $(0,0,1/2)$ $x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2)  |

For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)'	(4) $4^-$ ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)'
(5) $2'$ (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)'	(6) $2'$ (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)'	(7) $2$ (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)	(8) $2$ x, $\bar{x}+1/2,0$ (2 <sub>xy</sub>   1/2,1/2,0)
(9) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)	(10) $n$ (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)'
(13) $a'$ (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)'	(14) $b'$ (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)'	(15) $m$ x+1/2, $\bar{x},z$ (m <sub>xy</sub>   1/2,1/2,0)	(16) $g$ (1/2,1/2,0) x,x,z (m <sub>xy</sub>   1/2,1/2,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	m	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(6) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) y,x, $\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(13) x, $\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},\bar{v},w$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(16) y,x,z+1/2 [ $\bar{v},\bar{u},\bar{w}$ ]
16	l	..m	x,x+1/2,z [ $\bar{u},\bar{u},0$ ]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,z$ [ $\bar{u},\bar{u},0$ ]	x+1/2, $\bar{x},z$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},x+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]	x+1/2,x, $\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,\bar{x},\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]
16	k	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0, $\bar{w}$ ]	y, $\bar{x},0$ [0,0, $\bar{w}$ ]
			$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0,w]	y,x,1/2 [0,0, $\bar{w}$ ]	$\bar{y},\bar{x},1/2$ [0,0, $\bar{w}$ ]
16	j	.2'	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	0,x,1/4 [v,0, $\bar{w}$ ]	0, $\bar{x},1/4$ [ $\bar{v},0,\bar{w}$ ]
			$\bar{x},0,3/4$ [0, $\bar{v},w$ ]	x,0,3/4 [0,v,w]	0, $\bar{x},3/4$ [v,0, $\bar{w}$ ]	0,x,3/4 [ $\bar{v},0,\bar{w}$ ]
16	i	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/4$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	x,x,3/4 [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},0$ ]
8	h	m.2m	x,x+1/2,0 [0,0,0]	$\bar{x},\bar{x}+1/2,0$ [0,0,0]	$\bar{x}+1/2,x,0$ [0,0,0]	x+1/2, $\bar{x},0$ [0,0,0]
8	g	2.mm	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]
8	f	4'..	0,0,z [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0,z+1/2 [0,0,0]
8	e	..2/m	1/4,1/4,1/4 [u,u,0]	3/4,3/4,1/4 [ $\bar{u},\bar{u},0$ ]	3/4,1/4,1/4 [u, $\bar{u},0$ ]	1/4,3/4,1/4 [ $\bar{u},\bar{u},0$ ]
4	d	m.mm	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		

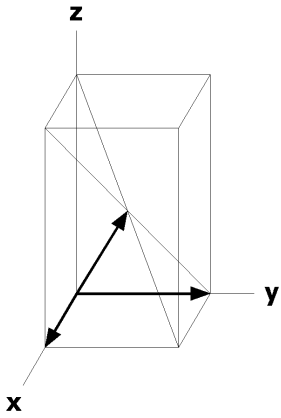
4	c	4'/m..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]
4	b	$\bar{4}$ '2'm	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	a	4'2'2	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p4'mm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



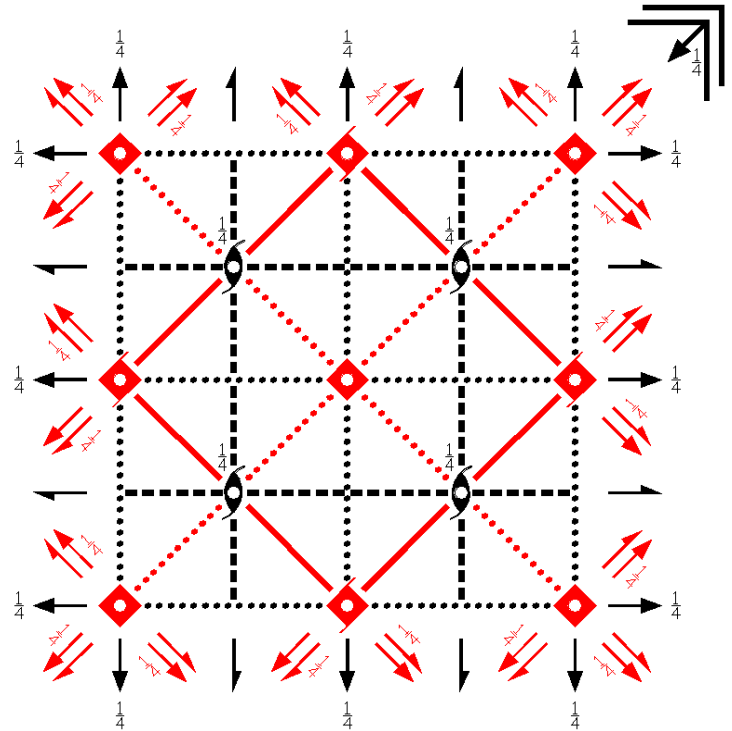
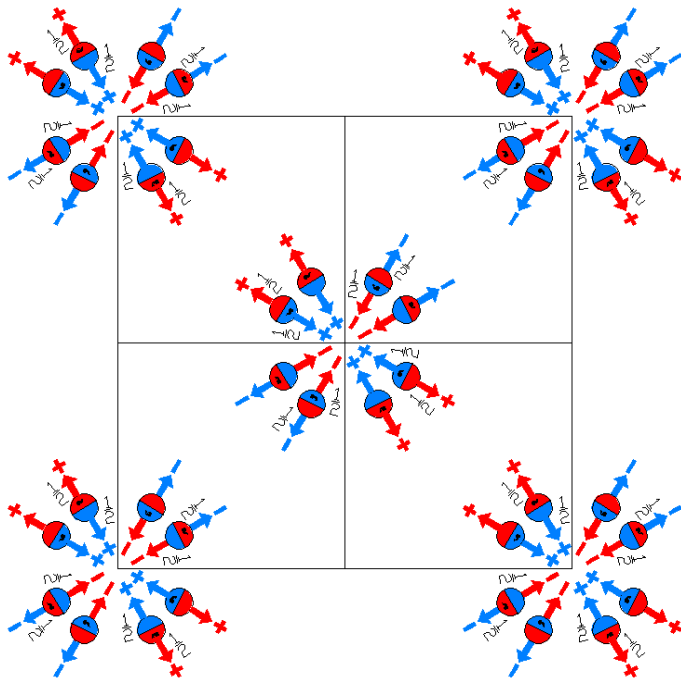
$I4'/mcm'$

140.5.1200

$4'/mmm'$

$I4'/m2/c2'/m'$

Tetragonal



Origin at center ( $4'/m$ ) at  $4'/mc2_1'/c'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)              | (3) $4^+$ $0,0,z$<br>( $4_z^+$  0,0,0)'                     | (4) $4^-$ $0,0,z$<br>( $4_z^-$  0,0,0)'                     |
| (5) 2 $0,y,1/4$<br>( $2_y$  0,0,1/2)          | (6) 2 $x,0,1/4$<br>( $2_x$  0,0,1/2)          | (7) $2'$ $x,x,1/4$<br>( $2_{xy}$  0,0,1/2)'                 | (8) $2'$ $x,\bar{x},1/4$<br>( $2_{\bar{xy}}$  0,0,1/2)'     |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)  | (10) m $x,y,0$<br>( $m_z$  0,0,0)             | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^+$  0,0,0)' | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^-$  0,0,0)' |
| (13) c (0,0,1/2) $x,0,z$<br>( $m_y$  0,0,1/2) | (14) c (0,0,1/2) $0,y,z$<br>( $m_x$  0,0,1/2) | (15) $c'$ (0,0,1/2) $x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2)'  | (16) $c'$ (0,0,1/2) $x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2)'  |

## For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)'	(4) $4^-$ ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)'
(5) $2$ (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)	(6) $2$ (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)	(7) $2'$ (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)'	(8) $2'$ x, $\bar{x}$ +1/2,0 (2 <sub>xy</sub>   1/2,1/2,0)'
(9) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)	(10) $n$ (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)'
(13) $a$ (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)	(14) $b$ (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)	(15) $m'$ x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,0)'	(16) $g'$ (1/2,1/2,0) x,x,z (m <sub>xy</sub>   1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	m	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
			(13) x, $\bar{y},z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(16) y,x,z+1/2 [v,u,w]
16	l	..m'	x,x+1/2,z [u,u,w]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,z$ [u, $\bar{u},\bar{w}$ ]	x+1/2, $\bar{x},z$ [ $\bar{u},u,\bar{w}$ ]
			$\bar{x},x+1/2,\bar{z}+1/2$ [ $\bar{u},u,\bar{w}$ ]	x, $\bar{x}+1/2,\bar{z}+1/2$ [u, $\bar{u},\bar{w}$ ]	x+1/2,x, $\bar{z}+1/2$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,\bar{x},\bar{z}+1/2$ [u,u,w]
16	k	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0, $\bar{w}$ ]	y, $\bar{x},0$ [0,0, $\bar{w}$ ]
			$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]	y,x,1/2 [0,0,w]	$\bar{y},\bar{x},1/2$ [0,0,w]
16	j	.2.	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	0,x,1/4 [0, $\bar{u},0$ ]	0, $\bar{x},1/4$ [0,u,0]
			$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [u,0,0]	0, $\bar{x},3/4$ [0, $\bar{u},0$ ]	0,x,3/4 [0,u,0]
16	i	..2'	x,x,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [u, $\bar{u},w$ ]	$\bar{x},x,1/4$ [u,u, $\bar{w}$ ]	x, $\bar{x},1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x},\bar{x},3/4$ [ $\bar{u},u,w$ ]	x,x,3/4 [u, $\bar{u},w$ ]	x, $\bar{x},3/4$ [u,u, $\bar{w}$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
8	h	m.2'm'	x,x+1/2,0 [0,0,w]	$\bar{x},\bar{x}+1/2,0$ [0,0,w]	$\bar{x}+1/2,x,0$ [0,0, $\bar{w}$ ]	x+1/2, $\bar{x},0$ [0,0, $\bar{w}$ ]
8	g	2.m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0,w]
8	f	4..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]
8	e	..2'/m'	1/4,1/4,1/4 [ $\bar{u},u,w$ ]	3/4,3/4,1/4 [u, $\bar{u},w$ ]	3/4,1/4,1/4 [u,u, $\bar{w}$ ]	1/4,3/4,1/4 [ $\bar{u},\bar{u},\bar{w}$ ]
4	d	m.m'm'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0, $\bar{w}$ ]		

4	c	4'/m..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]
4	b	$\bar{4}'2m'$	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	a	4'22'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]

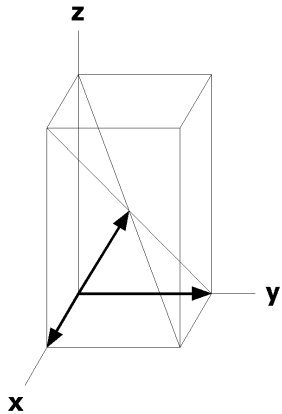
### Symmetry of Special Projections

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_c2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,0

Along [1,1,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0





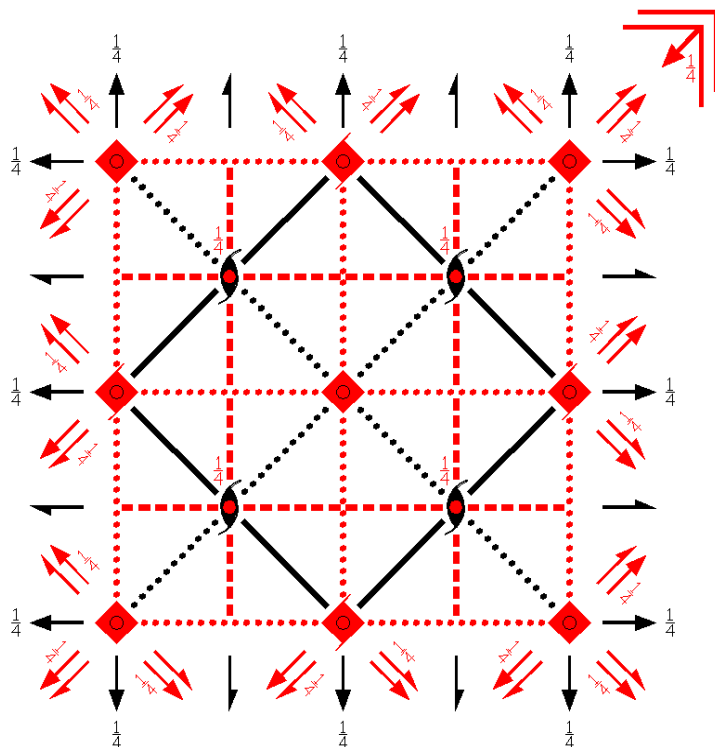
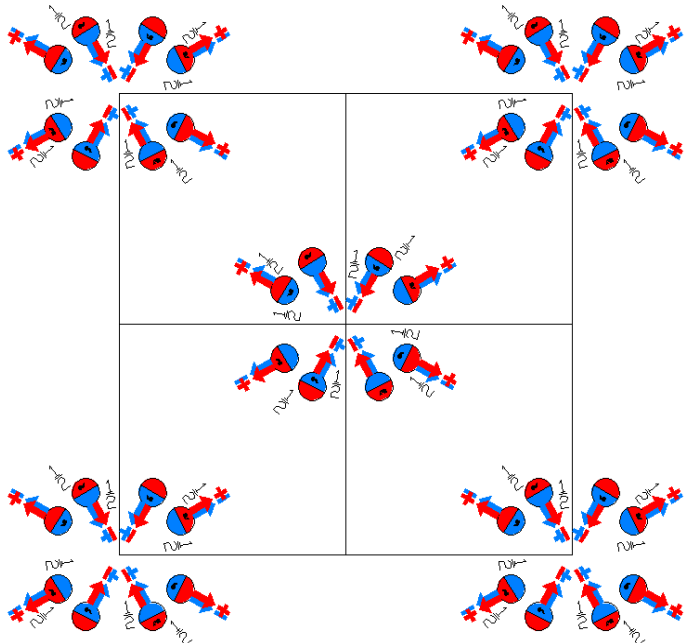
$I4'/m'c'm$

140.6.1201

$4'/m'm'm$

$I4'/m'2/c'2'/m$

Tetragonal



Origin at center ( $4'/m'$ ) at  $4'/m'c'2_1'/c$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $y \leq 1/2 - x$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                                    | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'        | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'        |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)            | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)            | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'               | (8) 2' x,x̄,1/4<br>(2 <sub>xȳ</sub>  0,0,1/2)'                           |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'                           | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'             | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub>  0,0,0) | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (14) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' | (15) c (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)       | (16) c (0,0,1/2) x,x,z<br>(m <sub>xȳ</sub>  0,0,1/2)                     |

For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)'	(4) $4^-$ ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)'
(5) $2$ (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)	(6) $2$ (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)	(7) $2'$ (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)'	(8) $2'$ x, $\bar{x}$ +1/2,0 (2 <sub>xy</sub> <sup>-1</sup>   1/2,1/2,0)'
(9) $\bar{1}$ ' 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)'	(10) $n'$ (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)'	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)
(13) $a'$ (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)'	(14) $b'$ (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)'	(15) $m$ x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,0)	(16) $g$ (1/2,1/2,0) x,x,z (m <sub>xy</sub> <sup>-1</sup>   1/2,1/2,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	m	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},u,\bar{w}$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(13) x, $\bar{y},z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ]	(16) y,x,z+1/2 [ $\bar{v},\bar{u},\bar{w}$ ]
16	l	..m	x,x+1/2,z [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,z$ [ $\bar{u},u,0$ ]	x+1/2, $\bar{x},z$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},x+1/2,\bar{z}+1/2$ [ $\bar{u},u,0$ ]	x, $\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]	x+1/2,x, $\bar{z}+1/2$ [ $\bar{u},u,0$ ]	$\bar{x}+1/2,\bar{x},\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]
16	k	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},\bar{u},0$ ]	y, $\bar{x},0$ [ $\bar{v},u,0$ ]
			$\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	x, $\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	y,x,1/2 [ $\bar{v},\bar{u},0$ ]	$\bar{y},\bar{x},1/2$ [ $\bar{v},u,0$ ]
16	j	.2.	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	0,x,1/4 [0, $\bar{u},0$ ]	0, $\bar{x},1/4$ [0,u,0]
			$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [u,0,0]	0, $\bar{x},3/4$ [0, $\bar{u},0$ ]	0,x,3/4 [0,u,0]
16	i	..2'	x,x,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,1/4$ [ $\bar{u},u,\bar{w}$ ]	x, $\bar{x},1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x},\bar{x},3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	x,x,3/4 [ $\bar{u},u,\bar{w}$ ]	x, $\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,3/4$ [ $\bar{u},u,\bar{w}$ ]
8	h	m'.2'm	x,x+1/2,0 [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}+1/2,0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,0$ [ $\bar{u},u,0$ ]	x+1/2, $\bar{x},0$ [ $\bar{u},\bar{u},0$ ]
8	g	2.mm	0,1/2,z [0,0,0]	1/2,0,z [0,0,0]	0,1/2, $\bar{z}+1/2$ [0,0,0]	1/2,0, $\bar{z}+1/2$ [0,0,0]
8	f	4'..	0,0,z [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0,z+1/2 [0,0,0]
8	e	..2'/m	1/4,1/4,1/4 [ $\bar{u},u,w$ ]	3/4,3/4,1/4 [ $\bar{u},\bar{u},w$ ]	3/4,1/4,1/4 [ $\bar{u},u,\bar{w}$ ]	1/4,3/4,1/4 [ $\bar{u},\bar{u},\bar{w}$ ]
4	d	m'.mm	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		

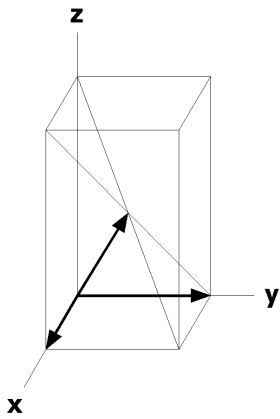
4	c	$4'/m'..$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]
4	b	$\overline{4}2m$	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	a	$4'22'$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p4'mm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



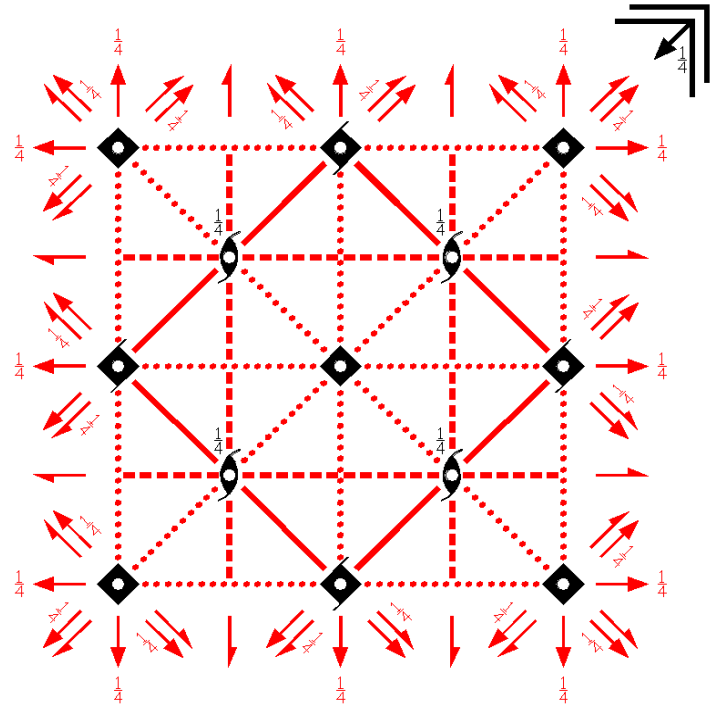
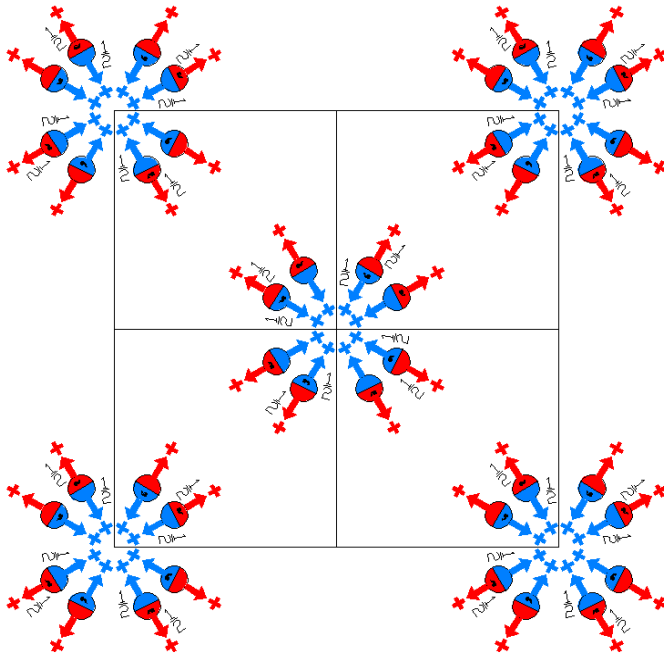
$I4/mc'm'$

140.7.1202

$4/mm'm'$

$I4/m2'/c2'/m'$

Tetragonal



Origin at center ( $4/m$ ) at  $4/mc'2_1/c'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                                    | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                      | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)         |
| (5) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'          | (6) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'          | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                            | (8) 2' x,x̄,1/4<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,1/2)'              |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)                            | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)               | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (14) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' | (15) c' (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)'                  | (16) c' (0,0,1/2) x,x,z<br>(m <sub>xy</sub> <sup>-1</sup>  0,0,1/2)'      |

## For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)	(4) $4^-$ (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)
(5) $2'$ (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)'	(6) $2'$ (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)'	(7) $2'$ (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)'	(8) $2'$ x, $\bar{x}$ +1/2,0 (2 <sub>xy</sub> <sup>-</sup>   1/2,1/2,0)'
(9) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)	(10) $n$ (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)
(13) $a'$ (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)'	(14) $b'$ (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)'	(15) $m'$ x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,0)'	(16) $g'$ (1/2,1/2,0) x,x,z (m <sub>xy</sub> <sup>-</sup>   1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	m	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [v, $\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(6) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) y,x, $\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [v,u,w]
			(9) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [v, $\bar{u},w$ ]
			(13) x, $\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},\bar{v},w$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) y,x,z+1/2 [v,u,w]
16	l	..m'	x,x+1/2,z [u,u,w]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,z$ [ $\bar{u},u,w$ ]	x+1/2, $\bar{x},z$ [u, $\bar{u},w$ ]
			$\bar{x},x+1/2,\bar{z}+1/2$ [u, $\bar{u},w$ ]	x, $\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{u},u,w$ ]	x+1/2,x, $\bar{z}+1/2$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,\bar{x},\bar{z}+1/2$ [u,u,w]
16	k	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0,w]	y, $\bar{x},0$ [0,0,w]
			$\bar{x},y,1/2$ [0,0,w]	x, $\bar{y},1/2$ [0,0,w]	y,x,1/2 [0,0,w]	$\bar{y},\bar{x},1/2$ [0,0,w]
16	j	.2'	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	0,x,1/4 [ $\bar{v},0,w$ ]	0, $\bar{x},1/4$ [v,0,w]
			$\bar{x},0,3/4$ [0, $\bar{v},w$ ]	x,0,3/4 [0,v,w]	0, $\bar{x},3/4$ [ $\bar{v},0,w$ ]	0,x,3/4 [v,0,w]
16	i	..2'	x,x,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [u, $\bar{u},w$ ]	$\bar{x},x,1/4$ [ $\bar{u},\bar{u},w$ ]	x, $\bar{x},1/4$ [u,u,w]
			$\bar{x},\bar{x},3/4$ [ $\bar{u},u,w$ ]	x,x,3/4 [u, $\bar{u},w$ ]	x, $\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,3/4$ [u,u,w]
8	h	m.2'm'	x,x+1/2,0 [0,0,w]	$\bar{x},\bar{x}+1/2,0$ [0,0,w]	$\bar{x}+1/2,x,0$ [0,0,w]	x+1/2, $\bar{x},0$ [0,0,w]
8	g	2.m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0,w]
8	f	4..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0,w]
8	e	..2'/m'	1/4,1/4,1/4 [ $\bar{u},u,w$ ]	3/4,3/4,1/4 [u, $\bar{u},w$ ]	3/4,1/4,1/4 [ $\bar{u},\bar{u},w$ ]	1/4,3/4,1/4 [u,u,w]
4	d	m.m'm'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]		

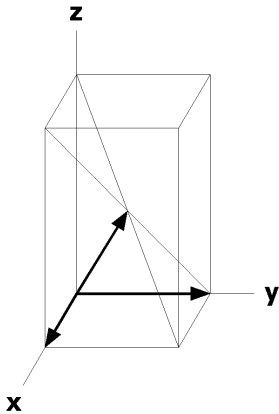
4	c	4/m..	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]
4	b	$\overline{4}2'm'$	0,1/2,1/4 [0,0,w]	1/2,0,1/4 [0,0,w]
4	a	42'2'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]

### Symmetry of Special Projections

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [1,1,0]  $p2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



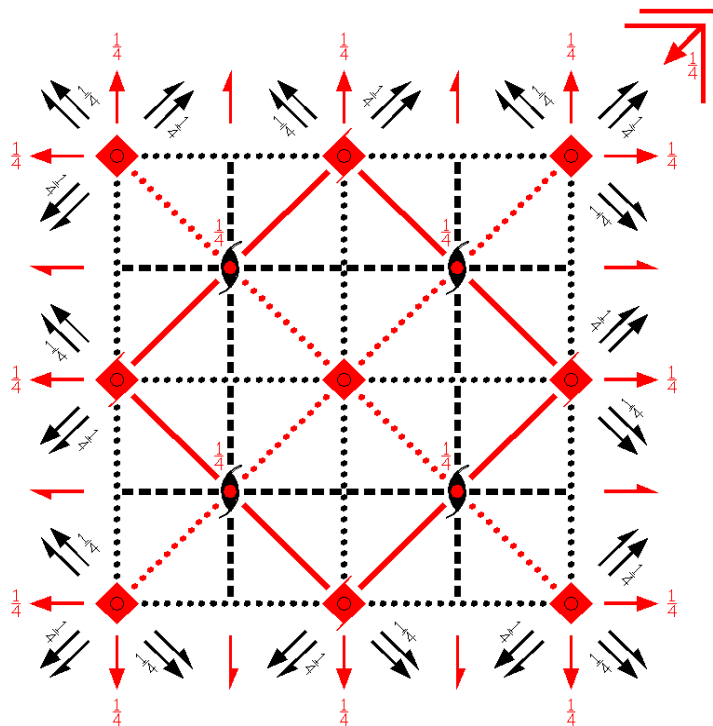
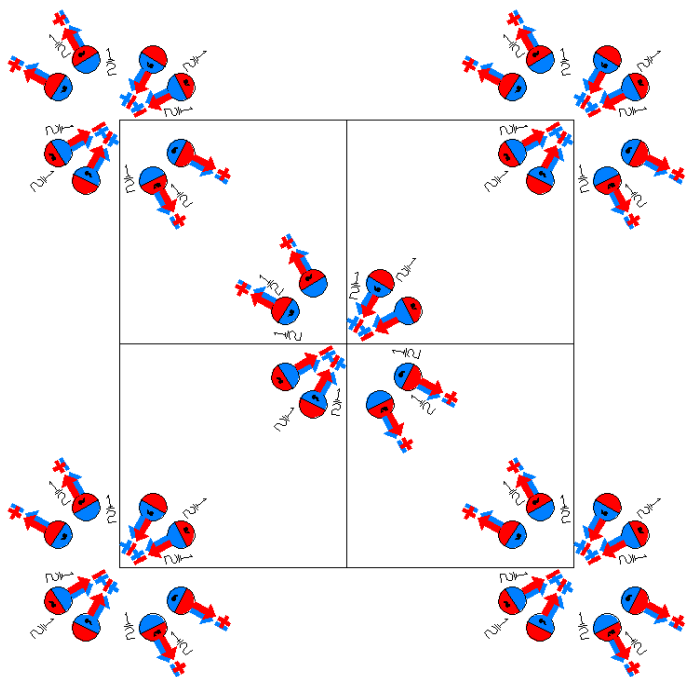
$I4'/m'cm'$

140.8.1203

$4'/m'mm'$

$I4'/m'2'/c2/m'$

Tetragonal



Origin at center ( $4'/m'$ ) at  $4'/m'c2_1/c'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; y \leq 1/2 - x$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)              | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)'        | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)'        |
| (5) 2' 0,y,1/4<br>(2 <sub>y</sub> ' 0,0,1/2)'       | (6) 2' x,0,1/4<br>(2 <sub>x</sub> ' 0,0,1/2)'       | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                              | (8) 2 x,x̄,1/4<br>(2 <sub>xȳ</sub>  0,0,1/2)                            |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'                         | (10) m' x,y,0<br>(m <sub>z</sub> ' 0,0,0)'          | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0) |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (15) c' (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub> ' 0,0,1/2)'                 | (16) c' (0,0,1/2) x,x,z<br>(m <sub>xȳ</sub> ' 0,0,1/2)'                 |

For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)'	(4) $4^-$ (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)'
(5) $2'$ (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)'	(6) $2'$ (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)'	(7) $2$ (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)	(8) $2$ x, $\bar{x}+1/2,0$ (2 <sub>xy</sub>   1/2,1/2,0)
(9) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)'	(10) $n'$ (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)'	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)
(13) $a$ (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)	(14) $b$ (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)	(15) $m'$ x+1/2, $\bar{x},z$ (m <sub>xy</sub>   1/2,1/2,0)'	(16) $g'$ (1/2,1/2,0) x,x,z (m <sub>xy</sub>   1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	m	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(6) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(7) y,x, $\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]
			(13) x, $\bar{y},z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) y,x,z+1/2 [ $\bar{v},\bar{u},w$ ]
16	l	..m'	x,x+1/2,z [u,u,w]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,z$ [u, $\bar{u},\bar{w}$ ]	x+1/2, $\bar{x},z$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x},x+1/2,\bar{z}+1/2$ [u, $\bar{u},w$ ]	x, $\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},w$ ]	x+1/2,x, $\bar{z}+1/2$ [u,u, $\bar{w}$ ]	$\bar{x}+1/2,\bar{x},\bar{z}+1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]
16	k	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},\bar{u},0$ ]	y, $\bar{x},0$ [ $\bar{v},\bar{u},0$ ]
			$\bar{x},y,1/2$ [u, $\bar{v},0$ ]	x, $\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	y,x,1/2 [v,u,0]	$\bar{y},\bar{x},1/2$ [ $\bar{v},\bar{u},0$ ]
16	j	.2'	x,0,1/4 [0,v,w]	$\bar{x},0,1/4$ [0, $\bar{v},w$ ]	0,x,1/4 [v,0, $\bar{w}$ ]	0, $\bar{x},1/4$ [ $\bar{v},0,\bar{w}$ ]
			$\bar{x},0,3/4$ [0, $\bar{v},w$ ]	x,0,3/4 [0,v,w]	0, $\bar{x},3/4$ [v,0, $\bar{w}$ ]	0,x,3/4 [ $\bar{v},0,\bar{w}$ ]
16	i	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/4$ [u, $\bar{u},0$ ]	x, $\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	x,x,3/4 [u,u,0]	x, $\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,3/4$ [u, $\bar{u},0$ ]
8	h	m'.2m'	x,x+1/2,0 [u,u,0]	$\bar{x},\bar{x}+1/2,0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,0$ [u, $\bar{u},0$ ]	x+1/2, $\bar{x},0$ [ $\bar{u},\bar{u},0$ ]
8	g	2.m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/2$ [0,0,w]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
8	f	4'..	0,0,z [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0,z+1/2 [0,0,0]
8	e	..2/m'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]
4	d	m'.m'm'	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		



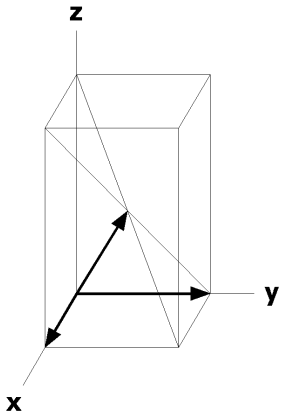
4	c	4'/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]
4	b	$\sqrt{2}$ m'	0,1/2,1/4 [0,0,w]	1/2,0,1/4 [0,0, $\bar{w}$ ]
4	a	4'2'2	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p4'm'm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_c2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,1/4

Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



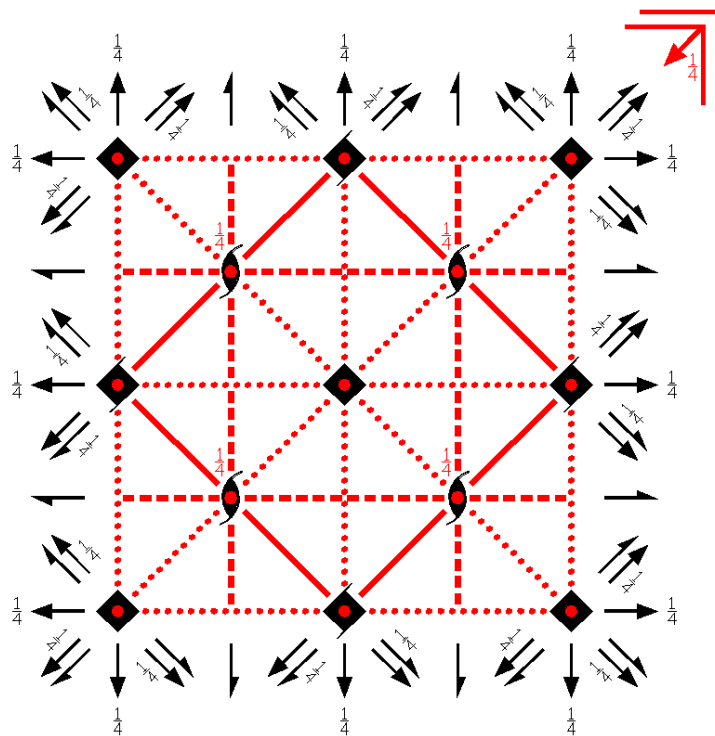
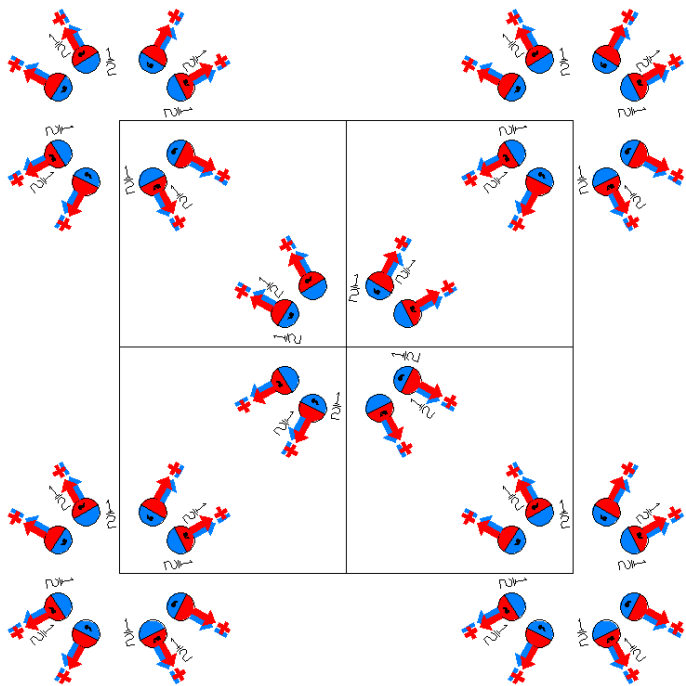
14/m'c'm'

140.9.1204

4/m'm'm'

14/m'2/c'2/m'

Tetragonal



Origin at center ( $4/m'$ ) at  $4/m'c'2_1/c'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                                    | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)          |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)            | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)            | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                      | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)  |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)'           | (10) m' x,y,0<br>(m <sub>z</sub> ' 0,0,0)'            | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'        | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                 |
| (13) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (14) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' | (15) c' (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2)' | (16) c' (0,0,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,1/2)' |

For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)	(4) $4^-$ (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)
(5) $2$ (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)	(6) $2$ (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)	(7) $2$ (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)	(8) $2$ x, $\bar{x}$ +1/2,0 (2 <sub>xy</sub> <sup>-1</sup>   1/2,1/2,0)
(9) $\bar{1}$ ' 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)'	(10) $n'$ (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)'	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)'
(13) $a'$ (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)'	(14) $b'$ (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)'	(15) $m'$ x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,0)'	(16) $g'$ (1/2,1/2,0) x,x,z (m <sub>xy</sub> <sup>-1</sup>   1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	m	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(13) x, $\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},\bar{v},w$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(16) y,x,z+1/2 [ $\bar{v},\bar{u},w$ ]
16	l	..m'	x,x+1/2,z [u,u,w]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,z$ [ $\bar{u},u,w$ ]	x+1/2, $\bar{x},z$ [ $\bar{u},\bar{u},w$ ]
			$\bar{x},x+1/2,\bar{z}+1/2$ [ $\bar{u},u,\bar{w}$ ]	x, $\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]	x+1/2,x, $\bar{z}+1/2$ [ $\bar{u},u,\bar{w}$ ]	$\bar{x}+1/2,\bar{x},\bar{z}+1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]
16	k	m'..	x,y,0 [u,v,0]	$\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x,0$ [ $\bar{v},u,0$ ]	y, $\bar{x},0$ [ $\bar{v},\bar{u},0$ ]
			$\bar{x},y,1/2$ [ $\bar{u},v,0$ ]	x, $\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	y,x,1/2 [ $\bar{v},u,0$ ]	$\bar{y},\bar{x},1/2$ [ $\bar{v},\bar{u},0$ ]
16	j	.2.	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	0,x,1/4 [0,u,0]	0, $\bar{x},1/4$ [0, $\bar{u},0$ ]
			$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [u,0,0]	0, $\bar{x},3/4$ [0,u,0]	0,x,3/4 [0, $\bar{u},0$ ]
16	i	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/4$ [ $\bar{u},u,0$ ]	x, $\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	x,x,3/4 [u,u,0]	x, $\bar{x},3/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]
8	h	m'.2m'	x,x+1/2,0 [u,u,0]	$\bar{x},\bar{x}+1/2,0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x}+1/2,x,0$ [ $\bar{u},u,0$ ]	x+1/2, $\bar{x},0$ [ $\bar{u},\bar{u},0$ ]
8	g	2.m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
8	f	4..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]
8	e	..2/m'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]
4	d	m'.m'm'	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		

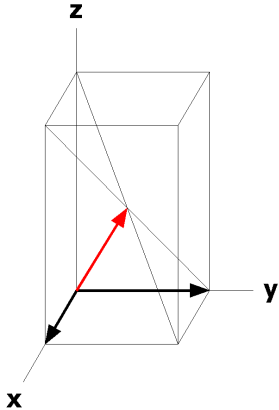
4	c	4/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]
4	b	$\bar{4}$ '2m'	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	a	422	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



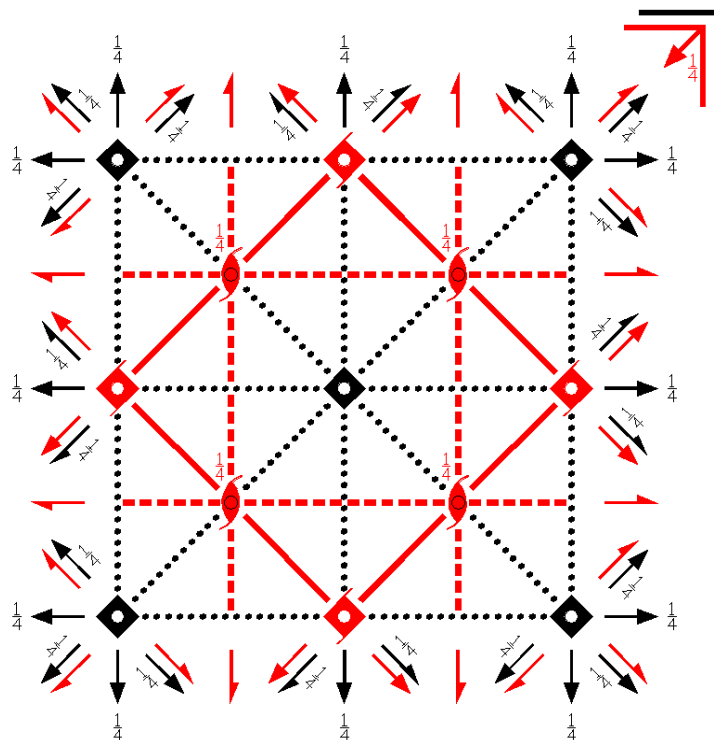
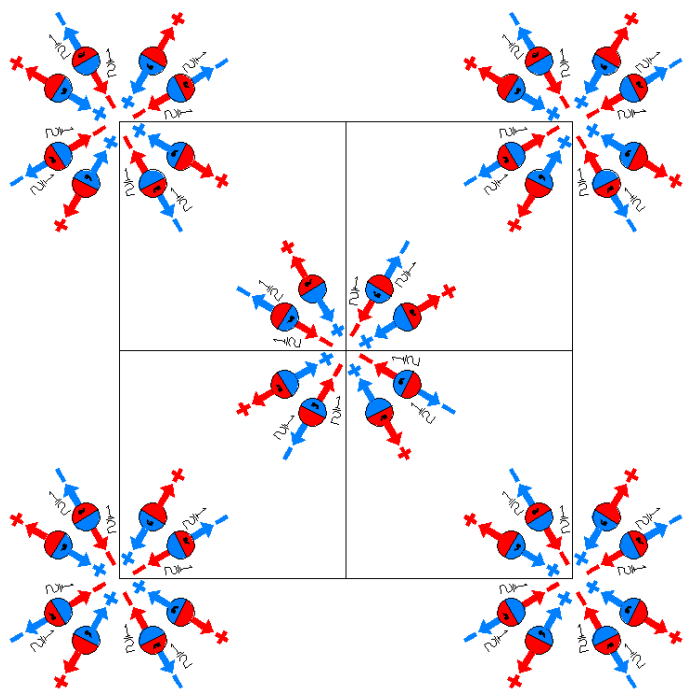
$I_P 4/mcm$

140.10.1205

$4/mmm1'$

$I_P 4/m2/c2/m$

Tetragonal



Origin at center ( $4/m$ ) at  $4/mc2_1/c$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                                | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                  | (3) $4^+$ $0,0,z$<br>( $4_z$  0,0,0)                       | (4) $4^-$ $0,0,z$<br>( $4_z^{-1}$  0,0,0)                     |
| (5) 2 $0,y,1/4$<br>( $2_y$  0,0,1/2)              | (6) 2 $x,0,1/4$<br>( $2_x$  0,0,1/2)              | (7) 2 $x,x,1/4$<br>( $2_{xy}$  0,0,1/2)                    | (8) 2 $x,\bar{x},1/4$<br>( $2_{\bar{xy}}$  0,0,1/2)           |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)      | (10) $m$ $x,y,0$<br>( $m_z$  0,0,0)               | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z$  0,0,0)   | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (13) $c$ $(0,0,1/2) \ x,0,z$<br>( $m_y$  0,0,1/2) | (14) $c$ $(0,0,1/2) \ 0,y,z$<br>( $m_x$  0,0,1/2) | (15) $c$ $(0,0,1/2) \ x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2) | (16) $c$ $(0,0,1/2) \ x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2)    |

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (1   1/2,1/2,1/2)'	(2) 2' (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)'	(3) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>   1/2,1/2,1/2)'	(4) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)'
(5) 2' (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)'	(6) 2' (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)'	(7) 2' (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)'	(8) 2' x, $\bar{x}$ +1/2,0 (2 <sub>xy</sub> <sup>-</sup>   1/2,1/2,0)'
(9) $\bar{1}$ ' 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)'	(10) n' (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>   1/2,1/2,1/2)'	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$   1/2,1/2,1/2)'
(13) a' (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)'	(14) b' (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)'	(15) m' x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,0)'	(16) g' (1/2,1/2,0) x,x,z (m <sub>xy</sub> <sup>-</sup>   1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (9).**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	m	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x,z$ [ $\bar{v},u,w$ ]	(4) y, $\bar{x},z$ [ $\bar{v},\bar{u},w$ ]
			(5) $\bar{x},y,\bar{z}+1/2$ [ $\bar{u},v,\bar{w}$ ]	(6) x, $\bar{y},\bar{z}+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(7) y,x, $\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]
			(9) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},v,w$ ]	(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(11) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]
			(13) x, $\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},u,\bar{w}$ ]	(16) y,x,z+1/2 [ $\bar{v},\bar{u},\bar{w}$ ]
16	l	..m'	x,x+1/2,z [u,u,w]	$\bar{x},\bar{x}+1/2,z$ [ $\bar{u},\bar{u},w$ ]	$\bar{x}+1/2,x,z$ [ $\bar{u},u,w$ ]	x+1/2, $\bar{x},z$ [ $\bar{u},\bar{u},w$ ]
			$\bar{x},x+1/2,\bar{z}+1/2$ [ $\bar{u},u,\bar{w}$ ]	x, $\bar{x}+1/2,\bar{z}+1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]	x+1/2,x, $\bar{z}+1/2$ [ $\bar{u},u,\bar{w}$ ]	$\bar{x}+1/2,\bar{x},\bar{z}+1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]
16	k	m..	x,y,0 [0,0,w]	$\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x,0$ [0,0,w]	y, $\bar{x},0$ [0,0,w]
			$\bar{x},y,1/2$ [0,0, $\bar{w}$ ]	x, $\bar{y},1/2$ [0,0, $\bar{w}$ ]	y,x,1/2 [0,0, $\bar{w}$ ]	$\bar{y},\bar{x},1/2$ [0,0, $\bar{w}$ ]
16	j	.2.	x,0,1/4 [u,0,0]	$\bar{x},0,1/4$ [ $\bar{u},0,0$ ]	0,x,1/4 [0,u,0]	0, $\bar{x},1/4$ [0, $\bar{u},0$ ]
			$\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	x,0,3/4 [u,0,0]	0, $\bar{x},3/4$ [0,u,0]	0,x,3/4 [0, $\bar{u},0$ ]
16	i	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x,1/4$ [ $\bar{u},u,0$ ]	x, $\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},\bar{x},3/4$ [u,u,0]	x,x,3/4 [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},3/4$ [ $\bar{u},u,0$ ]	$\bar{x},x,3/4$ [u, $\bar{u},0$ ]
8	h	m.2'm'	x,x+1/2,0 [0,0,w]	$\bar{x},\bar{x}+1/2,0$ [0,0,w]	$\bar{x}+1/2,x,0$ [0,0,w]	x+1/2, $\bar{x},0$ [0,0,w]
8	g	2.m'm'	0,1/2,z [0,0,w]	1/2,0,z [0,0,w]	0,1/2, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/2,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
8	f	4..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]
8	e	..2/m'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]
4	d	m.m'm'	0,1/2,0 [0,0,w]	1/2,0,0 [0,0,w]		

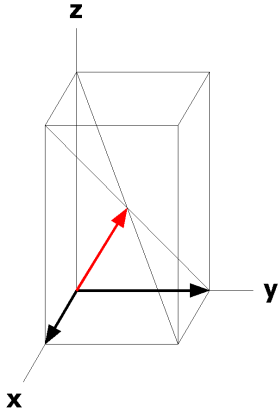
4	c	4/m..	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]
4	b	$\bar{4}'2m'$	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	a	422	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,1/4

Along [1,1,0]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



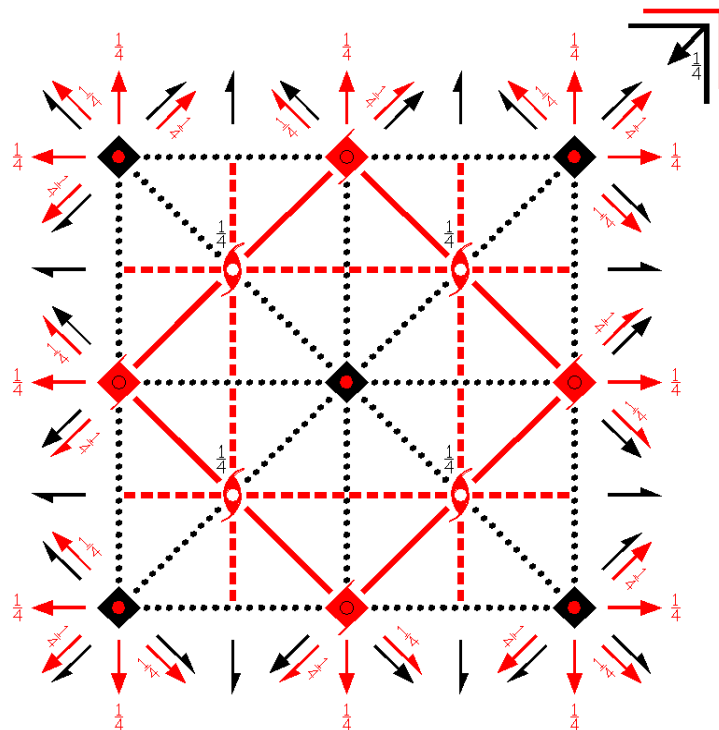
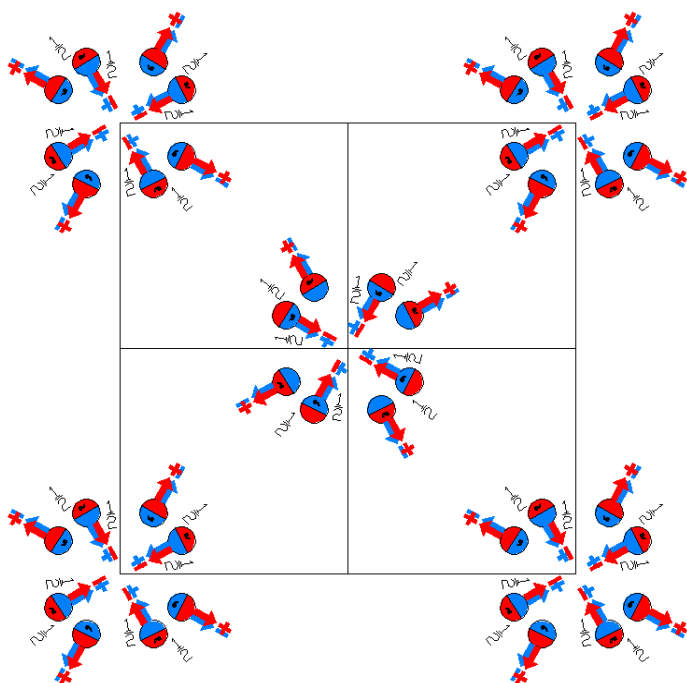
$I_p 4/m'cm$

140.11.1206

$4/mmm1'$

$I_p 4/m'2'/c2'/m$

Tetragonal



Origin at center ( $4/m'$ ) at  $4/m'c2_1'/c$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)              | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)                       | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)          |
| (5) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'        | (6) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'        | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                             | (8) 2' x,x̄,1/4<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,1/2)'               |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'                         | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'           | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)' | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (15) c (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)                     | (16) c (0,0,1/2) x,x,z<br>(m <sub>xy</sub> <sup>-1</sup>  0,0,1/2)         |



For  $(1/2, 1/2, 1/2)'$  + set

(1) $t' (1/2, 1/2, 1/2)$ $(1   1/2, 1/2, 1/2)'$	(2) $2' (0, 0, 1/2) \quad 1/4, 1/4, z$ $(2_z   1/2, 1/2, 1/2)'$	(3) $4^+ (0, 0, 1/2) \quad 0, 1/2, z$ $(4_z   1/2, 1/2, 1/2)'$	(4) $4^- (0, 0, 1/2) \quad 1/2, 0, z$ $(4_z^{-1}   1/2, 1/2, 1/2)'$
(5) $2 (0, 1/2, 0) \quad 1/4, y, 0$ $(2_y   1/2, 1/2, 0)$	(6) $2 (1/2, 0, 0) \quad x, 1/4, 0$ $(2_x   1/2, 1/2, 0)$	(7) $2 (1/2, 1/2, 0) \quad x, x, 0$ $(2_{xy}   1/2, 1/2, 0)$	(8) $2 \quad x, \bar{x} + 1/2, 0$ $(2_{\bar{xy}}   1/2, 1/2, 0)$
(9) $\bar{1} \quad 1/4, 1/4, 1/4$ $(\bar{1}   1/2, 1/2, 1/2)$	(10) $n (1/2, 1/2, 0) \quad x, y, 1/4$ $(m_z   1/2, 1/2, 1/2)$	(11) $\bar{4}^+ \quad 1/2, 0, z; \quad 1/2, 0, 1/4$ $(\bar{4}_z   1/2, 1/2, 1/2)$	(12) $\bar{4}^- \quad 0, 1/2, z; \quad 0, 1/2, 1/4$ $(\bar{4}_z^{-1}   1/2, 1/2, 1/2)$
(13) $a' (1/2, 0, 0) \quad x, 1/4, z$ $(m_y   1/2, 1/2, 0)'$	(14) $b' (0, 1/2, 0) \quad 1/4, y, z$ $(m_x   1/2, 1/2, 0)'$	(15) $m' \quad x + 1/2, \bar{x}, z$ $(m_{xy}   1/2, 1/2, 0)'$	(16) $g' (1/2, 1/2, 0) \quad x, x, z$ $(m_{\bar{xy}}   1/2, 1/2, 0)'$

**Generators selected** (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ;  $t'(1/2, 1/2, 1/2)$ ; (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0, 0, 0) +	$(1/2, 1/2, 1/2)'$ +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	m	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{y}, x, z [\bar{v}, u, w]$	(4) $y, \bar{x}, z [v, \bar{u}, w]$
			(5) $\bar{x}, y, \bar{z} + 1/2 [u, \bar{v}, w]$	(6) $x, \bar{y}, \bar{z} + 1/2 [\bar{u}, v, w]$	(7) $y, x, \bar{z} + 1/2 [\bar{v}, \bar{u}, w]$	(8) $\bar{y}, \bar{x}, \bar{z} + 1/2 [v, u, w]$
			(9) $\bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$	(10) $x, y, \bar{z} [u, v, \bar{w}]$	(11) $y, \bar{x}, \bar{z} [v, \bar{u}, \bar{w}]$	(12) $\bar{y}, x, \bar{z} [\bar{v}, u, \bar{w}]$
			(13) $x, \bar{y}, z + 1/2 [\bar{u}, v, \bar{w}]$	(14) $\bar{x}, y, z + 1/2 [u, \bar{v}, \bar{w}]$	(15) $\bar{y}, \bar{x}, z + 1/2 [v, u, \bar{w}]$	(16) $y, x, z + 1/2 [v, \bar{u}, \bar{w}]$
16	l	..m'	$x, x + 1/2, z [u, u, w]$	$\bar{x}, \bar{x} + 1/2, z [\bar{u}, \bar{u}, w]$	$\bar{x} + 1/2, x, z [\bar{u}, u, w]$	$x + 1/2, \bar{x}, z [u, \bar{u}, w]$
			$\bar{x}, x + 1/2, \bar{z} + 1/2 [u, \bar{u}, w]$	$x, \bar{x} + 1/2, \bar{z} + 1/2 [\bar{u}, u, w]$	$x + 1/2, x, \bar{z} + 1/2 [\bar{u}, \bar{u}, w]$	$\bar{x} + 1/2, \bar{x}, \bar{z} + 1/2 [u, u, w]$
16	k	m'..	$x, y, 0 [u, v, 0]$	$\bar{x}, \bar{y}, 0 [\bar{u}, \bar{v}, 0]$	$\bar{y}, x, 0 [v, \bar{u}, 0]$	$y, \bar{x}, 0 [\bar{v}, u, 0]$
			$\bar{x}, y, 1/2 [u, \bar{v}, 0]$	$x, \bar{y}, 1/2 [\bar{u}, v, 0]$	$y, x, 1/2 [v, \bar{u}, 0]$	$\bar{y}, \bar{x}, 1/2 [\bar{v}, u, 0]$
16	j	.2'	$x, 0, 1/4 [0, v, w]$	$\bar{x}, 0, 1/4 [0, \bar{v}, w]$	$0, x, 1/4 [v, 0, w]$	$0, \bar{x}, 1/4 [\bar{v}, 0, w]$
			$\bar{x}, 0, 3/4 [0, \bar{v}, w]$	$x, 0, 3/4 [0, v, w]$	$0, \bar{x}, 3/4 [v, 0, w]$	$0, x, 3/4 [\bar{v}, 0, w]$
16	i	..2'	$x, x, 1/4 [\bar{u}, u, w]$	$\bar{x}, \bar{x}, 1/4 [u, \bar{u}, w]$	$\bar{x}, x, 1/4 [\bar{u}, \bar{u}, w]$	$x, \bar{x}, 1/4 [u, u, w]$
			$\bar{x}, \bar{x}, 3/4 [u, \bar{u}, \bar{w}]$	$x, x, 3/4 [\bar{u}, u, \bar{w}]$	$x, \bar{x}, 3/4 [u, u, \bar{w}]$	$\bar{x}, x, 3/4 [\bar{u}, \bar{u}, \bar{w}]$
8	h	m'.2m'	$x, x + 1/2, 0 [u, u, 0]$	$\bar{x}, \bar{x} + 1/2, 0 [\bar{u}, \bar{u}, 0]$	$\bar{x} + 1/2, x, 0 [\bar{u}, u, 0]$	$x + 1/2, \bar{x}, 0 [u, \bar{u}, 0]$
8	g	2.m'm'	$0, 1/2, z [0, 0, w]$	$1/2, 0, z [0, 0, w]$	$0, 1/2, \bar{z} + 1/2 [0, 0, w]$	$1/2, 0, \bar{z} + 1/2 [0, 0, w]$
8	f	4..	$0, 0, z [0, 0, w]$	$0, 0, \bar{z} + 1/2 [0, 0, w]$	$0, 0, \bar{z} [0, 0, \bar{w}]$	$0, 0, z + 1/2 [0, 0, \bar{w}]$
8	e	..2'/m'	$1/4, 1/4, 1/4 [\bar{u}, u, w]$	$3/4, 3/4, 1/4 [u, \bar{u}, w]$	$3/4, 1/4, 1/4 [\bar{u}, \bar{u}, w]$	$1/4, 3/4, 1/4 [u, u, w]$
4	d	m.m'm'	$0, 1/2, 0 [0, 0, w]$	$1/2, 0, 0 [0, 0, w]$		

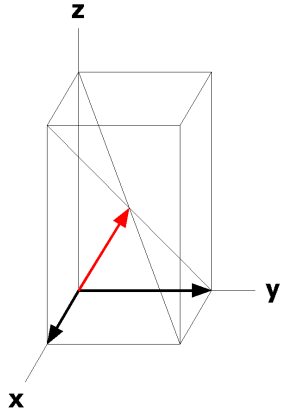
4	c	$4/m'..$	$0,0,0 [0,0,0]$	$0,0,1/2 [0,0,0]$
4	b	$\overline{4}2'm'$	$0,1/2,1/4 [0,0,w]$	$1/2,0,1/4 [0,0,w]$
4	a	$42'2'$	$0,0,1/4 [0,0,w]$	$0,0,3/4 [0,0,\overline{w}]$

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_p \cdot 4mm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,0,0$

Along  $[1,1,0]$   $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,0$



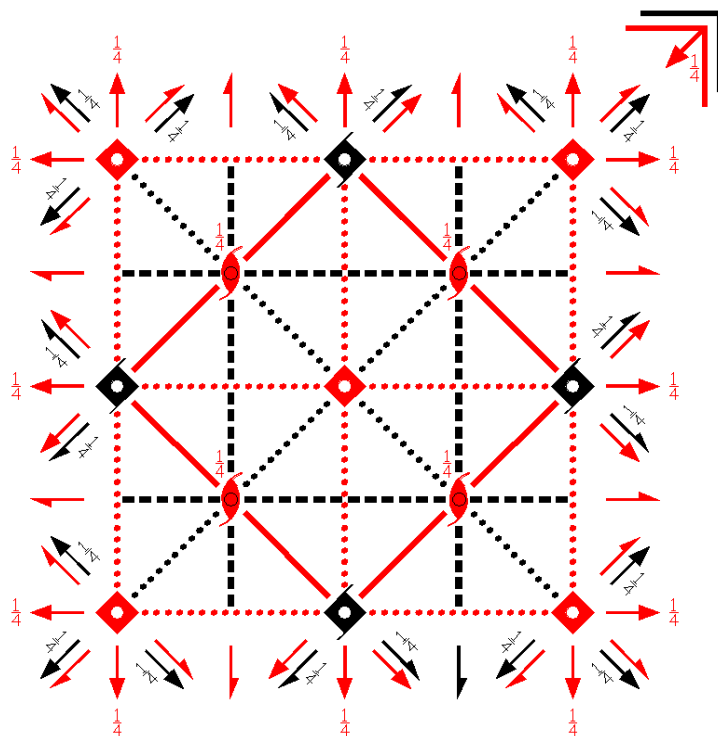
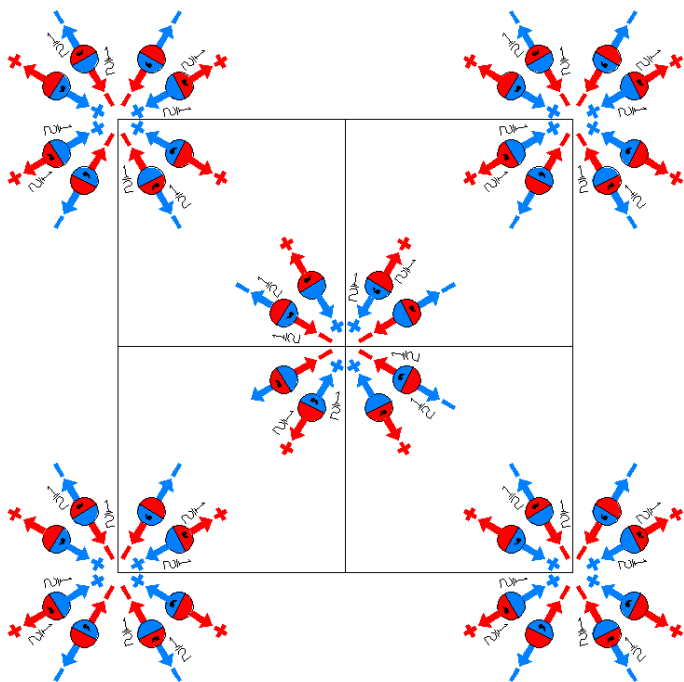
$I_p 4'/mc'm$

140.12.1207

$4/mmm1'$

$I_p 4'/m2'/c'2/m$

Tetragonal



Origin at center ( $4'/m$ ) at  $4'/mc'2_1/c$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                              | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                | (3) $4^+ 0,0,z$<br>( $4_z^+$  0,0,0)'                     | (4) $4^- 0,0,z$<br>( $4_z^-$  0,0,0)'                     |
| (5) $2' 0,y,1/4$<br>( $2_y$  0,0,1/2)'          | (6) $2' x,0,1/4$<br>( $2_x$  0,0,1/2)'          | (7) 2 $x,x,1/4$<br>( $2_{xy}$  0,0,1/2)                   | (8) 2 $x,\bar{x},1/4$<br>( $2_{\bar{xy}}$  0,0,1/2)       |
| (9) $\bar{1} 0,0,0$<br>( $\bar{1}$  0,0,0)      | (10) m $x,y,0$<br>( $m_z$  0,0,0)               | (11) $\bar{4}^+ 0,0,z; 0,0,0$<br>( $\bar{4}_z^+$  0,0,0)' | (12) $\bar{4}^- 0,0,z; 0,0,0$<br>( $\bar{4}_z^-$  0,0,0)' |
| (13) $c' (0,0,1/2) x,0,z$<br>( $m_y$  0,0,1/2)' | (14) $c' (0,0,1/2) 0,y,z$<br>( $m_x$  0,0,1/2)' | (15) $c (0,0,1/2) x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2)    | (16) $c (0,0,1/2) x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2)    |

For  $(1/2, 1/2, 1/2)'$  + set

(1) $t' (1/2, 1/2, 1/2)$ $(1   1/2, 1/2, 1/2)'$	(2) $2' (0, 0, 1/2) \quad 1/4, 1/4, z$ $(2_z   1/2, 1/2, 1/2)'$	(3) $4^+ (0, 0, 1/2) \quad 0, 1/2, z$ $(4_z   1/2, 1/2, 1/2)$	(4) $4^- (0, 0, 1/2) \quad 1/2, 0, z$ $(4_z^{-1}   1/2, 1/2, 1/2)$
(5) $2 (0, 1/2, 0) \quad 1/4, y, 0$ $(2_y   1/2, 1/2, 0)$	(6) $2 (1/2, 0, 0) \quad x, 1/4, 0$ $(2_x   1/2, 1/2, 0)$	(7) $2' (1/2, 1/2, 0) \quad x, x, 0$ $(2_{xy}   1/2, 1/2, 0)'$	(8) $2' \quad x, \bar{x} + 1/2, 0$ $(2_{\bar{xy}}   1/2, 1/2, 0)'$
(9) $\bar{1}' \quad 1/4, 1/4, 1/4$ $(\bar{1}   1/2, 1/2, 1/2)'$	(10) $n' (1/2, 1/2, 0) \quad x, y, 1/4$ $(m_z   1/2, 1/2, 1/2)'$	(11) $\bar{4}^+ \quad 1/2, 0, z; \quad 1/2, 0, 1/4$ $(\bar{4}_z   1/2, 1/2, 1/2)$	(12) $\bar{4}^- \quad 0, 1/2, z; \quad 0, 1/2, 1/4$ $(\bar{4}_z^{-1}   1/2, 1/2, 1/2)$
(13) $a (1/2, 0, 0) \quad x, 1/4, z$ $(m_y   1/2, 1/2, 0)$	(14) $b (0, 1/2, 0) \quad 1/4, y, z$ $(m_x   1/2, 1/2, 0)$	(15) $m' \quad x + 1/2, \bar{x}, z$ $(m_{xy}   1/2, 1/2, 0)'$	(16) $g' (1/2, 1/2, 0) \quad x, x, z$ $(m_{\bar{xy}}   1/2, 1/2, 0)'$

**Generators selected** (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ;  $t'(1/2, 1/2, 1/2)$ ; (2); (3); (5); (9).

**Positions**

			Coordinates			
			$(0, 0, 0) +$		$(1/2, 1/2, 1/2)'$ +	
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	m	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{y}, x, z [v, \bar{u}, \bar{w}]$	(4) $y, \bar{x}, z [\bar{v}, u, \bar{w}]$
			(5) $\bar{x}, y, \bar{z} + 1/2 [u, \bar{v}, w]$	(6) $x, \bar{y}, \bar{z} + 1/2 [\bar{u}, v, w]$	(7) $y, x, \bar{z} + 1/2 [v, u, \bar{w}]$	(8) $\bar{y}, \bar{x}, \bar{z} + 1/2 [\bar{v}, \bar{u}, \bar{w}]$
			(9) $\bar{x}, \bar{y}, \bar{z} [u, v, w]$	(10) $x, y, z [\bar{u}, \bar{v}, w]$	(11) $y, \bar{x}, \bar{z} [v, \bar{u}, \bar{w}]$	(12) $\bar{y}, x, z [\bar{v}, u, \bar{w}]$
			(13) $x, \bar{y}, z + 1/2 [u, \bar{v}, w]$	(14) $\bar{x}, y, z + 1/2 [\bar{u}, v, w]$	(15) $\bar{y}, \bar{x}, z + 1/2 [v, u, \bar{w}]$	(16) $y, x, z + 1/2 [\bar{v}, \bar{u}, \bar{w}]$
16	l	..m'	$x, x + 1/2, z [u, u, w]$	$\bar{x}, \bar{x} + 1/2, z [\bar{u}, \bar{u}, w]$	$\bar{x} + 1/2, x, z [u, \bar{u}, \bar{w}]$	$x + 1/2, \bar{x}, z [\bar{u}, u, \bar{w}]$
			$\bar{x}, x + 1/2, \bar{z} + 1/2 [u, \bar{u}, w]$	$x, \bar{x} + 1/2, \bar{z} + 1/2 [\bar{u}, u, w]$	$x + 1/2, x, \bar{z} + 1/2 [u, u, \bar{w}]$	$\bar{x} + 1/2, \bar{x}, \bar{z} + 1/2 [\bar{u}, \bar{u}, \bar{w}]$
16	k	m..	$x, y, 0 [0, 0, w]$	$\bar{x}, \bar{y}, 0 [0, 0, w]$	$\bar{y}, x, 0 [0, 0, \bar{w}]$	$y, \bar{x}, 0 [0, 0, \bar{w}]$
			$\bar{x}, y, 1/2 [0, 0, w]$	$x, \bar{y}, 1/2 [0, 0, w]$	$y, x, 1/2 [0, 0, \bar{w}]$	$\bar{y}, \bar{x}, 1/2 [0, 0, \bar{w}]$
16	j	.2'	$x, 0, 1/4 [0, v, w]$	$\bar{x}, 0, 1/4 [0, \bar{v}, w]$	$0, x, 1/4 [v, 0, \bar{w}]$	$0, \bar{x}, 1/4 [\bar{v}, 0, \bar{w}]$
			$\bar{x}, 0, 3/4 [0, \bar{v}, w]$	$x, 0, 3/4 [0, v, w]$	$0, \bar{x}, 3/4 [v, 0, \bar{w}]$	$0, x, 3/4 [\bar{v}, 0, \bar{w}]$
16	i	..2	$x, x, 1/4 [u, u, 0]$	$\bar{x}, \bar{x}, 1/4 [\bar{u}, \bar{u}, 0]$	$\bar{x}, x, 1/4 [u, \bar{u}, 0]$	$x, \bar{x}, 1/4 [\bar{u}, u, 0]$
			$\bar{x}, \bar{x}, 3/4 [u, \bar{u}, 0]$	$x, x, 3/4 [\bar{u}, u, 0]$	$x, \bar{x}, 3/4 [u, u, 0]$	$\bar{x}, x, 3/4 [\bar{u}, \bar{u}, 0]$
8	h	m.2'm'	$x, x + 1/2, 0 [0, 0, w]$	$\bar{x}, \bar{x} + 1/2, 0 [0, 0, w]$	$\bar{x} + 1/2, x, 0 [0, 0, \bar{w}]$	$x + 1/2, \bar{x}, 0 [0, 0, \bar{w}]$
8	g	2.m'm'	$0, 1/2, z [0, 0, w]$	$1/2, 0, z [0, 0, \bar{w}]$	$0, 1/2, \bar{z} + 1/2 [0, 0, w]$	$1/2, 0, \bar{z} + 1/2 [0, 0, \bar{w}]$
8	f	4'..	$0, 0, z [0, 0, 0]$	$0, 0, \bar{z} + 1/2 [0, 0, 0]$	$0, 0, \bar{z} [0, 0, 0]$	$0, 0, z + 1/2 [0, 0, 0]$
8	e	..2/m'	$1/4, 1/4, 1/4 [0, 0, 0]$	$3/4, 3/4, 1/4 [0, 0, 0]$	$3/4, 1/4, 1/4 [0, 0, 0]$	$1/4, 3/4, 1/4 [0, 0, 0]$
4	d	m.m'm'	$0, 1/2, 0 [0, 0, w]$	$1/2, 0, 0 [0, 0, \bar{w}]$		

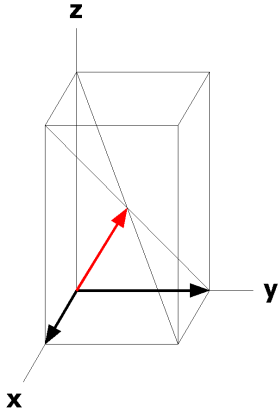
4	c	$4'/m..$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]
4	b	$\overline{4}2'm'$	0,1/2,1/4 [0,0,w]	1/2,0,1/4 [0,0, $\overline{w}$ ]
4	a	$4'2'2$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a'}2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,0

Along [1,1,0]  $p_{2a'}2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



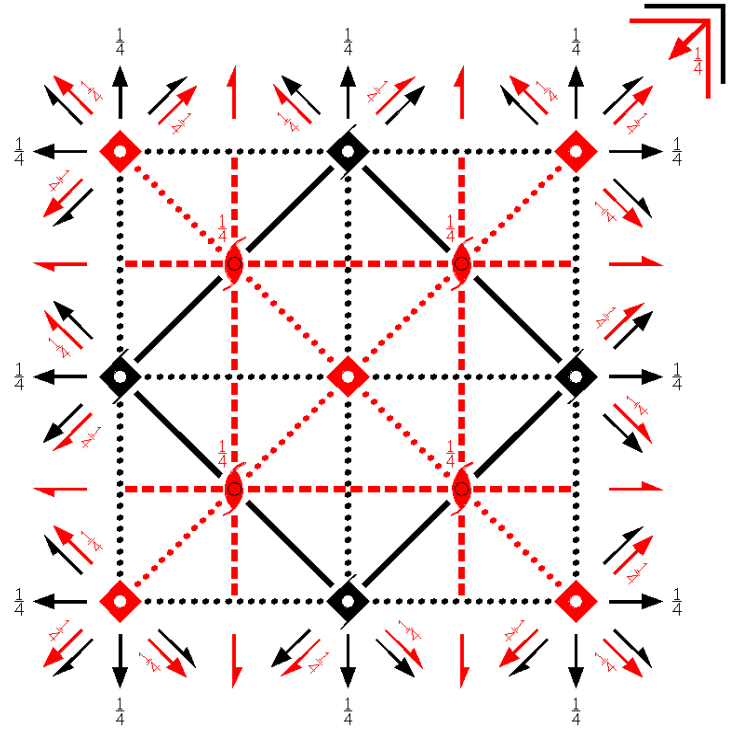
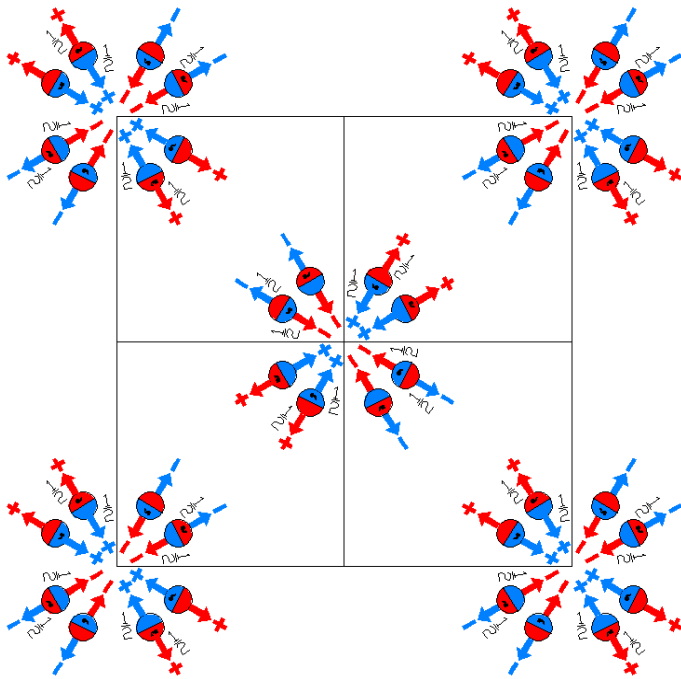
$I_P 4'/mcm'$

140.13.1208

$4/mmm1'$

$I_P 4'/m2/c2'/m'$

Tetragonal



Origin at center ( $4'/m$ ) at  $4'/mc2_1'/c'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                  | (3) $4^+$ $0,0,z$<br>( $4_z$  0,0,0)'                        | (4) $4^-$ $0,0,z$<br>( $4_z^{-1}$  0,0,0)'                     |
| (5) 2 $0,y,1/4$<br>( $2_y$  0,0,1/2)              | (6) 2 $x,0,1/4$<br>( $2_x$  0,0,1/2)              | (7) $2'$ $x,x,1/4$<br>( $2_{xy}$  0,0,1/2)'                  | (8) $2'$ $x,\bar{x},1/4$<br>( $2_{\bar{xy}}$  0,0,1/2)'        |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)      | (10) $m$ $x,y,0$<br>( $m_z$  0,0,0)               | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z$  0,0,0)'    | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1}$  0,0,0)' |
| (13) $c$ $(0,0,1/2) \ x,0,z$<br>( $m_y$  0,0,1/2) | (14) $c$ $(0,0,1/2) \ 0,y,z$<br>( $m_x$  0,0,1/2) | (15) $c'$ $(0,0,1/2) \ x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2)' | (16) $c'$ $(0,0,1/2) \ x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2)'   |

For  $(1/2, 1/2, 1/2)'$  + set

(1) $t' (1/2, 1/2, 1/2)$ $(1   1/2, 1/2, 1/2)'$	(2) $2' (0, 0, 1/2) \quad 1/4, 1/4, z$ $(2_z   1/2, 1/2, 1/2)'$	(3) $4^+ (0, 0, 1/2) \quad 0, 1/2, z$ $(4_z   1/2, 1/2, 1/2)$	(4) $4^- (0, 0, 1/2) \quad 1/2, 0, z$ $(4_z^{-1}   1/2, 1/2, 1/2)$
(5) $2' (0, 1/2, 0) \quad 1/4, y, 0$ $(2_y   1/2, 1/2, 0)'$	(6) $2' (1/2, 0, 0) \quad x, 1/4, 0$ $(2_x   1/2, 1/2, 0)'$	(7) $2 (1/2, 1/2, 0) \quad x, x, 0$ $(2_{xy}   1/2, 1/2, 0)$	(8) $2 \quad x, \bar{x} + 1/2, 0$ $(2_{\bar{xy}}   1/2, 1/2, 0)$
(9) $\bar{1}' \quad 1/4, 1/4, 1/4$ $(\bar{1}   1/2, 1/2, 1/2)'$	(10) $n' (1/2, 1/2, 0) \quad x, y, 1/4$ $(m_z   1/2, 1/2, 1/2)'$	(11) $\bar{4}^+ \quad 1/2, 0, z; \quad 1/2, 0, 1/4$ $(\bar{4}_z   1/2, 1/2, 1/2)$	(12) $\bar{4}^- \quad 0, 1/2, z; \quad 0, 1/2, 1/4$ $(\bar{4}_z^{-1}   1/2, 1/2, 1/2)$
(13) $a' (1/2, 0, 0) \quad x, 1/4, z$ $(m_y   1/2, 1/2, 0)'$	(14) $b' (0, 1/2, 0) \quad 1/4, y, z$ $(m_x   1/2, 1/2, 0)'$	(15) $m \quad x + 1/2, \bar{x}, z$ $(m_{xy}   1/2, 1/2, 0)$	(16) $g (1/2, 1/2, 0) \quad x, x, z$ $(m_{\bar{xy}}   1/2, 1/2, 0)$

**Generators selected** (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ;  $t'(1/2, 1/2, 1/2)$ ; (2); (3); (5); (9).**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			$(0, 0, 0) +$	$(1/2, 1/2, 1/2)'$ +		
32	m	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{y}, x, z [v, \bar{u}, \bar{w}]$	(4) $y, \bar{x}, z [\bar{v}, u, \bar{w}]$
			(5) $\bar{x}, y, \bar{z} + 1/2 [\bar{u}, v, \bar{w}]$	(6) $x, \bar{y}, \bar{z} + 1/2 [u, \bar{v}, \bar{w}]$	(7) $y, x, \bar{z} + 1/2 [\bar{v}, \bar{u}, w]$	(8) $\bar{y}, \bar{x}, \bar{z} + 1/2 [v, u, w]$
			(9) $\bar{x}, \bar{y}, \bar{z} [u, v, w]$	(10) $x, y, \bar{z} [\bar{u}, \bar{v}, w]$	(11) $y, \bar{x}, \bar{z} [v, \bar{u}, \bar{w}]$	(12) $\bar{y}, x, \bar{z} [\bar{v}, u, \bar{w}]$
			(13) $x, \bar{y}, z + 1/2 [\bar{u}, v, \bar{w}]$	(14) $\bar{x}, y, z + 1/2 [u, \bar{v}, \bar{w}]$	(15) $\bar{y}, \bar{x}, z + 1/2 [\bar{v}, \bar{u}, w]$	(16) $y, x, z + 1/2 [v, u, w]$
16	l	..m	$x, x + 1/2, z [\bar{u}, u, 0]$	$\bar{x}, \bar{x} + 1/2, z [u, \bar{u}, 0]$	$\bar{x} + 1/2, x, z [u, u, 0]$	$x + 1/2, \bar{x}, z [\bar{u}, \bar{u}, 0]$
			$\bar{x}, x + 1/2, \bar{z} + 1/2 [u, u, 0]$	$x, \bar{x} + 1/2, \bar{z} + 1/2 [\bar{u}, \bar{u}, 0]$	$x + 1/2, x, \bar{z} + 1/2 [\bar{u}, u, 0]$	$\bar{x} + 1/2, \bar{x}, \bar{z} + 1/2 [u, \bar{u}, 0]$
16	k	m..	$x, y, 0 [0, 0, w]$	$\bar{x}, \bar{y}, 0 [0, 0, w]$	$\bar{y}, x, 0 [0, 0, \bar{w}]$	$y, \bar{x}, 0 [0, 0, \bar{w}]$
			$\bar{x}, y, 1/2 [0, 0, \bar{w}]$	$x, \bar{y}, 1/2 [0, 0, \bar{w}]$	$y, x, 1/2 [0, 0, w]$	$\bar{y}, \bar{x}, 1/2 [0, 0, w]$
16	j	.2.	$x, 0, 1/4 [u, 0, 0]$	$\bar{x}, 0, 1/4 [\bar{u}, 0, 0]$	$0, x, 1/4 [0, \bar{u}, 0]$	$0, \bar{x}, 1/4 [0, u, 0]$
			$\bar{x}, 0, 3/4 [\bar{u}, 0, 0]$	$x, 0, 3/4 [u, 0, 0]$	$0, \bar{x}, 3/4 [0, \bar{u}, 0]$	$0, x, 3/4 [0, u, 0]$
16	i	..2'	$x, x, 1/4 [\bar{u}, u, w]$	$\bar{x}, \bar{x}, 1/4 [u, \bar{u}, w]$	$\bar{x}, x, 1/4 [u, u, \bar{w}]$	$x, \bar{x}, 1/4 [\bar{u}, \bar{u}, \bar{w}]$
			$\bar{x}, \bar{x}, 3/4 [\bar{u}, u, w]$	$x, x, 3/4 [u, \bar{u}, w]$	$x, \bar{x}, 3/4 [u, u, \bar{w}]$	$\bar{x}, x, 3/4 [\bar{u}, \bar{u}, \bar{w}]$
8	h	m.2m	$x, x + 1/2, 0 [0, 0, 0]$	$\bar{x}, \bar{x} + 1/2, 0 [0, 0, 0]$	$\bar{x} + 1/2, x, 0 [0, 0, 0]$	$x + 1/2, \bar{x}, 0 [0, 0, 0]$
8	g	2.mm	$0, 1/2, z [0, 0, 0]$	$1/2, 0, z [0, 0, 0]$	$0, 1/2, \bar{z} + 1/2 [0, 0, 0]$	$1/2, 0, \bar{z} + 1/2 [0, 0, 0]$
8	f	4..	$0, 0, z [0, 0, w]$	$0, 0, \bar{z} + 1/2 [0, 0, \bar{w}]$	$0, 0, \bar{z} [0, 0, w]$	$0, 0, z + 1/2 [0, 0, \bar{w}]$
8	e	..2'/m	$1/4, 1/4, 1/4 [0, 0, 0]$	$3/4, 3/4, 1/4 [0, 0, 0]$	$3/4, 1/4, 1/4 [0, 0, 0]$	$1/4, 3/4, 1/4 [0, 0, 0]$
4	d	m.mm	$0, 1/2, 0 [0, 0, 0]$	$1/2, 0, 0 [0, 0, 0]$		

4	c	$4'/m..$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]
4	b	$\overline{4}2m$	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	a	$4'22'$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]

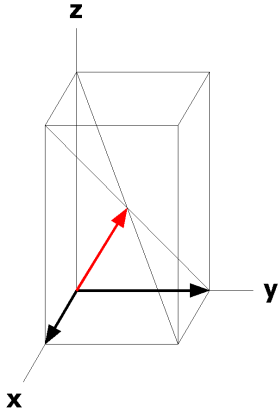
**Symmetry of Special Projections**

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}2m'm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,1/4

Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0





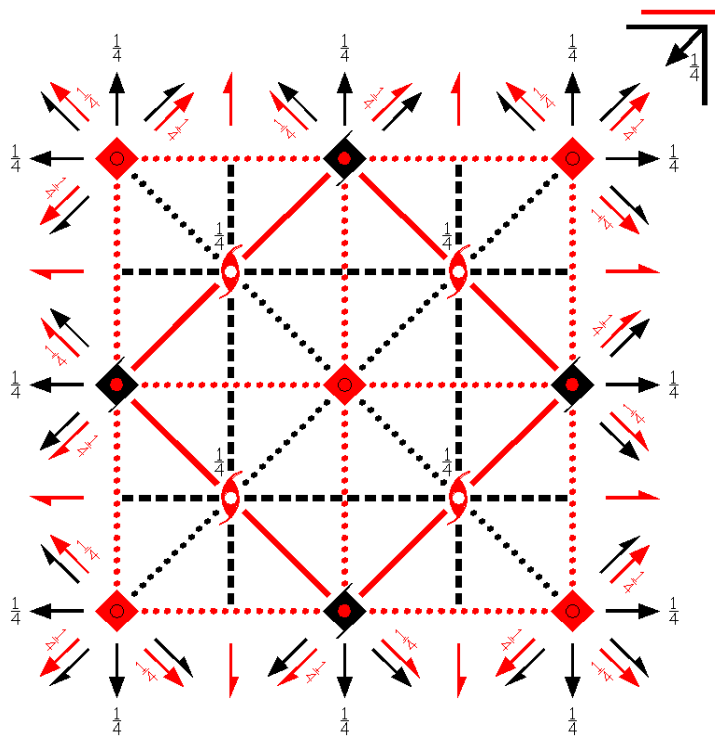
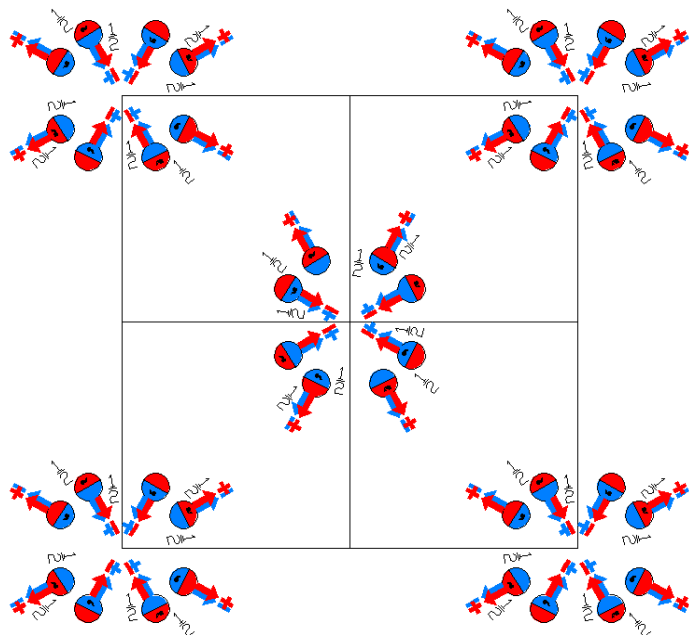
$I_p 4'/m'c'm$

140.14.1209

$4/mmm1'$

$I_p 4'/m'2/c'2'/m$

Tetragonal



Origin at center ( $4'/m'$ ) at  $4'/m'c'2'_1/c$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                    | (3) $4^+$ $0,0,z$<br>( $4_z^+$  0,0,0)'                    | (4) $4^-$ $0,0,z$<br>( $4_z^-$  0,0,0)'                    |
| (5) 2 $0,y,1/4$<br>( $2_y$  0,0,1/2)                | (6) 2 $x,0,1/4$<br>( $2_x$  0,0,1/2)                | (7) $2'$ $x,x,1/4$<br>( $2_{xy}$  0,0,1/2)'                | (8) $2'$ $x,\bar{x},1/4$<br>( $2_{\bar{xy}}$  0,0,1/2)'    |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)'       | (10) $m'$ $x,y,0$<br>( $m_z$  0,0,0)'               | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^+$  0,0,0) | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^-$  0,0,0) |
| (13) $c'$ $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2)' | (14) $c'$ $(0,0,1/2)$ $0,y,z$<br>( $m_x$  0,0,1/2)' | (15) $c$ $(0,0,1/2)$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2) | (16) $c$ $(0,0,1/2)$ $x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2) |

For  $(1/2, 1/2, 1/2)'$  + set

(1) $t' (1/2, 1/2, 1/2)$ $(1   1/2, 1/2, 1/2)'$	(2) $2' (0, 0, 1/2) \quad 1/4, 1/4, z$ $(2_z   1/2, 1/2, 1/2)'$	(3) $4^+ (0, 0, 1/2) \quad 0, 1/2, z$ $(4_z   1/2, 1/2, 1/2)$	(4) $4^- (0, 0, 1/2) \quad 1/2, 0, z$ $(4_z^{-1}   1/2, 1/2, 1/2)$
(5) $2' (0, 1/2, 0) \quad 1/4, y, 0$ $(2_y   1/2, 1/2, 0)'$	(6) $2' (1/2, 0, 0) \quad x, 1/4, 0$ $(2_x   1/2, 1/2, 0)'$	(7) $2 (1/2, 1/2, 0) \quad x, x, 0$ $(2_{xy}   1/2, 1/2, 0)$	(8) $2 \quad x, \bar{x} + 1/2, 0$ $(2_{\bar{xy}}   1/2, 1/2, 0)$
(9) $\bar{1} \quad 1/4, 1/4, 1/4$ $(\bar{1}   1/2, 1/2, 1/2)$	(10) $n (1/2, 1/2, 0) \quad x, y, 1/4$ $(m_z   1/2, 1/2, 1/2)$	(11) $\bar{4}^+ \quad 1/2, 0, z; \quad 1/2, 0, 1/4$ $(\bar{4}_z   1/2, 1/2, 1/2)'$	(12) $\bar{4}^- \quad 0, 1/2, z; \quad 0, 1/2, 1/4$ $(\bar{4}_z^{-1}   1/2, 1/2, 1/2)'$
(13) $a (1/2, 0, 0) \quad x, 1/4, z$ $(m_y   1/2, 1/2, 0)$	(14) $b (0, 1/2, 0) \quad 1/4, y, z$ $(m_x   1/2, 1/2, 0)$	(15) $m' \quad x + 1/2, \bar{x}, z$ $(m_{xy}   1/2, 1/2, 0)'$	(16) $g' (1/2, 1/2, 0) \quad x, x, z$ $(m_{\bar{xy}}   1/2, 1/2, 0)'$

**Generators selected** (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ;  $t'(1/2, 1/2, 1/2)$ ; (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0, 0, 0) +	(1/2, 1/2, 1/2)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	m	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{y}, x, z [v, \bar{u}, \bar{w}]$	(4) $y, \bar{x}, z [\bar{v}, u, \bar{w}]$
			(5) $\bar{x}, y, \bar{z} + 1/2 [\bar{u}, v, \bar{w}]$	(6) $x, \bar{y}, \bar{z} + 1/2 [u, \bar{v}, \bar{w}]$	(7) $y, x, \bar{z} + 1/2 [\bar{v}, \bar{u}, w]$	(8) $\bar{y}, \bar{x}, \bar{z} + 1/2 [v, u, w]$
			(9) $\bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$	(10) $x, y, \bar{z} [u, v, \bar{w}]$	(11) $y, \bar{x}, \bar{z} [\bar{v}, u, w]$	(12) $\bar{y}, x, \bar{z} [v, \bar{u}, w]$
			(13) $x, \bar{y}, z + 1/2 [u, \bar{v}, w]$	(14) $\bar{x}, y, z + 1/2 [\bar{u}, v, w]$	(15) $\bar{y}, \bar{x}, z + 1/2 [v, u, \bar{w}]$	(16) $y, x, z + 1/2 [v, \bar{u}, \bar{w}]$
16	l	..m'	$x, x + 1/2, z [u, u, w]$	$\bar{x}, \bar{x} + 1/2, z [\bar{u}, \bar{u}, w]$	$\bar{x} + 1/2, x, z [u, \bar{u}, \bar{w}]$	$x + 1/2, \bar{x}, z [\bar{u}, u, \bar{w}]$
			$\bar{x}, x + 1/2, \bar{z} + 1/2 [\bar{u}, u, \bar{w}]$	$x, \bar{x} + 1/2, \bar{z} + 1/2 [u, \bar{u}, \bar{w}]$	$x + 1/2, x, \bar{z} + 1/2 [\bar{u}, \bar{u}, w]$	$\bar{x} + 1/2, \bar{x}, \bar{z} + 1/2 [u, u, w]$
16	k	m'..	$x, y, 0 [u, v, 0]$	$\bar{x}, \bar{y}, 0 [\bar{u}, \bar{v}, 0]$	$\bar{y}, x, 0 [v, \bar{u}, 0]$	$y, \bar{x}, 0 [\bar{v}, u, 0]$
			$\bar{x}, y, 1/2 [\bar{u}, v, 0]$	$x, \bar{y}, 1/2 [u, \bar{v}, 0]$	$y, x, 1/2 [v, \bar{u}, 0]$	$\bar{y}, \bar{x}, 1/2 [\bar{v}, u, 0]$
16	j	.2.	$x, 0, 1/4 [u, 0, 0]$	$\bar{x}, 0, 1/4 [\bar{u}, 0, 0]$	$0, x, 1/4 [0, \bar{u}, 0]$	$0, \bar{x}, 1/4 [0, u, 0]$
			$\bar{x}, 0, 3/4 [\bar{u}, 0, 0]$	$x, 0, 3/4 [u, 0, 0]$	$0, \bar{x}, 3/4 [0, \bar{u}, 0]$	$0, x, 3/4 [0, u, 0]$
16	i	..2'	$x, x, 1/4 [\bar{u}, u, w]$	$\bar{x}, \bar{x}, 1/4 [u, \bar{u}, w]$	$\bar{x}, x, 1/4 [u, u, \bar{w}]$	$x, \bar{x}, 1/4 [\bar{u}, \bar{u}, \bar{w}]$
			$\bar{x}, \bar{x}, 3/4 [u, \bar{u}, \bar{w}]$	$x, x, 3/4 [\bar{u}, u, w]$	$x, \bar{x}, 3/4 [\bar{u}, \bar{u}, w]$	$\bar{x}, x, 3/4 [u, u, w]$
8	h	m'.2m'	$x, x + 1/2, 0 [u, u, 0]$	$\bar{x}, \bar{x} + 1/2, 0 [\bar{u}, \bar{u}, 0]$	$\bar{x} + 1/2, x, 0 [u, \bar{u}, 0]$	$x + 1/2, \bar{x}, 0 [\bar{u}, u, 0]$
8	g	2.m'm'	$0, 1/2, z [0, 0, w]$	$1/2, 0, z [0, 0, \bar{w}]$	$0, 1/2, \bar{z} + 1/2 [0, 0, \bar{w}]$	$1/2, 0, \bar{z} + 1/2 [0, 0, w]$
8	f	4'..	$0, 0, z [0, 0, 0]$	$0, 0, \bar{z} + 1/2 [0, 0, 0]$	$0, 0, \bar{z} [0, 0, 0]$	$0, 0, z + 1/2 [0, 0, 0]$
8	e	..2'/m'	$1/4, 1/4, 1/4 [u, v, 0]$	$3/4, 3/4, 1/4 [\bar{u}, \bar{v}, 0]$	$3/4, 1/4, 1/4 [v, \bar{u}, 0]$	$1/4, 3/4, 1/4 [\bar{v}, u, 0]$
4	d	m'.m'm'	$0, 1/2, 0 [0, 0, 0]$	$1/2, 0, 0 [0, 0, 0]$		

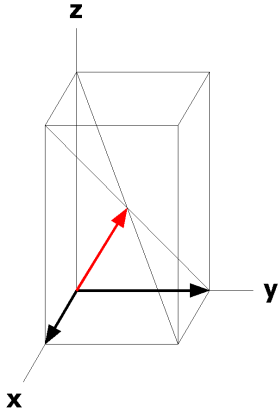
4	c	$4'/m'..$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]
4	b	$\overline{4}'2m'$	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	a	$4'22'$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $p_p \cdot 4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,1/2,z

Along [1,0,0]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

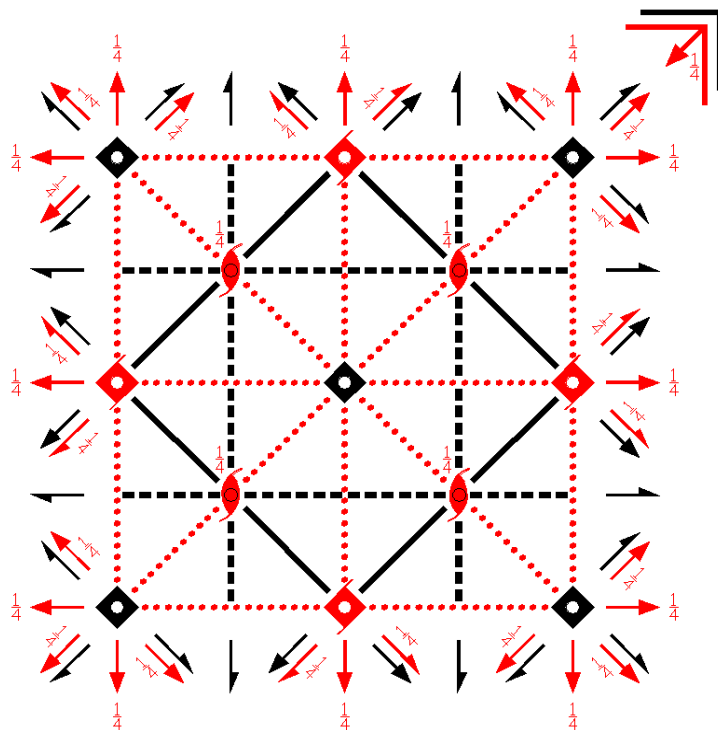
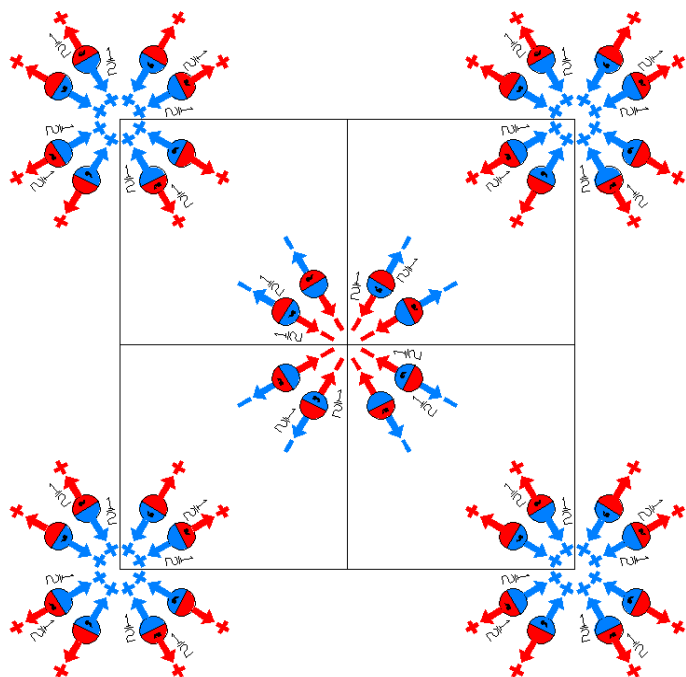
Along [1,1,0]  $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$I_P 4/mc'm'$   
140.15.1210

$4/mmm1'$   
 $I_P 4/m2'/c2'/m'$

Tetragonal



Origin at center ( $4/m$ ) at  $4/mc'2_1/c'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                    | (3) $4^+$ $0,0,z$<br>( $4_z$  0,0,0)                         | (4) $4^-$ $0,0,z$<br>( $4_z^{-1}$  0,0,0)                     |
| (5) $2'$ $0,y,1/4$<br>( $2_y$  0,0,1/2)'            | (6) $2'$ $x,0,1/4$<br>( $2_x$  0,0,1/2)'            | (7) $2'$ $x,x,1/4$<br>( $2_{xy}$  0,0,1/2)'                  | (8) $2'$ $x,\bar{x},1/4$<br>( $2_{\bar{xy}}$  0,0,1/2)'       |
| (9) $\bar{1}$ $0,0,0$<br>( $\bar{1}$  0,0,0)        | (10) $m$ $x,y,0$<br>( $m_z$  0,0,0)                 | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z$  0,0,0)     | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1}$  0,0,0) |
| (13) $c'$ $(0,0,1/2)$ $x,0,z$<br>( $m_y$  0,0,1/2)' | (14) $c'$ $(0,0,1/2)$ $0,y,z$<br>( $m_x$  0,0,1/2)' | (15) $c'$ $(0,0,1/2)$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2)' | (16) $c'$ $(0,0,1/2)$ $x,x,z$<br>( $m_{\bar{xy}}$  0,0,1/2)'  |

For  $(1/2, 1/2, 1/2)'$  + set

(1) $t' (1/2, 1/2, 1/2)$ $(1   1/2, 1/2, 1/2)'$	(2) $2' (0, 0, 1/2) \quad 1/4, 1/4, z$ $(2_z   1/2, 1/2, 1/2)'$	(3) $4^+ (0, 0, 1/2) \quad 0, 1/2, z$ $(4_z   1/2, 1/2, 1/2)'$	(4) $4^- (0, 0, 1/2) \quad 1/2, 0, z$ $(4_z^{-1}   1/2, 1/2, 1/2)'$
(5) $2 (0, 1/2, 0) \quad 1/4, y, 0$ $(2_y   1/2, 1/2, 0)$	(6) $2 (1/2, 0, 0) \quad x, 1/4, 0$ $(2_x   1/2, 1/2, 0)$	(7) $2 (1/2, 1/2, 0) \quad x, x, 0$ $(2_{xy}   1/2, 1/2, 0)$	(8) $2 \quad x, \bar{x} + 1/2, 0$ $(2_{\bar{xy}}   1/2, 1/2, 0)$
(9) $\bar{1}' \quad 1/4, 1/4, 1/4$ $(\bar{1}   1/2, 1/2, 1/2)'$	(10) $n' (1/2, 1/2, 0) \quad x, y, 1/4$ $(m_z   1/2, 1/2, 1/2)'$	(11) $\bar{4}^+ (1/2, 0, z; 1/2, 0, 1/4)$ $(\bar{4}_z   1/2, 1/2, 1/2)'$	(12) $\bar{4}^- (0, 1/2, z; 0, 1/2, 1/4)$ $(\bar{4}_z^{-1}   1/2, 1/2, 1/2)'$
(13) $a (1/2, 0, 0) \quad x, 1/4, z$ $(m_y   1/2, 1/2, 0)$	(14) $b (0, 1/2, 0) \quad 1/4, y, z$ $(m_x   1/2, 1/2, 0)$	(15) $m \quad x + 1/2, \bar{x}, z$ $(m_{xy}   1/2, 1/2, 0)$	(16) $g (1/2, 1/2, 0) \quad x, x, z$ $(m_{\bar{xy}}   1/2, 1/2, 0)$

**Generators selected** (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ;  $t'(1/2, 1/2, 1/2)$ ; (2); (3); (5); (9).**Positions**

			Coordinates			
			(0, 0, 0) +	$(1/2, 1/2, 1/2)'$ +		
Multiplicity,						
Wyckoff letter,						
Site Symmetry.						
32	m	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{y}, x, z [\bar{v}, u, w]$	(4) $y, \bar{x}, z [v, \bar{u}, w]$
			(5) $\bar{x}, y, \bar{z} + 1/2 [u, \bar{v}, w]$	(6) $x, \bar{y}, \bar{z} + 1/2 [\bar{u}, v, w]$	(7) $y, x, \bar{z} + 1/2 [\bar{v}, \bar{u}, w]$	(8) $\bar{y}, \bar{x}, \bar{z} + 1/2 [v, u, w]$
			(9) $\bar{x}, \bar{y}, \bar{z} [u, v, w]$	(10) $x, y, z [\bar{u}, \bar{v}, w]$	(11) $y, \bar{x}, \bar{z} [\bar{v}, u, w]$	(12) $\bar{y}, x, z [v, \bar{u}, w]$
			(13) $x, \bar{y}, z + 1/2 [u, \bar{v}, w]$	(14) $\bar{x}, y, z + 1/2 [\bar{u}, v, w]$	(15) $\bar{y}, \bar{x}, z + 1/2 [\bar{v}, \bar{u}, w]$	(16) $y, x, z + 1/2 [v, u, w]$
16	l	..m	$x, x + 1/2, z [\bar{u}, u, 0]$	$\bar{x}, \bar{x} + 1/2, z [u, \bar{u}, 0]$	$\bar{x} + 1/2, x, z [\bar{u}, \bar{u}, 0]$	$x + 1/2, \bar{x}, z [u, u, 0]$
			$\bar{x}, x + 1/2, \bar{z} + 1/2 [\bar{u}, \bar{u}, 0]$	$x, \bar{x} + 1/2, \bar{z} + 1/2 [u, u, 0]$	$x + 1/2, x, \bar{z} + 1/2 [\bar{u}, u, 0]$	$\bar{x} + 1/2, \bar{x}, \bar{z} + 1/2 [u, \bar{u}, 0]$
16	k	m..	$x, y, 0 [0, 0, w]$	$\bar{x}, \bar{y}, 0 [0, 0, w]$	$\bar{y}, x, 0 [0, 0, w]$	$y, \bar{x}, 0 [0, 0, w]$
			$\bar{x}, y, 1/2 [0, 0, w]$	$x, \bar{y}, 1/2 [0, 0, w]$	$y, x, 1/2 [0, 0, w]$	$\bar{y}, \bar{x}, 1/2 [0, 0, w]$
16	j	.2'	$x, 0, 1/4 [0, v, w]$	$\bar{x}, 0, 1/4 [0, \bar{v}, w]$	$0, x, 1/4 [\bar{v}, 0, w]$	$0, \bar{x}, 1/4 [v, 0, w]$
			$\bar{x}, 0, 3/4 [0, \bar{v}, w]$	$x, 0, 3/4 [0, v, w]$	$0, \bar{x}, 3/4 [\bar{v}, 0, w]$	$0, x, 3/4 [v, 0, w]$
16	i	..2'	$x, x, 1/4 [\bar{u}, u, w]$	$\bar{x}, \bar{x}, 1/4 [u, \bar{u}, w]$	$\bar{x}, x, 1/4 [\bar{u}, \bar{u}, w]$	$x, \bar{x}, 1/4 [u, u, w]$
			$\bar{x}, \bar{x}, 3/4 [\bar{u}, u, w]$	$x, x, 3/4 [u, \bar{u}, w]$	$x, \bar{x}, 3/4 [\bar{u}, \bar{u}, w]$	$\bar{x}, x, 3/4 [u, u, w]$
8	h	m.2m	$x, x + 1/2, 0 [0, 0, 0]$	$\bar{x}, \bar{x} + 1/2, 0 [0, 0, 0]$	$\bar{x} + 1/2, x, 0 [0, 0, 0]$	$x + 1/2, \bar{x}, 0 [0, 0, 0]$
8	g	2.mm	$0, 1/2, z [0, 0, 0]$	$1/2, 0, z [0, 0, 0]$	$0, 1/2, \bar{z} + 1/2 [0, 0, 0]$	$1/2, 0, \bar{z} + 1/2 [0, 0, 0]$
8	f	4..	$0, 0, z [0, 0, w]$	$0, 0, \bar{z} + 1/2 [0, 0, w]$	$0, 0, \bar{z} [0, 0, w]$	$0, 0, z + 1/2 [0, 0, w]$
8	e	..2'/m	$1/4, 1/4, 1/4 [0, 0, 0]$	$3/4, 3/4, 1/4 [0, 0, 0]$	$3/4, 1/4, 1/4 [0, 0, 0]$	$1/4, 3/4, 1/4 [0, 0, 0]$
4	d	m.mm	$0, 1/2, 0 [0, 0, 0]$	$1/2, 0, 0 [0, 0, 0]$		

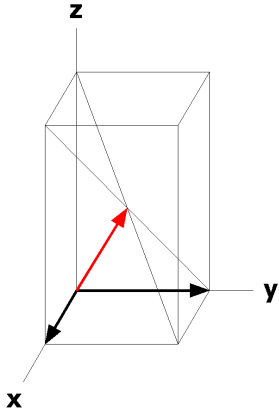
4	c	4/m..	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]
4	b	$\bar{4}'2'm$	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	a	42'2'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]

**Symmetry of Special Projections**

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a'}2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,0

Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



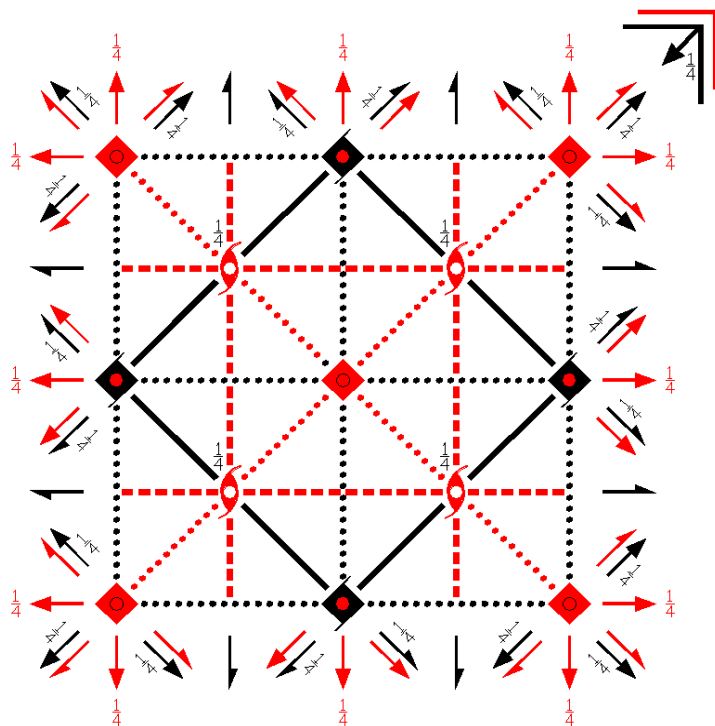
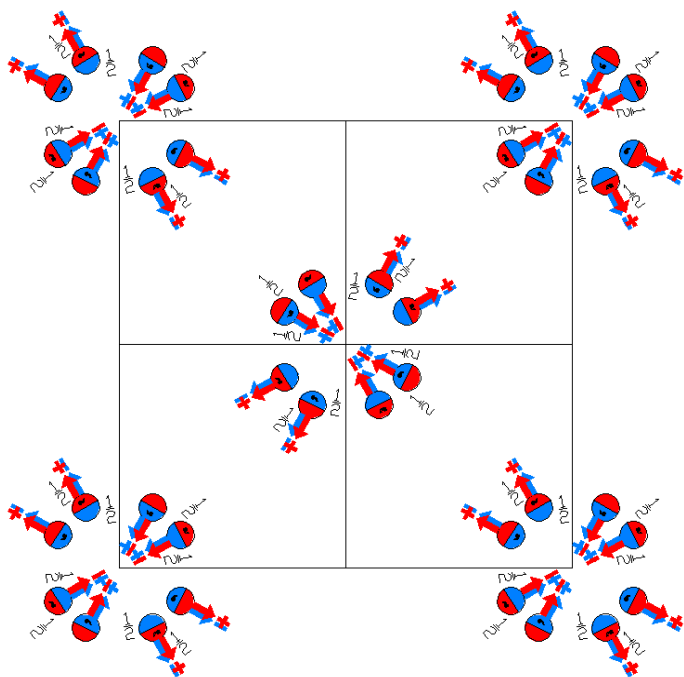
$I_P 4'/m'cm'$

140.16.1211

$4/mmm1'$

$I_P 4'/m'2'/c2/m'$

Tetragonal



Origin at center ( $4'/m'$ ) at  $4'/m'c2_1/c'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)              | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub>  0,0,0)'                     | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'        |
| (5) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'        | (6) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'        | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                              | (8) 2 x,x̄,1/4<br>(2 <sub>xȳ</sub>  0,0,1/2)                             |
| (9) 1̄ 0,0,0<br>(1̄ 0,0,0)'                         | (10) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'           | (11) 4 <sup>+</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (12) 4 <sup>-</sup> 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) c (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2) | (14) c (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2) | (15) c' (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)'                  | (16) c' (0,0,1/2) x,x,z<br>(m <sub>xȳ</sub>  0,0,1/2)'                   |

For  $(1/2, 1/2, 1/2)'$  + set

(1) $t' (1/2, 1/2, 1/2)$ $(1   1/2, 1/2, 1/2)'$	(2) $2' (0, 0, 1/2) \quad 1/4, 1/4, z$ $(2_z   1/2, 1/2, 1/2)'$	(3) $4^+ (0, 0, 1/2) \quad 0, 1/2, z$ $(4_z   1/2, 1/2, 1/2)$	(4) $4^- (0, 0, 1/2) \quad 1/2, 0, z$ $(4_z^{-1}   1/2, 1/2, 1/2)$
(5) $2 (0, 1/2, 0) \quad 1/4, y, 0$ $(2_y   1/2, 1/2, 0)$	(6) $2 (1/2, 0, 0) \quad x, 1/4, 0$ $(2_x   1/2, 1/2, 0)$	(7) $2' (1/2, 1/2, 0) \quad x, x, 0$ $(2_{xy}   1/2, 1/2, 0)'$	(8) $2' \quad x, \bar{x} + 1/2, 0$ $(2_{\bar{xy}}   1/2, 1/2, 0)'$
(9) $\bar{1} \quad 1/4, 1/4, 1/4$ $(\bar{1}   1/2, 1/2, 1/2)$	(10) $n (1/2, 1/2, 0) \quad x, y, 1/4$ $(m_z   1/2, 1/2, 1/2)$	(11) $\bar{4}^+ \quad 1/2, 0, z; \quad 1/2, 0, 1/4$ $(\bar{4}_z   1/2, 1/2, 1/2)'$	(12) $\bar{4}^- \quad 0, 1/2, z; \quad 0, 1/2, 1/4$ $(\bar{4}_z^{-1}   1/2, 1/2, 1/2)'$
(13) $a' (1/2, 0, 0) \quad x, 1/4, z$ $(m_y   1/2, 1/2, 0)'$	(14) $b' (0, 1/2, 0) \quad 1/4, y, z$ $(m_x   1/2, 1/2, 0)'$	(15) $m \quad x + 1/2, \bar{x}, z$ $(m_{xy}   1/2, 1/2, 0)$	(16) $g (1/2, 1/2, 0) \quad x, x, z$ $(m_{\bar{xy}}   1/2, 1/2, 0)$

**Generators selected** (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ;  $t'(1/2, 1/2, 1/2)$ ; (2); (3); (5); (9).**Positions**

			Coordinates			
			(0, 0, 0) +	$(1/2, 1/2, 1/2)'$ +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	m	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{y}, x, z [v, \bar{u}, \bar{w}]$	(4) $y, \bar{x}, z [\bar{v}, u, \bar{w}]$
			(5) $\bar{x}, y, \bar{z} + 1/2 [u, \bar{v}, w]$	(6) $x, \bar{y}, \bar{z} + 1/2 [\bar{u}, v, w]$	(7) $y, x, \bar{z} + 1/2 [v, u, \bar{w}]$	(8) $\bar{y}, \bar{x}, \bar{z} + 1/2 [\bar{v}, \bar{u}, \bar{w}]$
			(9) $\bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$	(10) $x, y, \bar{z} [u, v, \bar{w}]$	(11) $y, \bar{x}, \bar{z} [v, u, \bar{w}]$	(12) $\bar{y}, x, \bar{z} [v, \bar{u}, w]$
			(13) $x, \bar{y}, z + 1/2 [\bar{u}, v, \bar{w}]$	(14) $\bar{x}, y, z + 1/2 [u, \bar{v}, \bar{w}]$	(15) $\bar{y}, \bar{x}, z + 1/2 [\bar{v}, \bar{u}, w]$	(16) $y, x, z + 1/2 [v, u, w]$
16	l	..m	$x, x + 1/2, z [\bar{u}, u, 0]$	$\bar{x}, \bar{x} + 1/2, z [u, \bar{u}, 0]$	$\bar{x} + 1/2, x, z [u, u, 0]$	$x + 1/2, \bar{x}, z [\bar{u}, \bar{u}, 0]$
			$\bar{x}, x + 1/2, \bar{z} + 1/2 [\bar{u}, \bar{u}, 0]$	$x, \bar{x} + 1/2, \bar{z} + 1/2 [u, u, 0]$	$x + 1/2, x, \bar{z} + 1/2 [u, \bar{u}, 0]$	$\bar{x} + 1/2, \bar{x}, \bar{z} + 1/2 [\bar{u}, u, 0]$
16	k	m'..	$x, y, 0 [u, v, 0]$	$\bar{x}, \bar{y}, 0 [\bar{u}, \bar{v}, 0]$	$\bar{y}, x, 0 [v, \bar{u}, 0]$	$y, \bar{x}, 0 [\bar{v}, u, 0]$
			$\bar{x}, y, 1/2 [u, \bar{v}, 0]$	$x, \bar{y}, 1/2 [\bar{u}, v, 0]$	$y, x, 1/2 [v, u, 0]$	$\bar{y}, \bar{x}, 1/2 [\bar{v}, \bar{u}, 0]$
16	j	.2'	$x, 0, 1/4 [0, v, w]$	$\bar{x}, 0, 1/4 [0, \bar{v}, w]$	$0, x, 1/4 [v, 0, \bar{w}]$	$0, \bar{x}, 1/4 [\bar{v}, 0, \bar{w}]$
			$\bar{x}, 0, 3/4 [0, \bar{v}, w]$	$x, 0, 3/4 [0, v, w]$	$0, \bar{x}, 3/4 [v, 0, \bar{w}]$	$0, x, 3/4 [\bar{v}, 0, \bar{w}]$
16	i	..2	$x, x, 1/4 [u, u, 0]$	$\bar{x}, \bar{x}, 1/4 [\bar{u}, \bar{u}, 0]$	$\bar{x}, x, 1/4 [\bar{u}, \bar{u}, 0]$	$x, \bar{x}, 1/4 [u, u, 0]$
			$\bar{x}, \bar{x}, 3/4 [\bar{u}, \bar{u}, 0]$	$x, x, 3/4 [u, u, 0]$	$x, \bar{x}, 3/4 [\bar{u}, u, 0]$	$\bar{x}, x, 3/4 [u, \bar{u}, 0]$
8	h	m'.2'm	$x, x + 1/2, 0 [\bar{u}, u, 0]$	$\bar{x}, \bar{x} + 1/2, 0 [u, \bar{u}, 0]$	$\bar{x} + 1/2, x, 0 [u, u, 0]$	$x + 1/2, \bar{x}, 0 [\bar{u}, \bar{u}, 0]$
8	g	2.mm	$0, 1/2, z [0, 0, 0]$	$1/2, 0, z [0, 0, 0]$	$0, 1/2, \bar{z} + 1/2 [0, 0, 0]$	$1/2, 0, \bar{z} + 1/2 [0, 0, 0]$
8	f	4'..	$0, 0, z [0, 0, 0]$	$0, 0, \bar{z} + 1/2 [0, 0, 0]$	$0, 0, \bar{z} [0, 0, 0]$	$0, 0, z + 1/2 [0, 0, 0]$
8	e	..2/m	$1/4, 1/4, 1/4 [0, 0, w]$	$3/4, 3/4, 1/4 [0, 0, w]$	$3/4, 1/4, 1/4 [0, 0, \bar{w}]$	$1/4, 3/4, 1/4 [0, 0, \bar{w}]$
4	d	m'.mm	$0, 1/2, 0 [0, 0, 0]$	$1/2, 0, 0 [0, 0, 0]$		



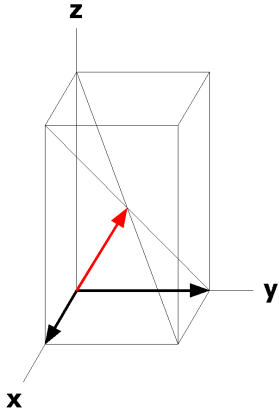
4	c	$4'/m'$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]
4	b	$\overline{4}'2'm$	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	a	$4'2'2$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $p_p \cdot 4mm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b} \cdot 2m'm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,0

Along [1,1,0]  $p_{2mm}1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



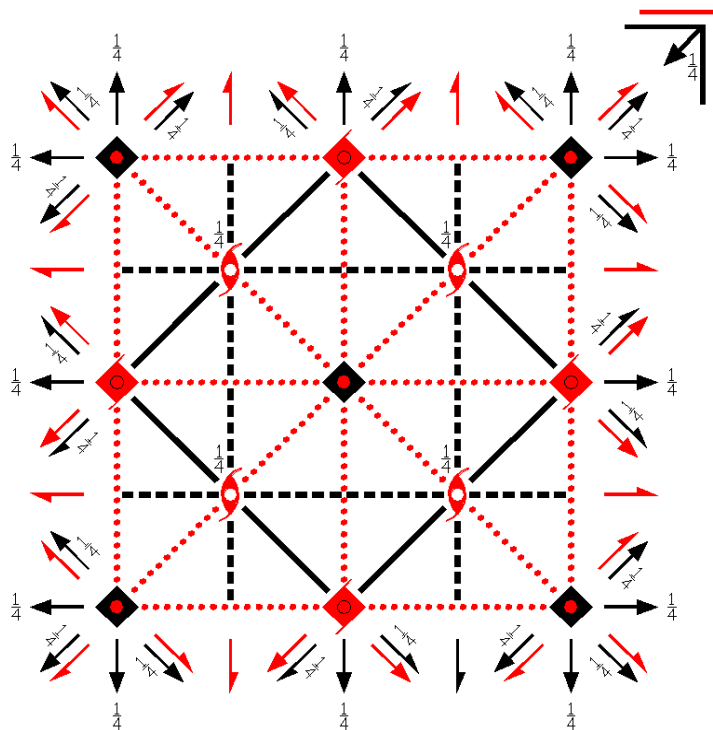
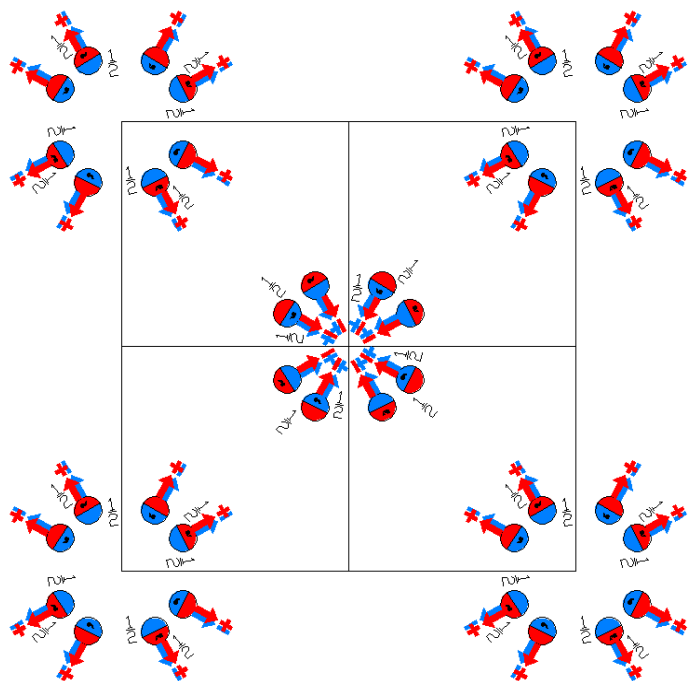
$I_P 4/m'c'm'$

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$4/mmm1'$

$I_P 4/m'2/c'2/m'$

Tetragonal



Origin at center ( $4/m'$ ) at  $4/m'c'2_1/c'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $y \leq 1/2 - x$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)                                    | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)          |
| (5) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)            | (6) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)            | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                      | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)  |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)'           | (10) m' x,y,0<br>(m <sub>z</sub> ' 0,0,0)'            | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'        | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                 |
| (13) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)' | (14) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)' | (15) c' (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2)' | (16) c' (0,0,1/2) x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,0,1/2)' |

For  $(1/2, 1/2, 1/2)'$  + set

(1) $t' (1/2, 1/2, 1/2)$ $(1   1/2, 1/2, 1/2)'$	(2) $2' (0, 0, 1/2) \quad 1/4, 1/4, z$ $(2_z   1/2, 1/2, 1/2)'$	(3) $4^{+} (0, 0, 1/2) \quad 0, 1/2, z$ $(4_z   1/2, 1/2, 1/2)'$	(4) $4^{-} (0, 0, 1/2) \quad 1/2, 0, z$ $(4_z^{-1}   1/2, 1/2, 1/2)'$
(5) $2' (0, 1/2, 0) \quad 1/4, y, 0$ $(2_y   1/2, 1/2, 0)'$	(6) $2' (1/2, 0, 0) \quad x, 1/4, 0$ $(2_x   1/2, 1/2, 0)'$	(7) $2' (1/2, 1/2, 0) \quad x, x, 0$ $(2_{xy}   1/2, 1/2, 0)'$	(8) $2' \quad x, \bar{x} + 1/2, 0$ $(2_{\bar{xy}}   1/2, 1/2, 0)'$
(9) $\bar{1} \quad 1/4, 1/4, 1/4$ $(\bar{1}   1/2, 1/2, 1/2)$	(10) $n (1/2, 1/2, 0) \quad x, y, 1/4$ $(m_z   1/2, 1/2, 1/2)$	(11) $\bar{4}^{+} \quad 1/2, 0, z; \quad 1/2, 0, 1/4$ $(\bar{4}_z   1/2, 1/2, 1/2)$	(12) $\bar{4}^{-} \quad 0, 1/2, z; \quad 0, 1/2, 1/4$ $(\bar{4}_z^{-1}   1/2, 1/2, 1/2)$
(13) $a (1/2, 0, 0) \quad x, 1/4, z$ $(m_y   1/2, 1/2, 0)$	(14) $b (0, 1/2, 0) \quad 1/4, y, z$ $(m_x   1/2, 1/2, 0)$	(15) $m \quad x + 1/2, \bar{x}, z$ $(m_{xy}   1/2, 1/2, 0)$	(16) $g (1/2, 1/2, 0) \quad x, x, z$ $(m_{\bar{xy}}   1/2, 1/2, 0)$

**Generators selected** (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ;  $t'(1/2, 1/2, 1/2)$ ; (2); (3); (5); (9).**Positions**

			Coordinates			
			(0, 0, 0) +	$(1/2, 1/2, 1/2)'$ +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	m	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{y}, x, z [\bar{v}, u, w]$	(4) $y, \bar{x}, z [v, \bar{u}, w]$
			(5) $\bar{x}, y, \bar{z} + 1/2 [\bar{u}, v, \bar{w}]$	(6) $x, \bar{y}, \bar{z} + 1/2 [u, v, \bar{w}]$	(7) $y, x, \bar{z} + 1/2 [v, u, \bar{w}]$	(8) $\bar{y}, \bar{x}, \bar{z} + 1/2 [\bar{v}, \bar{u}, \bar{w}]$
			(9) $\bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$	(10) $x, y, \bar{z} [\bar{u}, \bar{v}, w]$	(11) $y, \bar{x}, \bar{z} [v, \bar{u}, \bar{w}]$	(12) $\bar{y}, x, \bar{z} [\bar{v}, u, \bar{w}]$
			(13) $x, \bar{y}, z + 1/2 [u, \bar{v}, w]$	(14) $\bar{x}, y, z + 1/2 [\bar{u}, v, w]$	(15) $\bar{y}, \bar{x}, z + 1/2 [\bar{v}, \bar{u}, w]$	(16) $y, x, z + 1/2 [v, u, w]$
16	l	..m	$x, x + 1/2, z [\bar{u}, u, 0]$	$\bar{x}, \bar{x} + 1/2, z [u, \bar{u}, 0]$	$\bar{x} + 1/2, x, z [\bar{u}, \bar{u}, 0]$	$x + 1/2, \bar{x}, z [u, u, 0]$
			$\bar{x}, x + 1/2, \bar{z} + 1/2 [u, u, 0]$	$x, \bar{x} + 1/2, \bar{z} + 1/2 [\bar{u}, \bar{u}, 0]$	$x + 1/2, x, \bar{z} + 1/2 [u, \bar{u}, 0]$	$\bar{x} + 1/2, \bar{x}, \bar{z} + 1/2 [\bar{u}, \bar{u}, 0]$
16	k	m'..	$x, y, 0 [u, v, 0]$	$\bar{x}, \bar{y}, 0 [\bar{u}, \bar{v}, 0]$	$\bar{y}, x, 0 [\bar{v}, u, 0]$	$y, \bar{x}, 0 [v, \bar{u}, 0]$
			$\bar{x}, y, 1/2 [\bar{u}, v, 0]$	$x, \bar{y}, 1/2 [u, \bar{v}, 0]$	$y, x, 1/2 [v, u, 0]$	$\bar{y}, \bar{x}, 1/2 [\bar{v}, \bar{u}, 0]$
16	j	.2.	$x, 0, 1/4 [u, 0, 0]$	$\bar{x}, 0, 1/4 [\bar{u}, 0, 0]$	$0, x, 1/4 [0, u, 0]$	$0, \bar{x}, 1/4 [0, \bar{u}, 0]$
			$\bar{x}, 0, 3/4 [\bar{u}, 0, 0]$	$x, 0, 3/4 [u, 0, 0]$	$0, \bar{x}, 3/4 [0, u, 0]$	$0, x, 3/4 [0, \bar{u}, 0]$
16	i	..2	$x, x, 1/4 [u, u, 0]$	$\bar{x}, \bar{x}, 1/4 [\bar{u}, \bar{u}, 0]$	$\bar{x}, x, 1/4 [\bar{u}, u, 0]$	$x, \bar{x}, 1/4 [u, \bar{u}, 0]$
			$\bar{x}, \bar{x}, 3/4 [\bar{u}, \bar{u}, 0]$	$x, x, 3/4 [u, u, 0]$	$x, \bar{x}, 3/4 [u, \bar{u}, 0]$	$\bar{x}, x, 3/4 [\bar{u}, u, 0]$
8	h	m'.2'm	$x, x + 1/2, 0 [\bar{u}, u, 0]$	$\bar{x}, \bar{x} + 1/2, 0 [u, \bar{u}, 0]$	$\bar{x} + 1/2, x, 0 [\bar{u}, \bar{u}, 0]$	$x + 1/2, \bar{x}, 0 [u, u, 0]$
8	g	2.mm	$0, 1/2, z [0, 0, 0]$	$1/2, 0, z [0, 0, 0]$	$0, 1/2, \bar{z} + 1/2 [0, 0, 0]$	$1/2, 0, \bar{z} + 1/2 [0, 0, 0]$
8	f	4..	$0, 0, z [0, 0, w]$	$0, 0, \bar{z} + 1/2 [0, 0, \bar{w}]$	$0, 0, \bar{z} [0, 0, \bar{w}]$	$0, 0, z + 1/2 [0, 0, w]$
8	e	..2/m	$1/4, 1/4, 1/4 [0, 0, w]$	$3/4, 3/4, 1/4 [0, 0, w]$	$3/4, 1/4, 1/4 [0, 0, w]$	$1/4, 3/4, 1/4 [0, 0, w]$
4	d	m'.mm	$0, 1/2, 0 [0, 0, 0]$	$1/2, 0, 0 [0, 0, 0]$		

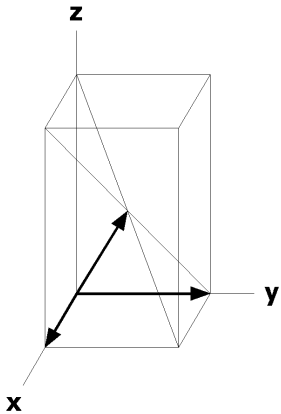
4	c	$4/m'..$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]
4	b	$\overline{4}2m$	0,1/2,1/4 [0,0,0]	1/2,0,1/4 [0,0,0]
4	a	422	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $p_p$   $4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}$   $2m'm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

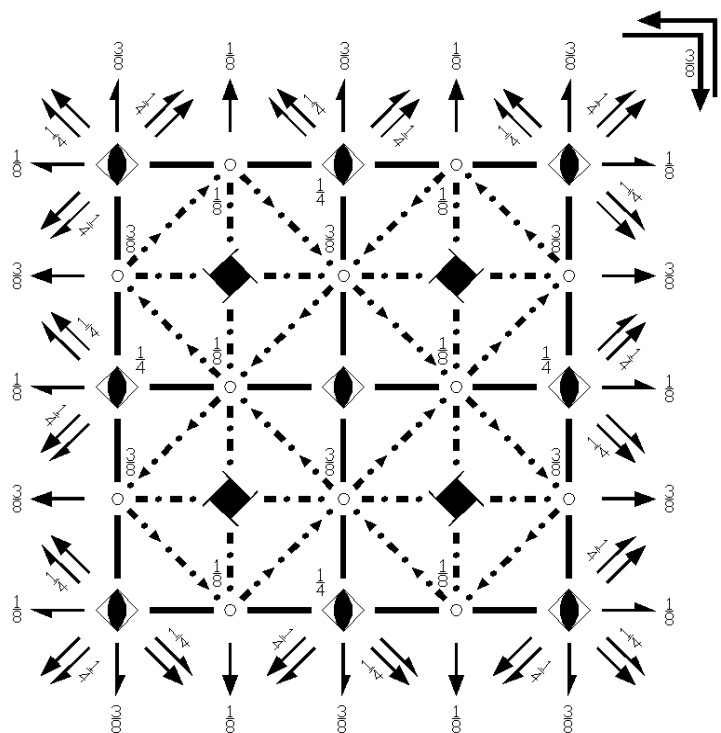
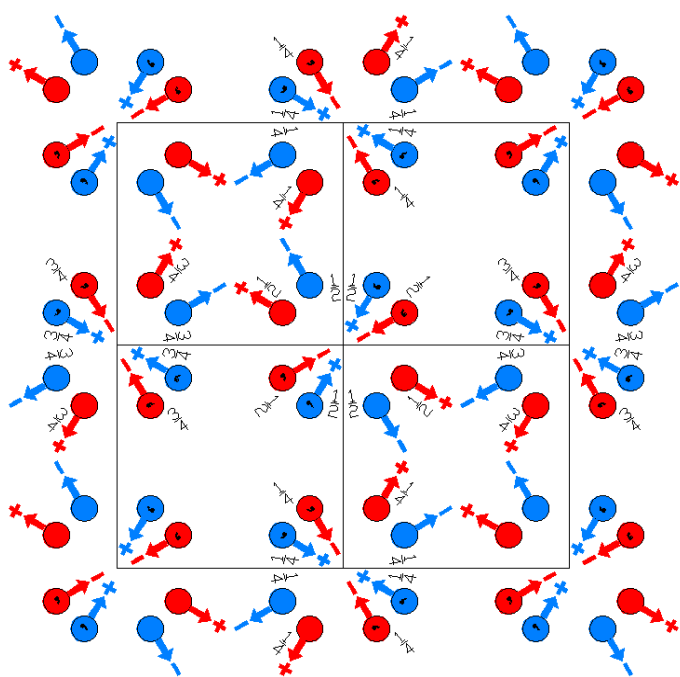
Along [1,1,0]  $p_{2mm}1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I4_1/amd$   
141.1.1213

$4/mmm$   
 $I4_1/a2/m2/d$

Tetragonal



Origin at  $\bar{4}m2$  at  $0, 1/4, -1/8$  from center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |   |  |  |
|--|---|--|--|
| (1) 1<br>(1 0,0,0)                                   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                  | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>( $4_z$  0,1/2,1/4)  | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>( $4_z^{-1}$  0,1/2,1/4)      |
| (5) 2 $(0,1/2,0) 0,y,1/8$<br>( $2_y$  0,1/2,1/4)     | (6) 2 $x,1/4,1/8$<br>( $2_x$  0,1/2,1/4)          | (7) 2 $x,x,0$<br>( $2_{xy}$  0,0,0)                      | (8) 2 $x,\bar{x},0$<br>( $2_{\bar{xy}}$  0,0,0)                  |
| (9) $\bar{1}$ $0,1/4,1/8$<br>( $\bar{1}$  0,1/2,1/4) | (10) b $(0,1/2,0) x,y,1/8$<br>( $m_z$  0,1/2,1/4) | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z$  0,0,0) | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1}$  0,0,0)    |
| (13) m $x,0,z$<br>( $m_y$  0,0,0)                    | (14) m $0,y,z$<br>( $m_x$  0,0,0)                 | (15) d $(-1/4,1/4,1/4) x+1/4,\bar{x},z$                  | (16) d $(1/4,1/4,1/4) x-1/4,x,z$<br>( $m_{\bar{xy}}$  0,1/2,1/4) |

For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>   1/2,0,3/4)	(4) $4^-$ (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4)
(5) $2$ 1/4,y,3/8 (2 <sub>y</sub>   1/2,0,3/4)	(6) $2$ (1/2,0,0) x,0,3/8 (2 <sub>x</sub>   1/2,0,3/4)	(7) $2$ (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)	(8) $2$ x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)
(9) $\bar{1}$ 1/4,0,3/8 ( $\bar{1}$   1/2,0,3/4)	(10) $a$ (1/2,0,0) x,y,3/8 (m <sub>z</sub>   1/2,0,3/4)	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)
(13) $n$ (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)	(14) $n$ (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)	(15) $d$ (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,0,3/4)	(16) $d$ (1/4,1/4,3/4) x+1/4,x,z (m <sub><math>\bar{xy}</math></sub>   1/2,0,3/4)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [ $u,v,w$ ]	(10) $x,y+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]		
			(13) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y},\bar{x}+1/2,z+1/4$ [ $v,u,\bar{w}$ ]	(16) $y,x+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]		
16	h	.m.	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},1/2,z+1/4$ [0,u,0]	$y,1/2,z+1/4$ [0, $\bar{u},0$ ]
			0,y+1/2, $\bar{z}+1/4$ [ $\bar{u},0,0$ ]	0, $\bar{y}+1/2,\bar{z}+1/4$ [u,0,0]	$y,0,\bar{z}$ [0,u,0]	$\bar{y},0,\bar{z}$ [0, $\bar{u},0$ ]
16	g	..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,1/4$ [ $\bar{u},u,0$ ]	$x,\bar{x}+1/2,1/4$ [u, $\bar{u},0$ ]
			$\bar{x},\bar{x}+1/2,1/4$ [u,u,0]	$x,x+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},0$ [ $\bar{u},u,0$ ]	$\bar{x},x,0$ [u, $\bar{u},0$ ]
16	f	.2.	x,1/4,1/8 [u,0,0]	$\bar{x},3/4,1/8$ [ $\bar{u},0,0$ ]	3/4,x+1/2,3/8 [0,u,0]	1/4, $\bar{x}+1/2,3/8$ [0, $\bar{u},0$ ]
			$\bar{x},1/4,1/8$ [u,0,0]	$x,3/4,1/8$ [ $\bar{u},0,0$ ]	1/4, $\bar{x},7/8$ [0,u,0]	3/4,x,7/8 [0, $\bar{u},0$ ]
8	e	2mm.	0,0,z [0,0,0]	0,1/2,z+1/4 [0,0,0]	0,1/2, $\bar{z}+1/4$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]
8	d	.2/m.	0,1/4,5/8 [u,0,0]	0,3/4,5/8 [ $\bar{u},0,0$ ]	3/4,1/2,7/8 [0,u,0]	1/4,1/2,7/8 [0, $\bar{u},0$ ]
8	c	.2/m.	0,1/4,1/8 [u,0,0]	0,3/4,1/8 [ $\bar{u},0,0$ ]	3/4,1/2,3/8 [0,u,0]	1/4,1/2,3/8 [0, $\bar{u},0$ ]

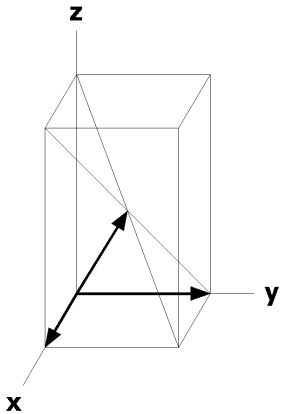
4	b	$\sqrt{2}m$	0,0,1/2 [0,0,0]	0,1/2,3/4 [0,0,0]
4	a	$\sqrt{2}m$	0,0,0 [0,0,0]	0,1/2,1/4 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p_2$ , 4m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,1/4,z

Along [1,0,0]  $c2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

Along [1,1,0]  $c_2$ , 2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I4_1/amd1'$

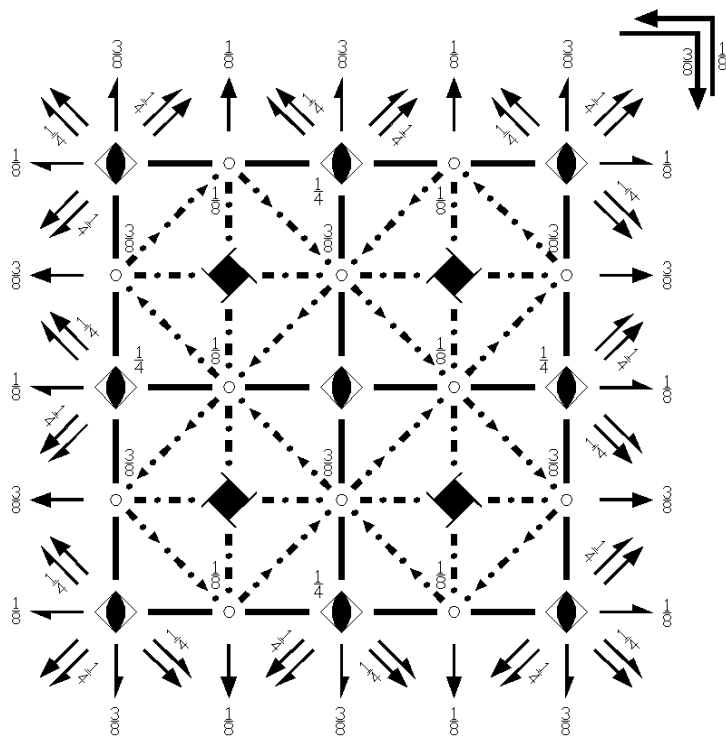
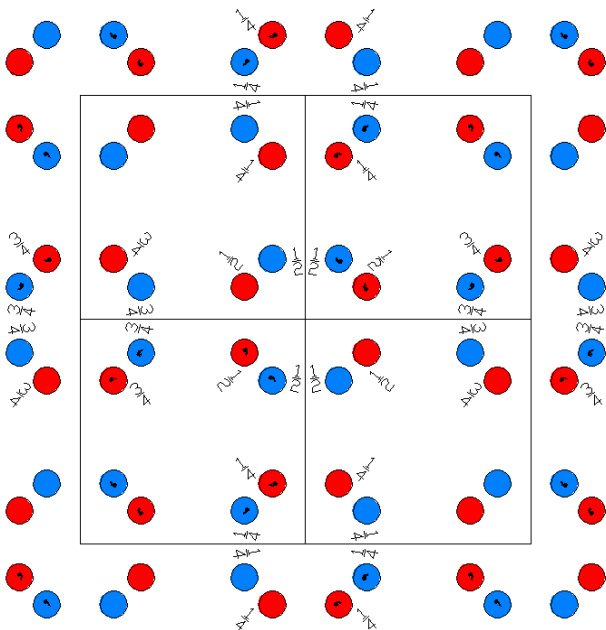
141.2.1214

$4/mmm1'$

$I4_1/a2/m2/d1'$

Tetragonal

$1'$



Origin at  $\bar{4}m2$  at  $0, 1/4, -1/8$  from center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

Symmetry Operations

For  $(0,0,0)$  + set

- |  |   |  |  |
|--|---|--|--|
| (1) $1$<br>$(1 0,0,0)$                             | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                  | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>$(4_z 0,1/2,1/4)$  | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>$(4_z^{-1} 0,1/2,1/4)$        |
| (5) $2$ $(0,1/2,0) 0,y,1/8$<br>$(2_y 0,1/2,1/4)$   | (6) $2$ $x,1/4,1/8$<br>$(2_x 0,1/2,1/4)$          | (7) $2$ $x,x,0$<br>$(2_{xy} 0,0,0)$                    | (8) $2$ $x,\bar{x},0$<br>$(2_{\bar{xy}} 0,0,0)$                  |
| (9) $\bar{1}$ $0,1/4,1/8$<br>$(\bar{1} 0,1/2,1/4)$ | (10) $b$ $(0,1/2,0) x,y,1/8$<br>$(m_z 0,1/2,1/4)$ | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z 0,0,0)$ | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1} 0,0,0)$      |
| (13) $m$ $x,0,z$<br>$(m_y 0,0,0)$                  | (14) $m$ $0,y,z$<br>$(m_x 0,0,0)$                 | (15) $d$ $(-1/4,1/4,1/4) x+1/4,\bar{x},z$              | (16) $d$ $(1/4,1/4,1/4) x-1/4,x,z$<br>$(m_{\bar{xy}} 0,1/2,1/4)$ |



## For (1/2,1/2,1/2) + set

- |  |  |  |   |
|--|--|--|---|
| (1) t (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)                     | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2)  | (3) 4 <sup>+</sup> (0,0,3/4) 1/4,1/4,z<br>(4 <sub>z</sub>   1/2,0,3/4)     | (4) 4 <sup>-</sup> (0,0,3/4) 1/4,-1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4) |
| (5) 2 1/4,y,3/8<br>(2 <sub>y</sub>   1/2,0,3/4)              | (6) 2 (1/2,0,0) x,0,3/8<br>(2 <sub>x</sub>   1/2,0,3/4)      | (7) 2 (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>   1/2,1/2,1/2)               | (8) 2 x, $\bar{x}$ +1/2,1/4<br>(2 <sub>xy</sub>   1/2,1/2,1/2)                        |
| (9) $\bar{1}$ 1/4,0,3/8<br>( $\bar{1}$   1/2,0,3/4)          | (10) a (1/2,0,0) x,y,3/8<br>(m <sub>z</sub>   1/2,0,3/4)     | (11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$   1/2,1/2,1/2)        | (12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)     |
| (13) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,1/2) | (14) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,1/2) | (15) d (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>   1/2,0,3/4) | (16) d (1/4,1/4,3/4) x+1/4,x,z<br>(m <sub>xy</sub>   1/2,0,3/4)                       |

## For (0,0,0)' + set

- |   |  |  |   |
|---|--|--|---|
| (1) 1'<br>(1   0,0,0)'                                    | (2) 2' 0,0,z<br>(2 <sub>z</sub>   0,0,0)'                  | (3) 4 <sup>+</sup> ' (0,0,1/4) -1/4,1/4,z<br>(4 <sub>z</sub>   0,1/2,1/4)'   | (4) 4 <sup>-</sup> ' (0,0,1/4) 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>   0,1/2,1/4)' |
| (5) 2' (0,1/2,0) 0,y,1/8<br>(2 <sub>y</sub>   0,1/2,1/4)' | (6) 2' x,1/4,1/8<br>(2 <sub>x</sub>   0,1/2,1/4)'          | (7) 2' x,x,0<br>(2 <sub>xy</sub>   0,0,0)'                                   | (8) 2' x, $\bar{x}$ ,0<br>(2 <sub>xy</sub>   0,0,0)'                                    |
| (9) $\bar{1}$ ' 0,1/4,1/8<br>( $\bar{1}$   0,1/2,1/4)'    | (10) b' (0,1/2,0) x,y,1/8<br>(m <sub>z</sub>   0,1/2,1/4)' | (11) $\bar{4}^+$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z$   0,0,0)'                   | (12) $\bar{4}^-$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z$ <sup>-1</sup>   0,0,0)'                |
| (13) m' x,0,z<br>(m <sub>y</sub>   0,0,0)'                | (14) m' 0,y,z<br>(m <sub>x</sub>   0,0,0)'                 | (15) d' (-1/4,1/4,1/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>   0,1/2,1/4)' | (16) d' (1/4,1/4,1/4) x-1/4,x,z<br>(m <sub>xy</sub>   0,1/2,1/4)'                       |

## For (1/2,1/2,1/2)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)'                     | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2)'  | (3) 4 <sup>+</sup> ' (0,0,3/4) 1/4,1/4,z<br>(4 <sub>z</sub>   1/2,0,3/4)'    | (4) 4 <sup>-</sup> ' (0,0,3/4) 1/4,-1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4)' |
| (5) 2' 1/4,y,3/8<br>(2 <sub>y</sub>   1/2,0,3/4)'              | (6) 2' (1/2,0,0) x,0,3/8<br>(2 <sub>x</sub>   1/2,0,3/4)'      | (7) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>   1/2,1/2,1/2)'               | (8) 2' x, $\bar{x}$ +1/2,1/4<br>(2 <sub>xy</sub>   1/2,1/2,1/2)'                         |
| (9) $\bar{1}$ ' 1/4,0,3/8<br>( $\bar{1}$   1/2,0,3/4)'         | (10) a' (1/2,0,0) x,y,3/8<br>(m <sub>z</sub>   1/2,0,3/4)'     | (11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$   1/2,1/2,1/2)'       | (12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)'     |
| (13) n' (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,1/2)' | (14) n' (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,1/2)' | (15) d' (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>   1/2,0,3/4)' | (16) d' (1/4,1/4,3/4) x+1/4,x,z<br>(m <sub>xy</sub>   1/2,0,3/4)'                        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

(0,0,0) + (1/2,1/2,1/2) +  
(0,0,0)' + (1/2,1/2,1/2)' +

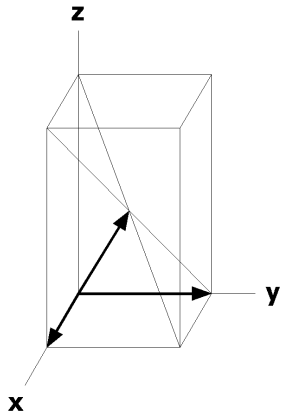
32	i	11'	(1) $x,y,z$ [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]		
			(3) $\bar{y},x+1/2,z+1/4$ [0,0,0]	(4) $y,\bar{x}+1/2,z+1/4$ [0,0,0]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [0,0,0]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [0,0,0]		
			(7) $y,x,\bar{z}$ [0,0,0]	(8) $\bar{y},\bar{x},\bar{z}$ [0,0,0]		
			(9) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [0,0,0]	(10) $x,y+1/2,\bar{z}+1/4$ [0,0,0]		
			(11) $y,\bar{x},\bar{z}$ [0,0,0]	(12) $\bar{y},x,\bar{z}$ [0,0,0]		
			(13) $x,\bar{y},z$ [0,0,0]	(14) $\bar{x},y,z$ [0,0,0]		
			(15) $\bar{y},\bar{x}+1/2,z+1/4$ [0,0,0]	(16) $y,x+1/2,z+1/4$ [0,0,0]		
16	h	.m.1'	$0,y,z$ [0,0,0]	$0,\bar{y},z$ [0,0,0]	$\bar{y},1/2,z+1/4$ [0,0,0]	$y,1/2,z+1/4$ [0,0,0]
			$0,y+1/2,\bar{z}+1/4$ [0,0,0]	$0,\bar{y}+1/2,\bar{z}+1/4$ [0,0,0]	$y,0,\bar{z}$ [0,0,0]	$\bar{y},0,\bar{z}$ [0,0,0]
16	g	.21'	$x,x,0$ [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	$\bar{x},x+1/2,1/4$ [0,0,0]	$x,\bar{x}+1/2,1/4$ [0,0,0]
			$\bar{x},\bar{x}+1/2,1/4$ [0,0,0]	$x,x+1/2,1/4$ [0,0,0]	$x,\bar{x},0$ [0,0,0]	$\bar{x},x,0$ [0,0,0]
16	f	.2.1'	$x,1/4,1/8$ [0,0,0]	$\bar{x},3/4,1/8$ [0,0,0]	$3/4,x+1/2,3/8$ [0,0,0]	$1/4,\bar{x}+1/2,3/8$ [0,0,0]
			$\bar{x},1/4,1/8$ [0,0,0]	$x,3/4,1/8$ [0,0,0]	$1/4,\bar{x},7/8$ [0,0,0]	$3/4,x,7/8$ [0,0,0]
8	e	2mm.1'	$0,0,z$ [0,0,0]	$0,1/2,z+1/4$ [0,0,0]	$0,1/2,\bar{z}+1/4$ [0,0,0]	$0,0,\bar{z}$ [0,0,0]
8	d	.2/m.1'	$0,1/4,5/8$ [0,0,0]	$0,3/4,5/8$ [0,0,0]	$3/4,1/2,7/8$ [0,0,0]	$1/4,1/2,7/8$ [0,0,0]
8	c	.2/m.1'	$0,1/4,1/8$ [0,0,0]	$0,3/4,1/8$ [0,0,0]	$3/4,1/2,3/8$ [0,0,0]	$1/4,1/2,3/8$ [0,0,0]
4	b	$\sqrt{2}m1'$	$0,0,1/2$ [0,0,0]	$0,1/2,3/4$ [0,0,0]		
4	a	$\sqrt{2}m1'$	$0,0,0$ [0,0,0]	$0,1/2,1/4$ [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

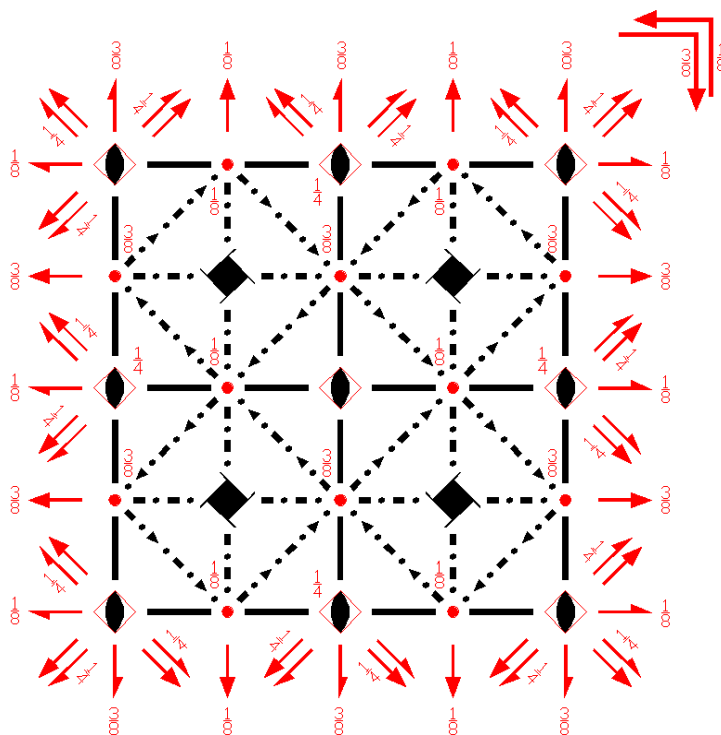
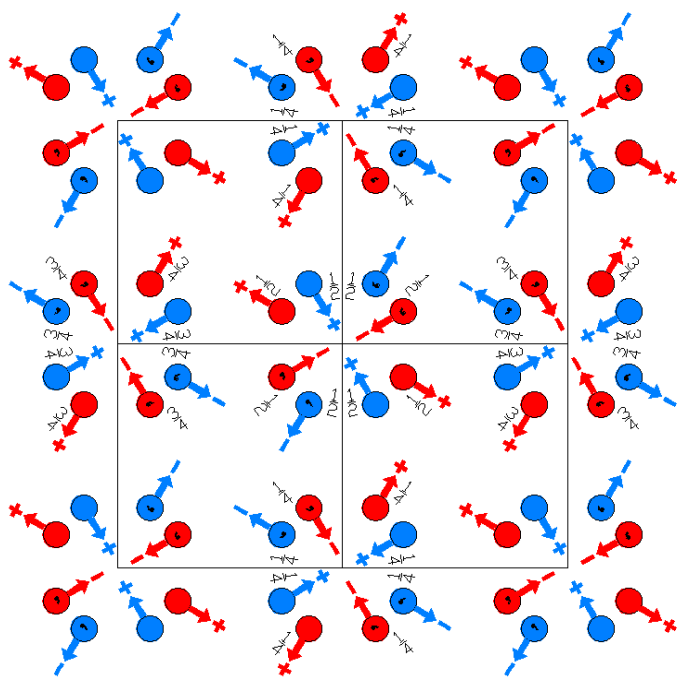
Along [1,1,0]  $c2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I4_1/a'md$   
141.3.1215

$4/m'mm$   
 $I4_1/a'2'/m2'/d$

Tetragonal



Origin at  $\bar{4}'m2'$  at  $0, 1/4, -1/8$  from center ( $2'/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

### Symmetry Operations

For (0,0,0) + set

- |  |   |  |   |
|--|---|--|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                    | (3) 4 <sup>+</sup> (0,0,1/4) -1/4,1/4,z<br>(4 <sub>z</sub>  0,1/2,1/4) | (4) 4 <sup>-</sup> (0,0,1/4) 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4) |
| (5) 2' (0,1/2,0) 0,y,1/8<br>(2 <sub>y</sub>  0,1/2,1/4)' | (6) 2' x,1/4,1/8<br>(2 <sub>x</sub>  0,1/2,1/4)'          | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                              | (8) 2' x,x̄,0<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,0)'                            |
| (9) $\bar{1}'$ 0,1/4,1/8<br>( $\bar{1}$  0,1/2,1/4)'     | (10) b' (0,1/2,0) x,y,1/8<br>(m <sub>z</sub>  0,1/2,1/4)' | (11) $\bar{4}^+$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'            | (12) $\bar{4}^-$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                         |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)                  | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)                   | (15) d (-1/4,1/4,1/4) x+1/4,x̄,z<br>(m <sub>xy</sub>  0,1/2,1/4)       | (16) d (1/4,1/4,1/4) x-1/4,x,z<br>(m <sub>xy</sub>  0,1/2,1/4)                      |

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) 2 (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) 4 <sup>+</sup> (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>   1/2,0,3/4)	(4) 4 <sup>-</sup> (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4)
(5) 2' 1/4,y,3/8 (2 <sub>y</sub>   1/2,0,3/4)'	(6) 2' (1/2,0,0) x,0,3/8 (2 <sub>x</sub>   1/2,0,3/4)'	(7) 2' (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)'	(8) 2' x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)'
(9) $\bar{1}$ ' 1/4,0,3/8 ( $\bar{1}$   1/2,0,3/4)'	(10) a' (1/2,0,0) x,y,3/8 (m <sub>z</sub>   1/2,0,3/4)'	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$   1/2,1/2,1/2)'
(13) n (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)	(14) n (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)	(15) d (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,0,3/4)	(16) d (1/4,1/4,3/4) x+1/4,x,z (m <sub><math>\bar{xy}</math></sub>   1/2,0,3/4)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

			(0,0,0) +	(1/2,1/2,1/2) +		
32	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},v,w$ ]		
			(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},z$ [ $v,u,w$ ]		
			(9) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y+1/2,\bar{z}+1/4$ [ $u,v,\bar{w}$ ]		
			(11) $y,\bar{x},z$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,z$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y},\bar{x}+1/2,z+1/4$ [ $v,u,\bar{w}$ ]	(16) $y,x+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]		
16	h	.m.	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},1/2,z+1/4$ [0,u,0]	$y,1/2,z+1/4$ [0, $\bar{u},0$ ]
			0,y+1/2, $\bar{z}+1/4$ [u,0,0]	0, $\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},0,0$ ]	$y,0,\bar{z}$ [0, $\bar{u},0$ ]	$\bar{y},0,z$ [0,u,0]
16	g	..2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [ $u,\bar{u},w$ ]	$\bar{x},x+1/2,1/4$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x}+1/2,1/4$ [ $u,u,w$ ]
			$\bar{x},\bar{x}+1/2,1/4$ [ $u,\bar{u},\bar{w}$ ]	$x,x+1/2,1/4$ [ $\bar{u},u,\bar{w}$ ]	$x,\bar{x},0$ [ $u,u,\bar{w}$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},\bar{w}$ ]
16	f	.2'	x,1/4,1/8 [0,v,w]	$\bar{x},3/4,1/8$ [0, $\bar{v},w$ ]	3/4,x+1/2,3/8 [ $\bar{v},0,w$ ]	1/4, $\bar{x}+1/2,3/8$ [ $v,0,w$ ]
			$\bar{x},1/4,1/8$ [0, $\bar{v},\bar{w}$ ]	$x,3/4,1/8$ [0,v, $\bar{w}$ ]	1/4, $\bar{x},7/8$ [ $v,0,\bar{w}$ ]	3/4,x,7/8 [ $\bar{v},0,\bar{w}$ ]
8	e	2mm.	0,0,z [0,0,0]	0,1/2,z+1/4 [0,0,0]	0,1/2, $\bar{z}+1/4$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]
8	d	.2/m'	0,1/4,5/8 [0,0,0]	0,3/4,5/8 [0,0,0]	3/4,1/2,7/8 [0,0,0]	1/4,1/2,7/8 [0,0,0]
8	c	.2/m'	0,1/4,1/8 [0,0,0]	0,3/4,1/8 [0,0,0]	3/4,1/2,3/8 [0,0,0]	1/4,1/2,3/8 [0,0,0]

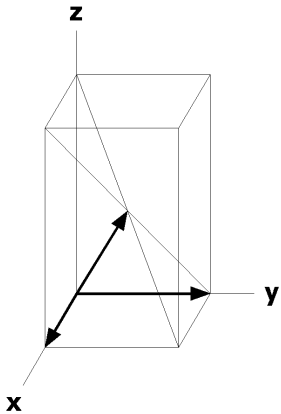
4	b	$\sqrt{4} \cdot 2' m$	0,0,1/2 [0,0,0]	0,1/2,3/4 [0,0,0]
4	a	$\sqrt{4} \cdot 2' m$	0,0,0 [0,0,0]	0,1/2,1/4 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c2mm1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

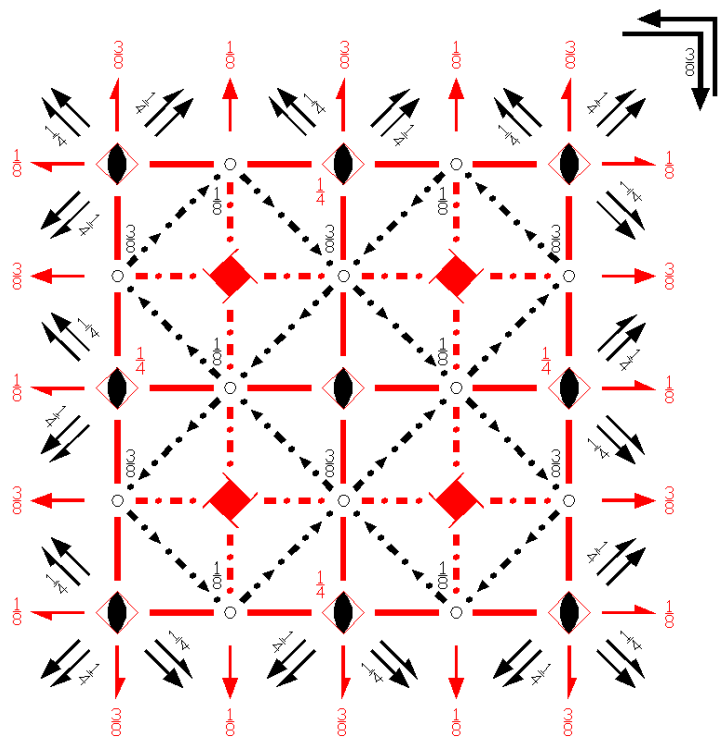
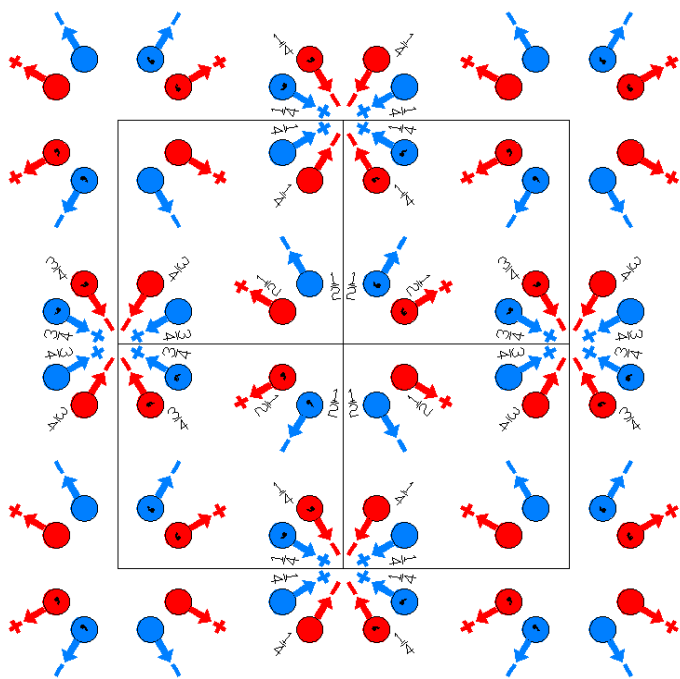
Along [1,1,0] c<sub>2v</sub> 2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$I4_1'/am'd$   
141.4.1216

$4'/mm'm$   
 $I4_1'/a2'/m'2/d$

Tetragonal



Origin at  $\bar{4}'m'2$  at  $0, 1/4, -1/8$  from center ( $2'/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

### Symmetry Operations

For (0,0,0) + set

- |  |   |   |  |
|--|---|---|--|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                  | (3) 4 <sup>+</sup> (0,0,1/4) -1/4,1/4,z<br>(4 <sub>z</sub>  0,1/2,1/4)'   | (4) 4 <sup>-</sup> (0,0,1/4) 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4)' |
| (5) 2' (0,1/2,0) 0,y,1/8<br>(2 <sub>y</sub>  0,1/2,1/4)' | (6) 2' x,1/4,1/8<br>(2 <sub>x</sub>  0,1/2,1/4)'        | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                   | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)                 |
| (9) $\bar{1}$ 0,1/4,1/8<br>( $\bar{1}$  0,1/2,1/4)       | (10) b (0,1/2,0) x,y,1/8<br>(m <sub>z</sub>  0,1/2,1/4) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'                 | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                            |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)'                | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)'               | (15) d (-1/4,1/4,1/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,1/2,1/4) | (16) d (1/4,1/4,1/4) x-1/4,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,1/2,1/4)    |

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) 2 (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) 4 <sup>+</sup> ' (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>   1/2,0,3/4)'	(4) 4 <sup>-</sup> ' (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4)'
(5) 2' 1/4,y,3/8 (2 <sub>y</sub>   1/2,0,3/4)'	(6) 2' (1/2,0,0) x,0,3/8 (2 <sub>x</sub>   1/2,0,3/4)'	(7) 2 (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)	(8) 2 x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)
(9) $\bar{1}$ 1/4,0,3/8 ( $\bar{1}$   1/2,0,3/4)	(10) a (1/2,0,0) x,y,3/8 (m <sub>z</sub>   1/2,0,3/4)	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z^+$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^-$   1/2,1/2,1/2)'
(13) n' (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)'	(14) n' (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)'	(15) d (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,0,3/4)	(16) d (1/4,1/4,3/4) x+1/4,x,z (m <sub><math>\bar{xy}</math></sub>   1/2,0,3/4)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},v,w$ ]		
			(7) y,x, $\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [ $u,v,w$ ]	(10) x,y+1/2, $\bar{z}+1/4$ [ $\bar{u},\bar{v},w$ ]		
			(11) y, $\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
			(13) x, $\bar{y},z$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y},\bar{x}+1/2,z+1/4$ [ $\bar{v},u,\bar{w}$ ]	(16) $y,x+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]		
16	h	.m'	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	$\bar{y},1/2,z+1/4$ [ $\bar{v},0,\bar{w}$ ]	$y,1/2,z+1/4$ [ $\bar{v},0,\bar{w}$ ]
			0,y+1/2, $\bar{z}+1/4$ [0, $\bar{v},w$ ]	0, $\bar{y}+1/2,\bar{z}+1/4$ [0,v,w]	y,0, $\bar{z}$ [ $\bar{v},0,\bar{w}$ ]	$\bar{y},0,\bar{z}$ [ $\bar{v},0,\bar{w}$ ]
16	g	..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,1/4$ [ $u,\bar{u},0$ ]	$x,\bar{x}+1/2,1/4$ [ $\bar{u},u,0$ ]
			$\bar{x},\bar{x}+1/2,1/4$ [ $u,u,0$ ]	x,x+1/2,1/4 [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},0$ [ $u,\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]
16	f	.2'	x,1/4,1/8 [0,v,w]	$\bar{x},3/4,1/8$ [0, $\bar{v},w$ ]	3/4,x+1/2,3/8 [ $\bar{v},0,\bar{w}$ ]	1/4, $\bar{x}+1/2,3/8$ [ $\bar{v},0,\bar{w}$ ]
			$\bar{x},1/4,1/8$ [0,v,w]	x,3/4,1/8 [0, $\bar{v},w$ ]	1/4, $\bar{x},7/8$ [ $\bar{v},0,\bar{w}$ ]	3/4,x,7/8 [ $\bar{v},0,\bar{w}$ ]
8	e	2mm.	0,0,z [0,0,0]	0,1/2,z+1/4 [0,0,0]	0,1/2, $\bar{z}+1/4$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]
8	d	.2'/m'	0,1/4,5/8 [0,v,w]	0,3/4,5/8 [0, $\bar{v},w$ ]	3/4,1/2,7/8 [ $\bar{v},0,\bar{w}$ ]	1/4,1/2,7/8 [ $\bar{v},0,\bar{w}$ ]
8	c	.2'/m'	0,1/4,1/8 [0,v,w]	0,3/4,1/8 [0, $\bar{v},w$ ]	3/4,1/2,3/8 [ $\bar{v},0,\bar{w}$ ]	1/4,1/2,3/8 [ $\bar{v},0,\bar{w}$ ]

4	b	$\sqrt{4} \cdot 2'm$	0,0,1/2 [0,0,0]	0,1/2,3/4 [0,0,0]
4	a	$\sqrt{4} \cdot 2'm$	0,0,0 [0,0,0]	0,1/2,1/4 [0,0,0]

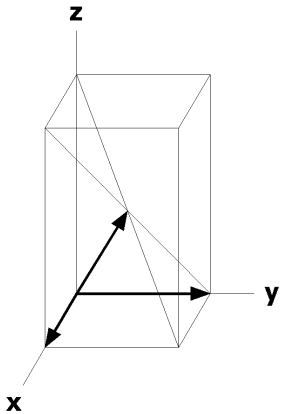
### Symmetry of Special Projections

Along [0,0,1]  $p_0 \cdot 4mm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2m'm'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

Along [1,1,0]  $c_0 \cdot 2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

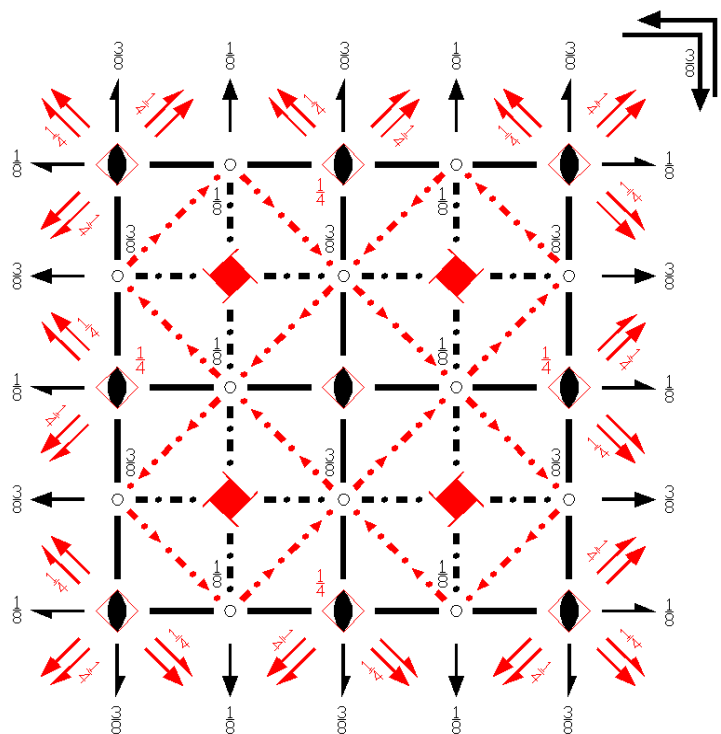
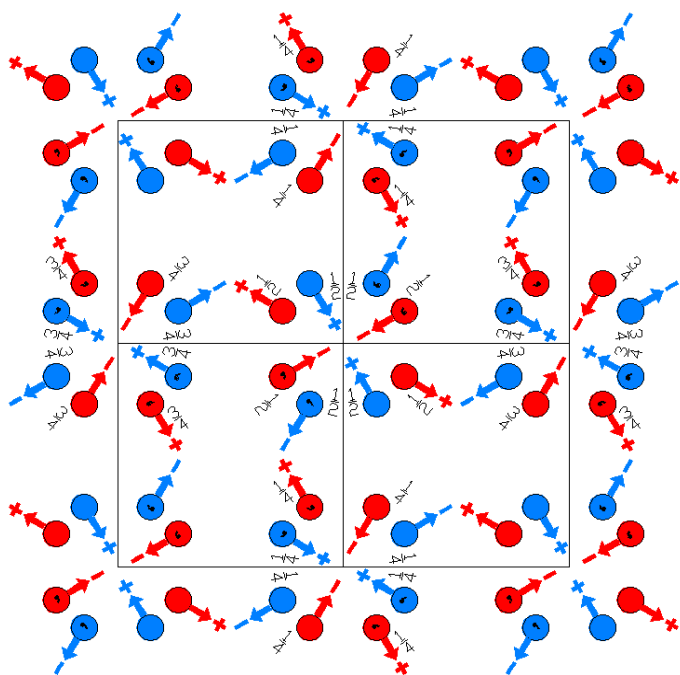




$I4_1'/amd'$   
141.5.1217

$4'/mmm'$   
 $I4_1'/a2/m2'/d'$

Tetragonal



Origin at  $\bar{4}'m2'$  at  $0, 1/4, -1/8$  from center ( $2/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |   |   |  |
|--|---|---|--|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                      | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>( $4_z$   $0,1/2,1/4$ )'              | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>( $4_z^{-1}$   $0,1/2,1/4$ )'         |
| (5) 2 $(0,1/2,0) 0,y,1/8$<br>( $2_y$   $0,1/2,1/4$ )     | (6) 2 $x,1/4,1/8$<br>( $2_x$   $0,1/2,1/4$ )          | (7) $2'$ $x,x,0$<br>( $2_{xy}$   $0,0,0$ )'                               | (8) $2'$ $x,\bar{x},0$<br>( $2_{\bar{xy}}$   $0,0,0$ )'                  |
| (9) $\bar{1}$ $0,1/4,1/8$<br>( $\bar{1}$   $0,1/2,1/4$ ) | (10) b $(0,1/2,0) x,y,1/8$<br>( $m_z$   $0,1/2,1/4$ ) | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z$   $0,0,0$ )'             | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1}$   $0,0,0$ )'       |
| (13) m $x,0,z$<br>( $m_y$   $0,0,0$ )                    | (14) m $0,y,z$<br>( $m_x$   $0,0,0$ )                 | (15) $d'$ $(-1/4,1/4,1/4) x+1/4,\bar{x},z$<br>( $m_{xy}$   $0,1/2,1/4$ )' | (16) $d'$ $(1/4,1/4,1/4) x-1/4,x,z$<br>( $m_{\bar{xy}}$   $0,1/2,1/4$ )' |

For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ ' (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>   1/2,0,3/4)'	(4) $4^-$ ' (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4)'
(5) $2$ 1/4,y,3/8 (2 <sub>y</sub>   1/2,0,3/4)	(6) $2$ (1/2,0,0) x,0,3/8 (2 <sub>x</sub>   1/2,0,3/4)	(7) $2'$ (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)'	(8) $2'$ x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub> <sup>-</sup>   1/2,1/2,1/2)'
(9) $\bar{1}$ 1/4,0,3/8 ( $\bar{1}$   1/2,0,3/4)	(10) $a$ (1/2,0,0) x,y,3/8 (m <sub>z</sub>   1/2,0,3/4)	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)'
(13) $n$ (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)	(14) $n$ (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)	(15) $d'$ (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,0,3/4)'	(16) $d'$ (1/4,1/4,3/4) x+1/4,x,z (m <sub>xy</sub> <sup>-</sup>   1/2,0,3/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

			(0,0,0) +	(1/2,1/2,1/2) +		
32	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]		
			(9) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [u,v,w]	(10) $x,y+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x,\bar{y},z$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y},\bar{x}+1/2,z+1/4$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x+1/2,z+1/4$ [ $v,u,w$ ]		
16	h	.m.	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},1/2,z+1/4$ [0, $\bar{u},0$ ]	$y,1/2,z+1/4$ [0,u,0]
			0,y+1/2, $\bar{z}+1/4$ [ $\bar{u},0,0$ ]	0, $\bar{y}+1/2,\bar{z}+1/4$ [u,0,0]	$y,0,\bar{z}$ [0, $\bar{u},0$ ]	$\bar{y},0,\bar{z}$ [0,u,0]
16	g	..2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [u, $\bar{u},w$ ]	$\bar{x},x+1/2,1/4$ [u,u, $\bar{w}$ ]	$x,\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},u,w$ ]	$x,x+1/2,1/4$ [u, $\bar{u},w$ ]	$x,\bar{x},0$ [u,u, $\bar{w}$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},\bar{w}$ ]
16	f	.2.	x,1/4,1/8 [u,0,0]	$\bar{x},3/4,1/8$ [ $\bar{u},0,0$ ]	3/4,x+1/2,3/8 [0, $\bar{u},0$ ]	1/4, $\bar{x}+1/2,3/8$ [0,u,0]
			$\bar{x},1/4,1/8$ [u,0,0]	$x,3/4,1/8$ [ $\bar{u},0,0$ ]	1/4, $\bar{x},7/8$ [0, $\bar{u},0$ ]	3/4,x,7/8 [0,u,0]
8	e	2mm.	0,0,z [0,0,0]	0,1/2,z+1/4 [0,0,0]	0,1/2, $\bar{z}+1/4$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]
8	d	.2/m.	0,1/4,5/8 [0,v,w]	0,3/4,5/8 [0, $\bar{v},w$ ]	3/4,1/2,7/8 [v,0, $\bar{w}$ ]	1/4,1/2,7/8 [ $\bar{v},0,\bar{w}$ ]
8	c	.2/m.	0,1/4,1/8 [0,v,w]	0,3/4,1/8 [0, $\bar{v},w$ ]	3/4,1/2,3/8 [v,0, $\bar{w}$ ]	1/4,1/2,3/8 [ $\bar{v},0,\bar{w}$ ]

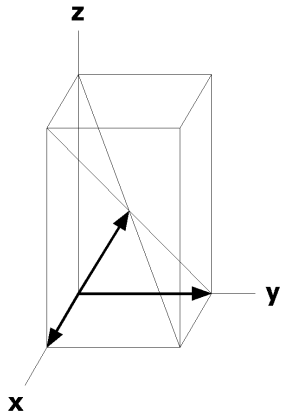
4	b	$\bar{4}'2m'$	0,0,1/2 [0,0,0]	0,1/2,3/4 [0,0,0]
4	a	$\bar{4}'2m'$	0,0,0 [0,0,0]	0,1/2,1/4 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $p_2'$  4mm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

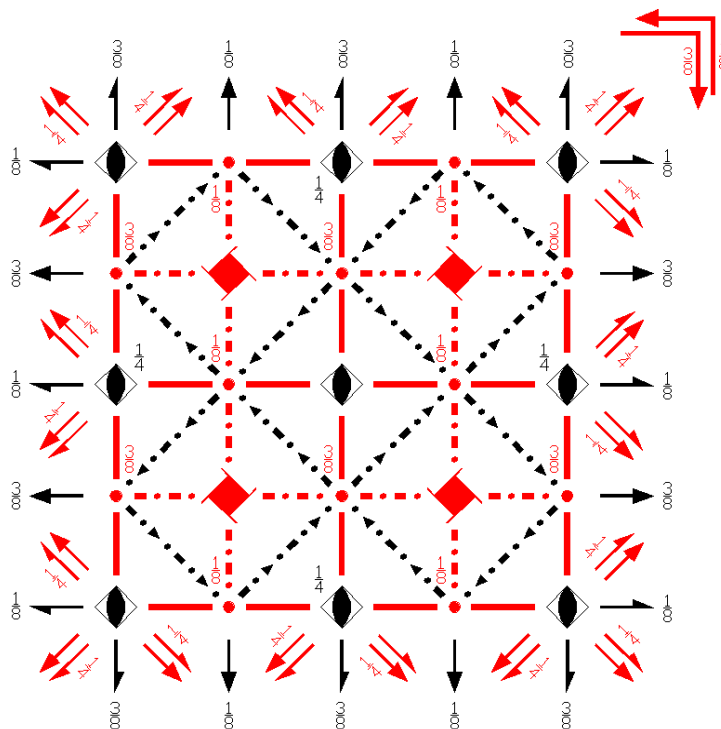
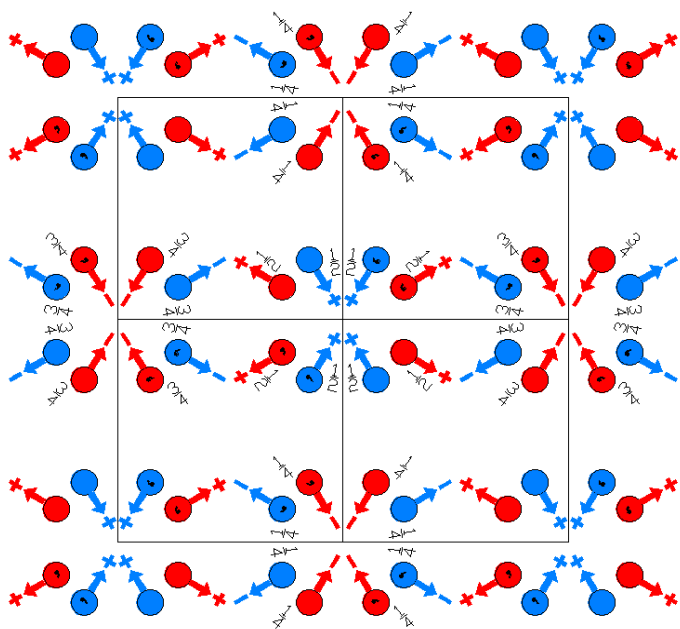
Along [1,1,0]  $c2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$I4_1'/a'm'd$   
141.6.1218

$4/m'm'm$   
 $I4_1'/a'2/m'2'/d$

Tetragonal



Origin at  $\bar{4}m'2'$  at  $0, 1/4, -1/8$  from center ( $2/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

### Symmetry Operations

For (0,0,0) + set

- |  |   |   |  |
|--|---|---|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                    | (3) 4 <sup>+</sup> (0,0,1/4) -1/4,1/4,z<br>(4 <sub>z</sub>  0,1/2,1/4)'   | (4) 4 <sup>-</sup> (0,0,1/4) 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4)' |
| (5) 2 (0,1/2,0) 0,y,1/8<br>(2 <sub>y</sub>  0,1/2,1/4) | (6) 2 x,1/4,1/8<br>(2 <sub>x</sub>  0,1/2,1/4)            | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                                 | (8) 2' x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)'               |
| (9) $\bar{1}$ 0,1/4,1/8<br>( $\bar{1}$  0,1/2,1/4)'    | (10) b' (0,1/2,0) x,y,1/8<br>(m <sub>z</sub>  0,1/2,1/4)' | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)                    | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)                          |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)'              | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)'                 | (15) d (-1/4,1/4,1/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,1/2,1/4) | (16) d (1/4,1/4,1/4) x-1/4,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,1/2,1/4)    |

For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>   1/2,0,3/4)'	(4) $4^-$ (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4)'
(5) $2$ 1/4,y,3/8 (2 <sub>y</sub>   1/2,0,3/4)	(6) $2$ (1/2,0,0) x,0,3/8 (2 <sub>x</sub>   1/2,0,3/4)	(7) $2'$ (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)'	(8) $2'$ x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)'
(9) $\bar{1}$ ' 1/4,0,3/8 ( $\bar{1}$   1/2,0,3/4)'	(10) $a'$ (1/2,0,0) x,y,3/8 (m <sub>z</sub>   1/2,0,3/4)'	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)
(13) $n'$ (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)'	(14) $n'$ (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)'	(15) $d$ (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,0,3/4)	(16) $d$ (1/4,1/4,3/4) x+1/4,x,z (m <sub><math>\bar{xy}</math></sub>   1/2,0,3/4)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},\bar{w}$ ]		
			(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},w$ ]		
			(9) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},\bar{w}$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]		
			(13) $x,\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},\bar{v},w$ ]		
			(15) $\bar{y},\bar{x}+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]	(16) $y,x+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]		
16	h	.m'	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	$\bar{y},1/2,z+1/4$ [ $\bar{v},0,\bar{w}$ ]	$y,1/2,z+1/4$ [ $\bar{v},0,\bar{w}$ ]
			0,y+1/2, $\bar{z}+1/4$ [0,v, $\bar{w}$ ]	0, $\bar{y}+1/2,\bar{z}+1/4$ [0, $\bar{v},\bar{w}$ ]	$y,0,\bar{z}$ [ $\bar{v},0,w$ ]	$\bar{y},0,\bar{z}$ [ $\bar{v},0,w$ ]
16	g	..2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x+1/2,1/4$ [ $\bar{u},u,\bar{w}$ ]	$x,\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	$x,x+1/2,1/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	$x,\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,0$ [ $\bar{u},\bar{u},w$ ]
16	f	.2.	x,1/4,1/8 [u,0,0]	$\bar{x},3/4,1/8$ [ $\bar{u},0,0$ ]	3/4,x+1/2,3/8 [0, $\bar{u},0$ ]	1/4, $\bar{x}+1/2,3/8$ [0,u,0]
			$\bar{x},1/4,1/8$ [ $\bar{u},0,0$ ]	x,3/4,1/8 [u,0,0]	1/4, $\bar{x},7/8$ [0,u,0]	3/4,x,7/8 [0, $\bar{u},0$ ]
8	e	2m'm'	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/4$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]
8	d	.2/m'	0,1/4,5/8 [0,0,0]	0,3/4,5/8 [0,0,0]	3/4,1/2,7/8 [0,0,0]	1/4,1/2,7/8 [0,0,0]
8	c	.2/m'	0,1/4,1/8 [0,0,0]	0,3/4,1/8 [0,0,0]	3/4,1/2,3/8 [0,0,0]	1/4,1/2,3/8 [0,0,0]

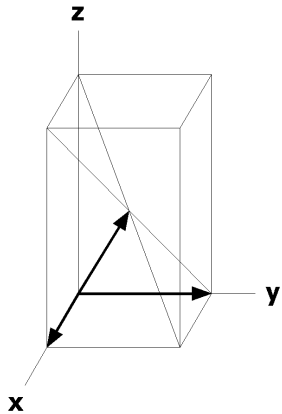
4	b	$\sqrt{2}m$	0,0,1/2 [0,0,0]	0,1/2,3/4 [0,0,0]
4	a	$\sqrt{2}m$	0,0,0 [0,0,0]	0,1/2,1/4 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  $p_2, 4m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2 \quad \mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2m'm'$   
 $\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

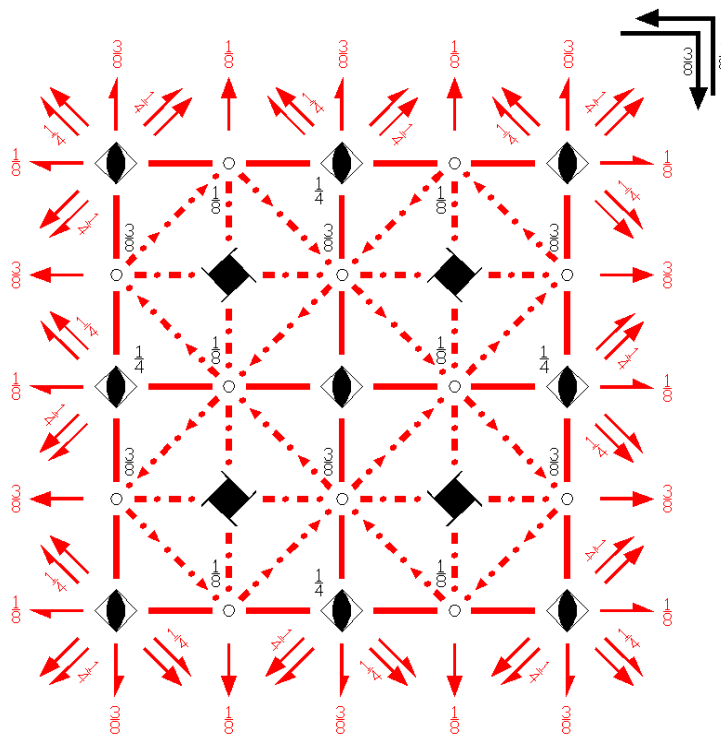
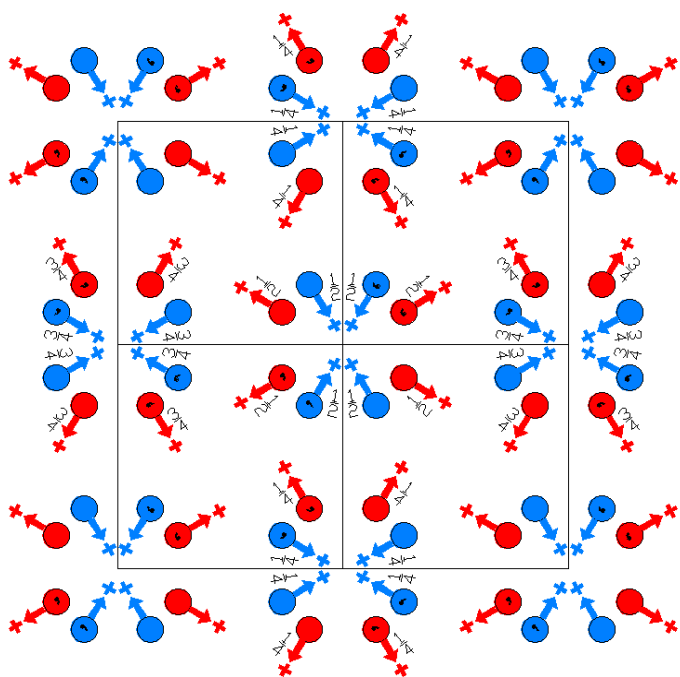
Along [1,1,0]  $c_2, 2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2 \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$I4_1/am'd'$   
141.7.1219

$4/mm'm'$   
 $I4_1/a2'/m'2'/d'$

Tetragonal



Origin at  $\bar{4}m'2'$  at  $0, 1/4, -1/8$  from center ( $2'/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

### Symmetry Operations

For (0,0,0) + set

- |  |   |  |   |
|--|---|--|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                  | (3) 4 <sup>+</sup> (0,0,1/4) -1/4,1/4,z<br>(4 <sub>z</sub>  0,1/2,1/4) | (4) 4 <sup>-</sup> (0,0,1/4) 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4) |
| (5) 2' (0,1/2,0) 0,y,1/8<br>(2 <sub>y</sub>  0,1/2,1/4)' | (6) 2' x,1/4,1/8<br>(2 <sub>x</sub>  0,1/2,1/4)'        | (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'                              | (8) 2' x,x̄,0<br>(2 <sub>xy</sub> <sup>-1</sup>  0,0,0)'                            |
| (9) $\bar{1}$ 0,1/4,1/8<br>( $\bar{1}$  0,1/2,1/4)       | (10) b (0,1/2,0) x,y,1/8<br>(m <sub>z</sub>  0,1/2,1/4) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)                 | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)                         |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)'                | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)'               | (15) d' (-1/4,1/4,1/4) x+1/4,x̄,z<br>(m <sub>xy</sub>  0,1/2,1/4)'     | (16) d'(1/4,1/4,1/4) x-1/4,x,z<br>(m <sub>xy</sub> <sup>-1</sup>  0,1/2,1/4)'       |

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) 2 (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) 4 <sup>+</sup> (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>   1/2,0,3/4)	(4) 4 <sup>-</sup> (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4)
(5) 2' 1/4,y,3/8 (2 <sub>y</sub>   1/2,0,3/4)'	(6) 2' (1/2,0,0) x,0,3/8 (2 <sub>x</sub>   1/2,0,3/4)'	(7) 2' (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)'	(8) 2' x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)'
(9) $\bar{1}$ 1/4,0,3/8 ( $\bar{1}$   1/2,0,3/4)	(10) a (1/2,0,0) x,y,3/8 (m <sub>z</sub>   1/2,0,3/4)	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)
(13) n' (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)'	(14) n' (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)'	(15) d' (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,0,3/4)'	(16) d' (1/4,1/4,3/4) x+1/4,x,z (m <sub><math>\bar{xy}</math></sub>   1/2,0,3/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +		(1/2,1/2,1/2) +	
32 i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $v,\bar{u},w$ ]
	(5) $\bar{x},y+1/2,\bar{z}+1/4$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $v,u,w$ ]
	(9) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [ $u,v,w$ ]	(10) $x,y+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
	(13) $x,\bar{y},z$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},v,w$ ]	(15) $\bar{y},\bar{x}+1/2,z+1/4$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x+1/2,z+1/4$ [ $v,u,w$ ]
16 h .m'	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	$\bar{y},1/2,z+1/4$ [ $\bar{v},0,w$ ]	$y,1/2,z+1/4$ [ $v,0,w$ ]
	0,y+1/2, $\bar{z}+1/4$ [0,v,w]	0, $\bar{y}+1/2,\bar{z}+1/4$ [0, $\bar{v},w$ ]	$y,0,\bar{z}$ [ $\bar{v},0,w$ ]	$\bar{y},0,\bar{z}$ [ $v,0,w$ ]
16 g ..2'	x,x,0 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},0$ [ $u,\bar{u},w$ ]	$\bar{x},x+1/2,1/4$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x}+1/2,1/4$ [ $u,u,w$ ]
	$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},u,w$ ]	$x,x+1/2,1/4$ [ $u,\bar{u},w$ ]	$x,\bar{x},0$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,0$ [ $u,u,w$ ]
16 f .2'	x,1/4,1/8 [0,v,w]	$\bar{x},3/4,1/8$ [0, $\bar{v},w$ ]	3/4,x+1/2,3/8 [ $\bar{v},0,w$ ]	1/4, $\bar{x}+1/2,3/8$ [ $v,0,w$ ]
	$\bar{x},1/4,1/8$ [0,v,w]	$x,3/4,1/8$ [0, $\bar{v},w$ ]	1/4, $\bar{x},7/8$ [ $\bar{v},0,w$ ]	3/4,x,7/8 [ $v,0,w$ ]
8 e 2m'm'	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0,w]	0,1/2, $\bar{z}+1/4$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]
8 d .2'/m'	0,1/4,5/8 [0,0,w]	0,3/4,5/8 [0,0,w]	3/4,1/2,7/8 [0,0,w]	1/4,1/2,7/8 [0,0,w]
8 c .2'/m'	0,1/4,1/8 [0,0,w]	0,3/4,1/8 [0,0,w]	3/4,1/2,3/8 [0,0,w]	1/4,1/2,3/8 [0,0,w]



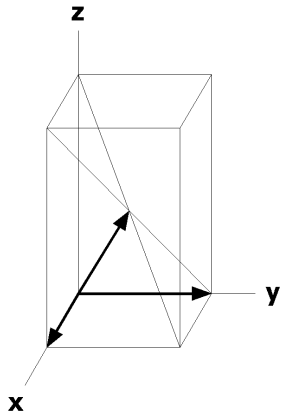
4	b	$\sqrt{2}m'$	0,0,1/2 [0,0,w]	0,1/2,3/4 [0,0,w]
4	a	$\sqrt{2}m'$	0,0,0 [0,0,w]	0,1/2,1/4 [0,0,w]

**Symmetry of Special Projections**

Along [0,0,1]  $p_2, 4m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,1/4,z

Along [1,0,0]  $c2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at x,0,3/8

Along [1,1,0]  $c2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



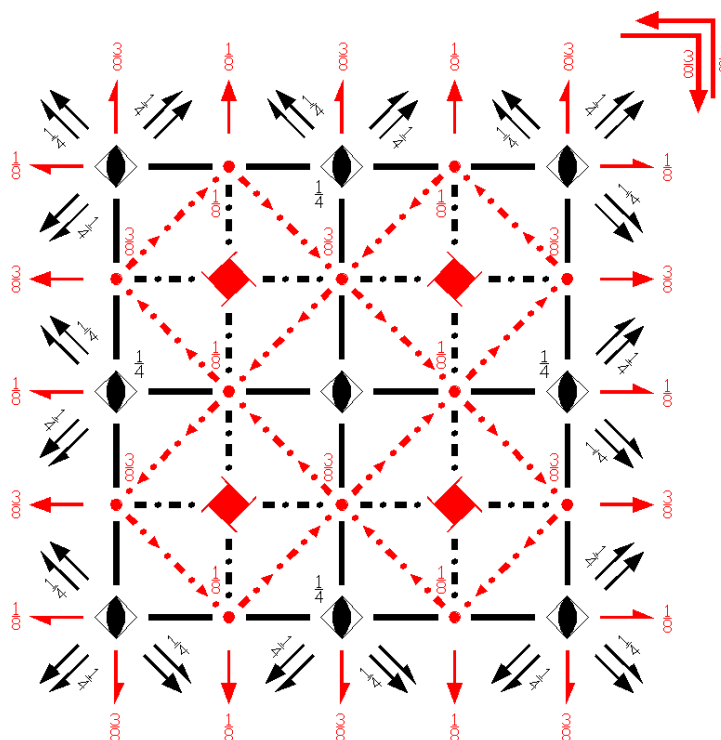
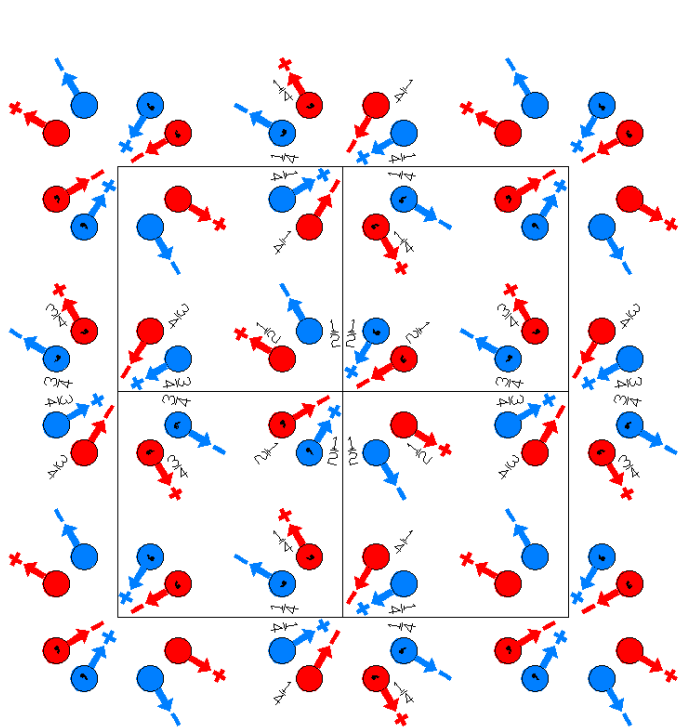
$I4_1'/a'md'$

141.8.1220

$4'/m'mm'$

$I4_1'/a'2'/m2/d'$

Tetragonal



Origin at  $\bar{4}m2$  at  $0, 1/4, -1/8$  from center ( $2'/m$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

### Symmetry Operations

For (0,0,0) + set

- |  |   |  |  |
|--|---|--|--|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                    | (3) 4 <sup>+</sup> (0,0,1/4) -1/4,1/4,z<br>(4 <sub>z</sub>  0,1/2,1/4)'      | (4) 4 <sup>-</sup> (0,0,1/4) 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4)'       |
| (5) 2' (0,1/2,0) 0,y,1/8<br>(2 <sub>y</sub>  0,1/2,1/4)' | (6) 2' x,1/4,1/8<br>(2 <sub>x</sub>  0,1/2,1/4)'          | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                      | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)                       |
| (9) $\bar{1}$ ' 0,1/4,1/8<br>( $\bar{1}$  0,1/2,1/4)'    | (10) b' (0,1/2,0) x,y,1/8<br>(m <sub>z</sub>  0,1/2,1/4)' | (11) $\bar{4}$ <sup>+</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub>  0,0,0) | (12) $\bar{4}$ <sup>-</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)                  | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0)                   | (15) d' (-1/4,1/4,1/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,1/2,1/4)'  | (16) d' (1/4,1/4,1/4) x-1/4,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,1/2,1/4)'        |

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) 2 (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) 4 <sup>+</sup> (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>   1/2,0,3/4)'	(4) 4 <sup>-</sup> (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4)'
(5) 2' 1/4,y,3/8 (2 <sub>y</sub>   1/2,0,3/4)'	(6) 2' (1/2,0,0) x,0,3/8 (2 <sub>x</sub>   1/2,0,3/4)'	(7) 2 (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)	(8) 2 x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)
(9) $\bar{1}$ ' 1/4,0,3/8 ( $\bar{1}$   1/2,0,3/4)'	(10) a' (1/2,0,0) x,y,3/8 (m <sub>z</sub>   1/2,0,3/4)'	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$   1/2,1/2,1/2)
(13) n (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)	(14) n (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)	(15) d' (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,0,3/4)'	(16) d' (1/4,1/4,3/4) x+1/4,x,z (m <sub><math>\bar{xy}</math></sub>   1/2,0,3/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

		(0,0,0) +		(1/2,1/2,1/2) +	
32	i 1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $\bar{v},u,\bar{w}$ ]
		(5) $\bar{x},y+1/2,\bar{z}+1/4$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
		(9) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y+1/2,\bar{z}+1/4$ [ $u,v,\bar{w}$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]
		(13) $x,\bar{y},z$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x}+1/2,z+1/4$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x+1/2,z+1/4$ [ $v,u,w$ ]
16	h .m.	0,y,z [u,0,0]	0, $\bar{y},z$ [ $\bar{u},0,0$ ]	$\bar{y},1/2,z+1/4$ [0, $\bar{u},0$ ]	$y,1/2,z+1/4$ [0,u,0]
		0,y+1/2, $\bar{z}+1/4$ [u,0,0]	0, $\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},0,0$ ]	$y,0,\bar{z}$ [0,u,0]	$\bar{y},0,\bar{z}$ [0, $\bar{u},0$ ]
16	g ..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,1/4$ [u, $\bar{u},0$ ]	$x,\bar{x}+1/2,1/4$ [ $\bar{u},u,0$ ]
		$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$x,x+1/2,1/4$ [u,u,0]	$x,\bar{x},0$ [ $\bar{u},u,0$ ]	$\bar{x},x,0$ [u, $\bar{u},0$ ]
16	f .2'	x,1/4,1/8 [0,v,w]	$\bar{x},3/4,1/8$ [0, $\bar{v},w$ ]	3/4,x+1/2,3/8 [v,0, $\bar{w}$ ]	1/4, $\bar{x}+1/2,3/8$ [ $\bar{v},0,\bar{w}$ ]
		$\bar{x},1/4,1/8$ [0, $\bar{v},\bar{w}$ ]	$x,3/4,1/8$ [0,v, $\bar{w}$ ]	1/4, $\bar{x},7/8$ [ $\bar{v},0,w$ ]	3/4,x,7/8 [v,0,w]
8	e 2mm.	0,0,z [0,0,0]	0,1/2,z+1/4 [0,0,0]	0,1/2, $\bar{z}+1/4$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]
8	d .2'/m.	0,1/4,5/8 [0,0,0]	0,3/4,5/8 [0,0,0]	3/4,1/2,7/8 [0,0,0]	1/4,1/2,7/8 [0,0,0]
8	c .2'/m.	0,1/4,1/8 [0,0,0]	0,3/4,1/8 [0,0,0]	3/4,1/2,3/8 [0,0,0]	1/4,1/2,3/8 [0,0,0]

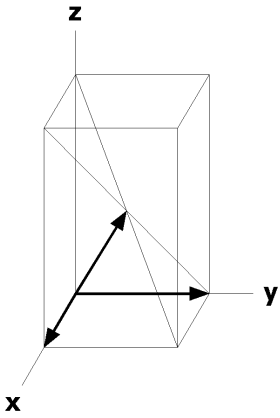
4	b	$\bar{4}2'm'$	0,0,1/2 [0,0,w]	0,1/2,3/4 [0,0, $\bar{w}$ ]
4	a	$\bar{4}2'm'$	0,0,0 [0,0,w]	0,1/2,1/4 [0,0, $\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1]  $p4'mm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]  $c2mm1'$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

Along [1,1,0]  $c2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



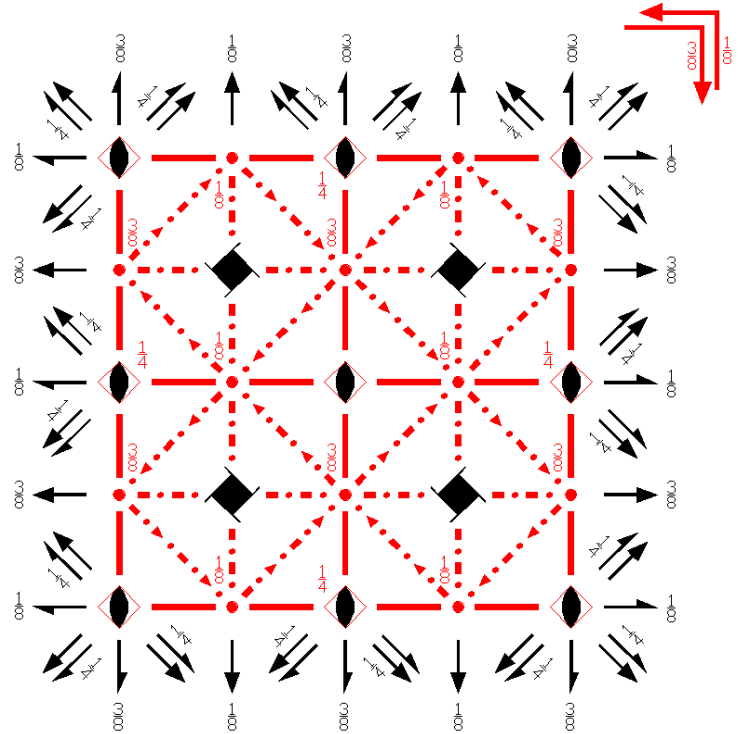
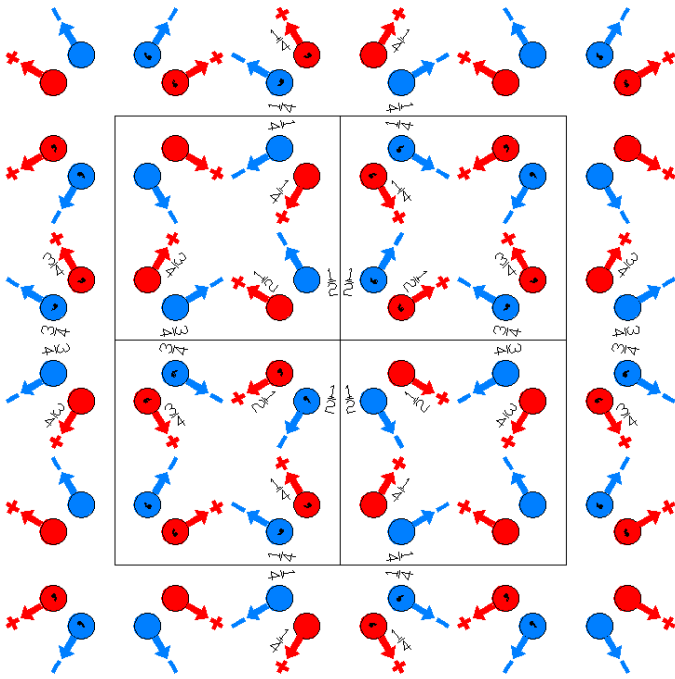
$I4_1/a'm'd'$

141.9.1221

$4/m'm'm'$

$I4_1/a'2/m'2/d'$

Tetragonal



Origin at  $\bar{4}'m'2$  at  $0, 1/4, -1/8$  from center ( $2/m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                    | (3) 4 <sup>+</sup> (0,0,1/4) -1/4,1/4,z<br>(4 <sub>z</sub>  0,1/2,1/4)      | (4) 4 <sup>-</sup> (0,0,1/4) 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4) |
| (5) 2 (0,1/2,0) 0,y,1/8<br>(2 <sub>y</sub>  0,1/2,1/4) | (6) 2 x,1/4,1/8<br>(2 <sub>x</sub>  0,1/2,1/4)            | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                                     | (8) 2 x, $\bar{x}$ ,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,0)                |
| (9) $\bar{1}'$ 0,1/4,1/8<br>( $\bar{1}'$  0,1/2,1/4)'  | (10) b' (0,1/2,0) x,y,1/8<br>(m <sub>z</sub>  0,1/2,1/4)' | (11) $\bar{4}^+$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)'                 | (12) $\bar{4}^-$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)'                         |
| (13) m' x,0,z<br>(m <sub>y</sub>  0,0,0)'              | (14) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)'                 | (15) d' (-1/4,1/4,1/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,1/2,1/4)' | (16) d' (1/4,1/4,1/4) x-1/4,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,1/2,1/4)' |

For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>   1/2,0,3/4)	(4) $4^-$ (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4)
(5) $2$ 1/4,y,3/8 (2 <sub>y</sub>   1/2,0,3/4)	(6) $2$ (1/2,0,0) x,0,3/8 (2 <sub>x</sub>   1/2,0,3/4)	(7) $2$ (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>   1/2,1/2,1/2)	(8) $2$ x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,1/2)
(9) $\bar{1}$ ' 1/4,0,3/8 ( $\bar{1}$   1/2,0,3/4)'	(10) $a'$ (1/2,0,0) x,y,3/8 (m <sub>z</sub>   1/2,0,3/4)'	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)'
(13) $n'$ (1/2,0,1/2) x,1/4,z (m <sub>y</sub>   1/2,1/2,1/2)'	(14) $n'$ (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>   1/2,1/2,1/2)'	(15) $d'$ (1/4,-1/4,3/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,0,3/4)'	(16) $d'$ (1/4,1/4,3/4) x+1/4,x,z (m <sub><math>\bar{xy}</math></sub>   1/2,0,3/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	i	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+1/4$ [ $\bar{u},v,\bar{w}$ ]	(6) $x,\bar{y}+1/2,\bar{z}+1/4$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y+1/2,\bar{z}+1/4$ [ $u,v,\bar{w}$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x,\bar{y},z$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y},\bar{x}+1/2,z+1/4$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x+1/2,z+1/4$ [ $v,u,w$ ]		
16	h	.m'	0,y,z [0,v,w]	0, $\bar{y},z$ [0, $\bar{v},w$ ]	$\bar{y},1/2,z+1/4$ [ $\bar{v},0,w$ ]	$y,1/2,z+1/4$ [ $v,0,w$ ]
			0,y+1/2, $\bar{z}+1/4$ [0,v, $\bar{w}$ ]	0, $\bar{y}+1/2,\bar{z}+1/4$ [0, $\bar{v},\bar{w}$ ]	$y,0,\bar{z}$ [ $v,0,\bar{w}$ ]	$\bar{y},0,\bar{z}$ [ $\bar{v},0,\bar{w}$ ]
16	g	..2	x,x,0 [u,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,1/4$ [ $\bar{u},u,0$ ]	$x,\bar{x}+1/2,1/4$ [ $u,\bar{u},0$ ]
			$\bar{x},\bar{x}+1/2,1/4$ [ $\bar{u},\bar{u},0$ ]	$x,x+1/2,1/4$ [ $u,u,0$ ]	$x,\bar{x},0$ [ $u,\bar{u},0$ ]	$\bar{x},x,0$ [ $\bar{u},u,0$ ]
16	f	.2.	x,1/4,1/8 [u,0,0]	$\bar{x},3/4,1/8$ [ $\bar{u},0,0$ ]	3/4,x+1/2,3/8 [0,u,0]	1/4, $\bar{x}+1/2,3/8$ [0, $\bar{u},0$ ]
			$\bar{x},1/4,1/8$ [ $\bar{u},0,0$ ]	$x,3/4,1/8$ [ $u,0,0$ ]	1/4, $\bar{x},7/8$ [0, $\bar{u},0$ ]	3/4,x,7/8 [0,u,0]
8	e	2m'm'	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0,w]	0,1/2, $\bar{z}+1/4$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
8	d	.2/m'	0,1/4,5/8 [0,0,0]	0,3/4,5/8 [0,0,0]	3/4,1/2,7/8 [0,0,0]	1/4,1/2,7/8 [0,0,0]
8	c	.2/m'	0,1/4,1/8 [0,0,0]	0,3/4,1/8 [0,0,0]	3/4,1/2,3/8 [0,0,0]	1/4,1/2,3/8 [0,0,0]

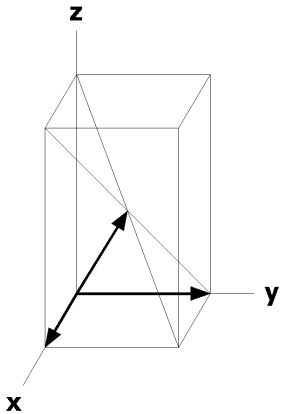
4	b	$\bar{4}'2m'$	0,0,1/2 [0,0,0]	0,1/2,3/4 [0,0,0]
4	a	$\bar{4}'2m'$	0,0,0 [0,0,0]	0,1/2,1/4 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] c2m'm'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,3/8

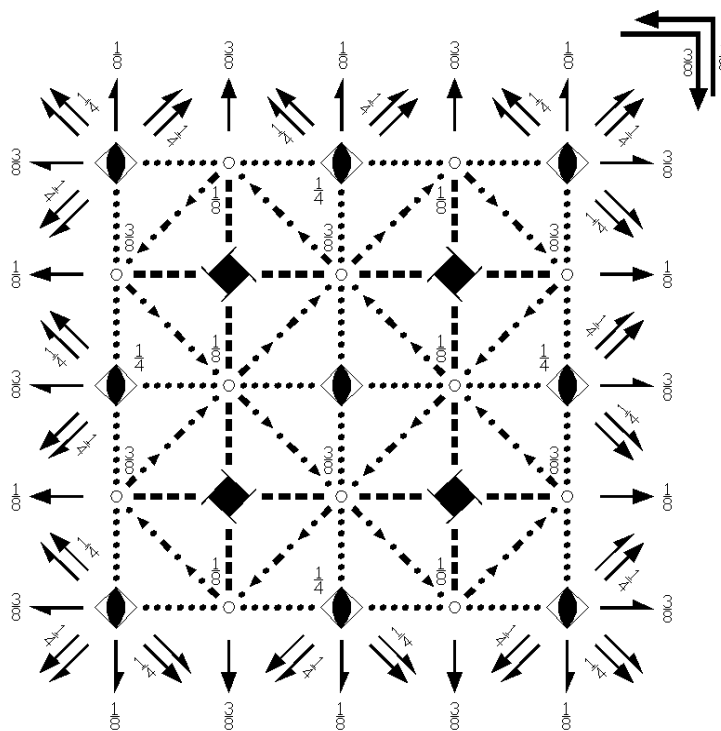
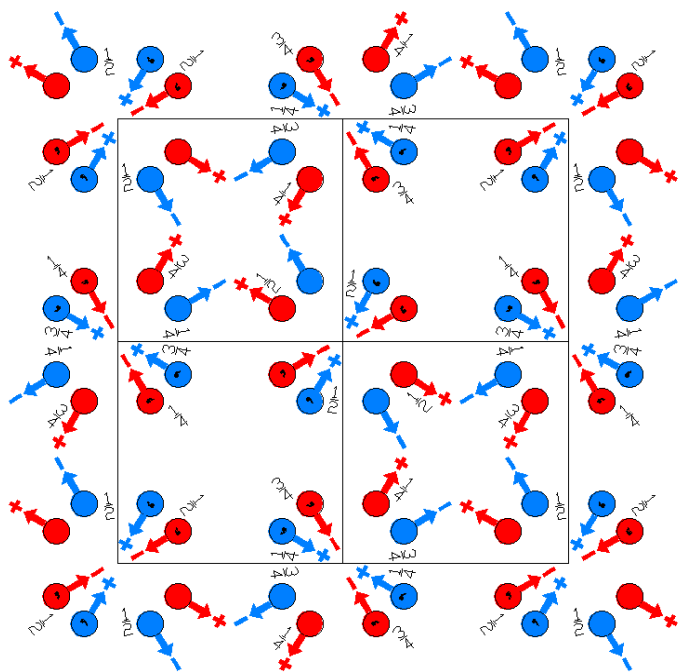
Along [1,1,0] c2'mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$I4_1/acd$   
142.1.1222

$4/mmm$   
 $I4_1/a2/c2/d$

Tetragonal



Origin at  $\bar{4}c2_1$ , at  $0, 1/4, -1/8$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |   |   |  |
|--|---|---|--|
| (1) 1<br>(1 0,0,0)                                   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                  | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>( $4_z$  0,1/2,1/4)           | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>( $4_z^{-1}$  0,1/2,1/4)      |
| (5) 2 $(0,1/2,0) 0,y,3/8$<br>( $2_y$  0,1/2,3/4)     | (6) 2 $x,1/4,3/8$<br>( $2_x$  0,1/2,3/4)          | (7) 2 $x,x,1/4$<br>( $2_{xy}$  0,0,1/2)                           | (8) 2 $x,\bar{x},1/4$<br>( $2_{\bar{xy}}$  0,0,1/2)              |
| (9) $\bar{1}$ $0,1/4,1/8$<br>( $\bar{1}$  0,1/2,1/4) | (10) b $(0,1/2,0) x,y,1/8$<br>( $m_z$  0,1/2,1/4) | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z$  0,0,0)          | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1}$  0,0,0)    |
| (13) c $(0,0,1/2) x,0,z$<br>( $m_y$  0,0,1/2)        | (14) c $(0,0,1/2) 0,y,z$<br>( $m_x$  0,0,1/2)     | (15) d $(-1/4,1/4,3/4) x+1/4,\bar{x},z$<br>( $m_{xy}$  0,1/2,3/4) | (16) d $(1/4,1/4,3/4) x-1/4,x,z$<br>( $m_{\bar{xy}}$  0,1/2,3/4) |



For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>   1/2,0,3/4)	(4) $4^-$ (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4)
(5) $2$ 1/4,y,1/8 (2 <sub>y</sub>   1/2,0,1/4)	(6) $2$ (1/2,0,0) x,0,1/8 (2 <sub>x</sub>   1/2,0,1/4)	(7) $2$ (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)	(8) $2$ x, $\bar{x}$ +1/2,0 (2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,0)
(9) $\bar{1}$ 1/4,0,3/8 ( $\bar{1}$   1/2,0,3/4)	(10) $a$ (1/2,0,0) x,y,3/8 (m <sub>z</sub>   1/2,0,3/4)	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)
(13) $a$ (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)	(14) $b$ (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)	(15) $d$ (1/4,-1/4,1/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,0,1/4)	(16) $d$ (1/4,1/4,1/4) x+1/4,x,z (m <sub><math>\bar{xy}</math></sub>   1/2,0,1/4)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates															
			(0,0,0) +		(1/2,1/2,1/2) +													
Multiplicity,	Wyckoff letter,	Site Symmetry.																
32	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $v,\bar{u},w$ ]	(5) $\bar{x},y+1/2,\bar{z}+3/4$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,\bar{y}+1/2,\bar{z}+3/4$ [ $u,\bar{v},\bar{w}$ ]	(7) $y,x,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [ $u,v,w$ ]	(10) $x,y+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]	(13) $x,\bar{y},z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]	(15) $\bar{y},\bar{x}+1/2,z+3/4$ [ $v,u,\bar{w}$ ]	(16) $y,x+1/2,z+3/4$ [ $\bar{v},\bar{u},\bar{w}$ ]
16	f	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,1/2$ [ $\bar{u},u,0$ ]	$x,\bar{x}+1/2,1/2$ [ $u,\bar{u},0$ ]	$\bar{x},\bar{x}+1/2,0$ [u,u,0]	$x,x+1/2,0$ [ $\bar{u},\bar{u},0$ ]	$x,\bar{x},3/4$ [ $\bar{u},u,0$ ]	$\bar{x},x,3/4$ [ $u,\bar{u},0$ ]								
16	e	.2.	1/4,y,1/8 [0,v,0]	3/4, $\bar{y},1/8$ [0, $\bar{v},0$ ]	$\bar{y},3/4,3/8$ [ $\bar{v},0,0$ ]	$y,1/4,3/8$ [ $v,0,0$ ]	3/4, $\bar{y}+1/2,1/8$ [0,v,0]	1/4,y+1/2,1/8 [0, $\bar{v},0$ ]	$y,3/4,7/8$ [ $\bar{v},0,0$ ]	$\bar{y},1/4,7/8$ [ $v,0,0$ ]								
16	d	2..	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0,w]	0,1/2, $\bar{z}+3/4$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/4$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2,z+3/4 [0,0, $\bar{w}$ ]								
16	c	$\bar{1}$	0,1/4,1/8 [u,v,w]	0,3/4,1/8 [ $\bar{u},\bar{v},w$ ]	3/4,1/2,3/8 [ $\bar{v},u,w$ ]	1/4,1/2,3/8 [ $v,\bar{u},w$ ]	0,3/4,5/8 [ $\bar{u},\bar{v},\bar{w}$ ]	0,1/4,5/8 [ $u,\bar{v},\bar{w}$ ]	1/4,0,3/8 [ $v,u,\bar{w}$ ]	3/4,0,3/8 [ $\bar{v},\bar{u},\bar{w}$ ]								
8	b	2.22	0,0,1/4 [0,0,0]	0,1/2,1/2 [0,0,0]	0,1/2,0 [0,0,0]	0,0,3/4 [0,0,0]												

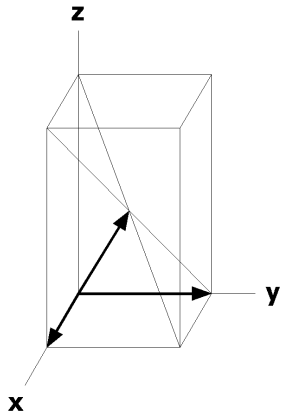
4    a     $\bar{4}..$     0,0,0 [0,0,w]    0,1/2,1/4 [0,0,w]    0,1/2,3/4 [0,0, $\bar{w}$ ]    0,0,1/2 [0,0, $\bar{w}$ ]

### Symmetry of Special Projections

Along [0,0,1]     $p_p^* 4m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$      $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,1/4,z

Along [1,0,0]     $p_c^* 2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$      $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,1/8

Along [1,1,0]     $c_p^* 2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$      $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

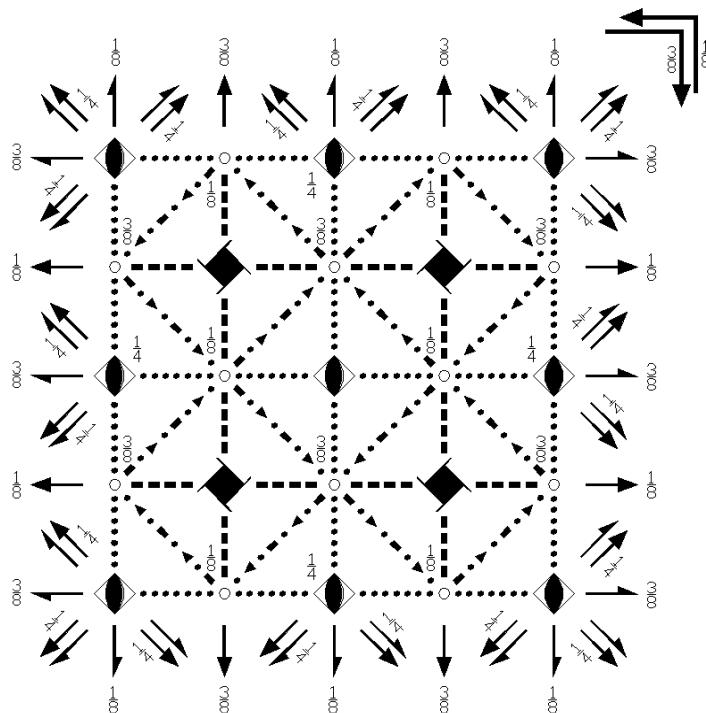
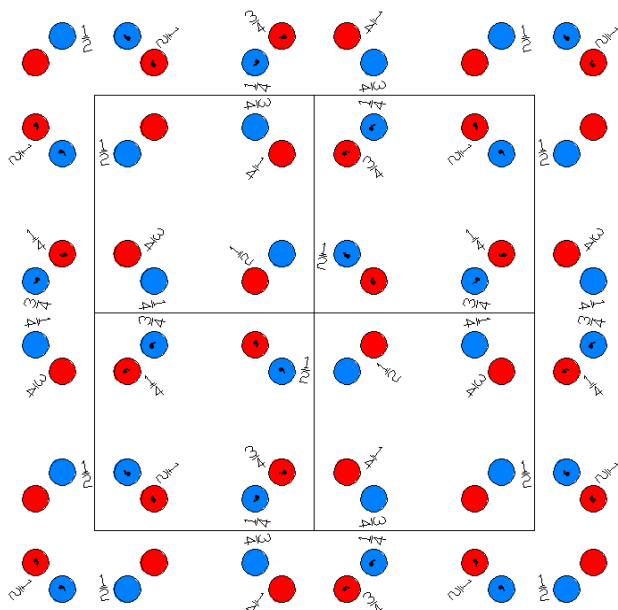


$I4_1/acd1'$   
142.2.1223

$4/mmm1'$   
 $I4_1/a2/c2/d1'$

Tetragonal

$1'$



Origin at  $\bar{4}c2_11'$  at  $0, 1/4, -1/8$  from  $\bar{1}1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

Symmetry Operations

For  $(0,0,0) +$  set

- |  |   |   |  |
|--|---|---|--|
| (1) $1$<br>$(1 0,0,0)$                             | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                  | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>$(4_z^+ 0,1/2,1/4)$           | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>$(4_z^- 0,1/2,1/4)$           |
| (5) $2$ $(0,1/2,0) 0,y,3/8$<br>$(2_y 0,1/2,3/4)$   | (6) $2$ $x,1/4,3/8$<br>$(2_x 0,1/2,3/4)$          | (7) $2$ $x,x,1/4$<br>$(2_{xy} 0,0,1/2)$                           | (8) $2$ $x,\bar{x},1/4$<br>$(2_{\bar{xy}} 0,0,1/2)$              |
| (9) $\bar{1}$ $0,1/4,1/8$<br>$(\bar{1} 0,1/2,1/4)$ | (10) $b$ $(0,1/2,0) x,y,1/8$<br>$(m_z 0,1/2,1/4)$ | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^+ 0,0,0)$          | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^- 0,0,0)$         |
| (13) $c$ $(0,0,1/2) x,0,z$<br>$(m_y 0,0,1/2)$      | (14) $c$ $(0,0,1/2) 0,y,z$<br>$(m_x 0,0,1/2)$     | (15) $d$ $(-1/4,1/4,3/4) x+1/4,\bar{x},z$<br>$(m_{xy} 0,1/2,3/4)$ | (16) $d$ $(1/4,1/4,3/4) x-1/4,x,z$<br>$(m_{\bar{xy}} 0,1/2,3/4)$ |

## For (1/2,1/2,1/2) + set

- |  |   |  |   |
|--|---|--|---|
| (1) t (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)                 | (2) 2 (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2) | (3) 4 <sup>+</sup> (0,0,3/4) 1/4,1/4,z<br>(4 <sub>z</sub>   1/2,0,3/4)     | (4) 4 <sup>-</sup> (0,0,3/4) 1/4,-1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4) |
| (5) 2 1/4,y,1/8<br>(2 <sub>y</sub>   1/2,0,1/4)          | (6) 2 (1/2,0,0) x,0,1/8<br>(2 <sub>x</sub>   1/2,0,1/4)     | (7) 2 (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>   1/2,1/2,0)                   | (8) 2 x, $\bar{x}$ +1/2,0<br>(2 <sub>xy</sub>   1/2,1/2,0)                            |
| (9) $\bar{1}$ 1/4,0,3/8<br>( $\bar{1}$   1/2,0,3/4)      | (10) a (1/2,0,0) x,y,3/8<br>(m <sub>z</sub>   1/2,0,3/4)    | (11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$   1/2,1/2,1/2)        | (12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)     |
| (13) a (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0) | (14) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)    | (15) d (1/4,-1/4,1/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>   1/2,0,1/4) | (16) d (1/4,1/4,1/4) x+1/4,x,z<br>(m <sub>xy</sub>   1/2,0,1/4)                       |

## For (0,0,0)' + set

- |   |  |  |   |
|---|--|--|---|
| (1) 1'<br>(1   0,0,0)'                                    | (2) 2' 0,0,z<br>(2 <sub>z</sub>   0,0,0)'                  | (3) 4 <sup>+</sup> ' (0,0,1/4) -1/4,1/4,z<br>(4 <sub>z</sub>   0,1/2,1/4)'   | (4) 4 <sup>-</sup> ' (0,0,1/4) 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>   0,1/2,1/4)' |
| (5) 2' (0,1/2,0) 0,y,3/8<br>(2 <sub>y</sub>   0,1/2,3/4)' | (6) 2' x,1/4,3/8<br>(2 <sub>x</sub>   0,1/2,3/4)'          | (7) 2' x,x,1/4<br>(2 <sub>xy</sub>   0,0,1/2)'                               | (8) 2' x, $\bar{x}$ ,1/4<br>(2 <sub>xy</sub>   0,0,1/2)'                                |
| (9) $\bar{1}$ ' 0,1/4,1/8<br>( $\bar{1}$   0,1/2,1/4)'    | (10) b' (0,1/2,0) x,y,1/8<br>(m <sub>z</sub>   0,1/2,1/4)' | (11) $\bar{4}^+$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z$   0,0,0)'                   | (12) $\bar{4}^-$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z$ <sup>-1</sup>   0,0,0)'                |
| (13) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>   0,0,1/2)'    | (14) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>   0,0,1/2)'     | (15) d' (-1/4,1/4,3/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>   0,1/2,3/4)' | (16) d' (1/4,1/4,3/4) x-1/4,x,z<br>(m <sub>xy</sub>   0,1/2,3/4)'                       |

## For (1/2,1/2,1/2)' + set

- |  |   |  |  |
|--|---|--|--|
| (1) t' (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)'                 | (2) 2' (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2)' | (3) 4 <sup>+</sup> ' (0,0,3/4) 1/4,1/4,z<br>(4 <sub>z</sub>   1/2,0,3/4)'    | (4) 4 <sup>-</sup> ' (0,0,3/4) 1/4,-1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4)' |
| (5) 2' 1/4,y,1/8<br>(2 <sub>y</sub>   1/2,0,1/4)'          | (6) 2' (1/2,0,0) x,0,1/8<br>(2 <sub>x</sub>   1/2,0,1/4)'     | (7) 2' (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>   1/2,1/2,0)'                   | (8) 2' x, $\bar{x}$ +1/2,0<br>(2 <sub>xy</sub>   1/2,1/2,0)'                             |
| (9) $\bar{1}$ ' 1/4,0,3/8<br>( $\bar{1}$   1/2,0,3/4)'     | (10) a' (1/2,0,0) x,y,3/8<br>(m <sub>z</sub>   1/2,0,3/4)'    | (11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$   1/2,1/2,1/2)'       | (12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)'     |
| (13) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0)' | (14) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)'    | (15) d' (1/4,-1/4,1/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>   1/2,0,1/4)' | (16) d' (1/4,1/4,1/4) x+1/4,x,z<br>(m <sub>xy</sub>   1/2,0,1/4)'                        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

(0,0,0) + (1/2,1/2,1/2) +  
(0,0,0)' + (1/2,1/2,1/2)' +

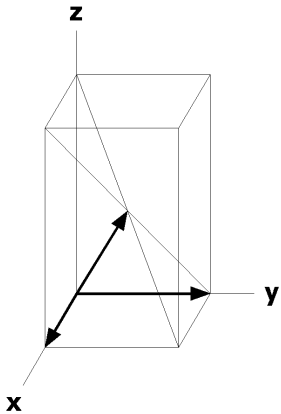
32	g	11'	(1) $x, y, z$ [0,0,0]	(2) $\bar{x}, \bar{y}, z$ [0,0,0]		
			(3) $\bar{y}, x+1/2, z+1/4$ [0,0,0]	(4) $y, \bar{x}+1/2, z+1/4$ [0,0,0]		
			(5) $\bar{x}, y+1/2, \bar{z}+3/4$ [0,0,0]	(6) $x, \bar{y}+1/2, \bar{z}+3/4$ [0,0,0]		
			(7) $y, x, \bar{z}+1/2$ [0,0,0]	(8) $\bar{y}, \bar{x}, \bar{z}+1/2$ [0,0,0]		
			(9) $\bar{x}, \bar{y}+1/2, \bar{z}+1/4$ [0,0,0]	(10) $x, y+1/2, \bar{z}+1/4$ [0,0,0]		
			(11) $y, \bar{x}, \bar{z}$ [0,0,0]	(12) $\bar{y}, x, \bar{z}$ [0,0,0]		
			(13) $x, \bar{y}, z+1/2$ [0,0,0]	(14) $\bar{x}, y, z+1/2$ [0,0,0]		
			(15) $\bar{y}, \bar{x}+1/2, z+3/4$ [0,0,0]	(16) $y, x+1/2, z+3/4$ [0,0,0]		
16	f	..21'	$x, x, 1/4$ [0,0,0]	$\bar{x}, \bar{x}, 1/4$ [0,0,0]	$\bar{x}, x+1/2, 1/2$ [0,0,0]	$x, \bar{x}+1/2, 1/2$ [0,0,0]
			$\bar{x}, \bar{x}+1/2, 0$ [0,0,0]	$x, x+1/2, 0$ [0,0,0]	$x, \bar{x}, 3/4$ [0,0,0]	$\bar{x}, x, 3/4$ [0,0,0]
16	e	.2.1'	$1/4, y, 1/8$ [0,0,0]	$3/4, \bar{y}, 1/8$ [0,0,0]	$\bar{y}, 3/4, 3/8$ [0,0,0]	$y, 1/4, 3/8$ [0,0,0]
			$3/4, \bar{y}+1/2, 1/8$ [0,0,0]	$1/4, y+1/2, 1/8$ [0,0,0]	$y, 3/4, 7/8$ [0,0,0]	$\bar{y}, 1/4, 7/8$ [0,0,0]
16	d	2..1'	$0, 0, z$ [0,0,0]	$0, 1/2, z+1/4$ [0,0,0]	$0, 1/2, \bar{z}+3/4$ [0,0,0]	$0, 0, \bar{z}+1/2$ [0,0,0]
			$0, 1/2, \bar{z}+1/4$ [0,0,0]	$0, 0, \bar{z}$ [0,0,0]	$0, 0, z+1/2$ [0,0,0]	$0, 1/2, z+3/4$ [0,0,0]
16	c	$\bar{1}$ 1'	$0, 1/4, 1/8$ [0,0,0]	$0, 3/4, 1/8$ [0,0,0]	$3/4, 1/2, 3/8$ [0,0,0]	$1/4, 1/2, 3/8$ [0,0,0]
			$0, 3/4, 5/8$ [0,0,0]	$0, 1/4, 5/8$ [0,0,0]	$1/4, 0, 3/8$ [0,0,0]	$3/4, 0, 3/8$ [0,0,0]
8	b	2.221'	$0, 0, 1/4$ [0,0,0]	$0, 1/2, 1/2$ [0,0,0]	$0, 1/2, 0$ [0,0,0]	$0, 0, 3/4$ [0,0,0]
4	a	$\bar{4}$ ..1'	$0, 0, 0$ [0,0,0]	$0, 1/2, 1/4$ [0,0,0]	$0, 1/2, 3/4$ [0,0,0]	$0, 0, 1/2$ [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,1/8

Along [1,1,0] c2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



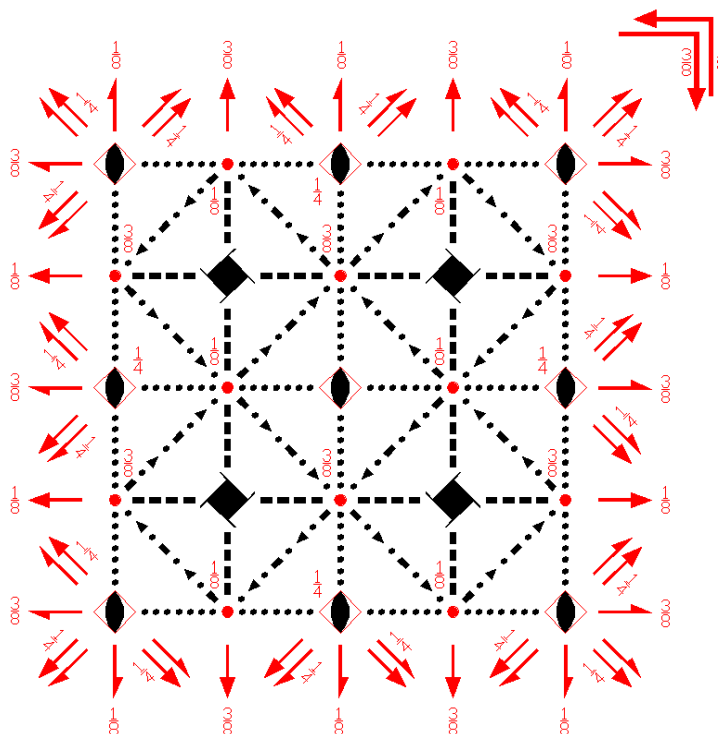
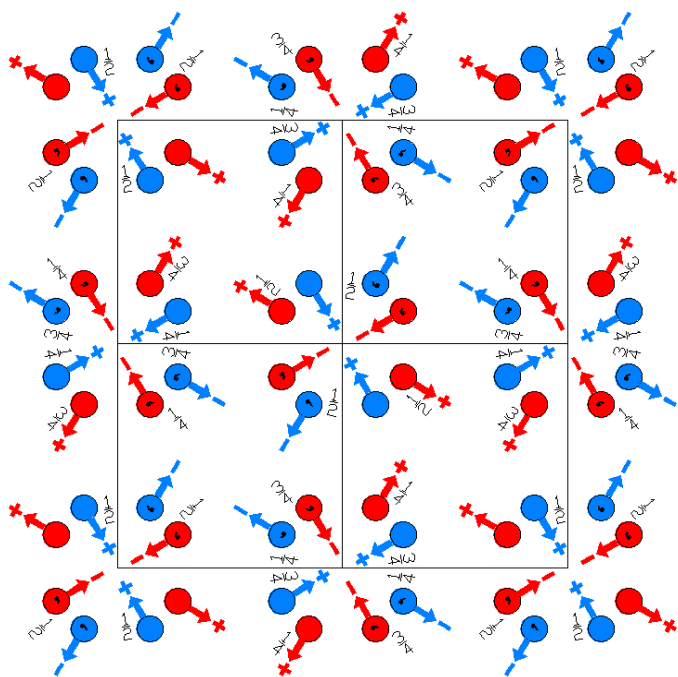
$I4_1/a'cd$

142.3.1224

$4/m'mm$

$I4_1/a'2'/c2'/d$

Tetragonal



Origin at  $\bar{4}'c2_1'$  at  $0, 1/4, -1/8$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |   |   |  |
|--|---|---|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                      | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>( $4_z$  0,1/2,1/4)             | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>( $4_z^{-1}$  0,1/2,1/4)        |
| (5) $2'$ $(0,1/2,0) 0,y,3/8$<br>( $2_y$  0,1/2,3/4)'   | (6) $2'$ $x,1/4,3/8$<br>( $2_x$  0,1/2,3/4)'          | (7) $2'$ $x,x,1/4$<br>( $2_{xy}$  0,0,1/2)'                         | (8) $2'$ $x,\bar{x},1/4$<br>( $2_{\bar{xy}}$  0,0,1/2)'            |
| (9) $\bar{1}'$ $0,1/4,1/8$<br>( $\bar{1}$  0,1/2,1/4)' | (10) $b'$ $(0,1/2,0) x,y,1/8$<br>( $m_z$  0,1/2,1/4)' | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z$  0,0,0)'           | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1}$  0,0,0)'     |
| (13) $c$ $(0,0,1/2) x,0,z$<br>( $m_y$  0,0,1/2)        | (14) $c$ $(0,0,1/2) 0,y,z$<br>( $m_x$  0,0,1/2)       | (15) $d$ $(-1/4,1/4,3/4) x+1/4,\bar{x},z$<br>( $m_{xy}$  0,1/2,3/4) | (16) $d$ $(1/4,1/4,3/4) x-1/4,x,z$<br>( $m_{\bar{xy}}$  0,1/2,3/4) |

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) 2 (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) 4 <sup>+</sup> (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>   1/2,0,3/4)	(4) 4 <sup>-</sup> (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4)
(5) 2' 1/4,y,1/8 (2 <sub>y</sub>   1/2,0,1/4)'	(6) 2' (1/2,0,0) x,0,1/8 (2 <sub>x</sub>   1/2,0,1/4)'	(7) 2' (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)'	(8) 2' x, $\bar{x}$ +1/2,0 (2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,0)'
(9) $\bar{1}$ ' 1/4,0,3/8 ( $\bar{1}$   1/2,0,3/4)'	(10) a' (1/2,0,0) x,y,3/8 (m <sub>z</sub>   1/2,0,3/4)'	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$   1/2,1/2,1/2)'
(13) a (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)	(14) b (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)	(15) d (1/4,-1/4,1/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,0,1/4)	(16) d (1/4,1/4,1/4) x+1/4,x,z (m <sub><math>\bar{xy}</math></sub>   1/2,0,1/4)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

			(0,0,0) +	(1/2,1/2,1/2) +		
32	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+3/4$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y}+1/2,\bar{z}+3/4$ [ $\bar{u},v,w$ ]		
			(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $v,u,w$ ]		
			(9) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y+1/2,\bar{z}+1/4$ [ $u,v,\bar{w}$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x,\bar{y},z+1/2$ [ $\bar{u},v,\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y},\bar{x}+1/2,z+3/4$ [ $v,u,\bar{w}$ ]	(16) $y,x+1/2,z+3/4$ [ $\bar{v},\bar{u},\bar{w}$ ]		
16	f	..2'	x,x,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [ $u,\bar{u},w$ ]	$\bar{x},x+1/2,1/2$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x}+1/2,1/2$ [ $u,u,w$ ]
			$\bar{x},\bar{x}+1/2,0$ [ $u,\bar{u},\bar{w}$ ]	$x,x+1/2,0$ [ $\bar{u},u,\bar{w}$ ]	$x,\bar{x},3/4$ [ $u,u,\bar{w}$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
16	e	.2'	1/4,y,1/8 [u,0,w]	3/4, $\bar{y},1/8$ [ $\bar{u},0,w$ ]	$\bar{y},3/4,3/8$ [0,u,w]	y,1/4,3/8 [0, $\bar{u},w$ ]
			3/4, $\bar{y}+1/2,1/8$ [ $\bar{u},0,\bar{w}$ ]	1/4,y+1/2,1/8 [u,0, $\bar{w}$ ]	y,3/4,7/8 [0, $\bar{u},\bar{w}$ ]	$\bar{y},1/4,7/8$ [0,u, $\bar{w}$ ]
16	d	2..	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0,w]	0,1/2, $\bar{z}+3/4$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]
			0,1/2, $\bar{z}+1/4$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2,z+3/4 [0,0, $\bar{w}$ ]
16	c	$\bar{1}$ '	0,1/4,1/8 [0,0,0]	0,3/4,1/8 [0,0,0]	3/4,1/2,3/8 [0,0,0]	1/4,1/2,3/8 [0,0,0]
			0,3/4,5/8 [0,0,0]	0,1/4,5/8 [0,0,0]	1/4,0,3/8 [0,0,0]	3/4,0,3/8 [0,0,0]
8	b	2.2'2'	0,0,1/4 [0,0,w]	0,1/2,1/2 [0,0,w]	0,1/2,0 [0,0, $\bar{w}$ ]	0,0,3/4 [0,0, $\bar{w}$ ]

Continued

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$I4_1/a'cd$

4    a     $\bar{4}$ '..    0,0,0 [0,0,0]    0,1/2,1/4 [0,0,0]    0,1/2,3/4 [0,0,0]    0,0,1/2 [0,0,0]

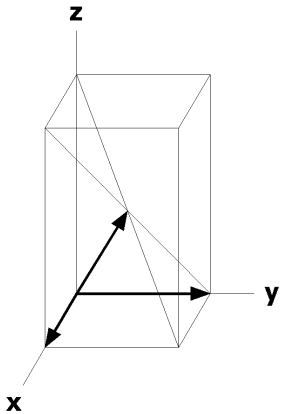
### Symmetry of Special Projections

Along [0,0,1]     $p4mm$   
 $\mathbf{a}^* = \mathbf{a}/2$      $\mathbf{b}^* = \mathbf{b}/2$   
Origin at 0,0,z

Along [1,0,0]     $p_2 \times 2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$      $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,1/4,3/8

Along [1,1,0]     $c_2 \times 2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$      $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
Origin at x,x,0





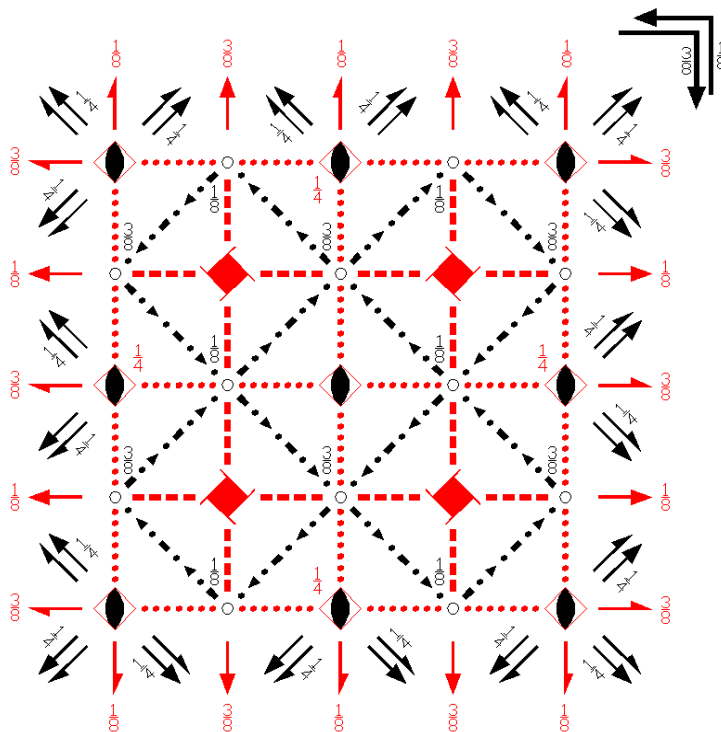
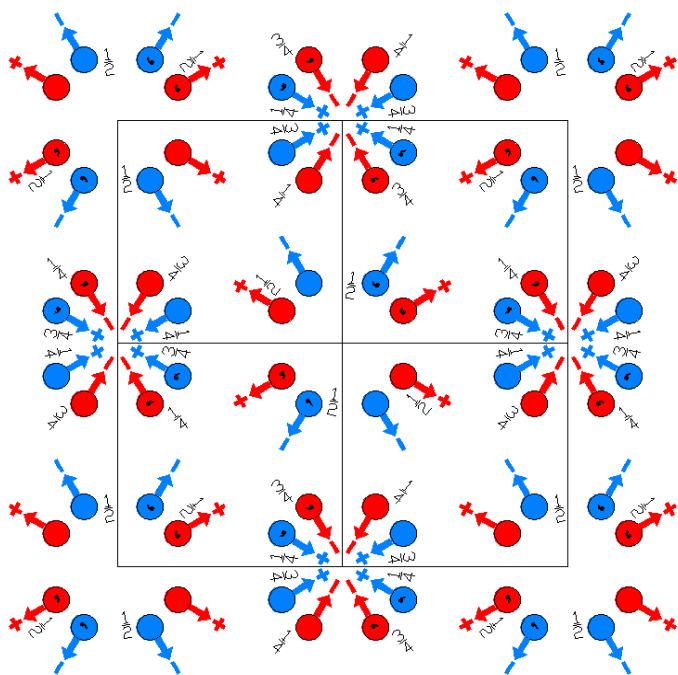
$I4_1'/ac'd$

142.4.1225

$4'/mm'm$

$I4_1'/a2'/c'2'/d$

Tetragonal



Origin at  $\bar{4}'c'2_1$  at  $0, 1/4, -1/8$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

### Symmetry Operations

For (0,0,0) + set

- |  |   |   |  |
|--|---|---|--|
| (1) $1$<br>( $1 0,0,0$ )                             | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                  | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>( $4_z 0,1/2,1/4$ )'            | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>( $4_z^{-1} 0,1/2,1/4$ )'       |
| (5) $2'$ $(0,1/2,0) 0,y,3/8$<br>( $2_y 0,1/2,3/4$ )' | (6) $2'$ $x,1/4,3/8$<br>( $2_x 0,1/2,3/4$ )'        | (7) $2$ $x,x,1/4$<br>( $2_{xy} 0,0,1/2$ )                           | (8) $2$ $x,\bar{x},1/4$<br>( $2_{\bar{xy}} 0,0,1/2$ )              |
| (9) $\bar{1}$ $0,1/4,1/8$<br>( $\bar{1} 0,1/2,1/4$ ) | (10) $b$ $(0,1/2,0) x,y,1/8$<br>( $m_z 0,1/2,1/4$ ) | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )'           | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ )'     |
| (13) $c'$ $(0,0,1/2) x,0,z$<br>( $m_y 0,0,1/2$ )'    | (14) $c'$ $(0,0,1/2) 0,y,z$<br>( $m_x 0,0,1/2$ )'   | (15) $d$ $(-1/4,1/4,3/4) x+1/4,\bar{x},z$<br>( $m_{xy} 0,1/2,3/4$ ) | (16) $d$ $(1/4,1/4,3/4) x-1/4,x,z$<br>( $m_{\bar{xy}} 0,1/2,3/4$ ) |

For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>   1/2,0,3/4)'	(4) $4^-$ (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4)'
(5) $2'$ 1/4,y,1/8 (2 <sub>y</sub>   1/2,0,1/4)'	(6) $2'$ (1/2,0,0) x,0,1/8 (2 <sub>x</sub>   1/2,0,1/4)'	(7) $2$ (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)	(8) $2$ x, $\bar{x}$ +1/2,0 (2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,0)
(9) $\bar{1}$ 1/4,0,3/8 ( $\bar{1}$   1/2,0,3/4)	(10) $a$ (1/2,0,0) x,y,3/8 (m <sub>z</sub>   1/2,0,3/4)	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)'
(13) $a'$ (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)'	(14) $b'$ (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)'	(15) $d$ (1/4,-1/4,1/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,0,1/4)	(16) $d$ (1/4,1/4,1/4) x+1/4,x,z (m <sub><math>\bar{xy}</math></sub>   1/2,0,1/4)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates															
			(0,0,0) +		(1/2,1/2,1/2) +													
Multiplicity,	Wyckoff letter,	Site Symmetry.																
32	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $\bar{v},u,\bar{w}$ ]	(5) $\bar{x},y+1/2,\bar{z}+3/4$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y}+1/2,\bar{z}+3/4$ [ $\bar{u},v,w$ ]	(7) $y,x,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(9) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [ $u,v,w$ ]	(10) $x,y+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},w$ ]	(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]	(13) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]	(15) $\bar{y},\bar{x}+1/2,z+3/4$ [ $\bar{v},\bar{u},\bar{w}$ ]	(16) $y,x+1/2,z+3/4$ [ $\bar{v},u,\bar{w}$ ]
16	f	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,1/2$ [ $u,\bar{u},0$ ]	$x,\bar{x}+1/2,1/2$ [ $\bar{u},u,0$ ]	$\bar{x},\bar{x}+1/2,0$ [u,u,0]	x,x+1/2,0 [ $\bar{u},\bar{u},0$ ]	x, $\bar{x}$ ,3/4 [u, $\bar{u},0$ ]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]								
16	e	.2'	1/4,y,1/8 [u,0,w]	3/4, $\bar{y},1/8$ [ $\bar{u},0,w$ ]	$\bar{y},3/4,3/8$ [0, $\bar{u},\bar{w}$ ]	y,1/4,3/8 [0,u, $\bar{w}$ ]	3/4, $\bar{y}+1/2,1/8$ [u,0,w]	1/4,y+1/2,1/8 [ $\bar{u},0,w$ ]	y,3/4,7/8 [0, $\bar{u},\bar{w}$ ]	$\bar{y},1/4,7/8$ [0,u, $\bar{w}$ ]								
16	d	2..	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+3/4$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+1/4$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]	0,1/2,z+3/4 [0,0, $\bar{w}$ ]								
16	c	$\bar{1}$	0,1/4,1/8 [u,v,w]	0,3/4,1/8 [ $\bar{u},\bar{v},w$ ]	3/4,1/2,3/8 [v, $\bar{u},\bar{w}$ ]	1/4,1/2,3/8 [ $\bar{v},u,\bar{w}$ ]	0,3/4,5/8 [u, $\bar{v},w$ ]	0,1/4,5/8 [ $\bar{u},v,w$ ]	1/4,0,3/8 [v,u, $\bar{w}$ ]	3/4,0,3/8 [ $\bar{v},\bar{u},\bar{w}$ ]								
8	b	2.22	0,0,1/4 [0,0,0]	0,1/2,1/2 [0,0,0]	0,1/2,0 [0,0,0]	0,0,3/4 [0,0,0]												

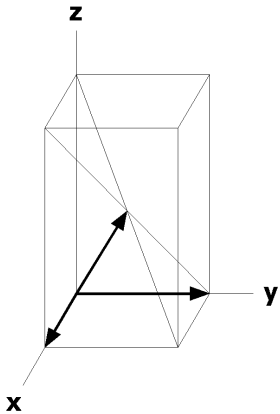
4    a     $\bar{4}'..$     0,0,0 [0,0,0]    0,1/2,1/4 [0,0,0]    0,1/2,3/4 [0,0,0]    0,0,1/2 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]     $p_p^* 4m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$      $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]     $p_c^* 2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$      $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,1/8

Along [1,1,0]     $c_p^* 2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$      $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



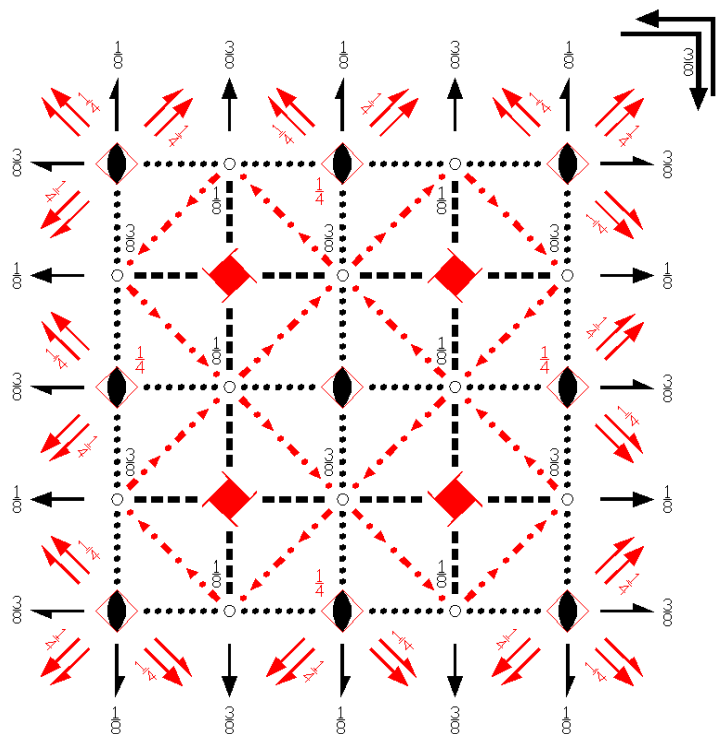
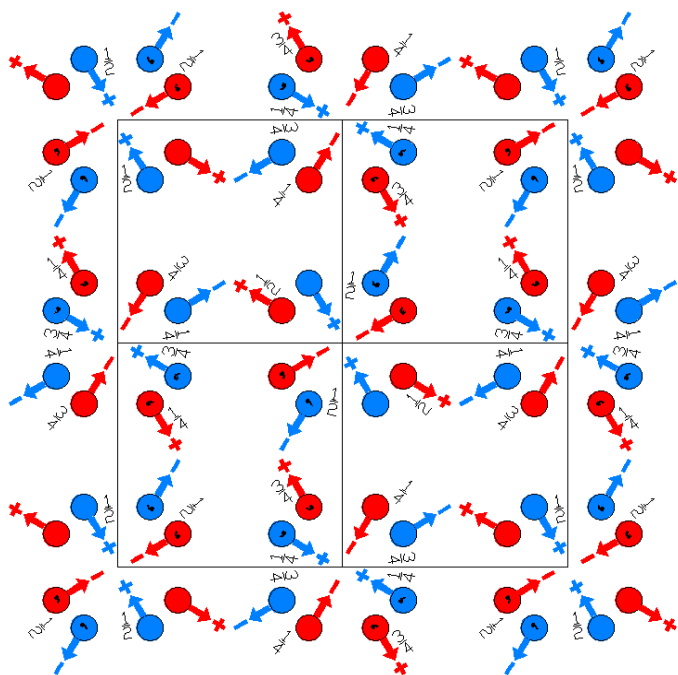
$I4_1'/acd'$

142.5.1226

$4'/mmm'$

$I4_1'/a2/c2'/d'$

Tetragonal



Origin at  $\bar{4}'c2_1'$  at  $0, 1/4, -1/8$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |   |   |  |
|--|---|---|--|
| (1) $1$<br>$(1 0,0,0)$                             | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                  | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>$(4_z 0,1/2,1/4)'$              | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>$(4_z^{-1} 0,1/2,1/4)'$         |
| (5) $2$ $(0,1/2,0) 0,y,3/8$<br>$(2_y 0,1/2,3/4)$   | (6) $2$ $x,1/4,3/8$<br>$(2_x 0,1/2,3/4)$          | (7) $2'$ $x,x,1/4$<br>$(2_{xy} 0,0,1/2)'$                           | (8) $2'$ $x,\bar{x},1/4$<br>$(2_{\bar{xy}} 0,0,1/2)'$              |
| (9) $\bar{1}$ $0,1/4,1/8$<br>$(\bar{1} 0,1/2,1/4)$ | (10) $b$ $(0,1/2,0) x,y,1/8$<br>$(m_z 0,1/2,1/4)$ | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z 0,0,0)'$             | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1} 0,0,0)'$       |
| (13) $c$ $(0,0,1/2) x,0,z$<br>$(m_y 0,0,1/2)$      | (14) $c$ $(0,0,1/2) 0,y,z$<br>$(m_x 0,0,1/2)$     | (15) $d'$ $(-1/4,1/4,3/4) x+1/4,\bar{x},z$<br>$(m_{xy} 0,1/2,3/4)'$ | (16) $d'$ $(1/4,1/4,3/4) x-1/4,x,z$<br>$(m_{\bar{xy}} 0,1/2,3/4)'$ |

For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ ' (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>   1/2,0,3/4)'	(4) $4^-$ ' (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4)'
(5) $2$ 1/4,y,1/8 (2 <sub>y</sub>   1/2,0,1/4)	(6) $2$ (1/2,0,0) x,0,1/8 (2 <sub>x</sub>   1/2,0,1/4)	(7) $2'$ (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)'	(8) $2'$ x, $\bar{x}$ +1/2,0 (2 <sub>xy</sub>   1/2,1/2,0)'
(9) $\bar{1}$ 1/4,0,3/8 ( $\bar{1}$   1/2,0,3/4)	(10) $a$ (1/2,0,0) x,y,3/8 (m <sub>z</sub>   1/2,0,3/4)	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)'
(13) $a$ (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)	(14) $b$ (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)	(15) $d'$ (1/4,-1/4,1/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,0,1/4)'	(16) $d'$ (1/4,1/4,1/4) x+1/4,x,z (m <sub>xy</sub>   1/2,0,1/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

			(0,0,0) +	(1/2,1/2,1/2) +		
32	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},\bar{u},\bar{w}$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $\bar{v},u,\bar{w}$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+3/4$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,\bar{y}+1/2,\bar{z}+3/4$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $v,u,w$ ]		
			(9) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [u,v,w]	(10) $x,y+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x,\bar{y},z+1/2$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $\bar{x},y,z+1/2$ [ $u,\bar{v},\bar{w}$ ]		
			(15) $\bar{y},\bar{x}+1/2,z+3/4$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x+1/2,z+3/4$ [ $v,u,w$ ]		
16	f	..2'	x,x,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x+1/2,1/2$ [ $u,u,\bar{w}$ ]	$x,\bar{x}+1/2,1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]
			$\bar{x},\bar{x}+1/2,0$ [ $\bar{u},u,w$ ]	$x,x+1/2,0$ [ $u,\bar{u},w$ ]	$x,\bar{x},3/4$ [ $u,u,\bar{w}$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]
16	e	.2.	1/4,y,1/8 [0,v,0]	3/4, $\bar{y},1/8$ [0, $\bar{v},0$ ]	$\bar{y},3/4,3/8$ [v,0,0]	y,1/4,3/8 [ $\bar{v},0,0$ ]
			3/4, $\bar{y}+1/2,1/8$ [0,v,0]	1/4,y+1/2,1/8 [0, $\bar{v},0$ ]	y,3/4,7/8 [v,0,0]	$\bar{y},1/4,7/8$ [ $\bar{v},0,0$ ]
16	d	2..	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0, $\bar{w}$ ]	0,1/2, $\bar{z}+3/4$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0,w]
			0,1/2, $\bar{z}+1/4$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,1/2,z+3/4 [0,0,w]
16	c	$\bar{1}$	0,1/4,1/8 [u,v,w]	0,3/4,1/8 [ $\bar{u},\bar{v},w$ ]	3/4,1/2,3/8 [v, $\bar{u},\bar{w}$ ]	1/4,1/2,3/8 [ $\bar{v},u,\bar{w}$ ]
			0,3/4,5/8 [ $\bar{u},\bar{v},\bar{w}$ ]	0,1/4,5/8 [u, $\bar{v},\bar{w}$ ]	1/4,0,3/8 [ $\bar{v},\bar{u},w$ ]	3/4,0,3/8 [v,u,w]
8	b	2.2'2'	0,0,1/4 [0,0,w]	0,1/2,1/2 [0,0, $\bar{w}$ ]	0,1/2,0 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]

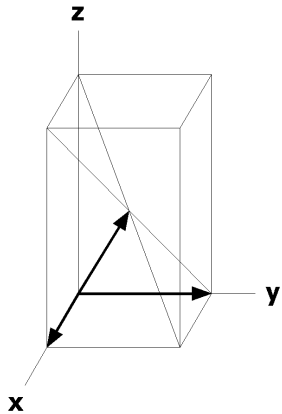
4    a     $\bar{4}'..$     0,0,0 [0,0,0]    0,1/2,1/4 [0,0,0]    0,1/2,3/4 [0,0,0]    0,0,1/2 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]     $p_p^* 4mm$   
 $\mathbf{a}^* = \mathbf{a}/2$      $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,0,0]     $p_c^* 2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$      $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,1/4,1/8

Along [1,1,0]     $c 2'mm'$   
 $\mathbf{a}^* = -\mathbf{c}/2$      $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



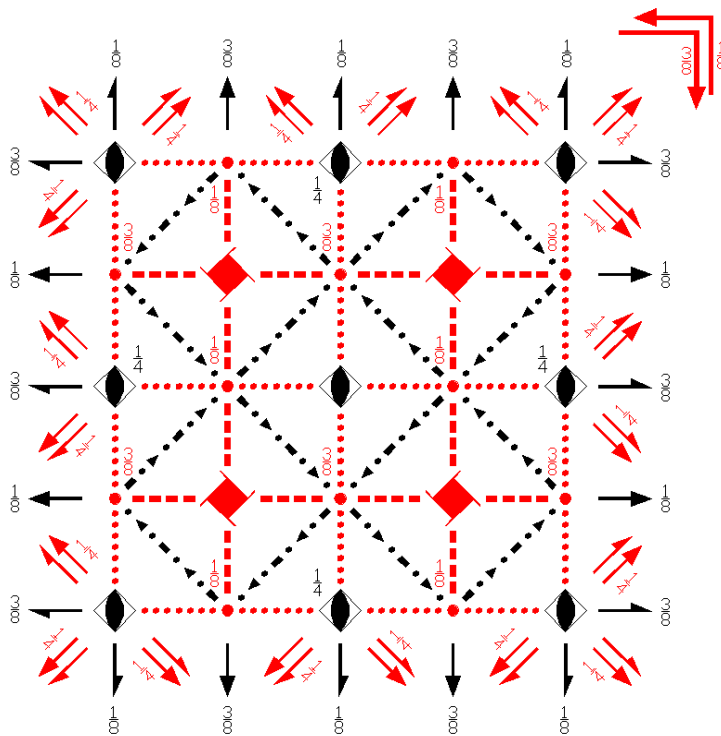
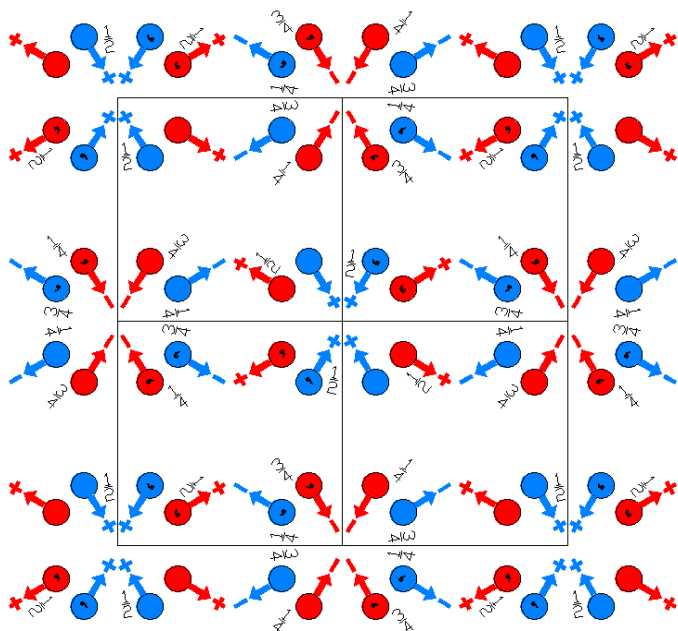
$I4_1'/a'c'd$

142.6.1227

$4/m'm'm$

$I4_1'/a'2/c'2'/d$

Tetragonal



Origin at  $\bar{4}c'2_1'$  at  $0, 1/4, -1/8$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

### Symmetry Operations

For  $(0,0,0)$  + set

- |  |   |   |  |
|--|---|---|--|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                        | (3) $4^+ 1' (0,0,1/4) -1/4,1/4,z$<br>( $4_z$   $0,1/2,1/4$ )'         | (4) $4^- 1' (0,0,1/4) 1/4,1/4,z$<br>( $4_z^{-1}$   $0,1/2,1/4$ )'    |
| (5) 2 $(0,1/2,0) 0,y,3/8$<br>( $2_y$   $0,1/2,3/4$ )     | (6) 2 $x,1/4,3/8$<br>( $2_x$   $0,1/2,3/4$ )            | (7) $2' x,x,1/4$<br>( $2_{xy}$   $0,0,1/2$ )'                         | (8) $2' x,\bar{x},1/4$<br>( $2_{\bar{xy}}$   $0,0,1/2$ )'            |
| (9) $\bar{1}' 0,1/4,1/8$<br>( $\bar{1}$   $0,1/2,1/4$ )' | (10) $b' (0,1/2,0) x,y,1/8$<br>( $m_z$   $0,1/2,1/4$ )' | (11) $\bar{4}^+ 0,0,z; 0,0,0$<br>( $\bar{4}_z$   $0,0,0$ )            | (12) $\bar{4}^- 0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1}$   $0,0,0$ )      |
| (13) $c' (0,0,1/2) x,0,z$<br>( $m_y$   $0,0,1/2$ )'      | (14) $c' (0,0,1/2) 0,y,z$<br>( $m_x$   $0,0,1/2$ )'     | (15) $d (-1/4,1/4,3/4) x+1/4,\bar{x},z$<br>( $m_{xy}$   $0,1/2,3/4$ ) | (16) $d (1/4,1/4,3/4) x-1/4,x,z$<br>( $m_{\bar{xy}}$   $0,1/2,3/4$ ) |

For  $(1/2,1/2,1/2)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t (1/2,1/2,1/2)$<br>(1  $1/2,1/2,1/2$ ) | (2) 2 $(0,0,1/2) 1/4,1/4,z$<br>( $2_z$   $1/2,1/2,1/2$ ) | (3) $4^+ 1' (0,0,3/4) 1/4,1/4,z$<br>( $4_z$   $1/2,0,3/4$ )' | (4) $4^- 1' (0,0,3/4) 1/4,-1/4,z$<br>( $4_z^{-1}$   $1/2,0,3/4$ )' |
|--|--|--|--|

(5) $2 \begin{matrix} 1/4, y, 1/8 \\ (2_y   1/2, 0, 1/4) \end{matrix}$	(6) $2 \begin{matrix} (1/2, 0, 0) \quad x, 0, 1/8 \\ (2_x   1/2, 0, 1/4) \end{matrix}$	(7) $2' \begin{matrix} (1/2, 1/2, 0) \quad x, x, 0 \\ (2_{xy}   1/2, 1/2, 0)' \end{matrix}$	(8) $2' \begin{matrix} x, \bar{x} + 1/2, 0 \\ (2_{\bar{xy}}   1/2, 1/2, 0)' \end{matrix}$
(9) $\bar{1}' \begin{matrix} 1/4, 0, 3/8 \\ (\bar{1}   1/2, 0, 3/4)' \end{matrix}$	(10) $a' \begin{matrix} (1/2, 0, 0) \quad x, y, 3/8 \\ (m_z   1/2, 0, 3/4)' \end{matrix}$	(11) $\bar{4}^+ \begin{matrix} 1/2, 0, z; 1/2, 0, 1/4 \\ (\bar{4}_z   1/2, 1/2, 1/2) \end{matrix}$	(12) $\bar{4}^- \begin{matrix} 0, 1/2, z; 0, 1/2, 1/4 \\ (\bar{4}_z^{-1}   1/2, 1/2, 1/2) \end{matrix}$
(13) $a' \begin{matrix} (1/2, 0, 0) \quad x, 1/4, z \\ (m_y   1/2, 1/2, 0)' \end{matrix}$	(14) $b' \begin{matrix} (0, 1/2, 0) \quad 1/4, y, z \\ (m_x   1/2, 1/2, 0)' \end{matrix}$	(15) $d \begin{matrix} (1/4, -1/4, 1/4) \quad x + 1/4, \bar{x}, z \\ (m_{xy}   1/2, 0, 1/4) \end{matrix}$	(16) $d \begin{matrix} (1/4, 1/4, 1/4) \quad x + 1/4, x, z \\ (m_{\bar{xy}}   1/2, 0, 1/4) \end{matrix}$

Continued

142.6.1227

 $I4_1'/a'c'd$ 

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,1/2)$ ; (2); (3); (5); (9).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1/2,1/2,1/2) +		
32	g	1	(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$		
			(3) $\bar{y}, x + 1/2, z + 1/4 [v, \bar{u}, \bar{w}]$	(4) $y, \bar{x} + 1/2, z + 1/4 [\bar{v}, u, \bar{w}]$		
			(5) $\bar{x}, y + 1/2, \bar{z} + 3/4 [\bar{u}, v, \bar{w}]$	(6) $x, \bar{y} + 1/2, \bar{z} + 3/4 [u, \bar{v}, \bar{w}]$		
			(7) $y, x, \bar{z} + 1/2 [\bar{v}, \bar{u}, w]$	(8) $\bar{y}, \bar{x}, \bar{z} + 1/2 [v, u, w]$		
			(9) $\bar{x}, \bar{y} + 1/2, \bar{z} + 1/4 [\bar{u}, \bar{v}, \bar{w}]$	(10) $x, y + 1/2, \bar{z} + 1/4 [u, v, \bar{w}]$		
			(11) $y, \bar{x}, \bar{z} [\bar{v}, u, w]$	(12) $\bar{y}, x, \bar{z} [v, \bar{u}, w]$		
			(13) $x, \bar{y}, z + 1/2 [u, \bar{v}, w]$	(14) $\bar{x}, y, z + 1/2 [\bar{u}, v, w]$		
			(15) $\bar{y}, \bar{x} + 1/2, z + 3/4 [v, u, \bar{w}]$	(16) $y, x + 1/2, z + 3/4 [\bar{v}, \bar{u}, \bar{w}]$		
16	f	..2'	$x, x, 1/4 [\bar{u}, u, w]$	$\bar{x}, \bar{x}, 1/4 [u, \bar{u}, w]$	$\bar{x}, x + 1/2, 1/2 [u, u, \bar{w}]$	$x, \bar{x} + 1/2, 1/2 [\bar{u}, \bar{u}, \bar{w}]$
			$\bar{x}, \bar{x} + 1/2, 0 [u, \bar{u}, \bar{w}]$	$x, x + 1/2, 0 [\bar{u}, u, \bar{w}]$	$x, \bar{x}, 3/4 [\bar{u}, \bar{u}, w]$	$\bar{x}, x, 3/4 [u, u, w]$
16	e	.2.	$1/4, y, 1/8 [0, v, 0]$	$3/4, \bar{y}, 1/8 [0, \bar{v}, 0]$	$\bar{y}, 3/4, 3/8 [v, 0, 0]$	$y, 1/4, 3/8 [\bar{v}, 0, 0]$
			$3/4, \bar{y} + 1/2, 1/8 [0, \bar{v}, 0]$	$1/4, y + 1/2, 1/8 [0, v, 0]$	$y, 3/4, 7/8 [\bar{v}, 0, 0]$	$\bar{y}, 1/4, 7/8 [v, 0, 0]$
16	d	2..	$0, 0, z [0, 0, w]$	$0, 1/2, z + 1/4 [0, 0, \bar{w}]$	$0, 1/2, \bar{z} + 3/4 [0, 0, \bar{w}]$	$0, 0, \bar{z} + 1/2 [0, 0, w]$
			$0, 1/2, \bar{z} + 1/4 [0, 0, \bar{w}]$	$0, 0, \bar{z} [0, 0, w]$	$0, 0, z + 1/2 [0, 0, w]$	$0, 1/2, z + 3/4 [0, 0, \bar{w}]$
16	c	$\bar{1}'$	$0, 1/4, 1/8 [0, 0, 0]$	$0, 3/4, 1/8 [0, 0, 0]$	$3/4, 1/2, 3/8 [0, 0, 0]$	$1/4, 1/2, 3/8 [0, 0, 0]$
			$0, 3/4, 5/8 [0, 0, 0]$	$0, 1/4, 5/8 [0, 0, 0]$	$1/4, 0, 3/8 [0, 0, 0]$	$3/4, 0, 3/8 [0, 0, 0]$
8	b	2.2'2'	$0, 0, 1/4 [0, 0, w]$	$0, 1/2, 1/2 [0, 0, \bar{w}]$	$0, 1/2, 0 [0, 0, \bar{w}]$	$0, 0, 3/4 [0, 0, w]$
4	a	$\bar{4}..$	$0, 0, 0 [0, 0, w]$	$0, 1/2, 1/4 [0, 0, \bar{w}]$	$0, 1/2, 3/4 [0, 0, \bar{w}]$	$0, 0, 1/2 [0, 0, w]$

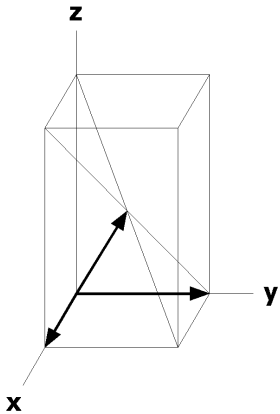


## Symmetry of Special Projections

Along  $[0,0,1]$   $p4'm'm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at  $x,0,1/8$

Along  $[1,1,0]$   $c_2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at  $x,x,0$



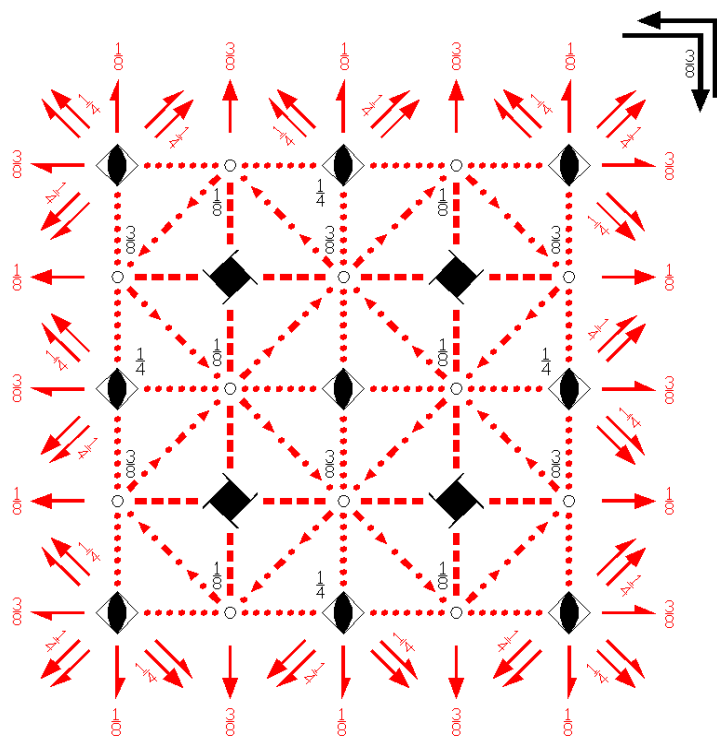
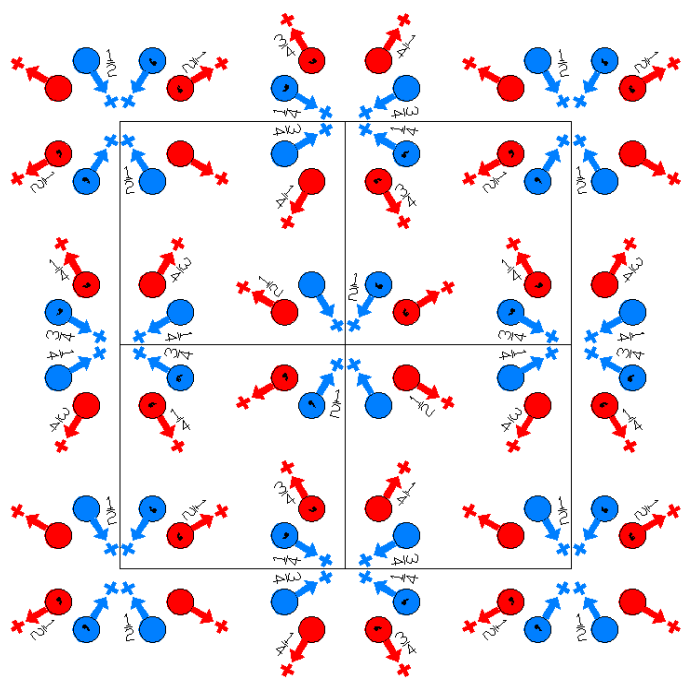
$I4_1/ac'd'$

142.7.1228

$4/mm'm'$

$I4_1/a2'/c2'/d'$

Tetragonal



Origin at  $\bar{4}c'2'_1$  at  $0, 1/4, -1/8$  from  $\bar{1}$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

### Symmetry Operations

For  $(0,0,0) +$  set

- |  |   |   |  |
|--|---|---|--|
| (1) $1$<br>$(1 0,0,0)$                             | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$                  | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>$(4_z 0,1/2,1/4)$               | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>$(4_z^{-1} 0,1/2,1/4)$          |
| (5) $2'$ $(0,1/2,0) 0,y,3/8$<br>$(2_y 0,1/2,3/4)'$ | (6) $2'$ $x,1/4,3/8$<br>$(2_x 0,1/2,3/4)'$        | (7) $2'$ $x,x,1/4$<br>$(2_{xy} 0,0,1/2)'$                           | (8) $2'$ $x,\bar{x},1/4$<br>$(2_{\bar{xy}} 0,0,1/2)'$              |
| (9) $\bar{1}$ $0,1/4,1/8$<br>$(\bar{1} 0,1/2,1/4)$ | (10) $b$ $(0,1/2,0) x,y,1/8$<br>$(m_z 0,1/2,1/4)$ | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z 0,0,0)$              | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1} 0,0,0)$        |
| (13) $c'$ $(0,0,1/2) x,0,z$<br>$(m_y 0,0,1/2)'$    | (14) $c'$ $(0,0,1/2) 0,y,z$<br>$(m_x 0,0,1/2)'$   | (15) $d'$ $(-1/4,1/4,3/4) x+1/4,\bar{x},z$<br>$(m_{xy} 0,1/2,3/4)'$ | (16) $d'$ $(1/4,1/4,3/4) x-1/4,x,z$<br>$(m_{\bar{xy}} 0,1/2,3/4)'$ |

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) 2 (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) 4 <sup>+</sup> (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>   1/2,0,3/4)	(4) 4 <sup>-</sup> (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4)
(5) 2' 1/4,y,1/8 (2 <sub>y</sub>   1/2,0,1/4)'	(6) 2' (1/2,0,0) x,0,1/8 (2 <sub>x</sub>   1/2,0,1/4)'	(7) 2' (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)'	(8) 2' x, $\bar{x}+1/2,0$ (2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,0)'
(9) $\bar{1}$ 1/4,0,3/8 ( $\bar{1}$   1/2,0,3/4)	(10) a (1/2,0,0) x,y,3/8 (m <sub>z</sub>   1/2,0,3/4)	(11) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)	(12) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$   1/2,1/2,1/2)
(13) a' (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)'	(14) b' (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)'	(15) d' (1/4,-1/4,1/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,0,1/4)'	(16) d' (1/4,1/4,1/4) x+1/4,x,z (m <sub><math>\bar{xy}</math></sub>   1/2,0,1/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

			Coordinates			
			(0,0,0) +	(1/2,1/2,1/2) +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
32	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+3/4$ [ $u,\bar{v},w$ ]	(6) $x,\bar{y}+1/2,\bar{z}+3/4$ [ $\bar{u},v,w$ ]		
			(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $v,u,w$ ]		
			(9) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [ $u,v,w$ ]	(10) $x,y+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},w$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(12) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]		
			(13) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y},\bar{x}+1/2,z+3/4$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x+1/2,z+3/4$ [ $v,u,w$ ]		
16	f	..2'	x,x,1/4 [ $\bar{u},u,w$ ]	$\bar{x},\bar{x},1/4$ [ $u,\bar{u},w$ ]	$\bar{x},x+1/2,1/2$ [ $\bar{u},\bar{u},w$ ]	$x,\bar{x}+1/2,1/2$ [ $u,u,w$ ]
			$\bar{x},\bar{x}+1/2,0$ [ $\bar{u},u,w$ ]	$x,x+1/2,0$ [ $u,\bar{u},w$ ]	$x,\bar{x},3/4$ [ $\bar{u},\bar{u},w$ ]	$\bar{x},x,3/4$ [ $u,u,w$ ]
16	e	.2'	1/4,y,1/8 [u,0,w]	3/4, $\bar{y},1/8$ [ $\bar{u},0,w$ ]	$\bar{y},3/4,3/8$ [0,u,w]	y,1/4,3/8 [0, $\bar{u},w$ ]
			3/4, $\bar{y}+1/2,1/8$ [u,0,w]	1/4,y+1/2,1/8 [ $\bar{u},0,w$ ]	y,3/4,7/8 [0,u,w]	$\bar{y},1/4,7/8$ [0, $\bar{u},w$ ]
16	d	2..	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0,w]	0,1/2, $\bar{z}+3/4$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]
			0,1/2, $\bar{z}+1/4$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0,w]	0,1/2,z+3/4 [0,0,w]
16	c	$\bar{1}$	0,1/4,1/8 [u,v,w]	0,3/4,1/8 [ $\bar{u},\bar{v},w$ ]	3/4,1/2,3/8 [ $\bar{v},u,w$ ]	1/4,1/2,3/8 [ $v,\bar{u},w$ ]
			0,3/4,5/8 [u, $\bar{v},w$ ]	0,1/4,5/8 [ $\bar{u},v,w$ ]	1/4,0,3/8 [ $\bar{v},\bar{u},w$ ]	3/4,0,3/8 [ $v,u,w$ ]
8	b	2.2'2'	0,0,1/4 [0,0,w]	0,1/2,1/2 [0,0,w]	0,1/2,0 [0,0,w]	0,0,3/4 [0,0,w]

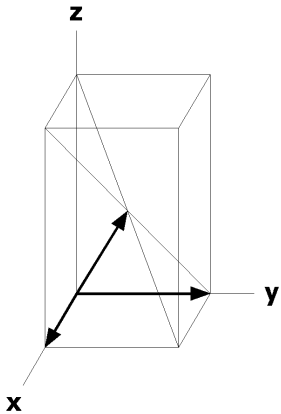
4    a     $\bar{4}..$     0,0,0 [0,0,w]    0,1/2,1/4 [0,0,w]    0,1/2,3/4 [0,0,w]    0,0,1/2 [0,0,w]

### Symmetry of Special Projections

Along [0,0,1]     $p_4$  4m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$      $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,1/4,z

Along [1,0,0]     $p2'$  mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$      $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,0,1/8

Along [1,1,0]     $c2'$  mm'  
 $\mathbf{a}^* = -\mathbf{c}/2$      $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



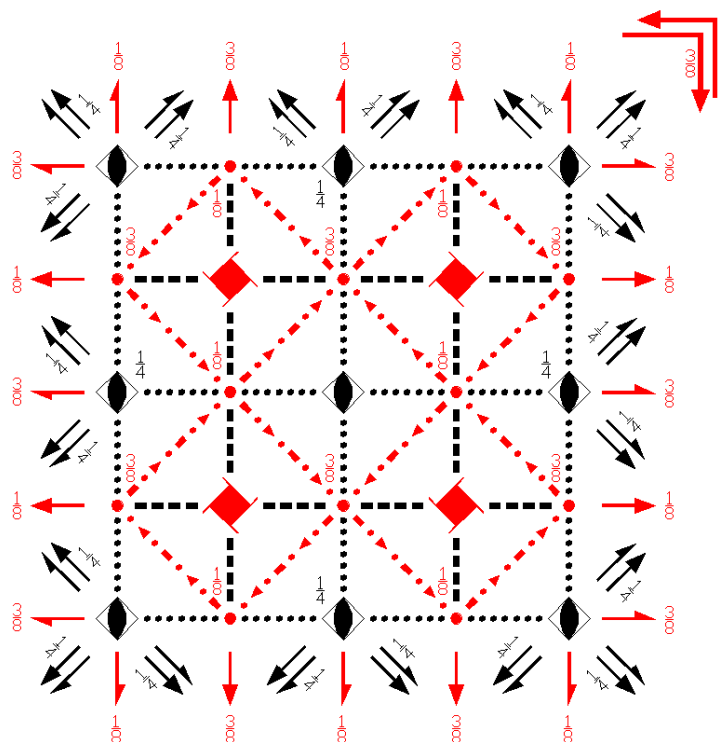
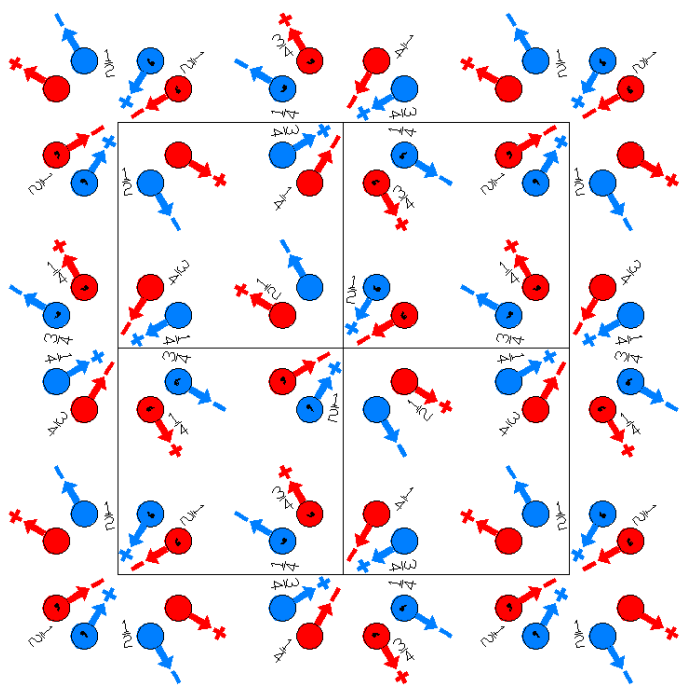
$I4_1'/a'cd'$

142.8.1229

$4'/m'mm'$

$I4_1'/a'2'/c2'/d'$

Tetragonal



Origin at  $\bar{4}c2_1$ , at  $0, 1/4, -1/8$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

### Symmetry Operations

For (0,0,0) + set

- |   |   |   |  |
|---|---|---|--|
| (1) $1$<br>( $1 0,0,0$ )                                | (2) $2$ $0,0,z$<br>( $2_z 0,0,0$ )                    | (3) $4^+$ $(0,0,1/4) -1/4,1/4,z$<br>( $4_z 0,1/2,1/4$ )'              | (4) $4^-$ $(0,0,1/4) 1/4,1/4,z$<br>( $4_z^{-1} 0,1/2,1/4$ )'         |
| (5) $2'$ $(0,1/2,0) 0,y,3/8$<br>( $2_y 0,1/2,3/4$ )'    | (6) $2'$ $x,1/4,3/8$<br>( $2_x 0,1/2,3/4$ )'          | (7) $2$ $x,x,1/4$<br>( $2_{xy} 0,0,1/2$ )                             | (8) $2$ $x,\bar{x},1/4$<br>( $2_{\bar{xy}} 0,0,1/2$ )                |
| (9) $\bar{1}'$ $0,1/4,1/8$<br>( $\bar{1}' 0,1/2,1/4$ )' | (10) $b'$ $(0,1/2,0) x,y,1/8$<br>( $m_z 0,1/2,1/4$ )' | (11) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )              | (12) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ )        |
| (13) $c$ $(0,0,1/2) x,0,z$<br>( $m_y 0,0,1/2$ )         | (14) $c$ $(0,0,1/2) 0,y,z$<br>( $m_x 0,0,1/2$ )       | (15) $d'$ $(-1/4,1/4,3/4) x+1/4,\bar{x},z$<br>( $m_{xy} 0,1/2,3/4$ )' | (16) $d'$ $(1/4,1/4,3/4) x-1/4,x,z$<br>( $m_{\bar{xy}} 0,1/2,3/4$ )' |

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) 2 (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) 4 <sup>+</sup> (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>   1/2,0,3/4)'	(4) 4 <sup>-</sup> (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4)'
(5) 2' 1/4,y,1/8 (2 <sub>y</sub>   1/2,0,1/4)'	(6) 2' (1/2,0,0) x,0,1/8 (2 <sub>x</sub>   1/2,0,1/4)'	(7) 2 (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)	(8) 2 x, x̄+1/2,0 (2 <sub>xy</sub>   1/2,1/2,0)
(9) 1̄' 1/4,0,3/8 (1̄   1/2,0,3/4)'	(10) a' (1/2,0,0) x,y,3/8 (m <sub>z</sub>   1/2,0,3/4)'	(11) 4 <sup>+</sup> 1/2,0,z; 1/2,0,1/4 (4 <sub>z</sub>   1/2,1/2,1/2)	(12) 4 <sup>-</sup> 0,1/2,z; 0,1/2,1/4 (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)
(13) a (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)	(14) b (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)	(15) d' (1/4,-1/4,1/4) x+1/4,x̄,z (m <sub>xy</sub>   1/2,0,1/4)'	(16) d' (1/4,1/4,1/4) x+1/4,x,z (m <sub>xy</sub>   1/2,0,1/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

			(0,0,0) +	(1/2,1/2,1/2) +		
32	g	1	(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w̄]		
			(3) ȳ,x+1/2,z+1/4 [v̄,ū,w̄]	(4) y,x̄+1/2,z+1/4 [v̄,ū,w̄]		
			(5) x̄,y+1/2,z̄+3/4 [ū,v̄,w̄]	(6) x,ȳ+1/2,z̄+3/4 [ū,v̄,w̄]		
			(7) y,x,z̄+1/2 [v̄,ū,w̄]	(8) ȳ,x̄,z̄+1/2 [v̄,ū,w̄]		
			(9) x̄,ȳ+1/2,z̄+1/4 [ū,v̄,w̄]	(10) x,y+1/2,z̄+1/4 [u,v,w̄]		
			(11) y,x̄,z̄ [v̄,ū,w̄]	(12) ȳ,x̄,z̄ [v̄,ū,w̄]		
			(13) x,ȳ,z+1/2 [ū,v̄,w̄]	(14) x̄,y,z+1/2 [u,v̄,w̄]		
			(15) ȳ,x̄+1/2,z+3/4 [v̄,ū,w̄]	(16) y,x+1/2,z+3/4 [v̄,ū,w̄]		
16	f	..2	x,x,1/4 [u,u,0]	x̄,x̄,1/4 [ū,ū,0]	x̄,x+1/2,1/2 [u,ū,0]	x,x̄+1/2,1/2 [ū,ū,0]
			x̄,x̄+1/2,0 [ū,ū,0]	x,x+1/2,0 [u,u,0]	x,x̄,3/4 [ū,ū,0]	x̄,x,3/4 [u,ū,0]
16	e	.2'	1/4,y,1/8 [u,0,w]	3/4,ȳ,1/8 [ū,0,w̄]	ȳ,3/4,3/8 [0,ū,w̄]	y,1/4,3/8 [0,u,w̄]
			3/4,ȳ+1/2,1/8 [ū,0,w̄]	1/4,y+1/2,1/8 [u,0,w̄]	y,3/4,7/8 [0,ū,w̄]	ȳ,1/4,7/8 [0,u,w̄]
16	d	2..	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0,w̄]	0,1/2,z̄+3/4 [0,0,w̄]	0,0,z̄+1/2 [0,0,w̄]
			0,1/2,z̄+1/4 [0,0,w̄]	0,0,z̄ [0,0,w̄]	0,0,z+1/2 [0,0,w̄]	0,1/2,z+3/4 [0,0,w̄]
16	c	1̄'	0,1/4,1/8 [0,0,0]	0,3/4,1/8 [0,0,0]	3/4,1/2,3/8 [0,0,0]	1/4,1/2,3/8 [0,0,0]
			0,3/4,5/8 [0,0,0]	0,1/4,5/8 [0,0,0]	1/4,0,3/8 [0,0,0]	3/4,0,3/8 [0,0,0]
8	b	2.22	0,0,1/4 [0,0,0]	0,1/2,1/2 [0,0,0]	0,1/2,0 [0,0,0]	0,0,3/4 [0,0,0]

Continued

142.8.1229

$I4_1'/a'cd'$

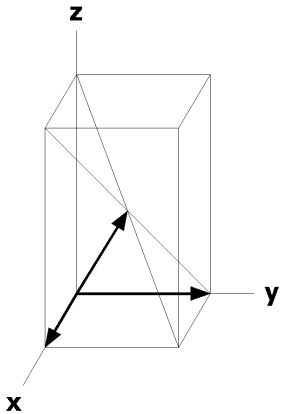
4    a     $\bar{4}..$     0,0,0 [0,0,w]    0,1/2,1/4 [0,0, $\bar{w}$ ]    0,1/2,3/4 [0,0,w]    0,0,1/2 [0,0, $\bar{w}$ ]

### Symmetry of Special Projections

Along [0,0,1]     $p4'mm'$   
 $\mathbf{a}^* = \mathbf{a}/2$      $\mathbf{b}^* = \mathbf{b}/2$   
Origin at 0,0,z

Along [1,0,0]     $p_c^*2mm$   
 $\mathbf{a}^* = \mathbf{b}/2$      $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,1/4,1/8

Along [1,1,0]     $c2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$      $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,x,0



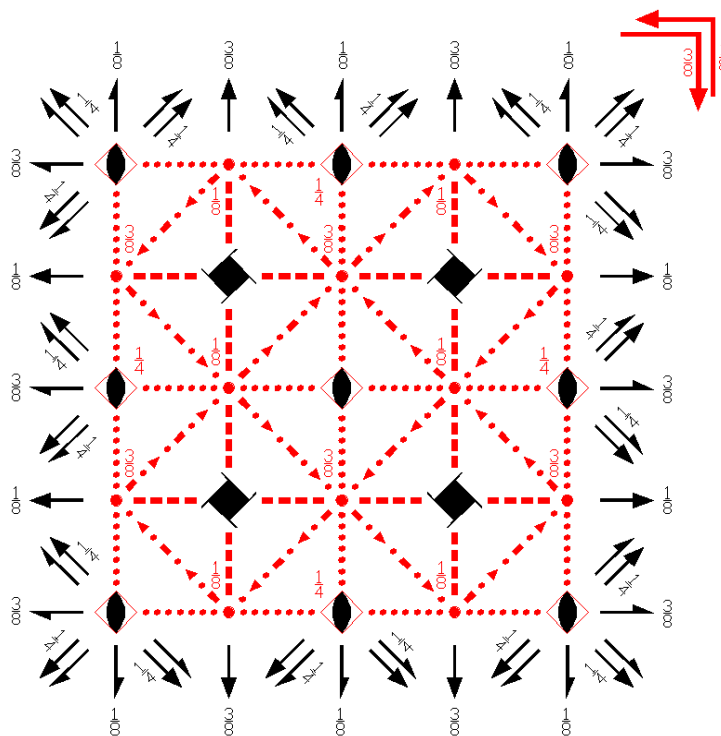
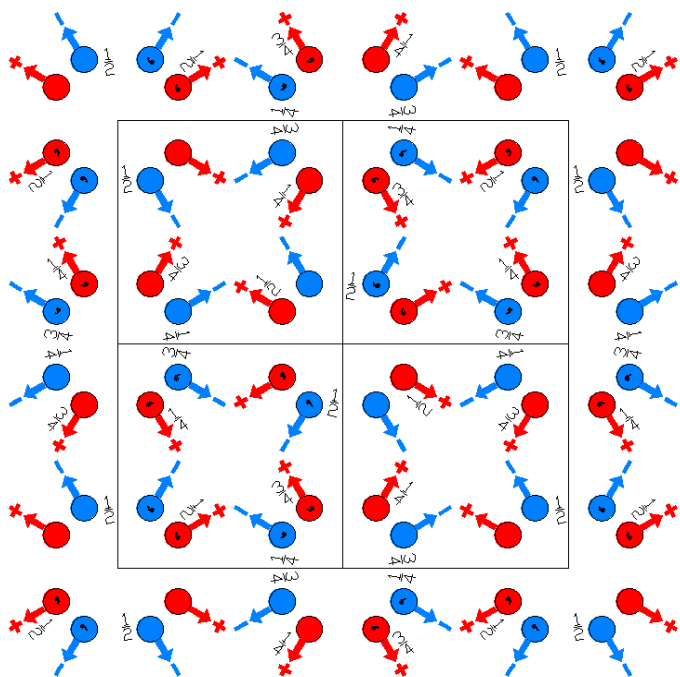
$I4_1/a'c'd'$

142.9.1230

$4/m'm'm'$

$I4_1/a'2/c'2/d'$

Tetragonal



Origin at  $\bar{4}'c'2_1$  at  $0, 1/4, -1/8$  from  $\bar{1}'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

### Symmetry Operations

For (0,0,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                    | (3) 4 <sup>+</sup> (0,0,1/4) -1/4,1/4,z<br>(4 <sub>z</sub>  0,1/2,1/4)      | (4) 4 <sup>-</sup> (0,0,1/4) 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/4) |
| (5) 2 (0,1/2,0) 0,y,3/8<br>(2 <sub>y</sub>  0,1/2,3/4) | (6) 2 x,1/4,3/8<br>(2 <sub>x</sub>  0,1/2,3/4)            | (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                                 | (8) 2 x, $\bar{x}$ ,1/4<br>(2 <sub><math>\bar{xy}</math></sub>  0,0,1/2)            |
| (9) $\bar{1}'$ 0,1/4,1/8<br>( $\bar{1}$  0,1/2,1/4)'   | (10) b' (0,1/2,0) x,y,1/8<br>(m <sub>z</sub>  0,1/2,1/4)' | (11) $\bar{4}'^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)'                    | (12) $\bar{4}'^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)'                       |
| (13) c' (0,0,1/2) x,0,z<br>(m <sub>y</sub>  0,0,1/2)'  | (14) c' (0,0,1/2) 0,y,z<br>(m <sub>x</sub>  0,0,1/2)'     | (15) d' (-1/4,1/4,3/4) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,1/2,3/4)' | (16) d' (1/4,1/4,3/4) x-1/4,x,z<br>(m <sub><math>\bar{xy}</math></sub>  0,1/2,3/4)' |



For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) $2$ (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $4^+$ (0,0,3/4) 1/4,1/4,z (4 <sub>z</sub>   1/2,0,3/4)	(4) $4^-$ (0,0,3/4) 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   1/2,0,3/4)
(5) $2$ 1/4,y,1/8 (2 <sub>y</sub>   1/2,0,1/4)	(6) $2$ (1/2,0,0) x,0,1/8 (2 <sub>x</sub>   1/2,0,1/4)	(7) $2$ (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)	(8) $2$ x, $\bar{x}$ +1/2,0 (2 <sub><math>\bar{xy}</math></sub>   1/2,1/2,0)
(9) $\bar{1}$ ' 1/4,0,3/8 ( $\bar{1}$   1/2,0,3/4)'	(10) $a'$ (1/2,0,0) x,y,3/8 (m <sub>z</sub>   1/2,0,3/4)'	(11) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'	(12) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,1/2)'
(13) $a'$ (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)'	(14) $b'$ (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)'	(15) $d'$ (1/4,-1/4,1/4) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,0,1/4)'	(16) $d'$ (1/4,1/4,1/4) x+1/4,x,z (m <sub><math>\bar{xy}</math></sub>   1/2,0,1/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

			(0,0,0) +	(1/2,1/2,1/2) +		
32	g	1	(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		
			(3) $\bar{y},x+1/2,z+1/4$ [ $\bar{v},u,w$ ]	(4) $y,\bar{x}+1/2,z+1/4$ [ $v,\bar{u},w$ ]		
			(5) $\bar{x},y+1/2,\bar{z}+3/4$ [ $\bar{u},\bar{v},\bar{w}$ ]	(6) $x,\bar{y}+1/2,\bar{z}+3/4$ [ $u,\bar{v},\bar{w}$ ]		
			(7) $y,x,\bar{z}+1/2$ [ $v,u,\bar{w}$ ]	(8) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]		
			(9) $\bar{x},\bar{y}+1/2,\bar{z}+1/4$ [ $\bar{u},\bar{v},\bar{w}$ ]	(10) $x,y+1/2,\bar{z}+1/4$ [ $u,v,\bar{w}$ ]		
			(11) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(12) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]		
			(13) $x,\bar{y},z+1/2$ [ $u,\bar{v},w$ ]	(14) $\bar{x},y,z+1/2$ [ $\bar{u},v,w$ ]		
			(15) $\bar{y},\bar{x}+1/2,z+3/4$ [ $\bar{v},\bar{u},w$ ]	(16) $y,x+1/2,z+3/4$ [ $v,u,w$ ]		
16	f	..2	x,x,1/4 [u,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},x+1/2,1/2$ [ $\bar{u},u,0$ ]	$x,\bar{x}+1/2,1/2$ [ $u,\bar{u},0$ ]
			$\bar{x},\bar{x}+1/2,0$ [ $\bar{u},\bar{u},0$ ]	$x,x+1/2,0$ [ $u,u,0$ ]	$x,\bar{x},3/4$ [ $u,\bar{u},0$ ]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]
16	e	.2.	1/4,y,1/8 [0,v,0]	3/4, $\bar{y},1/8$ [0, $\bar{v},0$ ]	$\bar{y},3/4,3/8$ [ $\bar{v},0,0$ ]	y,1/4,3/8 [v,0,0]
			3/4, $\bar{y}+1/2,1/8$ [0, $\bar{v},0$ ]	1/4,y+1/2,1/8 [0,v,0]	y,3/4,7/8 [v,0,0]	$\bar{y},1/4,7/8$ [ $\bar{v},0,0$ ]
16	d	2..	0,0,z [0,0,w]	0,1/2,z+1/4 [0,0,w]	0,1/2, $\bar{z}+3/4$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
			0,1/2, $\bar{z}+1/4$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]	0,1/2,z+3/4 [0,0,w]
16	c	$\bar{1}$ '	0,1/4,1/8 [0,0,0]	0,3/4,1/8 [0,0,0]	3/4,1/2,3/8 [0,0,0]	1/4,1/2,3/8 [0,0,0]
			0,3/4,5/8 [0,0,0]	0,1/4,5/8 [0,0,0]	1/4,0,3/8 [0,0,0]	3/4,0,3/8 [0,0,0]
8	b	2.22	0,0,1/4 [0,0,0]	0,1/2,1/2 [0,0,0]	0,1/2,0 [0,0,0]	0,0,3/4 [0,0,0]

Continued

142.9.1230

$I4_1/a'c'd'$

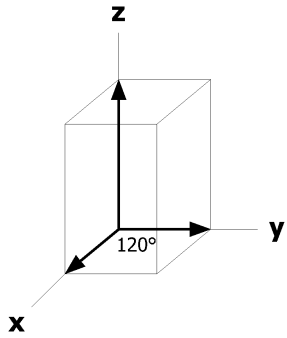
4    a     $\bar{4}'..$     0,0,0 [0,0,0]    0,1/2,1/4 [0,0,0]    0,1/2,3/4 [0,0,0]    0,0,1/2 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]     $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$      $\mathbf{b}^* = \mathbf{b}/2$   
Origin at 0,0,z

Along [1,0,0]     $p2m'm'$   
 $\mathbf{a}^* = \mathbf{b}/2$      $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,0,1/8

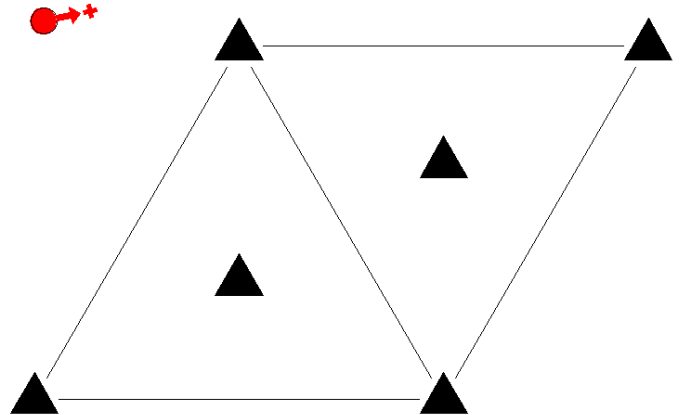
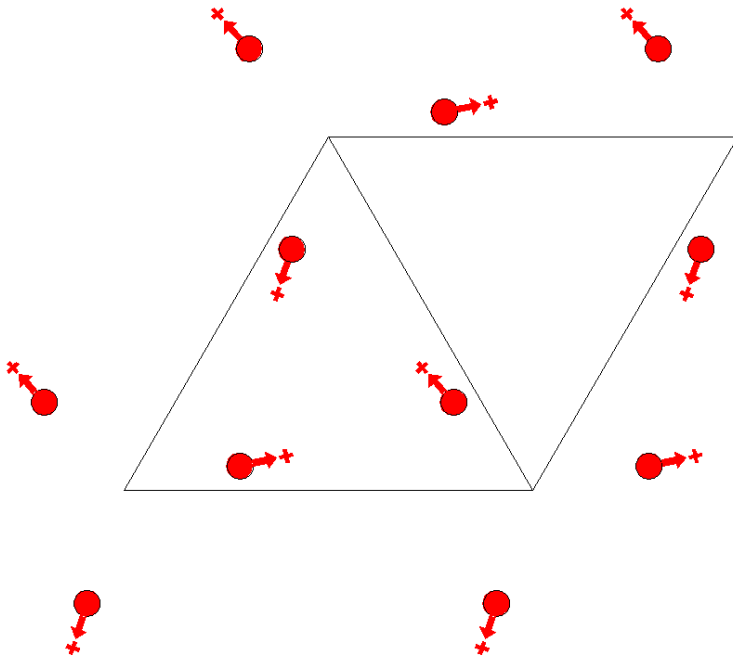
Along [1,1,0]     $c2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$      $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,x,0



P3  
143.1.1231

3  
P3

Trigonal



Origin on 3

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1	1/3,2/3,0 1/3,2/3,1	0,1/2,0 0,1/2,1

**Symmetry Operations**

- (1) 1  
(1|0,0,0)
- (2)  $3^+$  0,0,z  
( $3_z$ |0,0,0)
- (3)  $3^-$  0,0,z  
( $3_z^{-1}$ |0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

**Positions**

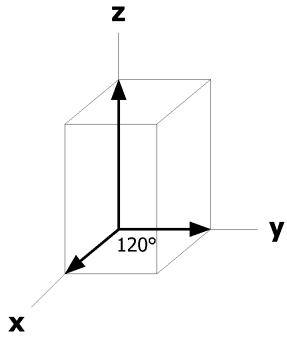
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
3	d	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
1	c	3..	2/3,1/3,z [0,0,w]		
1	b	3..	1/3,2/3,z [0,0,w]		
1	a	3..	0,0,z [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p3  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0

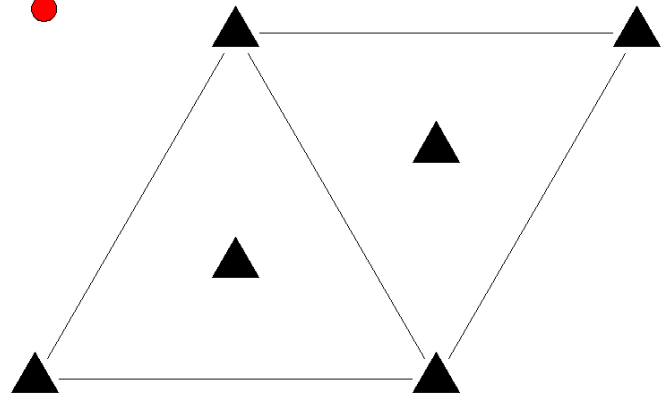
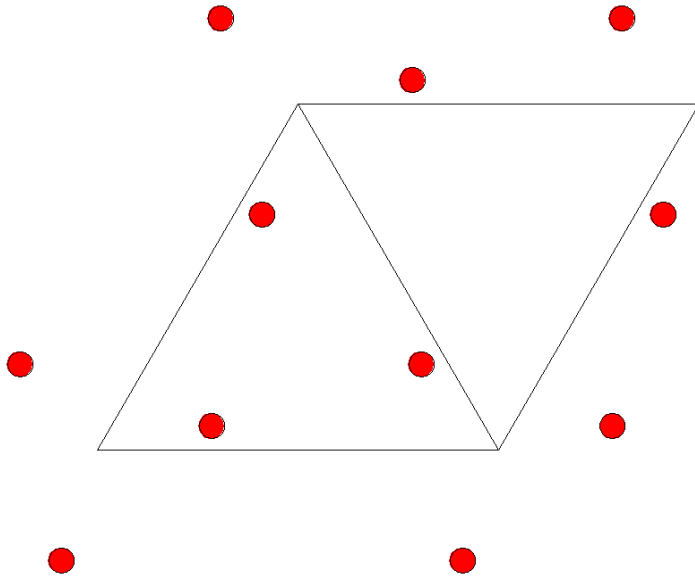


P31'  
143.2.1232

31'  
P31'

Trigonal

1'



Origin on 31'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1	1/3,2/3,0 1/3,2/3,1	0,1/2,0 0,1/2,1

**Symmetry Operations**

For 1 + set

- |                    |   |   |
|--------------------|---|---|
| (1) 1<br>(1 0,0,0) | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
|--------------------|---|---|

For 1' + set

- |                      |  |  |
|----------------------|--|--|
| (1) 1'<br>(1 0,0,0)' | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)' | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
|----------------------|--|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); 1'.

**Positions**

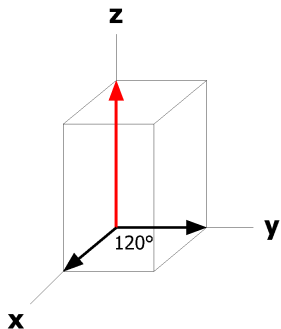
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates		
		1 +	1' +
3 d 11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x}$ ,z [0,0,0]
1 c 3..1'	2/3,1/3,z [0,0,0]		
1 b 3..1'	1/3,2/3,z [0,0,0]		
1 a 3..1'	0,0,z [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p31'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

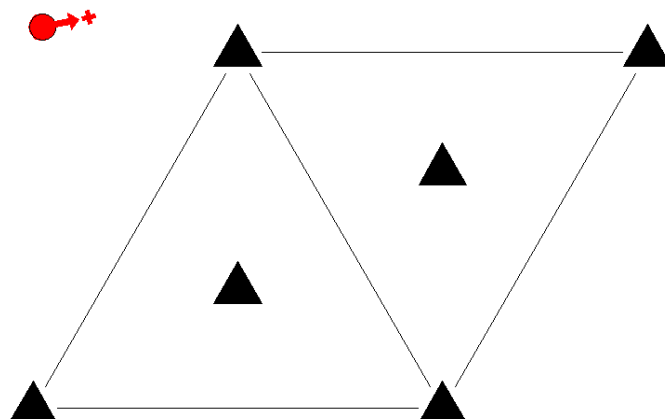
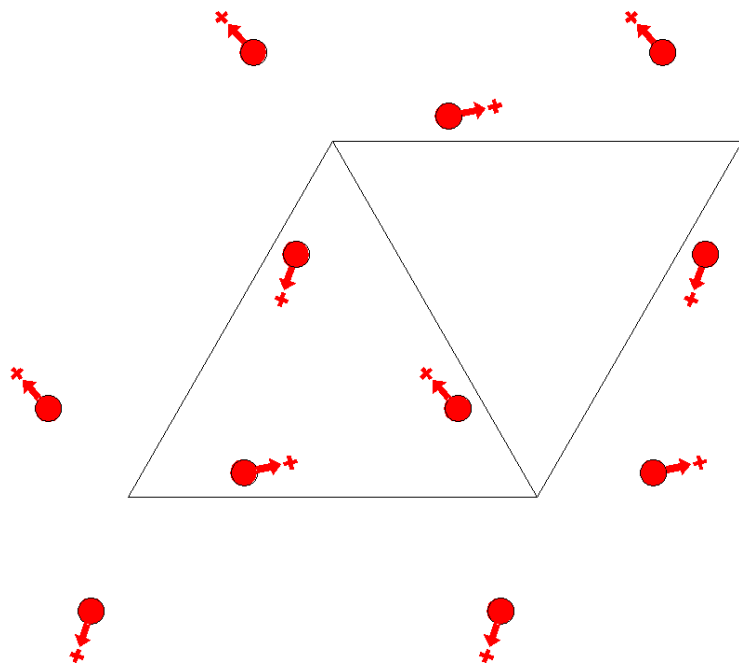
Along [2,1,0] p11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P_{2c} 3$   
143.3.1233

$31'$   
 $P_{2c} 3$

Trigonal



Origin on 3

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1	1/3,2/3,0 1/3,2/3,1	0,1/2,0 0,1/2,1

**Symmetry Operations**

For (0,0,0) +set

- |                    |                                    |   |
|--------------------|------------------------------------|---|
| (1) 1<br>(1 0,0,0) | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0) | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
|--------------------|------------------------------------|---|

For (0,0,1)' +set

- |                                |   |  |
|--------------------------------|---|--|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)' | (2) $3^{+ '}$ (0,0,1) 0,0,z<br>( $3_z$  0,0,1)' | (3) $3^{- '}$ (0,0,1) 0,0,z<br>( $3_z^{-1}$  0,0,1)' |
|--------------------------------|---|--|

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2).

**Positions**

				Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.				(0,0,0) +	(0,0,1)' +	
6	d	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]	
2	c	3..	2/3,1/3,z [0,0,w]			
2	b	3..	1/3,2/3,z [0,0,w]			
2	a	3..	0,0,z [0,0,w]			

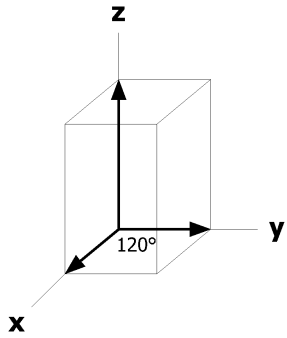
**Symmetry of Special Projections**

Along [0,0,1] p31'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>\* 1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p<sub>2a</sub>\* 1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0

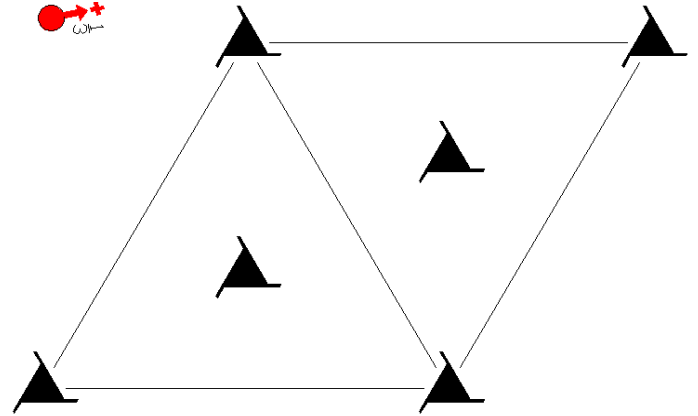
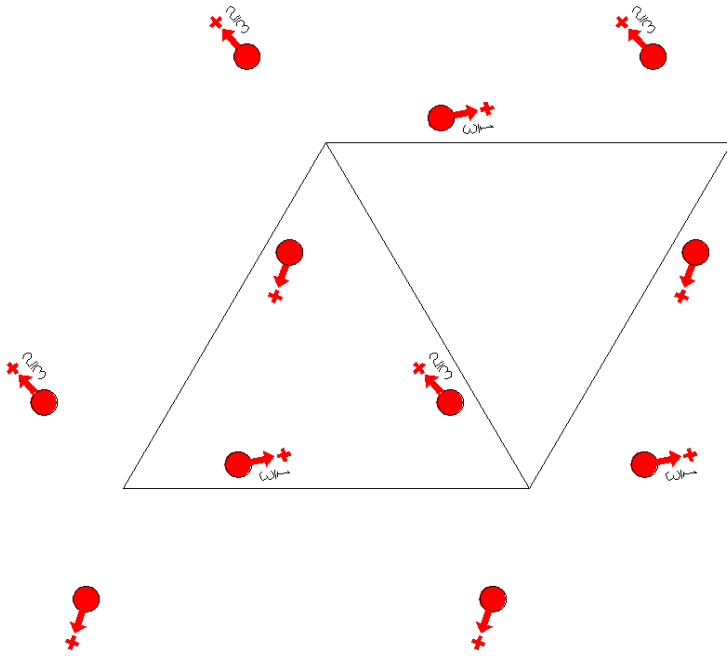




P3<sub>1</sub>  
144.1.1234

3  
P3<sub>1</sub>

Trigonal



Origin on 3<sub>1</sub>

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/3$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/3	1,0,1/3	1,1,1/3	0,1,1/3

**Symmetry Operations**

(1) 1 (1 0,0,0)	(2) 3 <sup>+</sup> (0,0,1/3) 0,0,z (3 <sub>z</sub>   0,0,1/3)	(3) 3 <sup>-</sup> (0,0,2/3) 0,0,z (3 <sub>z</sub> <sup>-1</sup>   0,0,2/3)
--------------------	--	--

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

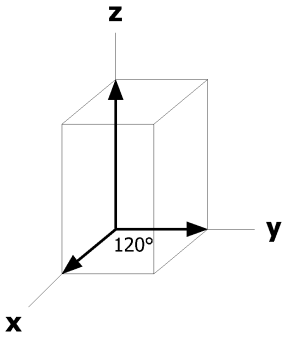
3	a	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z+1/3$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z+2/3$ [ $\bar{u}+v, \bar{u}, w$ ]
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**Symmetry of Special Projections**

Along [0,0,1] p3  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,0

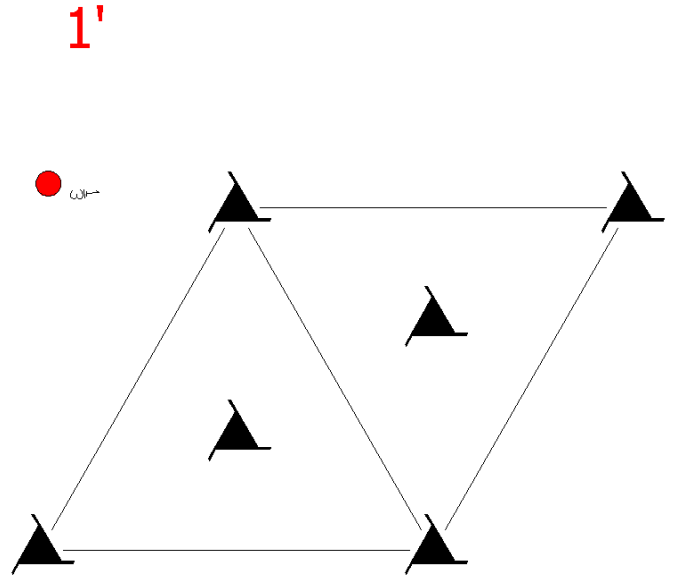
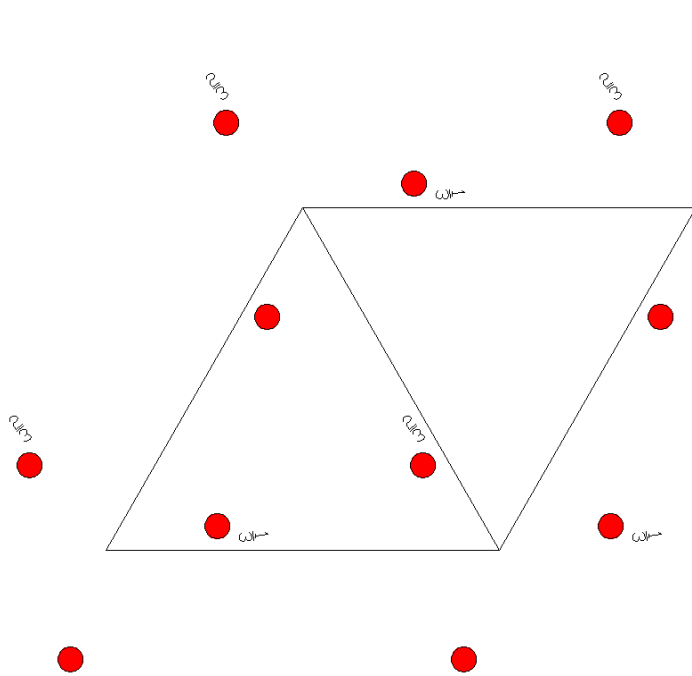
Along [2,1,0] p1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,x/2,0



$P3_11'$   
144.2.1235

$31'$   
 $P3_11'$

Trigonal



Origin on  $3_11'$

<b>Asymmetric unit</b>	$0 \leq x \leq 1;$	$0 \leq y \leq 1;$	$0 \leq z \leq 1/3$
Vertices	0,0,0	1,0,0	1,1,0
	0,0,1/3	1,0,1/3	1,1,1/3
			0,1,0
			0,1,1/3

**Symmetry Operations**

For  $1 + \text{set}$

- |                          |  |   |
|--------------------------|--|---|
| (1) $1$<br>( $1 0,0,0$ ) | (2) $3^+ (0,0,1/3)$ $0,0,z$<br>( $3_z 0,0,1/3$ ) | (3) $3^- (0,0,2/3)$ $0,0,z$<br>( $3_z^{-1} 0,0,2/3$ ) |
|--------------------------|--|---|

For  $1' + \text{set}$

- |                            |  |   |
|----------------------------|--|---|
| (1) $1'$<br>( $1 0,0,0$ )' | (2) $3^{+'} (0,0,1/3)$ $0,0,z$<br>( $3_z 0,0,1/3$ )' | (3) $3^{-'} (0,0,2/3)$ $0,0,z$<br>( $3_z^{-1} 0,0,2/3$ )' |
|----------------------------|--|---|

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2);  $1'$ .

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

1 +                      1' +

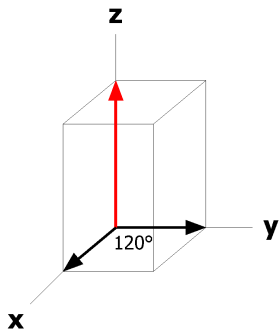
3    a    11'            (1) x,y,z [0,0,0]            (2)  $\bar{y},x-y,z+1/3$  [0,0,0]            (3)  $\bar{x}+y,\bar{x},z+2/3$  [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]    p31'  
 $\mathbf{a}^* = \mathbf{a}$     $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0]    p11'  
 $\mathbf{a}^* = \mathbf{c}$     $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,0

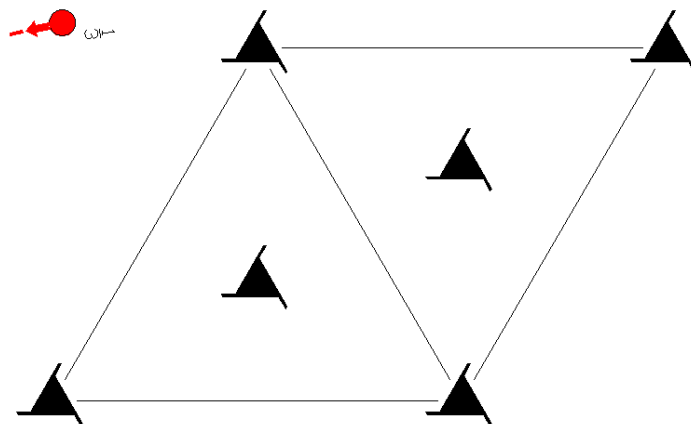
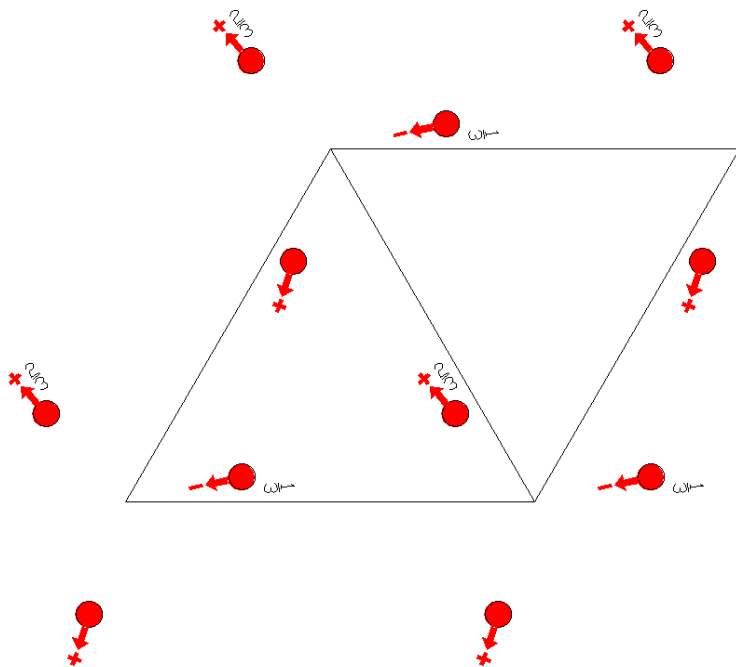
Along [2,1,0]    p11'  
 $\mathbf{a}^* = \mathbf{c}$     $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,x/2,0



$P_{2c} 3_2$   
144.3.1236

$31'$   
 $P_{2c} 3_2$

Trigonal



Origin on  $3_2$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/3$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/3	1,0,1/3	1,1,1/3	0,1,1/3

Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) $3^+ (0,0,1/3) \ 0,0,z$ $(3_z   0,0,1/3)'$	(3) $3^- (0,0,2/3) \ 0,0,z$ $(3_z^{-1}   0,0,2/3)$
--------------------	---	---

For (0,0,1)' + set

(1) $t' (0,0,1)$ (1 0,0,1)'	(2) $3^+ (0,0,4/3) \ 0,0,z$ $(3_z   0,0,4/3)$	(3) $3^- (0,0,5/3) \ 0,0,z$ $(3_z^{-1}   0,0,5/3)'$
--------------------------------	--	--

Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t'(0,0,1)$ ; (2).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

(0,0,0) +      (0,0,1)' +

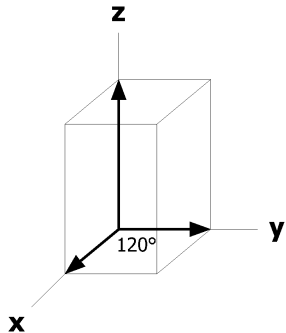
6      a      1      (1) x,y,z [u,v,w]      (2)  $\bar{y}, x-y, z+1/3$  [ $\bar{v}, \bar{u}+v, \bar{w}$ ]      (3)  $\bar{x}+y, \bar{x}, z+2/3$  [ $\bar{u}+v, \bar{u}, w$ ]

**Symmetry of Special Projections**

Along [0,0,1]      p31'  
**a\*** = **a**    **b\*** = **b**  
Origin at 0,0,z

Along [1,0,0]      p<sub>2a\*</sub> 1  
**a\*** = **c**    **b\*** = (**a** + **2b**)/2  
Origin at x,0,0

Along [2,1,0]      p<sub>2a\*</sub> 1  
**a\*** = **c**    **b\*** = **b**/2  
Origin at x,x/2,0



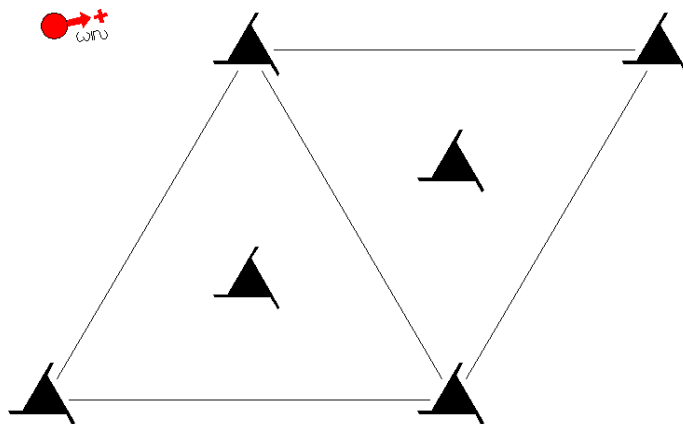
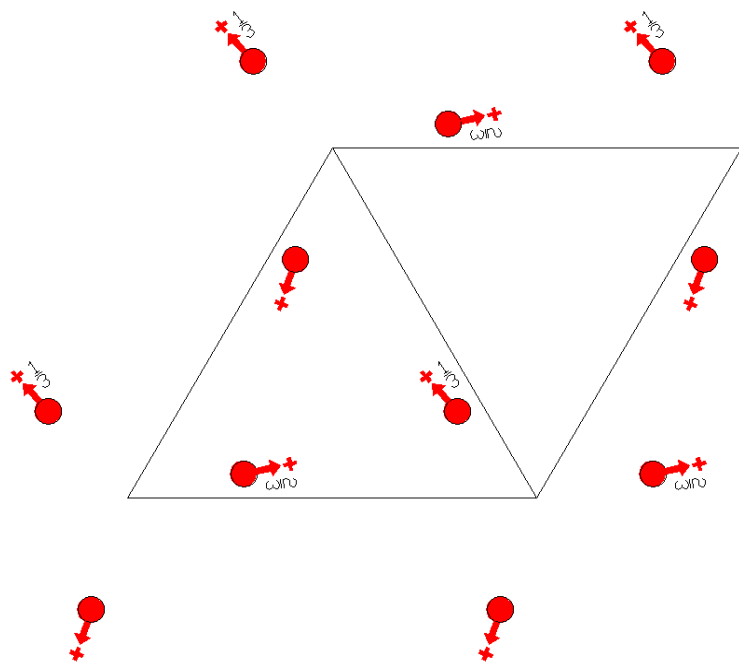
P3<sub>2</sub>

145.1.1237

3

P3<sub>2</sub>

Trigonal



Origin on 3<sub>2</sub>

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/3$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/3	1,0,1/3	1,1,1/3	0,1,1/3

Symmetry Operations

(1) 1 (1 0,0,0)	(2) 3 <sup>+</sup> (0,0,2/3) 0,0,z (3 <sub>z</sub>  0,0,2/3)	(3) 3 <sup>-</sup> (0,0,1/3) 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,1/3)
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Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

Positions

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

3	a	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z+2/3$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z+1/3$ [ $\bar{u}+v,\bar{u},w$ ]
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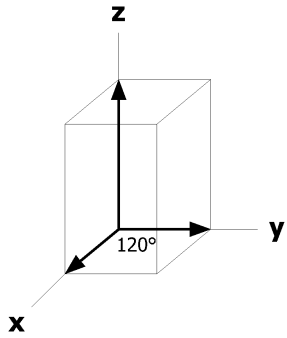
**Symmetry of Special Projections**

Along [0,0,1] p3  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,0

Along [2,1,0] p1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,x/2,0

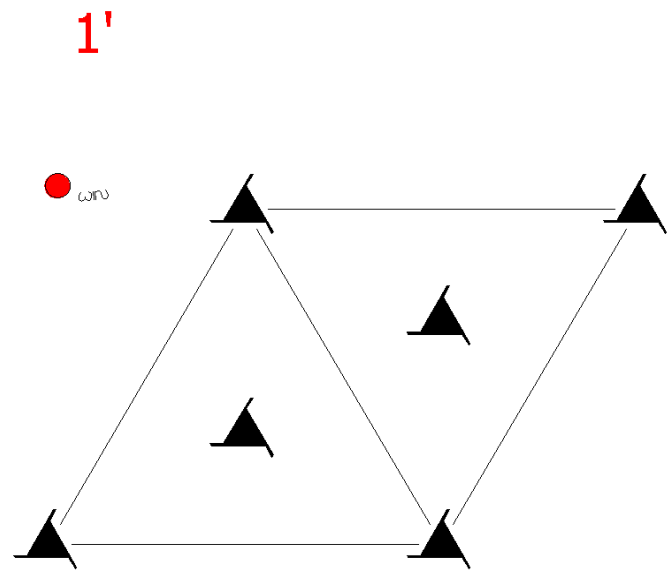
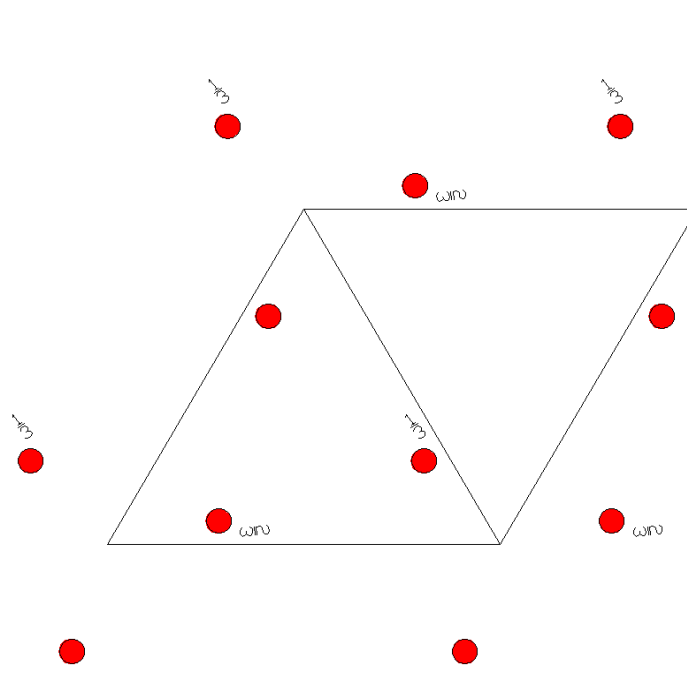




$P3_21'$   
145.2.1238

$31'$   
 $P3_21'$

Trigonal



Origin on  $3_21'$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/3$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/3	1,0,1/3	1,1,1/3	0,1,1/3

**Symmetry Operations**

For 1 + set

(1) 1 (1 0,0,0)	(2) $3^+$ (0,0,2/3) 0,0,z ( $3_z$  0,0,2/3)	(3) $3^-$ (0,0,1/3) 0,0,z ( $3_z^{-1}$  0,0,1/3)
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For 1' + set

(1) 1' (1 0,0,0)'	(2) $3^{+'}$ (0,0,2/3) 0,0,z ( $3_z$  0,0,2/3)'	(3) $3^{-'}$ (0,0,1/3) 0,0,z ( $3_z^{-1}$  0,0,1/3)'
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Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); 1'.

Continued

145.2.1238

P3<sub>2</sub>1'

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

1 +                      1' +

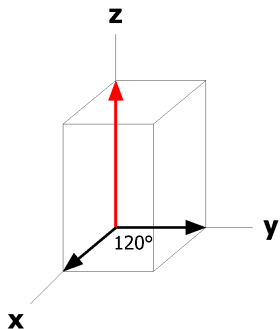
3    a    11'    (1) x,y,z [0,0,0]    (2)  $\bar{y}$ ,x-y,z+2/3 [0,0,0]    (3)  $\bar{x}+y,\bar{x},z+1/3$  [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]    p31'  
 $\mathbf{a}^* = \mathbf{a}$      $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0]    p11'  
 $\mathbf{a}^* = \mathbf{c}$      $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,0

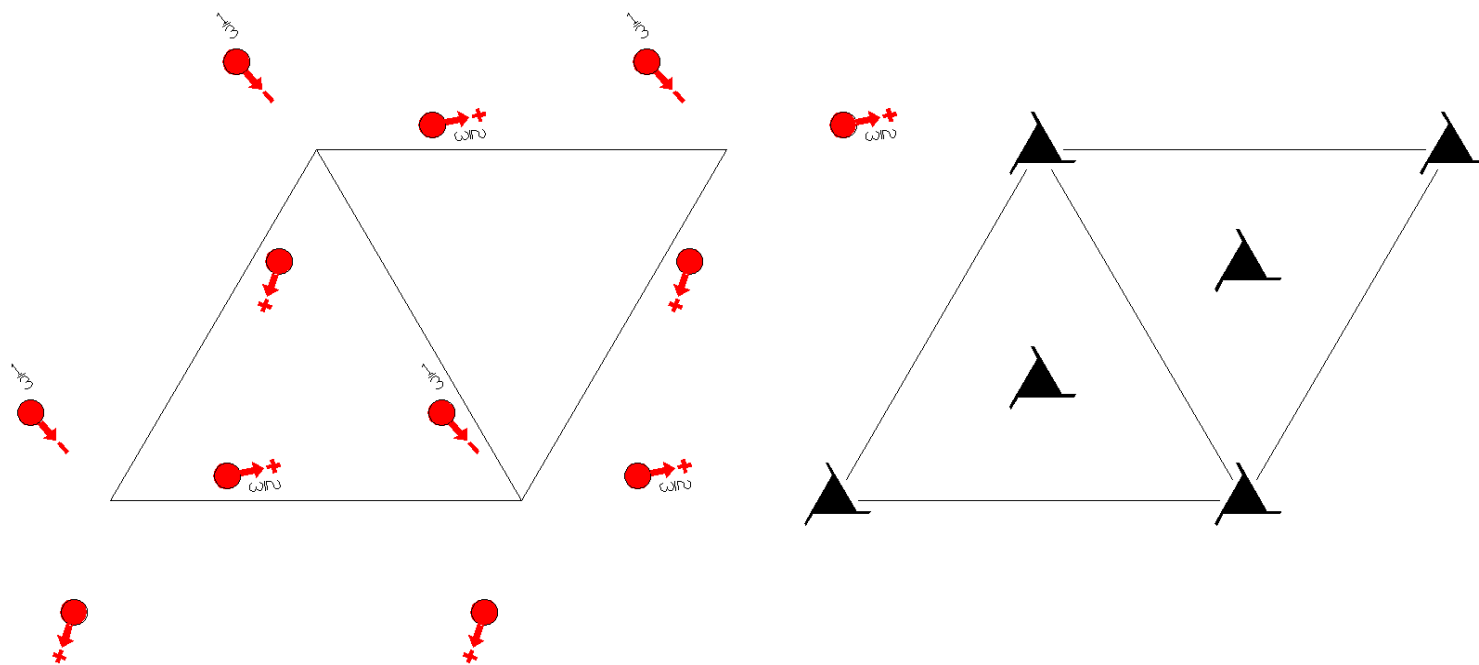
Along [2,1,0]    p11'  
 $\mathbf{a}^* = \mathbf{c}$      $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,x/2,0



$P_{2c} 3_1$   
145.3.1239

$31'$   
 $P_{2c} 3_1$

Trigonal



Origin on  $3_1$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/3$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/3	1,0,1/3	1,1,1/3	0,1,1/3

### Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) $3^+$ (0,0,2/3) 0,0,z ( $3_z$  0,0,2/3)	(3) $3^{-1}$ (0,0,1/3) 0,0,z ( $3_z^{-1}$  0,0,1/3)'
--------------------	--	---

For (0,0,1)' + set

(1) $t'$ (0,0,1) (1 0,0,1)'	(2) $3^+$ (0,0,5/3) 0,0,z ( $3_z$  0,0,5/3)'	(3) $3^-$ (0,0,4/3) 0,0,z ( $3_z^{-1}$  0,0,4/3)
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Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t'(0,0,1)$ ; (2).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

(0,0,0) +      (0,0,1)' +

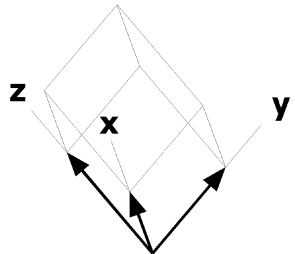
6      a      1      (1) x,y,z [u,v,w]      (2)  $\bar{y},x-y,z+2/3$  [ $\bar{v},u-v,w$ ]      (3)  $\bar{x}+y,\bar{x},z+1/3$  [u-v,u, $\bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1]      p31'  
 $\mathbf{a}^* = \mathbf{a}$     $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0]      p<sub>2a\*</sub> 1  
 $\mathbf{a}^* = \mathbf{c}$     $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,0

Along [2,1,0]      p<sub>2a\*</sub> 1  
 $\mathbf{a}^* = \mathbf{c}$     $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,x/2,0



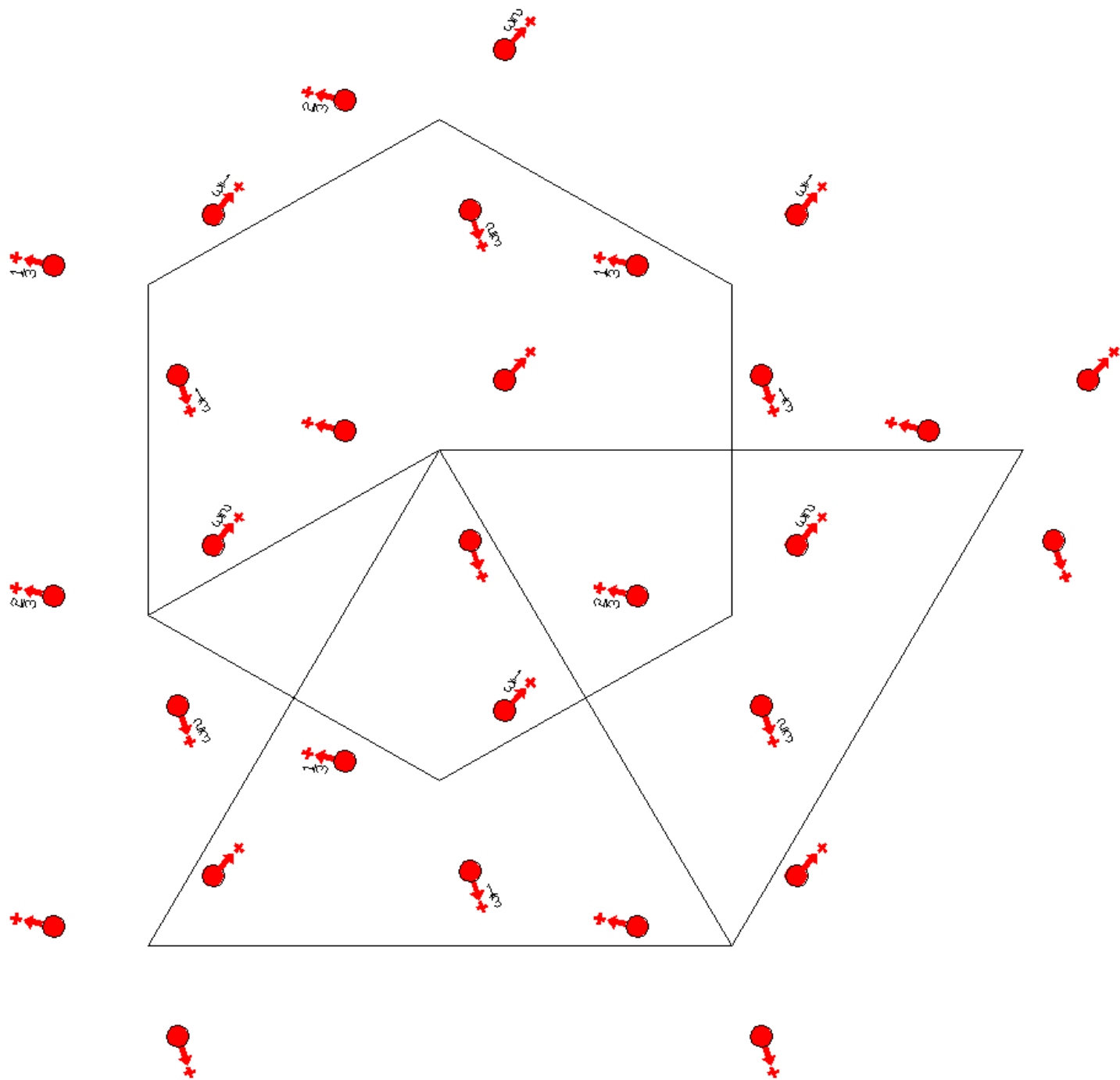
R3

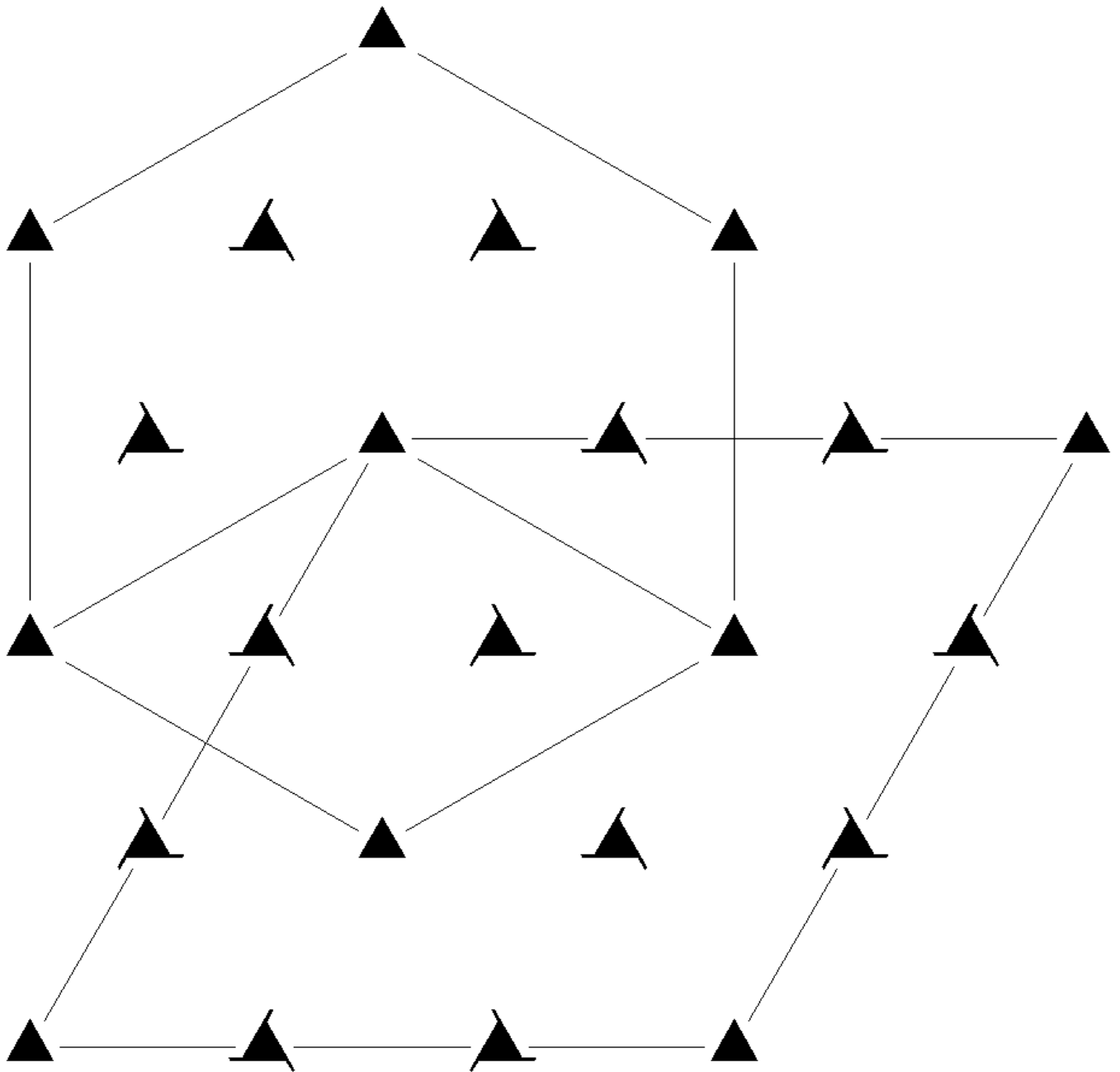
3

Trigonal

146.1.1240

R3





Origin on 3

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/3;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/3	1/2,0,0 1/2,0,1/3	2/3,1/3,0 2/3,1/3,1/3	1/3,2/3,0 1/3,2/3,1/3	0,1/2,0 0,1/2,1/3

## Symmetry Operations

For (0,0,0) + set

$$\begin{array}{lll}
 (1) 1 & (2) 3^+ \quad 0,0,z & (3) 3^- \quad 0,0,z \\
 (1 | 0,0,0) & (3_z | 0,0,0) & (3_z^{-1} | 0,0,0)
 \end{array}$$

For (2/3,1/3,1/3) + set

$$\begin{array}{lll}
 (1) t \quad (2/3,1/3,1/3) & (2) 3^+ \quad (0,0,1/3) \quad 1/3,1/3,z & (3) 3^- \quad (0,0,1/3) \quad 1/3,0,z \\
 (1 | 2/3,1/3,1/3) & (3_z | 2/3,1/3,1/3) & (3_z^{-1} | 2/3,1/3,1/3)
 \end{array}$$

For (1/3,2/3,2/3) + set

$$\begin{array}{lll}
 (1) t \quad (1/3,2/3,2/3) & (2) 3^+ \quad (0,0,2/3) \quad 0,1/3,z & (3) 3^- \quad (0,0,2/3) \quad 1/3,1/3,z \\
 (1 | 1/3,2/3,2/3) & (3_z | 1/3,2/3,2/3) & (3_z^{-1} | 1/3,2/3,2/3)
 \end{array}$$

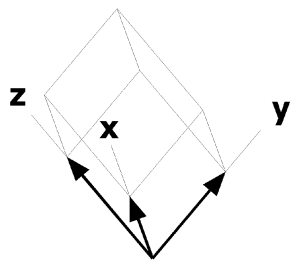
**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2).

## Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates		
	(0,0,0) +	(2/3,1/3,1/3) +	(1/3,2/3,2/3) +
9    b    1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
3    a    3..	0,0,z [0,0,w]		

## Symmetry of Special Projections

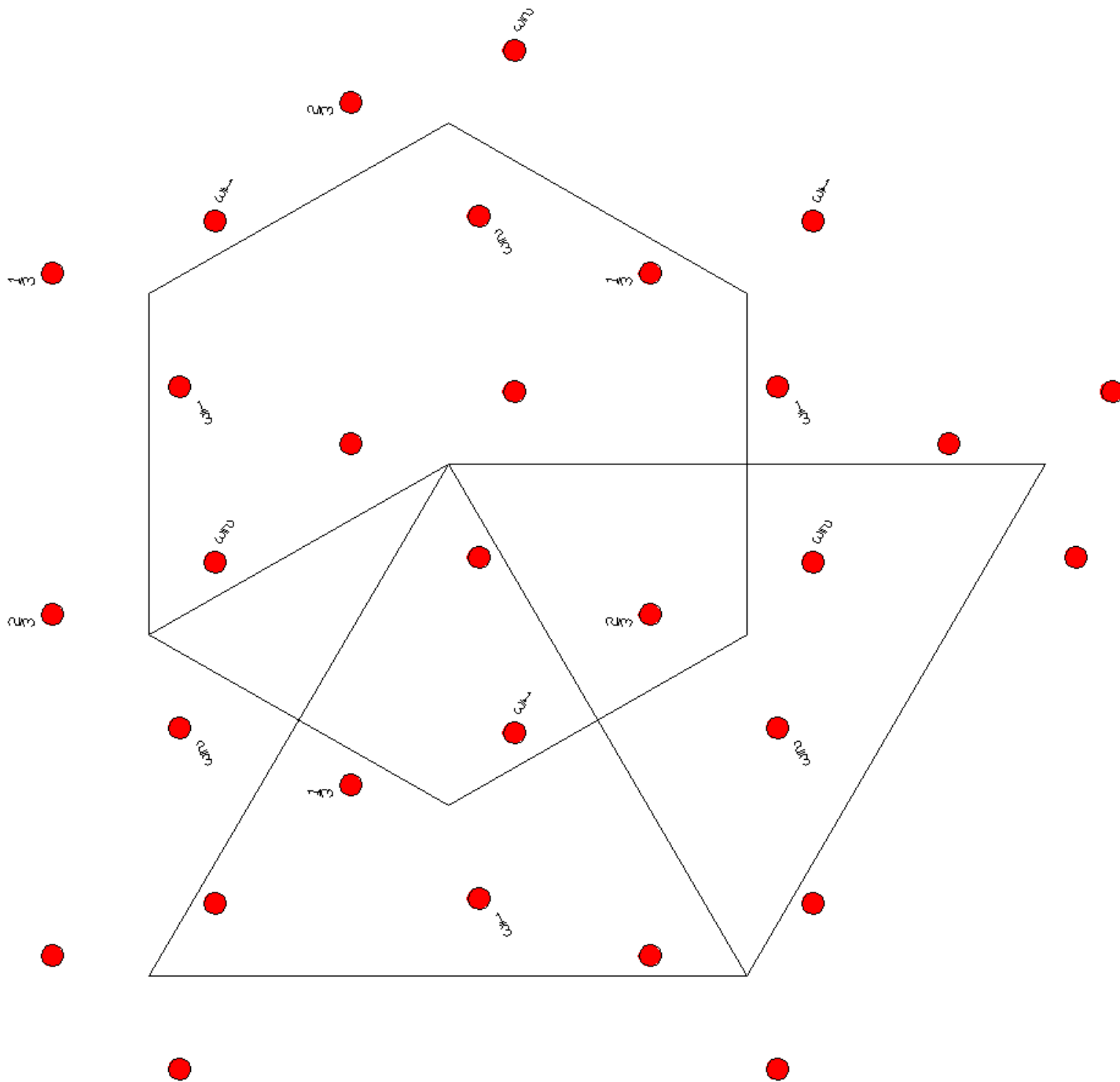
Along [0,0,1]    p3 $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$ Origin at 0,0,z	Along [1,0,0]    p1 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3 \quad \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$ Origin at x,0,0	Along [2,1,0]    p1 $\mathbf{a}^* = \mathbf{c}/3 \quad \mathbf{b}^* = \mathbf{b}/2$ Origin at x,x/2,0
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R31'  
146.2.1241

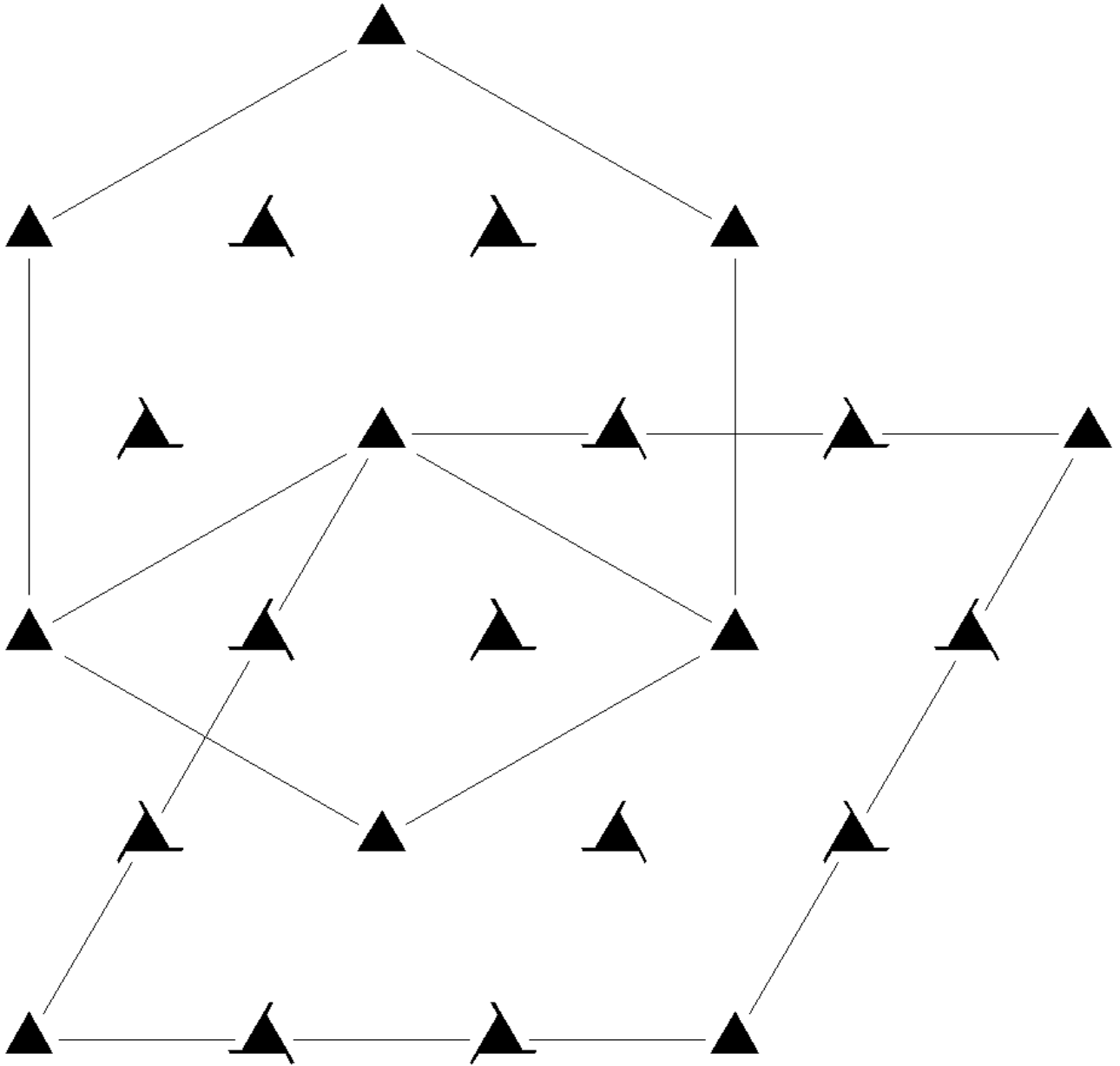
31'  
R31'

Trigonal





1'



Origin on 31'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/3;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/3	1/2,0,0 1/2,0,1/3	2/3,1/3,0 2/3,1/3,1/3	1/3,2/3,0 1/3,2/3,1/3	0,1/2,0 0,1/2,1/3

**Symmetry Operations**

For (0,0,0) + set

$$(1) 1 \quad (2) 3^+ \quad 0,0,z \quad (3) 3^- \quad 0,0,z$$

$$(1 | 0,0,0) \quad (3_z | 0,0,0) \quad (3_z^{-1} | 0,0,0)$$

For (2/3,1/3,1/3) + set

$$(1) t \quad (2/3, 1/3, 1/3) \quad (2) 3^+ \quad (0,0, 1/3) \quad 1/3, 1/3, z \quad (3) 3^- \quad (0,0, 1/3) \quad 1/3, 0, z$$

$$(1 | 2/3, 1/3, 1/3) \quad (3_z | 2/3, 1/3, 1/3) \quad (3_z^{-1} | 2/3, 1/3, 1/3)$$

For (1/3,2/3,2/3) + set

$$(1) t \quad (1/3, 2/3, 2/3) \quad (2) 3^+ \quad (0,0, 2/3) \quad 0, 1/3, z \quad (3) 3^- \quad (0,0, 2/3) \quad 1/3, 1/3, z$$

$$(1 | 1/3, 2/3, 2/3) \quad (3_z | 1/3, 2/3, 2/3) \quad (3_z^{-1} | 1/3, 2/3, 2/3)$$

For (0,0,0)' + set

$$(1) 1' \quad (2) 3^{+'} \quad 0,0,z \quad (3) 3^{-'} \quad 0,0,z$$

$$(1 | 0,0,0)' \quad (3_z | 0,0,0)'\quad (3_z^{-1} | 0,0,0)'$$

For (2/3,1/3,1/3)' + set

$$(1) t' \quad (2/3, 1/3, 1/3) \quad (2) 3^{+'} \quad (0,0, 1/3) \quad 1/3, 1/3, z \quad (3) 3^{-'} \quad (0,0, 1/3) \quad 1/3, 0, z$$

$$(1 | 2/3, 1/3, 1/3)'\quad (3_z | 2/3, 1/3, 1/3)'\quad (3_z^{-1} | 2/3, 1/3, 1/3)'$$

For (1/3,2/3,2/3)' + set

$$(1) t' \quad (1/3, 2/3, 2/3) \quad (2) 3^{+'} \quad (0,0, 2/3) \quad 0, 1/3, z \quad (3) 3^{-'} \quad (0,0, 2/3) \quad 1/3, 1/3, z$$

$$(1 | 1/3, 2/3, 2/3)'\quad (3_z | 1/3, 2/3, 2/3)'\quad (3_z^{-1} | 1/3, 2/3, 2/3)'$$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2);1'.**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

$$(0,0,0) + \quad (2/3, 1/3, 1/3) + \quad (1/3, 2/3, 2/3) +$$

$$(0,0,0)' + \quad (2/3, 1/3, 1/3)'\quad (1/3, 2/3, 2/3)'\quad +$$

$$9 \quad b \quad 11' \quad (1) \quad x,y,z \quad [0,0,0] \quad (2) \quad \bar{y}, x-y, z \quad [0,0,0] \quad (3) \quad \bar{x}+y, \bar{x}, z \quad [0,0,0]$$

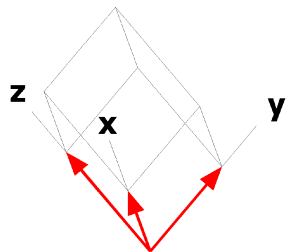
$$3 \quad a \quad 3..1' \quad 0,0,z \quad [0,0,0]$$

**Symmetry of Special Projections**

Along [0,0,1] p31'  
 $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p11'  
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3 \quad \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

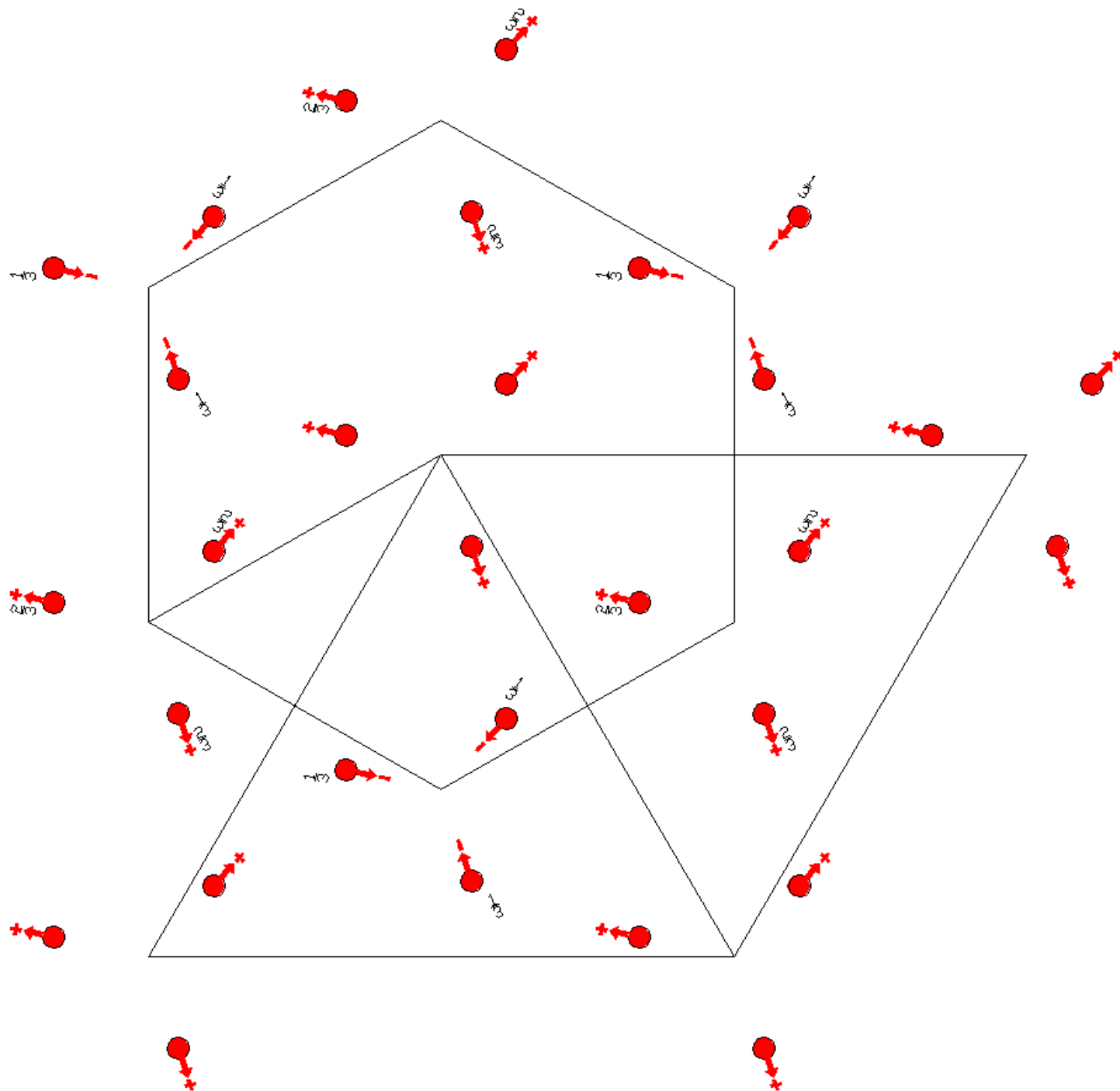
Along [2,1,0] p11'  
 $\mathbf{a}^* = \mathbf{c}/3 \quad \mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0

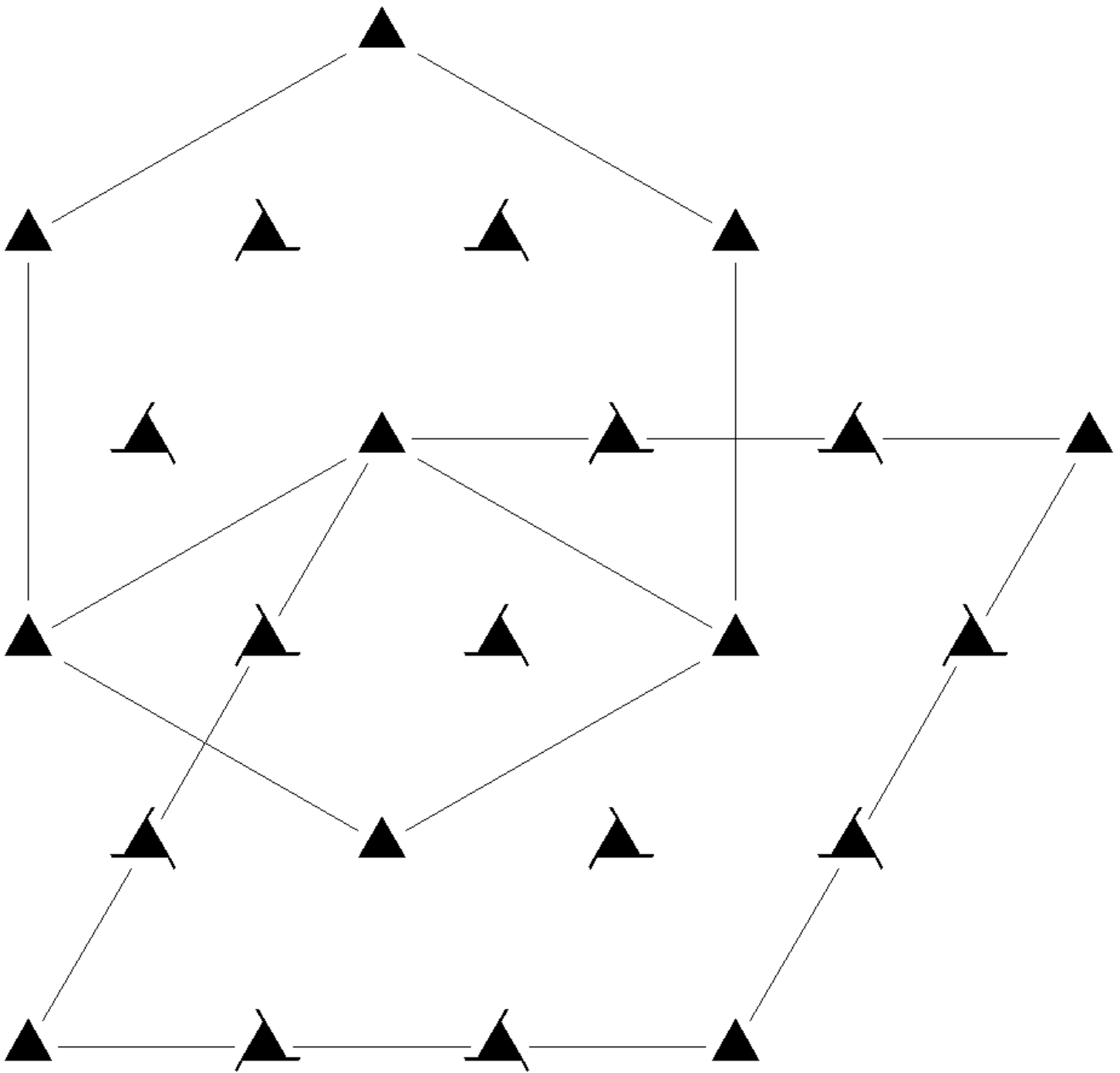


$R_R 3$   
146.3.1242

31'  
 $R_R 3$

Trigonal





Origin on 3

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/3;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/3	1/2,0,0 1/2,0,1/3	2/3,1/3,0 2/3,1/3,1/3	1/3,2/3,0 1/3,2/3,1/3	0,1/2,0 0,1/2,1/3

**Symmetry Operations**

For (0,0,0) + set

$$\begin{array}{lll}
 (1) 1 & (2) 3^+ \begin{array}{l} 0,0,z \\ (3_z | 0,0,0) \end{array} & (3) 3^- \begin{array}{l} 0,0,z \\ (3_z^{-1} | 0,0,0) \end{array} \\
 (1 | 0,0,0) & & 
 \end{array}$$

For (2/3,1/3,1/3)' + set

$$\begin{array}{lll}
 (1) t' \begin{array}{l} (2/3,1/3,1/3) \\ (1 | 2/3,1/3,1/3)' \end{array} & (2) 3^+ \begin{array}{l} (0,0,1/3) \quad 1/3,1/3,z \\ (3_z | 2/3,1/3,1/3)' \end{array} & (3) 3^- \begin{array}{l} (0,0,1/3) \quad 1/3,0,z \\ (3_z^{-1} | 2/3,1/3,1/3)' \end{array}
 \end{array}$$

For (1/3,2/3,2/3) + set

$$\begin{array}{lll}
 (1) t \begin{array}{l} (1/3,2/3,2/3) \\ (1 | 1/3,2/3,2/3) \end{array} & (2) 3^+ \begin{array}{l} (0,0,2/3) \quad 0,1/3,z \\ (3_z | 1/3,2/3,2/3) \end{array} & (3) 3^- \begin{array}{l} (0,0,2/3) \quad 1/3,1/3,z \\ (3_z^{-1} | 1/3,2/3,2/3) \end{array}
 \end{array}$$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(2/3,1/3,1/3);(2).**Positions**

Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

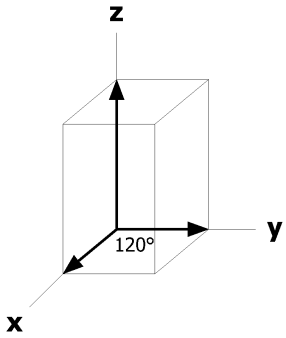
			(0,0,0) +	(2/3,1/3,1/3)' +	(1/3,2/3,2/3) +
9	b	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
3	a	3..	0,0,z [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1]  $p31'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a} 1$   
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

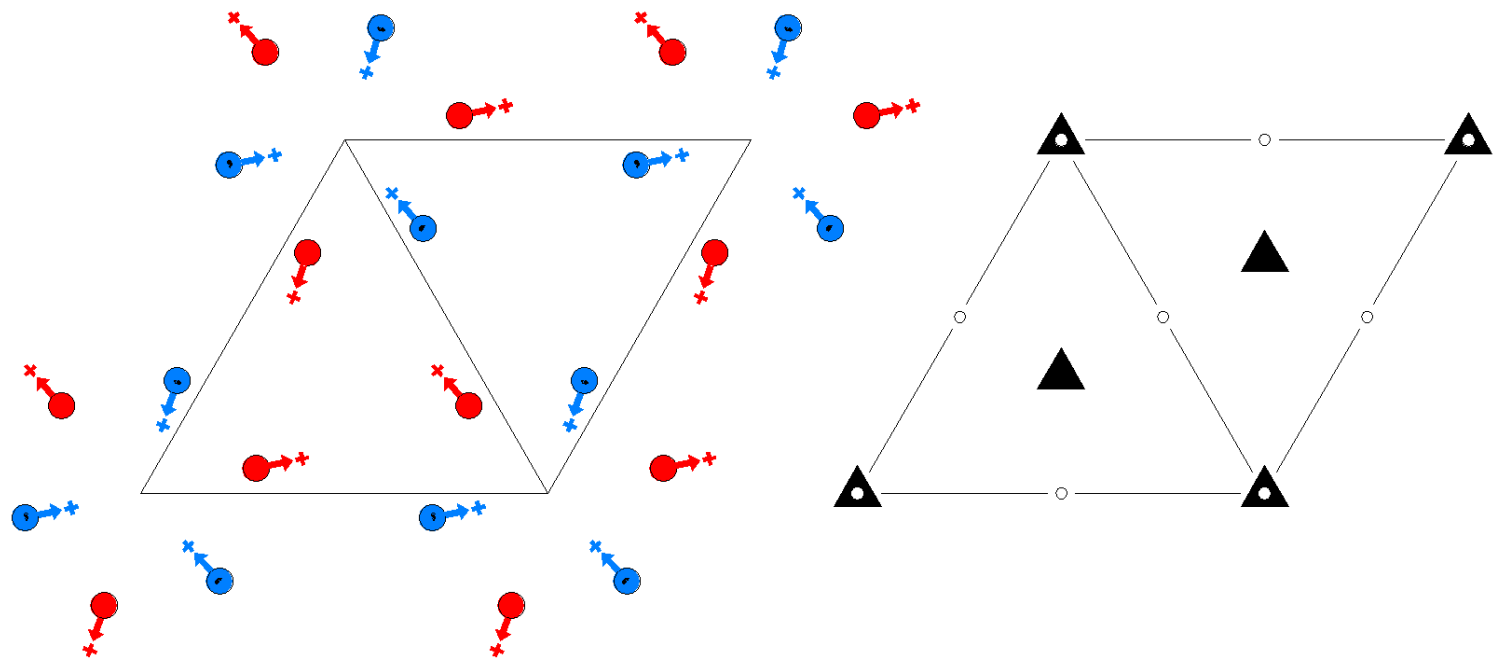
Along [2,1,0]  $p_{2a} 1$   
 $\mathbf{a}^* = \mathbf{c}/3$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P\bar{3}$   
147.1.1243

$\bar{3}$   
 $P\bar{3}$

Trigonal



Origin on  $\bar{3}$

**Asymmetric unit**     $0 \leq x \leq 2/3;$      $0 \leq y \leq 2/3;$      $0 \leq z \leq 1/2;$      $x \leq (1+y)/2;$      $y \leq \min(1-x, (1+x)/2)$

Vertices     $0,0,0$      $1/2,0,0$      $2/3,1/3,0$      $1/3,2/3,0$      $0,1/2,0$   
                   $0,0,1/2$      $1/2,0,1/2$      $2/3,1/3,1/2$      $1/3,2/3,1/2$      $0,1/2,1/2$

**Symmetry Operations**

- (1) 1  
(1|0,0,0)
- (2)  $3^+$  0,0,z  
( $3_z$ |0,0,0)
- (3)  $3^-$  0,0,z  
( $3_z^{-1}$ |0,0,0)
- (4)  $\bar{1}$   
( $\bar{1}$ |0,0,0)
- (5)  $\bar{3}^+$  0,0,z; 0,0,0  
( $\bar{3}_z$ |0,0,0)
- (6)  $\bar{3}^-$  0,0,z; 0,0,0  
( $\bar{3}_z^{-1}$ |0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

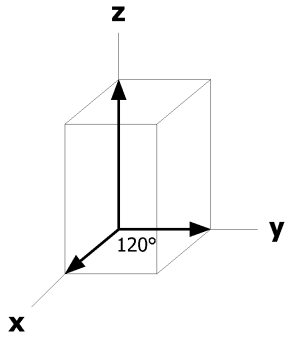
			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
6	g	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(5) y, $\bar{x}+y,\bar{z}$ [ $\bar{v}$ ,u-v,w]	(6) x-y,x, $\bar{z}$ [ $\bar{u}+v,\bar{u},w$ ]
3	f	$\bar{1}$	1/2,0,1/2 [u,v,w]	0,1/2,1/2 [ $\bar{v}$ ,u-v,w]	1/2,1/2,1/2 [ $\bar{u}+v,\bar{u},w$ ]
3	e	$\bar{1}$	1/2,0,0 [u,v,w]	0,1/2,0 [ $\bar{v}$ ,u-v,w]	1/2,1/2,0 [ $\bar{u}+v,\bar{u},w$ ]
2	d	3..	1/3,2/3,z [0,0,w]	2/3,1/3, $\bar{z}$ [0,0,w]	
2	c	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	
1	b	$\bar{3}..$	0,0,1/2 [0,0,w]		
1	a	$\bar{3}..$	0,0,0 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p6'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

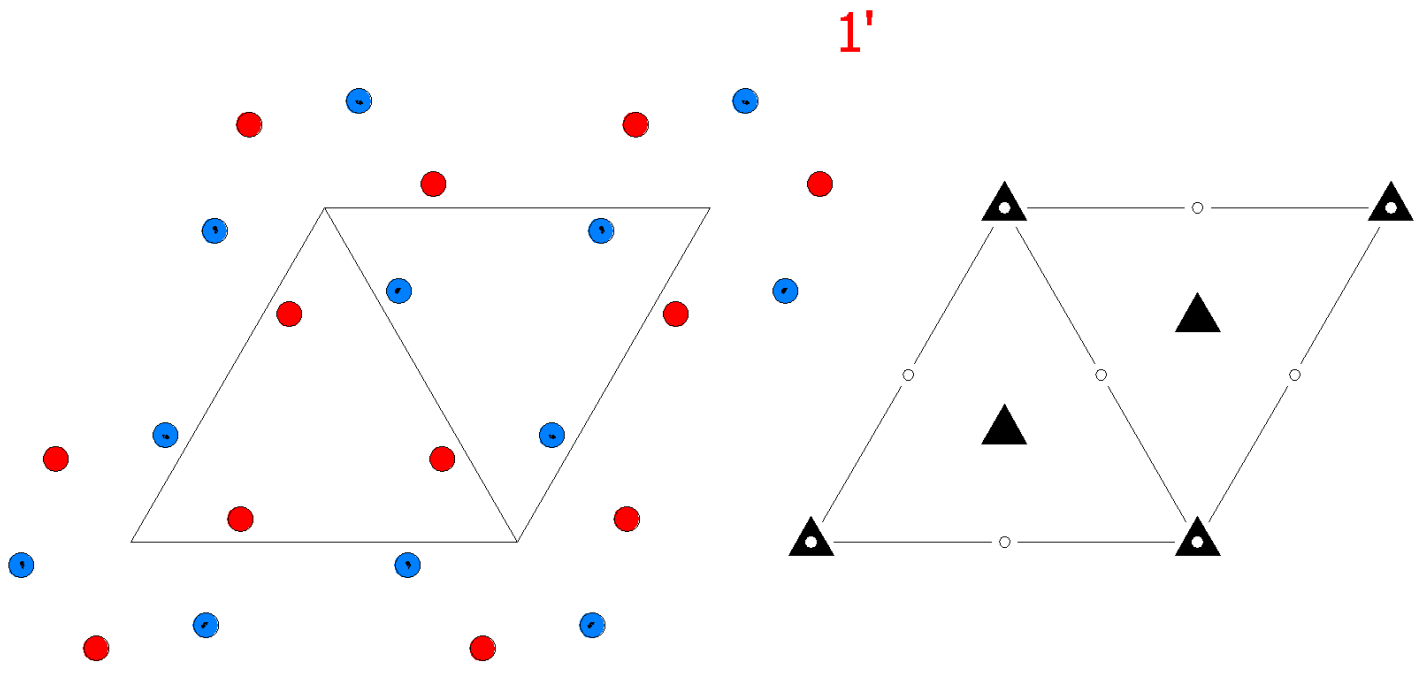
Along [2,1,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P\bar{3}1'$   
147.2.1244

$\bar{3}1'$   
 $P\bar{3}1'$

Trigonal



Origin on  $\bar{3}1'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/3,2/3,0 1/3,2/3,1/2	0,1/2,0 0,1/2,1/2

**Symmetry Operations**

For  $1$  +set

- |                                      |   |  |
|--------------------------------------|---|--|
| (1) $1$<br>(1 0,0,0)                 | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (5) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (6) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |

For  $1'$  +set

- |  |   |  |
|--|---|--|
| (1) $1'$<br>(1 0,0,0)'                 | (2) $3^{+'}$ 0,0,z<br>( $3_z$  0,0,0)'                    | (3) $3^{-'}$ 0,0,z<br>( $3_z^{-1}$  0,0,0)'                    |
| (4) $\bar{1}'$<br>( $\bar{1}$  0,0,0)' | (5) $\bar{3}^{+'}$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)' | (6) $\bar{3}^{-'}$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

**Positions**

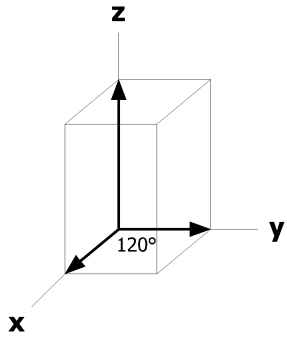
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			1 +	1' +	
6	g	11'	(1) x,y,z [0,0,0] (4) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(2) $\bar{y},x-y,z$ [0,0,0] (5) $y,\bar{x}+y,\bar{z}$ [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0] (6) $x-y,x,\bar{z}$ [0,0,0]
3	f	$\bar{1}1'$	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]
3	e	$\bar{1}1'$	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]
2	d	3..1'	1/3,2/3,z [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	
2	c	3..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	
1	b	$\bar{3}..1'$	0,0,1/2 [0,0,0]		
1	a	$\bar{3}..1'$	0,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

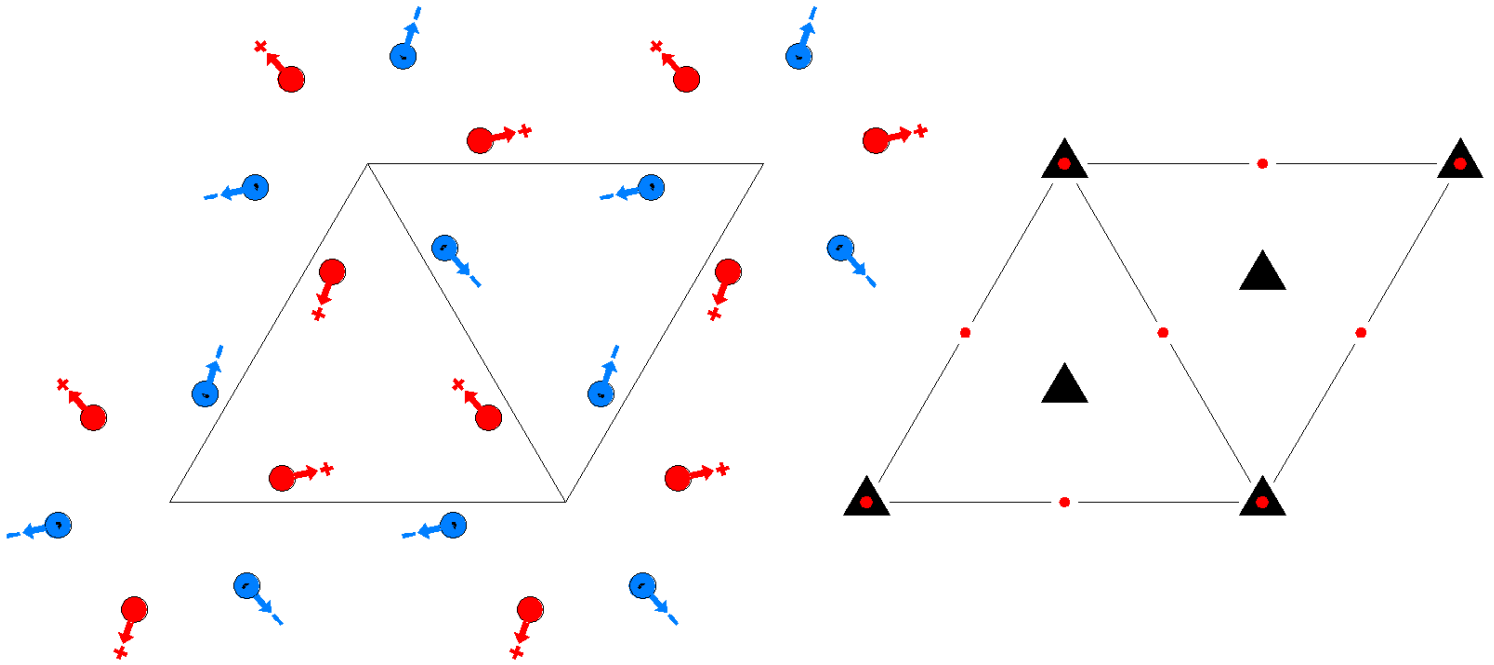
Along [2,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P\bar{3}'$   
147.3.1245

$\bar{3}'$   
 $P\bar{3}'$

Trigonal



Origin on  $\bar{3}'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/3,2/3,0 1/3,2/3,1/2	0,1/2,0 0,1/2,1/2

**Symmetry Operations**

- (1) 1  
(1|0,0,0)
- (2)  $3^+$  0,0,z  
( $3_z$ |0,0,0)
- (3)  $3^-$  0,0,z  
( $3_z^{-1}$ |0,0,0)
- (4)  $\bar{1}'$   
( $\bar{1}$ |0,0,0)'
- (5)  $\bar{3}^+$  0,0,z; 0,0,0  
( $\bar{3}_z$ |0,0,0)'
- (6)  $\bar{3}^-$  0,0,z; 0,0,0  
( $\bar{3}_z^{-1}$ |0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

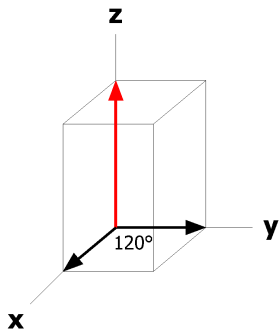
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	g	1	(1) x,y,z [u,v,w] (4) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $y,\bar{x}+y,\bar{z}$ [ $v,\bar{u}+v,\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $x-y,x,\bar{z}$ [ $u-v,u,\bar{w}$ ]
3	f	$\bar{1}'$	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]
3	e	$\bar{1}'$	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]
2	d	3..	1/3,2/3,z [0,0,w]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	
2	c	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	
1	b	$\bar{3}'..$	0,0,1/2 [0,0,0]		
1	a	$\bar{3}'..$	0,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p6  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

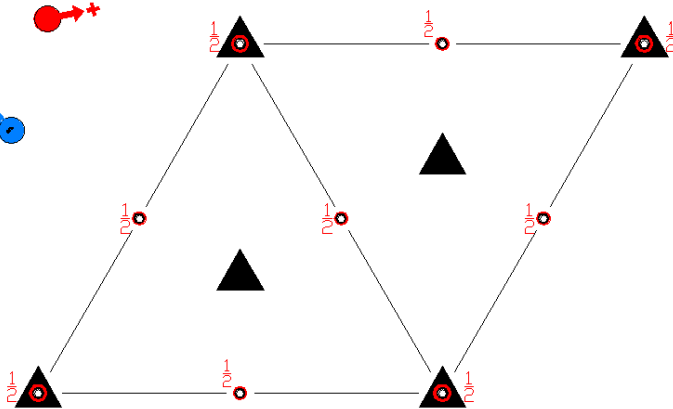
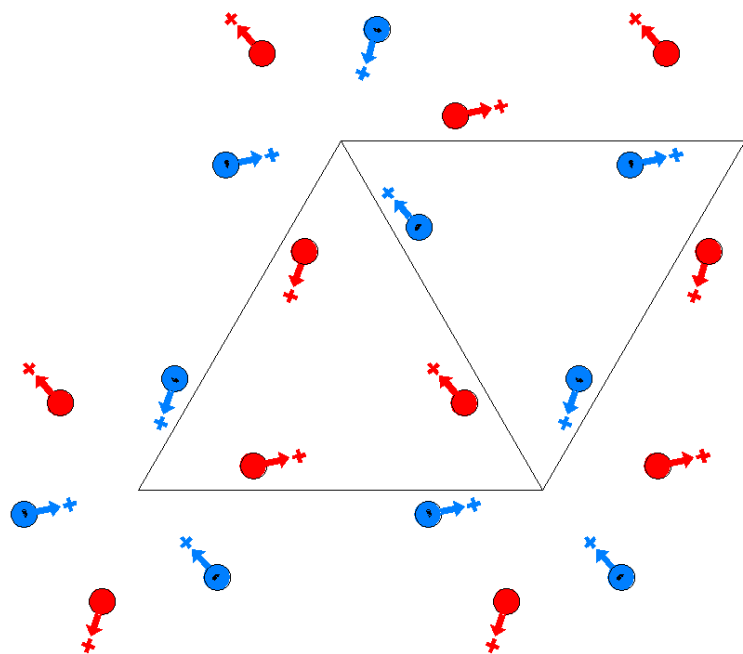
Along [2,1,0] p211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P_{2c} \bar{3}$   
147.4.1246

$\bar{3}1'$   
 $P_{2c} \bar{3}$

Trigonal



Origin on  $\bar{3}$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/3,2/3,0 1/3,2/3,1/2	0,1/2,0 0,1/2,1/2

**Symmetry Operations**

For (0,0,0) + set

- |                                      |   |  |
|--------------------------------------|---|--|
| (1) 1<br>(1 0,0,0)                   | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (5) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (6) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |

For (0,0,1)' + set

- |  |  |   |
|--|--|---|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'                 | (2) $3^+$ '(0,0,1) 0,0,z<br>( $3_z$  0,0,1)'               | (3) $3^-$ '(0,0,1) 0,0,z<br>( $3_z^{-1}$  0,0,1)'               |
| (4) $\bar{1}'$ 0,0,1/2<br>( $\bar{1}$  0,0,1)' | (5) $\bar{3}^+$ ' 0,0,z; 0,0,1/2<br>( $\bar{3}_z$  0,0,1)' | (6) $\bar{3}^-$ ' 0,0,z; 0,0,1/2<br>( $\bar{3}_z^{-1}$  0,0,1)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

**Positions**

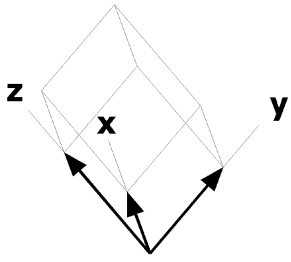
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			(0,0,0) +	(0,0,1)' +	
12	g	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(5) y, $\bar{x}+y,\bar{z}$ [ $\bar{v}$ ,u-v,w]	(6) x-y,x, $\bar{z}$ [ $\bar{u}+v,\bar{u},w$ ]
6	f	$\bar{1}'$	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]
6	e	$\bar{1}$	1/2,0,0 [u,v,w]	0,1/2,0 [ $\bar{v}$ ,u-v,w]	1/2,1/2,0 [ $\bar{u}+v,\bar{u},w$ ]
4	d	3..	1/3,2/3,z [0,0,w]	2/3,1/3, $\bar{z}$ [0,0,w]	
4	c	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	
2	b	$\bar{3}'..$	0,0,1/2 [0,0,0]		
2	a	$\bar{3}..$	0,0,0 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>\* 211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/2

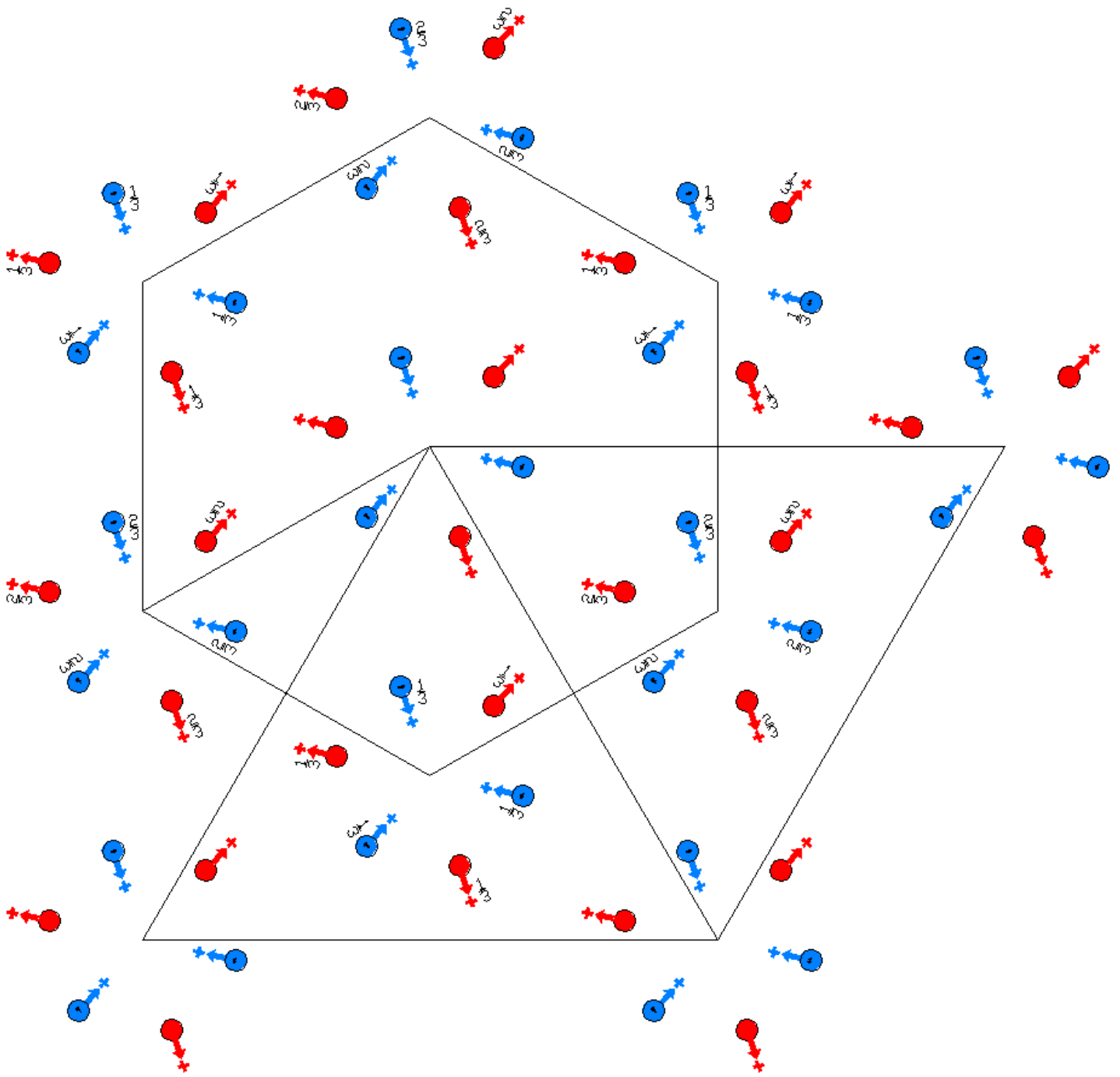
Along [2,1,0] p<sub>2a</sub>\* 211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/2

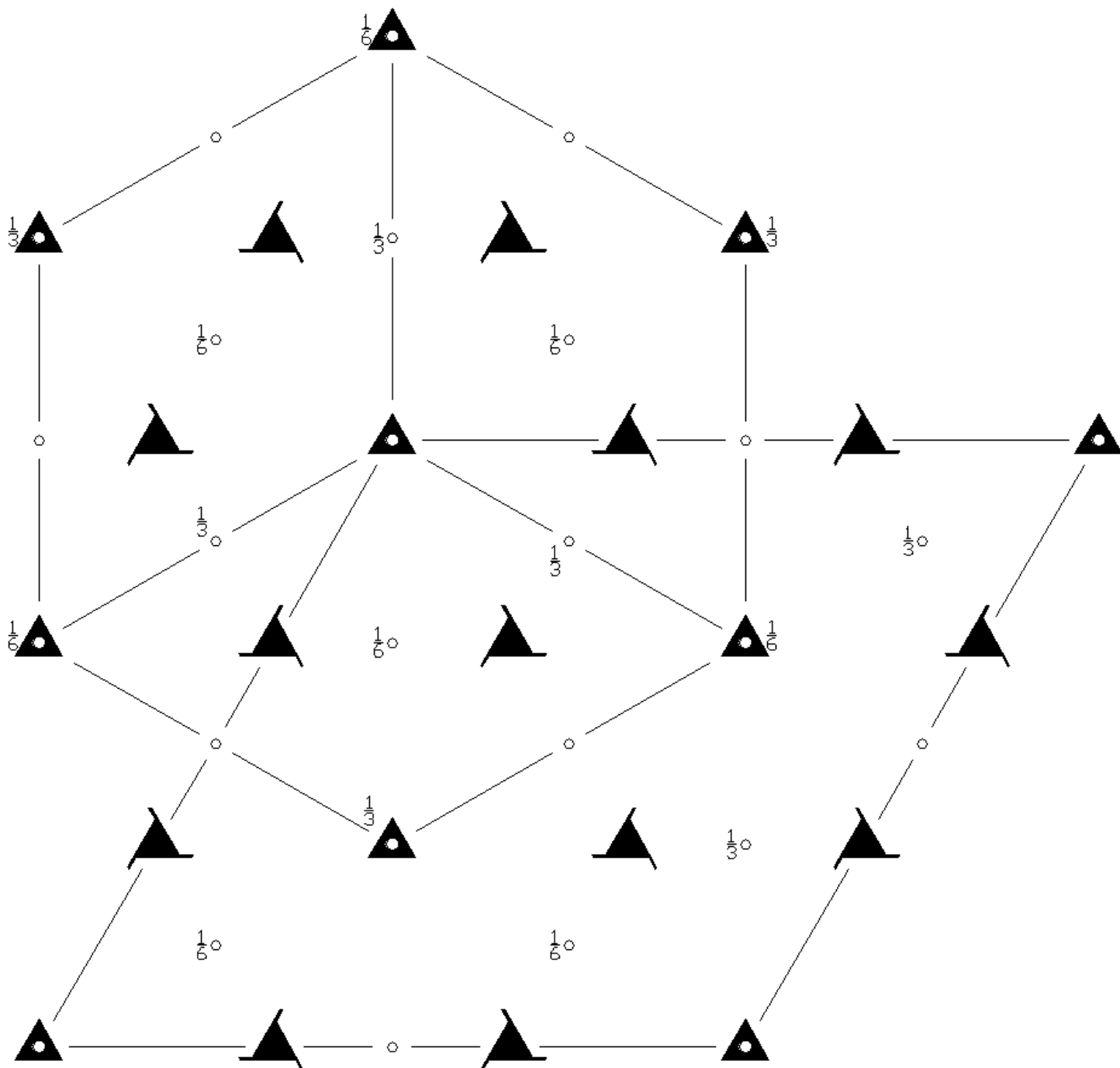


$R\bar{3}$   
148.1.1247

$\bar{3}$   
 $R\bar{3}$

Trigonal





Origin on  $\bar{3}$

Asymmetric unit	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/6;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/6	1/2,0,0 1/2,0,1/6	2/3,1/3,0 2/3,1/3,1/6	1/3,2/3,0 1/3,2/3,1/6	0,1/2,0 0,1/2,1/6

**Symmetry Operations**

For (0,0,0) + set

- |                                       |  |  |
|---------------------------------------|--|--|
| (1) 1<br>(1   0,0,0)                  | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>   0,0,0)   | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>   0,0,0) |
| (4) $\bar{1}$<br>( $\bar{1}$   0,0,0) | (5) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$   0,0,0) | (6) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$   0,0,0)        |

For (2/3,1/3,1/3) + set

- |   |  |  |
|---|--|--|
| (1) t (2/3,1/3,1/3)<br>(1   2/3,1/3,1/3)                | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>   2/3,1/3,1/3) | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>   2/3,1/3,1/3) |
| (4) $\bar{1}$ 1/3,1/6,1/6<br>( $\bar{1}$   2/3,1/3,1/3) | (5) $\bar{3}^+$ 1/3,-1/3,z; 1/3,-1/3,1/6<br>( $\bar{3}_z$   2/3,1/3,1/3) | (6) $\bar{3}^-$ 1/3,2/3,z; 1/3,2/3,1/6<br>( $\bar{3}_z^{-1}$   2/3,1/3,1/3)          |

For (1/3,2/3,2/3) + set

- |   |  |  |
|---|--|--|
| (1) t (1/3,2/3,2/3)<br>(1   1/3,2/3,2/3)                | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>   1/3,2/3,2/3) | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>   1/3,2/3,2/3) |
| (4) $\bar{1}$ 1/6,1/3,1/3<br>( $\bar{1}$   1/3,2/3,2/3) | (5) $\bar{3}^+$ 2/3,1/3,z; 2/3,1/3,1/3<br>( $\bar{3}_z$   1/3,2/3,2/3) | (6) $\bar{3}^-$ -1/3,1/3,z; -1/3,1/3,1/3<br>( $\bar{3}_z^{-1}$   1/3,2/3,2/3)          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4).**Positions**Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

			(0,0,0) +	(2/3,1/3,1/3) +	(1/3,2/3,2/3) +
18	f	1	(1) x,y,z [u,v,w] (4) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $y,\bar{x}+y,\bar{z}$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $x-y,x,\bar{z}$ [ $\bar{u}+v,\bar{u},w$ ]
9	e	$\bar{1}$	1/2,0,0 [u,v,w]	0,1/2,0 [ $\bar{v},u-v,w$ ]	1/2,1/2,0 [ $\bar{u}+v,\bar{u},w$ ]
9	d	$\bar{1}$	1/2,0,1/2 [u,v,w]	0,1/2,1/2 [ $\bar{v},u-v,w$ ]	1/2,1/2,1/2 [ $\bar{u}+v,\bar{u},w$ ]
6	c	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	
1	b	$\bar{3}..$	0,0,1/2 [0,0,w]		
1	a	$\bar{3}..$	0,0,0 [0,0,w]		

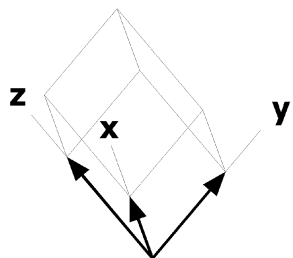
**Symmetry of Special Projections**

Along [0,0,1] p6'  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at 0,0,z

Along [1,0,0] p2'11  
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}/3$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0

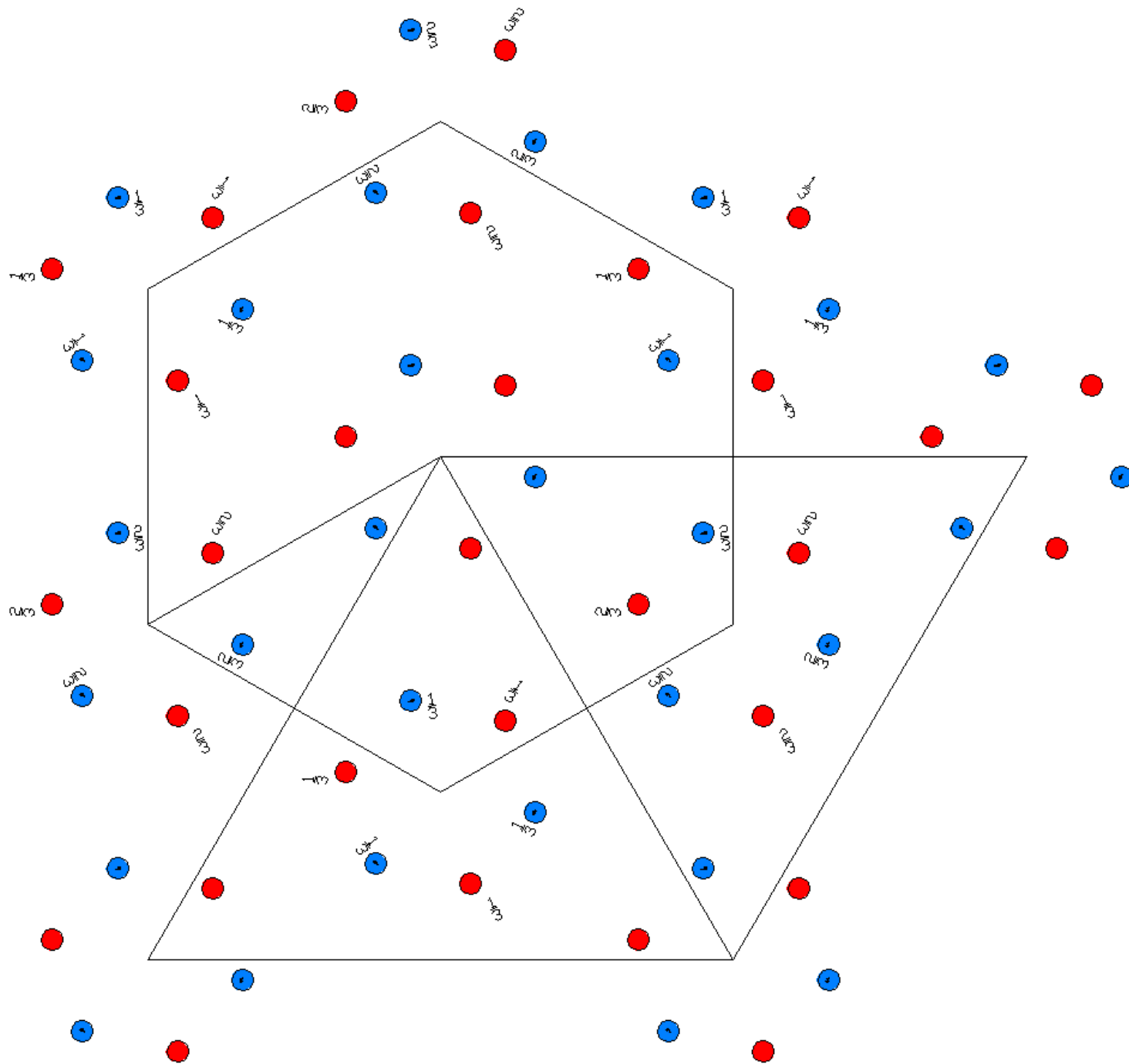




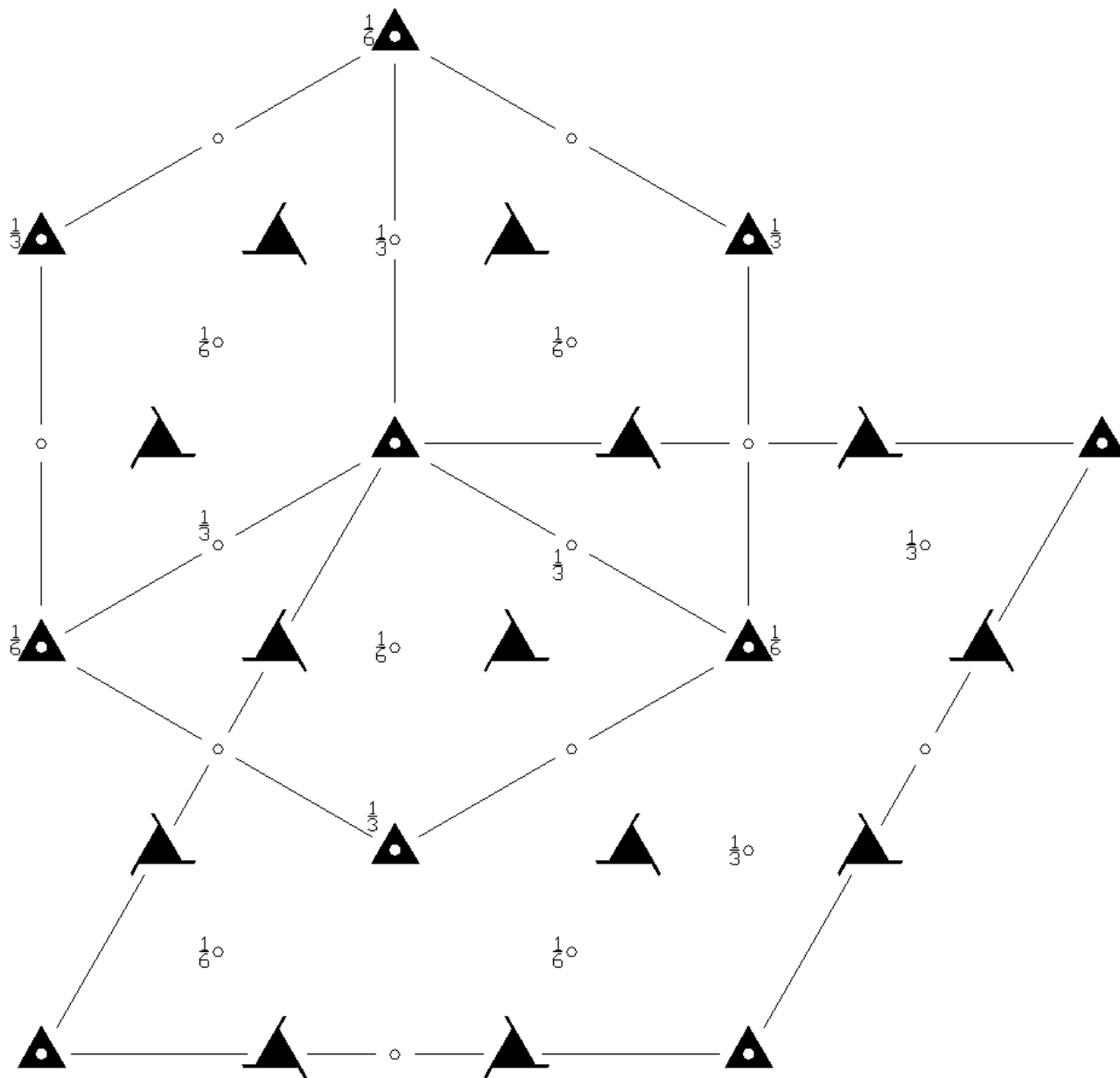
$R\bar{3}1'$   
148.2.1248

$\bar{3}1'$   
 $R\bar{3}1'$

Trigonal



1'

Origin on  $\bar{3}1'$ 

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/6;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/6	1/2,0,0 1/2,0,1/6	2/3,1/3,0 2/3,1/3,1/6	1/3,2/3,0 1/3,2/3,1/6	0,1/2,0 0,1/2,1/6

**Symmetry Operations**

For (0,0,0) + set

- |                                       |  |  |
|---------------------------------------|--|--|
| (1) 1<br>(1   0,0,0)                  | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>   0,0,0)   | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>   0,0,0) |
| (4) $\bar{1}$<br>( $\bar{1}$   0,0,0) | (5) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$   0,0,0) | (6) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$   0,0,0)        |

For (2/3,1/3,1/3) + set

- |   |  |  |
|---|--|--|
| (1) t (2/3,1/3,1/3)<br>(1   2/3,1/3,1/3)                | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>   2/3,1/3,1/3) | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>   2/3,1/3,1/3) |
| (4) $\bar{1}$ 1/3,1/6,1/6<br>( $\bar{1}$   2/3,1/3,1/3) | (5) $\bar{3}^+$ 1/3,-1/3,z; 1/3,-1/3,1/6<br>( $\bar{3}_z$   2/3,1/3,1/3) | (6) $\bar{3}^-$ 1/3,2/3,z; 1/3,2/3,1/6<br>( $\bar{3}_z^{-1}$   2/3,1/3,1/3)          |

For (1/3,2/3,2/3) + set

- |   |  |  |
|---|--|--|
| (1) t (1/3,2/3,2/3)<br>(1   1/3,2/3,2/3)                | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>   1/3,2/3,2/3) | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>   1/3,2/3,2/3) |
| (4) $\bar{1}$ 1/6,1/3,1/3<br>( $\bar{1}$   1/3,2/3,2/3) | (5) $\bar{3}^+$ 2/3,1/3,z; 2/3,1/3,1/3<br>( $\bar{3}_z$   1/3,2/3,2/3) | (6) $\bar{3}^-$ -1/3,1/3,z; -1/3,1/3,1/3<br>( $\bar{3}_z^{-1}$   1/3,2/3,2/3)          |

For (0,0,0)' + set

- |  |   |   |
|--|---|---|
| (1) 1'<br>(1   0,0,0)'                   | (2) 3 <sup>+</sup> ' 0,0,z<br>(3 <sub>z</sub>   0,0,0)'   | (3) 3 <sup>-</sup> ' 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>   0,0,0)' |
| (4) $\bar{1}$ '<br>( $\bar{1}$   0,0,0)' | (5) $\bar{3}^+$ ' 0,0,z; 0,0,0<br>( $\bar{3}_z$   0,0,0)' | (6) $\bar{3}^-$ ' 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$   0,0,0)'        |

For (2/3,1/3,1/3)' + set

- |  |   |   |
|--|---|---|
| (1) t' (2/3,1/3,1/3)<br>(1   2/3,1/3,1/3)'                 | (2) 3 <sup>+</sup> ' (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>   2/3,1/3,1/3)' | (3) 3 <sup>-</sup> ' (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>   2/3,1/3,1/3)' |
| (4) $\bar{1}$ ' 1/3,1/6,1/6<br>( $\bar{1}$   2/3,1/3,1/3)' | (5) $\bar{3}^+$ ' 1/3,-1/3,z; 1/3,-1/3,1/6<br>( $\bar{3}_z$   2/3,1/3,1/3)' | (6) $\bar{3}^-$ ' 1/3,2/3,z; 1/3,2/3,1/6<br>( $\bar{3}_z^{-1}$   2/3,1/3,1/3)'          |

For (1/3,2/3,2/3)' + set

- |  |   |   |
|--|---|---|
| (1) t' (1/3,2/3,2/3)<br>(1   1/3,2/3,2/3)'                 | (2) 3 <sup>+</sup> ' (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>   1/3,2/3,2/3)' | (3) 3 <sup>-</sup> ' (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>   1/3,2/3,2/3)' |
| (4) $\bar{1}$ ' 1/6,1/3,1/3<br>( $\bar{1}$   1/3,2/3,2/3)' | (5) $\bar{3}^+$ ' 2/3,1/3,z; 2/3,1/3,1/3<br>( $\bar{3}_z$   1/3,2/3,2/3)' | (6) $\bar{3}^-$ ' -1/3,1/3,z; -1/3,1/3,1/3<br>( $\bar{3}_z^{-1}$   1/3,2/3,2/3)'          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4);1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

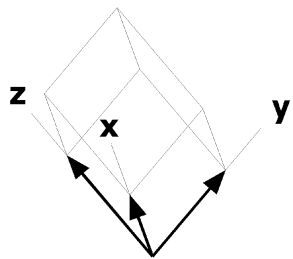
			(0,0,0) + (0,0,0)' +	(2/3,1/3,1/3) + (2/3,1/3,1/3)' +	(1/3,2/3,2/3) + (1/3,2/3,2/3)' +
18	f	11'	(1) x,y,z [0,0,0] (4) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(2) $\bar{y},x-y,z$ [0,0,0] (5) $y,\bar{x}+y,\bar{z}$ [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0] (6) $x-y,x,\bar{z}$ [0,0,0]
9	e	$\bar{1}1'$	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]
9	d	$\bar{1}1'$	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]
6	c	3..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	
1	b	$\bar{3}..1'$	0,0,1/2 [0,0,0]		
1	a	$\bar{3}..1'$	0,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p6'  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at 0,0,z

Along [1,0,0] p2111'  
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}/3$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



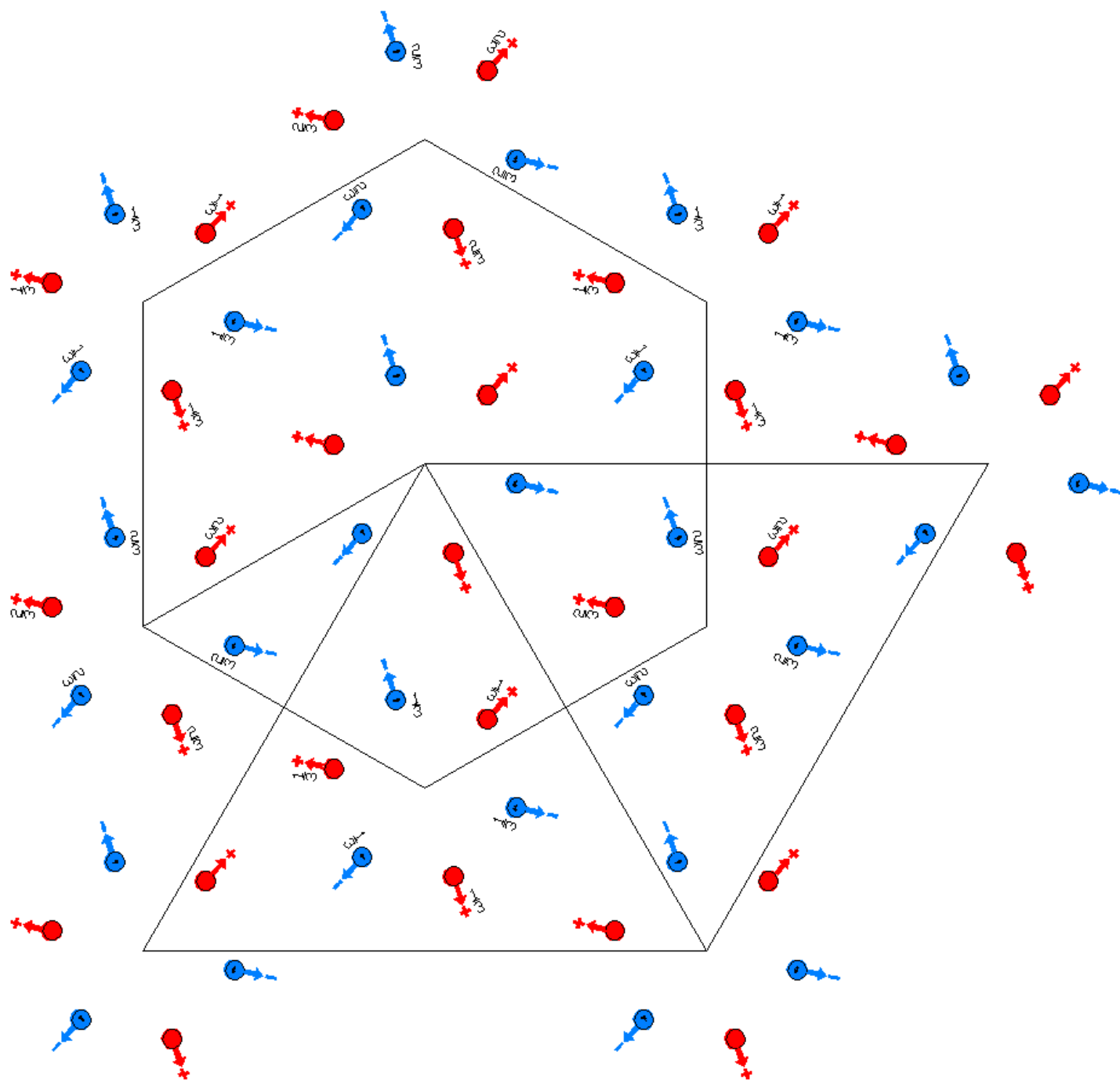
$R\bar{3}'$

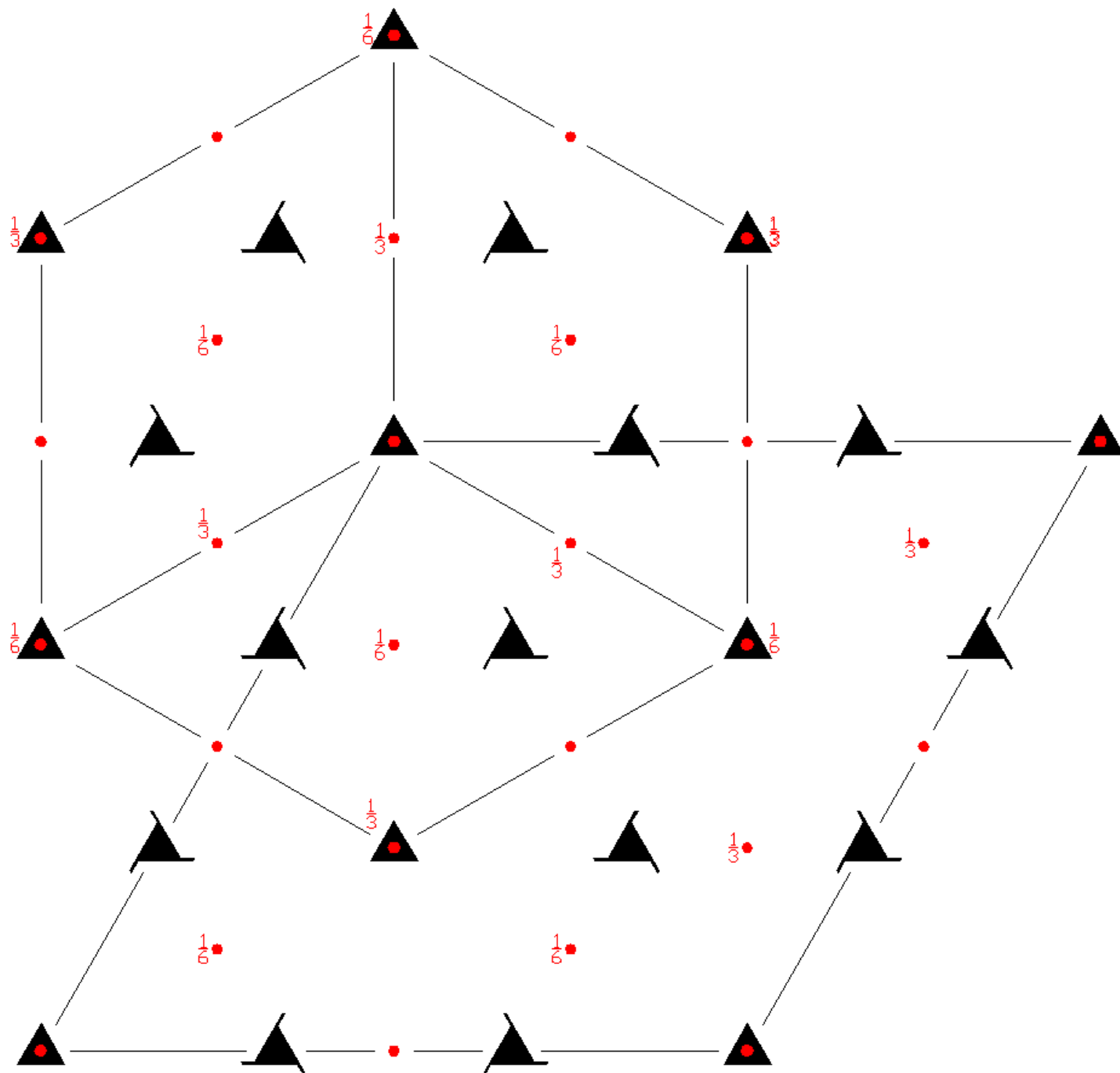
148.3.1249

$\bar{3}'$

$R\bar{3}'$

Trigonal





Origin on  $\bar{3}'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/6;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/6	1/2,0,0 1/2,0,1/6	2/3,1/3,0 2/3,1/3,1/6	1/3,2/3,0 1/3,2/3,1/6	0,1/2,0 0,1/2,1/6

## Symmetry Operations

For (0,0,0) + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1   0,0,0)                     | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>   0,0,0)                            | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>   0,0,0)                            |
| (4) $\bar{1}$ '<br>( $\bar{1}$   0,0,0)' | (5) $\bar{3}$ <sup>+</sup> ' 0,0,z; 0,0,0<br>( $\bar{3}$ <sub>z</sub>   0,0,0)' | (6) $\bar{3}$ <sup>-</sup> ' 0,0,z; 0,0,0<br>( $\bar{3}$ <sub>z</sub> <sup>-1</sup>   0,0,0)' |

For (2/3,1/3,1/3) + set

- |  |   |   |
|--|---|---|
| (1) t (2/3,1/3,1/3)<br>(1   2/3,1/3,1/3)                   | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>   2/3,1/3,1/3)                          | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>   2/3,1/3,1/3)                          |
| (4) $\bar{1}$ ' 1/3,1/6,1/6<br>( $\bar{1}$   2/3,1/3,1/3)' | (5) $\bar{3}$ <sup>+</sup> ' 1/3,-1/3,z; 1/3,-1/3,1/6<br>( $\bar{3}$ <sub>z</sub>   2/3,1/3,1/3)' | (6) $\bar{3}$ <sup>-</sup> ' 1/3,2/3,z; 1/3,2/3,1/6<br>( $\bar{3}$ <sub>z</sub> <sup>-1</sup>   2/3,1/3,1/3)' |

For (1/3,2/3,2/3) + set

- |  |   |   |
|--|---|---|
| (1) t (1/3,2/3,2/3)<br>(1   1/3,2/3,2/3)                   | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>   1/3,2/3,2/3)                          | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>   1/3,2/3,2/3)                          |
| (4) $\bar{1}$ ' 1/6,1/3,1/3<br>( $\bar{1}$   1/3,2/3,2/3)' | (5) $\bar{3}$ <sup>+</sup> ' 2/3,1/3,z; 2/3,1/3,1/3<br>( $\bar{3}$ <sub>z</sub>   1/3,2/3,2/3)' | (6) $\bar{3}$ <sup>-</sup> ' -1/3,1/3,z; -1/3,1/3,1/3<br>( $\bar{3}$ <sub>z</sub> <sup>-1</sup>   1/3,2/3,2/3)' |

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

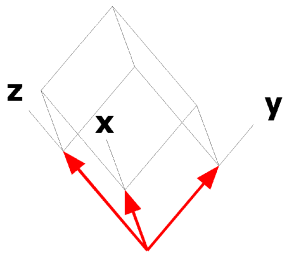
			(0,0,0) +	(2/3,1/3,1/3) +	(1/3,2/3,2/3) +
18	f	1	(1) x,y,z [u,v,w] (4) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $y,\bar{x}+y,\bar{z}$ [ $v,\bar{u}+v,\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $x-y,x,\bar{z}$ [ $u-v,u,\bar{w}$ ]
9	e	$\bar{1}$ '	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]
9	d	$\bar{1}$ '	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]
6	c	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	
1	b	$\bar{3}$ '..	0,0,1/2 [0,0,0]		
1	a	$\bar{3}$ '..	0,0,0 [0,0,0]		

## Symmetry of Special Projections

Along [0,0,1] p6  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at 0,0,z

Along [1,0,0] p211  
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

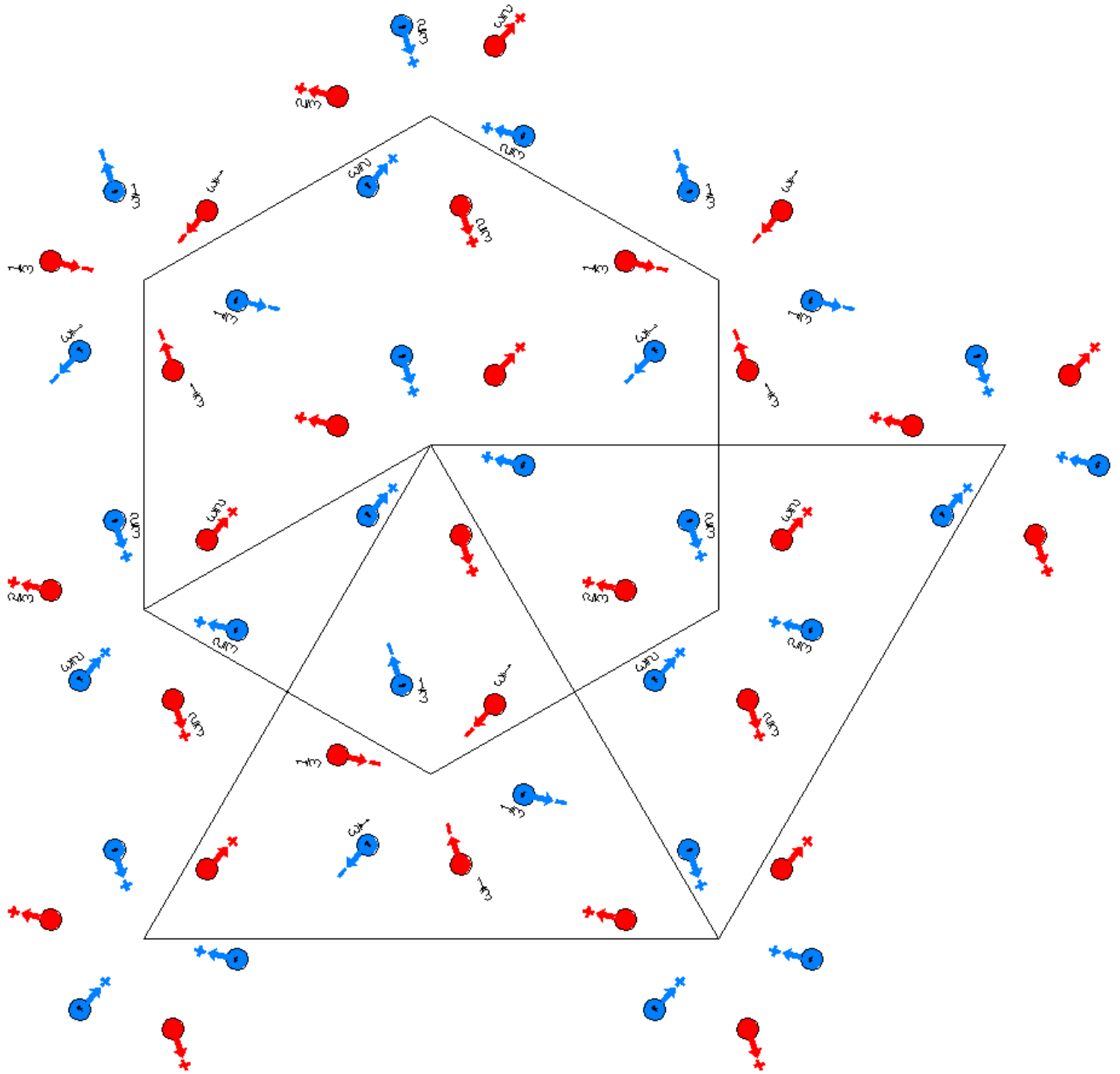
Along [2,1,0] p211  
 $\mathbf{a}^* = \mathbf{c}/3$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



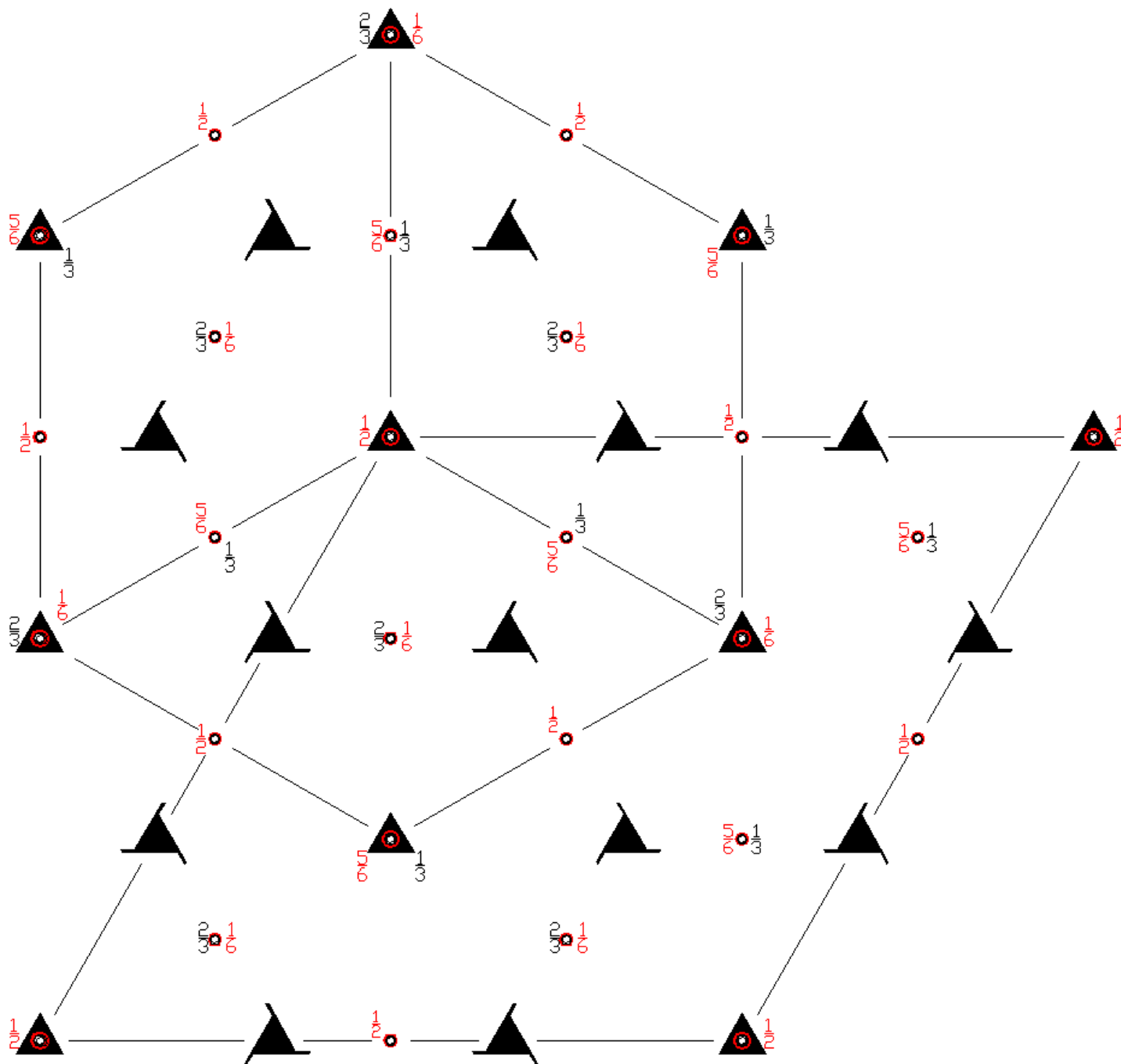
$R_{\bar{3}}$   
148.4.1250

$\bar{3}1'$   
 $R_{\bar{3}}$

Trigonal







Origin on  $\bar{3}$

Asymmetric unit	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/6;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/6	1/2,0,1/6	2/3,1/3,1/6	1/3,2/3,1/6	0,1/2,1/6

**Symmetry Operations**

For (0,0,0) + set

- |                                       |  |   |
|---------------------------------------|--|---|
| (1) 1<br>(1   0,0,0)                  | (2) $3^+$ 0,0,z<br>( $3_z$   0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$   0,0,0)                    |
| (4) $\bar{1}$<br>( $\bar{1}$   0,0,0) | (5) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$   0,0,0) | (6) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$   0,0,0) |

For (2/3,1/3,1/3)' + set

- |  |   |  |
|--|---|--|
| (1) t' (2/3,1/3,1/3)<br>(1   2/3,1/3,1/3)'                 | (2) $3^+$ ' (0,0,1/3) 1/3,1/3,z<br>( $3_z$   2/3,1/3,1/3)'                  | (3) $3^-$ ' (0,0,1/3) 1/3,0,z<br>( $3_z^{-1}$   2/3,1/3,1/3)'                  |
| (4) $\bar{1}$ ' 1/3,1/6,1/6<br>( $\bar{1}$   2/3,1/3,1/3)' | (5) $\bar{3}^+$ ' 1/3,-1/3,z; 1/3,-1/3,1/6<br>( $\bar{3}_z$   2/3,1/3,1/3)' | (6) $\bar{3}^-$ ' 1/3,2/3,z; 1/3,2/3,1/6<br>( $\bar{3}_z^{-1}$   2/3,1/3,1/3)' |

For (1/3,2/3,2/3) + set

- |   |  |   |
|---|--|---|
| (1) t (1/3,2/3,2/3)<br>(1   1/3,2/3,2/3)                | (2) $3^+$ (0,0,2/3) 0,1/3,z<br>( $3_z$   1/3,2/3,2/3)                  | (3) $3^-$ (0,0,2/3) 1/3,1/3,z<br>( $3_z^{-1}$   1/3,2/3,2/3)                  |
| (4) $\bar{1}$ 1/6,1/3,1/3<br>( $\bar{1}$   1/3,2/3,2/3) | (5) $\bar{3}^+$ 2/3,1/3,z; 2/3,1/3,1/3<br>( $\bar{3}_z$   1/3,2/3,2/3) | (6) $\bar{3}^-$ -1/3,1/3,z; -1/3,1/3,1/3<br>( $\bar{3}_z^{-1}$   1/3,2/3,2/3) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4).**Positions**Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

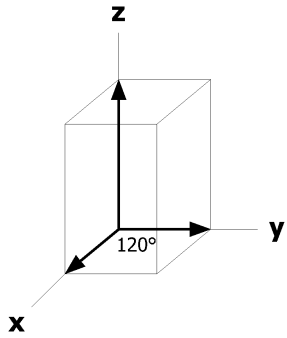
			(0,0,0) +	(2/3,1/3,1/3)' +	(1/3,2/3,2/3) +
18	f	1	(1) x,y,z [u,v,w] (4) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $y,\bar{x}+y,\bar{z}$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $x-y,x,\bar{z}$ [ $\bar{u}+v,\bar{u},w$ ]
9	e	$\bar{1}$	1/2,0,0 [u,v,w]	0,1/2,0 [ $\bar{v},u-v,w$ ]	1/2,1/2,0 [ $\bar{u}+v,\bar{u},w$ ]
9	d	$\bar{1}'$	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]
6	c	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	
1	b	$\bar{3}'..$	0,0,1/2 [0,0,0]		
1	a	$\bar{3}..$	0,0,0 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1]  $p61'$   
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}211$   
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/2

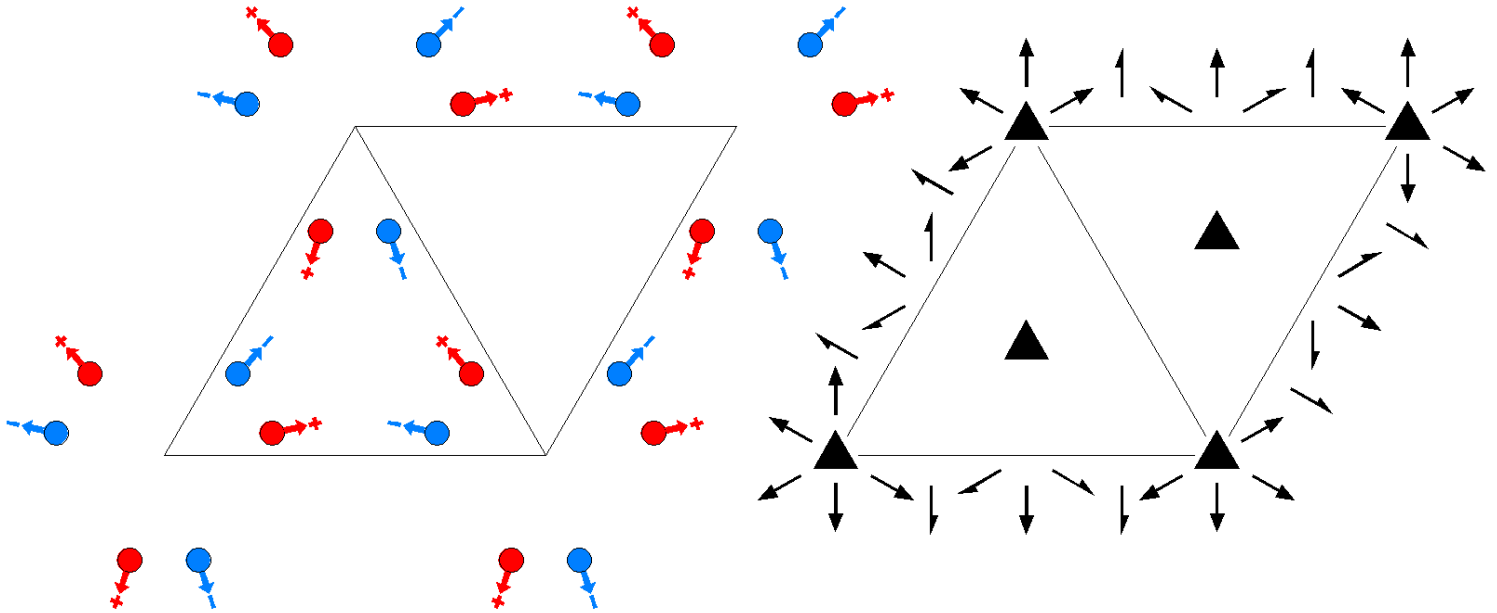
Along [2,1,0]  $p_{2a}211$   
 $\mathbf{a}^* = \mathbf{c}/3$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/2



P312  
149.1.1251

312  
P312

Trigonal



Origin on 312

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/3,2/3,0 1/3,2/3,1/2	0,1/2,0 0,1/2,1/2

**Symmetry Operations**

- |  |                                     |   |
|--|-------------------------------------|---|
| (1) 1<br>(1 0,0,0)                       | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) 2 $x, \bar{x}, 0$<br>( $2_3$  0,0,0) | (5) 2 $x, 2x, 0$<br>( $2_2$  0,0,0) | (6) 2 $2x, x, 0$<br>( $2_1$  0,0,0)     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

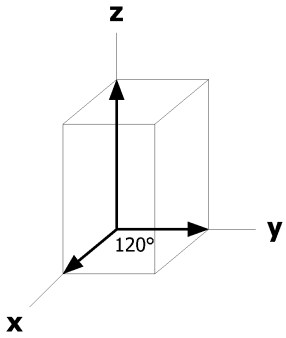
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	l	1	(1) $x,y,z$ [ $u,v,w$ ] (4) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $\bar{x}+y,y,\bar{z}$ [ $\bar{u}+v,v,\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $x,x-y,\bar{w}$ [ $u,u-v,\bar{w}$ ]
3	k	..2	$x,\bar{x},1/2$ [ $u,\bar{u},0$ ]	$x,2x,1/2$ [ $u,2u,0$ ]	$2\bar{x},\bar{x},1/2$ [ $2\bar{u},\bar{u},0$ ]
3	j	..2	$x,\bar{x},0$ [ $u,\bar{u},0$ ]	$x,2x,0$ [ $u,2u,0$ ]	$2\bar{x},\bar{x},0$ [ $2\bar{u},\bar{u},0$ ]
2	i	3..	$2/3,1/3,z$ [ $0,0,w$ ]	$2/3,1/3,\bar{z}$ [ $0,0,\bar{w}$ ]	
2	h	3..	$1/3,2/3,z$ [ $0,0,w$ ]	$1/3,2/3,\bar{z}$ [ $0,0,\bar{w}$ ]	
2	g	3..	$0,0,z$ [ $0,0,w$ ]	$0,0,\bar{z}$ [ $0,0,\bar{w}$ ]	
1	f	3.2	$2/3,1/3,1/2$ [ $0,0,0$ ]		
1	e	3.2	$2/3,1/3,0$ [ $0,0,0$ ]		
1	d	3.2	$1/3,2/3,1/2$ [ $0,0,0$ ]		
1	c	3.2	$1/3,2/3,0$ [ $0,0,0$ ]		
1	b	3.2	$0,0,1/2$ [ $0,0,0$ ]		
1	a	3.2	$0,0,0$ [ $0,0,0$ ]		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p3m'1$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p1m'1$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

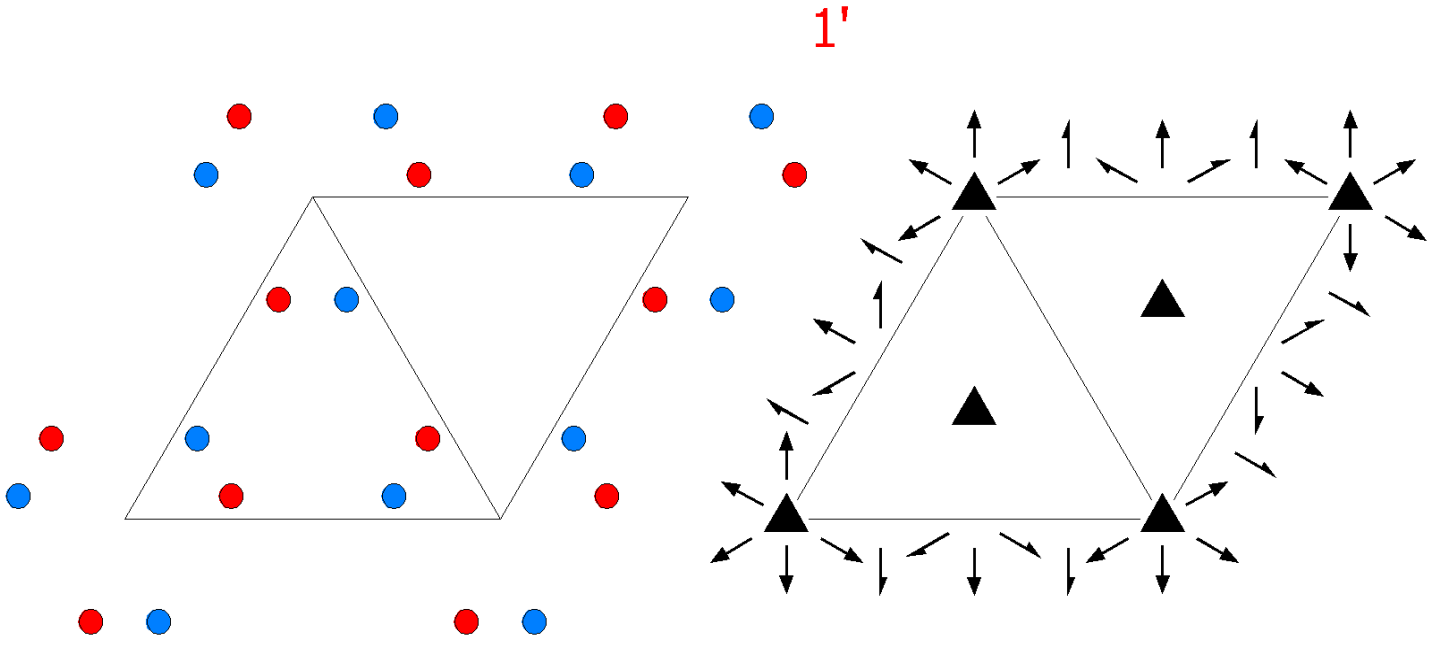
Along  $[2,1,0]$   $p211$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,0$



P3121'  
149.2.1252

3121'  
P3121'

Trigonal



Origin on 3121'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/3,2/3,0 1/3,2/3,1/2	0,1/2,0 0,1/2,1/2

**Symmetry Operations**

For 1 + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                      | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 x,x̄,0<br>(2 <sub>3</sub>  0,0,0) | (5) 2 x,2x,0<br>(2 <sub>2</sub>  0,0,0)             | (6) 2 2x,x,0<br>(2 <sub>1</sub>  0,0,0)                           |

For 1' + set

- |   |  |  |
|---|--|--|
| (1) 1'<br>(1 0,0,0)'                      | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)' | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (4) 2' x,x̄,0<br>(2 <sub>3</sub>  0,0,0)' | (2) 2' x,2x,0<br>(2 <sub>2</sub>  0,0,0)'            | (3) 2' 2x,x,0<br>(2 <sub>1</sub>  0,0,0)'                          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

### Positions

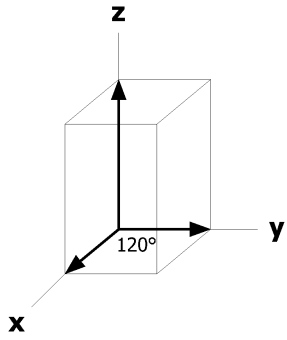
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			1 +	1' +	
6	l	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x}$ ,z [0,0,0]
			(4) $\bar{y},\bar{x},\bar{z}$ [0,0,0]	(5) $\bar{x}+y,y,\bar{z}$ [0,0,0]	(6) x,x-y, $\bar{w}$ [0,0,0]
3	k	..21'	x, $\bar{x}$ ,1/2 [0,0,0]	x,2x,1/2 [0,0,0]	2 $\bar{x},\bar{x}$ ,1/2 [0,0,0]
3	j	..21'	x, $\bar{x}$ ,0 [0,0,0]	x,2x,0 [0,0,0]	2 $\bar{x},\bar{x}$ ,0 [0,0,0]
2	i	3..1'	2/3,1/3,z [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	
2	h	3..1'	1/3,2/3,z [0,0,0]	1/3,2/3, $\bar{z}$ [0,0,0]	
2	g	3..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	
1	f	3.21'	2/3,1/3,1/2 [0,0,0]		
1	e	3.21'	2/3,1/3,0 [0,0,0]		
1	d	3.21'	1/3,2/3,1/2 [0,0,0]		
1	c	3.21'	1/3,2/3,0 [0,0,0]		
1	b	3.21'	0,0,1/2 [0,0,0]		
1	a	3.21'	0,0,0 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p3m11'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

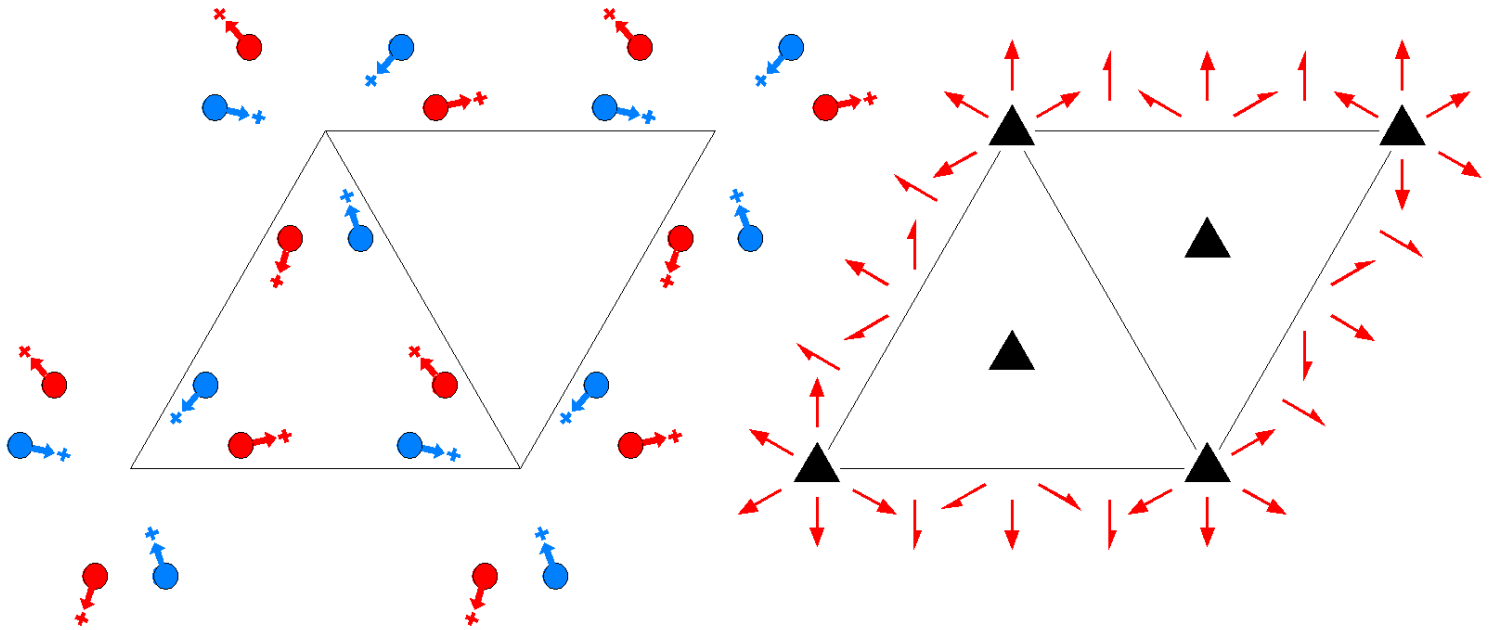
Along [2,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P312'  
149.3.1253

312'  
P312'

Trigonal



Origin on 312'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/3,2/3,1/2	0,1/2,1/2

**Symmetry Operations**

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                        | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' x,x̄,0<br>(2 <sub>3</sub>  0,0,0)' | (5) 2' x,2x,0<br>(2 <sub>2</sub>  0,0,0)'           | (6) 2' 2x,x,0<br>(2 <sub>1</sub>  0,0,0)'                         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	l	1	(1) $x,y,z$ [u,v,w] (4) $\bar{y},\bar{x},\bar{z}$ [v,u,w]	(2) $\bar{y},x-y,z$ [ $\bar{v}$ ,u-v,w] (5) $\bar{x}+y,y,\bar{z}$ [u-v, $\bar{v}$ ,w]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u}$ ,w] (6) $x,x-y,\bar{w}$ [ $\bar{u},\bar{u}+v,w$ ]
3	k	..2'	$x,\bar{x},1/2$ [u,u,w]	$x,2x,1/2$ [ $\bar{u},0,w$ ]	$2\bar{x},\bar{x},1/2$ [0, $\bar{u},w$ ]
3	j	..2'	$x,\bar{x},0$ [u,u,w]	$x,2x,0$ [ $\bar{u},0,w$ ]	$2\bar{x},\bar{x},0$ [0, $\bar{u},w$ ]
2	i	3..	$2/3,1/3,z$ [0,0,w]	$2/3,1/3,\bar{z}$ [0,0,w]	
2	h	3..	$1/3,2/3,z$ [0,0,w]	$1/3,2/3,\bar{z}$ [0,0,w]	
2	g	3..	$0,0,z$ [0,0,w]	$0,0,\bar{z}$ [0,0,w]	
1	f	3.2'	$2/3,1/3,1/2$ [0,0,w]		
1	e	3.2'	$2/3,1/3,0$ [0,0,w]		
1	d	3.2'	$1/3,2/3,1/2$ [0,0,w]		
1	c	3.2'	$1/3,2/3,0$ [0,0,w]		
1	b	3.2'	$0,0,1/2$ [0,0,w]		
1	a	3.2'	$0,0,0$ [0,0,w]		

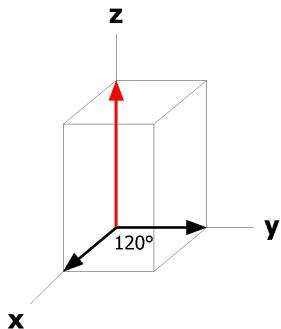
**Symmetry of Special Projections**

Along [0,0,1] p3m1  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0

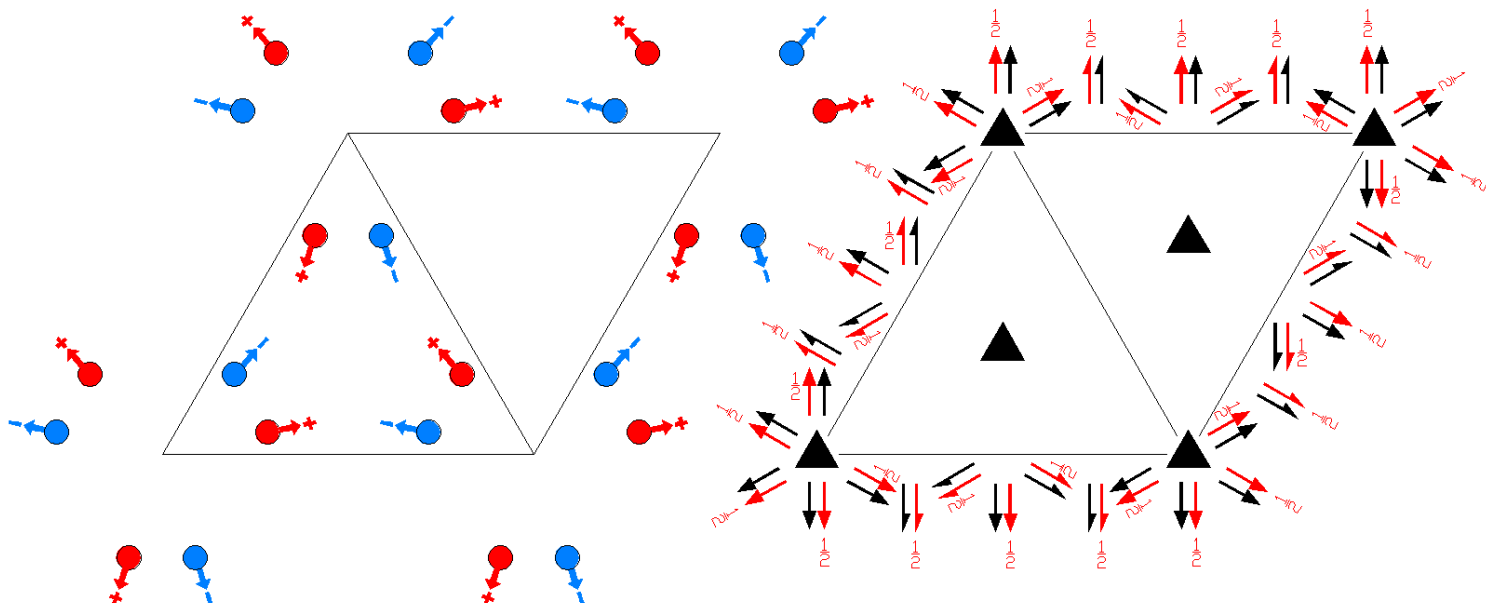




P<sub>2c</sub> 312  
149.4.1254

3121'  
P<sub>2c</sub> 312

Trigonal



Origin on 312

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/3,2/3,0 1/3,2/3,1/2	0,1/2,0 0,1/2,1/2

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                      | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 x,x̄,0<br>(2 <sub>3</sub>  0,0,0) | (5) 2 x,2x,0<br>(2 <sub>2</sub>  0,0,0)             | (6) 2 2x,x,0<br>(2 <sub>1</sub>  0,0,0)                           |

For (0,0,1)' + set

- |   |  |  |
|---|--|--|
| (1) t' (0,0,1)<br>(1 0,0,1)'                | (2) 3 <sup>+</sup> ' (0,0,1) 0,0,z<br>(3 <sub>z</sub>  0,0,1)' | (3) 3 <sup>-</sup> ' (0,0,1) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,1)' |
| (4) 2' x,x̄,1/2<br>(2 <sub>3</sub>  0,0,1)' | (5) 2' x,2x,1/2<br>(2 <sub>2</sub>  0,0,1)'                    | (6) 2' 2x,x,1/2<br>(2 <sub>1</sub>  0,0,1)'                                  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

**Positions**

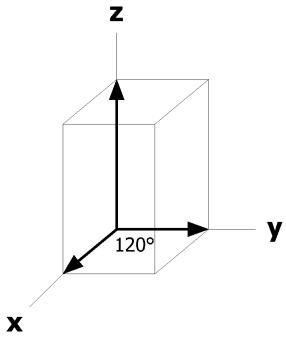
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
				(0,0,0) +	(0,0,1)' +
12	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(5) $\bar{x}+y,y,\bar{z}$ [ $\bar{u}+v,v,\bar{w}$ ]	(6) x,x-y, $\bar{w}$ [u,u-v, $\bar{w}$ ]
6	k	..2'	x, $\bar{x},1/2$ [u,u,w]	x,2x,1/2 [ $\bar{u},0,w$ ]	2 $\bar{x},\bar{x},1/2$ [0, $\bar{u},w$ ]
6	j	..2	x, $\bar{x},0$ [u, $\bar{u},0$ ]	x,2x,0 [u,2u,0]	2 $\bar{x},\bar{x},0$ [2 $\bar{u},\bar{u},0$ ]
4	i	3..	2/3,1/3,z [0,0,w]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	
4	h	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ [0,0, $\bar{w}$ ]	
4	g	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	
2	f	3.2'	2/3,1/3,1/2 [0,0,w]		
2	e	3.2	2/3,1/3,0 [0,0,0]		
2	d	3.2'	1/3,2/3,1/2 [0,0,w]		
2	c	3.2	1/3,2/3,0 [0,0,0]		
2	b	3.2'	0,0,1/2 [0,0,w]		
2	a	3.2	0,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p3m11'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>\*1m1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

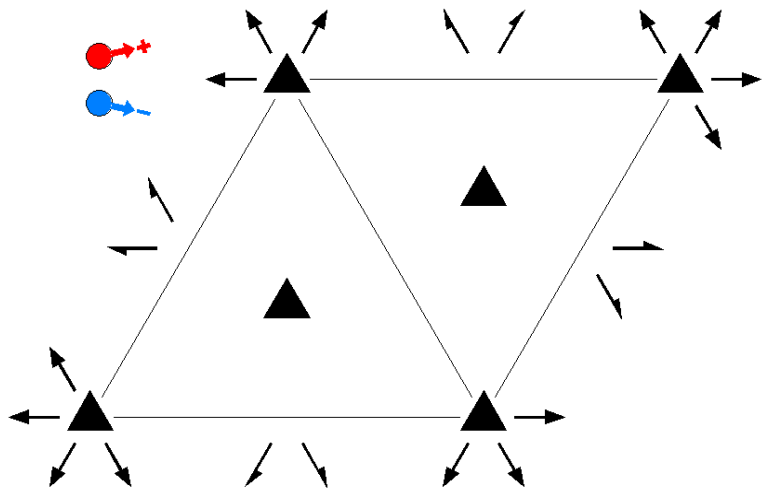
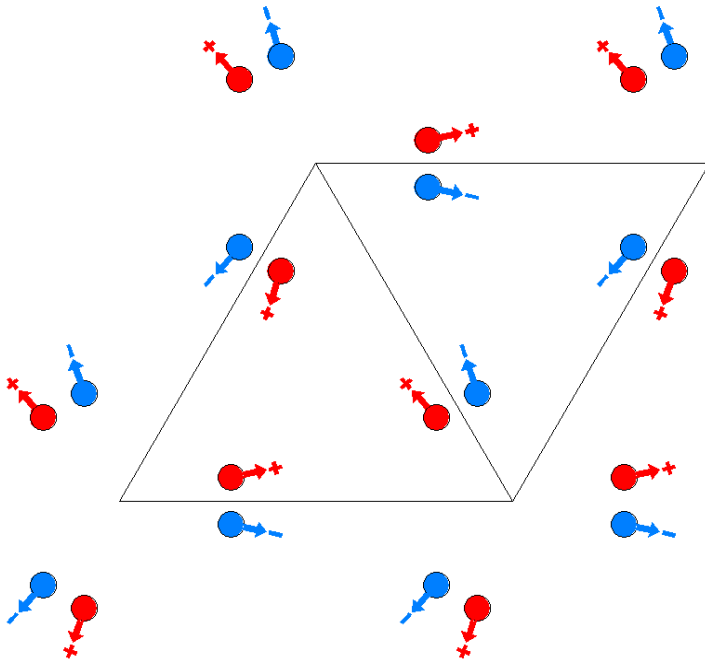
Along [2,1,0] p<sub>2a</sub>\*211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P321  
150.1.1255

321  
P321

Trigonal



**Origin on 321**

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/3,2/3,1/2	0,1/2,1/2

**Symmetry Operations**

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                      | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0) | (5) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)              | (6) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                            |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

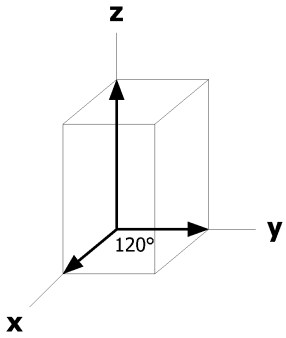
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	g	1	(1) x,y,z [u,v,w] (4) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w] (5) x-y, $\bar{y}$ , $\bar{z}$ [u-v, $\bar{v}$ , $\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x},\bar{x}+y,\bar{z}$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
3	f	.2.	x,0,1/2 [u,0,0]	0,x,1/2 [0,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]
3	g	.2.	x,0,0 [u,0,0]	0,x,0 [0,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]
2	d	3..	1/3,2/3,z [0,0,w]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	
2	c	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	
1	b	32.	0,0,1/2 [0,0,0]		
1	a	32.	0,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p31m'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

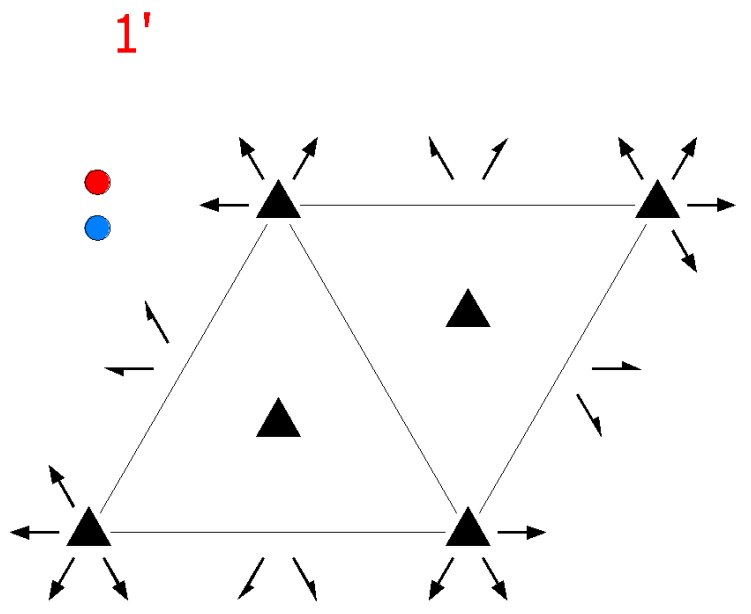
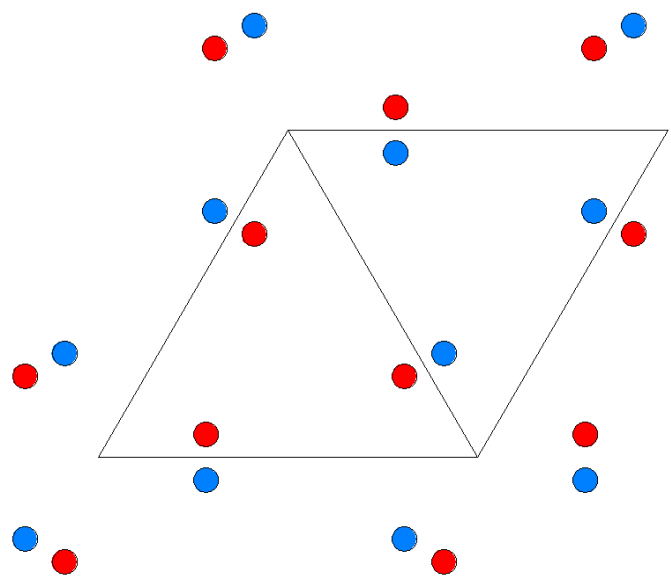
Along [2,1,0] p1m'1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P3211'  
150.2.1256

3211'  
P3211'

Trigonal



Origin on 3211'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/3,2/3,1/2	0,1/2,1/2

**Symmetry Operations**

For 1 + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                      | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0) | (5) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)              | (6) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                            |

For 1' + set

- |   |  |  |
|---|--|--|
| (1) 1'<br>(1 0,0,0)'                      | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)' | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (4) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)' | (5) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'             | (6) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                           |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2);(4); 1'.

**Positions**

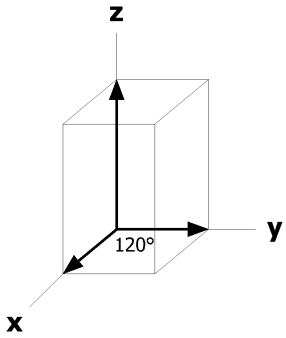
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			1 +	1' +	
6	g	11'	(1) x,y,z [0,0,0] (4) y,x, $\bar{z}$ [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0] (5) x-y, $\bar{y}$ , $\bar{z}$ [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0] (6) $\bar{x},\bar{x}+y,\bar{z}$ [0,0,0]
3	f	.2.1'	x,0,1/2 [0,0,0]	0,x,1/2 [0,0,0]	$\bar{x},\bar{x},1/2$ [0,0,0]
3	g	.2.1'	x,0,0 [0,0,0]	0,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]
2	d	3..1'	1/3,2/3,z [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	
2	c	3..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	
1	b	32.1'	0,0,1/2 [0,0,0]		
1	a	32.1'	0,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p31m1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

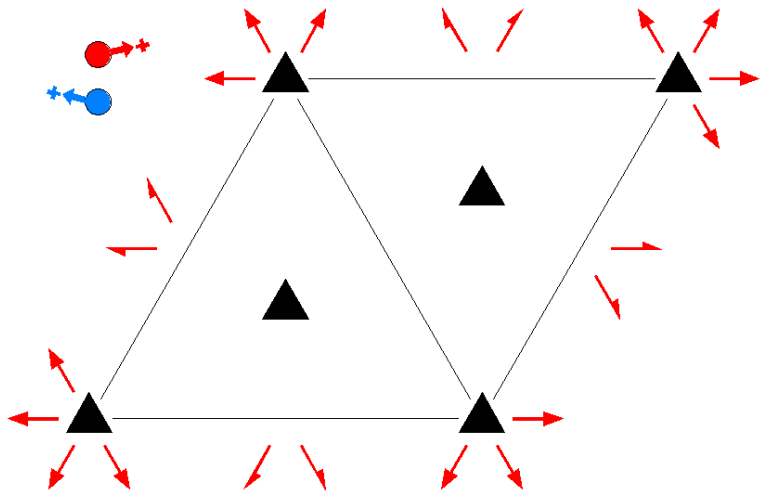
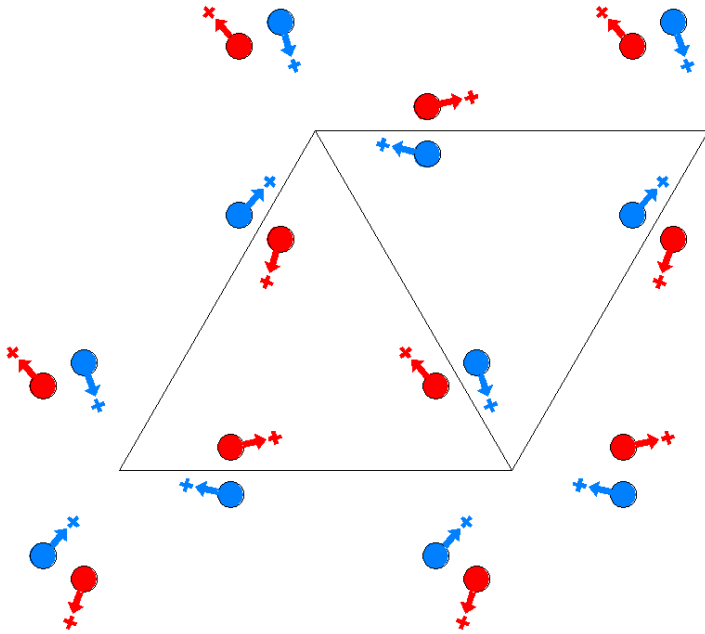
Along [2,1,0] p1m11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P32'1  
150.3.1257

32'1  
P32'1

Trigonal



Origin on 32'1

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/3,2/3,1/2	0,1/2,1/2

**Symmetry Operations**

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                        | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)' | (5) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'            | (6) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	g	1	(1) x,y,z [u,v,w] (4) y,x, $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ ,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w] (5) x-y, $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ +v,v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w] (6) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ [u,u-v,w]
3	f	.2'	x,0,1/2 [u,2u,w]	0,x,1/2 [2 $\bar{u}$ , $\bar{u}$ ,w]	$\bar{x}$ , $\bar{x}$ ,1/2 [u, $\bar{u}$ ,w]
3	g	.2'	x,0,0 [u,2u,w]	0,x,0 [2 $\bar{u}$ , $\bar{u}$ ,w]	$\bar{x}$ , $\bar{x}$ ,0 [u, $\bar{u}$ ,w]
2	d	3..	1/3,2/3,z [0,0,w]	2/3,1/3, $\bar{z}$ [0,0,w]	
2	c	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	
1	b	32'	0,0,1/2 [0,0,w]		
1	a	32'	0,0,0 [0,0,w]		

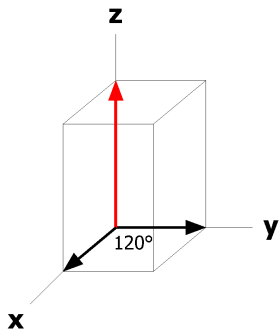
**Symmetry of Special Projections**

Along [0,0,1] p31m  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p1m1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0





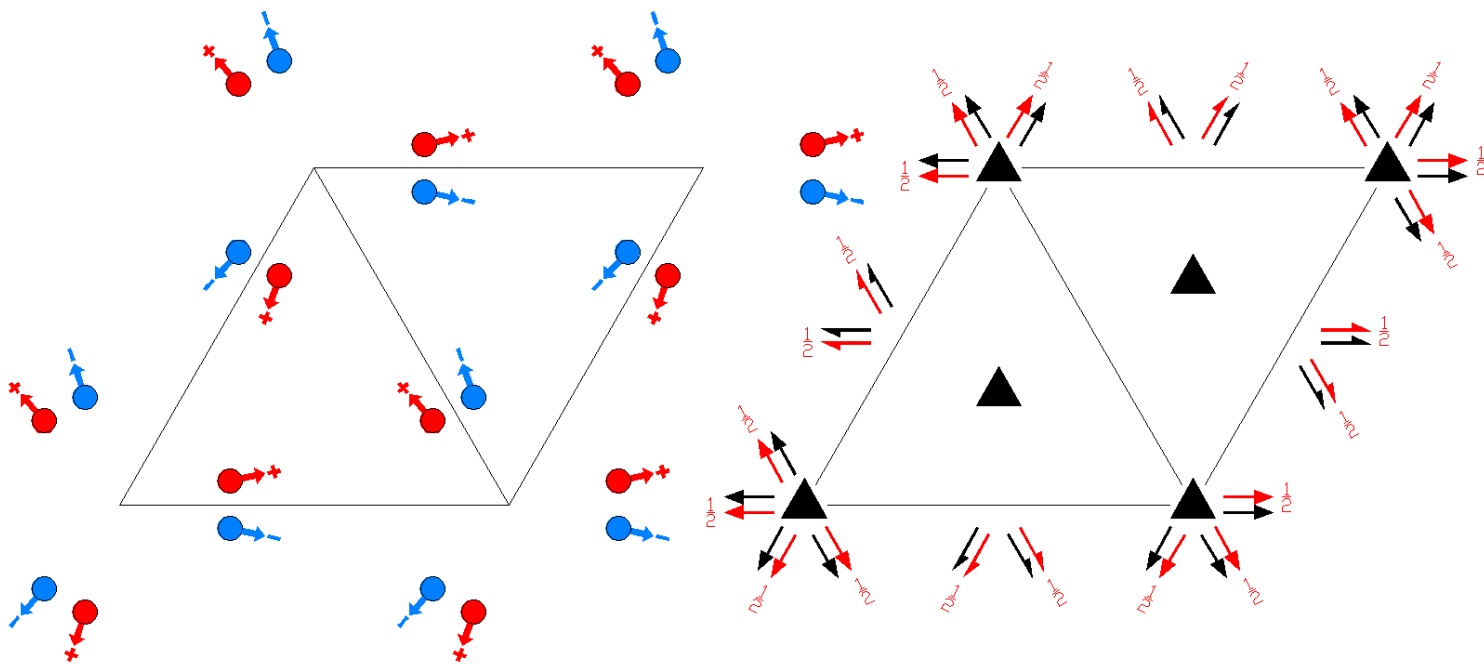
$P_{2c} 321$

150.4.1258

$3211'$

$P_{2c} 321$

Trigonal



Origin on 321

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/3,2/3,1/2	0,1/2,1/2

**Symmetry Operations**

For (0,0,0) + set

- |                                   |                                    |   |
|-----------------------------------|------------------------------------|---|
| (1) 1<br>(1 0,0,0)                | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0) | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) 2 x,x,0<br>( $2_{xy}$  0,0,0) | (5) 2 x,0,0<br>( $2_x$  0,0,0)     | (6) 2 0,y,0<br>( $2_y$  0,0,0)          |

For (0,0,1)' + set

- |   |   |  |
|---|---|--|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'          | (2) $3^+$ (0,0,1) 0,0,z<br>( $3_z$  0,0,1)' | (3) $3^-$ (0,0,1) 0,0,z<br>( $3_z^{-1}$  0,0,1)' |
| (4) $2'$ x,x,1/2<br>( $2_{xy}$  0,0,1)' | (5) $2'$ x,0,1/2<br>( $2_x$  0,0,1)'        | (6) $2'$ 0,y,1/2<br>( $2_y$  0,0,1)'             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

**Positions**

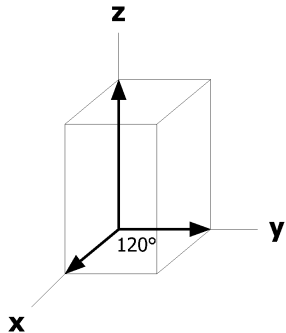
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			(0,0,0) +	(0,0,1)' +	
12	g	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(5) x-y, $\bar{y},\bar{z}$ [u-v, $\bar{v},\bar{w}$ ]	(6) $\bar{x},\bar{x}+y,\bar{z}$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
6	f	.2'	x,0,1/2 [u,2u,w]	0,x,1/2 [2 $\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},1/2$ [u, $\bar{u},w$ ]
6	g	.2.	x,0,0 [u,0,0]	0,x,0 [0,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]
4	d	3..	1/3,2/3,z [0,0,w]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	
4	c	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	
2	b	32'	0,0,1/2 [0,0,w]		
2	a	32.	0,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p31m1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>\*211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

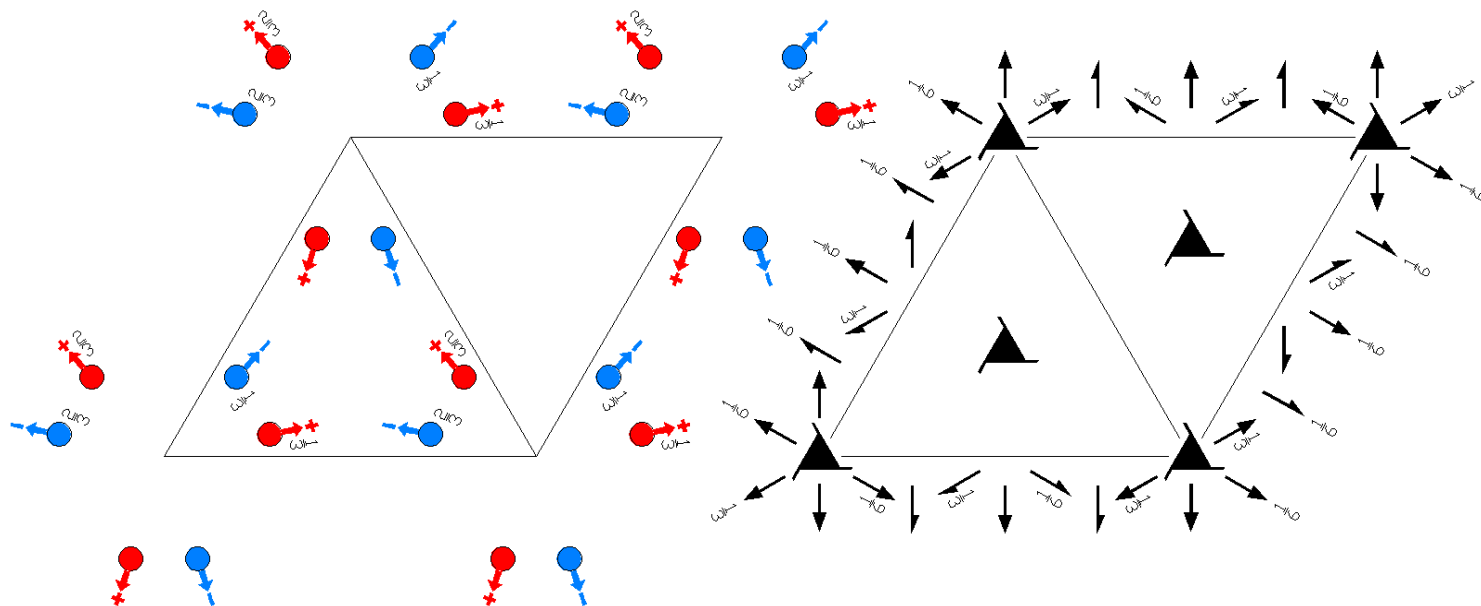
Along [2,1,0] p<sub>2a</sub>\*1m1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/2



P3<sub>1</sub>12  
151.1.1259

312  
P3<sub>1</sub>12

Trigonal



Origin on 2 [210] at 3<sub>1</sub>(1,1,2)

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

### Symmetry Operations

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                   | (2) 3 <sup>+</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub>  0,0,1/3) | (3) 3 <sup>-</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,2/3) |
| (4) 2 $x, \bar{x}, 1/3$<br>(2 <sub>3</sub>  0,0,2/3) | (5) 2 $x, 2x, 1/6$<br>(2 <sub>2</sub>  0,0,1/3)                 | (6) 2 $2x, x, 0$<br>(2 <sub>1</sub>  0,0,0)                                   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

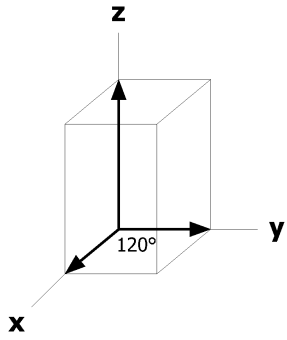
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	c	1	(1) $x, y, z$ [u, v, w]	(2) $\bar{y}, x-y, z+1/3$ [ $\bar{v}$ , u-v, w]	(3) $\bar{x}+y, \bar{x}, z+2/3$ [ $\bar{u}+v, \bar{u}$ , w]
			(4) $\bar{y}, \bar{x}, \bar{z}+2/3$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(5) $\bar{x}+y, y, \bar{z}+1/3$ [ $\bar{u}+v, v, \bar{w}$ ]	(6) $x, x-y, \bar{z}$ [u, u-v, $\bar{w}$ ]
3	b	..2	$x, \bar{x}, 5/6$ [u, $\bar{u}$ , 0]	$x, 2x, 1/6$ [u, 2u, 0]	$2\bar{x}, \bar{x}, 1/2$ [2 $\bar{u}$ , $\bar{u}$ , 0]
3	a	..2	$x, \bar{x}, 1/3$ [u, $\bar{u}$ , 0]	$x, 2x, 2/3$ [u, 2u, 0]	$2\bar{x}, \bar{x}, 0$ [2 $\bar{u}$ , $\bar{u}$ , 0]

**Symmetry of Special Projections**

Along [0,0,1] p3m'1  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/6

Along [2,1,0] p211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



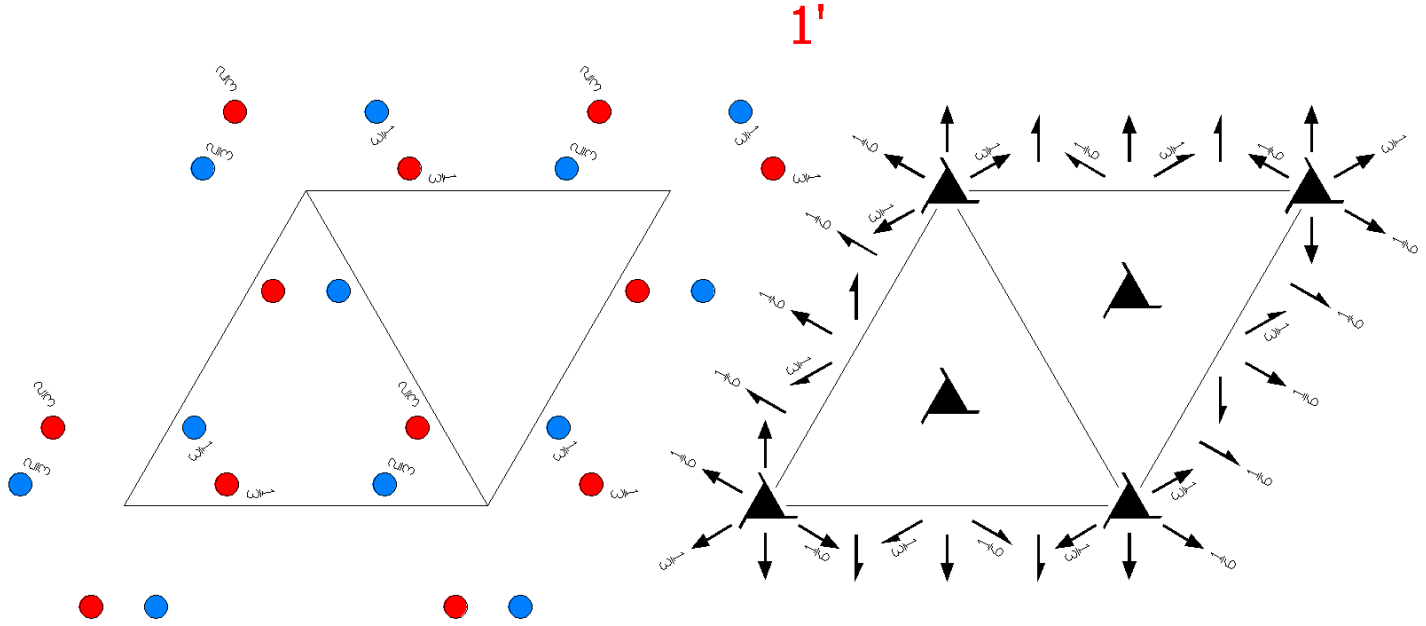
P3<sub>1</sub>121'

151.2.1260

3121'

P3<sub>1</sub>121'

Trigonal



Origin on 21' [210] at 3<sub>1</sub>1(1,1,2)1'

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

### Symmetry Operations

For 1 + set

(1) 1 (1 0,0,0)	(2) 3 <sup>+</sup> (0,0,1/3) 0,0,z (3 <sub>z</sub>  0,0,1/3)	(3) 3 <sup>-</sup> (0,0,2/3) 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,2/3)
--------------------	---	---

(4) 2 $x, \bar{x}, 1/3$ (2 <sub>3</sub>  0,0,2/3)	(5) 2 $x, 2x, 1/6$ (2 <sub>2</sub>  0,0,1/3)	(6) 2 $2x, x, 0$ (2 <sub>1</sub>  0,0,0)
--	---	---

For 1' + set

(1) 1' (1 0,0,0)'	(2) 3 <sup>+</sup> ' (0,0,1/3) 0,0,z (3 <sub>z</sub>  0,0,1/3)'	(3) 3 <sup>-</sup> ' (0,0,2/3) 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,2/3)'
----------------------	--	--

(4) 2' (2 <sub>3</sub>  0,0,2/3)'	(5) 2' (2 <sub>2</sub>  0,0,1/3)'	(6) 2' (2 <sub>1</sub>  0,0,0)'
--------------------------------------	--------------------------------------	------------------------------------

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

**Positions**

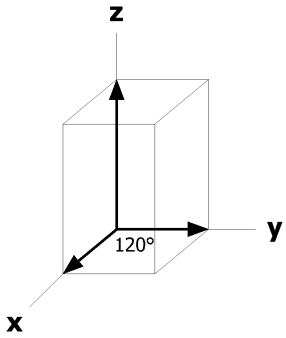
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			1 +	1' +	
6 c 11'	(1)	x,y,z [0,0,0]	(2)	$\bar{y}, x-y, z+1/3$ [0,0,0]	(3) $\bar{x}+y, \bar{x}, z+2/3$ [0,0,0]
	(4)	$\bar{y}, \bar{x}, \bar{z}+2/3$ [0,0,0]	(5)	$\bar{x}+y, y, \bar{z}+1/3$ [0,0,0]	(6) x,x-y, $\bar{z}$ [0,0,0]
3 b ..21'		x, $\bar{x}$ ,5/6 [0,0,0]		x,2x,1/6 [0,0,0]	2 $\bar{x}$ , $\bar{x}$ ,1/2 [0,0,0]
3 a ..21'		x, $\bar{x}$ ,1/3 [0,0,0]		x,2x,2/3 [0,0,0]	2 $\bar{x}$ , $\bar{x}$ ,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p3m11'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/6

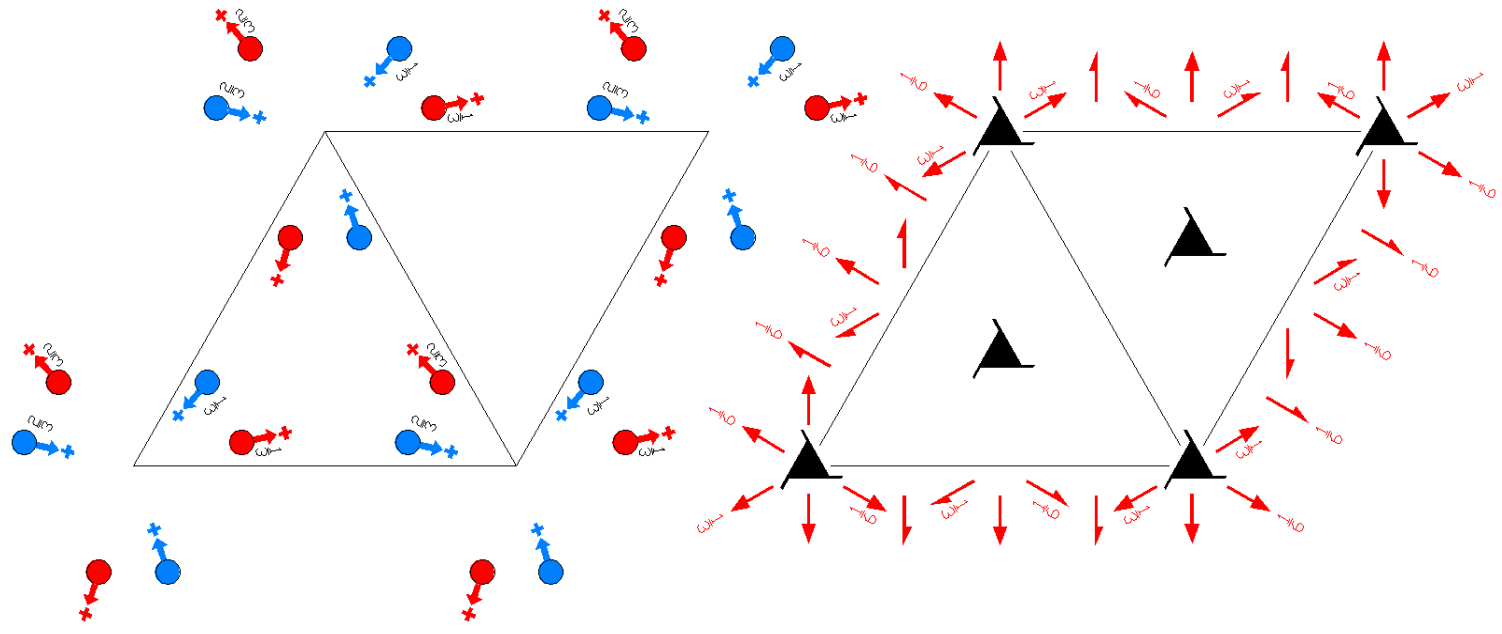
Along [2,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P3_112'$   
151.3.1261

$312'$   
 $P3_112'$

Trigonal



Origin on  $2'$   $[210]$  at  $3_11(1,1,2')$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

**Symmetry Operations**

- (1) 1  $(1|0,0,0)$
- (2)  $3^+$   $(0,0,1/3) 0,0,z$   
 $(3_z|0,0,1/3)$
- (3)  $3^-$   $(0,0,2/3) 0,0,z$   
 $(3_z^{-1}|0,0,2/3)$
- (4)  $2'$   $x, \bar{x}, 1/3$   
 $(2_3|0,0,2/3)'$
- (5)  $2'$   $x, 2x, 1/6$   
 $(2_2|0,0,1/3)'$
- (6)  $2'$   $2x, x, 0$   
 $(2_1|0,0,0)'$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	c	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{y}, x-y, z+1/3$ [ $\bar{v}$ , u-v, w]	(3) $\bar{x}+y, \bar{x}, z+2/3$ [ $\bar{u}+v, \bar{u}$ , w]
			(4) $\bar{y}, \bar{x}, \bar{z}+2/3$ [v, u, w]	(5) $\bar{x}+y, y, \bar{z}+1/3$ [u-v, $\bar{v}$ , w]	(6) $x, x-y, \bar{z}$ [ $\bar{u}$ , $\bar{u}+v$ , w]
3	b	..2'	$x, \bar{x}, 5/6$ [u, u, w]	$x, 2x, 1/6$ [ $\bar{u}$ , 0, w]	$2\bar{x}, \bar{x}, 1/2$ [0, $\bar{u}$ , w]
3	a	..2'	$x, \bar{x}, 1/3$ [u, u, w]	$x, 2x, 2/3$ [ $\bar{u}$ , 0, w]	$2\bar{x}, \bar{x}, 0$ [0, $\bar{u}$ , w]

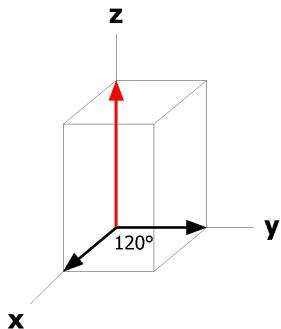
**Symmetry of Special Projections**

Along [0,0,1] p3m1  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/6

Along [2,1,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0





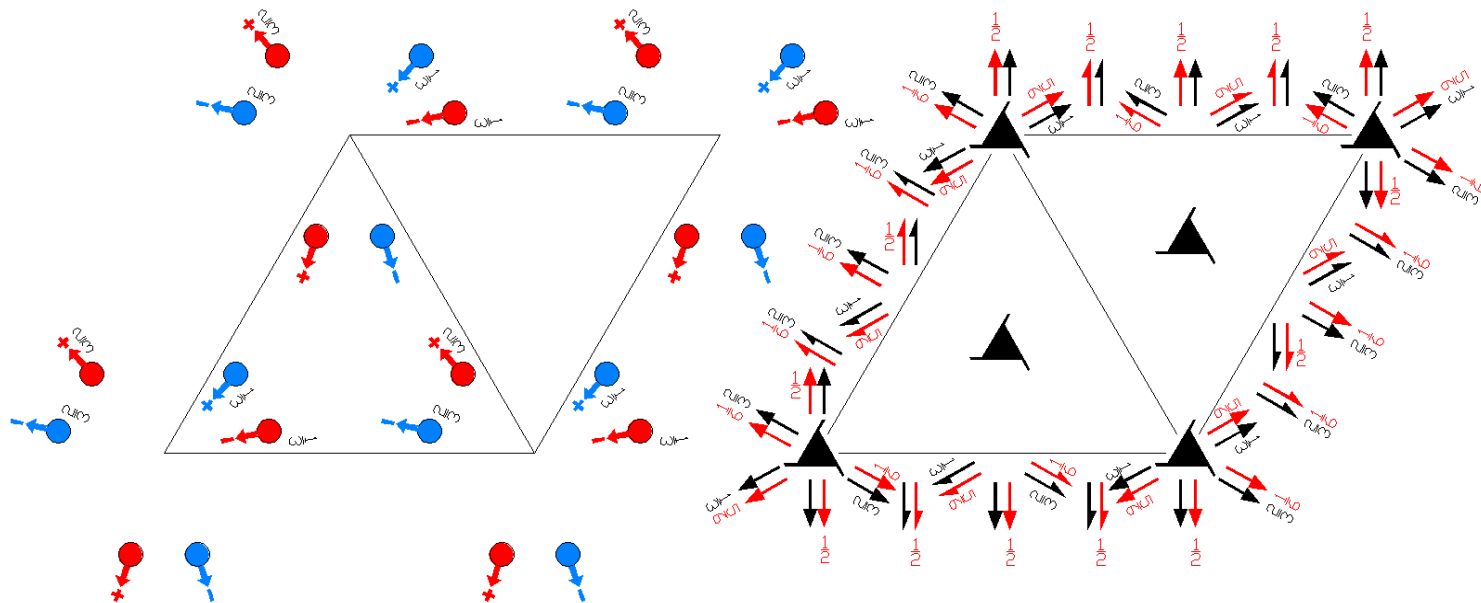
$P_{2c} 3_2 12$

151.4.1262

$3121'$

$P_{2c} 3_2 12$

Trigonal



Origin on 2 [210] at  $3_2 1(1,1,2)$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

### Symmetry Operations

For (0,0,0) + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                           | (2) $3^+ (0,0,1/3)$ 0,0,z<br>( $3_z$  0,0,1/3)' | (3) $3^- (0,0,2/3)$ 0,0,z<br>( $3_z^{-1}$  0,0,2/3) |
| (4) 2 $x, \bar{x}, 1/3$<br>( $2_3$  0,0,2/3) | (5) $2' x, 2x, 1/6$<br>( $2_2$  0,0,1/3)'       | (6) 2 $2x, x, 0$<br>( $2_1$  0,0,0)                 |

For (0,0,1)' + set

- |  |  |  |
|--|--|--|
| (1) $t' (0,0,1)$<br>(1 0,0,1)'                 | (2) $3^+ (0,0,4/3)$ 0,0,z<br>( $3_z$  0,0,4/3) | (3) $3^- (0,0,5/3)$ 0,0,z<br>( $3_z^{-1}$  0,0,5/3)' |
| (4) $2' x, \bar{x}, 5/6$<br>( $2_3$  0,0,5/3)' | (5) 2 $x, 2x, 2/3$<br>( $2_2$  0,0,4/3)        | (6) $2' 2x, x, 1/2$<br>( $2_1$  0,0,1)'              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

### Positions

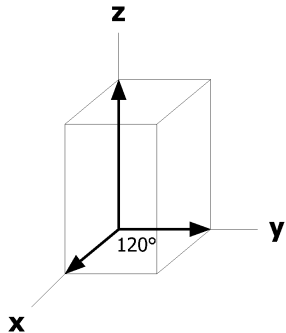
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			(0,0,0) +	(0,0,1)' +	
12	c	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z+1/3$ [ $\bar{v}, \bar{u}+v, \bar{w}$ ]	(3) $\bar{x}+y, \bar{x}, z+2/3$ [ $\bar{u}+v, \bar{u}, w$ ]
			(4) $\bar{y}, \bar{x}, \bar{z}+2/3$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(5) $\bar{x}+y, y, \bar{z}+1/3$ [ $u-v, \bar{v}, w$ ]	(6) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ]
6	b	..2'	x, $\bar{x}, 5/6$ [u,u,w]	x,2x,1/6 [ $\bar{u}, 0, w$ ]	2 $\bar{x}, \bar{x}, 1/2$ [0, $\bar{u}, \bar{w}$ ]
6	a	..2	x, $\bar{x}, 1/3$ [u, $\bar{u}, 0$ ]	x,2x,2/3 [ $\bar{u}, 2\bar{u}, 0$ ]	2 $\bar{x}, \bar{x}, 0$ [2u,u,0]

### Symmetry of Special Projections

Along [0,0,1] p3m11'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>\*1m1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/6

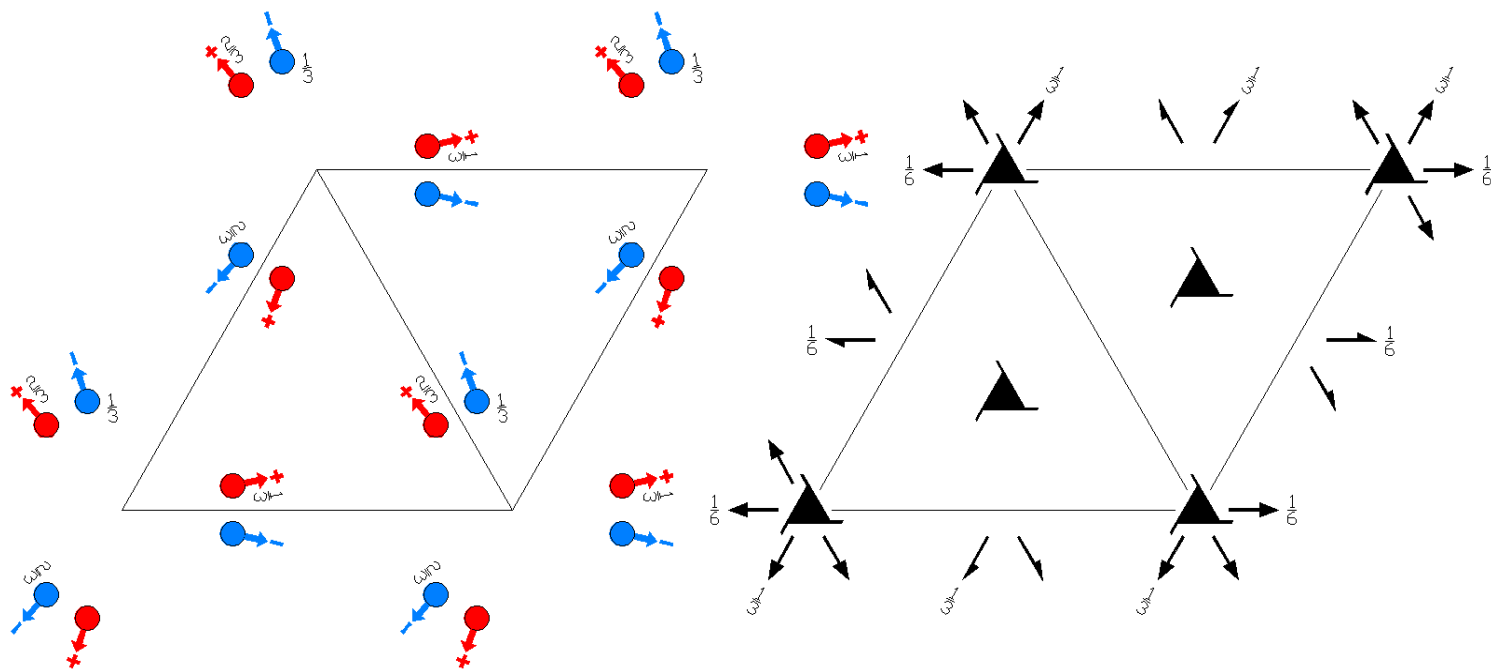
Along [2,1,0] p<sub>2a</sub>\*211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P3<sub>1</sub>21  
152.1.1263

321  
P3<sub>1</sub>21

Trigonal



Origin on 2 [110] at 3<sub>1</sub>(1,1,2) 1

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

### Symmetry Operations

- |  |  |  |
|--|--|--|
| (1) 1<br>(1 0,0,0)                       | (2) 3 <sup>+</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub>   0,0,1/3) | (3) 3 <sup>-</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>   0,0,2/3) |
| (4) 2 x,x,0<br>(2 <sub>xy</sub>   0,0,0) | (5) 2 x,0,1/3<br>(2 <sub>x</sub>   0,0,2/3)                      | (6) 2 0,y,1/6<br>(2 <sub>y</sub>   0,0,1/3)                                    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

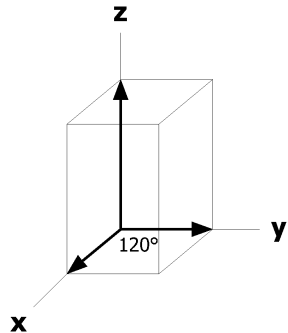
			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
6	c	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z+1/3$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z+2/3$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(5) $x-y,\bar{y},\bar{z}+2/3$ [ $u-v,\bar{v},\bar{w}$ ]	(6) $\bar{x},\bar{x}+y,\bar{z}+1/3$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
3	b	.2.	$x,0,5/6$ [u,0,0]	0,x,1/6 [0,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]
3	a	.2.	$x,0,1/3$ [u,0,0]	0,x,2/3 [0,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]

**Symmetry of Special Projections**

Along [0,0,1] p31m'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/3

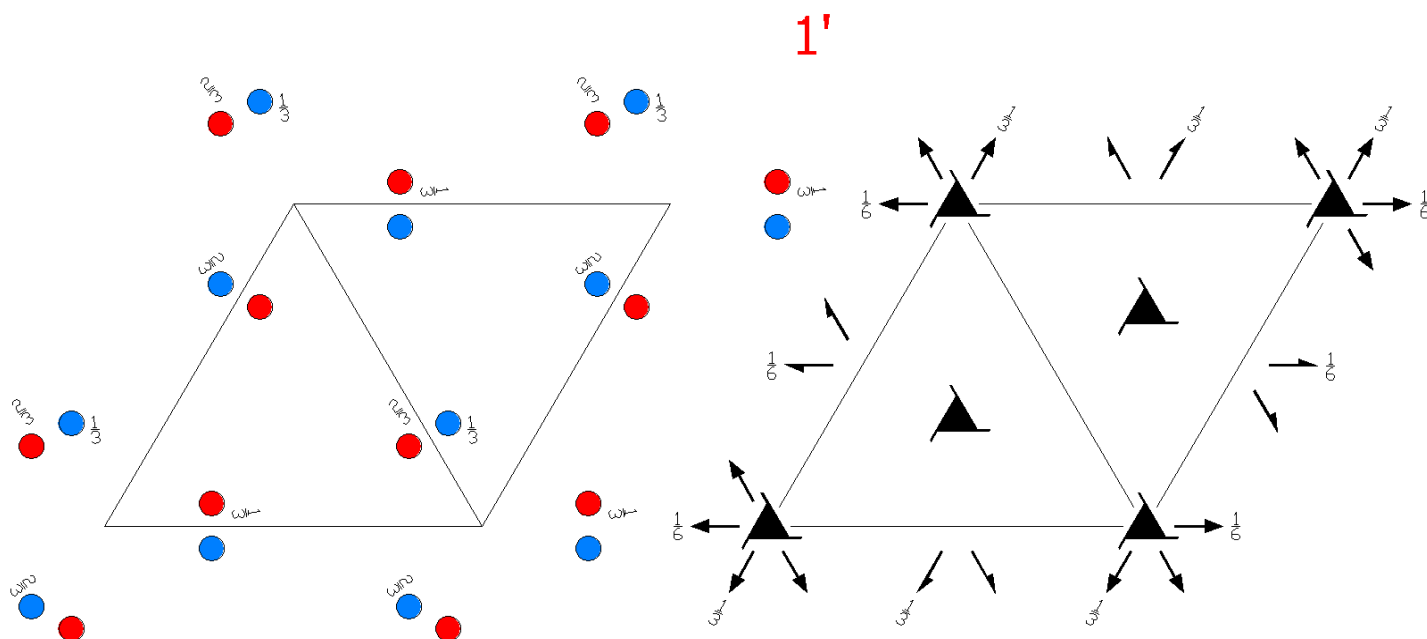
Along [2,1,0] p1m'1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/6



P3<sub>1</sub>211'  
152.2.1264

3211'  
P3<sub>1</sub>211'

Trigonal



<b>Asymmetric unit</b>	$0 \leq x \leq 1;$	$0 \leq y \leq 1;$	$0 \leq z \leq 1/6$
Vertices	0,0,0	1,0,0	1,1,0
	0,0,1/6	1,0,1/6	1,1,1/6
			0,1,0
			0,1,1/6

**Symmetry Operations**

For 1 + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                      | (2) 3 <sup>+</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub>  0,0,1/3) | (3) 3 <sup>-</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,2/3) |
| (4) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0) | (5) 2 x,0,1/3<br>(2 <sub>x</sub>  0,0,2/3)                      | (6) 2 0,y,1/6<br>(2 <sub>y</sub>  0,0,1/3)                                    |

For 1' + set

- |                                     |  |  |
|-------------------------------------|--|--|
| (1) 1'<br>(1 0,0,0)'                | (2) 3 <sup>+</sup> ' (0,0,1/3) 0,0,z<br>(3 <sub>z</sub>  0,0,1/3)' | (3) 3 <sup>-</sup> ' (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,2/3)' |
| (4) 2'<br>(2 <sub>xy</sub>  0,0,0)' | (5) 2'<br>(2 <sub>x</sub>  0,0,2/3)'                               | (6) 2'<br>(2 <sub>y</sub>  0,0,1/3)'   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

**Positions**

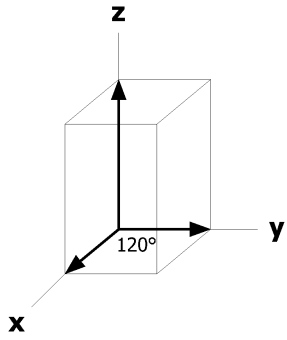
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			1 +	1' +	
6	c	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}, x-y, z+1/3$ [0,0,0]	(3) $\bar{x}+y, \bar{x}, z+2/3$ [0,0,0]
			(4) y,x, $\bar{z}$ [0,0,0]	(5) x-y, $\bar{y}, \bar{z}+2/3$ [0,0,0]	(6) $\bar{x}, \bar{x}+y, \bar{z}+1/3$ [0,0,0]
3	b	.2.1'	x,0,5/6 [0,0,0]	0,x,1/6 [0,0,0]	$\bar{x}, \bar{x}, 1/2$ [0,0,0]
3	a	.2.1'	x,0,1/3 [0,0,0]	0,x,2/3 [0,0,0]	$\bar{x}, \bar{x}, 0$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p31m1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/3

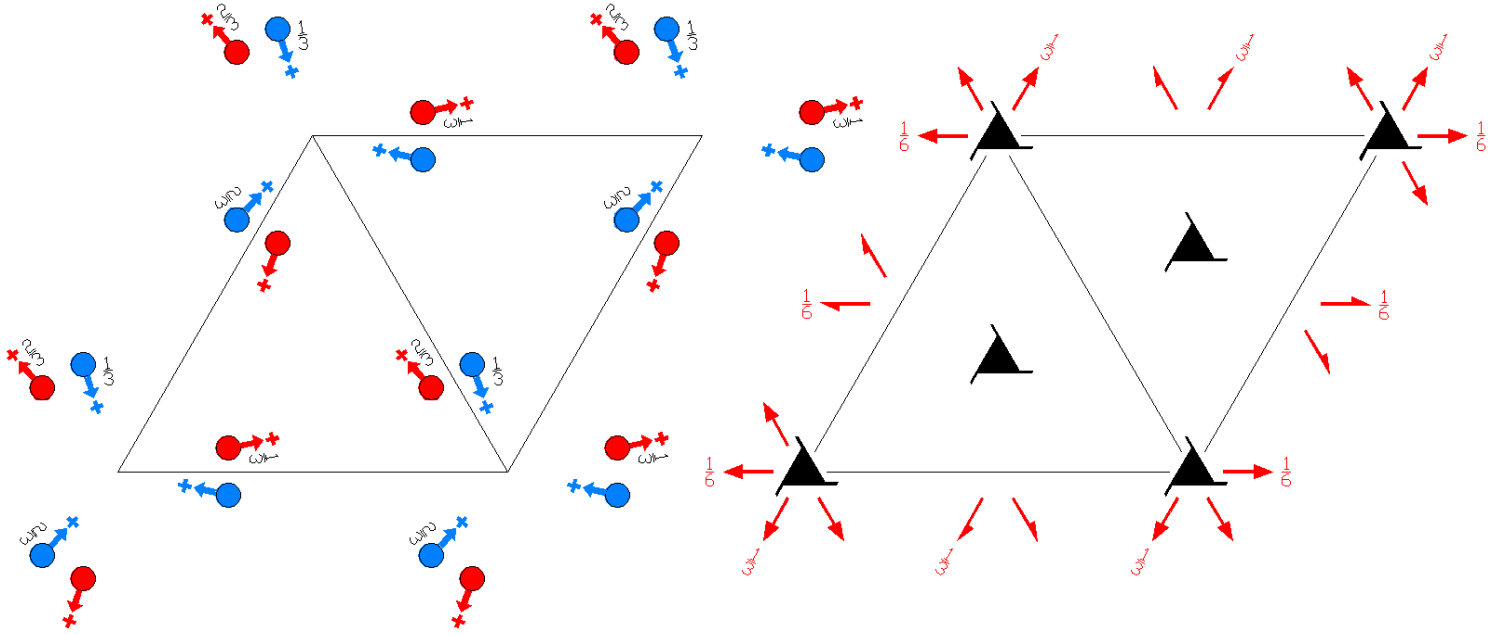
Along [2,1,0] p1m11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/6



P3<sub>1</sub>2'1  
152.3.1265

32'1  
P3<sub>1</sub>2'1

Trigonal



Origin on 2' [110] at 3<sub>1</sub>(1,1,2') 1

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

### Symmetry Operations

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                        | (2) 3 <sup>+</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub>  0,0,1/3) | (3) 3 <sup>-</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,2/3) |
| (4) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)' | (5) 2' x,0,1/3<br>(2 <sub>x</sub>  0,0,2/3)'                    | (6) 2' 0,y,1/6<br>(2 <sub>y</sub>  0,0,1/3)'                                  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	c	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z+1/3$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z+2/3$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(5) $x-y,\bar{y},\bar{z}+2/3$ [ $\bar{u}+v,v,w$ ]	(6) $\bar{x},\bar{x}+y,\bar{z}+1/3$ [u,u-v,w]
3	b	.2'	$x,0,5/6$ [u,2u,w]	$0,x,1/6$ [ $2\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},1/2$ [u, $\bar{u},w$ ]
3	a	.2'	$x,0,1/3$ [u,2u,w]	$0,x,2/3$ [ $2\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},0$ [u, $\bar{u},w$ ]

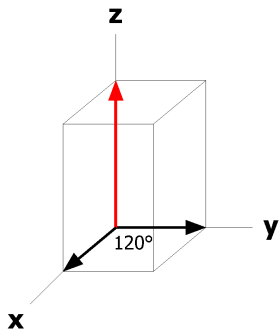
**Symmetry of Special Projections**

Along [0,0,1] p31m  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/3

Along [2,1,0] p1m1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/6





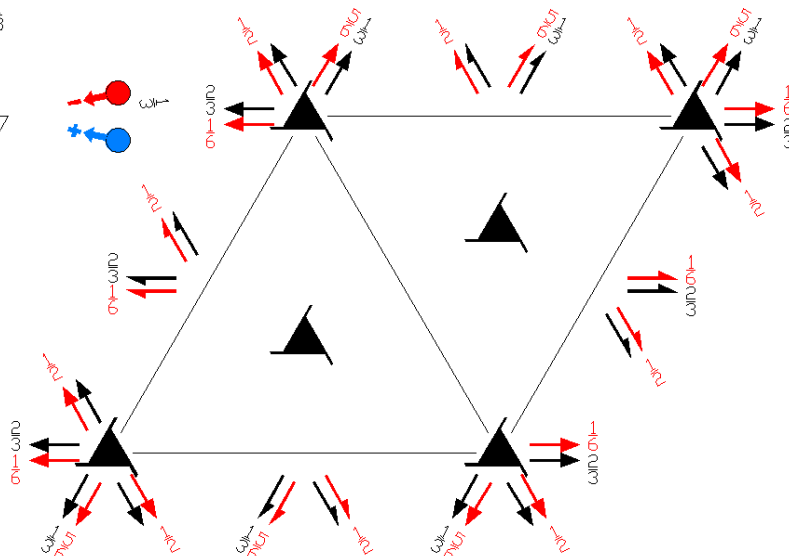
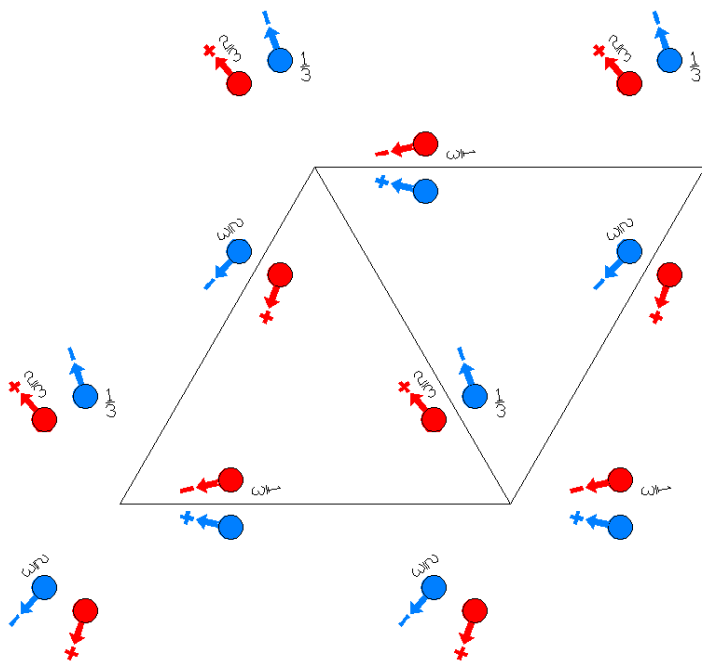
$P_{2c} 3_2 21$

152.4.1266

3211'

$P_{2c} 3_2 21$

Trigonal



Origin on 2 [110] at  $3_2(1,1,2)$  1

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

### Symmetry Operations

For (0,0,0) + set

- |                                   |   |   |
|-----------------------------------|---|---|
| (1) 1<br>(1 0,0,0)                | (2) $3^+$ (0,0,1/3) 0,0,z<br>( $3_z$  0,0,1/3)' | (3) $3^-$ (0,0,2/3) 0,0,z<br>( $3_z^{-1}$  0,0,2/3) |
| (4) 2 x,x,0<br>( $2_{xy}$  0,0,0) | (5) 2 x,0,1/3<br>( $2_x$  0,0,2/3)              | (6) $2'$ 0,y,1/6<br>( $2_y$  0,0,1/3)'              |

For (0,0,1)' + set

- |   |  |  |
|---|--|--|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'          | (2) $3^+$ (0,0,4/3) 0,0,z<br>( $3_z$  0,0,4/3) | (3) $3^-$ (0,0,5/3) 0,0,z<br>( $3_z^{-1}$  0,0,5/3)' |
| (4) $2'$ x,x,1/2<br>( $2_{xy}$  0,0,1)' | (5) $2'$ x,0,5/6<br>( $2_x$  0,0,5/3)'         | (6) 2 0,y,2/3<br>( $2_y$  0,0,4/3)'                  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

### Positions

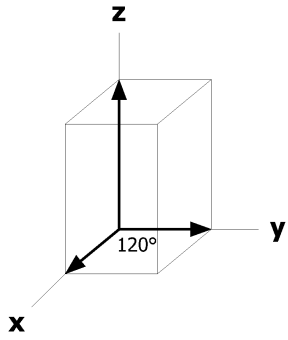
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			(0,0,0) +	(0,0,1)' +	
12	c	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z+1/3$ [v, $\bar{u}+v, \bar{w}$ ]	(3) $\bar{x}+y, \bar{x}, z+2/3$ [ $\bar{u}+v, \bar{u}, w$ ]
			(4) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(5) x-y, $\bar{y}, \bar{z}+2/3$ [u-v, $\bar{v}, \bar{w}$ ]	(6) $\bar{x}, \bar{x}+y, \bar{z}+1/3$ [u,u-v,w]
6	b	.2'	x,0,5/6 [u,2u,w]	0,x,1/6 [2 $\bar{u}, \bar{u}, w$ ]	$\bar{x}, \bar{x}, 1/2$ [ $\bar{u}, u, \bar{w}$ ]
6	a	.2.	x,0,1/3 [u,0,0]	0,x,2/3 [0, $\bar{u}, 0$ ]	$\bar{x}, \bar{x}, 0$ [u,u,0]

### Symmetry of Special Projections

Along [0,0,1] p31m1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>\*211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/3

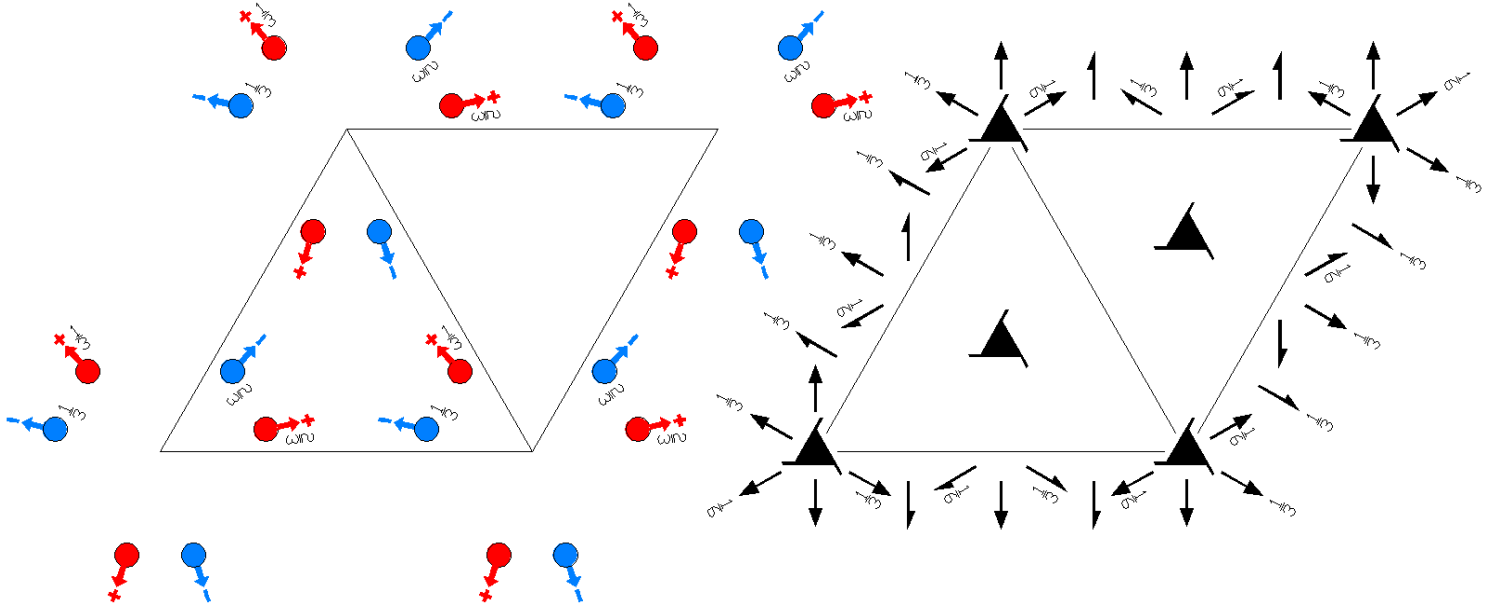
Along [2,1,0] p<sub>2a</sub>\*1m1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/6



$P3_212$   
153.1.1267

312  
 $P3_212$

Trigonal



Origin on 2 [210] at  $3_21(1,1,2)$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

### Symmetry Operations

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                           | (2) $3^+$ (0,0,2/3) 0,0,z<br>( $3_z$  0,0,2/3) | (3) $3^-$ (0,0,1/3) 0,0,z<br>( $3_z^{-1}$  0,0,1/3) |
| (4) 2 $x, \bar{x}, 1/6$<br>( $2_3$  0,0,1/3) | (5) 2 $x, 2x, 1/3$<br>( $2_2$  0,0,2/3)        | (6) 2 $2x, x, 0$<br>( $2_1$  0,0,0)                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

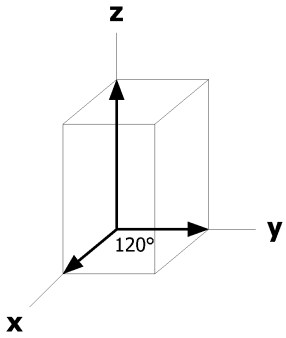
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	c	1	(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{y}, x-y, z+2/3$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z+1/3$ [ $\bar{u}+v, \bar{u}, w$ ]
			(4) $\bar{y}, \bar{x}, \bar{z}+1/3$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(5) $\bar{x}+y, y, \bar{z}+2/3$ [ $\bar{u}+v, v, \bar{w}$ ]	(6) $x, x-y, \bar{z}$ [ $u, u-v, \bar{w}$ ]
3	b	..2	$x, \bar{x}, 1/6$ [ $u, \bar{u}, 0$ ]	$x, 2x, 5/6$ [ $u, 2u, 0$ ]	$2\bar{x}, \bar{x}, 1/2$ [ $2\bar{u}, \bar{u}, 0$ ]
3	a	..2	$x, \bar{x}, 2/3$ [ $u, \bar{u}, 0$ ]	$x, 2x, 1/3$ [ $u, 2u, 0$ ]	$2\bar{x}, \bar{x}, 0$ [ $2\bar{u}, \bar{u}, 0$ ]

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p3m'1$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p1m'1$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,1/3$

Along  $[2,1,0]$   $p211$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,0$



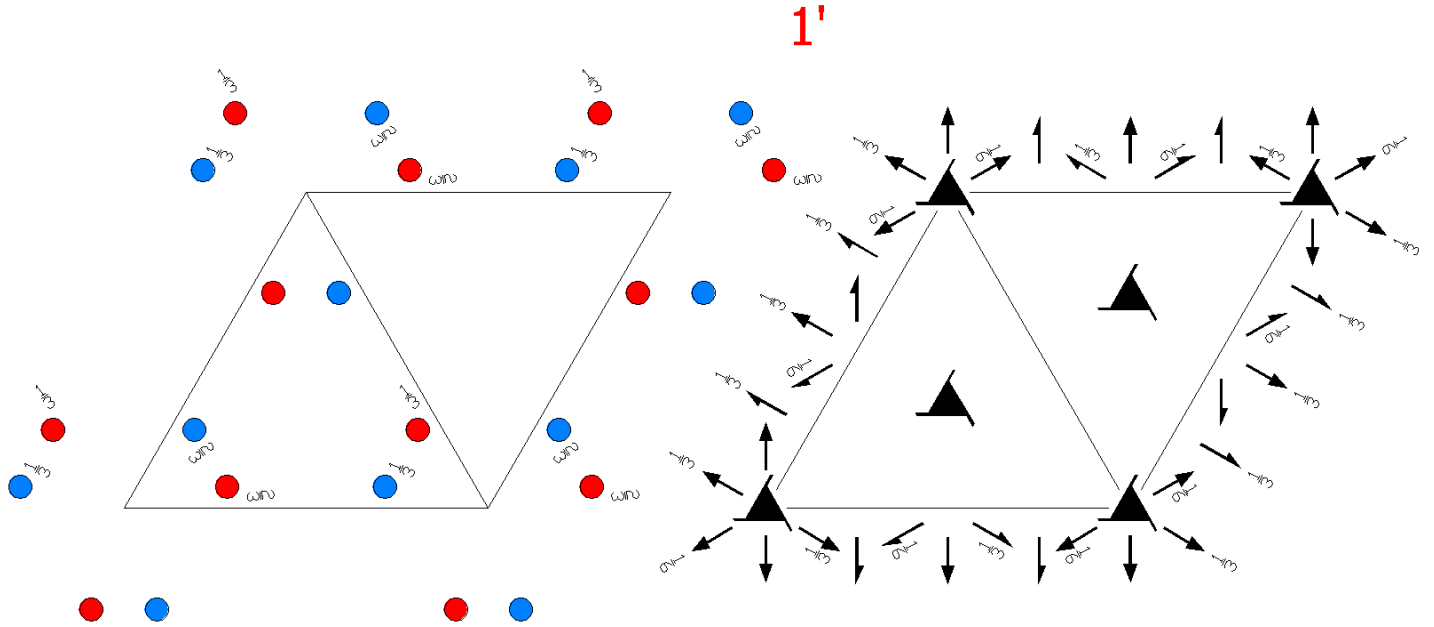
$P3_2121'$

153.2.1268

3121'

$P3_2121'$

Trigonal



Origin on  $21'$   $[210]$  at  $3_21(1,1,2)1'$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

**Symmetry Operations**

For  $1 + \text{set}$

(1) $1$ ( $1 0,0,0$ )	(2) $3^+ (0,0,2/3) 0,0,z$ ( $3_z 0,0,2/3$ )	(3) $3^- (0,0,1/3) 0,0,z$ ( $3_z^{-1} 0,0,1/3$ )
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(4) $2 \ x, \bar{x}, 1/6$ ( $2_3 0,0,1/3$ )	(5) $2 \ x, 2x, 1/3$ ( $2_2 0,0,2/3$ )	(6) $2 \ 2x, x, 0$ ( $2_1 0,0,0$ )
--	---	---------------------------------------

For  $1' + \text{set}$

(1) $1'$ ( $1 0,0,0$ )'	(2) $3^+ (0,0,2/3) 0,0,z$ ( $3_z 0,0,2/3$ )'	(3) $3^- (0,0,1/3) 0,0,z$ ( $3_z^{-1} 0,0,1/3$ )'
----------------------------	---	--

(4) $2'$ $x, \bar{x}, 1/6$ ( $2_3 0,0,1/3$ )'	(5) $2'$ $x, 2x, 1/3$ ( $2_2 0,0,2/3$ )'	(6) $2'$ $2x, x, 0$ ( $2_1 0,0,0$ )'
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**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

**Positions**

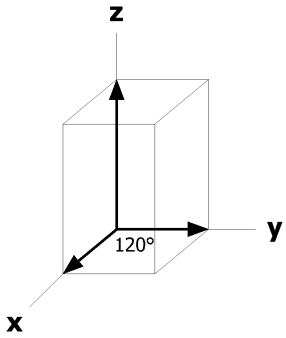
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			1 +	1' +	
6	c	11'	(1) x,y,z [0,0,0]	(2) $\bar{y},x-y,z+2/3$ [0,0,0]	(3) $\bar{x}+y,\bar{x},z+1/3$ [0,0,0]
			(4) $\bar{y},\bar{x},\bar{z}+1/3$ [0,0,0]	(5) $\bar{x}+y,y,\bar{z}+2/3$ [0,0,0]	(6) x,x-y, $\bar{z}$ [0,0,0]
3	b	..21'	x, $\bar{x},1/6$ [0,0,0]	x,2x,5/6 [0,0,0]	2 $\bar{x},\bar{x},1/2$ [0,0,0]
3	a	..21'	x, $\bar{x},2/3$ [0,0,0]	x,2x,1/3 [0,0,0]	2 $\bar{x},\bar{x},0$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p3m11'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/3

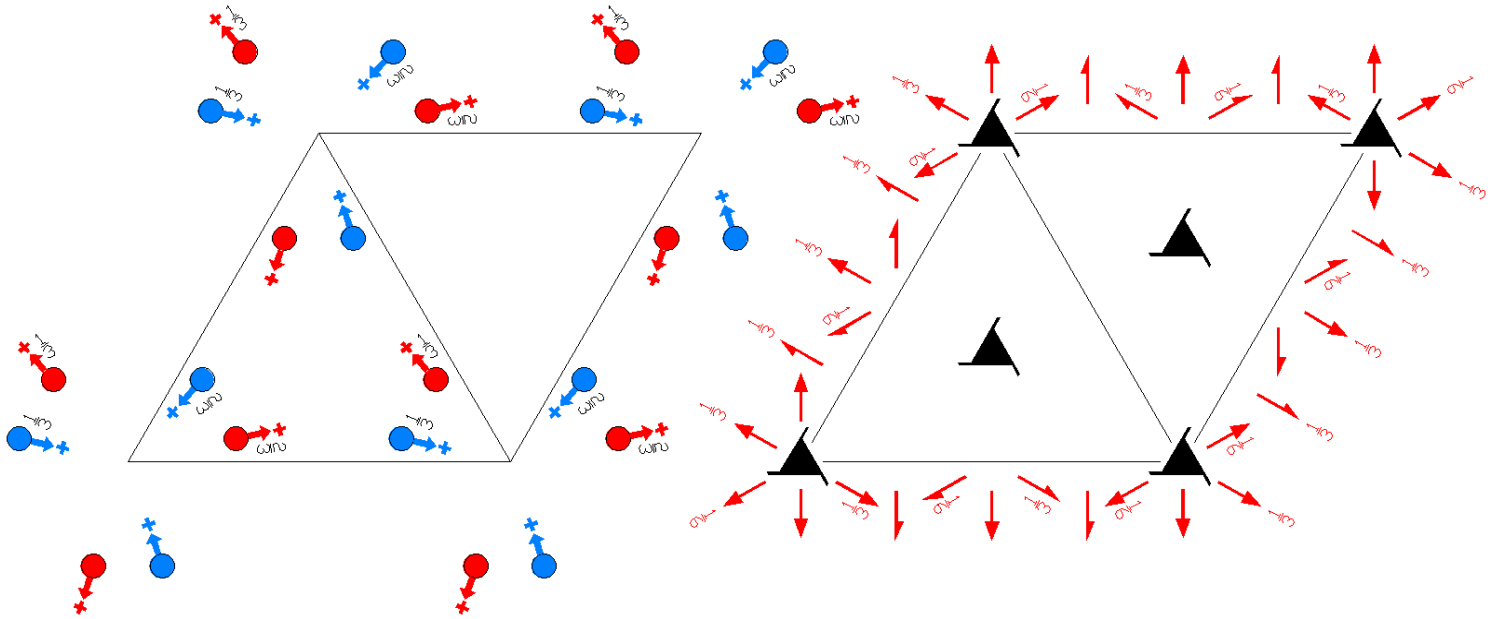
Along [2,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P3_212'$   
153.3.1269

$312'$   
 $P3_212'$

Trigonal



Origin on  $2'$   $[210]$  at  $3_21(1,1,2')$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

**Symmetry Operations**

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                               | (2) $3^+$ (0,0,2/3) 0,0,z<br>( $3_z$  0,0,2/3) | (3) $3^-$ (0,0,1/3) 0,0,z<br>( $3_z^{-1}$  0,0,1/3) |
| (4) $2'$ $x, \bar{x}, 1/6$<br>( $2_3$  0,0,1/3)' | (5) $2'$ $x, 2x, 1/3$<br>( $2_2$  0,0,2/3)'    | (6) $2'$ $2x, x, 0$<br>( $2_1$  0,0,0)'             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	c	1	(1) $x, y, z$ [u,v,w]	(2) $\bar{y}, x-y, z+2/3$ [ $\bar{v}$ , u-v, w]	(3) $\bar{x}+y, \bar{x}, z+1/3$ [ $\bar{u}+v, \bar{u}$ , w]
			(4) $\bar{y}, \bar{x}, \bar{z}+1/3$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(5) $\bar{x}+y, y, \bar{z}+2/3$ [ $\bar{u}+v, v, \bar{w}$ ]	(6) $x, x-y, \bar{z}$ [u, u-v, $\bar{w}$ ]
3	b	..2'	$x, \bar{x}, 1/6$ [u, u, w]	$x, 2x, 5/6$ [ $\bar{u}$ , 0, w]	$2\bar{x}, \bar{x}, 1/2$ [0, $\bar{u}$ , w]
3	a	..2'	$x, \bar{x}, 2/3$ [u, u, w]	$x, 2x, 1/3$ [ $\bar{u}$ , 0, w]	$2\bar{x}, \bar{x}, 0$ [0, $\bar{u}$ , w]

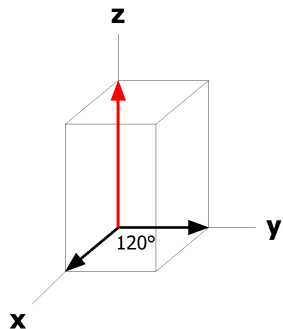
**Symmetry of Special Projections**

Along [0,0,1] p3m1  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/3

Along [2,1,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0





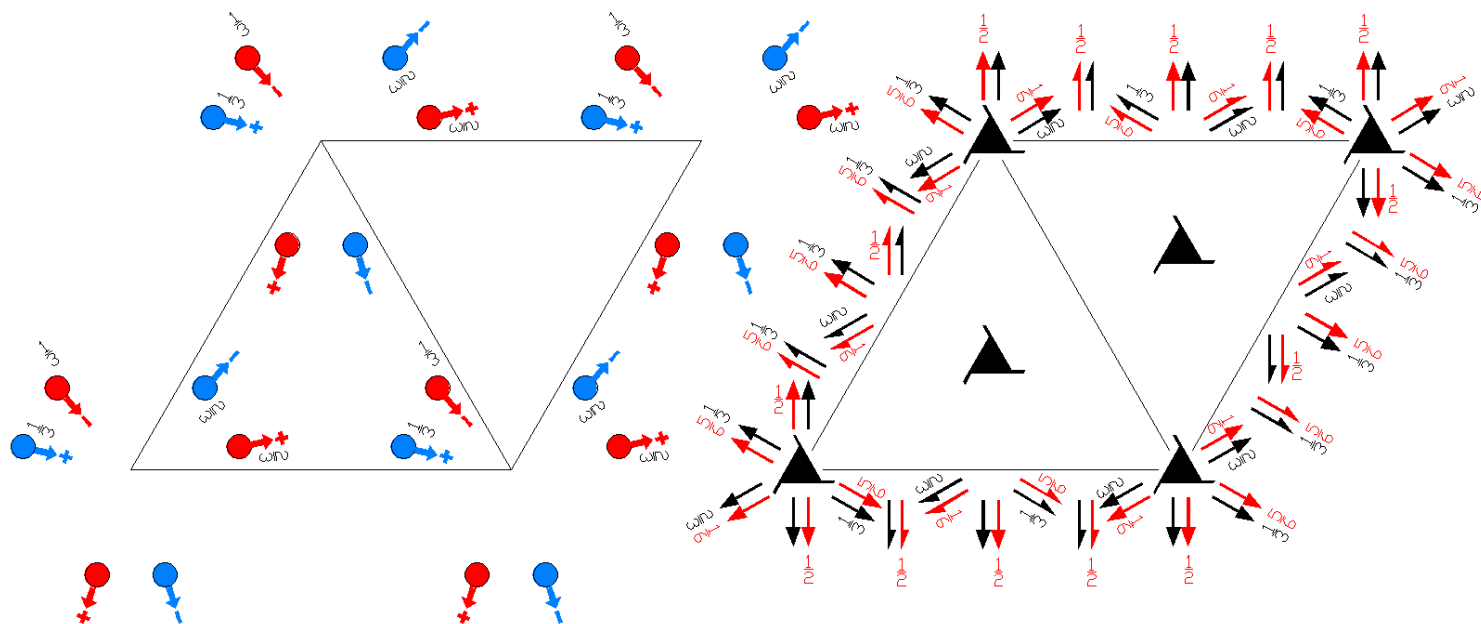
$P_{2c} 3_2 12$

153.4.1270

$3121'$

$P_{2c} 3_2 12$

Trigonal



Origin on 2 [210] at  $3_2 1(1,1,2)$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

### Symmetry Operations

For (0,0,0) + set

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                             | (2) $3^+ (0,0,2/3)$ 0,0,z<br>( $3_z$  0,0,2/3) | (3) $3^{-1} (0,0,1/3)$ 0,0,z<br>( $3_z^{-1}$  0,0,1/3)' |
| (4) $2' x, \bar{x}, 1/6$<br>( $2_3$  0,0,1/3)' | (5) $2 x, 2x, 1/3$<br>( $2_2$  0,0,2/3)        | (6) $2 2x, x, 0$<br>( $2_1$  0,0,0)                     |

For (0,0,1)' + set

- |  |   |   |
|--|---|---|
| (1) $t' (0,0,1)$<br>(1 0,0,1)'               | (2) $3^+ (0,0,5/3)$ 0,0,z<br>( $3_z$  0,0,5/3)' | (3) $3^- (0,0,4/3)$ 0,0,z<br>( $3_z^{-1}$  0,0,4/3) |
| (4) $2 x, \bar{x}, 2/3$<br>( $2_3$  0,0,4/3) | (5) $2' x, 2x, 5/6$<br>( $2_2$  0,0,5/3)'       | (6) $2' 2x, x, 1/2$<br>( $2_1$  0,0,1)'             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

### Positions

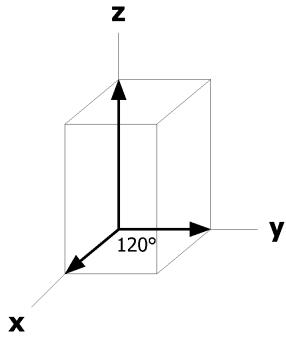
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
				(0,0,0) +	(0,0,1)' +
12	c	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z+2/3$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z+1/3$ [ $u-v, u, \bar{w}$ ]
			(4) $\bar{y}, \bar{x}, \bar{z}+1/3$ [ $v, u, w$ ]	(5) $\bar{x}+y, y, \bar{z}+2/3$ [ $\bar{u}+v, v, \bar{w}$ ]	(6) x,x-y, $\bar{z}$ [ $u, u-v, \bar{w}$ ]
6	b	..2'	x, $\bar{x}, 1/6$ [u,u,w]	x, 2x, 5/6 [ $\bar{u}, 0, w$ ]	2 $\bar{x}, \bar{x}, 1/2$ [0, $\bar{u}, w$ ]
6	a	..2	x, $\bar{x}, 2/3$ [u, $\bar{u}, 0$ ]	x, 2x, 1/3 [ $\bar{u}, 2\bar{u}, 0$ ]	2 $\bar{x}, \bar{x}, 0$ [2 $\bar{u}, \bar{u}, 0$ ]

### Symmetry of Special Projections

Along [0,0,1] p3m11'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a\*</sub>1m1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,5/6

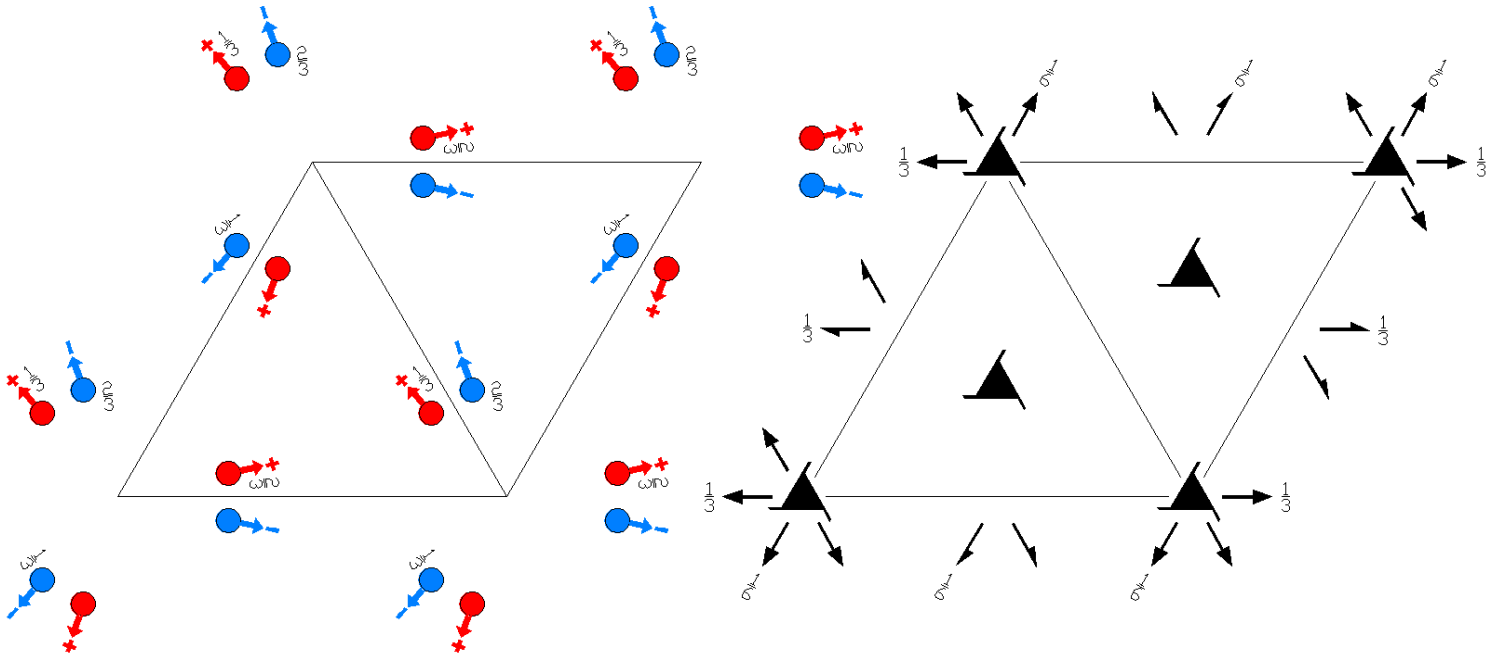
Along [2,1,0] p<sub>2a\*</sub>211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P3<sub>2</sub>21  
154.1.1271

321  
P3<sub>2</sub>21

Trigonal



Origin on 2 [110] at 3<sub>2</sub>(1,1,2) 1

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

### Symmetry Operations

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                      | (2) 3 <sup>+</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub>  0,0,2/3) | (3) 3 <sup>-</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,1/3) |
| (4) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0) | (5) 2 x,0,1/6<br>(2 <sub>x</sub>  0,0,1/3)                      | (6) 2 0,y,1/3<br>(2 <sub>y</sub>  0,0,2/3)                                    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

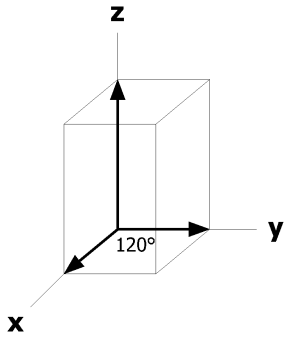
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	c	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z+2/3$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z+1/3$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $y,x,\bar{z}$ [ $v,u,\bar{w}$ ]	(5) $x-y,\bar{y},\bar{z}+1/3$ [ $u-v,\bar{v},\bar{w}$ ]	(6) $\bar{x},\bar{x}+y,\bar{z}+2/3$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
3	b	.2.	$x,0,1/6$ [u,0,0]	$0,x,5/6$ [0,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]
3	a	.2.	$x,0,2/3$ [u,0,0]	$0,x,1/3$ [0,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]

**Symmetry of Special Projections**

Along [0,0,1] p31m'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/6

Along [2,1,0] p1m'1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/3



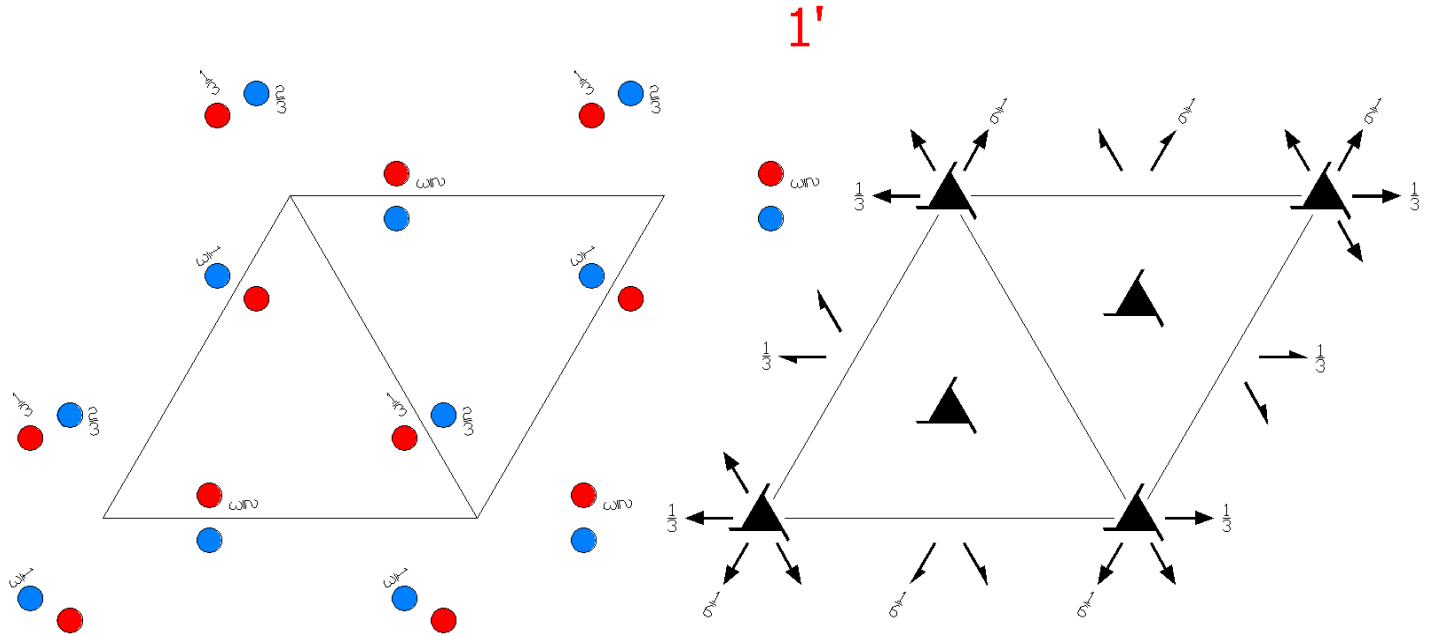
$P3_2 211'$

154.2.1272

$3211'$

$P3_2 211'$

Trigonal



Origin on  $21'$   $[110]$  at  $3_2(1,1,2)$   $11'$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

**Symmetry Operations**

For  $1 +$  set

(1) $1$ ( $1 0,0,0$ )	(2) $3^+$ (0,0,2/3) $0,0,z$ ( $3_z 0,0,2/3$ )	(3) $3^-$ (0,0,1/3) $0,0,z$ ( $3_z^{-1} 0,0,1/3$ )
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(4) $2$ $x,x,0$ ( $2_{xy} 0,0,0$ )	(5) $2$ $x,0,1/6$ ( $2_x 0,0,1/3$ )	(6) $2$ $0,y,1/3$ ( $2_y 0,0,2/3$ )
---------------------------------------	--	--

For  $1' +$  set

(1) $1'$ ( $1 0,0,0$ )'	(2) $3^{+'}$ (0,0,2/3) $0,0,z$ ( $3_z 0,0,2/3$ )'	(3) $3^{-'}$ (0,0,1/3) $0,0,z$ ( $3_z^{-1} 0,0,1/3$ )'
----------------------------	--	---

(4) $2'$ $x,x,0$ ( $2_{xy} 0,0,0$ )'	(5) $2'$ $x,0,1/6$ ( $2_x 0,0,1/3$ )'	(6) $2'$ $0,y,1/3$ ( $2_y 0,0,2/3$ )'
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**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

**Positions**

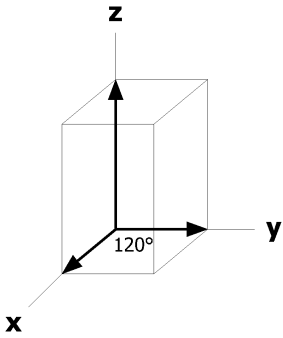
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			1 +	1' +	
6	c	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}, x-y, z+2/3$ [0,0,0]	(3) $\bar{x}+y, \bar{x}, z+1/3$ [0,0,0]
			(4) y,x, $\bar{z}$ [0,0,0]	(5) x-y, $\bar{y}, \bar{z}+1/3$ [0,0,0]	(6) $\bar{x}, \bar{x}+y, \bar{z}+2/3$ [0,0,0]
3	b	.2.1'	x,0,1/6 [0,0,0]	0,x,5/6 [0,0,0]	$\bar{x}, \bar{x}, 1/2$ [0,0,0]
3	a	.2.1'	x,0,2/3 [0,0,0]	0,x,1/3 [0,0,0]	$\bar{x}, \bar{x}, 0$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p31m1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/6

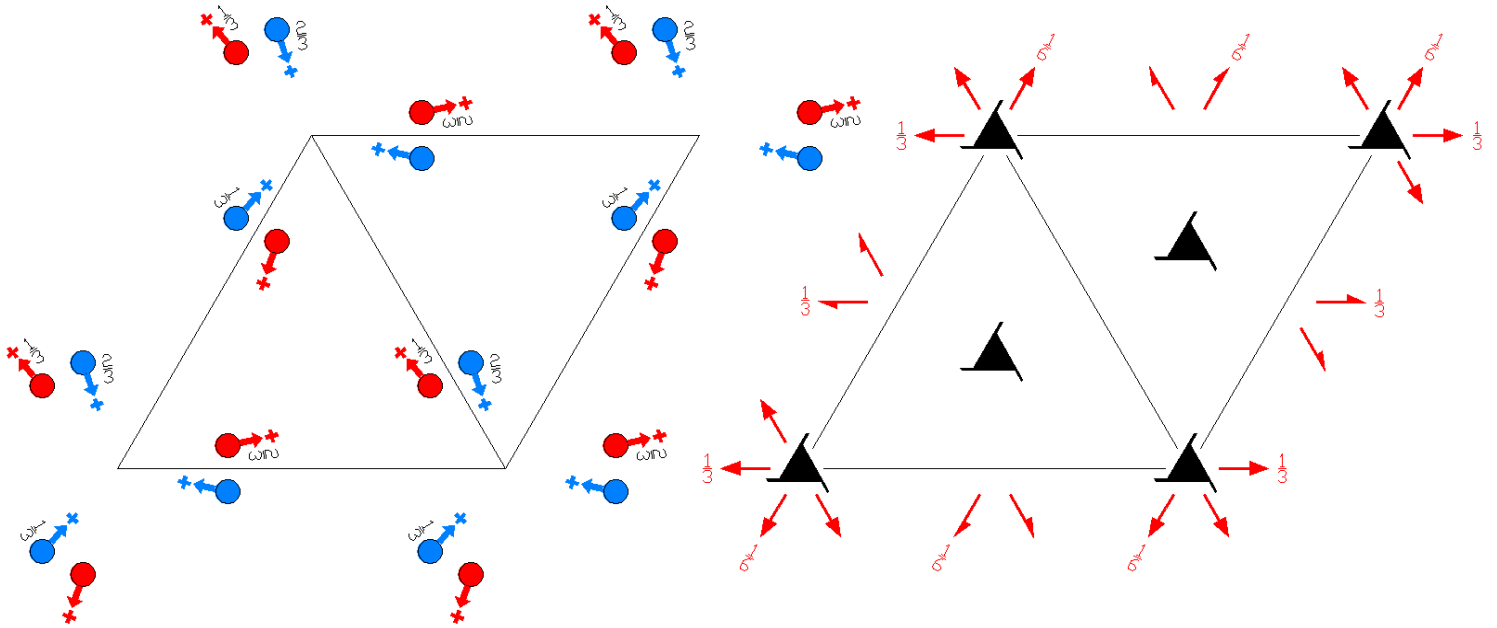
Along [2,1,0] p1m11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/3



$P3_2 2'1$   
154.3.1273

$32'1$   
 $P3_2 2'1$

Trigonal



Origin on  $2'$   $[110]$  at  $3_2(1,1,2')$   $1$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) $1$<br>( $1 0,0,0$ )                | (2) $3^+$ (0,0,2/3) $0,0,z$<br>( $3_z 0,0,2/3$ ) | (3) $3^-$ (0,0,1/3) $0,0,z$<br>( $3_z^{-1} 0,0,1/3$ ) |
| (4) $2'$ $x,x,0$<br>( $2_{xy} 0,0,0$ )' | (5) $2'$ $x,0,1/6$<br>( $2_x 0,0,1/3$ )'         | (6) $2'$ $0,y,1/3$<br>( $2_y 0,0,2/3$ )'              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	c	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z+2/3$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z+1/3$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(5) $x-y,\bar{y},\bar{z}+1/3$ [ $\bar{u}+v,v,w$ ]	(6) $\bar{x},\bar{x}+y,\bar{z}+2/3$ [u,u-v,w]
3	b	.2'	$x,0,1/6$ [u,2u,w]	$0,x,5/6$ [ $2\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},1/2$ [u, $\bar{u},w$ ]
3	a	.2'	$x,0,2/3$ [u,2u,w]	$0,x,1/3$ [ $2\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},0$ [u, $\bar{u},w$ ]

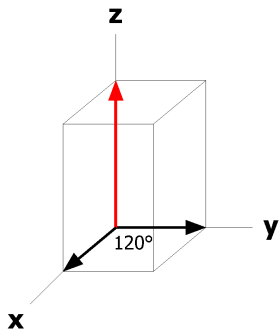
**Symmetry of Special Projections**

Along [0,0,1] p31m  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/6

Along [2,1,0] p1m1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/3

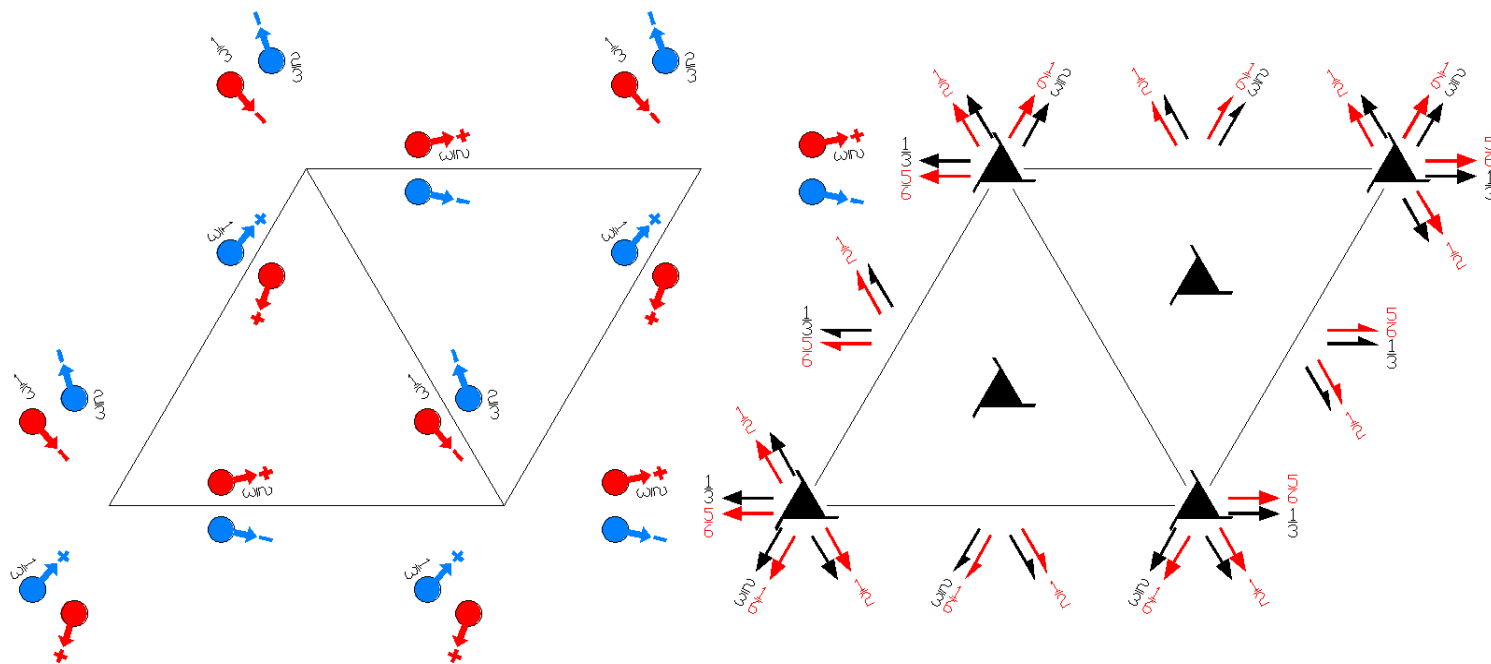




$P_{2c} 3_1 21$   
154.41274

$3211'$   
 $P_{2c} 3_1 21$

Trigonal



Origin on 2 [110] at  $3_1(1,1,2) 1$

Asymmetric unit  $0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

### Symmetry Operations

For (0,0,0) + set

- |                                     |  |  |
|-------------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                  | (2) $3^+ (0,0,2/3) \quad 0,0,z$<br>( $3_z$  0,0,2/3) | (3) $3^- (0,0,1/3) \quad 0,0,z$<br>( $3_z^{-1}$  0,0,1/3)' |
| (4) 2 $x,x,0$<br>( $2_{xy}$  0,0,0) | (5) $2' \quad x,0,1/6$<br>( $2_x$  0,0,1/3)'         | (6) 2 $0,y,1/3$<br>( $2_y$  0,0,2/3)                       |

For (0,0,1)' + set

- |   |   |   |
|---|---|---|
| (1) $t' (0,0,1)$<br>(1 0,0,1)'                | (2) $3^+ (0,0,5/3) \quad 0,0,z$<br>( $3_z$  0,0,5/3)' | (3) $3^- (0,0,4/3) \quad 0,0,z$<br>( $3_z^{-1}$  0,0,4/3) |
| (4) $2' \quad x,x,1/2$<br>( $2_{xy}$  0,0,1)' | (5) 2 $x,0,2/3$<br>( $2_x$  0,0,4/3)                  | (6) $2' \quad 0,y,5/6$<br>( $2_y$  0,0,5/3)'              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

### Positions

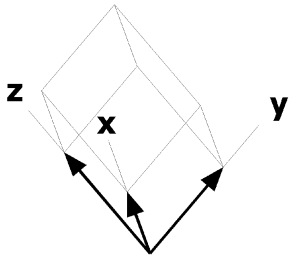
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			(0,0,0) +	(0,0,1)' +	
12	c	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z+2/3$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z+1/3$ [ $u-v, u, \bar{w}$ ]
			(4) y,x, $\bar{z}$ [ $v, u, \bar{w}$ ]	(5) x-y, $\bar{y}, \bar{z}+1/3$ [ $\bar{u}+v, v, w$ ]	(6) $\bar{x}, \bar{x}+y, \bar{z}+2/3$ [ $\bar{u}, \bar{u}+v, \bar{w}$ ]
6	b	.2'	x,0,1/6 [u,2u,w]	0,x,5/6 [2 $\bar{u}, \bar{u}, w$ ]	$\bar{x}, \bar{x}, 1/2$ [ $\bar{u}, u, w$ ]
6	a	.2	x,0,2/3 [u,0,0]	0,x,1/3 [0, $\bar{u}, 0$ ]	$\bar{x}, \bar{x}, 0$ [ $\bar{u}, \bar{u}, 0$ ]

### Symmetry of Special Projections

Along [0,0,1] p31m1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>\* 211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,2/3

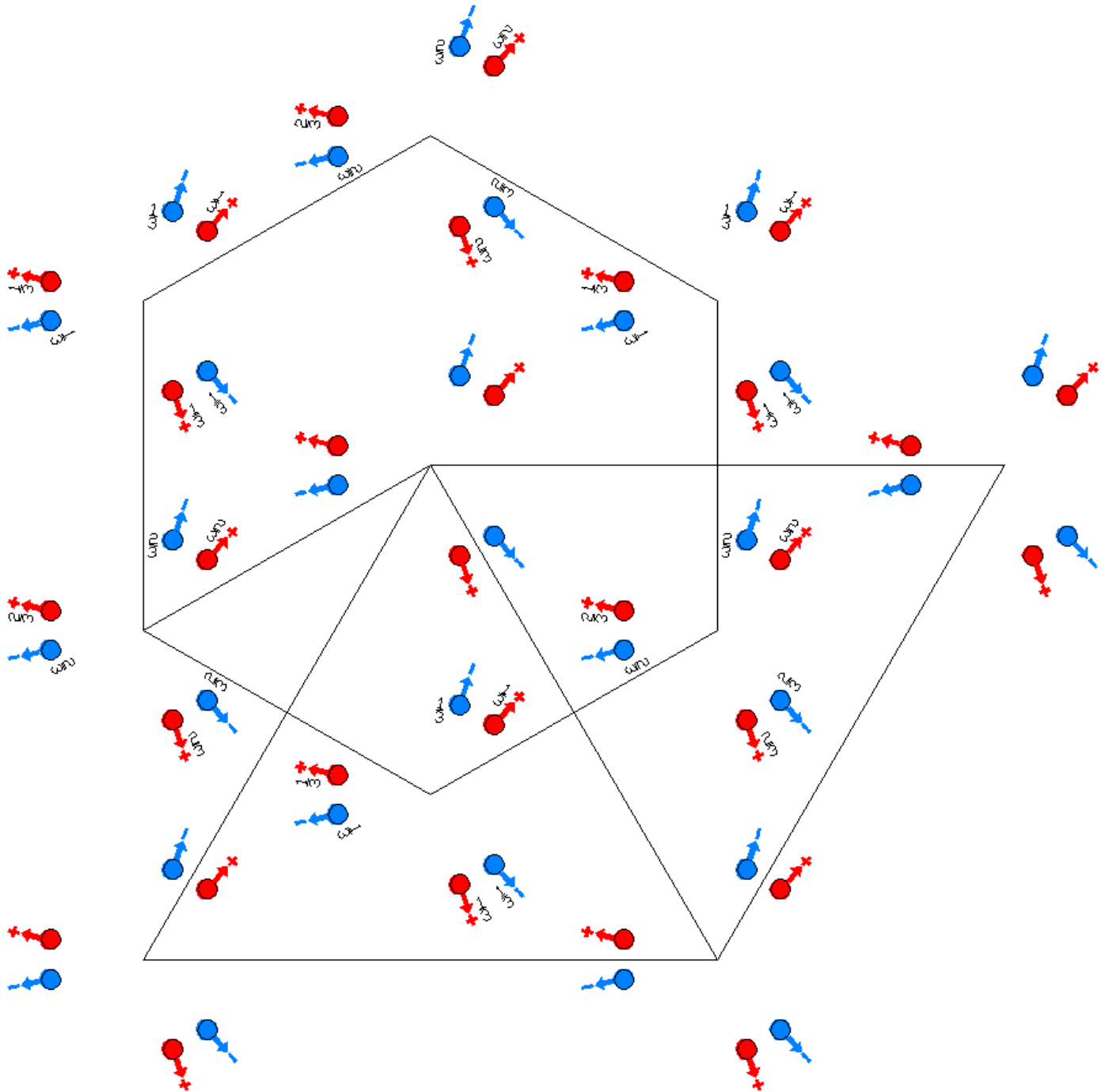
Along [2,1,0] p<sub>2a</sub>\*1m1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,5/6

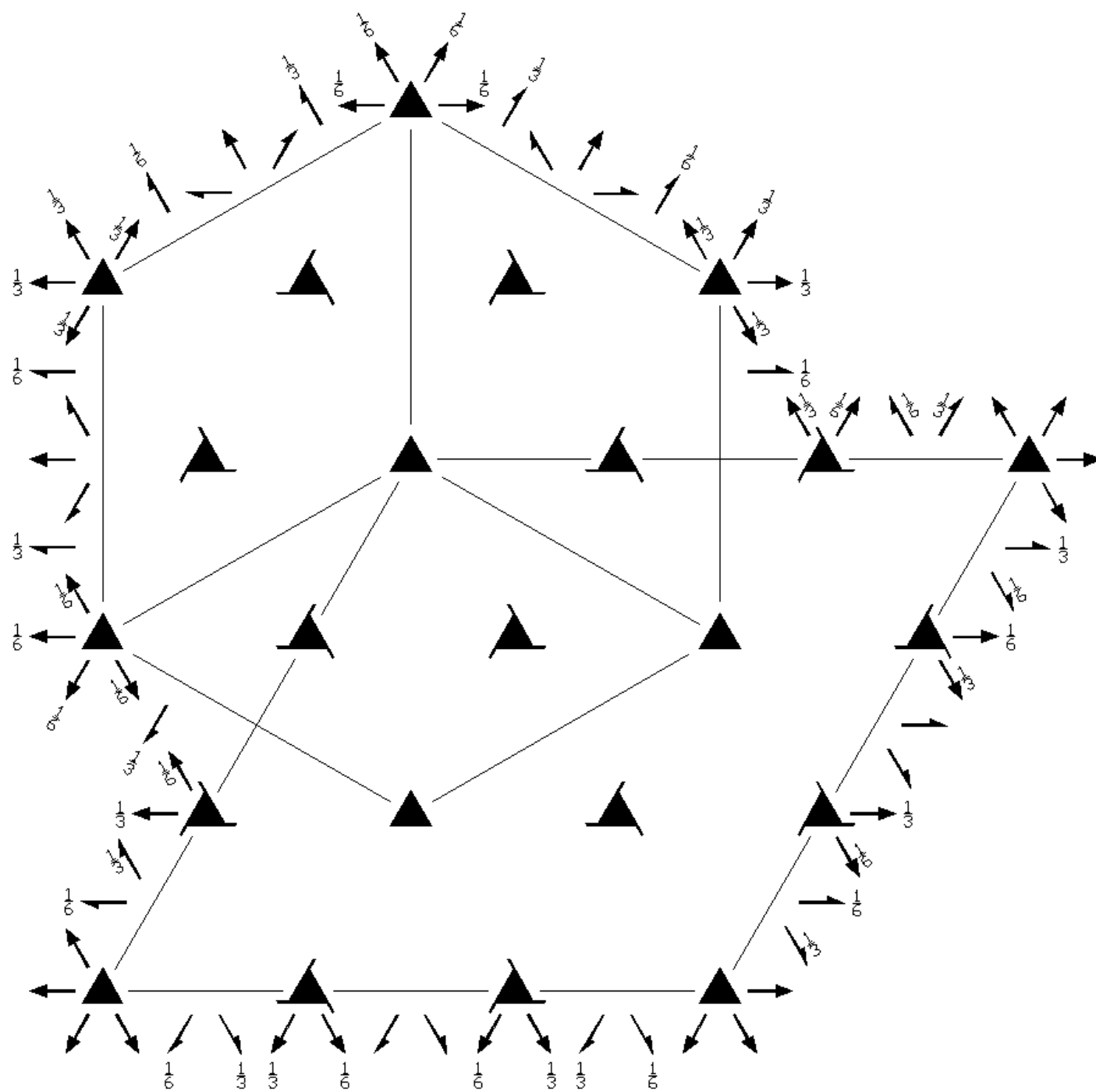


R32  
155.1.1275

32  
R32

Trigonal





Origin on 32

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/6;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/6	1/2,0,1/6	2/3,1/3,1/6	1/3,2/3,1/6	0,1/2,1/6

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                      | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0) | (5) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)              | (6) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                            |

For (2/3,1/3,1/3) + set

- |   |   |   |
|---|---|---|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)                          | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3) | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3) |
| (4) 2 (1/2,1/2,0) x,x-1/6,1/6<br>(2 <sub>xy</sub>  2/3,1/3,1/3) | (5) 2 (1/2,0,0) x,1/6,1/6<br>(2 <sub>x</sub>  2/3,1/3,1/3)              | (6) 2 1/3,y,1/6<br>(2 <sub>y</sub>  2/3,1/3,1/3)                                    |

For (1/3,2/3,2/3) + set

- |   |   |   |
|---|---|---|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)                          | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3) | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3) |
| (4) 2 (1/2,1/2,0) x,x+1/6,1/3<br>(2 <sub>xy</sub>  1/3,2/3,2/3) | (5) 2 x,1/3,1/3<br>(2 <sub>x</sub>  1/3,2/3,2/3)                      | (6) 2 (0,1/2,0) 1/6,y,1/3<br>(2 <sub>y</sub>  1/3,2/3,2/3)                            |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4).**Positions**Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

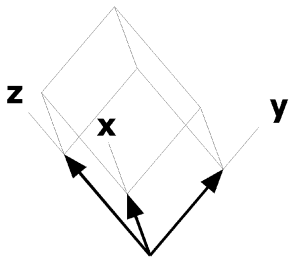
			(0,0,0) +	(2/3,1/3,1/3) +	(1/3,2/3,2/3) +
18	f	1	(1) x,y,z [u,v,w] (4) y,x,z̄ [v,u,w̄]	(2) $\bar{y}$ ,x-y,z [v̄,u-v,w]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x},\bar{x}+y,\bar{z}$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
9	e	.2.	x,0,1/2 [u,0,0]	0,x,1/2 [0,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]
9	d	.2.	x,0,0 [u,0,0]	0,x,0 [0,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]
6	c	3..	0,0,z [0,0,w]	0,0,z̄ [0,0,w̄]	
3	b	32.	0,0,1/2 [0,0,0]		
3	a	32.	0,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p3m'1  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at 0,0,z

Along [1,0,0] p211  
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

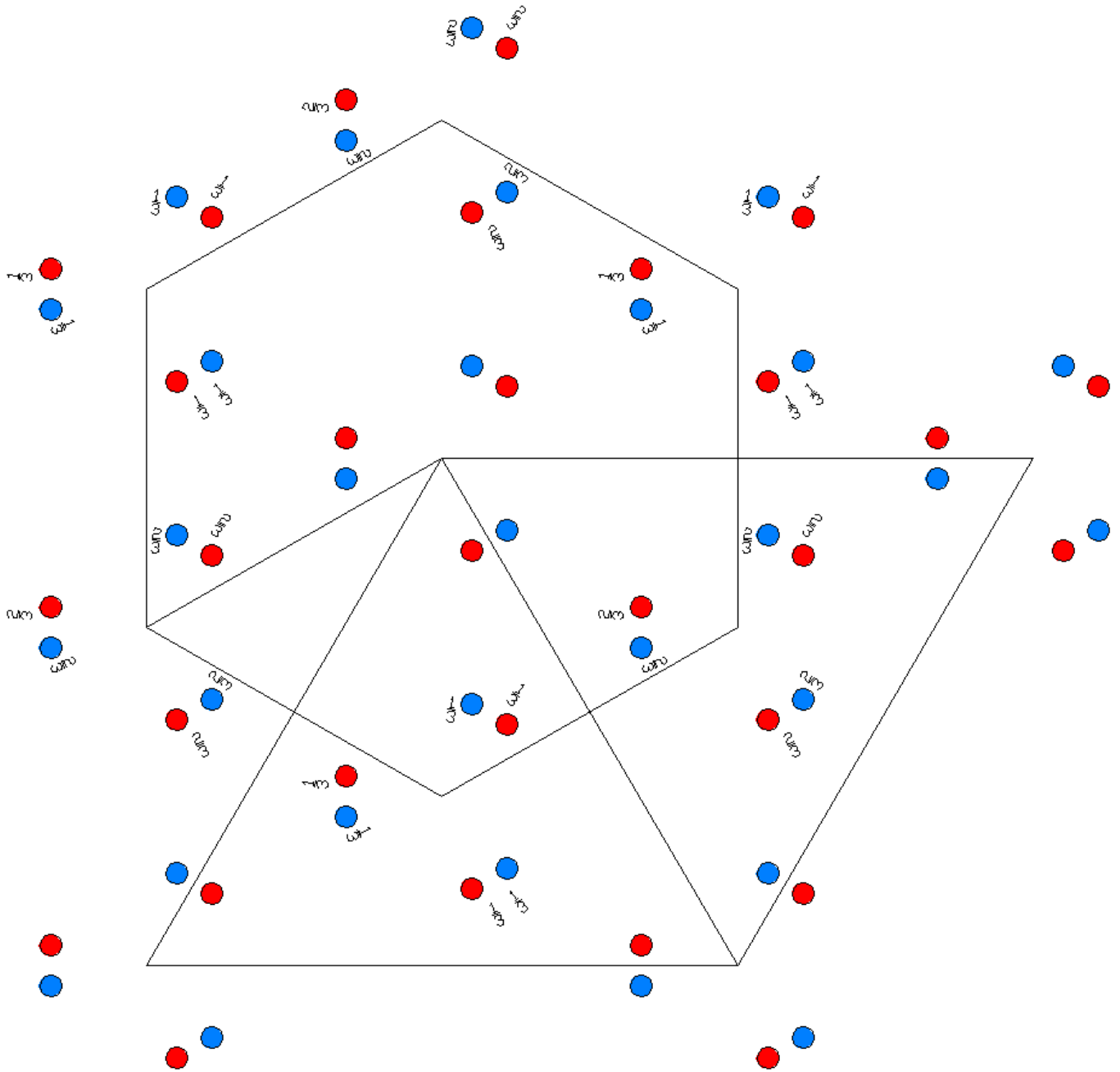
Along [2,1,0] p1m'1  
 $\mathbf{a}^* = \mathbf{c}/3$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



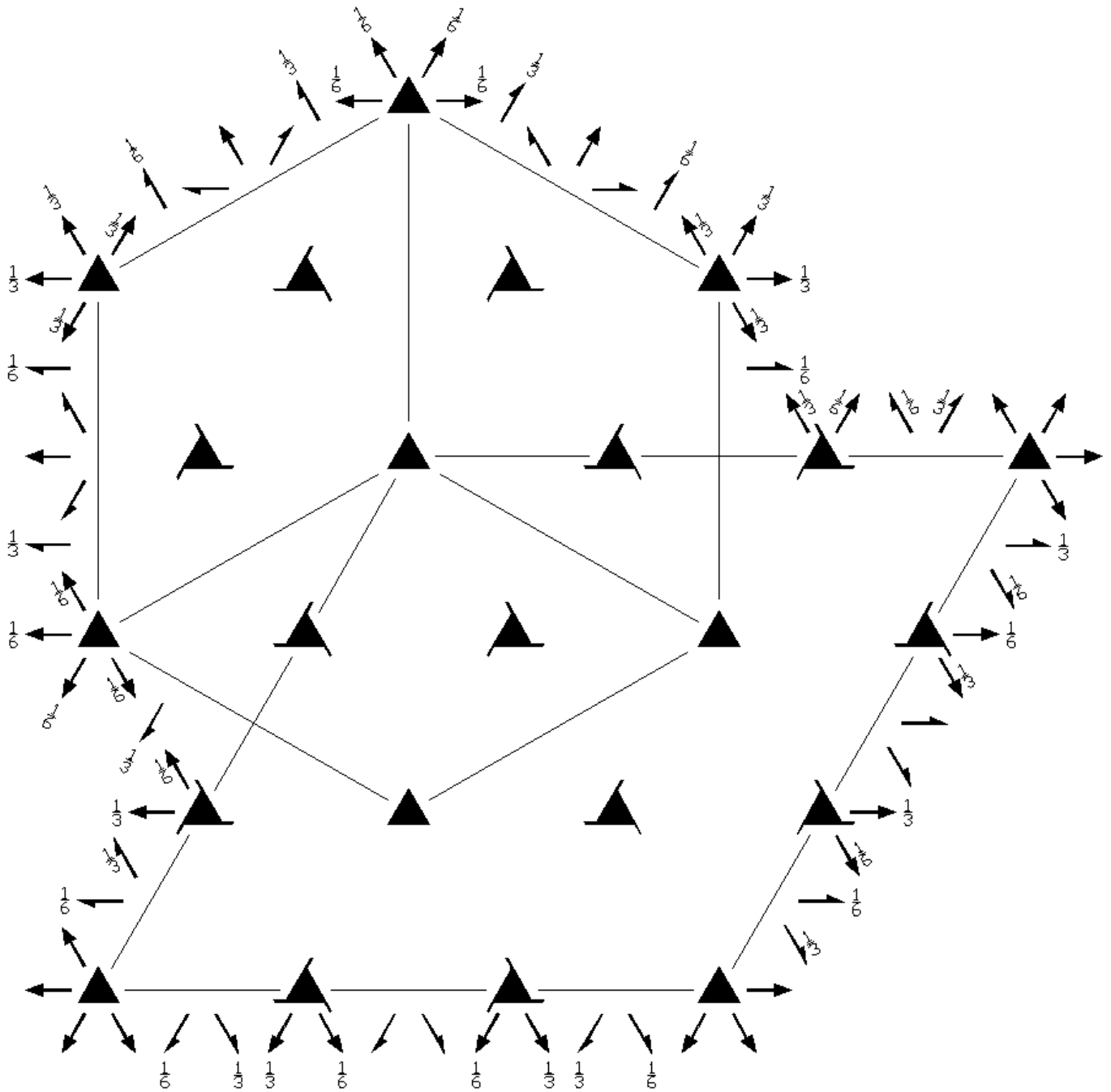
R321'  
155.2.1276

321'  
R321'

Trigonal



1'



Origin on 321'

**Asymmetric unit**      $0 \leq x \leq 2/3;$       $0 \leq y \leq 2/3;$       $0 \leq z \leq 1/6;$       $x \leq (1+y)/2;$       $y \leq \min(1-x, (1+x)/2)$

Vertices     0,0,0     1/2,0,0     2/3,1/3,0     1/3,2/3,0     0,1/2,0  
                  0,0,1/6     1/2,0,1/6     2/3,1/3,1/6     1/3,2/3,1/6     0,1/2,1/6

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                      | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0) | (5) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)              | (6) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                            |

For (2/3,1/3,1/3) + set

- |   |   |   |
|---|---|---|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)                          | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3) | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3) |
| (4) 2 (1/2,1/2,0) x,x-1/6,1/6<br>(2 <sub>xy</sub>  2/3,1/3,1/3) | (5) 2 (1/2,0,0) x,1/6,1/6<br>(2 <sub>x</sub>  2/3,1/3,1/3)              | (6) 2 1/3,y,1/6<br>(2 <sub>y</sub>  2/3,1/3,1/3)                                    |

For (1/3,2/3,2/3) + set

- |   |   |   |
|---|---|---|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)                          | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3) | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3) |
| (4) 2 (1/2,1/2,0) x,x+1/6,1/3<br>(2 <sub>xy</sub>  1/3,2/3,2/3) | (5) 2 x,1/3,1/3<br>(2 <sub>x</sub>  1/3,2/3,2/3)                      | (6) 2 (0,1/2,0) 1/6,y,1/3<br>(2 <sub>y</sub>  1/3,2/3,2/3)                            |

For (0,0,0)' + set

- |   |  |  |
|---|--|--|
| (1) 1'<br>(1 0,0,0)'                      | (2) 3 <sup>+</sup> ' 0,0,z<br>(3 <sub>z</sub>  0,0,0)' | (3) 3 <sup>-</sup> ' 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (4) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)' | (5) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'               | (6) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                             |

For (2/3,1/3,1/3)' + set

- |   |  |  |
|---|--|--|
| (1) t' (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)'                          | (2) 3 <sup>+</sup> ' (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3)' | (3) 3 <sup>-</sup> ' (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3)' |
| (4) 2' (1/2,1/2,0) x,x-1/6,1/6<br>(2 <sub>xy</sub>  2/3,1/3,1/3)' | (5) 2' (1/2,0,0) x,1/6,1/6<br>(2 <sub>x</sub>  2/3,1/3,1/3)'               | (6) 2' 1/3,y,1/6<br>(2 <sub>y</sub>  2/3,1/3,1/3)'                                     |

For (1/3,2/3,2/3)' + set

- |   |  |  |
|---|--|--|
| (1) t' (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)'                          | (2) 3 <sup>+</sup> ' (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3)' | (3) 3 <sup>-</sup> ' (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3)' |
| (4) 2' (1/2,1/2,0) x,x+1/6,1/3<br>(2 <sub>xy</sub>  1/3,2/3,2/3)' | (5) 2' x,1/3,1/3<br>(2 <sub>x</sub>  1/3,2/3,2/3)'                       | (6) 2' (0,1/2,0) 1/6,y,1/3<br>(2 <sub>y</sub>  1/3,2/3,2/3)'                             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4); 1'.



**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

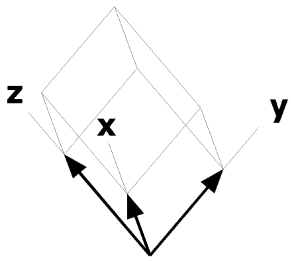
			$(0,0,0) +$ $(0,0,0)'$ +	$(2/3,1/3,1/3) +$ $(2/3,1/3,1/3)'$ +	$(1/3,2/3,2/3) +$ $(1/3,2/3,2/3)'$ +
18	f	11'	(1) $x,y,z$ [0,0,0] (4) $y,x,\bar{z}$ [0,0,0]	(2) $\bar{y},x-y,z$ [0,0,0] (5) $x-y,\bar{y},\bar{z}$ [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0] (6) $\bar{x},\bar{x}+y,\bar{z}$ [0,0,0]
9	e	.2.1'	$x,0,1/2$ [0,0,0]	$0,x,1/2$ [0,0,0]	$\bar{x},\bar{x},1/2$ [0,0,0]
9	d	.2.1'	$x,0,0$ [0,0,0]	$0,x,0$ [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]
6	c	3..1'	$0,0,z$ [0,0,0]	$0,0,\bar{z}$ [0,0,0]	
3	b	32.1'	$0,0,1/2$ [0,0,0]		
3	a	32.1'	$0,0,0$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p3m11'$   
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at 0,0,z

Along [1,0,0]  $p2111'$   
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

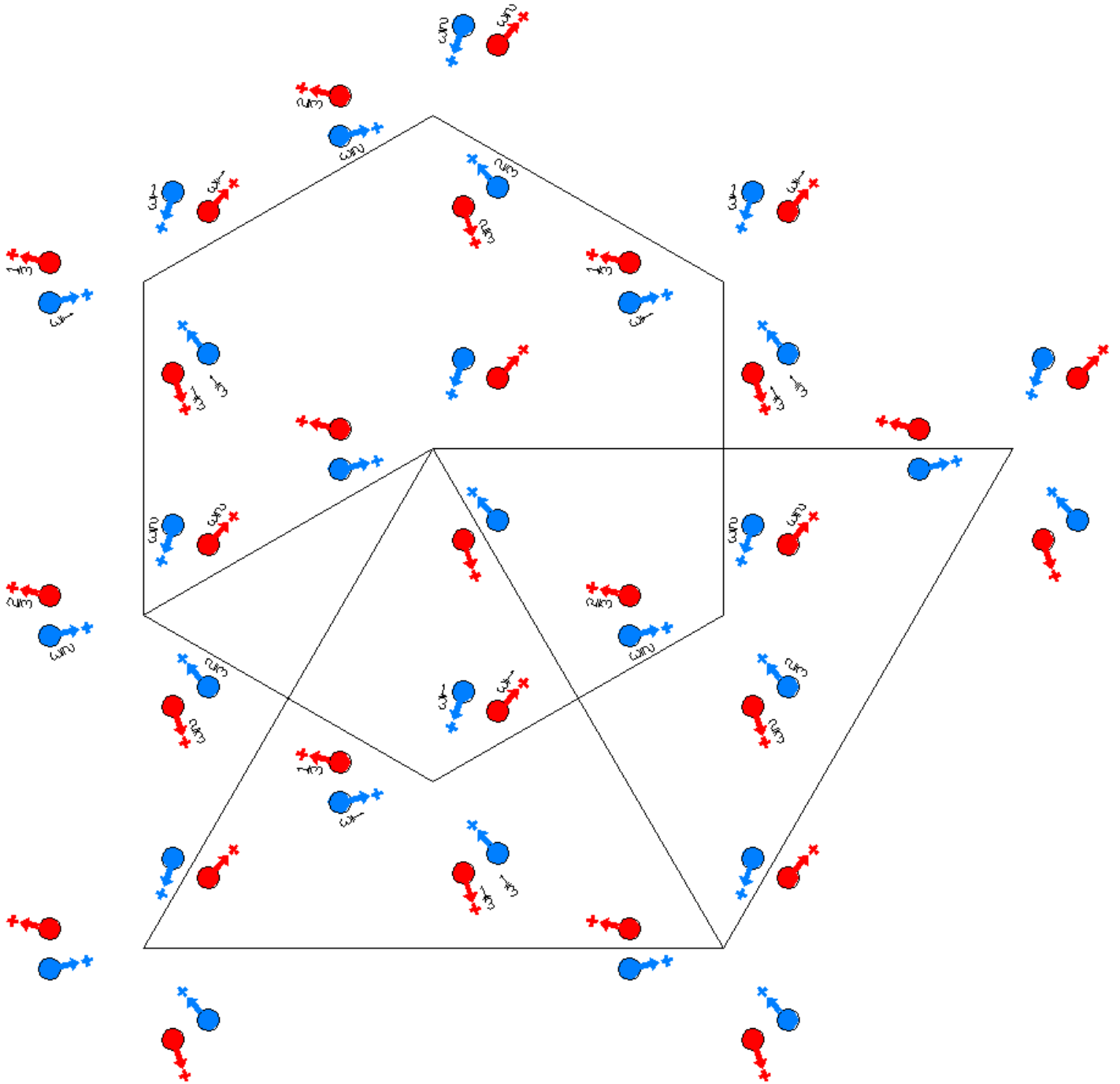
Along [2,1,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{c}/3$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0

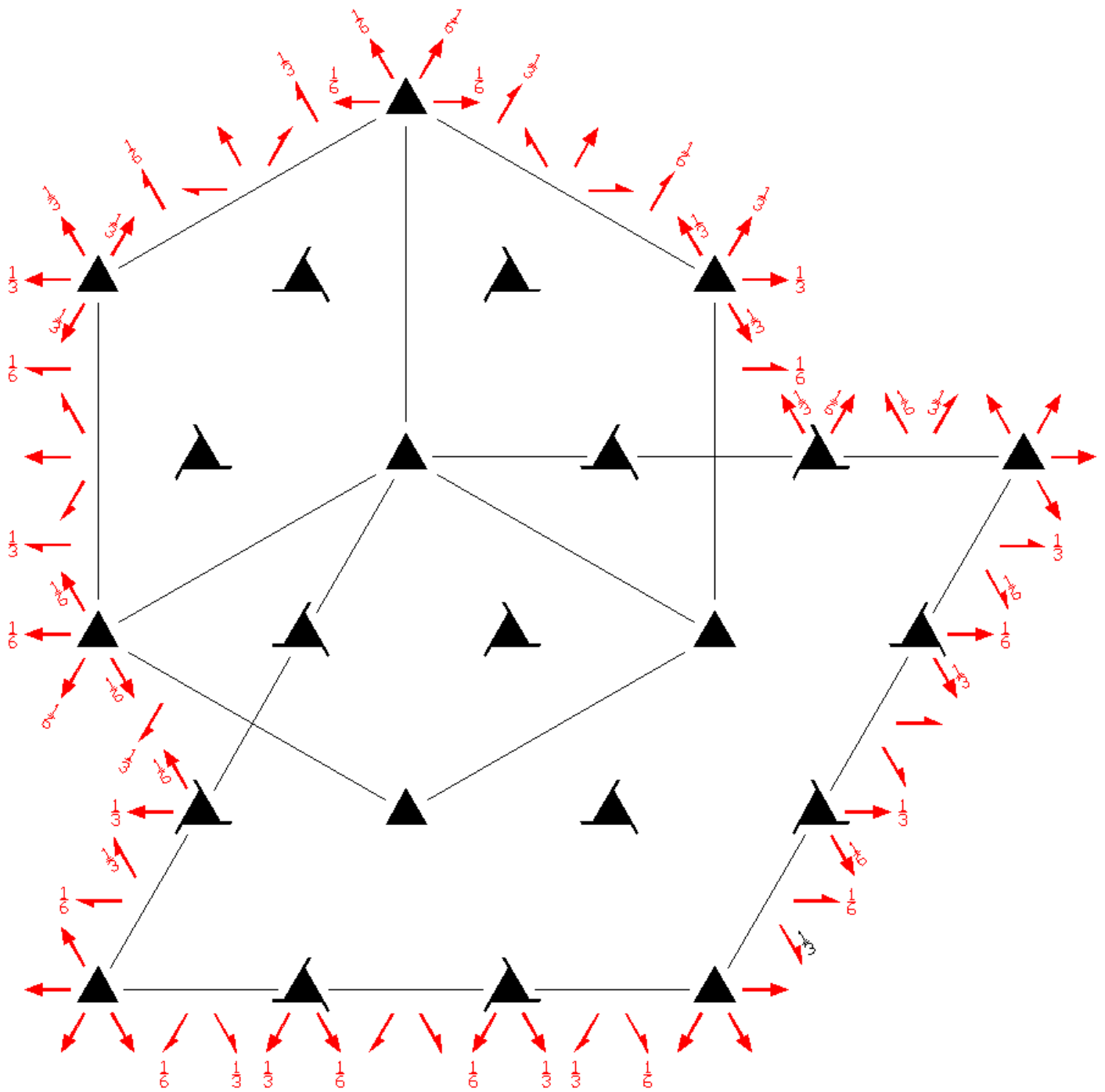


R32'  
155.3.1277

32'  
R32'

Trigonal





Origin on 32'

**Asymmetric unit**  $0 \leq x \leq 2/3;$   $0 \leq y \leq 2/3;$   $0 \leq z \leq 1/6;$   $x \leq (1+y)/2;$   $y \leq \min(1-x, (1+x)/2)$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/6	1/2,0,1/6	2/3,1/3,1/6	1/3,2/3,1/6	0,1/2,1/6

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                        | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)' | (5) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'            | (6) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                          |

For (2/3,1/3,1/3) + set

- |   |   |   |
|---|---|---|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)                            | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3) | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3) |
| (4) 2' (1/2,1/2,0) x,x-1/6,1/6<br>(2 <sub>xy</sub>  2/3,1/3,1/3)' | (5) 2' (1/2,0,0) x,1/6,1/6<br>(2 <sub>x</sub>  2/3,1/3,1/3)'            | (6) 2' 1/3,y,1/6<br>(2 <sub>y</sub>  2/3,1/3,1/3)'                                  |

For (1/3,2/3,2/3) + set

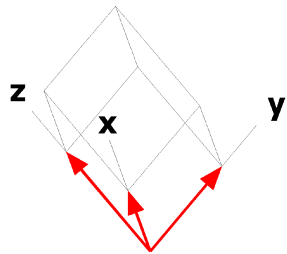
- |   |   |   |
|---|---|---|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)                            | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3) | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3) |
| (4) 2' (1/2,1/2,0) x,x+1/6,1/3<br>(2 <sub>xy</sub>  1/3,2/3,2/3)' | (5) 2' x,1/3,1/3<br>(2 <sub>x</sub>  1/3,2/3,2/3)'                    | (6) 2' (0,1/2,0) 1/6,y,1/3<br>(2 <sub>y</sub>  1/3,2/3,2/3)'                          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4).**Positions**Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

			(0,0,0) +	(2/3,1/3,1/3) +	(1/3,2/3,2/3) +
18	f	1	(1) x,y,z [u,v,w] (4) y,x,z̄ [v̄,ū,w]	(2) ȳ,x-y,z [v̄,u-v,w] (5) x-y,ȳ,z̄ [u+v,v,w]	(3) x̄+y,x̄,z [u+v,ū,w] (6) x̄,x̄+y,z̄ [u,u-v,w]
9	e	.2'	x,0,1/2 [u,2u,w]	0,x,1/2 [2ū,ū,w]	x̄,x̄,1/2 [u,ū,w]
9	d	.2'	x,0,0 [u,2u,w]	0,x,0 [2ū,ū,w]	x̄,x̄,0 [u,ū,w]
6	c	3..	0,0,z [0,0,w]	0,0,z̄ [0,0,w]	
3	b	32'	0,0,1/2 [0,0,w]		
3	a	32'	0,0,0 [0,0,w]		

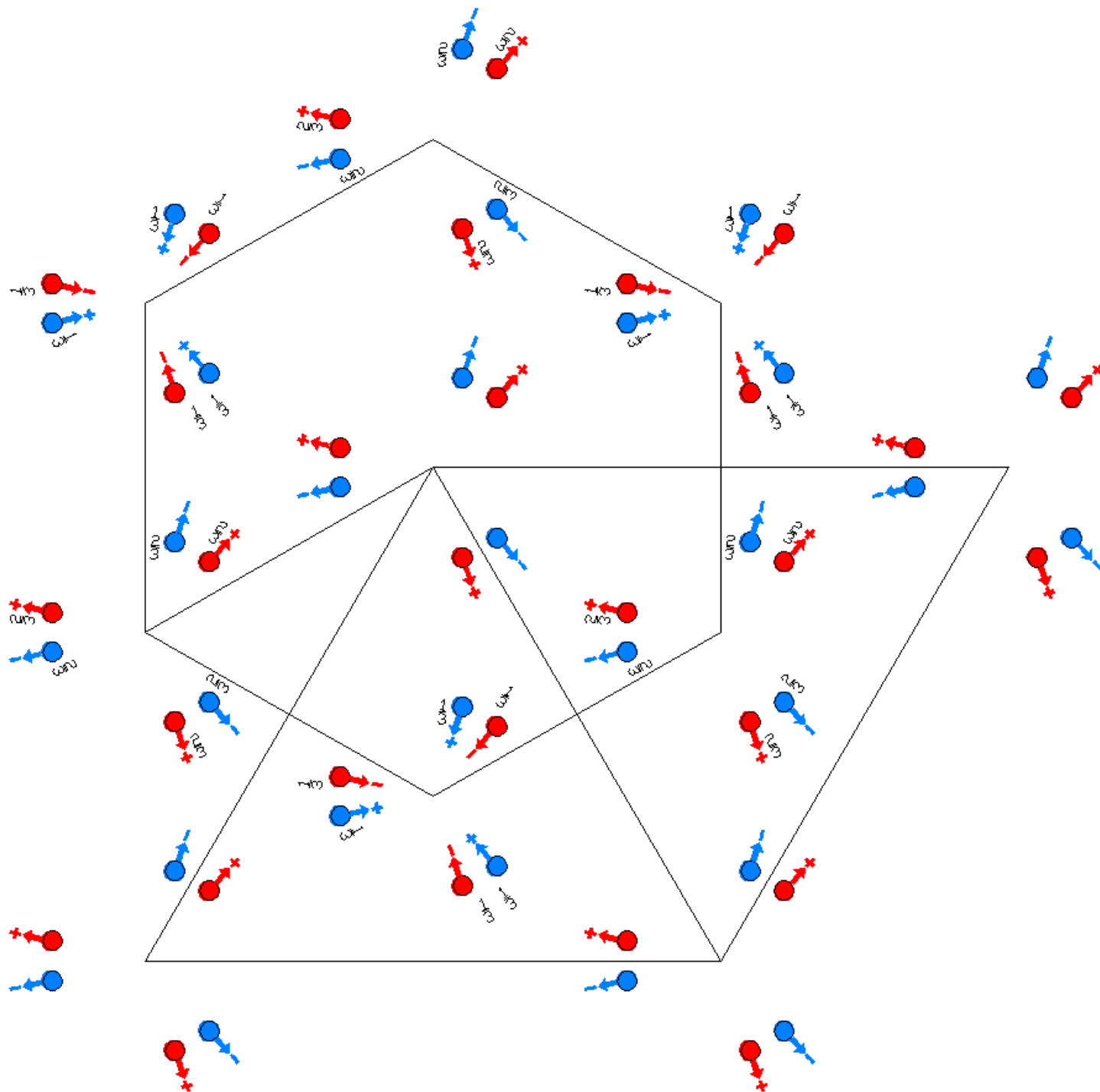
**Symmetry of Special Projections**Along [0,0,1] p3m1  
**a\*** = (2**a** + **b**)/3 **b\*** = (-**a** + **b**)/3  
Origin at 0,0,zAlong [1,0,0] p2'11  
**a\*** = (-**a** - 2**b** + **c**)/3 **b\*** = (**a** + 2**b**)/2  
Origin at x,0,0Along [2,1,0] p1m1  
**a\*** = **c**/3 **b\*** = **b**/2  
Origin at x,x/2,0

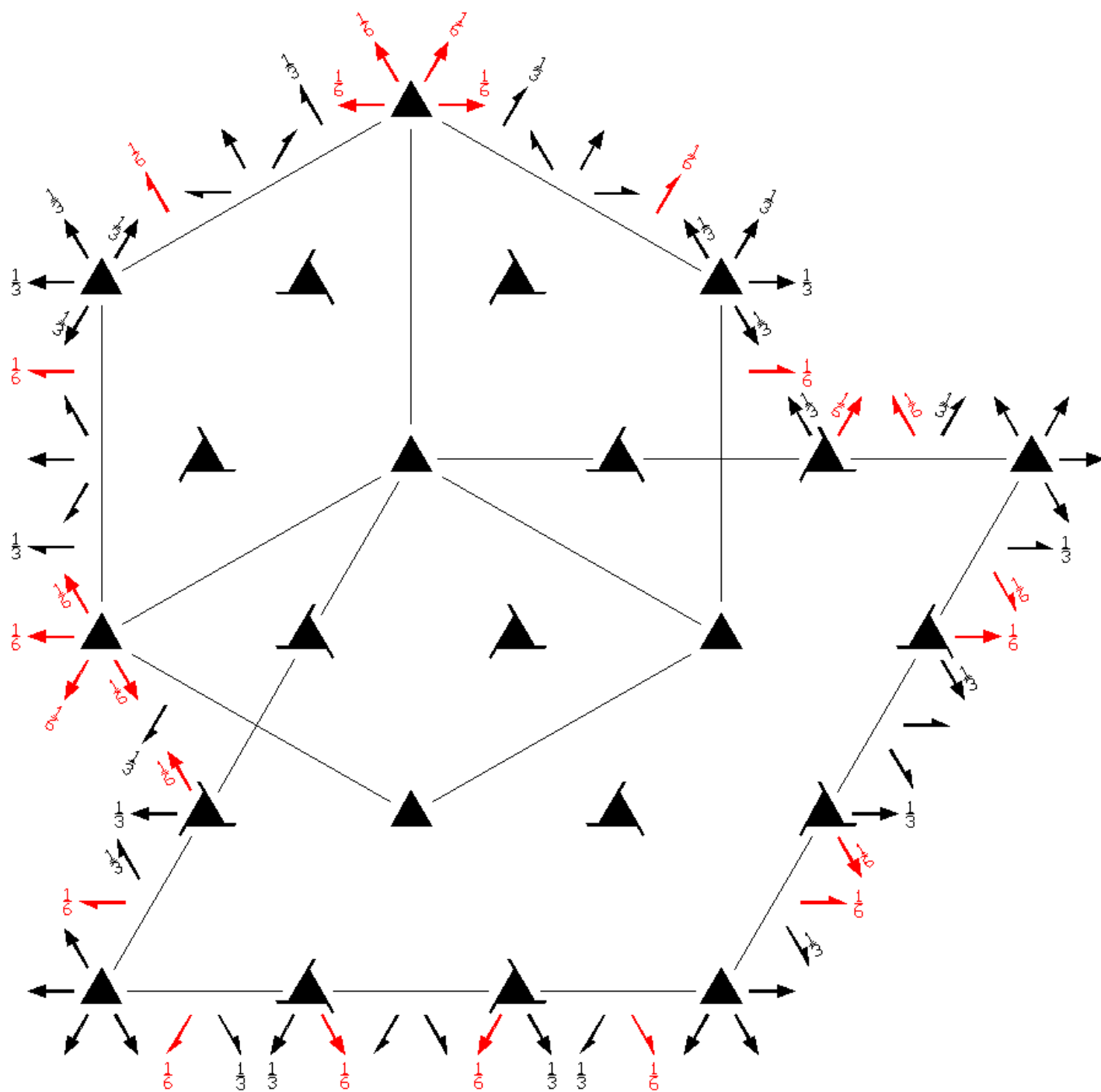


$R_R 32$   
155.4.1278

$321'$   
 $R_R 32$

Trigonal





Origin on 32

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/6;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/6	1/2,0,0 1/2,0,1/6	2/3,1/3,0 2/3,1/3,1/6	1/3,2/3,0 1/3,2/3,1/6	0,1/2,0 0,1/2,1/6

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                      | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0) | (5) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)              | (6) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                            |

For (2/3,1/3,1/3)' + set

- |   |  |  |
|---|--|--|
| (1) t' (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)'                          | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3)' | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3)' |
| (4) 2' (1/2,1/2,0) x,x-1/6,1/6<br>(2 <sub>xy</sub>  2/3,1/3,1/3)' | (5) 2' (1/2,0,0) x,1/6,1/6<br>(2 <sub>x</sub>  2/3,1/3,1/3)'             | (6) 2' 1/3,y,1/6<br>(2 <sub>y</sub>  2/3,1/3,1/3)'                                   |

For (1/3,2/3,2/3) + set

- |   |   |   |
|---|---|---|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)                          | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3) | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3) |
| (4) 2 (1/2,1/2,0) x,x+1/6,1/3<br>(2 <sub>xy</sub>  1/3,2/3,2/3) | (5) 2 x,1/3,1/3<br>(2 <sub>x</sub>  1/3,2/3,2/3)                      | (6) 2 (0,1/2,0) 1/6,y,1/3<br>(2 <sub>y</sub>  1/3,2/3,2/3)                            |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(2/3,1/3,1/3);(2); (4).**Positions**Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

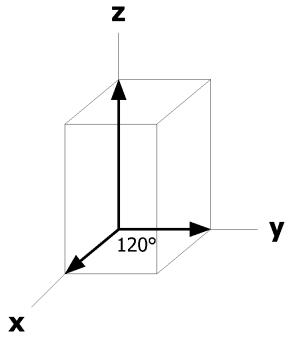
			(0,0,0) +	(2/3,1/3,1/3)' +	(1/3,2/3,2/3) +
18	f	1	(1) x,y,z [u,v,w] (4) y,x,z̄ [v,u,w̄]	(2) $\bar{y}$ ,x-y,z [v̄,u-v,w]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x},\bar{x}+y,\bar{z}$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
9	e	.2'	x,0,1/2 [u,2u,w]	0,x,1/2 [2 $\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},1/2$ [u, $\bar{u},w$ ]
9	d	.2.	x,0,0 [u,0,0]	0,x,0 [0,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]
6	c	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w̄]	
3	b	32'	0,0,1/2 [0,0,w]		
3	a	32.	0,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p3m1'  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub> 211  
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

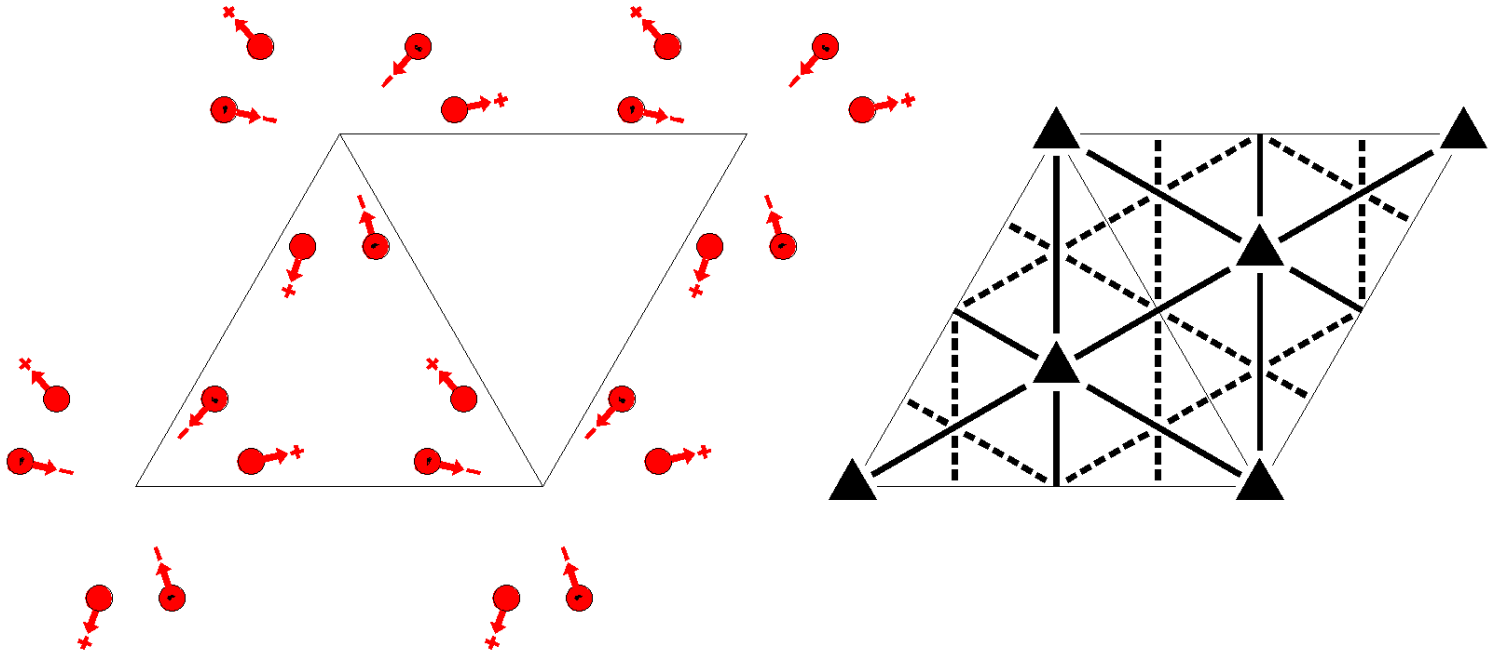
Along [2,1,0] p<sub>2a</sub> 1m1  
 $\mathbf{a}^* = \mathbf{c}/3$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P3m1  
156.1.1279

3m1  
P3m1

Trigonal



Origin on 3m1

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1;$	$x \leq 2y;$	$y \leq \min(1-x, 2x)$
Vertices	0,0,0 0,0,1	2/3,1/3,0 2/3,1/3,1	1/3,2/3,0 1/3,2/3,1		

**Symmetry Operations**

- |   |                                     |   |
|---|-------------------------------------|---|
| (1) 1<br>(1 0,0,0)                          | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) m $x, \bar{x}, z$<br>( $m_{xy}$  0,0,0) | (5) m $x, 2x, z$<br>( $m_x$  0,0,0) | (6) m $2x, x, z$<br>( $m_y$  0,0,0)     |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

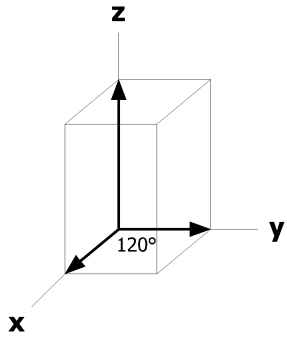
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	e	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$
			(4) $\bar{y},\bar{x},z [v,u,\bar{w}]$	(5) $\bar{x}+y,y,z [u-v,\bar{v},\bar{w}]$	(6) $x,x-y,z [\bar{u},\bar{u}+v,\bar{w}]$
3	d	.m.	$x,\bar{x},z [u,u,0]$	$x,2x,z [\bar{u},0,0]$	$2\bar{x},\bar{x},z [0,\bar{u},0]$
1	c	3m.	$2/3,1/3,z [0,0,0]$		
1	b	3m.	$1/3,2/3,z [0,0,0]$		
1	a	3m.	$0,0,z [0,0,0]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$  p3m1  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

Along  $[2,1,0]$  p1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x/2,0$

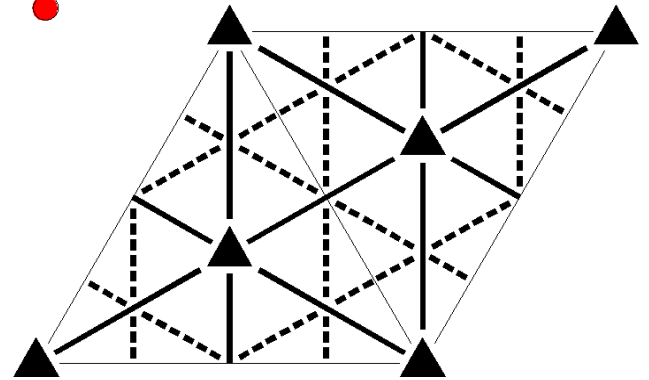
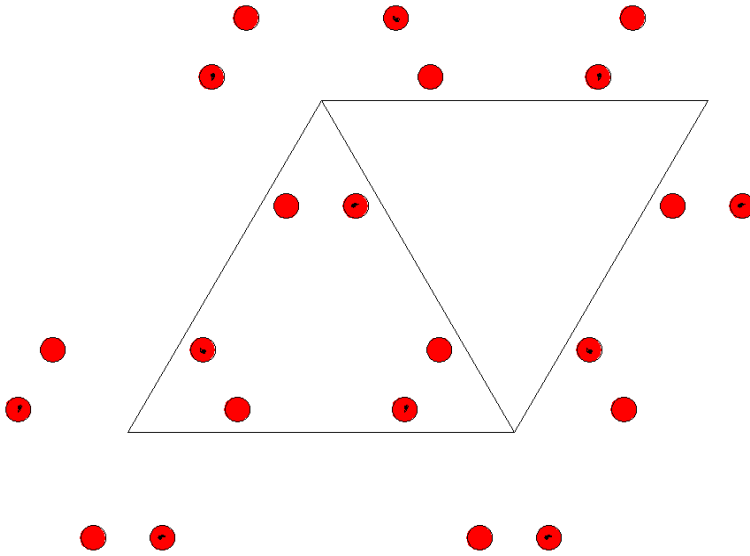


P3m11'  
156.2.1280

3m11'  
P3m11'

Trigonal

1'



Origin on 3m11'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1;$	$x \leq 2y;$	$y \leq \min(1-x, 2x)$
Vertices	0,0,0	2/3,1/3,0	1/3,2/3,0		
	0,0,1	2/3,1/3,1	1/3,2/3,1		

**Symmetry Operations**

For 1 + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                       | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0) | (5) m x,2x,z<br>(m <sub>x</sub>  0,0,0)             | (6) m 2x,x,z<br>(m <sub>y</sub>  0,0,0)                           |

For 1' + set

- |  |  |  |
|--|--|--|
| (1) 1'<br>(1 0,0,0)'                       | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)' | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (4) m' x,x̄,z<br>(m <sub>xy</sub>  0,0,0)' | (5) m' x,2x,z<br>(m <sub>x</sub>  0,0,0)'            | (6) m' 2x,x,z<br>(m <sub>y</sub>  0,0,0)'                          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

**Positions**

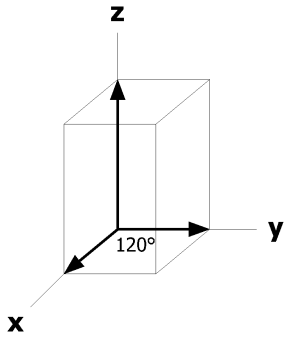
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			1 +	1' +	
6	e	11'	(1) x,y,z [0,0,0]	(2) $\bar{y},x-y,z$ [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0]
			(4) $\bar{y},\bar{x},z$ [0,0,0]	(5) $\bar{x}+y,y,z$ [0,0,0]	(6) x,x-y,z [0,0,0]
3	d	.m.1'	x, $\bar{x},z$ [0,0,0]	x,2x,z [0,0,0]	2 $\bar{x},\bar{x},z$ [0,0,0]
1	c	3m.1'	2/3,1/3,z [0,0,0]		
1	b	3m.1'	1/3,2/3,z [0,0,0]		
1	a	3m.1'	0,0,z [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p3m11'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

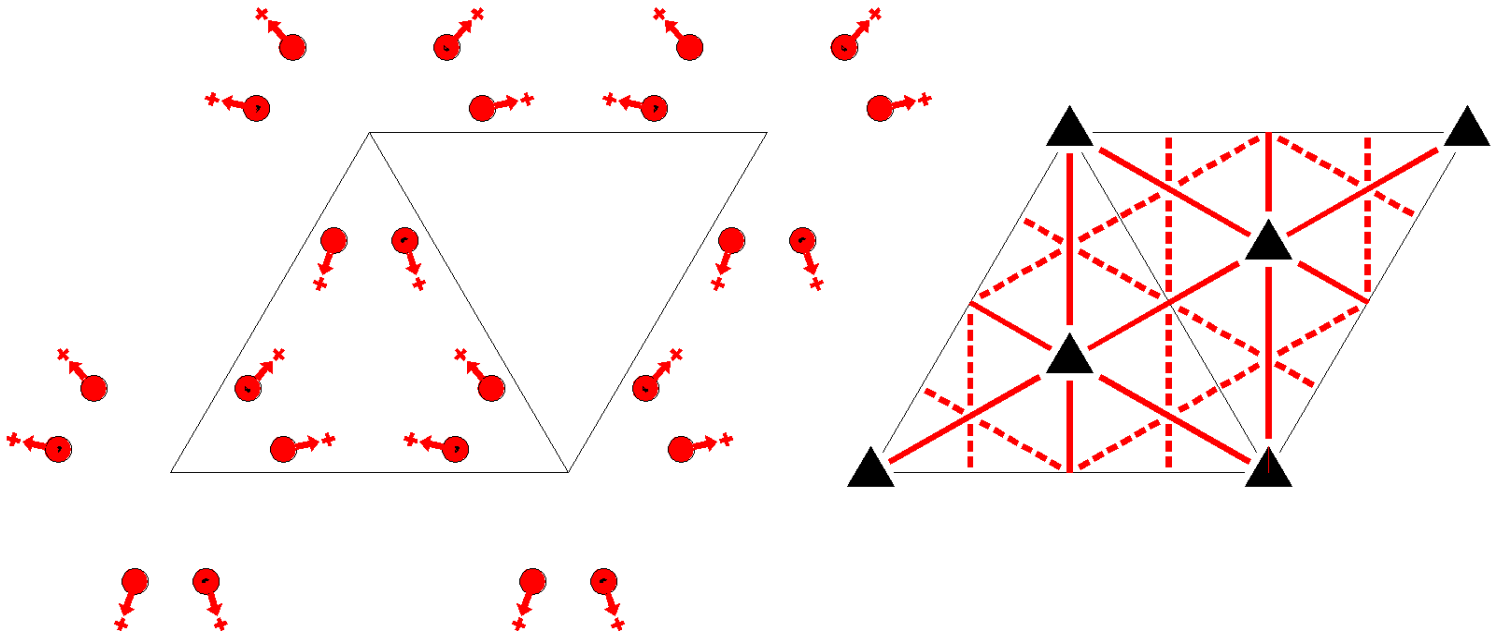
Along [2,1,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



P3m'1  
156.3.1281

3m'1  
P3m'1

Trigonal



Origin on 3m'1

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1;$	$x \leq 2y;$	$y \leq \min(1-x, 2x)$
Vertices	0,0,0 0,0,1	2/3,1/3,0 2/3,1/3,1	1/3,2/3,0 1/3,2/3,1		

**Symmetry Operations**

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                         | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) m' x,x̄,z<br>(m <sub>xy</sub>  0,0,0)' | (5) m' x,2x,z<br>(m <sub>x</sub>  0,0,0)'           | (6) m' 2x,x,z<br>(m <sub>y</sub>  0,0,0)'                         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

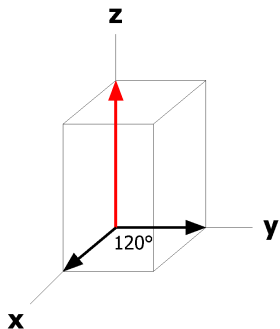
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	e	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$
			(4) $\bar{y},\bar{x},z [\bar{v},\bar{u},w]$	(5) $\bar{x}+y,y,z [\bar{u}+v,v,w]$	(6) $x,x-y,z [u,u-v,w]$
3	d	.m'	$x,\bar{x},z [u,\bar{u},w]$	$x,2x,z [u,2u,w]$	$2\bar{x},\bar{x},z [2\bar{u},\bar{u},w]$
1	c	3m'	$2/3,1/3,z [0,0,w]$		
1	b	3m'	$1/3,2/3,z [0,0,w]$		
1	a	3m'	$0,0,z [0,0,w]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p3m'1$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p1$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

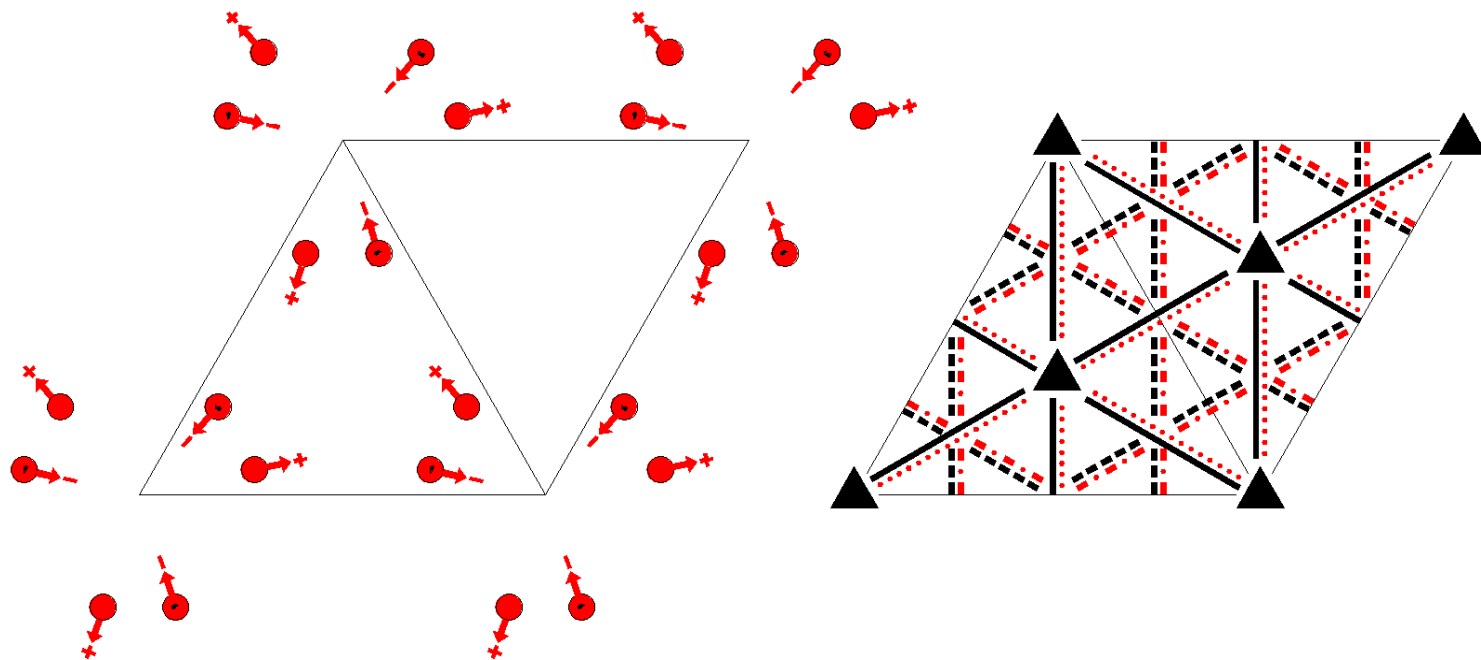
Along  $[2,1,0]$   $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x/2,0$



$P_{2c} 3m1$   
156.4.1282

$3m11'$   
 $P_{2c} 3m1$

Trigonal



Origin on  $3m1$

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $0 \leq z \leq 1$ ;  $x \leq 2y$ ;  $y \leq \min(1-x, 2x)$

Vertices	0,0,0	$2/3, 1/3, 0$	$1/3, 2/3, 0$
	0,0,1	$2/3, 1/3, 1$	$1/3, 2/3, 1$

Symmetry Operations

For (0,0,0) + set

- |   |                                     |   |
|---|-------------------------------------|---|
| (1) 1<br>(1 0,0,0)                          | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) m $x, \bar{x}, z$<br>( $m_{xy}$  0,0,0) | (5) m $x, 2x, z$<br>( $m_x$  0,0,0) | (6) m $2x, x, z$<br>( $m_y$  0,0,0)     |

For (0,0,1)' + set

- |   |   |  |
|---|---|--|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'                          | (2) $3^+$ ' (0,0,1) 0,0,z<br>( $3_z$  0,0,1)'   | (3) $3^-$ ' (0,0,1) 0,0,z<br>( $3_z^{-1}$  0,0,1)' |
| (4) $c'$ (0,0,1) $x, \bar{x}, z$<br>( $m_{xy}$  0,0,1)' | (5) $c'$ (0,0,1) $x, 2x, z$<br>( $m_x$  0,0,1)' | (6) $c'$ (0,0,1) $2x, x, z$<br>( $m_y$  0,0,1)'    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

### Positions

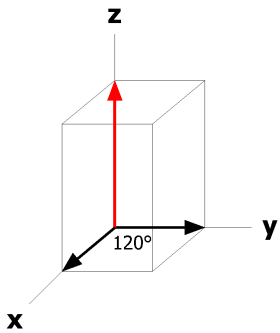
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			(0,0,0) +	(0,0,1)' +	
12	e	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$
			(4) $\bar{y},\bar{x},z [v,u,\bar{w}]$	(5) $\bar{x}+y,y,z [u-v,\bar{v},\bar{w}]$	(6) x,x-y,z [ $\bar{u},\bar{u}+v,\bar{w}$ ]
6	d	.m.	x, $\bar{x},z [u,u,0]$	x,2x,z [ $\bar{u},0,0]$	2 $\bar{x},\bar{x},z [0,\bar{u},0]$
2	c	3m.	2/3,1/3,z [0,0,0]		
2	b	3m.	1/3,2/3,z [0,0,0]		
2	a	3m.	0,0,z [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p3m11'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

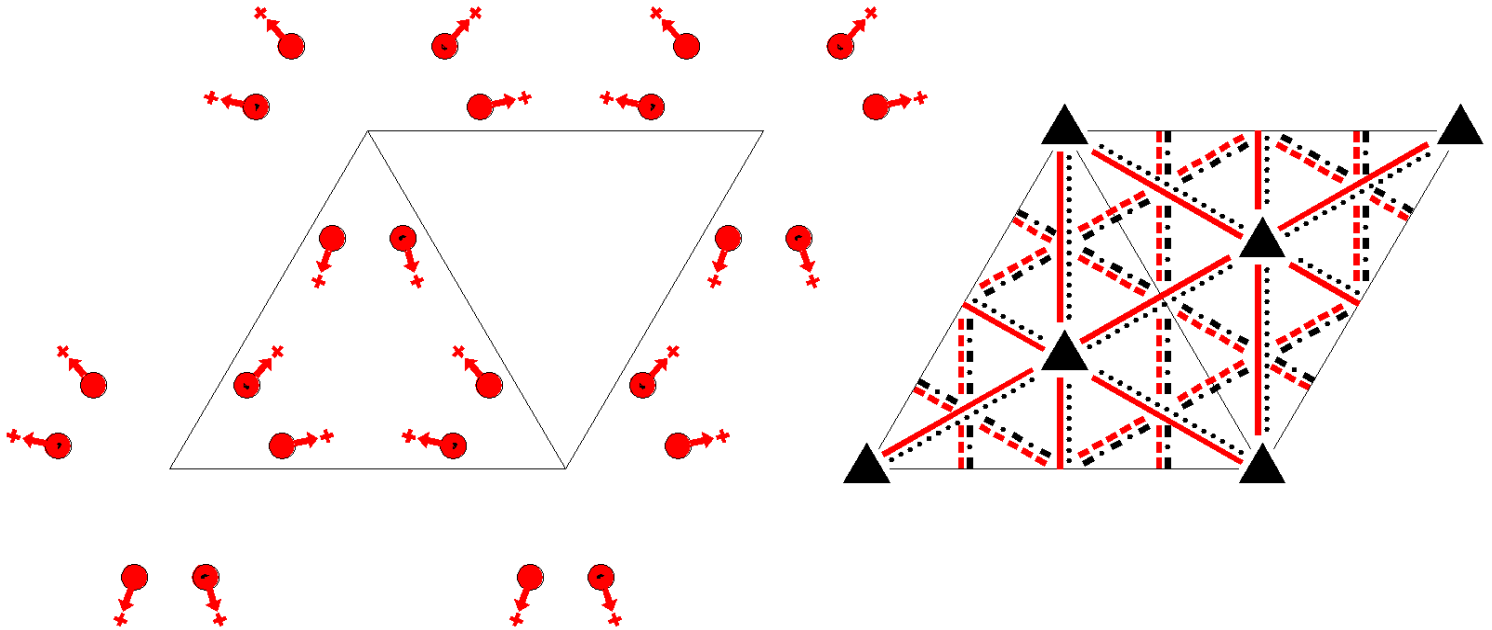
Along [2,1,0] p<sub>2b</sub>-1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$P_{2c} 3m'1'$   
156.5.1283

$3m'11'$   
 $P_{2c} 3m'1'$

Trigonal



Origin on  $3m'1'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1;$	$x \leq 2y;$	$y \leq \min(1-x, 2x)$
Vertices	0,0,0	$2/3, 1/3, 0$	$1/3, 2/3, 0$		
	0,0,1	$2/3, 1/3, 1$	$1/3, 2/3, 1$		

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                              | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)      | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) $m'$ $x, \bar{x}, z$<br>( $m_{xy}$  0,0,0)' | (5) $m'$ $x, 2x, z$<br>( $m_x$  0,0,0)' | (6) $m'$ $2x, x, z$<br>( $m_y$  0,0,0)' |

For (0,0,1)' + set

- |   |   |  |
|---|---|--|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'                        | (2) $3^+$ (0,0,1) 0,0,z<br>( $3_z$  0,0,1)'   | (3) $3^-$ (0,0,1) 0,0,z<br>( $3_z^{-1}$  0,0,1)' |
| (4) $c$ (0,0,1) $x, \bar{x}, z$<br>( $m_{xy}$  0,0,1) | (5) $c$ (0,0,1) $x, 2x, z$<br>( $m_x$  0,0,1) | (6) $c$ (0,0,1) $2x, x, z$<br>( $m_y$  0,0,1)    |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

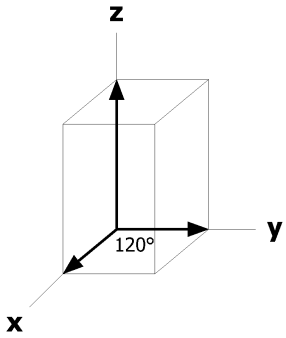
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.					
			(0,0,0) +	(0,0,1)' +	
12	e	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$
			(4) $\bar{y},\bar{x},z [\bar{v},\bar{u},w]$	(5) $\bar{x}+y,y,z [\bar{u}+v,v,w]$	(6) x,x-y,z [u,u-v,w]
6	d	.m'	x, $\bar{x},z [u,\bar{u},w]$	x,2x,z [u,2u,w]	2 $\bar{x},\bar{x},z [2\bar{u},\bar{u},w]$
2	c	3m'	2/3,1/3,z [0,0,w]		
2	b	3m'	1/3,2/3,z [0,0,w]		
2	a	3m'	0,0,z [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p3m11'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub> 1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

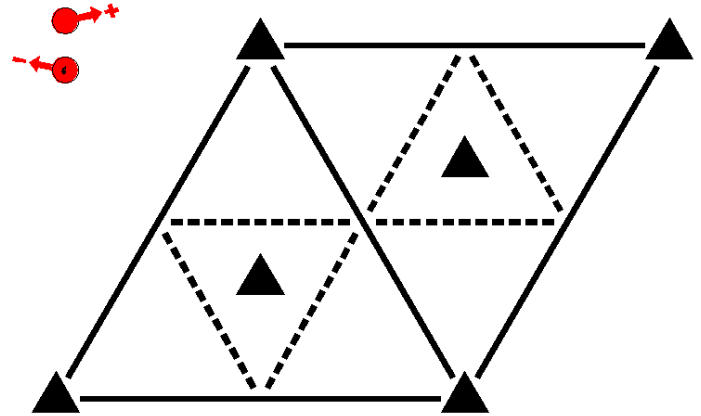
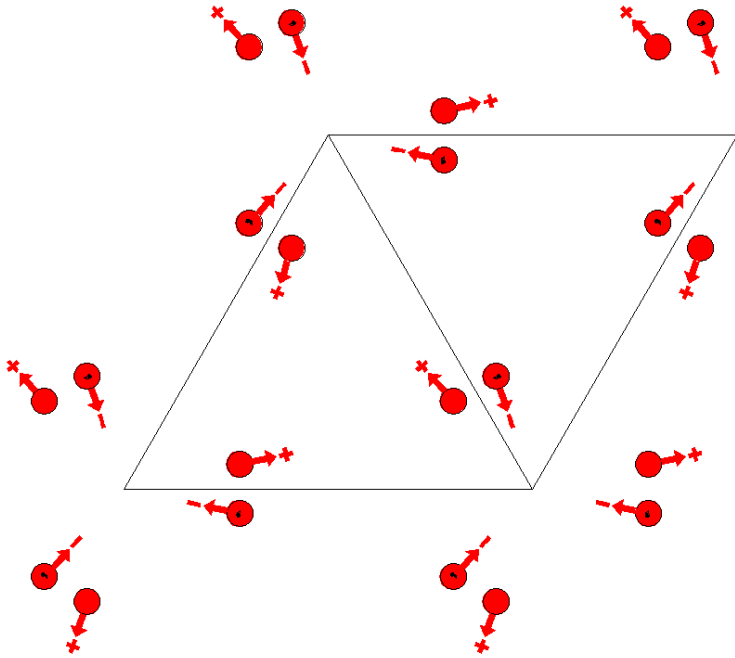
Along [2,1,0] p<sub>2b</sub> 1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



P31m  
157.1.1284

31m  
P31m

Trigonal



**Origin on 31m**

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1	1/2,0,1	2/3,1/3,1	1/2,1/2,1	

**Symmetry Operations**

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) m x,x,z<br>(m <sub>3</sub>  0,0,0) | (5) m x,0,z<br>(m <sub>2</sub>  0,0,0)              | (6) m 0,y,z<br>(m <sub>1</sub>  0,0,0)                            |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

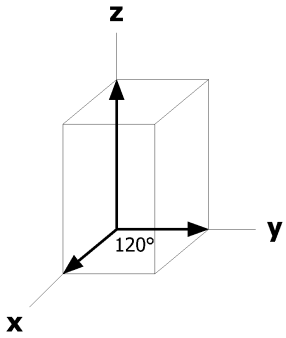
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	d	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$
			(4) $y,x,z [\bar{v},\bar{u},\bar{w}]$	(5) $x-y,\bar{y},z [\bar{u}+v,v,\bar{w}]$	(6) $\bar{x},\bar{x}+y,z [u,u-v,\bar{w}]$
3	c	..m	$x,0,z [u,2u,0]$	$0,x,z [2\bar{u},\bar{u},0]$	$\bar{x},\bar{x},z [u,\bar{u},0]$
2	b	3..	$1/3,2/3,z [0,0,w]$	$2/3,1/3,z [0,0,\bar{w}]$	
1	a	3.m	$0,0,z [0,0,0]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$  p31m  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p1m1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[2,1,0]$  p11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,0$

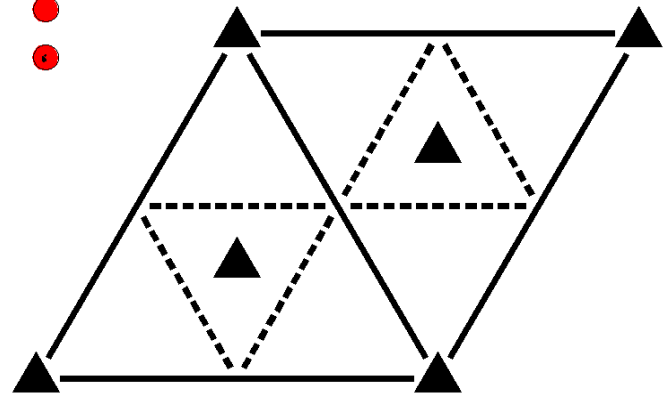
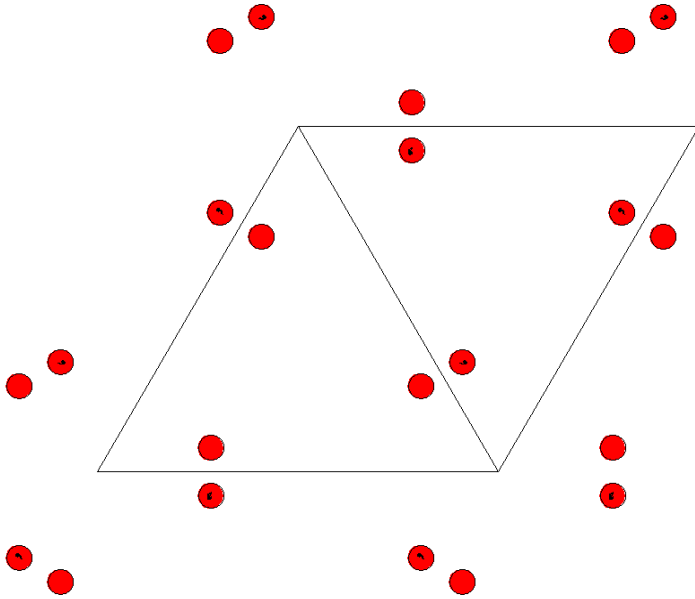


P31m1'  
157.2.1285

31m1'  
P31m1'

Trigonal

1'



Origin on 31m1'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1	1/2,1/2,0 1/2,1/2,1	

**Symmetry Operations**

For 1 + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                                  | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) m <sub>x</sub> x,x,z<br>(m <sub>3</sub>  0,0,0) | (5) m <sub>x</sub> x,0,z<br>(m <sub>2</sub>  0,0,0) | (6) m <sub>y</sub> 0,y,z<br>(m <sub>1</sub>  0,0,0)               |

For 1' + set

- |   |   |  |
|---|---|--|
| (1) 1'<br>(1 0,0,0)'                                  | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)'  | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (4) m' <sub>x</sub> x,x,z<br>(m <sub>3</sub>  0,0,0)' | (5) m' <sub>x</sub> x,0,z<br>(m <sub>2</sub>  0,0,0)' | (6) m' <sub>y</sub> 0,y,z<br>(m <sub>1</sub>  0,0,0)'              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

**Positions**

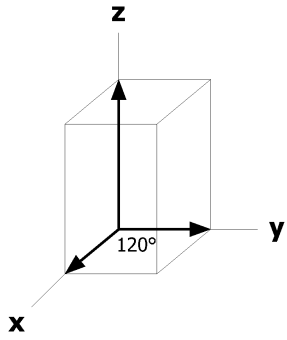
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			1 +	1' +	
6	d	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x}$ ,z [0,0,0]
			(4) y,x,z [0,0,0]	(5) x-y, $\bar{y}$ ,z [0,0,0]	(6) $\bar{x}$ , $\bar{x}+y$ ,z [0,0,0]
3	c	..m1'	x,0,z [0,0,0]	0,x,z [0,0,0]	$\bar{x},\bar{x}$ ,z [0,0,0]
2	b	3..1'	1/3,2/3,z [0,0,0]	2/3,1/3,z [0,0,0]	
1	a	3.m1'	0,0,z [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p31m1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

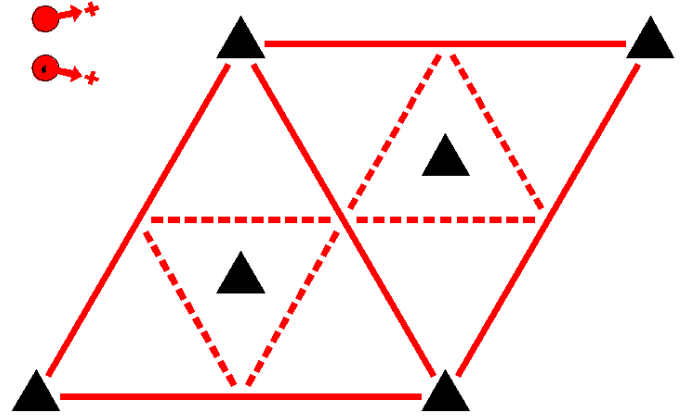
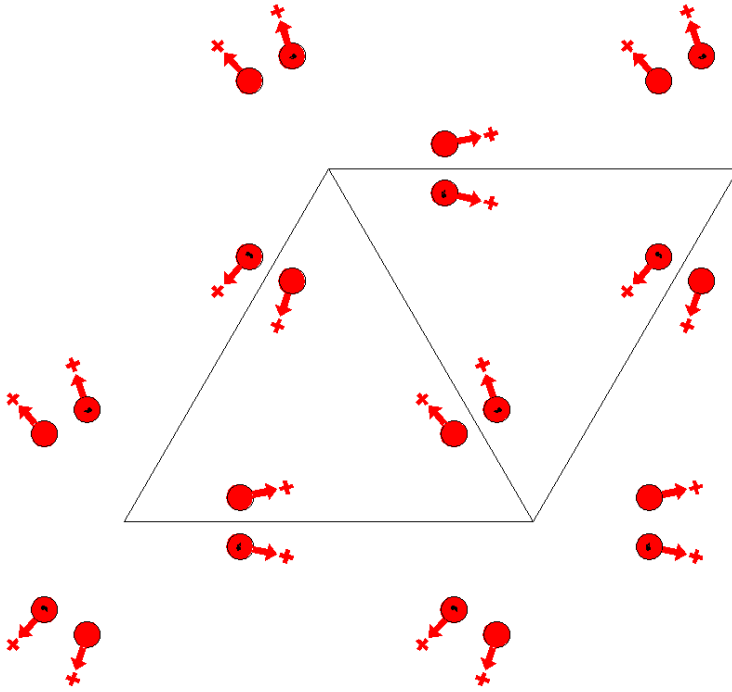
Along [2,1,0] p11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P31m'  
157.3.1286

31m'  
P31m'

Trigonal



Origin on 31m'

Asymmetric unit	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1	1/2,1/2,0 1/2,1/2,1	

**Symmetry Operations**

- (1) 1  
(1|0,0,0)
- (2) 3<sup>+</sup> 0,0,z  
(3<sub>z</sub>|0,0,0)
- (3) 3<sup>-</sup> 0,0,z  
(3<sub>z</sub><sup>-1</sup>|0,0,0)
- (4) m' x,x,z  
(m<sub>3</sub>|0,0,0)'
- (5) m' x,0,z  
(m<sub>2</sub>|0,0,0)'
- (6) m' 0,y,z  
(m<sub>1</sub>|0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

### Positions

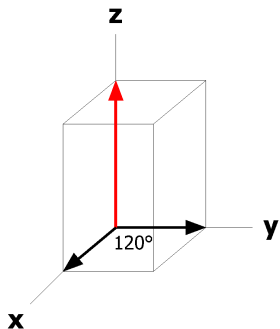
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	d	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$
			(4) y,x,z [v,u,w]	(5) x-y, $\bar{y},z [u-v,\bar{v},w]$	(6) $\bar{x},\bar{x}+y,z [\bar{u},\bar{u}+v,w]$
3	c	..m'	x,0,z [u,0,w]	0,x,z [0,u,w]	$\bar{x},\bar{x},z [\bar{u},\bar{u},w]$
2	b	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0,w]	
1	a	3.m'	0,0,z [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] p31m'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [2,1,0] p1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



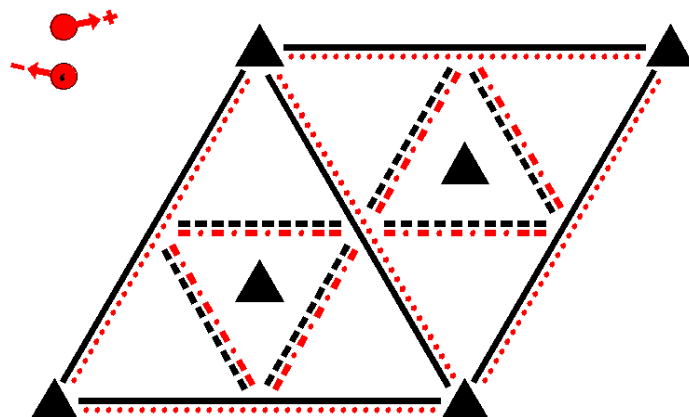
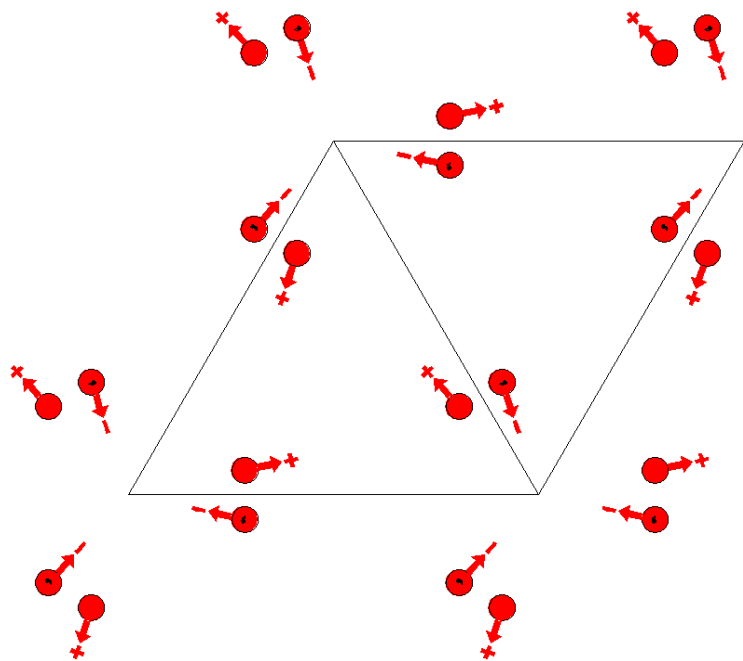
$P_{2c}$  31m

157.4.1287

31m1'

$P_{2c}$  31m

Trigonal



Origin on 31m

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1	1/2,0,1	2/3,1/3,1	1/2,1/2,1	

**Symmetry Operations**

For (0,0,0) + set

- |                                |                                    |   |
|--------------------------------|------------------------------------|---|
| (1) 1<br>(1 0,0,0)             | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0) | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) m x,x,z<br>( $m_3$  0,0,0) | (5) m x,0,z<br>( $m_2$  0,0,0)     | (6) m 0,y,z<br>( $m_1$  0,0,0)          |

For (0,0,1)' + set

- |  |  |   |
|--|--|---|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'             | (2) $3^+$ '(0,0,1) 0,0,z<br>( $3_z$  0,0,1)' | (3) $3^-$ '(0,0,1) 0,0,z<br>( $3_z^{-1}$  0,0,1)' |
| (4) $c'$ (0,0,1) x,x,z<br>( $m_3$  0,0,1)' | (5) $c'$ (0,0,1) x,0,z<br>( $m_2$  0,0,1)'   | (6) $c'$ (0,0,1) 0,y,z<br>( $m_1$  0,0,1)'        |



**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

### Positions

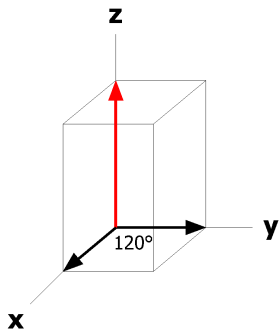
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			(0,0,0) +	(0,0,1)' +	
12	d	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$
			(4) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]	(5) x-y, $\bar{y},z [\bar{u}+v,v,\bar{w}]$	(6) $\bar{x},\bar{x}+y,z [u,u-v,\bar{w}]$
6	c	..m	x,0,z [u,2u,0]	0,x,z [2 $\bar{u},\bar{u},0]$	$\bar{x},\bar{x},z [u,\bar{u},0]$
4	b	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0, $\bar{w}$ ]	
2	a	3.m	0,0,z [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p31m1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>·1m1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

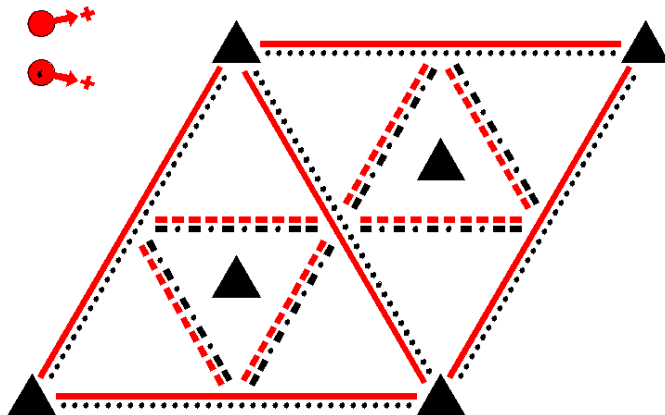
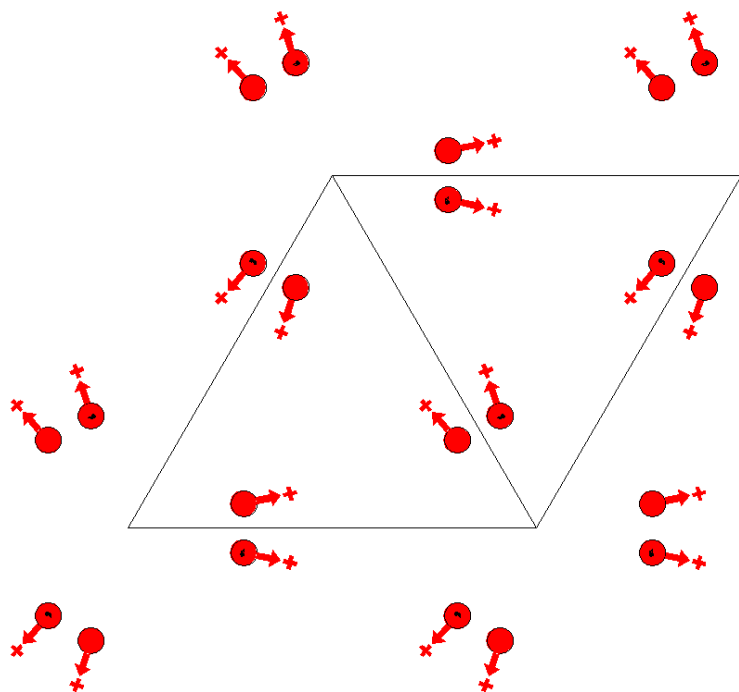
Along [2,1,0] p11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P_{2c}$  31m'  
157.5.1288

31m1'  
 $P_{2c}$  31m'

Trigonal



Origin on 31m'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1	1/2,0,1	2/3,1/3,1	1/2,1/2,1	

**Symmetry Operations**

For (0,0,0) + set

- |                                    |                                    |   |
|------------------------------------|------------------------------------|---|
| (1) 1<br>(1 0,0,0)                 | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0) | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) $m'$ x,x,z<br>( $m_3$  0,0,0)' | (5) $m'$ x,0,z<br>( $m_2$  0,0,0)' | (6) $m'$ 0,y,z<br>( $m_1$  0,0,0)'      |

For (0,0,1)' + set

- |  |  |   |
|--|--|---|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'         | (2) $3^+$ '(0,0,1) 0,0,z<br>( $3_z$  0,0,1)' | (3) $3^-$ '(0,0,1) 0,0,z<br>( $3_z^{-1}$  0,0,1)' |
| (4) c (0,0,1) x,x,z<br>( $m_3$  0,0,1) | (5) c (0,0,1) x,0,z<br>( $m_2$  0,0,1)       | (6) c (0,0,1) 0,y,z<br>( $m_1$  0,0,1)            |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

### Positions

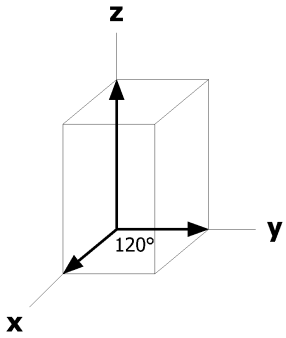
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
				(0,0,0) +	(0,0,1)' +
12	d	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z$ [ $\bar{u}+v, \bar{u}, w$ ]
			(4) y,x,z [v,u,w]	(5) x-y, $\bar{y}, z$ [u-v, $\bar{v}, w$ ]	(6) $\bar{x}, \bar{x}+y, z$ [ $\bar{u}, \bar{u}+v, w$ ]
6	c	..m'	x,0,z [u,0,w]	0,x,z [0,u,w]	$\bar{x}, \bar{x}, z$ [ $\bar{u}, \bar{u}, w$ ]
4	b	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0,w]	
2	a	3.m'	0,0,z [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] p31m1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>·1m'1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

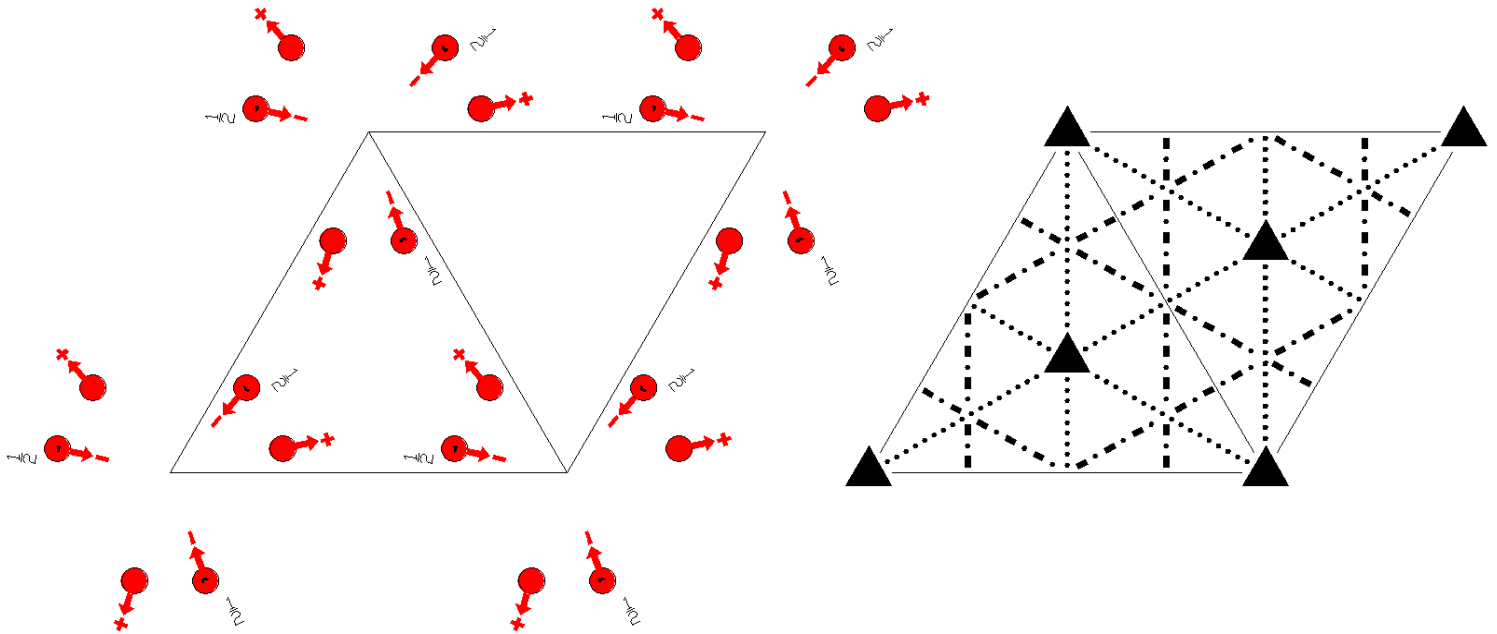
Along [2,1,0] p<sub>2a</sub>·1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P3c1  
158.1.1289

3m1  
P3c1

Trigonal



**Origin on 3c1**

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/3,2/3,1/2	0,1/2,1/2

**Symmetry Operations**

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                                      | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)              | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)         |
| (4) c (0,0,1/2) $x, \bar{x}, z$<br>( $m_{xy}$  0,0,1/2) | (5) c (0,0,1/2) $x, 2x, z$<br>( $m_x$  0,0,1/2) | (6) c (0,0,1/2) $2x, x, z$<br>( $m_y$  0,0,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

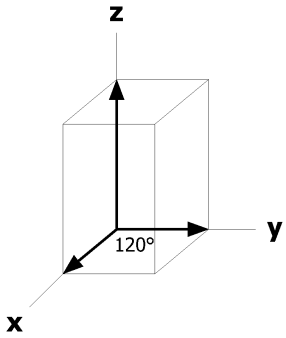
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	d	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{y},\bar{x},z+1/2$ [v,u, $\bar{w}$ ]	(5) $\bar{x}+y,y,z+1/2$ [u-v, $\bar{v},\bar{w}$ ]	(6) $x,x-y,z+1/2$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
2	c	3..	$2/3,1/3,z$ [0,0,w]	$2/3,1/3,z+1/2$ [0,0, $\bar{w}$ ]	
2	b	3..	$1/3,2/3,z$ [0,0,w]	$1/3,2/3,z+1/2$ [0,0, $\bar{w}$ ]	
2	a	3..	$0,0,z$ [0,0,w]	$0,0,z+1/2$ [0,0, $\bar{w}$ ]	

**Symmetry of Special Projections**

Along [0,0,1]  $p3m1$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a}1$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0]  $p1g1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



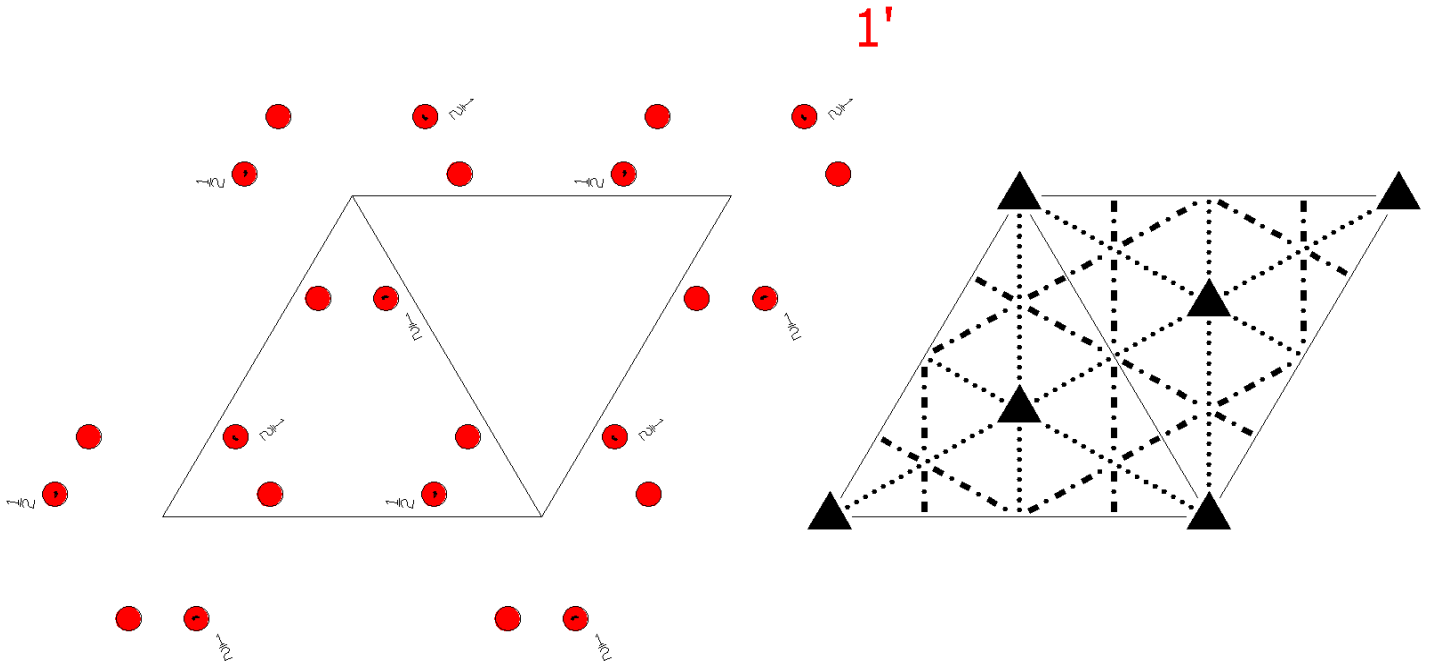
P3c11'

158.2.1290

3m11'

P3c11'

Trigonal



Origin on 3c11'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/3,2/3,1/2	0,1/2,1/2

**Symmetry Operations**

For 1 + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                   | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) c (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2) | (5) c (0,0,1/2) x,2x,z<br>(m <sub>x</sub>  0,0,1/2) | (6) c (0,0,1/2) 2x,x,z<br>(m <sub>y</sub>  0,0,1/2)               |

For 1' + set

- |  |   |  |
|--|---|--|
| (1) 1'<br>(1 0,0,0)'                                   | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)'  | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (4) c' (0,0,1/2) x,x̄,z<br>(m <sub>xy</sub>  0,0,1/2)' | (5) c' (0,0,1/2) x,2x,z<br>(m <sub>x</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 2x,x,z<br>(m <sub>y</sub>  0,0,1/2)'              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

**Positions**

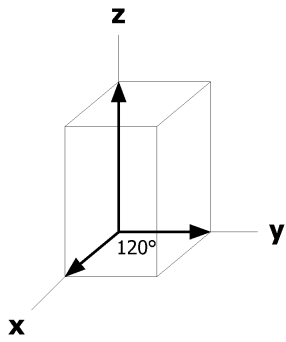
			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
			1 +	1' +	
6	d	11'	(1) x,y,z [0,0,0]	(2) $\bar{y},x-y,z$ [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0]
			(4) $\bar{y},\bar{x},z+1/2$ [0,0,0]	(5) $\bar{x}+y,y,z+1/2$ [0,0,0]	(6) x,x-y,z+1/2 [0,0,0]
2	c	3..1'	2/3,1/3,z [0,0,0]	2/3,1/3,z+1/2 [0,0,0]	
2	b	3..1'	1/3,2/3,z [0,0,0]	1/3,2/3,z+1/2 [0,0,0]	
2	a	3..1'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	

**Symmetry of Special Projections**

Along [0,0,1] p3m11'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p11'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

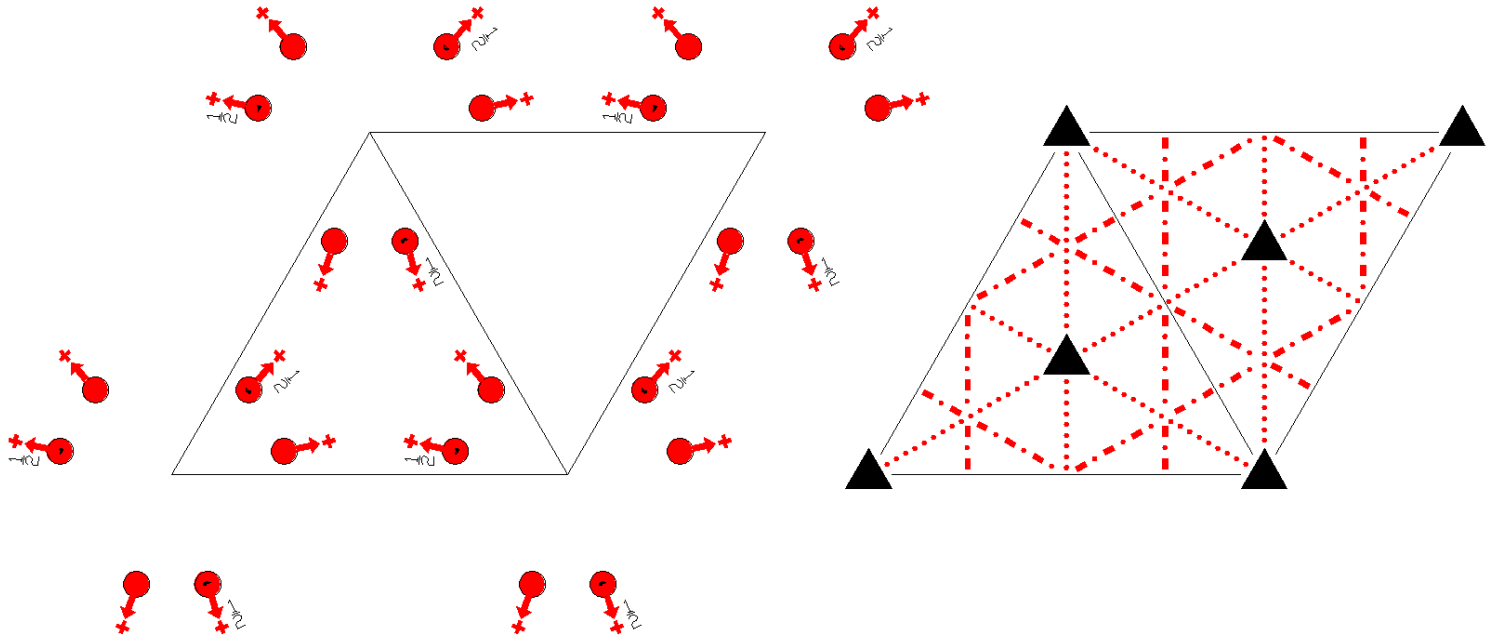
Along [2,1,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



P3c'1  
158.3.1291

3m'1  
P3c'1

Trigonal



Origin on 3c'1

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/3,2/3,0 1/3,2/3,1/2	0,1/2,0 0,1/2,1/2

**Symmetry Operations**

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)     | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) c' (0,0,1/2) x, x̄, z<br>(m <sub>xy</sub>  0,0,1/2)' | (5) c' (0,0,1/2) x, 2x, z<br>(m <sub>x</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 2x, x, z<br>(m <sub>y</sub>  0,0,1/2)'           |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

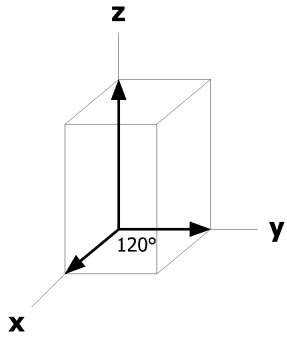
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	d	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(5) $\bar{x}+y,y,z+1/2$ [ $\bar{u}+v,v,w$ ]	(6) $x,x-y,z+1/2$ [u,u-v,w]
2	c	3..	$2/3,1/3,z$ [0,0,w]	$2/3,1/3,z+1/2$ [0,0,w]	
2	b	3..	$1/3,2/3,z$ [0,0,w]	$1/3,2/3,z+1/2$ [0,0,w]	
2	a	3..	$0,0,z$ [0,0,w]	$0,0,z+1/2$ [0,0,w]	

**Symmetry of Special Projections**

Along [0,0,1]  $p3m'1$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

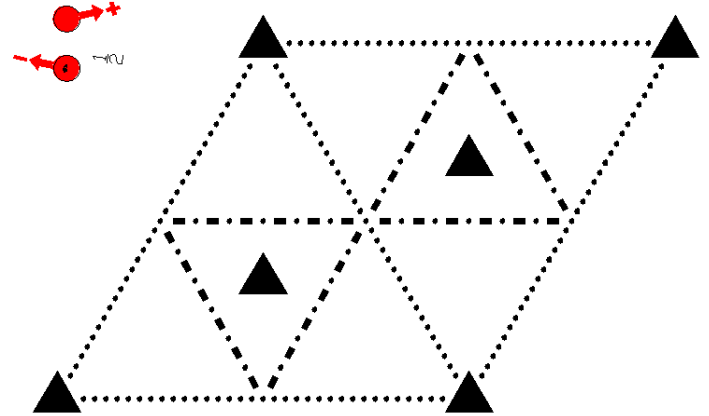
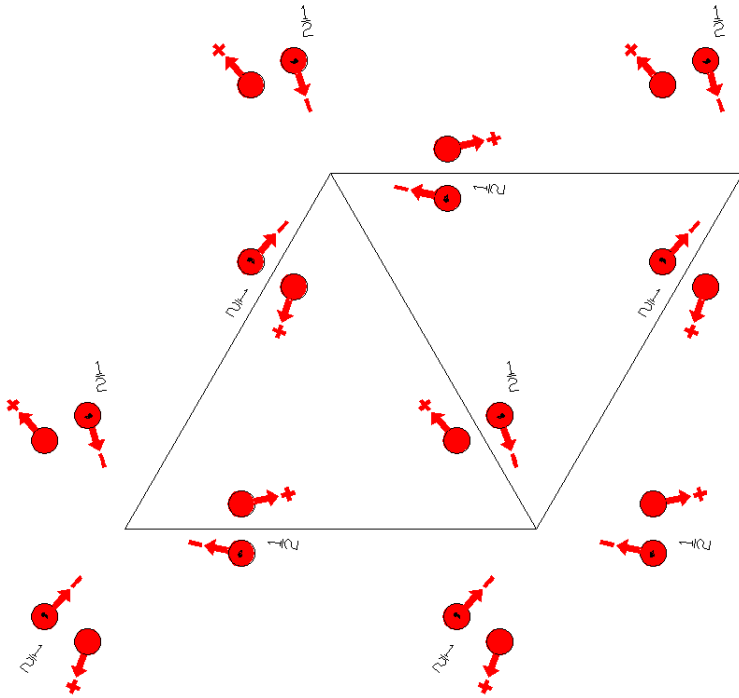
Along [2,1,0]  $p1g'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



P31c  
159.1.1292

31m  
P31c

Trigonal



Origin on 31c

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/3,2/3,1/2	0,1/2,1/2

**Symmetry Operations**

- |  |  |  |
|--|--|--|
| (1) 1<br>(1 0,0,0)                         | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)         | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)    |
| (4) c (0,0,1/2) x,x,z<br>( $m_3$  0,0,1/2) | (5) c (0,0,1/2) x,0,z<br>( $m_2$  0,0,1/2) | (6) c (0,0,1/2) 0,y,z<br>( $m_1$  0,0,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

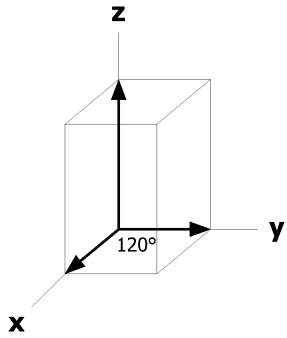
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	c	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $y,x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(5) $x-y,\bar{y},z+1/2$ [ $\bar{u}+v,v,\bar{w}$ ]	(6) $\bar{x},\bar{x}+y,z+1/2$ [u,u-v, $\bar{w}$ ]
2	b	3..	$1/3,2/3,z$ [0,0,w]	$2/3,1/3,z+1/2$ [0,0, $\bar{w}$ ]	
2	a	3..	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	

**Symmetry of Special Projections**

Along [0,0,1] p31m  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [2,1,0] p<sub>2a</sub>\* 1  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



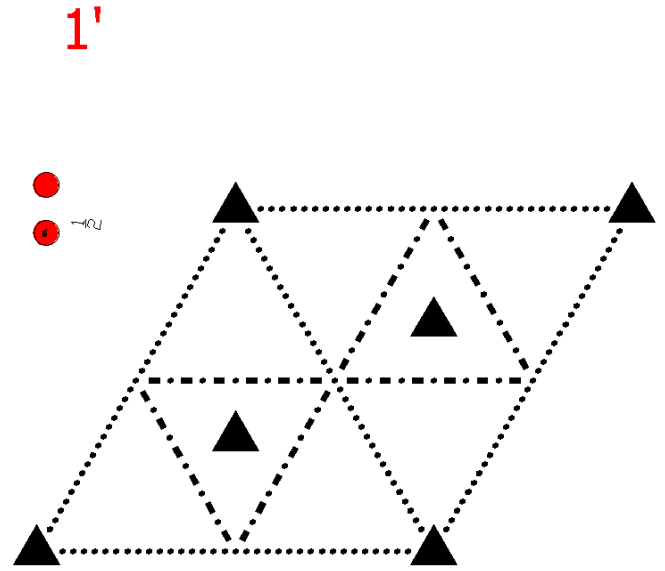
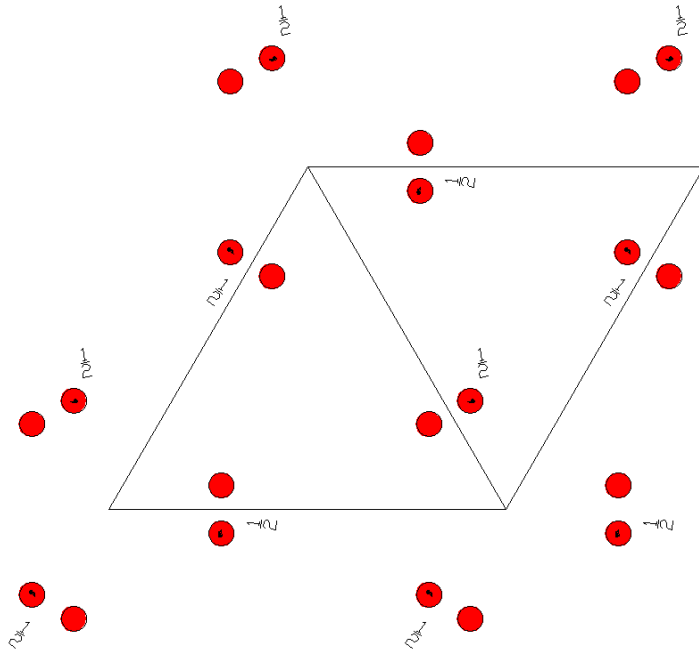
P31c1'

159.2.1293

31m1'

P31c1'

Trigonal



Origin on 31c1'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/3,2/3,1/2	0,1/2,1/2

**Symmetry Operations**

For 1 + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) c (0,0,1/2) x,x,z<br>(m <sub>3</sub>  0,0,1/2) | (5) c (0,0,1/2) x,0,z<br>(m <sub>2</sub>  0,0,1/2)  | (6) c (0,0,1/2) 0,y,z<br>(m <sub>1</sub>  0,0,1/2)                |

For 1' + set

- |  |  |  |
|--|--|--|
| (1) 1'<br>(1 0,0,0)'                                 | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)' | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (4) c' (0,0,1/2) x,x,z<br>(m <sub>3</sub>  0,0,1/2)' | (5) c' (0,0,1/2) x,0,z<br>(m <sub>2</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 0,y,z<br>(m <sub>1</sub>  0,0,1/2)'               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

**Positions**

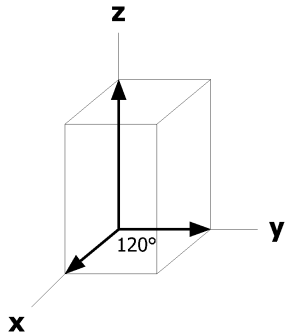
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			1 +	1' +	
6	c	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x}$ ,z [0,0,0]
			(4) y,x,z+1/2 [0,0,0]	(5) x-y, $\bar{y}$ ,z+1/2 [0,0,0]	(6) $\bar{x}$ , $\bar{x}+y$ ,z+1/2 [0,0,0]
2	b	3..1'	1/3,2/3,z [0,0,0]	2/3,1/3,z+1/2 [0,0,0]	
2	a	3..1'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	

**Symmetry of Special Projections**

Along [0,0,1] p31m1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

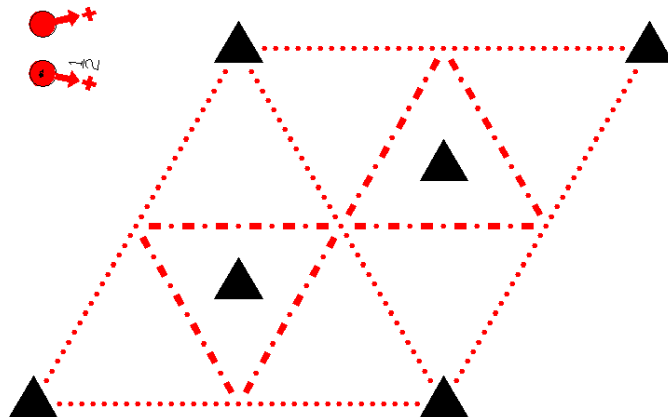
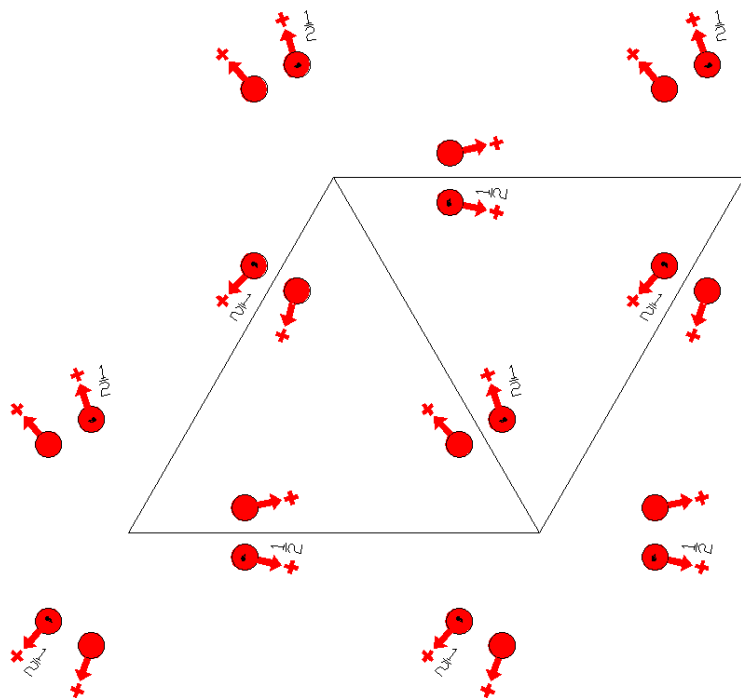
Along [2,1,0] p11'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P31c'  
159.3.1294

31m'  
P31c'

Trigonal



Origin on 31c'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/3,2/3,1/2	0,1/2,1/2

**Symmetry Operations**

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                                   | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)  | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) c' (0,0,1/2) x,x,z<br>(m <sub>3</sub>  0,0,1/2)' | (5) c' (0,0,1/2) x,0,z<br>(m <sub>2</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 0,y,z<br>(m <sub>1</sub>  0,0,1/2)'              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

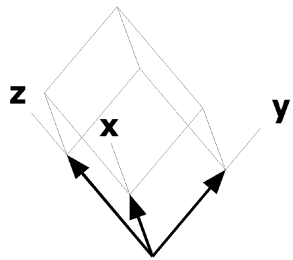
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	c	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) y,x,z+1/2 [v,u,w]	(5) x-y, $\bar{y},z+1/2$ [u-v, $\bar{v},w$ ]	(6) $\bar{x},\bar{x}+y,z+1/2$ [ $\bar{u},\bar{u}+v,w$ ]
2	b	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z+1/2 [0,0,w]	
2	a	3..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	

**Symmetry of Special Projections**

Along [0,0,1] p31m'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

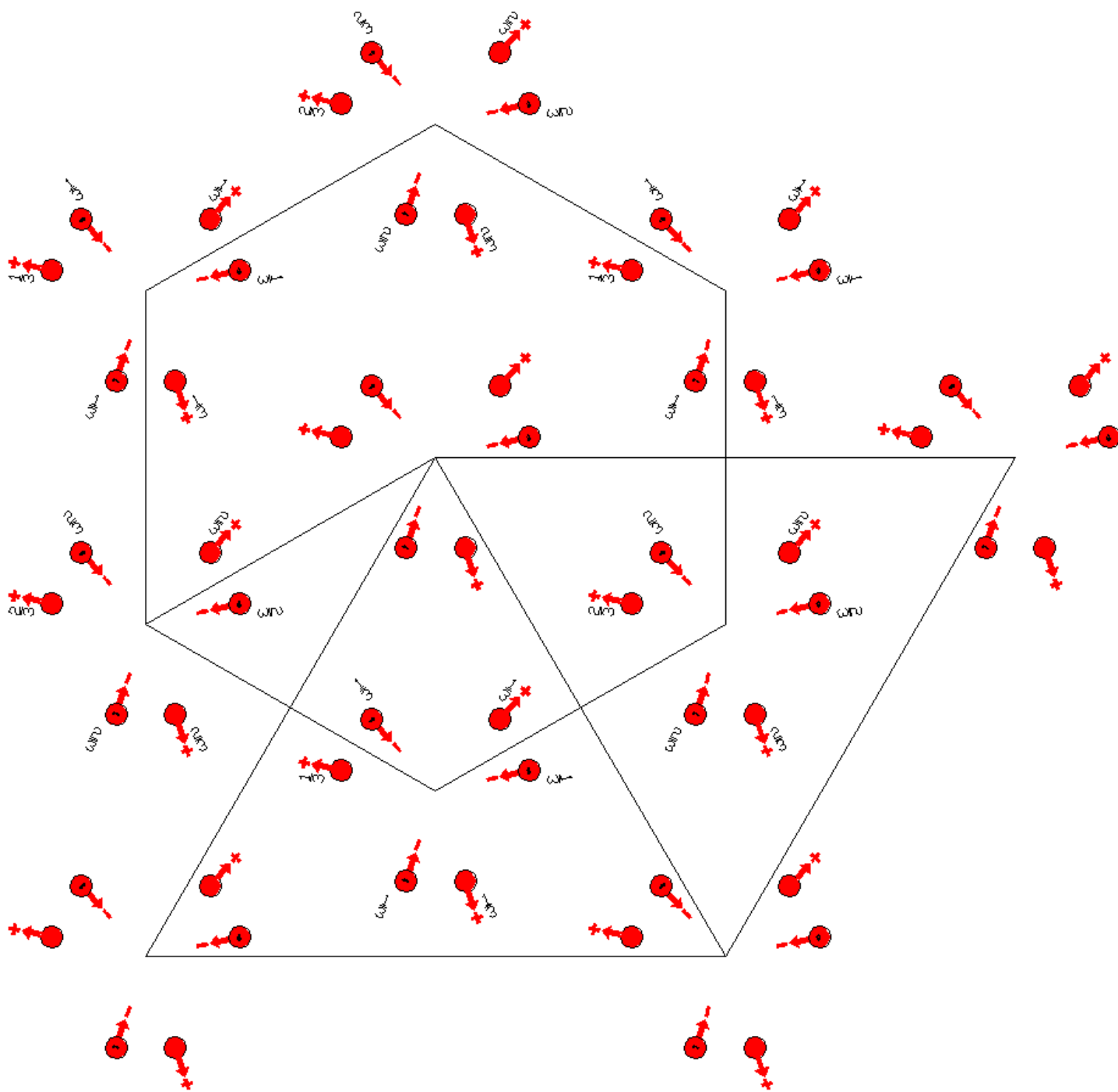
Along [2,1,0] p1  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



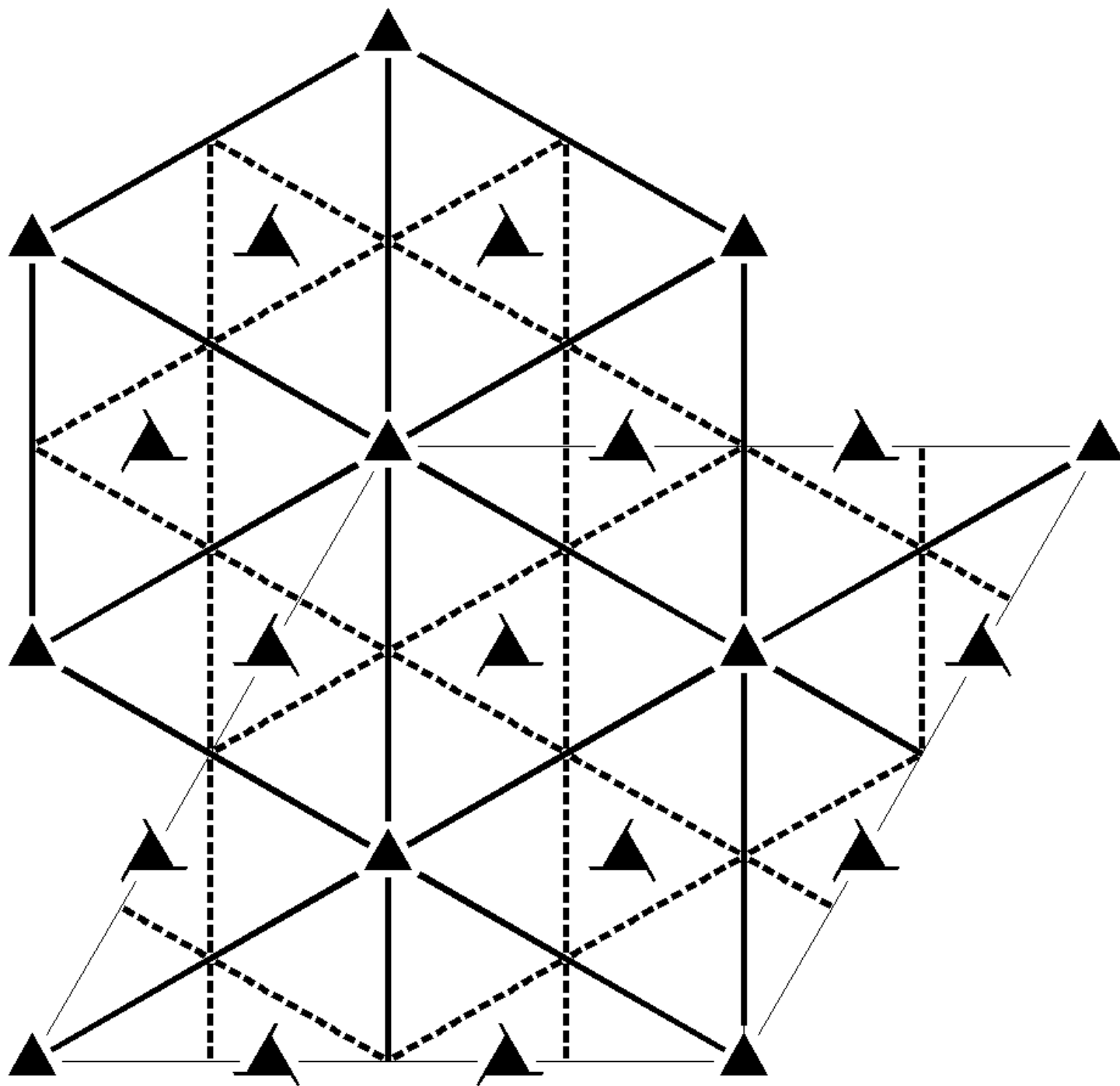
R3m  
160.1.1295

3m  
R3m

Trigonal







Origin on 3m

Asymmetric unit

$0 \leq x \leq 2/3;$      $0 \leq y \leq 2/3;$      $0 \leq z \leq 1/3;$      $x \leq 2y;$      $y \leq \min(1-x, 2x)$

Vertices

0,0,0            2/3,1/3,0            1/3,2/3,0  
 0,0,1/3        2/3,1/3,1/3        1/3,2/3,1/3

**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) m x, $\bar{x}$ , z<br>(m <sub>xy</sub>  0,0,0) | (5) m x, 2x, z<br>(m <sub>x</sub>  0,0,0)           | (6) m 2x, x, z<br>(m <sub>y</sub>  0,0,0)                         |

For (2/3,1/3,1/3) + set

- |   |   |   |
|---|---|---|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)                                      | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3) | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3) |
| (4) g (1/6,-1/6,1/3) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  2/3,1/3,1/3) | (5) g (1/6,1/3,1/3) x, 2x-1/2, z<br>(m <sub>x</sub>  2/3,1/3,1/3)       | (6) g (2/3,1/3,1/3) 2x, x, z<br>(m <sub>y</sub>  2/3,1/3,1/3)                       |

For (1/3,2/3,2/3) + set

- |   |   |   |
|---|---|---|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)                                      | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3) | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3) |
| (4) g (-1/6,1/6,2/3) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  1/3,2/3,2/3) | (5) g (1/3,2/3,2/3) x, 2x, z<br>(m <sub>x</sub>  1/3,2/3,2/3)         | (6) g (1/3,1/6,2/3) 2x-1/2, x, z<br>(m <sub>y</sub>  1/3,2/3,2/3)                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4).**Positions**

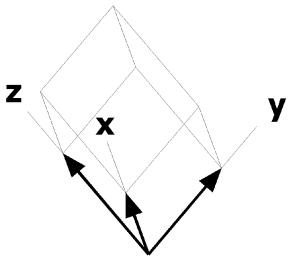
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(2/3,1/3,1/3) +	(1/3,2/3,2/3) +
18	c	1	(1) x,y,z [u,v,w] (4) $\bar{y}$ , $\bar{x}$ , z [v,u, $\bar{w}$ ]	(2) $\bar{y}$ , x-y, z [ $\bar{v}$ , u-v, w] (5) $\bar{x}$ +y, y, z [u-v, $\bar{v}$ , $\bar{w}$ ]	(3) $\bar{x}$ +y, $\bar{x}$ , z [ $\bar{u}$ +v, $\bar{u}$ , w] (6) x, x-y, z [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ]
9	b	.m	x, $\bar{x}$ , z [u,u,0]	x, 2x, z [ $\bar{u}$ , 0,0]	2 $\bar{x}$ , $\bar{x}$ , z [0, $\bar{u}$ , 0]
3	a	3m	0,0,z [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p31m  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at 0,0,z

Along [1,0,0] p11'  
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

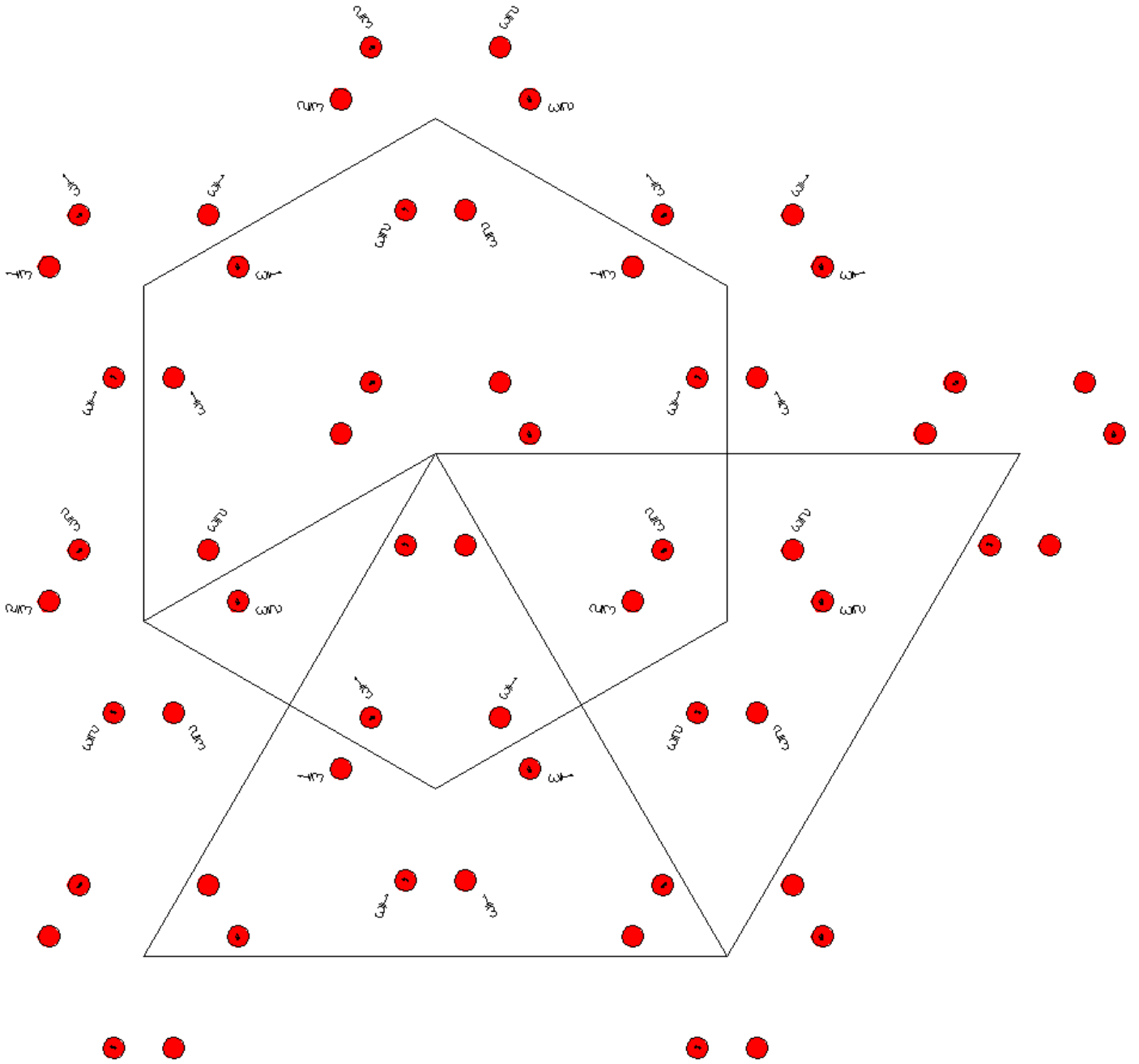
Along [2,1,0] p1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/3$   
 Origin at x,x/2,0



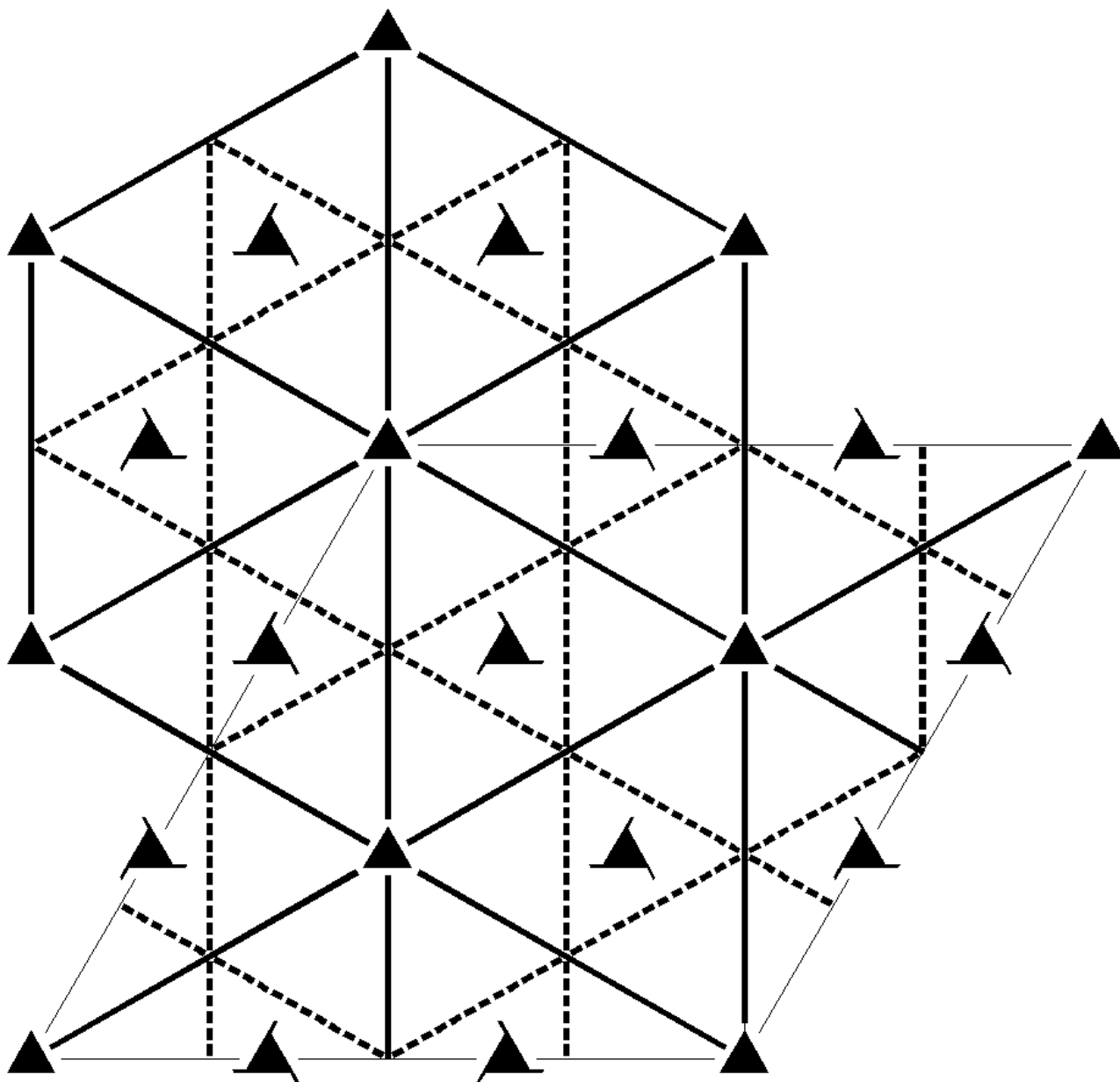
R3m1'  
160.2.1296

3m1'  
R3m1'

Trigonal



1'



Origin on 3m1'

**Asymmetric unit**     $0 \leq x \leq 2/3;$      $0 \leq y \leq 2/3;$      $0 \leq z \leq 1/3;$      $x \leq 2y;$      $y \leq \min(1-x, 2x)$

Vertices     $0,0,0$      $2/3,1/3,0$      $1/3,2/3,0$   
                $0,0,1/3$      $2/3,1/3,1/3$      $1/3,2/3,1/3$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) m x, $\bar{x}$ , z<br>(m <sub>xy</sub>  0,0,0) | (5) m x, 2x, z<br>(m <sub>x</sub>  0,0,0)           | (6) m 2x, x, z<br>(m <sub>y</sub>  0,0,0)                         |

For (2/3,1/3,1/3) + set

- |   |   |   |
|---|---|---|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)                                      | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3) | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3) |
| (4) g (1/6,-1/6,1/3) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  2/3,1/3,1/3) | (5) g (1/6,1/3,1/3) x, 2x-1/2, z<br>(m <sub>x</sub>  2/3,1/3,1/3)       | (6) g (2/3,1/3,1/3) 2x, x, z<br>(m <sub>y</sub>  2/3,1/3,1/3)                       |

For (1/3,2/3,2/3) + set

- |   |   |   |
|---|---|---|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)                                      | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3) | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3) |
| (4) g (-1/6,1/6,2/3) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  1/3,2/3,2/3) | (5) g (1/3,2/3,2/3) x, 2x, z<br>(m <sub>x</sub>  1/3,2/3,2/3)         | (6) g (1/3,1/6,2/3) 2x-1/2, x, z<br>(m <sub>y</sub>  1/3,2/3,2/3)                     |

For (0,0,0)' + set

- |  |  |  |
|--|--|--|
| (1) 1'<br>(1 0,0,0)'                                 | (2) 3 <sup>+</sup> ' 0,0,z<br>(3 <sub>z</sub>  0,0,0)' | (3) 3 <sup>-</sup> ' 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (4) m' x, $\bar{x}$ , z<br>(m <sub>xy</sub>  0,0,0)' | (5) m' x, 2x, z<br>(m <sub>x</sub>  0,0,0)'            | (6) m' 2x, x, z<br>(m <sub>y</sub>  0,0,0)'                          |

For (2/3,1/3,1/3)' + set

- |   |  |  |
|---|--|--|
| (1) t' (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)'                                      | (2) 3 <sup>+</sup> ' (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3)' | (3) 3 <sup>-</sup> ' (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3)' |
| (4) g' (1/6,-1/6,1/3) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  2/3,1/3,1/3)' | (5) g' (1/6,1/3,1/3) x, 2x-1/2, z<br>(m <sub>x</sub>  2/3,1/3,1/3)'        | (6) g' (2/3,1/3,1/3) 2x, x, z<br>(m <sub>y</sub>  2/3,1/3,1/3)'                        |

For (1/3,2/3,2/3)' + set

- |   |  |  |
|---|--|--|
| (1) t' (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)'                                      | (2) 3 <sup>+</sup> ' (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3)' | (3) 3 <sup>-</sup> ' (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3)' |
| (4) g' (-1/6,1/6,2/3) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  1/3,2/3,2/3)' | (5) g' (1/3,2/3,2/3) x, 2x, z<br>(m <sub>x</sub>  1/3,2/3,2/3)'          | (6) g' (1/3,1/6,2/3) 2x-1/2, x, z<br>(m <sub>y</sub>  1/3,2/3,2/3)'                      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4);1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

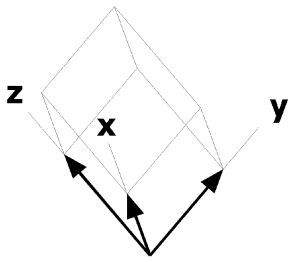
			(0,0,0) + (0,0,0)' +	(2/3,1/3,1/3) + (2/3,1/3,1/3)' +	(1/3,2/3,2/3) + (1/3,2/3,2/3)' +
18	c	11'	(1) x,y,z [0,0,0] (4) $\bar{y},\bar{x},z$ [0,0,0]	(2) $\bar{y},x-y,z$ [0,0,0] (5) $\bar{x}+y,y,z$ [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0] (6) x,x-y,z [0,0,0]
9	b	.m1'	x, $\bar{x},z$ [0,0,0]	x,2x,z [0,0,0]	2 $\bar{x},\bar{x},z$ [0,0,0]
3	a	3m1'	0,0,z [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p31m1'  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at 0,0,z

Along [1,0,0] p11'  
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

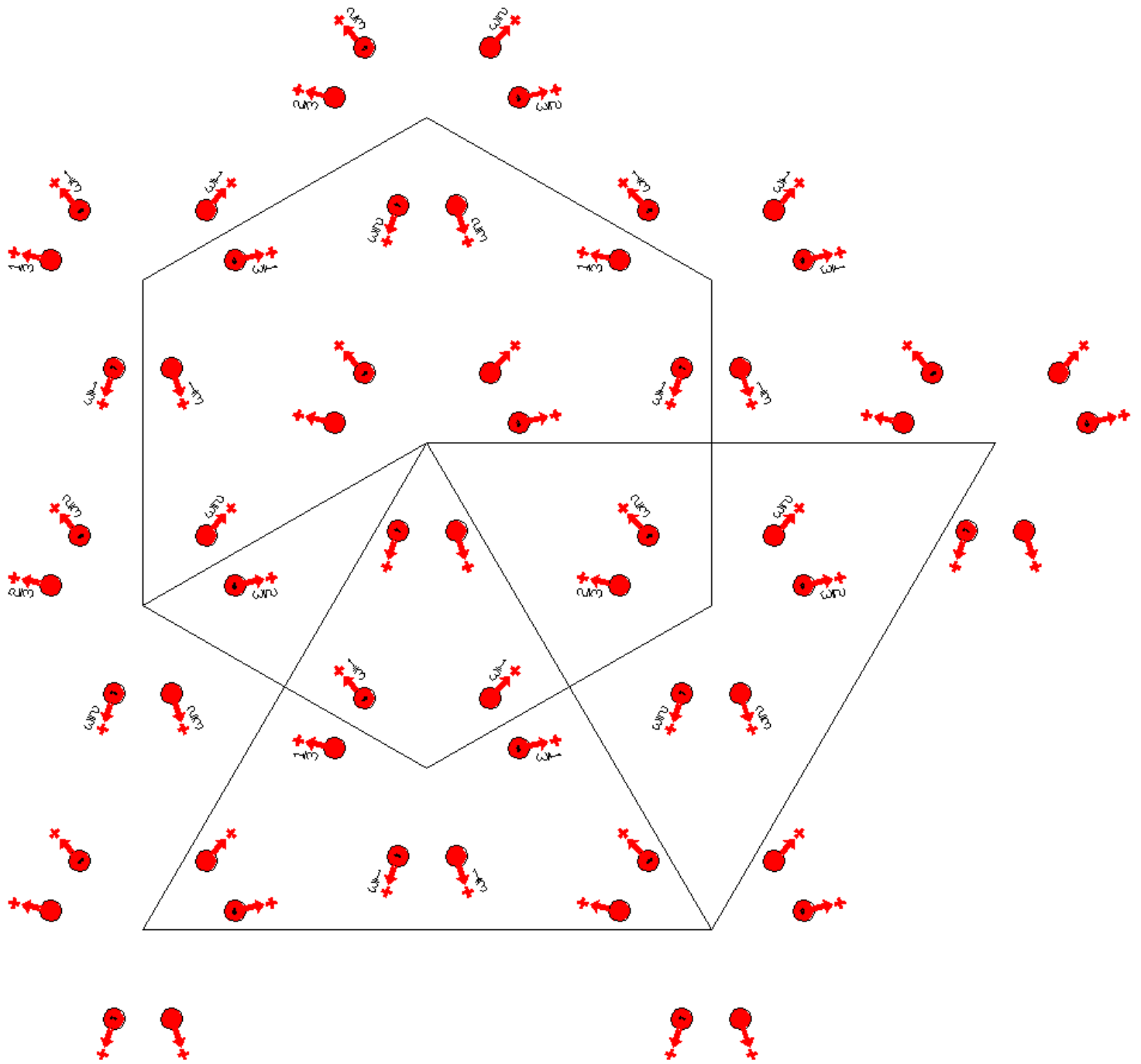
Along [2,1,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/3$   
 Origin at x,x/2,0

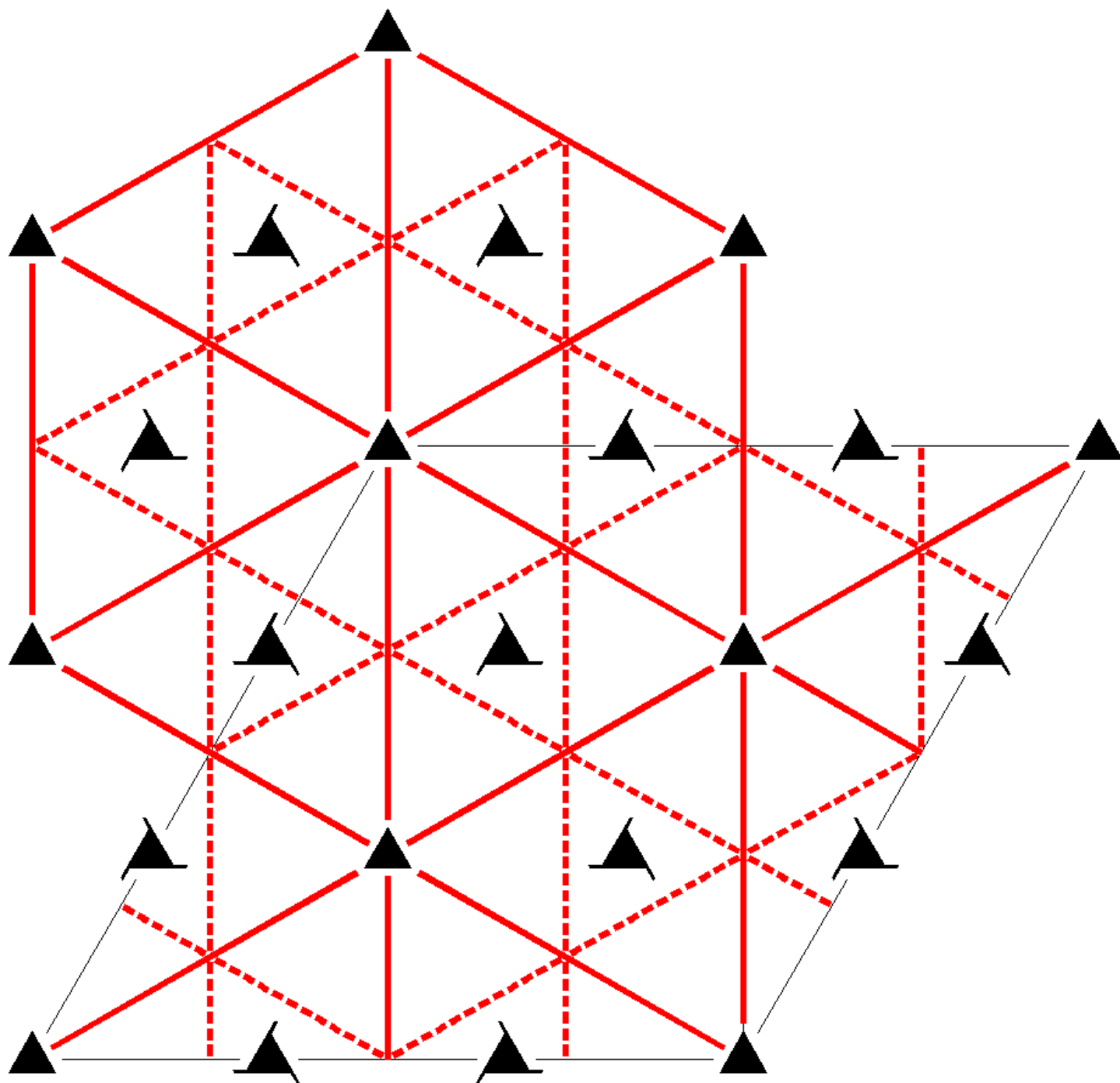


R3m'  
160.3.1297

3m'  
R3m'

Trigonal





Origin on 3m'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/3;$	$x \leq 2y;$	$y \leq \min(1-x, 2x)$
Vertices	0,0,0 0,0,1/3	2/3,1/3,0 2/3,1/3,1/3	1/3,2/3,0 1/3,2/3,1/3		



**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                   | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) m' x, $\bar{x}$ , z<br>(m <sub>xy</sub>  0,0,0)' | (5) m' x, 2x, z<br>(m <sub>x</sub>  0,0,0)'         | (6) m' 2x, x, z<br>(m <sub>y</sub>  0,0,0)'                       |

For (2/3,1/3,1/3) + set

- |   |   |   |
|---|---|---|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)  | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3) | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3) |
| (4) g' (1/6,-1/6,1/3) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  2/3,1/3,1/3)' | (5) g' (1/6,1/3,1/3) x, 2x-1/2, z<br>(m <sub>x</sub>  2/3,1/3,1/3)'     | (6) g' (2/3,1/3,1/3) 2x, x, z<br>(m <sub>y</sub>  2/3,1/3,1/3)'                     |

For (1/3,2/3,2/3) + set

- |   |   |   |
|---|---|---|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)  | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3) | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3) |
| (4) g' (-1/6,1/6,2/3) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  1/3,2/3,2/3)' | (5) g' (1/3,2/3,2/3) x, 2x, z<br>(m <sub>x</sub>  1/3,2/3,2/3)'       | (6) g' (1/3,1/6,2/3) 2x-1/2, x, z<br>(m <sub>y</sub>  1/3,2/3,2/3)'                   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4).**Positions**

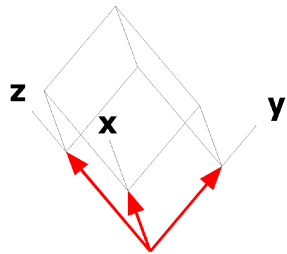
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(2/3,1/3,1/3) +	(1/3,2/3,2/3) +
18	c	1	(1) x,y,z [u,v,w] (4) $\bar{y}$ , $\bar{x}$ , z [ $\bar{v}$ , $\bar{u}$ , w]	(2) $\bar{y}$ , x-y, z [ $\bar{v}$ , u-v, w] (5) $\bar{x}$ +y, y, z [ $\bar{u}$ +v, v, w]	(3) $\bar{x}$ +y, $\bar{x}$ , z [ $\bar{u}$ +v, $\bar{u}$ , w] (6) x, x-y, z [u, u-v, w]
9	b	.m'	x, $\bar{x}$ , z [u, $\bar{u}$ , w]	x, 2x, z [u, 2u, w]	2 $\bar{x}$ , $\bar{x}$ , z [2 $\bar{u}$ , $\bar{u}$ , w]
3	a	3m'	0,0,z [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p31m'  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at 0,0,z

Along [1,0,0] p1  
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

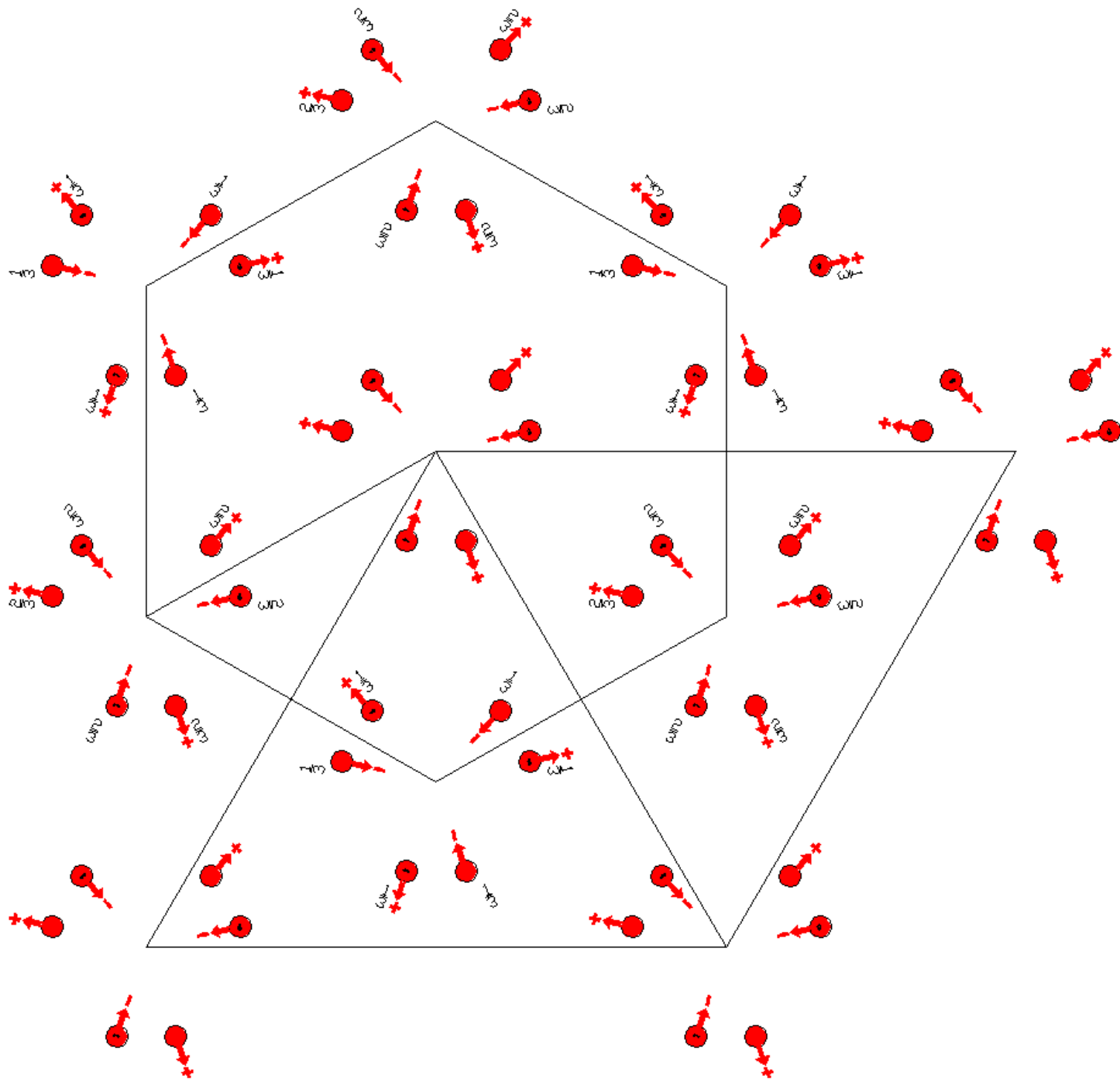
Along [2,1,0] p1m'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/3$   
 Origin at x,x/2,0

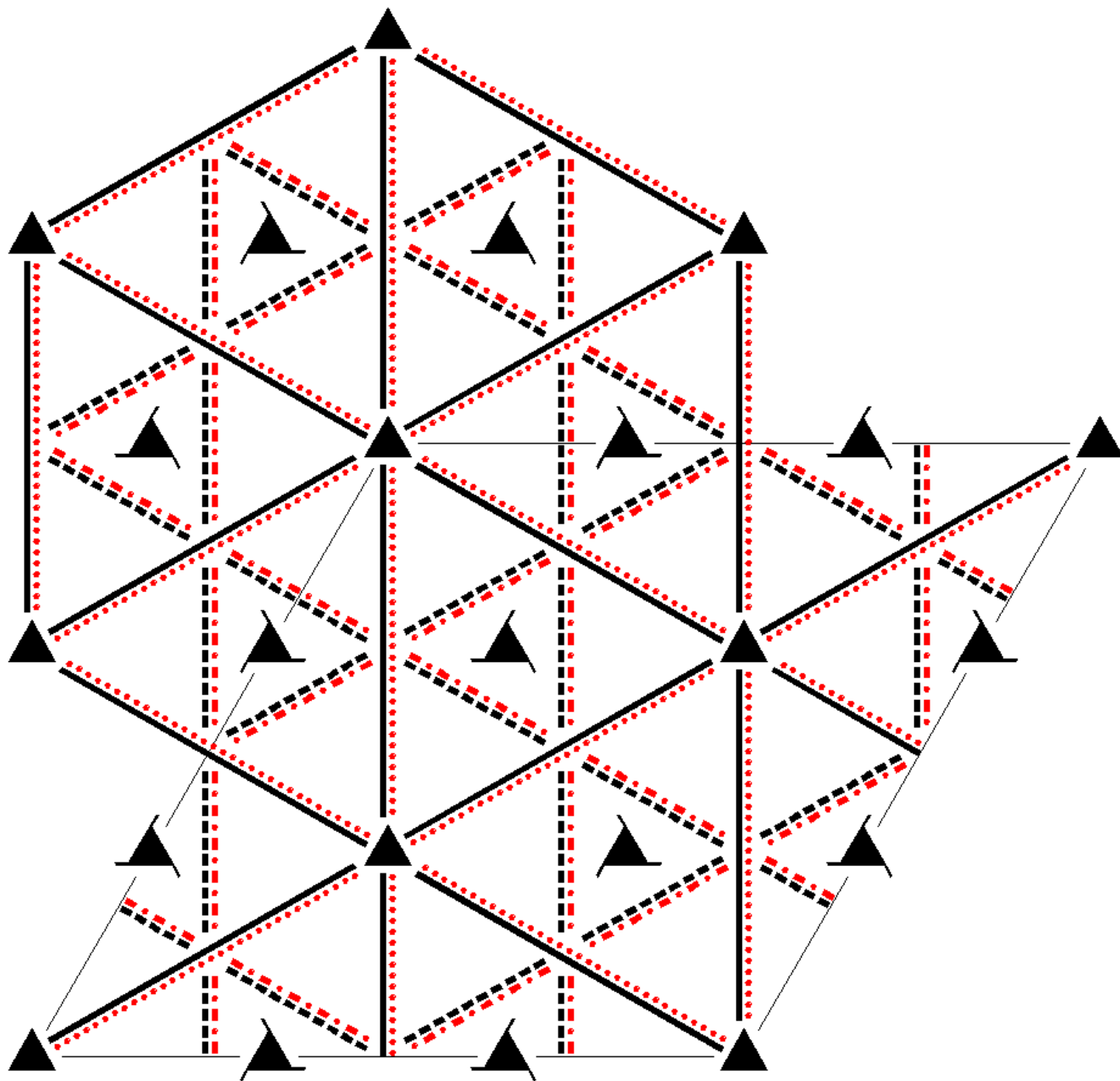


$R_R 3m$   
160.4.1298

$3m1'$   
 $R_R 3m$

Trigonal





Origin on  $3m$

Asymmetric unit

$$0 \leq x \leq 2/3;$$

$$0 \leq y \leq 2/3;$$

$$0 \leq z \leq 1/3;$$

$$x \leq 2y;$$

$$y \leq \min(1-x, 2x)$$

Vertices

$$0,0,0$$

$$2/3,1/3,0$$

$$1/3,2/3,0$$

$$0,0,1/3$$

$$2/3,1/3,1/3$$

$$1/3,2/3,1/3$$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |
|---|--|--|
| (1) 1<br>(1   0,0,0)                                | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>   0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>   0,0,0) |
| (4) m x, $\bar{x}$ , z<br>(m <sub>xy</sub>   0,0,0) | (5) m x, 2x, z<br>(m <sub>x</sub>   0,0,0)           | (6) m 2x, x, z<br>(m <sub>y</sub>   0,0,0)                         |

For (2/3,1/3,1/3)' + set

- |  |   |   |
|--|---|---|
| (1) t' (2/3,1/3,1/3)<br>(1   2/3,1/3,1/3)'                                     | (2) 3 <sup>+</sup> ' (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>   2/3,1/3,1/3)' | (3) 3 <sup>-</sup> ' (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>   2/3,1/3,1/3)' |
| (4) g' (1/6,-1/6,1/3) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>   2/3,1/3,1/3)' | (5) g' (1/6,1/3,1/3) x, 2x-1/2, z<br>(m <sub>x</sub>   2/3,1/3,1/3)'        | (6) g' (2/3,1/3,1/3) 2x, x, z<br>(m <sub>y</sub>   2/3,1/3,1/3)'                        |

For (1/3,2/3,2/3) + set

- |  |  |  |
|--|--|--|
| (1) t (1/3,2/3,2/3)<br>(1   1/3,2/3,2/3)                                     | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>   1/3,2/3,2/3) | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>   1/3,2/3,2/3) |
| (4) g (-1/6,1/6,2/3) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>   1/3,2/3,2/3) | (5) g (1/3,2/3,2/3) x, 2x, z<br>(m <sub>x</sub>   1/3,2/3,2/3)         | (6) g (1/3,1/6,2/3) 2x-1/2, x, z<br>(m <sub>y</sub>   1/3,2/3,2/3)                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(2/3,1/3,1/3); (2); (4).**Positions**

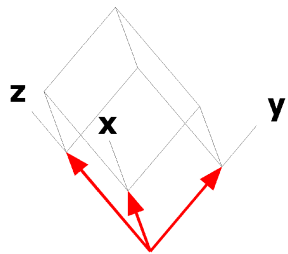
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(2/3,1/3,1/3)' +	(1/3,2/3,2/3) +
18	c	1	(1) x,y,z [u,v,w] (4) $\bar{y}$ , $\bar{x}$ , z [v,u, $\bar{w}$ ]	(2) $\bar{y}$ , x-y, z [ $\bar{v}$ , u-v, w] (5) $\bar{x}$ +y, y, z [u-v, $\bar{v}$ , $\bar{w}$ ]	(3) $\bar{x}$ +y, $\bar{x}$ , z [ $\bar{u}$ +v, $\bar{u}$ , w] (6) x, x-y, z [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ]
9	b	.m	x, $\bar{x}$ , z [u,u,0]	x, 2x, z [ $\bar{u}$ , 0, 0]	2 $\bar{x}$ , $\bar{x}$ , z [0, $\bar{u}$ , 0]
3	a	3m	0,0,z [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p31m1'  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at 0,0,z

Along [1,0,0] p11'  
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p<sub>2b</sub> 1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/3$   
 Origin at x,x/2,0



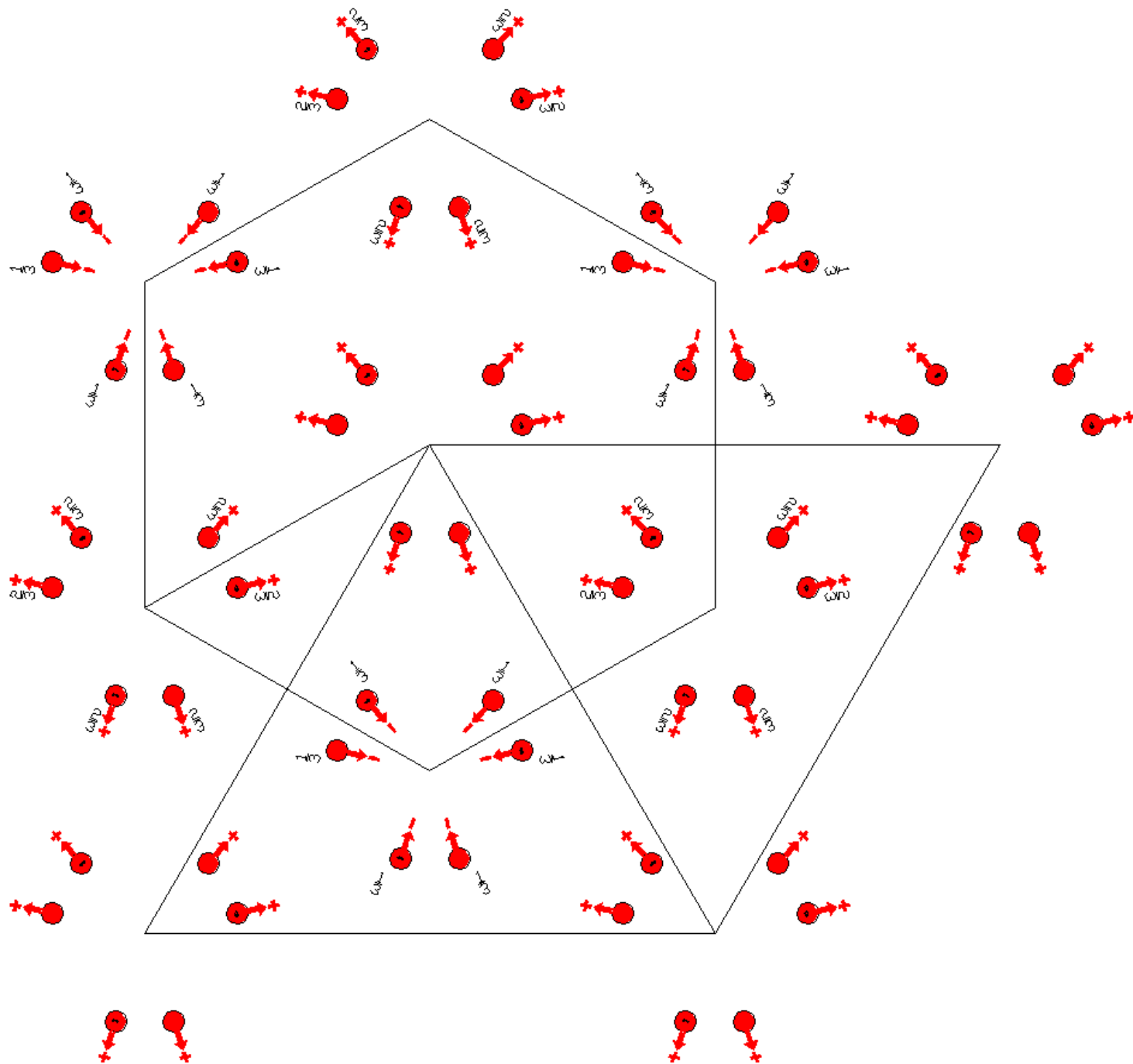
$R_R 3m'$

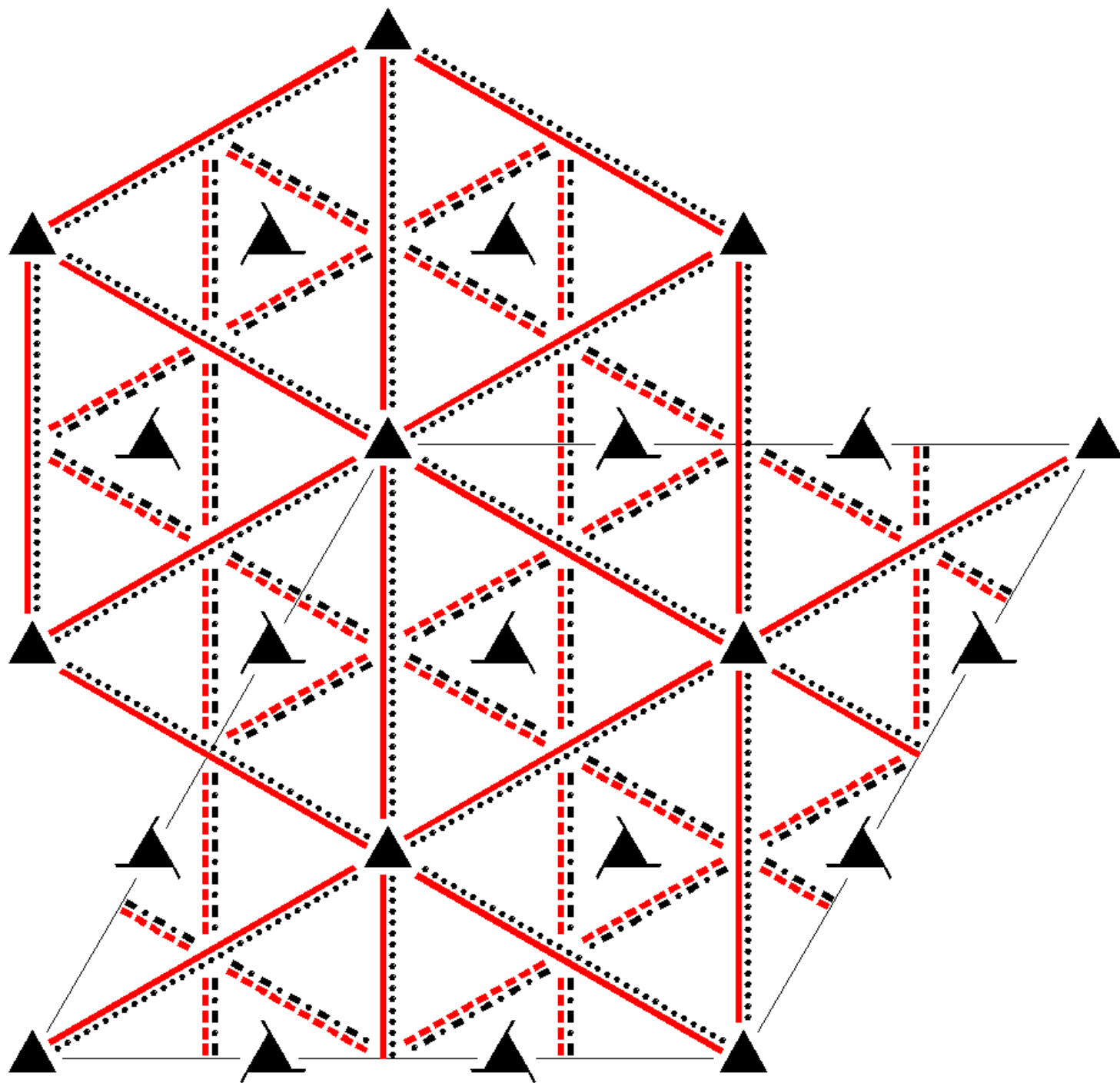
$3m1'$

Trigonal

160.5.1299

$R_R 3m'$





Origin on  $3m'$

Asymmetric unit

$$0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/3; \quad x \leq 2y; \quad y \leq \min(1-x, 2x)$$

Vertices

$$\begin{array}{lll} 0,0,0 & 2/3,1/3,0 & 1/3,2/3,0 \\ 0,0,1/3 & 2/3,1/3,1/3 & 1/3,2/3,1/3 \end{array}$$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                   | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) m' x, $\bar{x}$ , z<br>(m <sub>xy</sub>  0,0,0)' | (5) m' x, 2x, z<br>(m <sub>x</sub>  0,0,0)'         | (6) m' 2x, x, z<br>(m <sub>y</sub>  0,0,0)'                       |

For (2/3,1/3,1/3)' + set

- |   |  |  |
|---|--|--|
| (1) t' (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)'                                    | (2) 3 <sup>+</sup> ' (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3)' | (3) 3 <sup>-</sup> ' (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3)' |
| (4) g (1/6,-1/6,1/3) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  2/3,1/3,1/3) | (5) g (1/6,1/3,1/3) x, 2x-1/2, z<br>(m <sub>x</sub>  2/3,1/3,1/3)          | (6) g (2/3,1/3,1/3) 2x, x, z<br>(m <sub>y</sub>  2/3,1/3,1/3)                          |

For (1/3,2/3,2/3) + set

- |   |   |   |
|---|---|---|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)  | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3) | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3) |
| (4) g' (-1/6,1/6,2/3) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  1/3,2/3,2/3)' | (5) g' (1/3,2/3,2/3) x, 2x, z<br>(m <sub>x</sub>  1/3,2/3,2/3)'       | (6) g' (1/3,1/6,2/3) 2x-1/2, x, z<br>(m <sub>y</sub>  1/3,2/3,2/3)'                   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(2/3,1/3,1/3); (2); (4).**Positions**

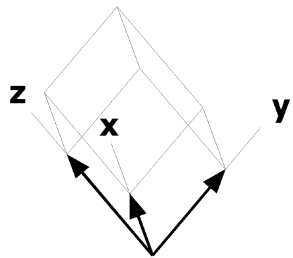
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(2/3,1/3,1/3)' +	(1/3,2/3,2/3) +
18	c	1	(1) x,y,z [u,v,w] (4) $\bar{y}$ , $\bar{x}$ , z [ $\bar{v}$ , $\bar{u}$ , w]	(2) $\bar{y}$ , x-y, z [ $\bar{v}$ , u-v, w] (5) $\bar{x}$ +y, y, z [ $\bar{u}$ +v, v, w]	(3) $\bar{x}$ +y, $\bar{x}$ , z [ $\bar{u}$ +v, $\bar{u}$ , w] (6) x, x-y, z [u, u-v, w]
9	b	.m'	x, $\bar{x}$ , z [u, $\bar{u}$ , w]	x, 2x, z [u, 2u, w]	2 $\bar{x}$ , $\bar{x}$ , z [2 $\bar{u}$ , $\bar{u}$ , w]
3	a	3m'	0,0,z [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p31m'  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>' 1  
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

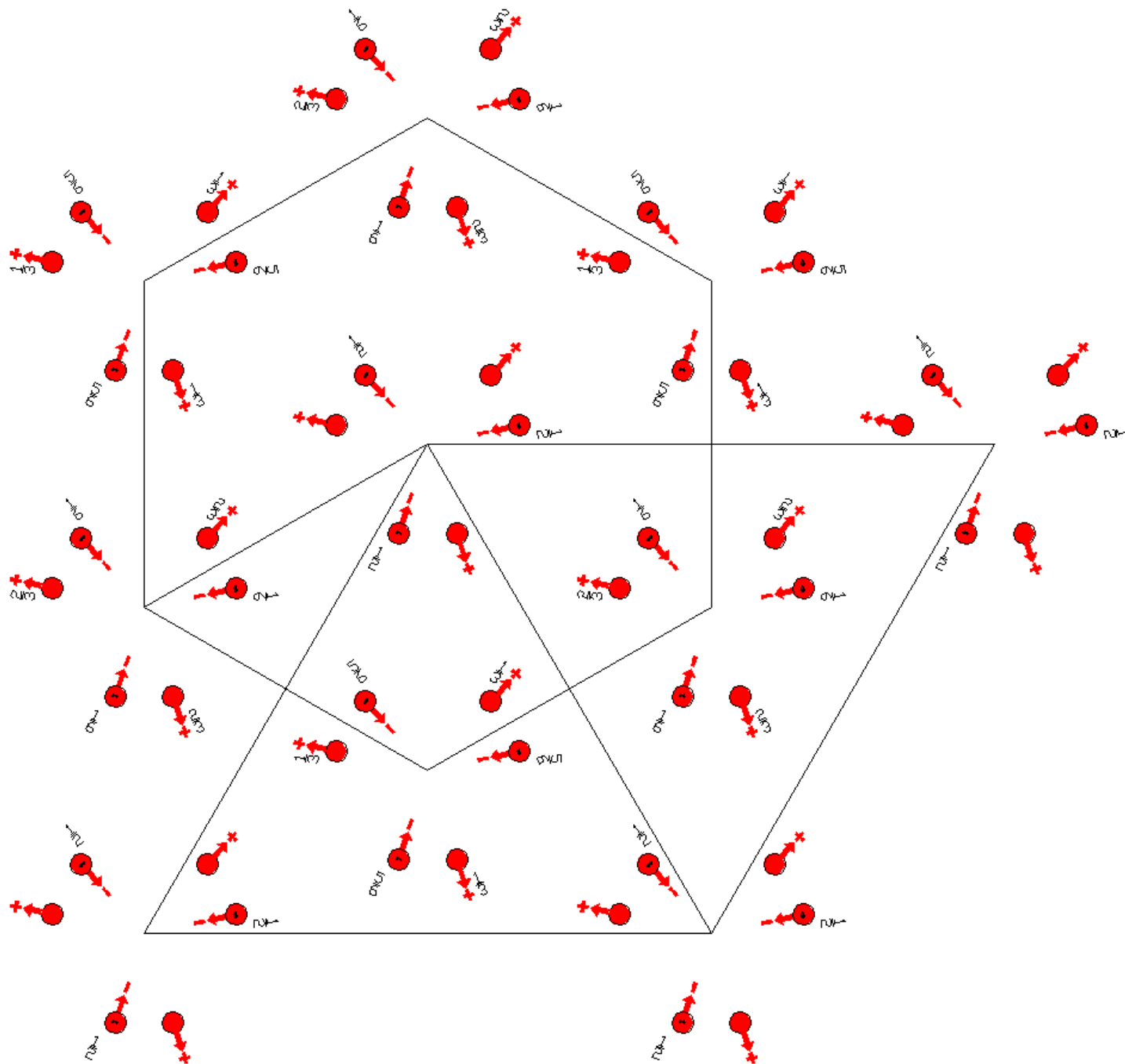
Along [2,1,0] p<sub>2b</sub>' 1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/3$   
 Origin at x,x/2,0



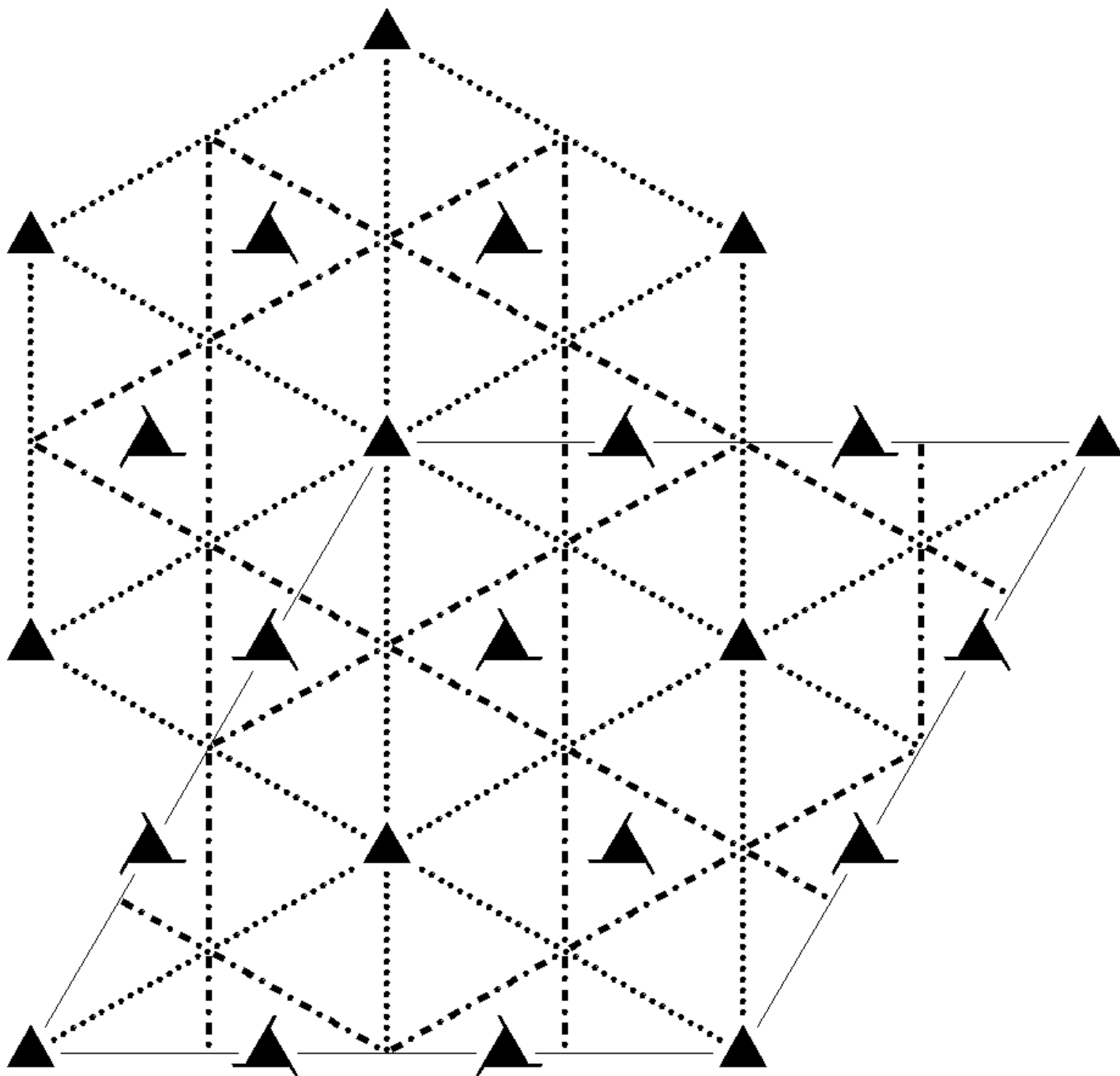
R3c  
161.1.1300

3m  
R3c

Trigonal







Origin on 3c

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/6;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/6	1/2,0,0 1/2,0,1/6	2/3,1/3,0 2/3,1/3,1/6	1/3,2/3,0 1/3,2/3,1/6	0,1/2,0 0,1/2,1/6

**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)   | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) c (0,0,1/2) x, $\bar{x}$ , z<br>(m <sub>xy</sub>  0,0,1/2) | (5) c (0,0,1/2) x, 2x, z<br>(m <sub>x</sub>  0,0,1/2) | (6) c (0,0,1/2) 2x, x, z<br>(m <sub>y</sub>  0,0,1/2)             |

For (2/3,1/3,1/3) + set

- |   |   |   |
|---|---|---|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)                                      | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3) | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3) |
| (4) g (1/6,-1/6,5/6) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  2/3,1/3,5/6) | (5) g (1/6,1/3,5/6) x, 2x-1/2, z<br>(m <sub>x</sub>  2/3,1/3,5/6)       | (6) g (2/3,1/3,5/6) 2x, x, z<br>(m <sub>y</sub>  2/3,1/3,5/6)                       |

For (1/3,2/3,2/3) + set

- |   |   |   |
|---|---|---|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)                                      | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3) | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3) |
| (4) g (-1/6,1/6,1/6) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  1/3,2/3,1/6) | (5) g (1/3,2/3,1/6) x, 2x, z<br>(m <sub>x</sub>  1/3,2/3,1/6)         | (6) g (1/3,1/6,1/6) 2x-1/2, x, z<br>(m <sub>y</sub>  1/3,2/3,1/6)                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4).**Positions**

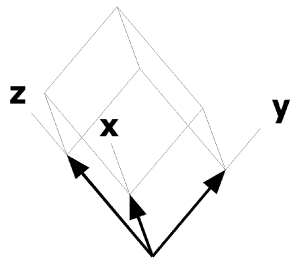
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(2/3,1/3,1/3) +	(1/3,2/3,2/3) +
18	b	1	(1) x,y,z [u,v,w] (4) $\bar{y}$ , $\bar{x}$ , z+1/2 [v,u, $\bar{w}$ ]	(2) $\bar{y}$ , x-y, z [ $\bar{v}$ , u-v, w] (5) $\bar{x}$ +y, y, z+1/2 [u-v, $\bar{v}$ , $\bar{w}$ ]	(3) $\bar{x}$ +y, $\bar{x}$ , z [ $\bar{u}$ +v, $\bar{u}$ , w] (6) x, x-y, z+1/2 [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ]
3	a	3.	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	

**Symmetry of Special Projections**

Along [0,0,1] p31m  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub> 1  
 $\mathbf{a}^* = (2\mathbf{a} + 4\mathbf{b} + \mathbf{c})/6$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

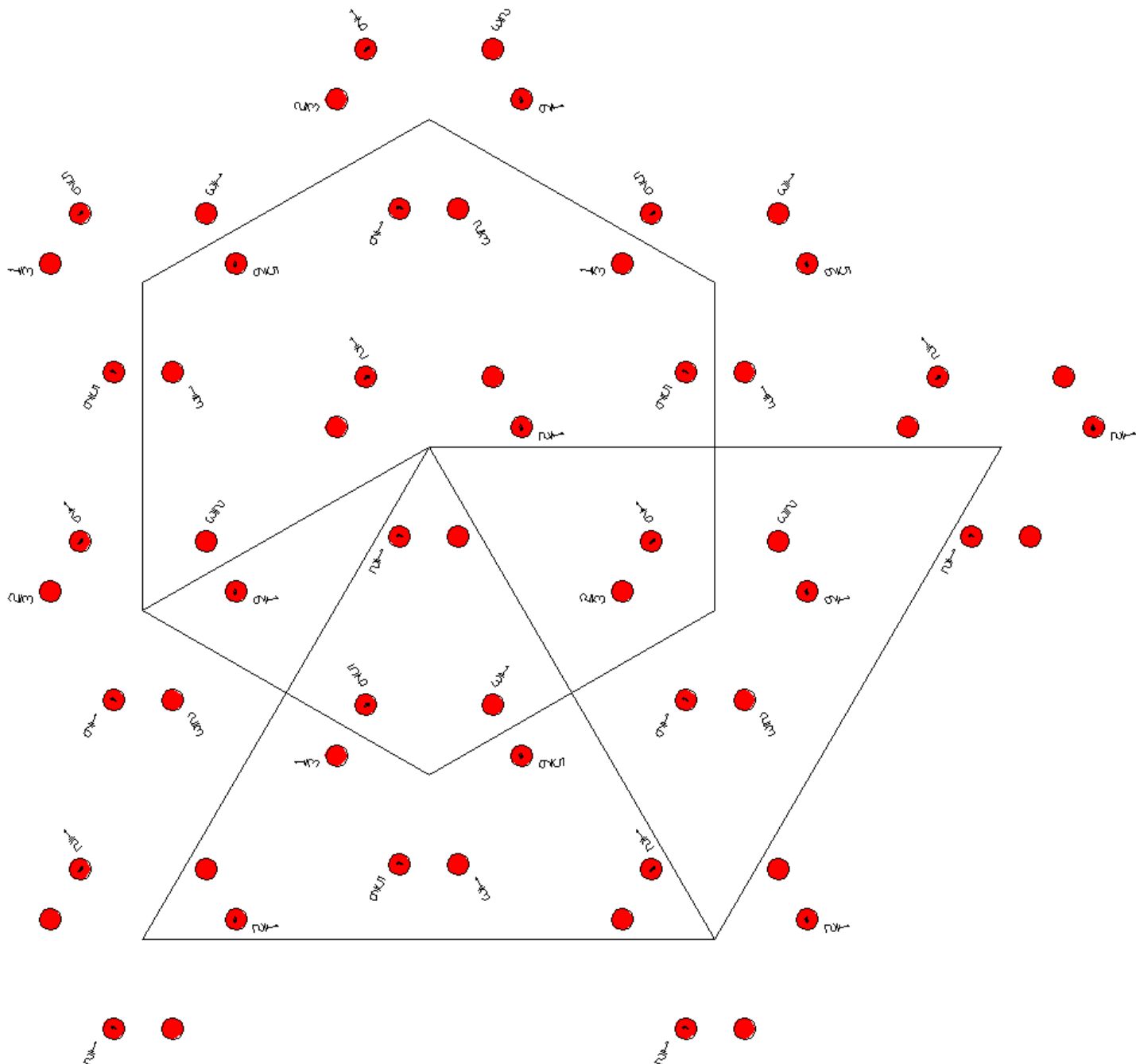
Along [2,1,0] p1g1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/3$   
 Origin at x,x/2,0



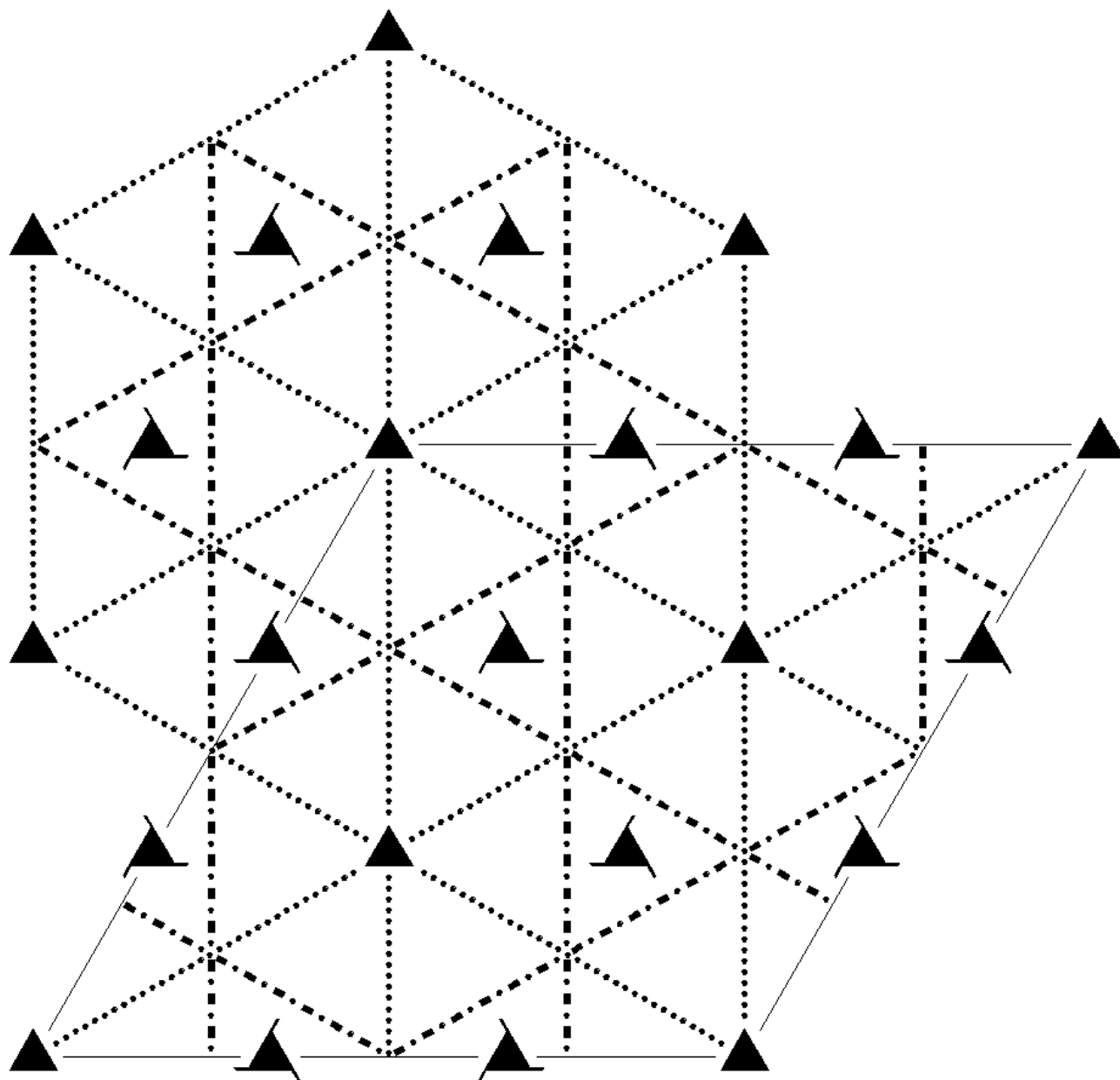
R3c1'  
161.2.1301

3m1'  
R3c1'

Trigonal



1'



Origin on 3c1'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/6;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/6	1/2,0,0 1/2,0,1/6	2/3,1/3,0 2/3,1/3,1/6	1/3,2/3,0 1/3,2/3,1/6	0,1/2,0 0,1/2,1/6

**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)   | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) c (0,0,1/2) x, $\bar{x}$ , z<br>(m <sub>xy</sub>  0,0,1/2) | (5) c (0,0,1/2) x, 2x, z<br>(m <sub>x</sub>  0,0,1/2) | (6) c (0,0,1/2) 2x, x, z<br>(m <sub>y</sub>  0,0,1/2)             |

For (2/3,1/3,1/3) + set

- |   |   |   |
|---|---|---|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)                                      | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3) | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3) |
| (4) g (1/6,-1/6,5/6) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  2/3,1/3,5/6) | (5) g (1/6,1/3,5/6) x, 2x-1/2, z<br>(m <sub>x</sub>  2/3,1/3,5/6)       | (6) g (2/3,1/3,5/6) 2x, x, z<br>(m <sub>y</sub>  2/3,1/3,5/6)                       |

For (1/3,2/3,2/3) + set

- |   |   |   |
|---|---|---|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)                                      | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3) | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3) |
| (4) g (-1/6,1/6,1/6) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  1/3,2/3,1/6) | (5) g (1/3,2/3,1/6) x, 2x, z<br>(m <sub>x</sub>  1/3,2/3,1/6)         | (6) g (1/3,1/6,1/6) 2x-1/2, x, z<br>(m <sub>y</sub>  1/3,2/3,1/6)                     |

For (0,0,0)' + set

- |  |   |  |
|--|---|--|
| (1) 1'<br>(1 0,0,0)'   | (2) 3 <sup>+</sup> ' 0,0,z<br>(3 <sub>z</sub>  0,0,0)'  | (3) 3 <sup>-</sup> ' 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (4) c' (0,0,1/2) x, $\bar{x}$ , z<br>(m <sub>xy</sub>  0,0,1/2)' | (5) c' (0,0,1/2) x, 2x, z<br>(m <sub>x</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 2x, x, z<br>(m <sub>y</sub>  0,0,1/2)'              |

For (2/3,1/3,1/3)' + set

- |   |  |  |
|---|--|--|
| (1) t' (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)'                                      | (2) 3 <sup>+</sup> ' (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3)' | (3) 3 <sup>-</sup> ' (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3)' |
| (4) g' (1/6,-1/6,5/6) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  2/3,1/3,5/6)' | (5) g' (1/6,1/3,5/6) x, 2x-1/2, z<br>(m <sub>x</sub>  2/3,1/3,5/6)'        | (6) g' (2/3,1/3,5/6) 2x, x, z<br>(m <sub>y</sub>  2/3,1/3,5/6)'                        |

For (1/3,2/3,2/3)' + set

- |   |  |  |
|---|--|--|
| (1) t' (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)'                                      | (2) 3 <sup>+</sup> ' (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3)' | (3) 3 <sup>-</sup> ' (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3)' |
| (4) g' (-1/6,1/6,1/6) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  1/3,2/3,1/6)' | (5) g' (1/3,2/3,1/6) x, 2x, z<br>(m <sub>x</sub>  1/3,2/3,1/6)'          | (6) g' (1/3,1/6,1/6) 2x-1/2, x, z<br>(m <sub>y</sub>  1/3,2/3,1/6)'                      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

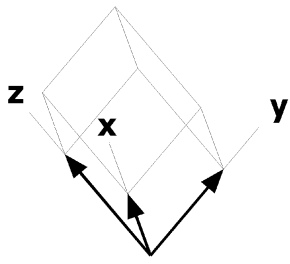
			(0,0,0) + (0,0,0)' +	(2/3,1/3,1/3) + (2/3,1/3,1/3)' +	(1/3,2/3,2/3) + (1/3,2/3,2/3)' +
18	b	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x}$ ,z [0,0,0]
			(4) $\bar{y},\bar{x}$ ,z+1/2 [0,0,0]	(5) $\bar{x}+y$ ,y,z+1/2 [0,0,0]	(6) x,x-y,z+1/2 [0,0,0]
3	a	3.1'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	

**Symmetry of Special Projections**

Along [0,0,1] p31m1'  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at 0,0,z

Along [1,0,0] p11'  
 $\mathbf{a}^* = (2\mathbf{a} + 4\mathbf{b} + \mathbf{c})/6$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

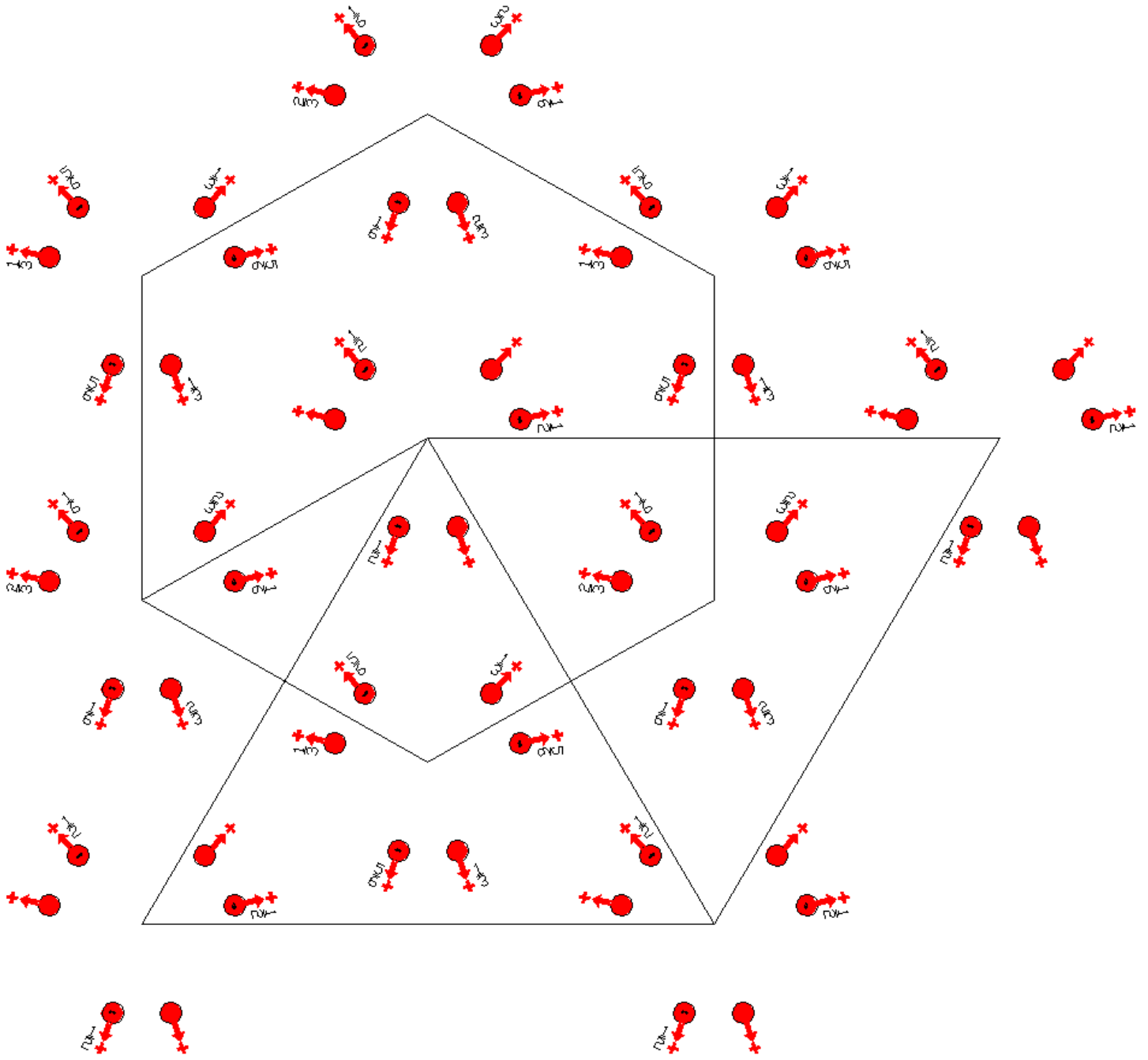
Along [2,1,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/3$   
 Origin at x,x/2,0

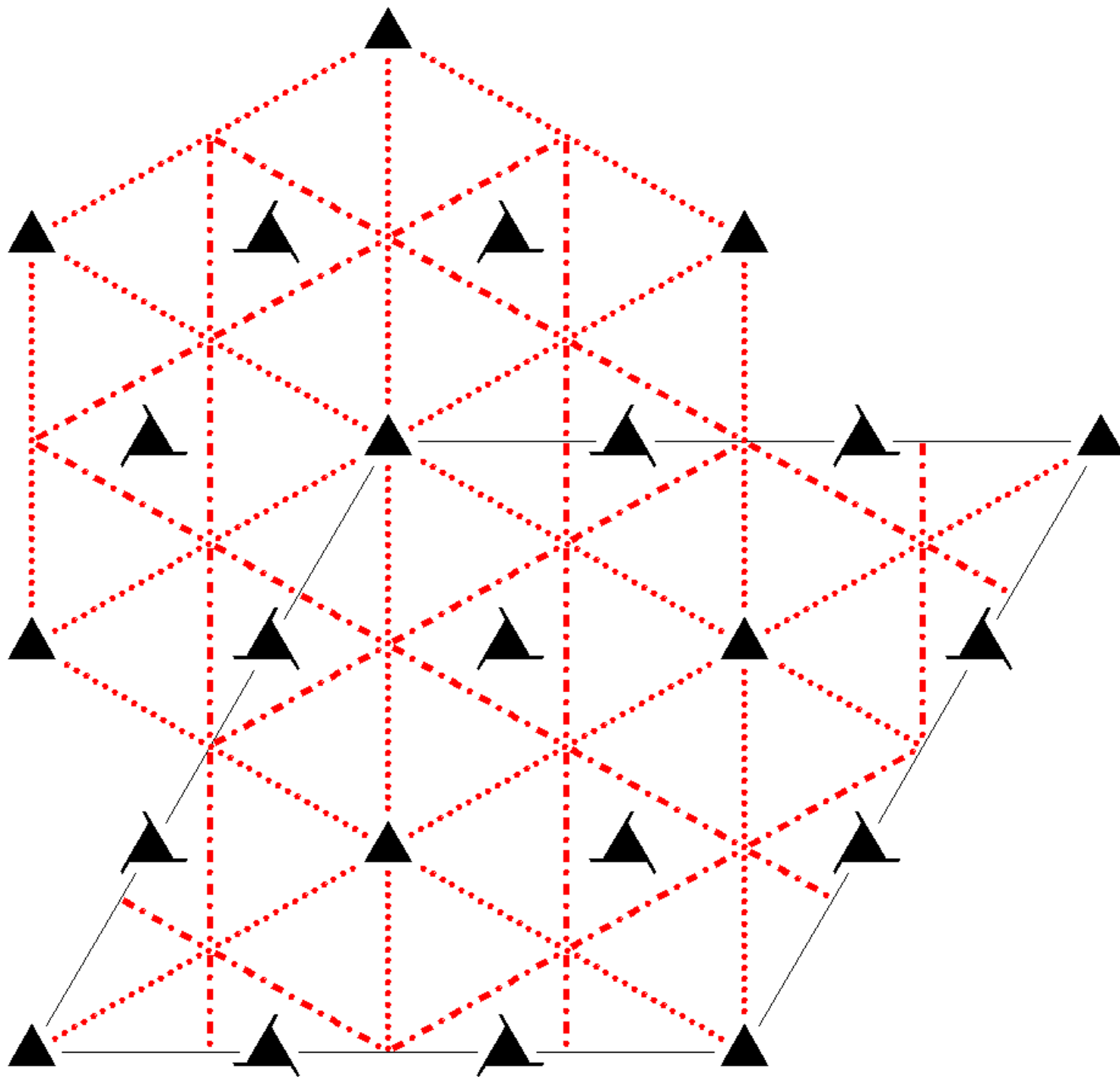


R3c'  
161.3.1302

3m'  
R3c'

Trigonal





**Origin** on  $3c'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/6;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/6	1/2,0,0 1/2,0,1/6	2/3,1/3,0 2/3,1/3,1/6	1/3,2/3,0 1/3,2/3,1/6	0,1/2,0 0,1/2,1/6



**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)     | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) c' (0,0,1/2) x, $\bar{x}$ , z<br>(m <sub>xy</sub>  0,0,1/2)' | (5) c' (0,0,1/2) x, 2x, z<br>(m <sub>x</sub>  0,0,1/2)' | (6) c' (0,0,1/2) 2x, x, z<br>(m <sub>y</sub>  0,0,1/2)'           |

For (2/3,1/3,1/3) + set

- |   |   |   |
|---|---|---|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)  | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3) | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3) |
| (4) g' (1/6,-1/6,5/6) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  2/3,1/3,5/6)' | (5) g' (1/6,1/3,5/6) x, 2x-1/2, z<br>(m <sub>x</sub>  2/3,1/3,5/6)'     | (6) g' (2/3,1/3,5/6) 2x, x, z<br>(m <sub>y</sub>  2/3,1/3,5/6)'                     |

For (1/3,2/3,2/3) + set

- |   |   |   |
|---|---|---|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)  | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3) | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3) |
| (4) g' (-1/6,1/6,1/6) x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>  1/3,2/3,1/6)' | (5) g' (1/3,2/3,1/6) x, 2x, z<br>(m <sub>x</sub>  1/3,2/3,1/6)'       | (6) g' (1/3,1/6,1/6) 2x-1/2, x, z<br>(m <sub>y</sub>  1/3,2/3,1/6)'                   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4).**Positions**

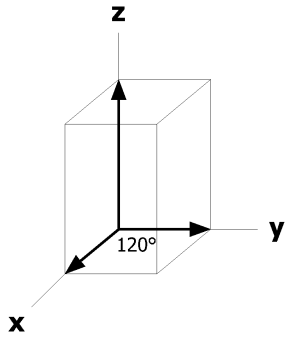
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(2/3,1/3,1/3) +	(1/3,2/3,2/3) +
18	b	1	(1) x,y,z [u,v,w] (4) $\bar{y}$ , $\bar{x}$ , z+1/2 [ $\bar{v}$ , $\bar{u}$ , w]	(2) $\bar{y}$ , x-y, z [ $\bar{v}$ , u-v, w] (5) $\bar{x}$ +y, y, z+1/2 [ $\bar{u}$ +v, v, w]	(3) $\bar{x}$ +y, $\bar{x}$ , z [ $\bar{u}$ +v, $\bar{u}$ , w] (6) x, x-y, z+1/2 [u, u-v, w]
3	a	3.	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	

**Symmetry of Special Projections**

Along [0,0,1] p31m'  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at 0,0,z

Along [1,0,0] p1  
 $\mathbf{a}^* = (2\mathbf{a} + 4\mathbf{b} + \mathbf{c})/6$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

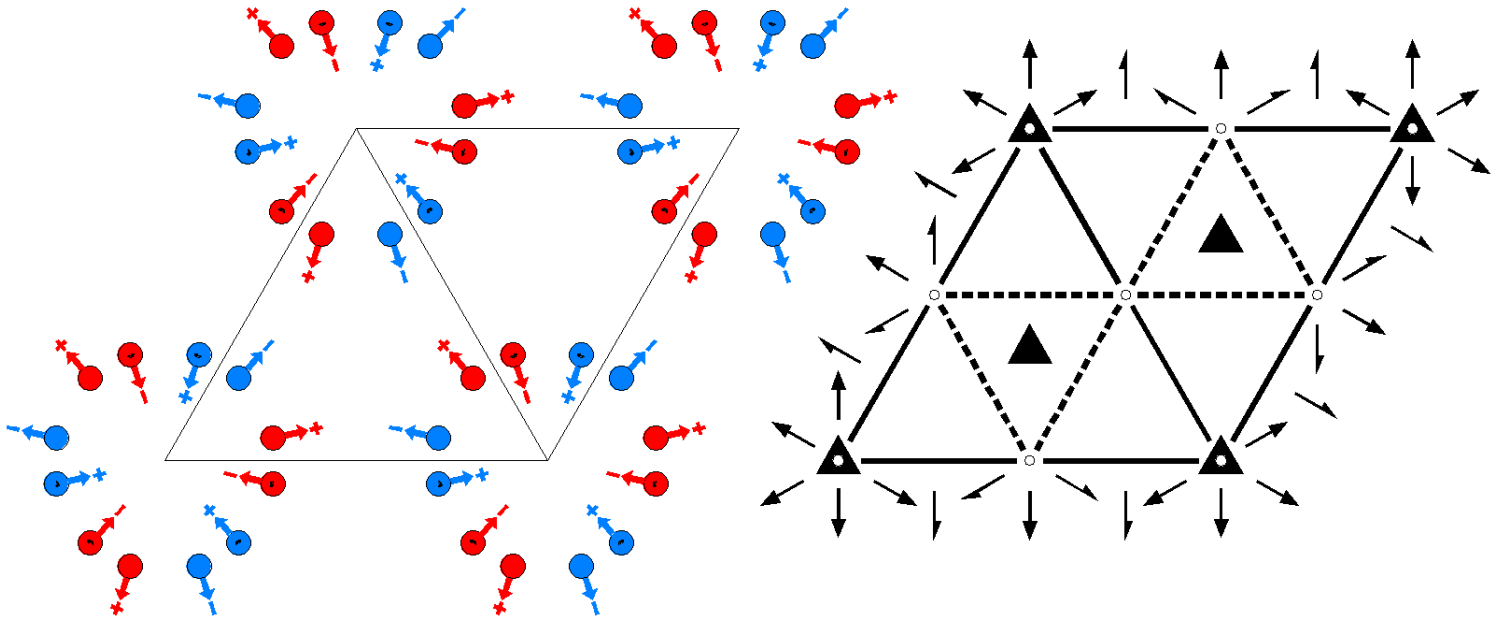
Along [2,1,0] p1g'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/3$   
 Origin at x,x/2,0



$P\bar{3}1m$   
162.1.1303

$\bar{3}1m$   
 $P\bar{3}12/m$

Trigonal



Origin on center ( $\bar{3}1m$ )

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

### Symmetry Operations

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                       | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) 2 $x, \bar{x}, 0$<br>( $2_3$  0,0,0) | (5) 2 $x, 2x, 0$<br>( $2_2$  0,0,0)                   | (6) 2 $2x, x, 0$<br>( $2_1$  0,0,0)                        |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)     | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) m $x, x, z$<br>( $m_3$  0,0,0)      | (11) m $x, 0, z$<br>( $m_2$  0,0,0)                   | (12) m $0, y, z$<br>( $m_1$  0,0,0)                        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

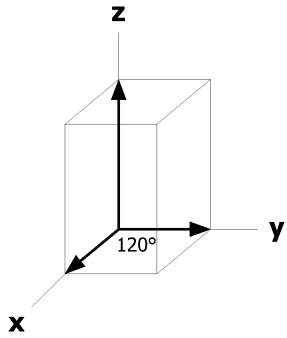
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	l	1	(1) x,y,z [u,v,w] (4) $\bar{y}, \bar{x}, \bar{z}$ [ $\bar{v}, \bar{u}, \bar{w}$ ] (7) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w] (10) y,x,z [ $\bar{v}, \bar{u}, \bar{w}$ ]	(2) $\bar{y}, x-y, z$ [ $\bar{v}, u-v, w$ ] (5) $\bar{x}+y, y, \bar{z}$ [ $\bar{u}+v, v, \bar{w}$ ] (8) y, $\bar{x}+y, \bar{z}$ [ $\bar{v}, u-v, w$ ] (11) x-y, $\bar{y}, \bar{z}$ [ $\bar{u}+v, v, \bar{w}$ ]	(3) $\bar{x}+y, \bar{x}, z$ [ $\bar{u}+v, \bar{u}, w$ ] (6) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ] (9) x-y,x, $\bar{z}$ [ $\bar{u}+v, \bar{u}, w$ ] (12) $\bar{x}, \bar{x}+y, z$ [u,u-v, $\bar{w}$ ]	
6	k	..m	x,0,z [u,2u,0] 0, $\bar{x}, \bar{z}$ [2 $\bar{u}, \bar{u}, 0$ ]	0,x,z [2 $\bar{u}, \bar{u}, 0$ ] $\bar{x}, 0, \bar{z}$ [u,2u,0]	$\bar{x}, \bar{x}, z$ [u, $\bar{u}, 0$ ] x,x, $\bar{z}$ [u, $\bar{u}, 0$ ]	
6	j	..2	x, $\bar{x}, 1/2$ [u, $\bar{u}, 0$ ] $\bar{x}, x, 1/2$ [u, $\bar{u}, 0$ ]	x,2x,1/2 [u,2u,0] $\bar{x}, 2\bar{x}, 1/2$ [u,2u,0]	2 $\bar{x}, \bar{x}, 1/2$ [2 $\bar{u}, \bar{u}, 0$ ] 2x,x,1/2 [2 $\bar{u}, \bar{u}, 0$ ]	
6	i	..2	x, $\bar{x}, 0$ [u, $\bar{u}, 0$ ] $\bar{x}, x, 0$ [u, $\bar{u}, 0$ ]	x,2x,0 [u,2u,0] $\bar{x}, 2\bar{x}, 0$ [u,2u,0]	2 $\bar{x}, \bar{x}, 0$ [2 $\bar{u}, \bar{u}, 0$ ] 2x,x,0 [2 $\bar{u}, \bar{u}, 0$ ]	
4	h	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0,w]      2/3,1/3,z [0,0, $\bar{w}$ ]	
3	g	..2/m	1/2,0,1/2 [u,2u,0]	0,1/2,1/2 [2 $\bar{u}, \bar{u}, 0$ ]	1/2,1/2,1/2 [u, $\bar{u}, 0$ ]	
3	f	..2/m	1/2,0,0 [u,2u,0]	0,1/2,0 [2 $\bar{u}, \bar{u}, 0$ ]	1/2,1/2,0 [u, $\bar{u}, 0$ ]	
2	e	3.m	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	d	3.2	1/3,2/3,1/2 [0,0,0]	2/3,1/3,1/2 [0,0,0]		
2	c	3.2	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]		
1	b	$\bar{3}.m$	0,0,1/2 [0,0,0]			
1	a	$\bar{3}.m$	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p6'm'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [2,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0

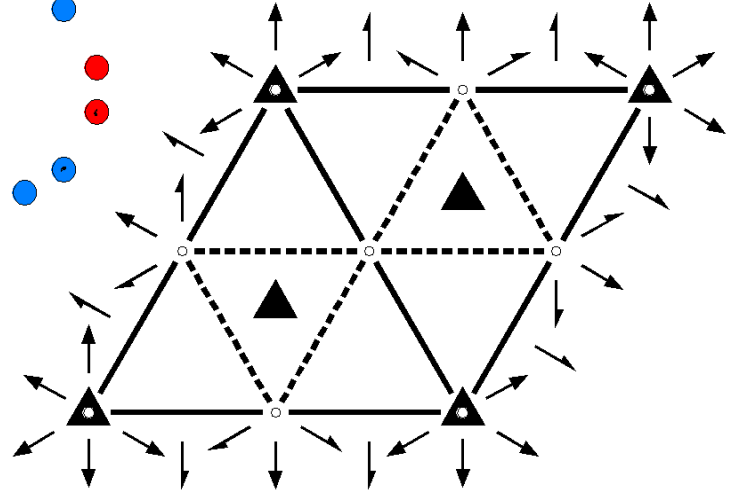
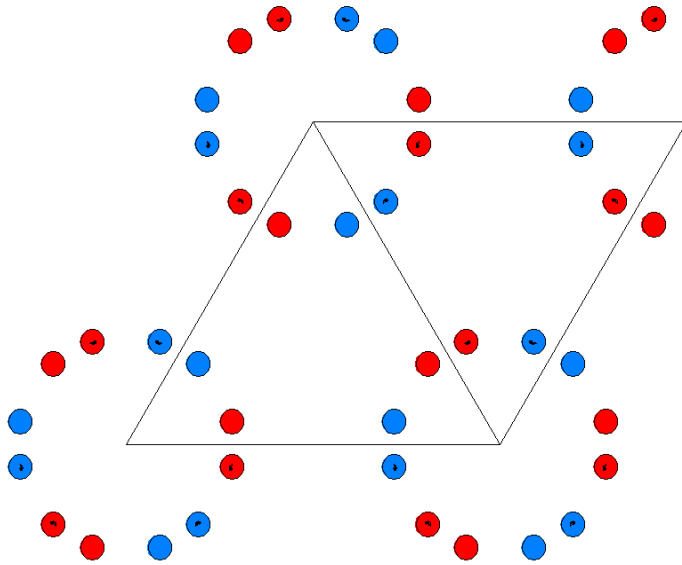


$P\bar{3}1m1'$   
162.2.1304

$\bar{3}1m1'$   
 $P\bar{3}12/m1'$

Trigonal

1'



Origin on center ( $\bar{3}1m1'$ )

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

**Symmetry Operations**

For 1 + set

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                       | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) 2 $x, \bar{x}, 0$<br>( $2_3$  0,0,0) | (5) 2 $x, 2x, 0$<br>( $2_2$  0,0,0)                   | (6) 2 $2x, x, 0$<br>( $2_1$  0,0,0)                        |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)     | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) m $x, x, z$<br>( $m_3$  0,0,0)      | (11) m $x, 0, z$<br>( $m_2$  0,0,0)                   | (12) m $0, y, z$<br>( $m_1$  0,0,0)                        |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 3 <sup>+</sup> 0,0,z (3 <sub>z</sub>  0,0,0)'	(3) 3 <sup>-</sup> 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(4) 2' x, $\bar{x}$ ,0 (2 <sub>3</sub>  0,0,0)'	(5) 2' x,2x,0 (2 <sub>2</sub>  0,0,0)'	(6) 2' 2x,x,0 (2 <sub>1</sub>  0,0,0)'
(7) $\bar{1}$ ' ( $\bar{1}$  0,0,0)'	(8) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(9) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(10) m' x,x,z (m <sub>3</sub>  0,0,0)'	(11) m' x,0,z (m <sub>2</sub>  0,0,0)'	(12) m' 0,y,z (m <sub>1</sub>  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			1 +	1' +		
12	l	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x,y,z [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0]	
			(4) $\bar{y},\bar{x},\bar{z}$ [0,0,0]	(5) $\bar{x}+y,\bar{y},\bar{z}$ [0,0,0]	(6) x,x-y, $\bar{z}$ [0,0,0]	
			(7) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(8) y, $\bar{x}+y,\bar{z}$ [0,0,0]	(9) x-y,x, $\bar{z}$ [0,0,0]	
			(10) y,x,z [0,0,0]	(11) x-y, $\bar{y},z$ [0,0,0]	(12) $\bar{x},\bar{x}+y,z$ [0,0,0]	
6	k	..m1'	x,0,z [0,0,0]	0,x,z [0,0,0]	$\bar{x},\bar{x},z$ [0,0,0]	
			0, $\bar{x},\bar{z}$ [0,0,0]	$\bar{x},0,\bar{z}$ [0,0,0]	x,x, $\bar{z}$ [0,0,0]	
6	j	..21'	x, $\bar{x},1/2$ [0,0,0]	x,2x,1/2 [0,0,0]	2 $\bar{x},\bar{x},1/2$ [0,0,0]	
			$\bar{x},x,1/2$ [0,0,0]	$\bar{x},2\bar{x},1/2$ [0,0,0]	2x,x,1/2 [0,0,0]	
6	i	..21'	x, $\bar{x},0$ [0,0,0]	x,2x,0 [0,0,0]	2 $\bar{x},\bar{x},0$ [0,0,0]	
			$\bar{x},x,0$ [0,0,0]	$\bar{x},2\bar{x},0$ [0,0,0]	2x,x,0 [0,0,0]	
4	h	3..1'	1/3,2/3,z [0,0,0]	1/3,2/3, $\bar{z}$ [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	2/3,1/3,z 0,0,0]
3	g	..2/m1'	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
3	f	..2/m1'	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
2	e	3.m1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	d	3.21'	1/3,2/3,1/2 [0,0,0]	2/3,1/3,1/2 [0,0,0]		
2	c	3.21'	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]		
1	b	$\bar{3}.m1'$	0,0,1/2 [0,0,0]			

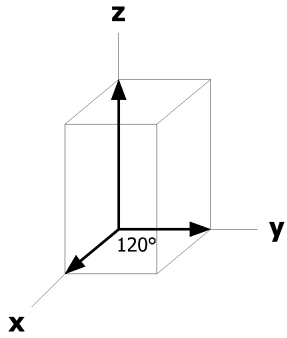
1      a       $\overline{3}.m1'$  0,0,0 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]       $p6mm1'$   
 $\mathbf{a}^* = \mathbf{a}$     $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]       $p2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$     $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

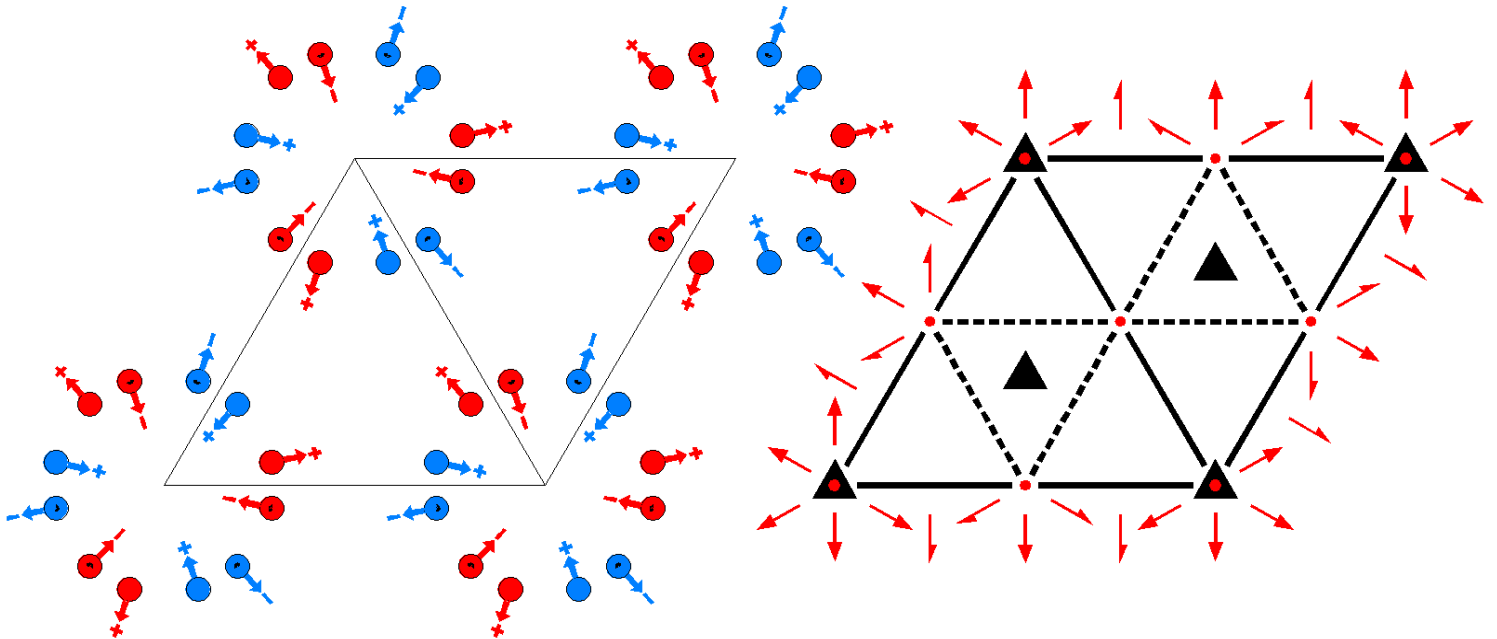
Along [2,1,0]       $p2111'$   
 $\mathbf{a}^* = \mathbf{c}$     $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P\bar{3}1m$   
162.3.1305

$\bar{3}1m$   
 $P\bar{3}12'/m$

Trigonal



Origin on center ( $\bar{3}1m$ )

Asymmetric unit	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

### Symmetry Operations

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                           | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                     | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                     |
| (4) $2'$ x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)' | (5) $2'$ x,2x,0<br>( $2_2$  0,0,0)'                    | (6) $2'$ 2x,x,0<br>( $2_1$  0,0,0)'                         |
| (7) $\bar{1}'$<br>( $\bar{1}$  0,0,0)'       | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)' | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)' |
| (10) m x,x,z<br>( $m_3$  0,0,0)              | (11) m x,0,z<br>( $m_2$  0,0,0)                        | (12) m 0,y,z<br>( $m_1$  0,0,0)                             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	l	1	(1) x,y,z [u,v,w] (4) $\bar{y}, \bar{x}, \bar{z}$ [v,u,w] (7) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ] (10) y,x,z [ $\bar{v}, \bar{u}, \bar{w}$ ]	(2) $\bar{y}, x-y, z$ [ $\bar{v}, u-v, w$ ] (5) $\bar{x}+y, y, \bar{z}$ [u-v, $\bar{v}, w$ ] (8) y, $\bar{x}+y, \bar{z}$ [v, $\bar{u}+v, \bar{w}$ ] (11) x-y, $\bar{y}, z$ [ $\bar{u}+v, v, \bar{w}$ ]	(3) $\bar{x}+y, \bar{x}, z$ [ $\bar{u}+v, \bar{u}, w$ ] (6) x, x-y, $\bar{z}$ [ $\bar{u}, \bar{u}+v, w$ ] (9) x-y, x, $\bar{z}$ [u-v, $\bar{u}, \bar{w}$ ] (12) $\bar{x}, \bar{x}+y, z$ [u, u-v, $\bar{w}$ ]	
6	k	..m	x,0,z [u,2u,0] 0, $\bar{x}, \bar{z}$ [2u,u,0]	0,x,z [2 $\bar{u}, \bar{u}, 0$ ] $\bar{x}, 0, \bar{z}$ [ $\bar{u}, 2\bar{u}, 0$ ]	$\bar{x}, \bar{x}, z$ [u, $\bar{u}, 0$ ] x, x, $\bar{z}$ [ $\bar{u}, u, 0$ ]	
6	j	..2'	x, $\bar{x}, 1/2$ [u,u,w] $\bar{x}, x, 1/2$ [ $\bar{u}, \bar{u}, \bar{w}$ ]	x, 2x, 1/2 [ $\bar{u}, 0, w$ ] $\bar{x}, 2\bar{x}, 1/2$ [u, 0, $\bar{w}$ ]	2 $\bar{x}, \bar{x}, 1/2$ [0, $\bar{u}, w$ ] 2x, x, 1/2 [0, u, $\bar{w}$ ]	
6	i	..2'	x, $\bar{x}, 0$ [u,u,w] $\bar{x}, x, 0$ [ $\bar{u}, \bar{u}, \bar{w}$ ]	x, 2x, 0 [ $\bar{u}, 0, w$ ] $\bar{x}, 2\bar{x}, 0$ [u, 0, $\bar{w}$ ]	2 $\bar{x}, \bar{x}, 0$ [0, $\bar{u}, w$ ] 2x, x, 0 [0, u, $\bar{w}$ ]	
4	h	3..	1/3, 2/3, z [0,0,w]	1/3, 2/3, $\bar{z}$ [0,0,w]	2/3, 1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	2/3, 1/3, z [0,0, $\bar{w}$ ]
3	g	..2'/m	1/2, 0, 1/2 [0,0,0]	0, 1/2, 1/2 [0,0,0]	1/2, 1/2, 1/2 [0,0,0]	
3	f	..2'/m	1/2, 0, 0 [0,0,0]	0, 1/2, 0 [0,0,0]	1/2, 1/2, 0 [0,0,0]	
2	e	3.m	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	d	3.2'	1/3, 2/3, 1/2 [0,0,w]	2/3, 1/3, 1/2 [0,0, $\bar{w}$ ]		
2	c	3.2'	1/3, 2/3, 0 [0,0,w]	2/3, 1/3, 0 [0,0, $\bar{w}$ ]		
1	b	$\bar{3}'$ .m	0,0, 1/2 [0,0,0]			
1	a	$\bar{3}'$ .m	0,0,0 [0,0,0]			

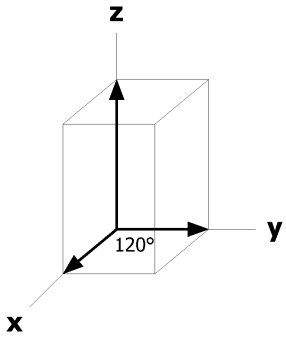
**Symmetry of Special Projections**

Along [0,0,1] p6mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0





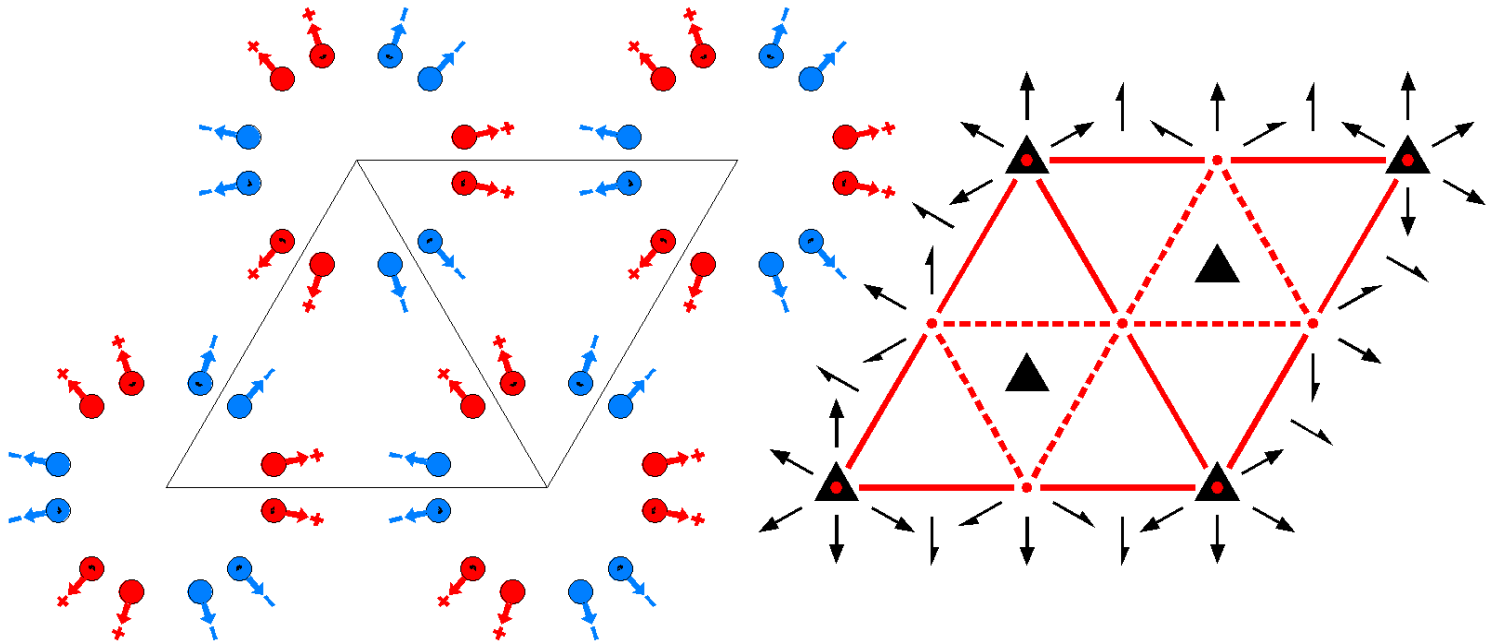
$P\bar{3}1m'$

162.4.1306

$\bar{3}1m'$

$P\bar{3}12/m'$

Trigonal



Origin on center ( $\bar{3}1m'$ )

Asymmetric unit	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

### Symmetry Operations

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                       | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                     | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                     |
| (4) 2 $x, \bar{x}, 0$<br>( $2_3$  0,0,0) | (5) 2 $x, 2x, 0$<br>( $2_2$  0,0,0)                    | (6) 2 $2x, x, 0$<br>( $2_1$  0,0,0)                         |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)'    | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)' | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)' |
| (10) $m'$ $x, x, z$<br>( $m_3$  0,0,0)'  | (11) $m'$ $x, 0, z$<br>( $m_2$  0,0,0)'                | (12) $m'$ $0, y, z$<br>( $m_1$  0,0,0)'                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

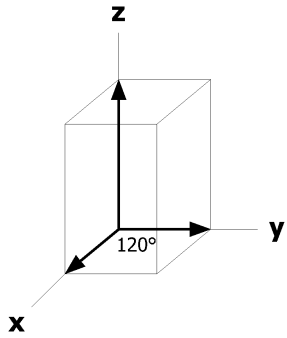
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	l	1	(1) x,y,z [u,v,w] (4) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ] (7) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (10) y,x,z [v,u,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $\bar{x}+y,y,\bar{z}$ [ $\bar{u}+v,v,\bar{w}$ ] (8) y, $\bar{x}+y,\bar{z}$ [v, $\bar{u}+v,\bar{w}$ ] (11) x-y, $\bar{y},\bar{z}$ [u-v, $\bar{v},w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ] (9) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ] (12) $\bar{x},\bar{x}+y,z$ [ $\bar{u},\bar{u}+v,w$ ]	
6	k	..m'	x,0,z [u,0,w] 0, $\bar{x},\bar{z}$ [0, $\bar{u},\bar{w}$ ]	0,x,z [0,u,w] $\bar{x},0,\bar{z}$ [ $\bar{u},0,\bar{w}$ ]	$\bar{x},\bar{x},z$ [u, $\bar{u},w$ ] x,x, $\bar{z}$ [u,u, $\bar{w}$ ]	
6	j	..2	x, $\bar{x},1/2$ [u, $\bar{u},0$ ] $\bar{x},x,1/2$ [ $\bar{u},u,0$ ]	x,2x,1/2 [u,2u,0] $\bar{x},2\bar{x},1/2$ [ $\bar{u},2\bar{u},0$ ]	2 $\bar{x},\bar{x},1/2$ [2 $\bar{u},\bar{u},0$ ] 2x,x,1/2 [2u,u,0]	
6	i	..2	x, $\bar{x},0$ [u, $\bar{u},0$ ] $\bar{x},x,0$ [ $\bar{u},u,0$ ]	x,2x,0 [u,2u,0] $\bar{x},2\bar{x},0$ [ $\bar{u},2\bar{u},0$ ]	2 $\bar{x},\bar{x},0$ [2 $\bar{u},\bar{u},0$ ] 2x,x,0 [2u,u,0]	
4	h	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	2/3,1/3,z [0,0,w]
3	g	..2/m'	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
3	f	..2/m'	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
2	e	3.m'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	d	3.2	1/3,2/3,1/2 [0,0,0]	2/3,1/3,1/2 [0,0,0]		
2	c	3.2	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]		
1	b	$\bar{3}$ 'm'	0,0,1/2 [0,0,0]			
1	a	$\bar{3}$ 'm'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p6m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p211  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



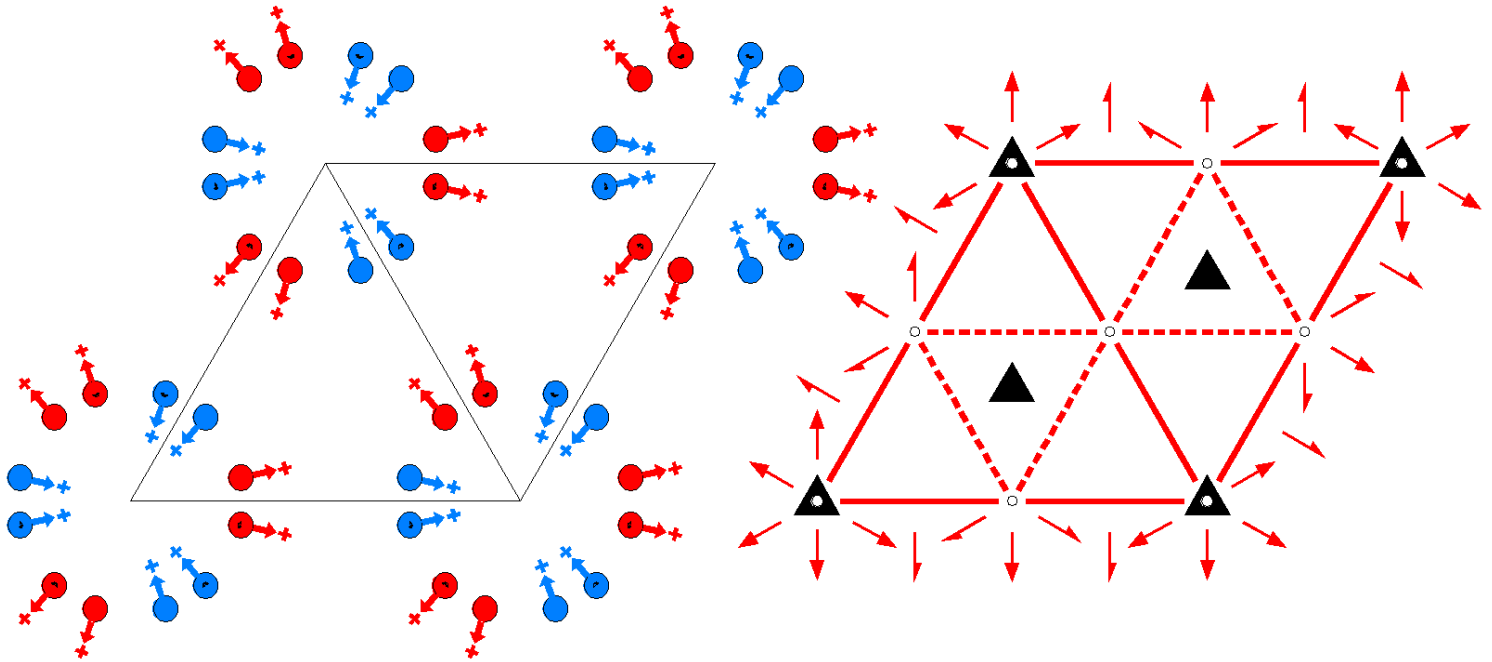
$P\bar{3}1m'$

162.5.1307

$\bar{3}1m'$

$P\bar{3}12'/m'$

Trigonal



Origin on center ( $\bar{3}1m'$ )

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

**Symmetry Operations**

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                           | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) $2'$ x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)' | (5) $2'$ x,2x,0<br>( $2_2$  0,0,0)'                   | (6) $2'$ 2x,x,0<br>( $2_1$  0,0,0)'                        |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)         | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) $m'$ x,x,z<br>( $m_3$  0,0,0)'          | (11) $m'$ x,0,z<br>( $m_2$  0,0,0)'                   | (12) $m'$ 0,y,z<br>( $m_1$  0,0,0)'                        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

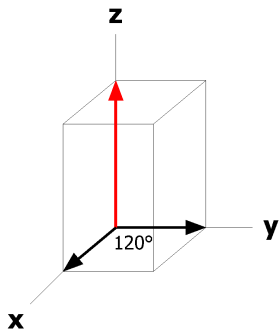
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	l	1	(1) x,y,z [u,v,w] (4) $\bar{y},\bar{x},\bar{z}$ [v,u,w] (7) $\bar{x},\bar{y},\bar{z}$ [u,v,w] (10) y,x,z [v,u,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $\bar{x}+y,y,\bar{z}$ [u-v, $\bar{v}$ ,w] (8) y, $\bar{x}+y,\bar{z}$ [ $\bar{v},u-v,w$ ] (11) x-y, $\bar{y},z$ [u-v, $\bar{v}$ ,w]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) x,x-y, $\bar{z}$ [ $\bar{u},\bar{u}+v,w$ ] (9) x-y,x, $\bar{z}$ [ $\bar{u}+v,\bar{u},w$ ] (12) $\bar{x},\bar{x}+y,z$ [ $\bar{u},\bar{u}+v,w$ ]	
6	k	..m'	x,0,z [u,0,w] 0, $\bar{x},\bar{z}$ [0,u,w]	0,x,z [0,u,w] $\bar{x},0,\bar{z}$ [u,0,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ] x,x, $\bar{z}$ [ $\bar{u},\bar{u},w$ ]	
6	j	..2'	x, $\bar{x},1/2$ [u,u,w] $\bar{x},x,1/2$ [u,u,w]	x,2x,1/2 [ $\bar{u},0,w$ ] $\bar{x},2\bar{x},1/2$ [ $\bar{u},0,w$ ]	2 $\bar{x},\bar{x},1/2$ [0, $\bar{u},w$ ] 2x,x,1/2 [0, $\bar{u},w$ ]	
6	i	..2'	x, $\bar{x},0$ [u,u,w] $\bar{x},x,0$ [u,u,w]	x,2x,0 [ $\bar{u},0,w$ ] $\bar{x},2\bar{x},0$ [ $\bar{u},0,w$ ]	2 $\bar{x},\bar{x},0$ [0, $\bar{u},w$ ] 2x,x,0 [0, $\bar{u},w$ ]	
4	h	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ [0,0,w]	2/3,1/3, $\bar{z}$ [0,0,w]	2/3,1/3,z [0,0,w]
3	g	..2'/m'	1/2,0,1/2 [u,0,w]	0,1/2,1/2 [0,u,w]	1/2,1/2,1/2 [ $\bar{u},\bar{u},w$ ]	
3	f	..2'/m'	1/2,0,0 [u,0,w]	0,1/2,0 [0,u,w]	1/2,1/2,0 [ $\bar{u},\bar{u},w$ ]	
2	e	3.m'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
2	d	3.2'	1/3,2/3,1/2 [0,0,w]	2/3,1/3,1/2 [0,0,w]		
2	c	3.2'	1/3,2/3,0 [0,0,w]	2/3,1/3,0 [0,0,w]		
1	b	$\bar{3}.m'$	0,0,1/2 [0,0,w]			
1	a	$\bar{3}.m'$	0,0,0 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] p6'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

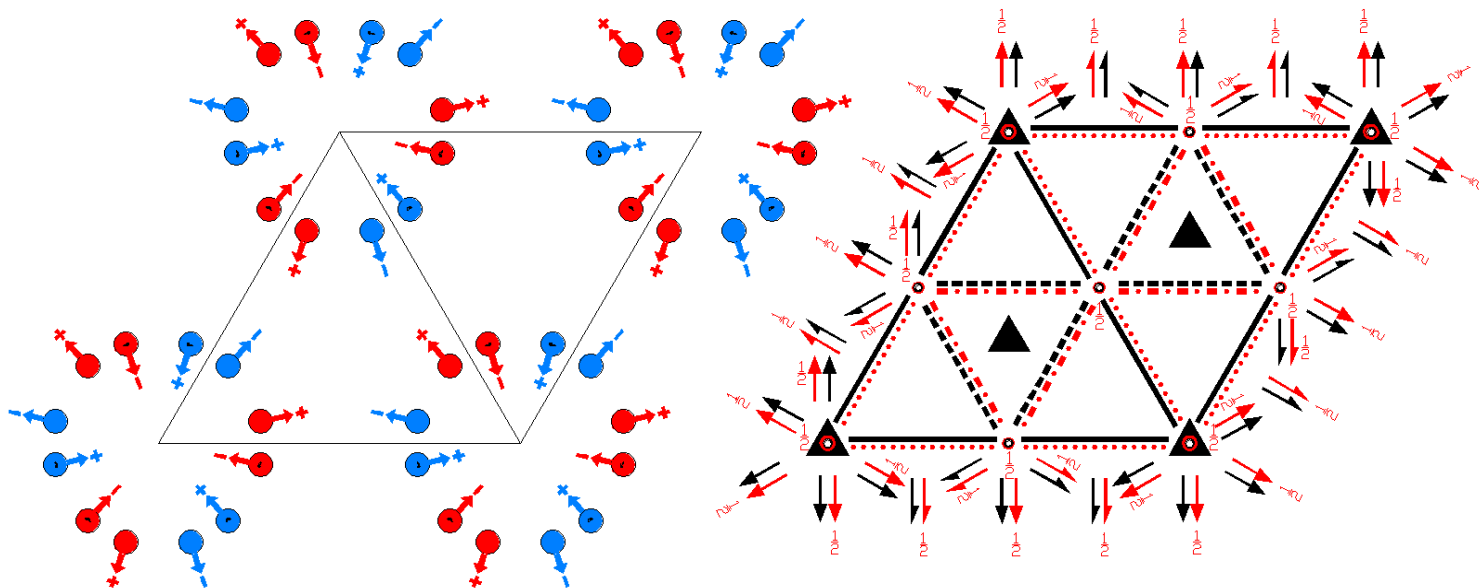
Along [2,1,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P_{2c}\bar{3}1m$   
162.6.1308

$\bar{3}1m1'$   
 $P_{2c}\bar{3}1m$

Trigonal



Origin on center ( $\bar{3}1m$ )

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$ ;  $x \leq (1+y)/2$ ;  $y \leq \min(1-x, x)$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/2,1/2,1/2

### Symmetry Operations

For (0,0,0) + set

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                       | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) 2 $x, \bar{x}, 0$<br>( $2_3$  0,0,0) | (5) 2 $x, 2x, 0$<br>( $2_2$  0,0,0)                   | (6) 2 $2x, x, 0$<br>( $2_1$  0,0,0)                        |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)     | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) m $x, x, z$<br>( $m_3$  0,0,0)      | (11) m $x, 0, z$<br>( $m_2$  0,0,0)                   | (12) m $0, y, z$<br>( $m_1$  0,0,0)                        |

## For (0,0,1)' +set

(1) t' (0,0,1) (1 0,0,1)'	(2) 3 <sup>+</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub>  0,0,1)'	(3) 3 <sup>-</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,1)'
(4) 2' x, $\bar{x}$ ,1/2 (2 <sub>3</sub>  0,0,1)'	(5) 2' x,2x,1/2 (2 <sub>2</sub>  0,0,1)'	(6) 2' 2x,x,1/2 (2 <sub>1</sub>  0,0,1)'
(4) $\bar{1}$ ' 0,0,1/2 ( $\bar{1}$  0,0,1)'	(5) $\bar{3}^+$ ' 0,0,z; 0,0,1/2 ( $\bar{3}_z$  0,0,1)'	(6) $\bar{3}^-$ ' 0,0,z; 0,0,1/2 ( $\bar{3}_z^{-1}$  0,0,1)'
(4) c' (0,0,1) x,x,z (m <sub>3</sub>  0,0,1)'	(5) c' (0,0,1) x,0,z (m <sub>2</sub>  0,0,1)'	(6) c' (0,0,1) 0,y,z (m <sub>1</sub>  0,0,1)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) + (0,0,1)'			
24	l	1	(1) x,y,z [u,v,w] (4) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ] (7) $\bar{x},\bar{y},\bar{z}$ [u,v,w] (10) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $\bar{x}+y,y,\bar{z}$ [ $\bar{u}+v,v,\bar{w}$ ] (8) y, $\bar{x}+y,\bar{z}$ [ $\bar{v},u-v,w$ ] (11) x-y, $\bar{y},\bar{z}$ [ $\bar{u}+v,v,\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},\bar{z}$ [ $\bar{u}+v,\bar{u},w$ ] (6) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ] (9) x-y,x, $\bar{z}$ [ $\bar{u}+v,\bar{u},w$ ] (12) $\bar{x},\bar{x}+y,z$ [u,u-v, $\bar{w}$ ]	
12	k	..m	x,0,z [u,2u,0] 0, $\bar{x},\bar{z}$ [2 $\bar{u},\bar{u},0$ ]	0,x,z [2 $\bar{u},\bar{u},0$ ] $\bar{x},0,\bar{z}$ [u,2u,0]	$\bar{x},\bar{x},\bar{z}$ [u, $\bar{u},0$ ] x,x, $\bar{z}$ [u, $\bar{u},0$ ]	
12	j	..2'	x, $\bar{x}$ ,1/2 [u,u,w] $\bar{x},x,1/2$ [ $\bar{u},\bar{u},\bar{w}$ ]	x,2x,1/2 [ $\bar{u},0,w$ ] $\bar{x},2\bar{x},1/2$ [u,0, $\bar{w}$ ]	2 $\bar{x},\bar{x},1/2$ [0, $\bar{u},w$ ] 2x,x,1/2 [0,u, $\bar{w}$ ]	
12	i	..2	x, $\bar{x}$ ,0 [u, $\bar{u},0$ ] $\bar{x},x,0$ [u, $\bar{u},0$ ]	x,2x,0 [u,2u,0] $\bar{x},2\bar{x},0$ [u,2u,0]	2 $\bar{x},\bar{x},0$ [0,u, $\bar{w}$ ] 2x,x,0 [2 $\bar{u},\bar{u},0$ ]	
8	h	3..	1/3,2/3,z [0,0,w] 1/3,2/3, $\bar{z}$ [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0,w] 2/3,1/3,z [0,0, $\bar{w}$ ]	2/3,1/3,z [0,0, $\bar{w}$ ]	
6	g	..2'/m	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
6	f	..2'/m	1/2,0,0 [u,2u,0]	0,1/2,0 [2 $\bar{u},\bar{u},0$ ]	1/2,1/2,0 [u, $\bar{u},0$ ]	
2	e	3.m	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4	d	3.2	1/3,2/3,1/2 [0,0,0]	2/3,1/3,1/2 [0,0,0]		
4	c	3.2	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]		
2	b	$\bar{3}.m$	0,0,1/2 [0,0,0]			

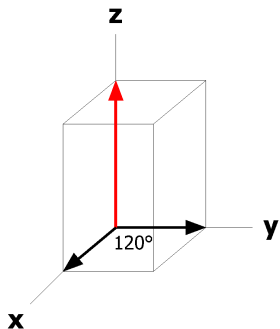
2      a       $\bar{3}.m$       0,0,0 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]       $p6mm1'$   
 $\mathbf{a}^* = \mathbf{a}$     $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]       $p_{2a^*}2mm$   
 $\mathbf{a}^* = \mathbf{c}$     $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/2

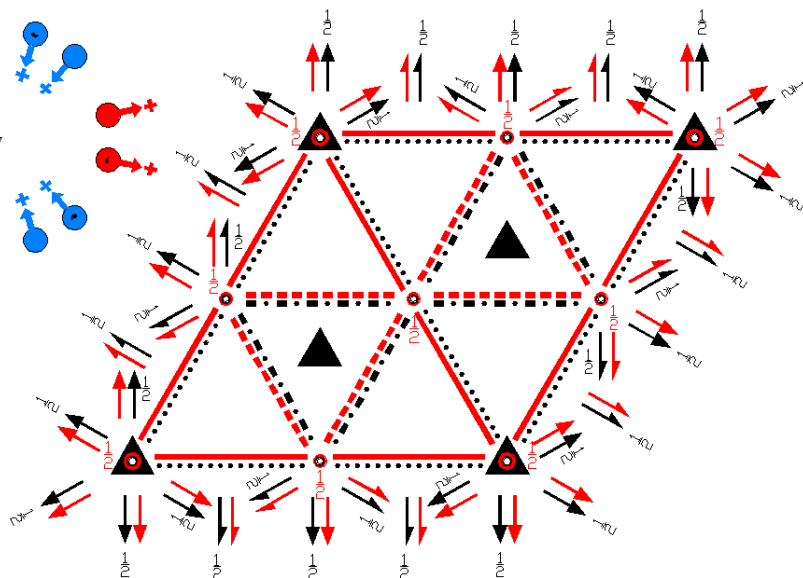
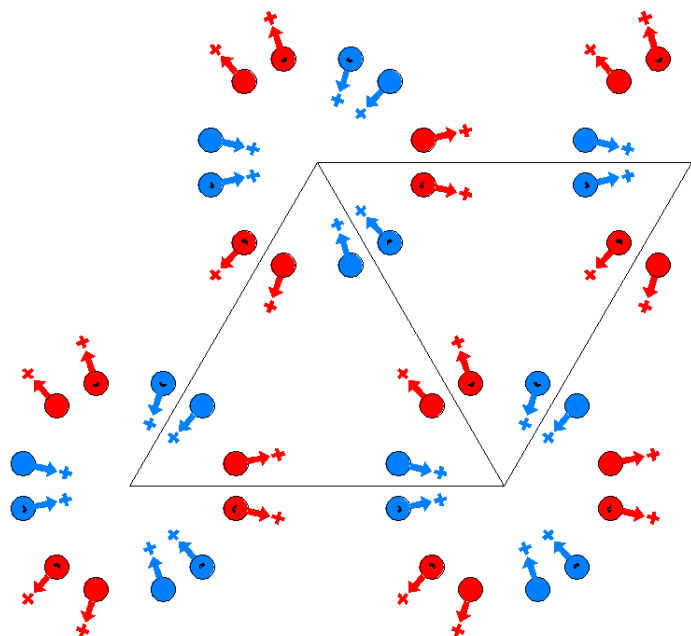
Along [2,1,0]       $p2111'$   
 $\mathbf{a}^* = \mathbf{c}$     $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P_{2c}\bar{3}1m'$   
162.7.1309

$\bar{3}1m'$   
 $P_{2c}\bar{3}1m'$

Trigonal



Origin on center ( $\bar{3}1m'$ )

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$ ;  $x \leq (1+y)/2$ ;  $y \leq \min(1-x, x)$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/2,1/2,1/2

### Symmetry Operations

For (0,0,0) + set

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                           | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) $2'$ x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)' | (5) $2'$ x,2x,0<br>( $2_2$  0,0,0)'                   | (6) $2'$ 2x,x,0<br>( $2_1$  0,0,0)'                        |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)         | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) $m'$ x,x,z<br>( $m_3$  0,0,0)'          | (11) $m'$ x,0,z<br>( $m_2$  0,0,0)'                   | (12) $m'$ 0,y,z<br>( $m_1$  0,0,0)'                        |



## For (0,0,1)' +set

(1) t' (0,0,1) (1 0,0,1)'	(2) $\bar{3}^+$ ' (0,0,1) 0,0,z ( $\bar{3}_z$  0,0,1)'	(3) $\bar{3}^-$ ' (0,0,1) 0,0,z ( $\bar{3}_z^{-1}$  0,0,1)'
(4) $2_{\bar{3}}$ x, $\bar{x}$ ,1/2 ( $2_{\bar{3}}$  0,0,1)	(5) $2_{\bar{2}}$ x,2x,1/2 ( $2_{\bar{2}}$  0,0,1)	(6) $2_{\bar{2}}$ 2x,x,1/2 ( $2_{\bar{2}}$  0,0,1)
(4) $\bar{1}$ ' 0,0,1/2 ( $\bar{1}$  0,0,1)'	(5) $\bar{3}^+$ ' 0,0,z; 0,0,1/2 ( $\bar{3}_z$  0,0,1)'	(6) $\bar{3}^-$ ' 0,0,z; 0,0,1/2 ( $\bar{3}_z^{-1}$  0,0,1)'
(4) c (0,0,1) x,x,z ( $m_3$  0,0,1)	(5) c (0,0,1) x,0,z ( $m_2$  0,0,1)	(6) c (0,0,1) 0,y,z ( $m_1$  0,0,1)

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

**Positions**

			Coordinates			
			(0,0,0) +	(0,0,1)' +		
Multiplicity,	Wyckoff letter,	Site Symmetry.				
24	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]	
			(4) $\bar{y},\bar{x},\bar{z}$ [v,u,w]	(5) $\bar{x}+y,y,\bar{z}$ [u-v, $\bar{v},w$ ]	(6) x,x-y, $\bar{z}$ [ $\bar{u},\bar{u}+v,w$ ]	
			(7) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(8) y, $\bar{x}+y,\bar{z}$ [ $\bar{v},u-v,w$ ]	(9) x-y,x, $\bar{z}$ [ $\bar{u}+v,\bar{u},w$ ]	
			(10) y,x,z [v,u,w]	(11) x-y, $\bar{y},z$ [u-v, $\bar{v},w$ ]	(12) $\bar{x},\bar{x}+y,z$ [ $\bar{u},\bar{u}+v,w$ ]	
12	k	..m'	x,0,z [u,0,w]	0,x,z [0,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	
			0, $\bar{x},\bar{z}$ [0,u,w]	$\bar{x},0,\bar{z}$ [u,0,w]	x,x, $\bar{z}$ [ $\bar{u},\bar{u},w$ ]	
12	j	..2	x, $\bar{x}$ ,1/2 [u, $\bar{u}$ ,0]	x,2x,1/2 [u,2u,0]	$2\bar{x},\bar{x},1/2$ [ $2\bar{u},\bar{u},0$ ]	
			$\bar{x},x,1/2$ [ $\bar{u},u,0$ ]	$\bar{x},2\bar{x},1/2$ [ $\bar{u},2\bar{u},0$ ]	2x,x,1/2 [2u,u,0]	
12	i	..2'	x, $\bar{x}$ ,0 [u,u,w]	x,2x,0 [ $\bar{u},0,w$ ]	$2\bar{x},\bar{x},0$ [0, $\bar{u},w$ ]	
			$\bar{x},x,0$ [u,u,w]	$\bar{x},2\bar{x},0$ [ $\bar{u},0,w$ ]	2x,x,0 [0, $\bar{u},w$ ]	
8	h	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ [0,0,w]	2/3,1/3, $\bar{z}$ [0,0,w]	2/3,1/3,z [0,0,w]
6	g	..2/m'	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
6	f	..2'/m'	1/2,0,0 [u,0,w]	0,1/2,0 [0,u,w]	1/2,1/2,0 [ $\bar{u},\bar{u},w$ ]	
4	e	3.m'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
4	d	3.2'	1/3,2/3,1/2 [0,0,w]	2/3,1/3,1/2 [0,0,w]		
4	c	3.2'	1/3,2/3,0 [0,0,w]	2/3,1/3,0 [0,0,w]		
2	b	$\bar{3}.m'$	0,0,1/2 [0,0,w]			

2      a       $\bar{3}.m'$     0,0,0 [0,0,w]

### Symmetry of Special Projections

Along [0,0,1]     $p6mm1'$

$\mathbf{a}^* = \mathbf{a}$     $\mathbf{b}^* = \mathbf{b}$

Origin at 0,0,z

Along [1,0,0]     $p_{2a}2m'm'$

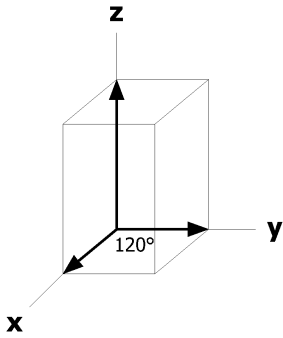
$\mathbf{a}^* = \mathbf{c}$     $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$

Origin at x,0,1/2

Along [2,1,0]     $p_{2a}211$

$\mathbf{a}^* = \mathbf{c}$     $\mathbf{b}^* = \mathbf{b}/2$

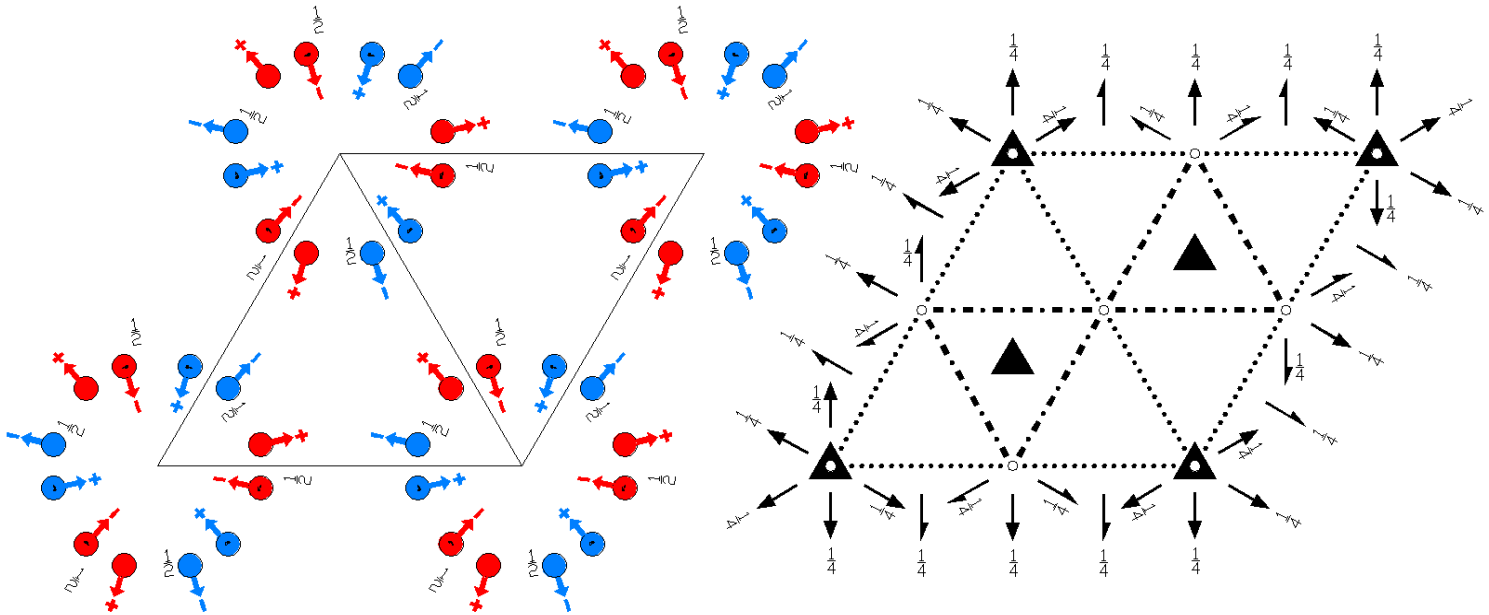
Origin at x,x/2,0



$P\bar{3}1c$   
163.1.1310

$\bar{3}1m$   
 $P\bar{3}12/c$

Trigonal



Origin at center ( $\bar{3}$ ) at  $\bar{3}1c$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

### Symmetry Operations

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                              | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) 2 $x, \bar{x}, 1/4$<br>( $2_3$  0,0,1/2)    | (5) 2 $x, 2x, 1/4$<br>( $2_2$  0,0,1/2)               | (6) 2 $2x, x, 1/4$<br>( $2_1$  0,0,1/2)                    |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)            | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) c (0,0,1/2) $x, x, z$<br>( $m_3$  0,0,1/2) | (11) c (0,0,1/2) $x, 0, z$<br>( $m_2$  0,0,1/2)       | (12) c (0,0,1/2) $0, y, z$<br>( $m_1$  0,0,1/2)            |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

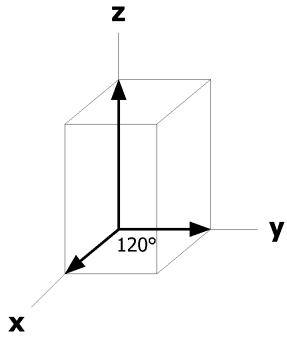
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	i	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]	
			(4) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(5) $\bar{x}+y,y,\bar{z}+1/2$ [ $\bar{u}+v,v,\bar{w}$ ]	(6) $x,x-y,\bar{z}+1/2$ [u,u-v, $\bar{w}$ ]	
			(7) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(8) $y,\bar{x}+y,\bar{z}$ [ $\bar{v},u-v,w$ ]	(9) $x-y,x,\bar{z}$ [ $\bar{u}+v,\bar{u},w$ ]	
			(10) $y,x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(11) $x-y,y,\bar{z}+1/2$ [ $\bar{u}+v,v,\bar{w}$ ]	(12) $\bar{x},\bar{x}+y,z+1/2$ [u,u-v, $\bar{w}$ ]	
6	h	..2	$x,\bar{x},1/4$ [u, $\bar{u},0$ ]	$x,2x,1/4$ [u,2u,0]	$2\bar{x},\bar{x},1/4$ [2 $\bar{u},\bar{u},0$ ]	
			$\bar{x},x,3/4$ [u, $\bar{u},0$ ]	$\bar{x},2\bar{x},3/4$ [u,2u,0]	$2x,x,3/4$ [2 $\bar{u},\bar{u},0$ ]	
6	g	$\bar{1}$	1/2,0,0 [u,v,w]	0,1/2,0 [ $\bar{v},u-v,w$ ]	1/2,1/2,0 [ $\bar{u}+v,\bar{u},w$ ]	
			0,1/2,1/2 [ $\bar{v},\bar{u},\bar{w}$ ]	1/2,0,1/2 [ $\bar{u}+v,v,\bar{w}$ ]	1/2,1/2,1/2 [u,u-v, $\bar{w}$ ]	
4	f	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0,w]	2/3,1/3,z+1/2 [0,0, $\bar{w}$ ]
4	e	3..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]
2	d	3.2	2/3,1/3,1/4 [0,0,0]	1/3,2/3,3/4 [0,0,0]		
2	c	3.2	1/3,2/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]		
2	b	$\bar{3}$ ..	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		
2	a	3.2	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p6'm'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p<sub>2a</sub><sup>-</sup>211  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/4



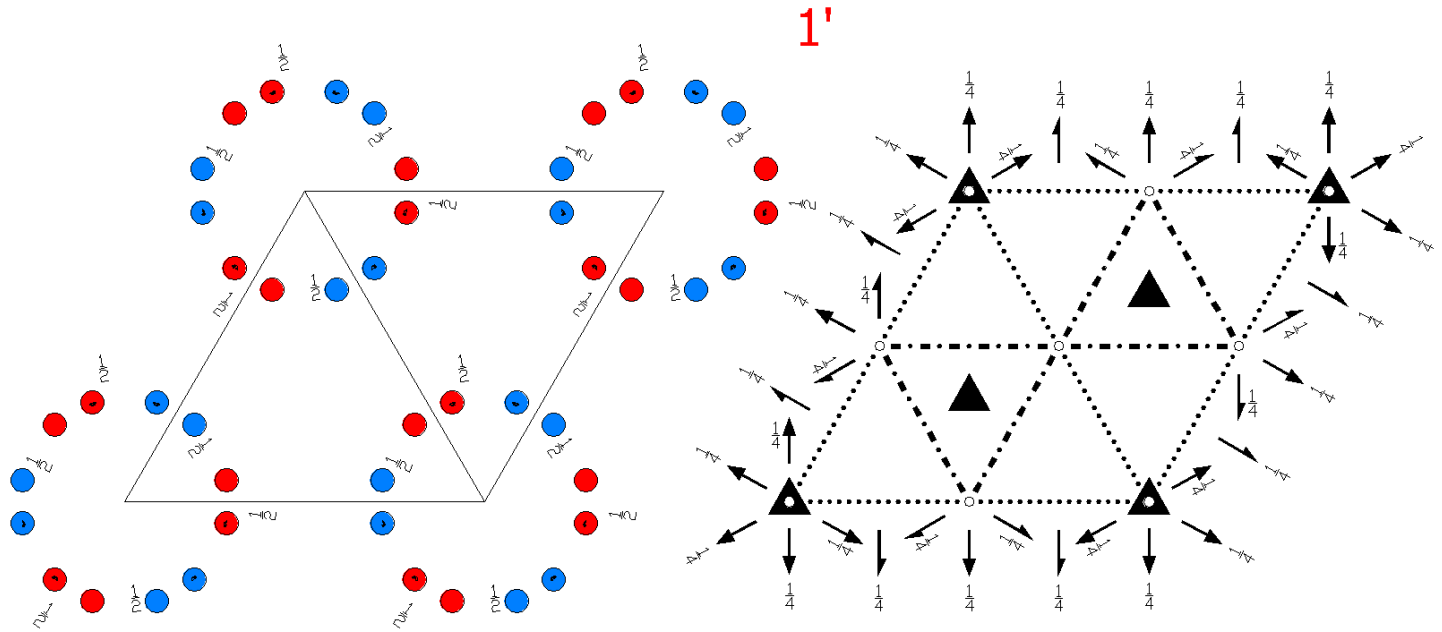
$P\bar{3}1c1'$

163.2.1311

$\bar{3}1m1'$

$P\bar{3}12/c1'$

Trigonal



Origin at center ( $\bar{3}1'$ ) at  $\bar{3}1c1'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/4	1/2,0,0 1/2,0,1/4	2/3,1/3,0 2/3,1/3,1/4	1/3,2/3,0 1/3,2/3,1/4	0,1/2,0 0,1/2,1/4

**Symmetry Operations**

For 1 + set

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                              | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) 2 $x, \bar{x}, 1/4$<br>( $2_3$  0,0,1/2)    | (5) 2 $x, 2x, 1/4$<br>( $2_2$  0,0,1/2)               | (6) 2 $2x, x, 1/4$<br>( $2_1$  0,0,1/2)                    |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)            | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) c (0,0,1/2) $x, x, z$<br>( $m_3$  0,0,1/2) | (11) c (0,0,1/2) $x, 0, z$<br>( $m_2$  0,0,1/2)       | (12) c (0,0,1/2) $0, y, z$<br>( $m_1$  0,0,1/2)            |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 3 <sup>+</sup> 0,0,z (3 <sub>z</sub>  0,0,0)'	(3) 3 <sup>-</sup> 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(4) 2' x, $\bar{x}$ ,1/4 (2 <sub>3</sub>  0,0,1/2)'	(5) 2' x,2x,1/4 (2 <sub>2</sub>  0,0,1/2)'	(6) 2' 2x,x,1/4 (2 <sub>1</sub>  0,0,1/2)'
(7) $\bar{1}$ ' ( $\bar{1}$  0,0,0)'	(8) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(9) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(10) c' (0,0,1/2) x,x,z (m <sub>3</sub>  0,0,1/2)'	(11) c' (0,0,1/2) x,0,z (m <sub>2</sub>  0,0,1/2)'	(12) c' (0,0,1/2) 0,y,z (m <sub>1</sub>  0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

**Positions**

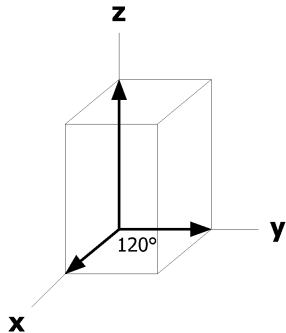
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			1 +	1' +		
12	i	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x,y,z [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0]	
			(4) $\bar{y},\bar{x},\bar{z}+1/2$ [0,0,0]	(5) $\bar{x}+y,y,\bar{z}+1/2$ [0,0,0]	(6) x,x-y, $\bar{z}+1/2$ [0,0,0]	
			(7) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(8) y, $\bar{x}+y,\bar{z}$ [0,0,0]	(9) x-y,x, $\bar{z}$ [0,0,0]	
			(10) y,x,z+1/2 [0,0,0]	(11) x-y, $\bar{y},z+1/2$ [0,0,0]	(12) $\bar{x},\bar{x}+y,z+1/2$ [0,0,0]	
6	h	..21'	x, $\bar{x}$ ,1/4 [0,0,0]	x,2x,1/4 [0,0,0]	2 $\bar{x},\bar{x}$ ,1/4 [0,0,0]	
			$\bar{x},x,3/4$ [0,0,0]	$\bar{x},2\bar{x},3/4$ [0,0,0]	2x,x,3/4 [0,0,0]	
6	g	$\bar{1}$ 1'	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
			0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
4	f	3..1'	1/3,2/3,z [0,0,0]	1/3,2/3, $\bar{z}+1/2$ [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	2/3,1/3,z+1/2 [0,0,0]
4	e	3..1'	0,0,z [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0,z+1/2 [0,0,0]
2	d	3.21'	2/3,1/3,1/4 [0,0,0]	1/3,2/3,3/4 [0,0,0]		
2	c	3.21'	1/3,2/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]		
1	b	$\bar{3}$ ..1'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
1	a	3.21'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mg1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at  $x,0,0$

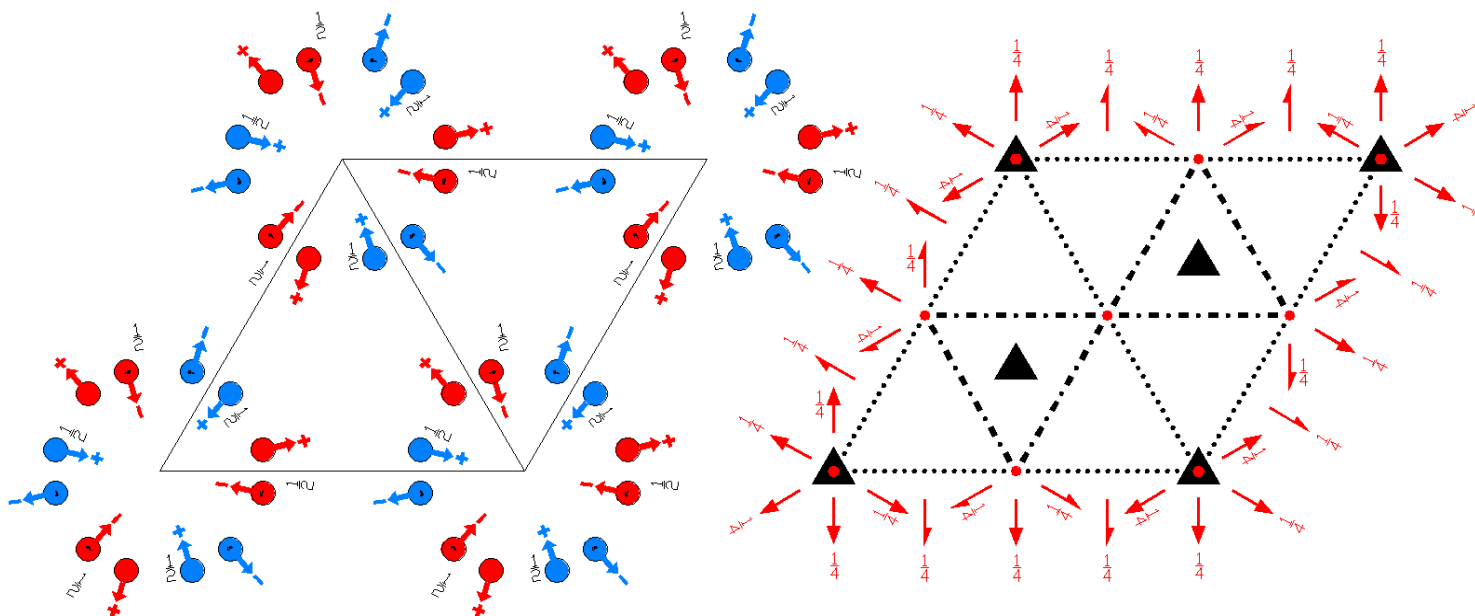
Along  $[2,1,0]$   $p2111'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $x,x/2,0$



$P\bar{3}'1c$   
163.3.1312

$\bar{3}'1m$   
 $P\bar{3}'12'/c$

Trigonal



Origin at center ( $\bar{3}'$ ) at  $\bar{3}'1c$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

### Symmetry Operations

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                               | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                       | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                       |
| (4) $2'$ $x, \bar{x}, 1/4$<br>( $2_3$  0,0,1/2)' | (5) $2'$ $x, 2x, 1/4$<br>( $2_2$  0,0,1/2)'              | (6) $2'$ $2x, x, 1/4$<br>( $2_1$  0,0,1/2)'                   |
| (7) $\bar{1}'$<br>( $\bar{1}$  0,0,0)'           | (8) $\bar{3}^+$ ' 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)' | (9) $\bar{3}^-$ ' 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)' |
| (10) c (0,0,1/2) $x, x, z$<br>( $m_3$  0,0,1/2)  | (11) c (0,0,1/2) $x, 0, z$<br>( $m_2$  0,0,1/2)          | (12) c (0,0,1/2) $0, y, z$<br>( $m_1$  0,0,1/2)               |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

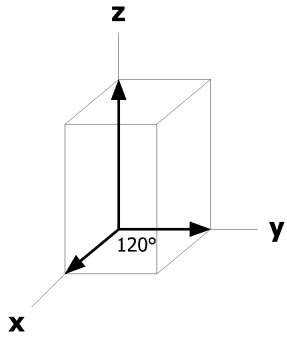
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	i	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w]	
			(4) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ +1/2 [v,u,w]	(5) $\bar{x}$ +y,y, $\bar{z}$ +1/2 [u-v, $\bar{v}$ ,w]	(6) x,x-y, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{u}$ +v,w]	
			(7) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(8) y, $\bar{x}$ +y, $\bar{z}$ [v, $\bar{u}$ +v, $\bar{w}$ ]	(9) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ]	
			(10) y,x,z+1/2 [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(11) x-y, $\bar{y}$ ,z+1/2 [ $\bar{u}$ +v,v, $\bar{w}$ ]	(12) $\bar{x}$ , $\bar{x}$ +y,z+1/2 [u,u-v, $\bar{w}$ ]	
6	h	..2'	x, $\bar{x}$ ,1/4 [u,u,w]	x,2x,1/4 [ $\bar{u}$ ,0,w]	2 $\bar{x}$ , $\bar{x}$ ,1/4 [0, $\bar{u}$ ,w]	
			$\bar{x}$ ,x,3/4 [ $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]	$\bar{x}$ ,2 $\bar{x}$ ,3/4 [u,0, $\bar{w}$ ]	2x,x,3/4 [0,u, $\bar{w}$ ]	
6	g	$\bar{1}$ '	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
			0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
4	f	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ +1/2 [0,0,w]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	2/3,1/3,z+1/2 [0,0, $\bar{w}$ ]
4	e	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ +1/2 [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]
2	d	3.2'	2/3,1/3,1/4 [0,0,w]	1/3,2/3,3/4 [0,0, $\bar{w}$ ]		
2	c	3.2'	1/3,2/3,1/4 [0,0,w]	2/3,1/3,3/4 [0,0, $\bar{w}$ ]		
1	b	$\bar{3}$ '..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
1	a	3.2'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p6mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

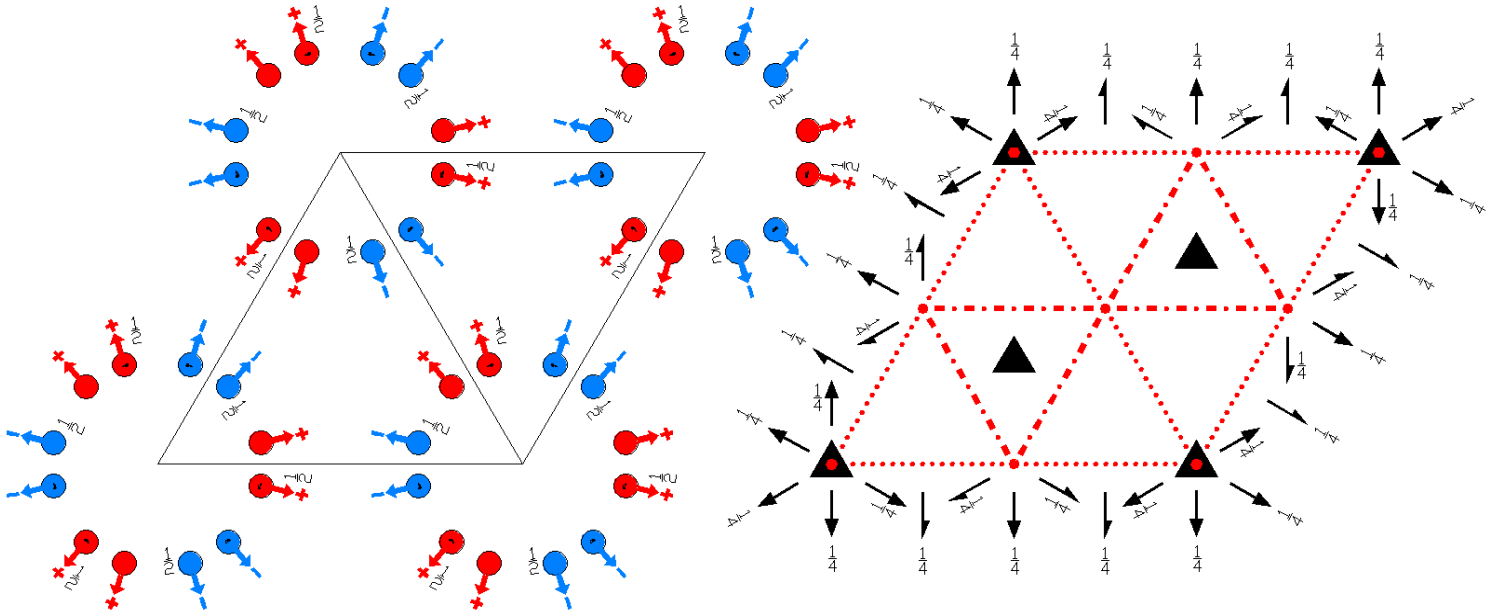
Along [2,1,0] p<sub>2a</sub>'-211  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$\bar{P}3'1c'$   
163.4.1313

$\bar{3}'1m'$   
 $\bar{P}3'12/c'$

Trigonal



Origin at center ( $\bar{3}'$ ) at  $\bar{3}'1c'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

### Symmetry Operations

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                                  | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                     | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                     |
| (4) 2 $x, \bar{x}, 1/4$<br>( $2_3$  0,0,1/2)        | (5) 2 $x, 2x, 1/4$<br>( $2_2$  0,0,1/2)                | (6) 2 $2x, x, 1/4$<br>( $2_1$  0,0,1/2)                     |
| (7) $\bar{1}'$<br>( $\bar{1}$  0,0,0)'              | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)' | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)' |
| (10) $c'$ (0,0,1/2) $x, x, z$<br>( $m_3$  0,0,1/2)' | (11) $c'$ (0,0,1/2) $x, 0, z$<br>( $m_2$  0,0,1/2)'    | (12) $c'$ (0,0,1/2) $0, y, z$<br>( $m_1$  0,0,1/2)'         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

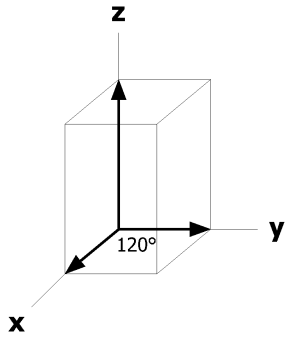
Multiplicity, Wyckoff letter, Site Symmetry.				Coordinates		
12	i	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]	
			(4) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(5) $\bar{x}+y,y,\bar{z}+1/2$ [ $\bar{u}+v,v,\bar{w}$ ]	(6) $x,x-y,\bar{z}+1/2$ [ $u,u-v,\bar{w}$ ]	
			(7) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(8) $y,\bar{x}+y,\bar{z}$ [ $v,\bar{u}+v,\bar{w}$ ]	(9) $x-y,x,\bar{z}$ [ $u-v,u,\bar{w}$ ]	
			(10) $y,x,z+1/2$ [ $v,u,w$ ]	(11) $x-y,\bar{y},\bar{z}+1/2$ [ $u-v,\bar{v},w$ ]	(12) $\bar{x},\bar{x}+y,z+1/2$ [ $\bar{u},\bar{u}+v,w$ ]	
6	h	..2	$x,\bar{x},1/4$ [ $u,\bar{u},0$ ]	$x,2x,1/4$ [ $u,2u,0$ ]	$2\bar{x},\bar{x},1/4$ [ $2\bar{u},\bar{u},0$ ]	
			$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]	$\bar{x},2\bar{x},3/4$ [ $\bar{u},2\bar{u},0$ ]	$2x,x,3/4$ [ $2u,u,0$ ]	
6	g	$\bar{1}'$	$1/2,0,0$ [ $0,0,0$ ]	$0,1/2,0$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]	
			$0,1/2,1/2$ [ $0,0,0$ ]	$1/2,0,1/2$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]	
4	f	3..	$1/3,2/3,z$ [ $0,0,w$ ]	$1/3,2/3,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$2/3,1/3,\bar{z}$ [ $0,0,\bar{w}$ ]	$2/3,1/3,z+1/2$ [ $0,0,w$ ]
4	e	3..	$0,0,z$ [ $0,0,w$ ]	$0,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]	$0,0,\bar{z}$ [ $0,0,\bar{w}$ ]	$0,0,z+1/2$ [ $0,0,w$ ]
2	d	3.2	$2/3,1/3,1/4$ [ $0,0,0$ ]	$1/3,2/3,3/4$ [ $0,0,0$ ]		
2	c	3.2	$1/3,2/3,1/4$ [ $0,0,0$ ]	$2/3,1/3,3/4$ [ $0,0,0$ ]		
1	b	$\bar{3}'..$	$0,0,0$ [ $0,0,0$ ]	$0,0,1/2$ [ $0,0,0$ ]		
1	a	3.2	$0,0,1/4$ [ $0,0,0$ ]	$0,0,3/4$ [ $0,0,0$ ]		

**Symmetry of Special Projections**

Along  $[0,0,1]$  p6m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p2m'g'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

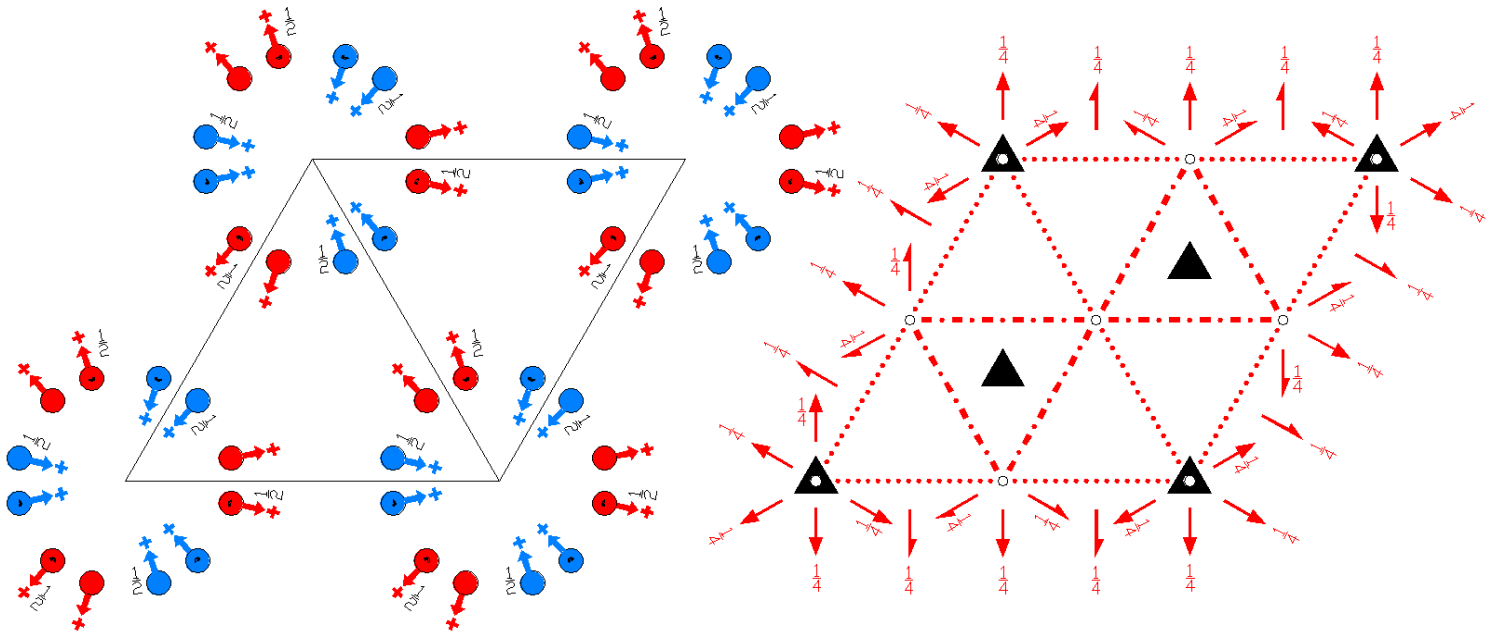
Along  $[2,1,0]$  p211  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,0$



$P\bar{3}1c'$   
163.5.1314

$\bar{3}1m'$   
 $P\bar{3}12'/c'$

Trigonal



Origin at center ( $\bar{3}$ ) at  $\bar{3}1c'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

### Symmetry Operations

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                                  | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) $2'$ $x, \bar{x}, 1/4$<br>( $2_3$  0,0,1/2)'    | (5) $2'$ $x, 2x, 1/4$<br>( $2_2$  0,0,1/2)'           | (6) $2'$ $2x, x, 1/4$<br>( $2_1$  0,0,1/2)'                |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)                | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) $c'$ (0,0,1/2) $x, x, z$<br>( $m_3$  0,0,1/2)' | (11) $c'$ (0,0,1/2) $x, 0, z$<br>( $m_2$  0,0,1/2)'   | (12) $c'$ (0,0,1/2) $0, y, z$<br>( $m_1$  0,0,1/2)'        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

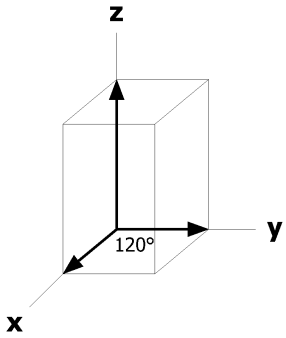
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
12	i	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y,\bar{x}$ ,z [ $\bar{u}+v,\bar{u}$ ,w]	
			(4) $\bar{y}$ , $\bar{x}$ , $\bar{z}+1/2$ [v,u,w]	(5) $\bar{x}+y,y,\bar{z}+1/2$ [u-v, $\bar{v}$ ,w]	(6) x,x-y, $\bar{z}+1/2$ [ $\bar{u}$ , $\bar{u}+v$ ,w]	
			(7) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(8) y, $\bar{x}+y,\bar{z}$ [ $\bar{v}$ ,u-v,w]	(9) x-y,x, $\bar{z}$ [ $\bar{u}+v,\bar{u}$ ,w]	
			(10) y,x, $\bar{z}+1/2$ [v,u,w]	(11) x-y, $\bar{y}$ , $\bar{z}+1/2$ [u-v, $\bar{v}$ ,w]	(12) $\bar{x}$ , $\bar{x}+y,\bar{z}+1/2$ [ $\bar{u}$ , $\bar{u}+v$ ,w]	
6	h	..2'	$x,\bar{x},1/4$ [u,u,w]	x,2x,1/4 [ $\bar{u}$ ,0,w]	$2\bar{x},\bar{x},1/4$ [0, $\bar{u}$ ,w]	
			$\bar{x},x,3/4$ [u,u,w]	$\bar{x},2\bar{x},3/4$ [ $\bar{u}$ ,0,w]	2x,x,3/4 [0, $\bar{u}$ ,w]	
6	g	$\bar{1}$	1/2,0,0 [u,v,w]	0,1/2,0 [ $\bar{v}$ ,u-v,w]	1/2,1/2,0 [ $\bar{u}+v,\bar{u}$ ,w]	
			0,1/2,1/2 [v,u,w]	1/2,0,1/2 [u-v, $\bar{v}$ ,w]	1/2,1/2,1/2 [ $\bar{u}$ , $\bar{u}+v$ ,w]	
4	f	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}+1/2$ [0,0,w]	2/3,1/3, $\bar{z}$ [0,0,w]	2/3,1/3, $\bar{z}+1/2$ [0,0,w]
4	e	3..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]
2	d	3.2'	2/3,1/3,1/4 [0,0,w]	1/3,2/3,3/4 [0,0,w]		
2	c	3.2'	1/3,2/3,1/4 [0,0,w]	2/3,1/3,3/4 [0,0,w]		
1	b	$\bar{3}..$	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]		
1	a	3.2'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p6'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

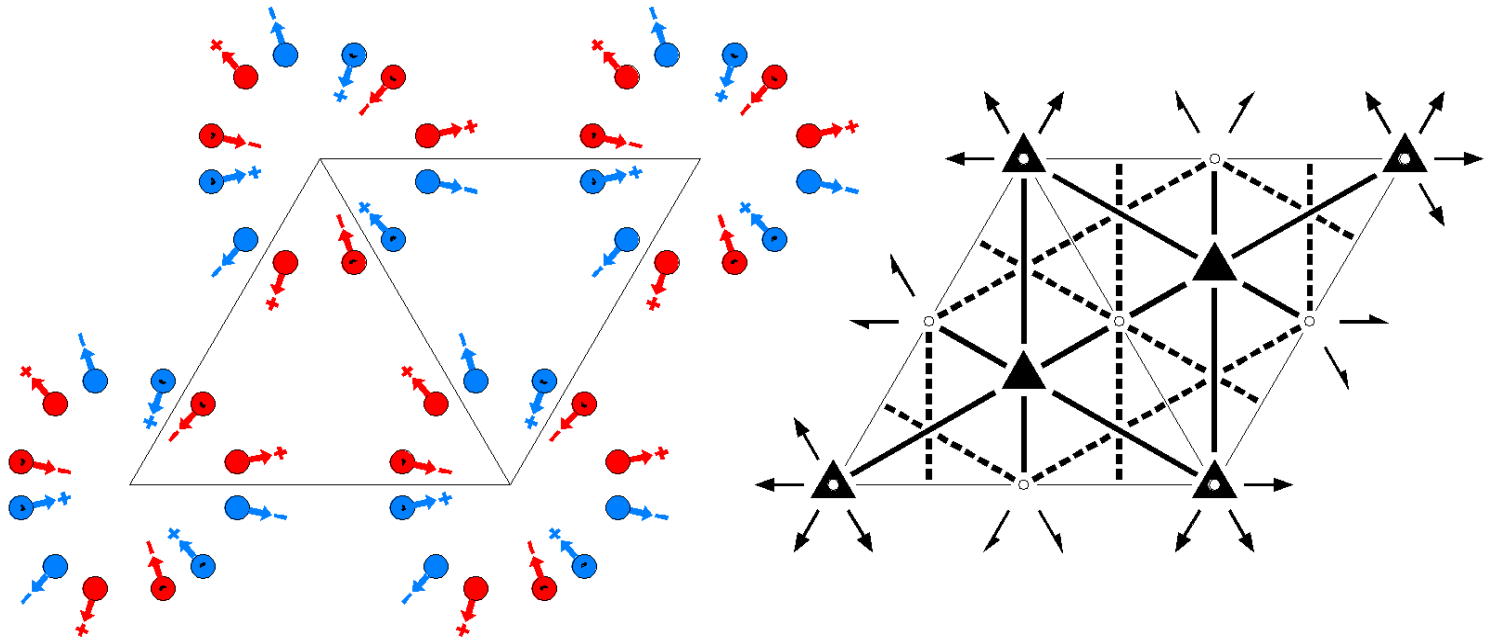
Along [2,1,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P\bar{3}m1$   
164.1.1315

$\bar{3}m1$   
 $P\bar{3}2/m1$

Trigonal



Origin on center ( $\bar{3}m1$ )

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1		

**Symmetry Operations**

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                           | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) 2 x,x,0<br>( $2_{xy}$  0,0,0)            | (5) 2 x,0,0<br>( $2_x$  0,0,0)                        | (6) 2 0,y,0<br>( $2_y$  0,0,0)                             |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)         | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) m x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0) | (11) m x,2x,z<br>( $m_x$  0,0,0)                      | (12) m 2x,x,z<br>( $m_y$  0,0,0)                           |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

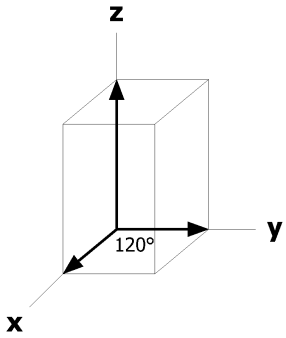
			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
12	j	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(4) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(5) x-y, $\bar{y}$ , $\bar{z}$ [u-v, $\bar{v}$ , $\bar{w}$ ]	(6) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ]
			(7) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(8) y, $\bar{x}$ +y, $\bar{z}$ [ $\bar{v}$ ,u-v,w]	(9) x-y,x, $\bar{z}$ [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(10) $\bar{y}$ , $\bar{x}$ ,z [v,u, $\bar{w}$ ]	(11) $\bar{x}$ +y,y,z [u-v, $\bar{v}$ , $\bar{w}$ ]	(12) x,x-y,z [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ]
6	i	.m.	x, $\bar{x}$ ,z [u,u,0]	x,2x,z [ $\bar{u}$ ,0,0]	2 $\bar{x}$ , $\bar{x}$ ,z [0, $\bar{u}$ ,0]
			$\bar{x}$ ,x, $\bar{z}$ [u,u,0]	2x,x, $\bar{z}$ [0, $\bar{u}$ ,0]	$\bar{x}$ ,2 $\bar{x}$ , $\bar{z}$ [ $\bar{u}$ ,0,0]
6	h	.2.	x,0,1/2 [u,0,0]	0,x,1/2 [0,u,0]	$\bar{x}$ , $\bar{x}$ ,1/2 [ $\bar{u}$ , $\bar{u}$ ,0]
			$\bar{x}$ ,0,1/2 [u,0,0]	0, $\bar{x}$ ,1/2 [0,u,0]	x,x,1/2 [ $\bar{u}$ , $\bar{u}$ ,0]
6	g	.2.	x,0,0 [u,0,0]	0,x,0 [0,u,0]	$\bar{x}$ , $\bar{x}$ ,0 [ $\bar{u}$ , $\bar{u}$ ,0]
			$\bar{x}$ ,0,0 [u,0,0]	0, $\bar{x}$ ,0 [0,u,0]	x,x,0 [ $\bar{u}$ , $\bar{u}$ ,0]
3	f	.2/m.	1/2,0,1/2 [u,0,0]	0,1/2,1/2 [0,u,0]	1/2,1/2,1/2 [ $\bar{u}$ , $\bar{u}$ ,0]
3	e	.2/m.	1/2,0,0 [u,0,0]	0,1/2,0 [0,u,0]	1/2,1/2,0 [ $\bar{u}$ , $\bar{u}$ ,0]
2	d	3m.	1/3,2/3,z [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	
2	c	3m.	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	
1	b	$\bar{3}$ m.	0,0,1/2 [0,0,0]		
1	a	$\bar{3}$ m.	0,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p6'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

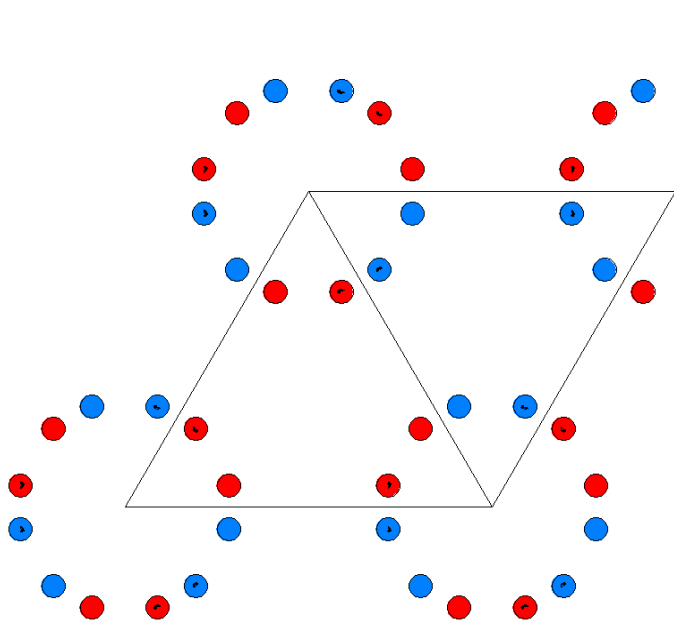
Along [2,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



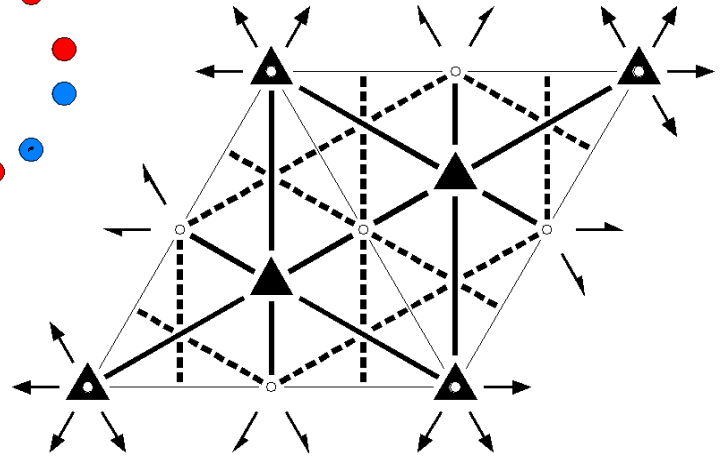
$P\bar{3}m11'$   
164.2.1316

$\bar{3}m11'$   
 $P\bar{3}2/m11'$

Trigonal



1'



Origin on center ( $\bar{3}m11'$ )

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1		

**Symmetry Operations**

For 1 + set

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                           | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) 2 x,x,0<br>( $2_{xy}$  0,0,0)            | (5) 2 x,0,0<br>( $2_x$  0,0,0)                        | (6) 2 0,y,0<br>( $2_y$  0,0,0)                             |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)         | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) m x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0) | (11) m x,2x,z<br>( $m_x$  0,0,0)                      | (12) m 2x,x,z<br>( $m_y$  0,0,0)                           |



## For 1' + set

(1) 1' (1 0,0,0)'	(2) 3 <sup>+</sup> ' 0,0,z (3 <sub>z</sub>  0,0,0)'	(3) 3 <sup>-</sup> ' 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(4) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(5) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'	(6) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'
(7) $\bar{1}$ ' ( $\bar{1}$  0,0,0)'	(8) $\bar{3}^+$ ' 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(9) $\bar{3}^-$ ' 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(10) m' x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)'	(11) m' x,2x,z (m <sub>x</sub>  0,0,0)'	(12) m' 2x,x,z (m <sub>y</sub>  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

**Positions**

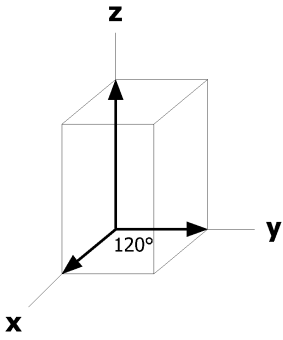
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			1 +	1' +	
12	j	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0]
			(4) y,x, $\bar{z}$ [0,0,0]	(5) x-y, $\bar{y},\bar{z}$ [0,0,0]	(6) $\bar{x},\bar{x}+y,\bar{z}$ [0,0,0]
			(7) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(8) y, $\bar{x}+y,\bar{z}$ [0,0,0]	(9) x-y,x, $\bar{z}$ [0,0,0]
			(10) $\bar{y},\bar{x},z$ [0,0,0]	(11) $\bar{x}+y,y,z$ [0,0,0]	(12) x,x-y,z [0,0,0]
6	i	.m.1'	x, $\bar{x},z$ [0,0,0]	x,2x,z [0,0,0]	2 $\bar{x},\bar{x},z$ [0,0,0]
			$\bar{x},x,\bar{z}$ [0,0,0]	2x,x, $\bar{z}$ [0,0,0]	$\bar{x},2\bar{x},\bar{z}$ [0,0,0]
6	h	.2.1'	x,0,1/2 [0,0,0]	0,x,1/2 [0,0,0]	$\bar{x},\bar{x},1/2$ [0,0,0]
			$\bar{x},0,1/2$ [0,0,0]	0, $\bar{x},1/2$ [0,0,0]	x,x,1/2 [0,0,0]
6	g	.2.1'	x,0,0 [0,0,0]	0,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]
			$\bar{x},0,0$ [0,0,0]	0, $\bar{x},0$ [0,0,0]	x,x,0 [0,0,0]
3	f	.2/m.1'	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]
3	e	.2/m.1'	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]
2	d	3m.1'	1/3,2/3,z [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	
2	c	3m.1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	
1	b	$\bar{3}m.1'$	0,0,1/2 [0,0,0]		
1	a	$\bar{3}m.1'$	0,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2111'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at  $x,0,0$

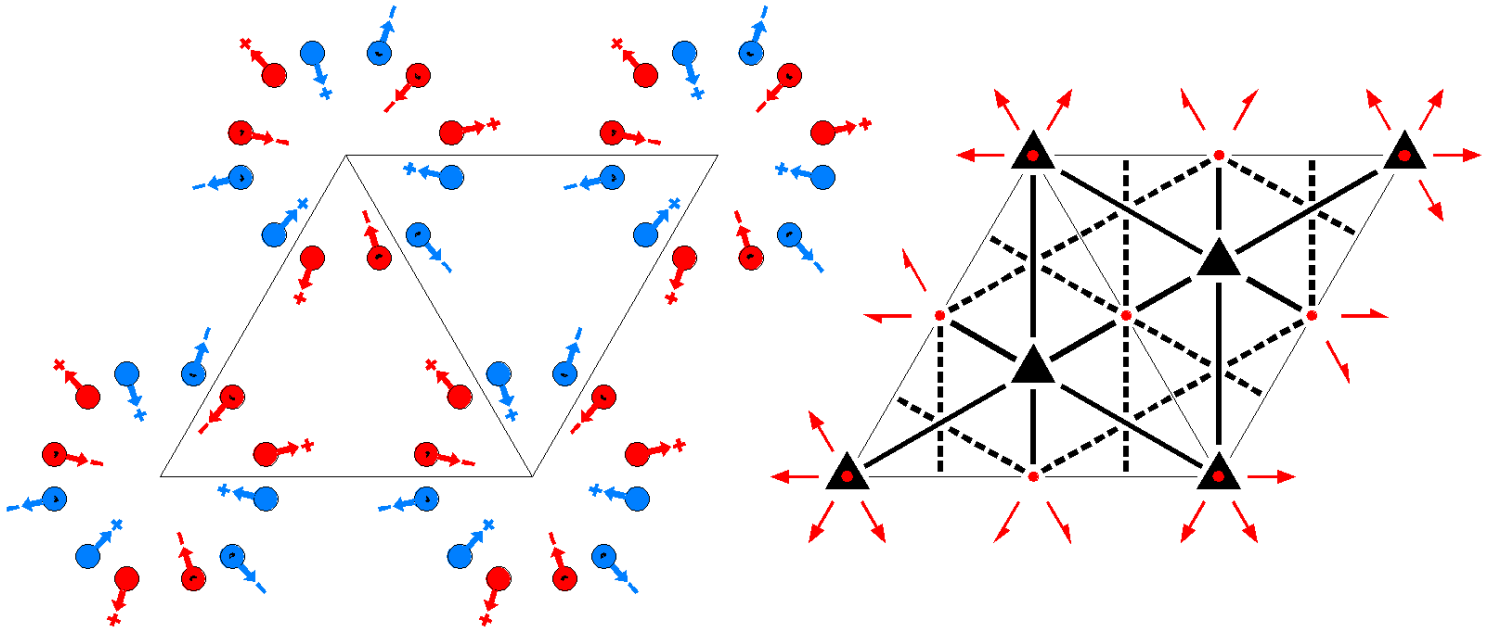
Along  $[2,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $x,x/2,0$



$P\bar{3}'m1$   
164.3.1317

$\bar{3}'m1$   
 $P\bar{3}'2'/m1$

Trigonal



Origin on center ( $\bar{3}'m1$ )

**Asymmetric unit**     $0 \leq x \leq 2/3$ ;     $0 \leq y \leq 1/3$ ;     $0 \leq z \leq 1$ ;     $x \leq (1+y)/2$ ;     $y \leq x/2$

Vertices             $0,0,0$              $1/2,0,0$              $2/3,1/3,0$   
                           $0,0,1$              $1/2,0,1$              $2/3,1/3,1$

**Symmetry Operations**

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                           | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                     | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                     |
| (4) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)'        | (5) $2'$ x,0,0<br>( $2_x$  0,0,0)'                     | (6) $2'$ 0,y,0<br>( $2_y$  0,0,0)'                          |
| (7) $\bar{1}'$<br>( $\bar{1}$  0,0,0)'       | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)' | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)' |
| (10) m x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0) | (11) m x,2x,z<br>( $m_x$  0,0,0)                       | (12) m 2x,x,z<br>( $m_y$  0,0,0)                            |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

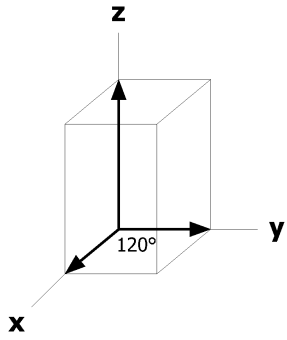
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	j	1	(1) x,y,z [u,v,w] (4) y,x, $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ ,w] (7) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ] (10) $\bar{y}$ , $\bar{x}$ ,z [v,u, $\bar{w}$ ]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w] (5) x-y, $\bar{y}$ , $\bar{z}$ [ $\bar{u}+v$ ,v,w] (8) y, $\bar{x}+y$ , $\bar{z}$ [v, $\bar{u}+v$ , $\bar{w}$ ] (11) $\bar{x}+y$ ,y,z [u-v, $\bar{v}$ , $\bar{w}$ ]	(3) $\bar{x}+y$ , $\bar{x}$ ,z [ $\bar{u}+v$ , $\bar{u}$ ,w] (6) $\bar{x}$ , $\bar{x}+y$ , $\bar{z}$ [u,u-v,w] (9) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ] (12) x,x-y,z [ $\bar{u}$ , $\bar{u}+v$ , $\bar{w}$ ]
6	i	.m.	x, $\bar{x}$ ,z [u,u,0] $\bar{x}$ ,x, $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ ,0]	x,2x,z [ $\bar{u}$ ,0,0] 2x,x, $\bar{z}$ [0,u,0]	2 $\bar{x}$ , $\bar{x}$ ,z [0, $\bar{u}$ ,0] $\bar{x}$ ,2 $\bar{x}$ , $\bar{z}$ [u,0,0]
6	h	.2'	x,0,1/2 [u,2u,w] $\bar{x}$ ,0,1/2 [ $\bar{u}$ ,2 $\bar{u}$ , $\bar{w}$ ]	0,x,1/2 [2 $\bar{u}$ , $\bar{u}$ ,w] 0, $\bar{x}$ ,1/2 [2u,u, $\bar{w}$ ]	$\bar{x}$ , $\bar{x}$ ,1/2 [u, $\bar{u}$ ,w] x,x,1/2 [ $\bar{u}$ ,u, $\bar{w}$ ]
6	g	.2'	x,0,0 [u,2u,w] $\bar{x}$ ,0,0 [ $\bar{u}$ ,2 $\bar{u}$ , $\bar{w}$ ]	0,x,0 [2 $\bar{u}$ , $\bar{u}$ ,w] 0, $\bar{x}$ ,0 [2u,u, $\bar{w}$ ]	$\bar{x}$ , $\bar{x}$ ,0 [u, $\bar{u}$ ,w] x,x,0 [ $\bar{u}$ ,u, $\bar{w}$ ]
3	f	.2'/m.	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]
3	e	.2'/m.	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]
2	d	3m.	1/3,2/3,z [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	
2	c	3m.	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	
1	b	$\bar{3}$ 'm.	0,0,1/2 [0,0,0]		
1	a	$\bar{3}$ 'm.	0,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p6mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

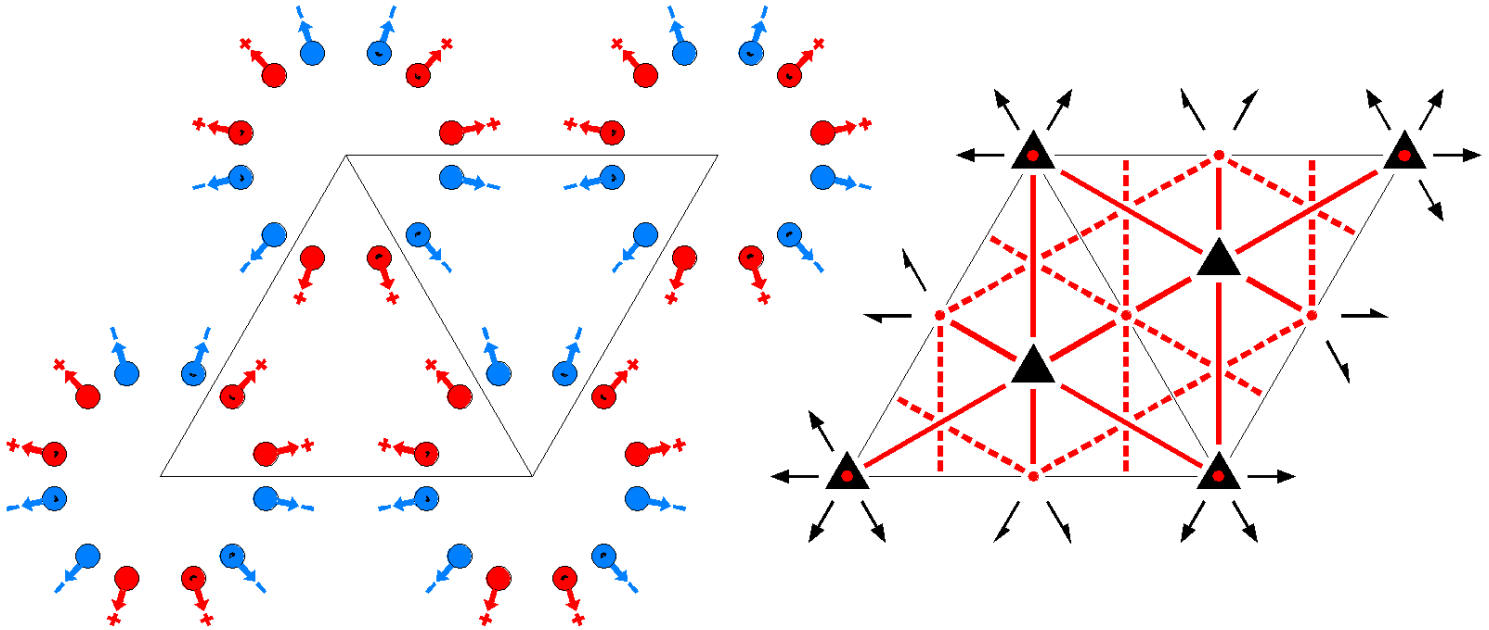
Along [2,1,0] p2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P\bar{3}'m'1$   
164.4.1318

$\bar{3}'m'1$   
 $P\bar{3}'2/m'1$

Trigonal



Origin on center ( $\bar{3}'m'1$ )

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1		

**Symmetry Operations**

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                               | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                     | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                     |
| (4) 2 x,x,0<br>( $2_{xy}$  0,0,0)                | (5) 2 x,0,0<br>( $2_x$  0,0,0)                         | (6) 2 0,y,0<br>( $2_y$  0,0,0)                              |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)'            | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)' | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)' |
| (10) $m'$ x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0)' | (11) $m'$ x,2x,z<br>( $m_x$  0,0,0)'                   | (12) $m'$ 2x,x,z<br>( $m_y$  0,0,0)'                        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

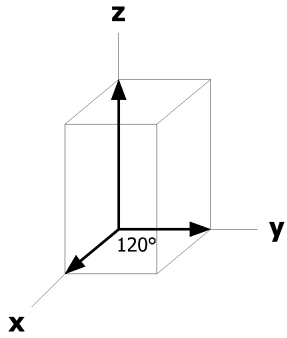
			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
12	j	1	(1) x,y,z [u,v,w] (4) y,x, $\bar{z}$ [v,u, $\bar{w}$ ] (7) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (10) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) x-y, $\bar{y},z$ [u-v, $\bar{v},\bar{w}$ ] (8) y, $\bar{x}+y,z$ [v, $\bar{u}+v,\bar{w}$ ] (11) $\bar{x}+y,y,z$ [ $\bar{u}+v,v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x},\bar{x}+y,z$ [ $\bar{u},\bar{u}+v,\bar{w}$ ] (9) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ] (12) x,x-y,z [u,u-v,w]
6	i	.m'	x, $\bar{x},z$ [u, $\bar{u},w$ ] $\bar{x},x,z$ [ $\bar{u},u,\bar{w}$ ]	x,2x,z [u,2u,w] 2x,x, $\bar{z}$ [2u,u, $\bar{w}$ ]	2 $\bar{x},\bar{x},z$ [2 $\bar{u},\bar{u},w$ ] $\bar{x},2\bar{x},\bar{z}$ [ $\bar{u},2\bar{u},\bar{w}$ ]
6	h	.2.	x,0,1/2 [u,0,0] $\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,1/2 [0,u,0] 0, $\bar{x},1/2$ [0, $\bar{u},0$ ]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ] x,x,1/2 [u,u,0]
6	g	.2.	x,0,0 [u,0,0] $\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0,u,0] 0, $\bar{x},0$ [0, $\bar{u},0$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ] x,x,0 [u,u,0]
3	f	.2/m'	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]
3	e	.2/m'	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]
2	d	3m'	1/3,2/3,z [0,0,w]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	
2	c	3m'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	
1	b	$\bar{3}'m'$	0,0,1/2 [0,0,0]		
1	a	$\bar{3}'m'$	0,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p6m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p211$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

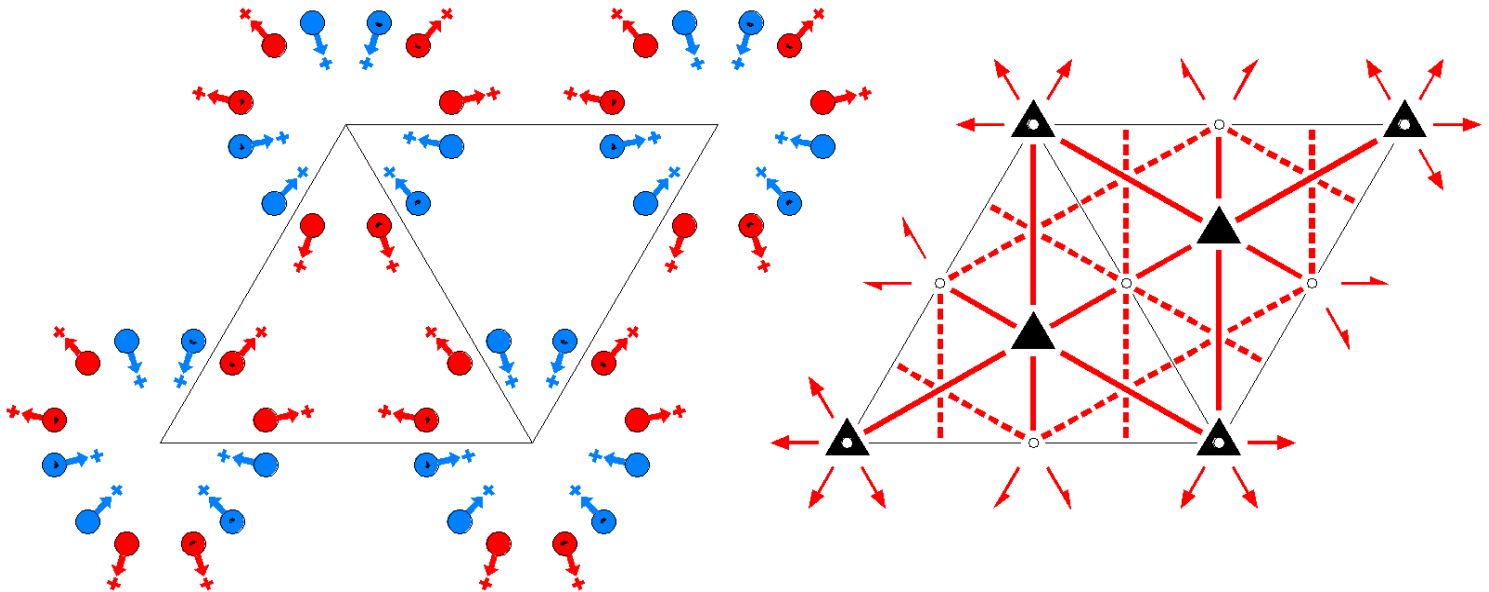
Along [2,1,0]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P\bar{3}m'1$   
164.5.1319

$\bar{3}m'1$   
 $P\bar{3}2'/m'1$

Trigonal



Origin on center ( $\bar{3}m'1$ )

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1		

**Symmetry Operations**

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                               | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)'            | (5) $2'$ x,0,0<br>( $2_x$  0,0,0)'                    | (6) $2'$ 0,y,0<br>( $2_y$  0,0,0)'                         |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)             | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) $m'$ x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0)' | (11) $m'$ x,2x,z<br>( $m_x$  0,0,0)'                  | (12) $m'$ 2x,x,z<br>( $m_y$  0,0,0)'                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	j	1	(1) x,y,z [u,v,w] (4) y,x, $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ ,w] (7) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w] (10) $\bar{y}$ , $\bar{x}$ ,z [ $\bar{v}$ , $\bar{u}$ ,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w] (5) x-y, $\bar{y}$ , $\bar{z}$ [ $\bar{u}+v$ ,v,w] (8) y, $\bar{x}+y$ , $\bar{z}$ [ $\bar{v}$ ,u-v,w] (11) $\bar{x}+y$ ,y,z [ $\bar{u}+v$ ,v,w]	(3) $\bar{x}+y$ , $\bar{x}$ ,z [ $\bar{u}+v$ , $\bar{u}$ ,w] (6) $\bar{x}$ , $\bar{x}+y$ , $\bar{z}$ [u,u-v,w] (9) x-y,x, $\bar{z}$ [ $\bar{u}+v$ , $\bar{u}$ ,w] (12) x,x-y,z [u,u-v,w]
6	i	.m'	x, $\bar{x}$ ,z [u, $\bar{u}$ ,w] $\bar{x}$ ,x, $\bar{z}$ [u, $\bar{u}$ ,w]	x,2x,z [u,2u,w] 2x,x, $\bar{z}$ [2 $\bar{u}$ , $\bar{u}$ ,w]	2 $\bar{x}$ , $\bar{x}$ ,z [2 $\bar{u}$ , $\bar{u}$ ,w] $\bar{x}$ ,2 $\bar{x}$ , $\bar{z}$ [u,2u,w]
6	h	.2'	x,0,1/2 [u,2u,w] $\bar{x}$ ,0,1/2 [u,2u,w]	0,x,1/2 [2 $\bar{u}$ , $\bar{u}$ ,w] 0, $\bar{x}$ ,1/2 [2 $\bar{u}$ , $\bar{u}$ ,w]	$\bar{x}$ , $\bar{x}$ ,1/2 [u, $\bar{u}$ ,w] x,x,1/2 [u, $\bar{u}$ ,w]
6	g	.2'	x,0,0 [u,2u,w] $\bar{x}$ ,0,0 [u,2u,w]	0,x,0 [2 $\bar{u}$ , $\bar{u}$ ,w] 0, $\bar{x}$ ,0 [2 $\bar{u}$ , $\bar{u}$ ,w]	$\bar{x}$ , $\bar{x}$ ,0 [u, $\bar{u}$ ,w] x,x,0 [u, $\bar{u}$ ,w]
3	f	.2'/m'	1/2,0,1/2 [u,2u,w]	0,1/2,1/2 [2 $\bar{u}$ , $\bar{u}$ ,w]	1/2,1/2,1/2 [u, $\bar{u}$ ,w]
3	e	.2'/m'	1/2,0,0 [u,2u,w]	0,1/2,0 [2 $\bar{u}$ , $\bar{u}$ ,w]	1/2,1/2,0 [u, $\bar{u}$ ,w]
2	d	3m'	1/3,2/3,z [0,0,w]	2/3,1/3, $\bar{z}$ [0,0,w]	
2	c	3m'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	
1	b	$\bar{3}m'$	0,0,1/2 [0,0,w]		
1	a	$\bar{3}m'$	0,0,0 [0,0,w]		

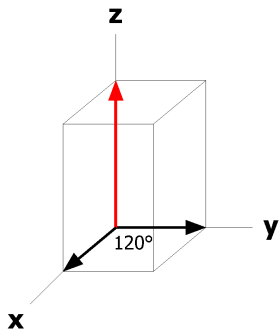
**Symmetry of Special Projections**

Along [0,0,1]  $p6'm'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p2'11$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0]  $p2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0





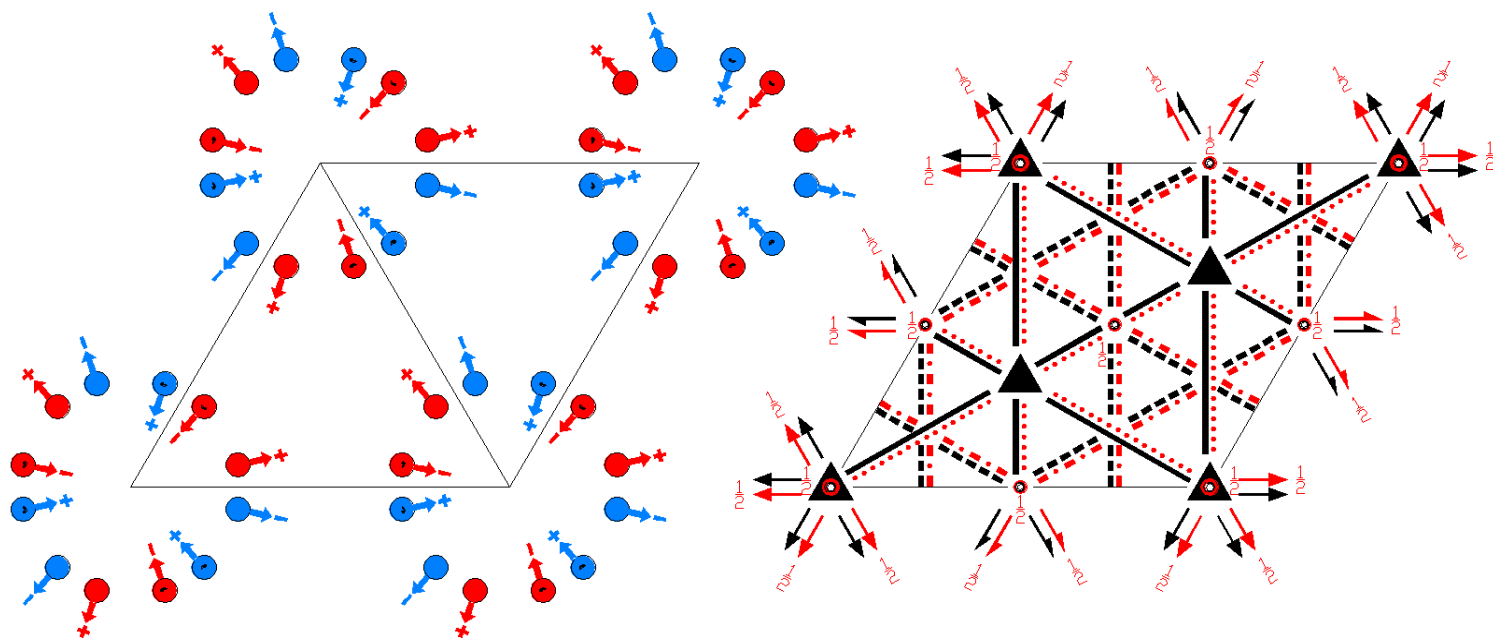
$P_{2c} \bar{3}m1$

164.6.1320

$\bar{3}m11'$

$P_{2c} \bar{3}2/m1$

Trigonal



Origin on center ( $\bar{3}m1$ )

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/3$ ;  $0 \leq z \leq 1$ ;  $x \leq (1+y)/2$ ;  $y \leq x/2$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0
	0,0,1	1/2,0,1	2/3,1/3,1

### Symmetry Operations

For (0,0,0) + set

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                           | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) 2 x,x,0<br>( $2_{xy}$  0,0,0)            | (5) 2 x,0,0<br>( $2_x$  0,0,0)                        | (6) 2 0,y,0<br>( $2_y$  0,0,0)                             |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)         | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) m x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0) | (11) m x,2x,z<br>( $m_x$  0,0,0)                      | (12) m 2x,x,z<br>( $m_y$  0,0,0)                           |

For (0,0,1)' + set

(1) $t' (0,0,1)$ $(1 0,0,1)'$	(2) $3^{+'} (0,0,1)$ 0,0,z $(3_z 0,0,1)'$	(3) $3^{-'} (0,0,1)$ 0,0,z $(3_z^{-1} 0,0,1)'$
(4) $2' x,x,1/2$ $(2_{xy} 0,0,1)'$	(5) $2' x,0,1/2$ $(2_x 0,0,1)'$	(6) $2' 0,y,1/2$ $(2_y 0,0,1)'$
(7) $\bar{1}' 0,0,1/2$ $(\bar{1} 0,0,1)'$	(8) $\bar{3}^{+'} 0,0,z; 0,0,1/2$ $(\bar{3}_z 0,0,1)'$	(9) $\bar{3}^{-'} 0,0,z; 0,0,1/2$ $(\bar{3}_z^{-1} 0,0,1)'$
(10) $c' (0,0,1)$ $x,\bar{x},z$ $(m_{xy} 0,0,1)'$	(11) $c' (0,0,1)$ $x,2x,z$ $(m_x 0,0,1)'$	(12) $c' (0,0,1)$ $2x,x,z$ $(m_y 0,0,1)'$

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).**Positions**

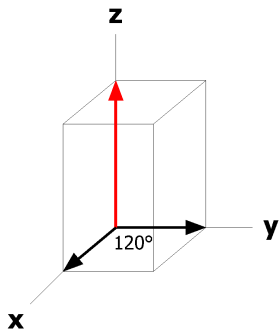
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(0,0,1)' +	
24	j	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$
			(4) $y,x,\bar{z} [v,u,\bar{w}]$	(5) $x-y,\bar{y},\bar{z} [u-v,\bar{v},\bar{w}]$	(6) $\bar{x},\bar{x}+y,\bar{z} [\bar{u},\bar{u}+v,\bar{w}]$
			(7) $\bar{x},\bar{y},\bar{z} [u,v,w]$	(8) $y,\bar{x}+y,\bar{z} [\bar{v},u-v,w]$	(9) $x-y,x,\bar{z} [\bar{u}+v,\bar{u},w]$
			(10) $\bar{y},\bar{x},z [v,u,\bar{w}]$	(11) $\bar{x}+y,y,z [u-v,\bar{v},\bar{w}]$	(12) $x,x-y,z [\bar{u},\bar{u}+v,\bar{w}]$
12	i	.m.	$x,\bar{x},z [u,u,0]$	$x,2x,z [\bar{u},0,0]$	$2\bar{x},\bar{x},z [0,\bar{u},0]$
			$\bar{x},x,\bar{z} [u,u,0]$	$2x,x,\bar{z} [0,\bar{u},0]$	$\bar{x},2\bar{x},\bar{z} [\bar{u},0,0]$
12	h	.2'	$x,0,1/2 [u,2u,w]$	$0,x,1/2 [2\bar{u},\bar{u},w]$	$\bar{x},\bar{x},1/2 [u,\bar{u},w]$
			$\bar{x},0,1/2 [\bar{u},2\bar{u},w]$	$0,\bar{x},1/2 [2u,u,w]$	$x,x,1/2 [\bar{u},u,w]$
12	g	.2.	$x,0,0 [u,0,0]$	$0,x,0 [0,u,0]$	$\bar{x},\bar{x},0 [\bar{u},\bar{u},0]$
			$\bar{x},0,0 [u,0,0]$	$0,\bar{x},0 [0,u,0]$	$x,x,0 [\bar{u},\bar{u},0]$
6	f	.2'/m.	$1/2,0,1/2 [0,0,0]$	$0,1/2,1/2 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$
6	e	.2/m.	$1/2,0,0 [u,0,0]$	$0,1/2,0 [0,u,0]$	$1/2,1/2,0 [\bar{u},\bar{u},0]$
4	d	3m.	$1/3,2/3,z [0,0,0]$	$2/3,1/3,\bar{z} [0,0,0]$	
4	c	3m.	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$	
2	b	$\bar{3}m.$	$0,0,1/2 [0,0,0]$		
2	a	$\bar{3}m.$	$0,0,0 [0,0,0]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2111'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at  $x,0,0$

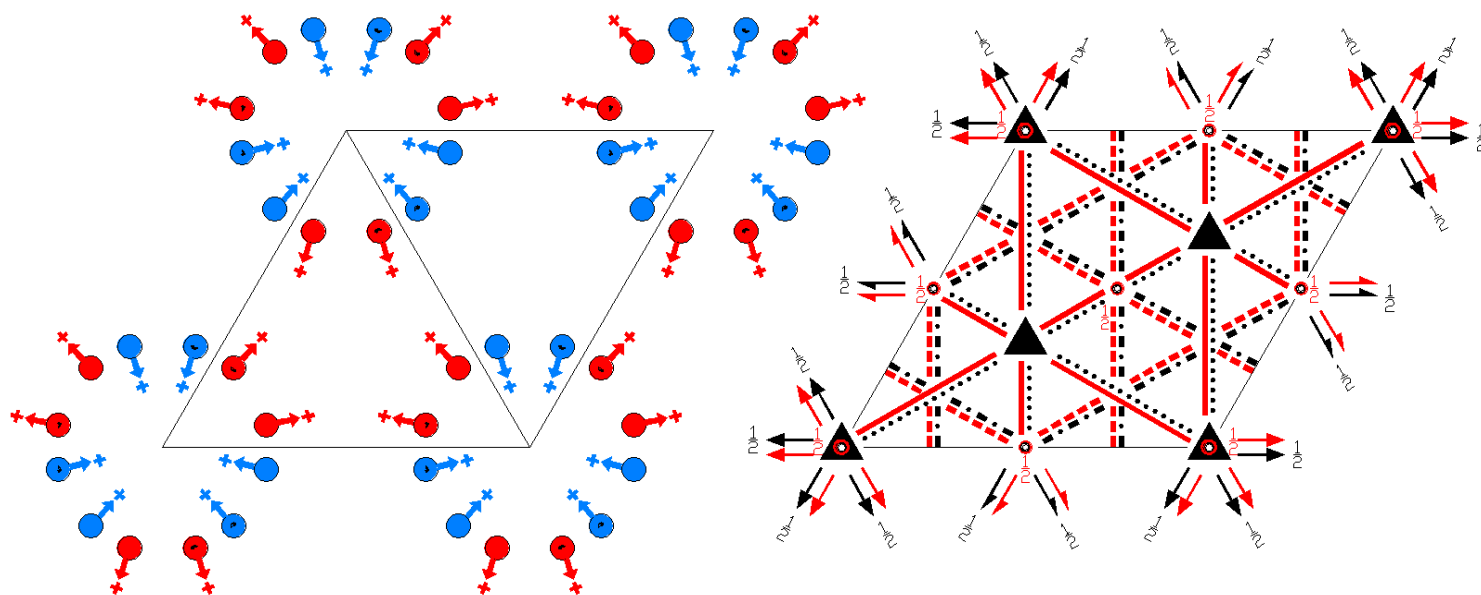
Along  $[2,1,0]$   $p_{2a}2mm$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $x,x/2,1/2$



$P_{2c} \bar{3}m'1$   
164.7.1321

$\bar{3}m'11'$   
 $P_{2c} \bar{3}2'/m'1$

Trigonal



Origin on center ( $\bar{3}m'1$ )

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/3$ ;  $0 \leq z \leq 1$ ;  $x \leq (1+y)/2$ ;  $y \leq x/2$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0
	0,0,1	1/2,0,1	2/3,1/3,1

### Symmetry Operations

For (0,0,0) + set

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                               | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)'            | (5) $2'$ x,0,0<br>( $2_x$  0,0,0)'                    | (6) $2'$ 0,y,0<br>( $2_y$  0,0,0)'                         |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)             | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) $m'$ x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0)' | (11) $m'$ x,2x,z<br>( $m_x$  0,0,0)'                  | (12) $m'$ 2x,x,z<br>( $m_y$  0,0,0)'                       |

## For (0,0,1)' + set

(1) $t' (0,0,1)$ $(1 0,0,1)'$	(2) $3^+ ' (0,0,1)$ 0,0,z $(3_z 0,0,1)'$	(3) $3^- ' (0,0,1)$ 0,0,z $(3_z^{-1} 0,0,1)'$
(4) $2_{xy} x,x,1/2$ $(2_{xy} 0,0,1)$	(5) $2_{xz} x,0,1/2$ $(2_{xz} 0,0,1)$	(6) $2_{yz} 0,y,1/2$ $(2_{yz} 0,0,1)$
(7) $\bar{1}' 0,0,1/2$ $(\bar{1} 0,0,1)'$	(8) $\bar{3}^+ ' 0,0,z; 0,0,1/2$ $(\bar{3}_z 0,0,1)'$	(9) $\bar{3}^- ' 0,0,z; 0,0,1/2$ $(\bar{3}_z^{-1} 0,0,1)'$
(10) $c (0,0,1) x,\bar{x},z$ $(m_{xy} 0,0,1)$	(11) $c (0,0,1) x,2x,z$ $(m_x 0,0,1)$	(12) $c (0,0,1) 2x,x,z$ $(m_y 0,0,1)$

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

**Positions**

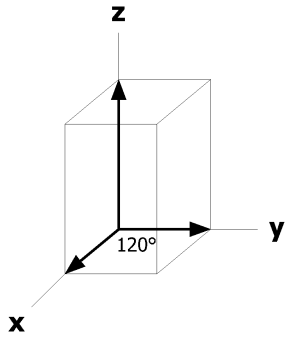
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) + (0,0,1)' +		
24	j	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$
			(4) $y,x,\bar{z} [\bar{v},\bar{u},w]$	(5) $x-y,\bar{y},\bar{z} [\bar{u}+v,v,w]$	(6) $\bar{x},\bar{x}+y,\bar{z} [u,u-v,w]$
			(7) $\bar{x},\bar{y},\bar{z} [u,v,w]$	(8) $y,\bar{x}+y,\bar{z} [\bar{v},u-v,w]$	(9) $x-y,x,\bar{z} [\bar{u}+v,\bar{u},w]$
			(10) $\bar{y},\bar{x},z [\bar{v},\bar{u},w]$	(11) $\bar{x}+y,y,z [\bar{u}+v,v,w]$	(12) $x,x-y,z [u,u-v,w]$
12	i	.m'	$x,\bar{x},z [u,\bar{u},w]$	$x,2x,z [u,2u,w]$	$2\bar{x},\bar{x},z [2\bar{u},\bar{u},w]$
			$\bar{x},x,\bar{z} [u,\bar{u},w]$	$2x,x,\bar{z} [2\bar{u},\bar{u},w]$	$\bar{x},2\bar{x},\bar{z} [u,2u,w]$
12	h	.2.	$x,0,1/2 [u,0,0]$	$0,x,1/2 [0,u,0]$	$\bar{x},\bar{x},1/2 [\bar{u},\bar{u},0]$
			$\bar{x},0,1/2 [\bar{u},0,0]$	$0,\bar{x},1/2 [0,\bar{u},0]$	$x,x,1/2 [u,u,0]$
12	g	.2'	$x,0,0 [u,2u,w]$	$0,x,0 [2\bar{u},\bar{u},w]$	$\bar{x},\bar{x},0 [u,\bar{u},w]$
			$\bar{x},0,0 [u,2u,w]$	$0,\bar{x},0 [2\bar{u},\bar{u},w]$	$x,x,0 [u,\bar{u},w]$
6	f	.2/m.	$1/2,0,1/2 [u,0,0]$	$0,1/2,1/2 [0,u,0]$	$1/2,1/2,1/2 [u,\bar{u},0]$
6	e	.2'/m'	$1/2,0,0 [u,2u,w]$	$0,1/2,0 [2\bar{u},\bar{u},w]$	$1/2,1/2,0 [\bar{u},\bar{u},0]$
4	d	3m'	$1/3,2/3,z [0,0,w]$	$2/3,1/3,\bar{z} [0,0,w]$	
4	c	3m'	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,w]$	
2	b	$\bar{3}m'$	$0,0,1/2 [0,0,w]$		
2	a	$\bar{3}m'$	$0,0,0 [0,0,w]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a'}211$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at  $x,0,1/2$

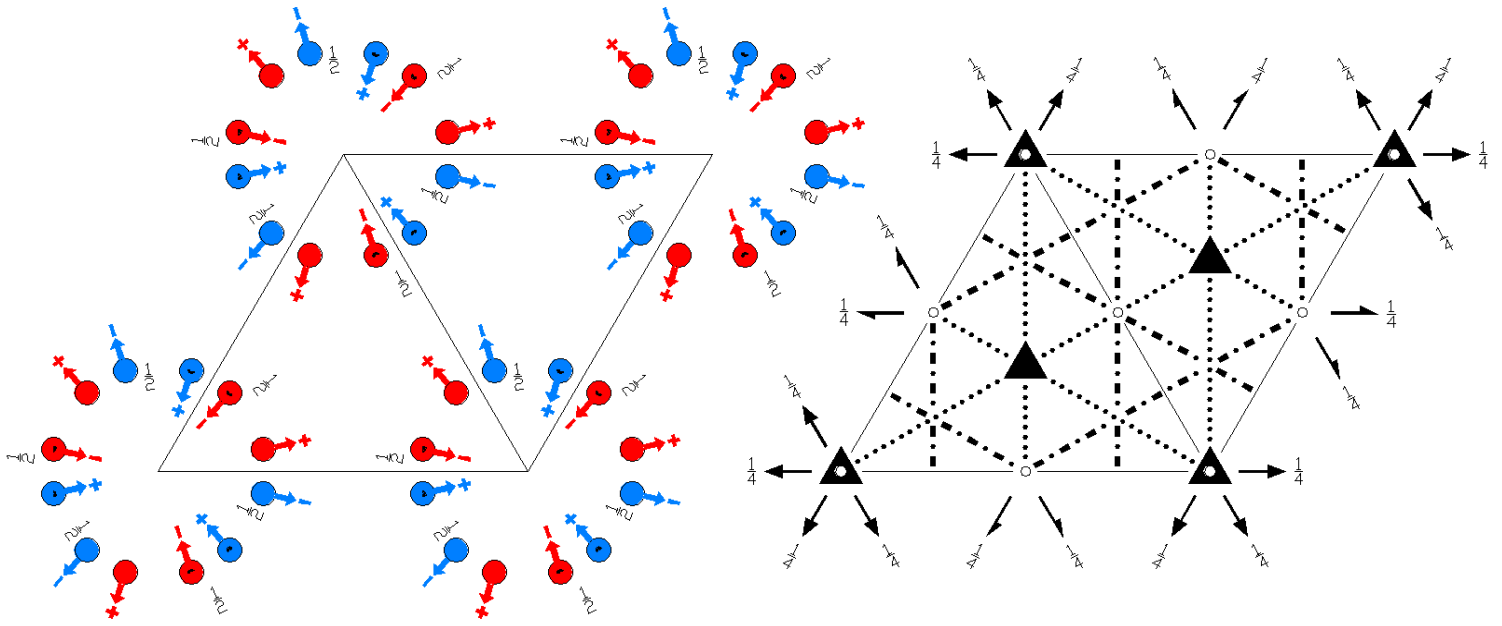
Along  $[2,1,0]$   $p_{2a'}2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $x,x/2,1/2$



$P\bar{3}c1$   
165.1.1322

$\bar{3}m1$   
 $P\bar{3}2/c1$

Trigonal



Origin on center ( $\bar{3}$ ) at  $\bar{3}c1$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

**Symmetry Operations**

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                                       | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) 2 x,x,1/4<br>( $2_{xy}$  0,0,1/2)                    | (5) 2 x,0,1/4<br>( $2_x$  0,0,1/2)                    | (6) 2 0,y,1/4<br>( $2_y$  0,0,1/2)                         |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)                     | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) c (0,0,1/2) x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,1/2) | (11) c (0,0,1/2) x,2x,z<br>( $m_x$  0,0,1/2)          | (12) c (0,0,1/2) 2x,x,z<br>( $m_y$  0,0,1/2)               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	g	1	(1) x,y,z [u,v,w] (4) y,x, $\bar{z}+1/2$ [v,u, $\bar{w}$ ] (7) $\bar{x},\bar{y},\bar{z}$ [u,v,w] (10) $\bar{y},\bar{x},z+1/2$ [v,u, $\bar{w}$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) x-y, $\bar{y},\bar{z}+1/2$ [u-v, $\bar{v},\bar{w}$ ] (8) y, $\bar{x}+y,\bar{z}$ [ $\bar{v},u-v,w$ ] (11) $\bar{x}+y,y,z+1/2$ [u-v, $\bar{v},\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x},\bar{x}+y,\bar{z}+1/2$ [ $\bar{u},\bar{u}+v,\bar{w}$ ] (9) x-y,x, $\bar{z}$ [ $\bar{u}+v,\bar{u},w$ ] (12) x,x-y,z+1/2 [ $\bar{u},\bar{u}+v,\bar{w}$ ]	
6	f	.2.	x,0,1/4 [u,0,0] $\bar{x},0,3/4$ [u,0,0]	0,x,1/4 [0,u,0] 0, $\bar{x},3/4$ [0,u,0]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ] x,x,3/4 [ $\bar{u},\bar{u},0$ ]	
6	e	$\bar{1}$	1/2,0,0 [u,v,w] 0,1/2,1/2 [v,u, $\bar{w}$ ]	0,1/2,0 [ $\bar{v},u-v,w$ ] 1/2,0,1/2 [u-v, $\bar{v},\bar{w}$ ]	1/2,1/2,0 [ $\bar{u}+v,\bar{u},w$ ] 1/2,1/2,1/2 [ $\bar{u},\bar{u}+v,\bar{w}$ ]	
4	d	3..	1/3,2/3,z [0,0,w]	2/3,1/3, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0,w]	1/3,2/3,z+1/2 [0,0, $\bar{w}$ ]
4	c	3..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]
2	b	$\bar{3}$ ..	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		
2	a	32.	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

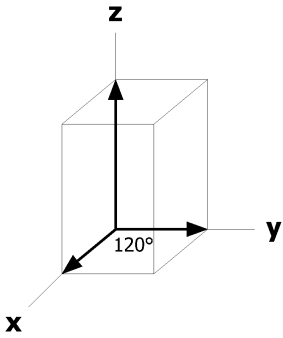
**Symmetry of Special Projections**

Along [0,0,1] p6'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>\* 211  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/4

Along [2,1,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0

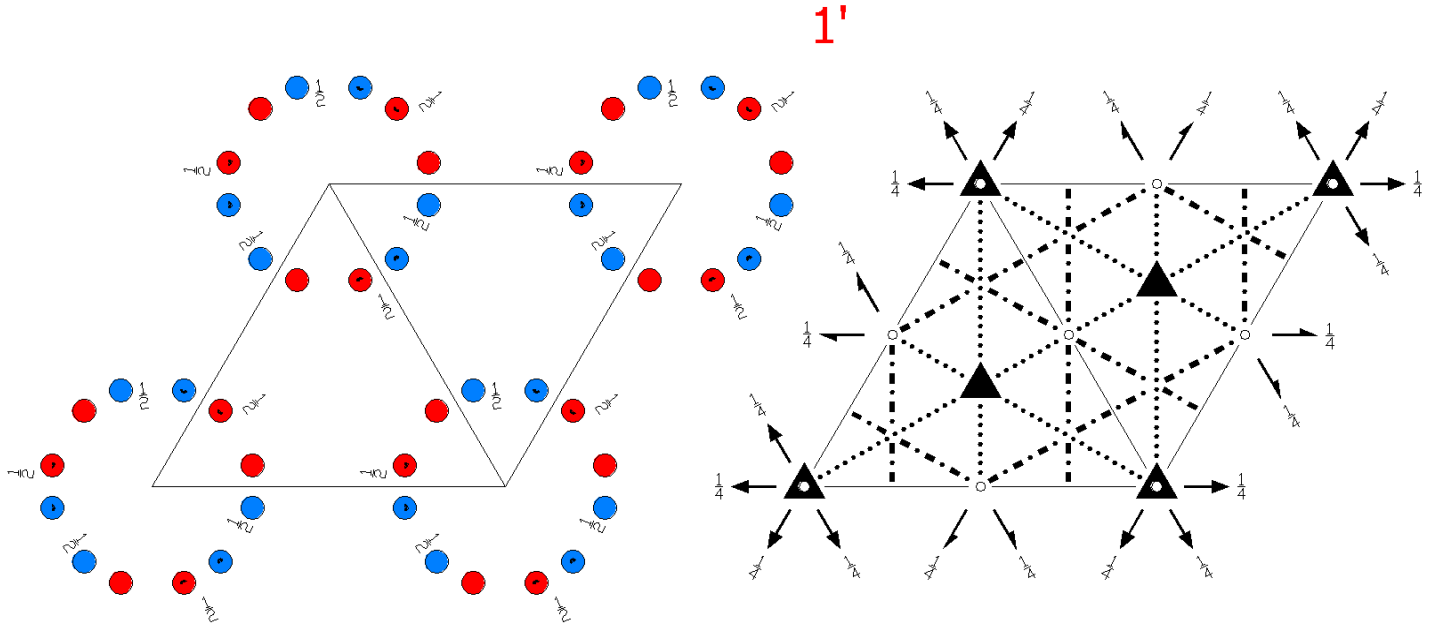




$P\bar{3}c11'$   
165.2.1323

$\bar{3}m11'$   
 $P\bar{3}2/c11'$

Trigonal



Origin on center ( $\bar{3}1'$ ) at  $\bar{3}c11'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

**Symmetry Operations**

For 1 + set

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                                       | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) 2 x,x,1/4<br>( $2_{xy}$  0,0,1/2)                    | (5) 2 x,0,1/4<br>( $2_x$  0,0,1/2)                    | (6) 2 0,y,1/4<br>( $2_y$  0,0,1/2)                         |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)                     | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) c (0,0,1/2) x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,1/2) | (11) c (0,0,1/2) x,2x,z<br>( $m_x$  0,0,1/2)          | (12) c (0,0,1/2) 2x,x,z<br>( $m_y$  0,0,1/2)               |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 3 <sup>+</sup> 0,0,z (3 <sub>z</sub>  0,0,0)'	(3) 3 <sup>-</sup> 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(4) 2' x,x,1/4 (2 <sub>xy</sub>  0,0,1/2)'	(5) 2' x,0,1/4 (2 <sub>x</sub>  0,0,1/2)'	(6) 2' 0,y,1/4 (2 <sub>y</sub>  0,0,1/2)'
(7) $\bar{1}$ ' ( $\bar{1}$  0,0,0)'	(8) $\bar{3}$ <sup>+</sup> 0,0,z; 0,0,0 ( $\bar{3}$ <sub>z</sub>  0,0,0)'	(9) $\bar{3}$ <sup>-</sup> 0,0,z; 0,0,0 ( $\bar{3}$ <sub>z</sub> <sup>-1</sup>  0,0,0)'
(10) c' (0,0,1/2) x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,1/2)'	(11) c' (0,0,1/2) x,2x,z (m <sub>x</sub>  0,0,1/2)'	(12) c' (0,0,1/2) 2x,x,z (m <sub>y</sub>  0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

**Positions**

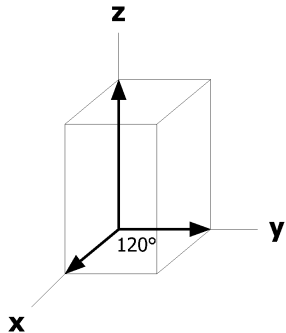
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			1 +	1' +		
12	g	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0]	
			(4) y,x, $\bar{z}+1/2$ [0,0,0]	(5) x-y, $\bar{y},\bar{z}+1/2$ [0,0,0]	(6) $\bar{x},\bar{x}+y,\bar{z}+1/2$ [0,0,0]	
			(7) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(8) y, $\bar{x}+y,\bar{z}$ [0,0,0]	(9) x-y,x, $\bar{z}$ [0,0,0]	
			(10) $\bar{y},\bar{x},z+1/2$ [0,0,0]	(11) $\bar{x}+y,y,z+1/2$ [0,0,0]	(12) x,x-y,z+1/2 [0,0,0]	
6	f	.2.1'	x,0,1/4 [0,0,0]	0,x,1/4 [0,0,0]	$\bar{x},\bar{x},1/4$ [0,0,0]	
			$\bar{x},0,3/4$ [0,0,0]	0, $\bar{x},3/4$ [0,0,0]	x,x,3/4 [0,0,0]	
6	e	$\bar{1}$ 1'	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
			0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
4	d	3..1'	1/3,2/3,z [0,0,0]	2/3,1/3, $\bar{z}+1/2$ [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	1/3,2/3,z+1/2 [0,0,0]
4	c	3..1'	0,0,z [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0,z+1/2 [0,0,0]
2	b	$\bar{3}$ ..1'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
2	a	32.1'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2111'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

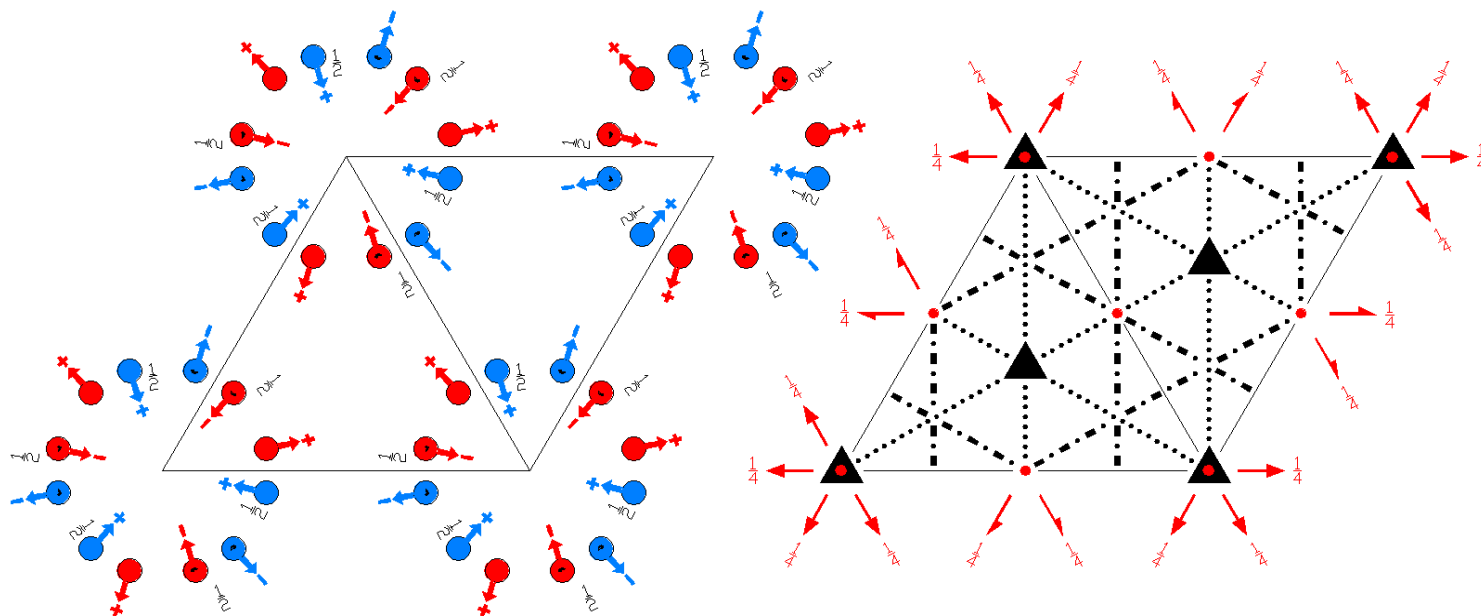
Along [2,1,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P\bar{3}'c1$   
165.3.1324

$\bar{3}'m1$   
 $P\bar{3}'2'/c1$

Trigonal



Origin on center ( $\bar{3}'$ ) at  $\bar{3}'c1$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

### Symmetry Operations

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                                       | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                     | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                     |
| (4) $2'$ x,x,1/4<br>( $2_{xy}$  0,0,1/2)'                | (5) $2'$ x,0,1/4<br>( $2_x$  0,0,1/2)'                 | (6) $2'$ 0,y,1/4<br>( $2_y$  0,0,1/2)'                      |
| (7) $\bar{1}'$<br>( $\bar{1}$  0,0,0)'                   | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)' | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)' |
| (10) c (0,0,1/2) x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,1/2) | (11) c (0,0,1/2) x,2x,z<br>( $m_x$  0,0,1/2)           | (12) c (0,0,1/2) 2x,x,z<br>( $m_y$  0,0,1/2)                |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

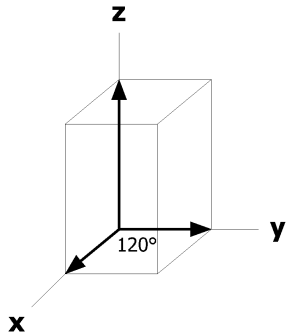
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
12	g	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y,\bar{x}$ ,z [ $\bar{u}+v,\bar{u}$ ,w]	
			(4) y,x, $\bar{z}+1/2$ [ $\bar{v}$ , $\bar{u}$ ,w]	(5) x-y, $\bar{y}$ , $\bar{z}+1/2$ [ $\bar{u}+v,v,w$ ]	(6) $\bar{x}$ , $\bar{x}+y,\bar{z}+1/2$ [u,u-v,w]	
			(7) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(8) y, $\bar{x}+y,\bar{z}$ [v, $\bar{u}+v,\bar{w}$ ]	(9) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ]	
			(10) $\bar{y},\bar{x},z+1/2$ [v,u, $\bar{w}$ ]	(11) $\bar{x}+y,y,z+1/2$ [u-v, $\bar{v},\bar{w}$ ]	(12) x,x-y,z+1/2 [ $\bar{u},\bar{u}+v,\bar{w}$ ]	
6	f	.2'	x,0,1/4 [u,2u,w]	0,x,1/4 [2 $\bar{u}$ , $\bar{u}$ ,w]	$\bar{x},\bar{x}$ ,1/4 [u, $\bar{u}$ ,w]	
			$\bar{x}$ ,0,3/4 [ $\bar{u}$ ,2 $\bar{u}$ , $\bar{w}$ ]	0, $\bar{x}$ ,3/4 [2u,u, $\bar{w}$ ]	x,x,3/4 [ $\bar{u}$ ,u, $\bar{w}$ ]	
6	e	$\bar{1}'$	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
			0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
4	d	3..	1/3,2/3,z [0,0,w]	2/3,1/3, $\bar{z}+1/2$ [0,0,w]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	1/3,2/3,z+1/2 [0,0, $\bar{w}$ ]
4	c	3..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]
2	b	$\bar{3}'$ ..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
2	a	32'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p6mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a\*</sub> 211  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

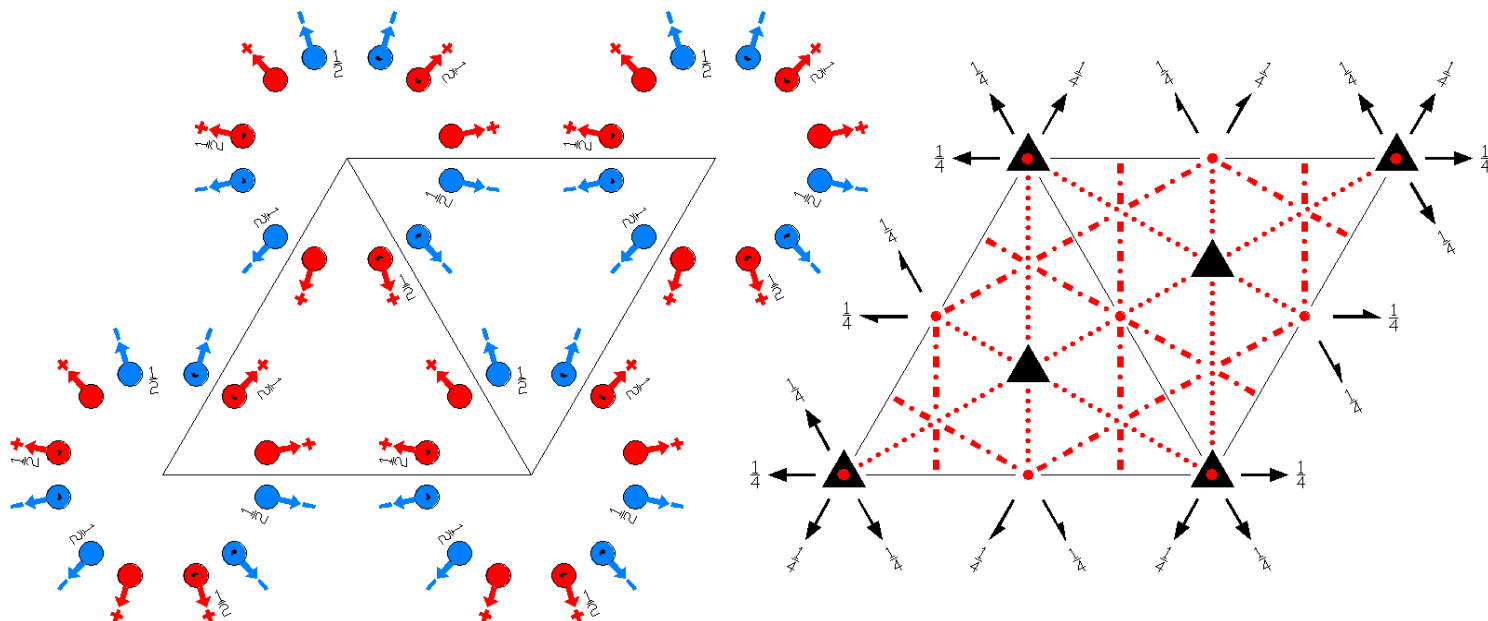
Along [2,1,0] p2mg  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P\bar{3}'c'1$   
165.4.1325

$\bar{3}'m'1$   
 $P\bar{3}'2/c'1$

Trigonal



Origin on center ( $\bar{3}'$ ) at  $\bar{3}'c'1$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

### Symmetry Operations

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)   | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                     | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                     |
| (4) 2 x,x,1/4<br>( $2_{xy}$  0,0,1/2)                        | (5) 2 x,0,1/4<br>( $2_x$  0,0,1/2)                     | (6) 2 0,y,1/4<br>( $2_y$  0,0,1/2)                          |
| (7) $\bar{1}'$<br>( $\bar{1}$  0,0,0)'                       | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)' | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)' |
| (10) $c'$ (0,0,1/2) x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,1/2)' | (11) $c'$ (0,0,1/2) x,2x,z<br>( $m_x$  0,0,1/2)'       | (12) $c'$ (0,0,1/2) 2x,x,z<br>( $m_y$  0,0,1/2)'            |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

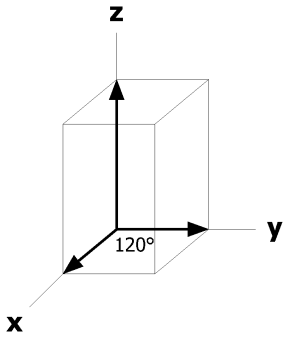
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates				
12	g	1	(1) x,y,z [u,v,w] (4) y,x, $\bar{z}+1/2$ [v,u, $\bar{w}$ ] (7) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (10) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) x-y, $\bar{y},\bar{z}+1/2$ [u-v, $\bar{v},\bar{w}$ ] (8) y, $\bar{x}+y,\bar{z}$ [v, $\bar{u}+v,\bar{w}$ ] (11) $\bar{x}+y,y,z+1/2$ [ $\bar{u}+v,v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x},\bar{x}+y,\bar{z}+1/2$ [ $\bar{u},\bar{u}+v,\bar{w}$ ] (9) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ] (12) x,x-y,z+1/2 [u,u-v,w]		
6	f	.2.	x,0,1/4 [u,0,0] $\bar{x},0,3/4$ [ $\bar{u},0,0$ ]	0,x,1/4 [0,u,0] 0, $\bar{x},3/4$ [0, $\bar{u},0$ ]	$\bar{x},\bar{x},1/4$ [ $\bar{u},\bar{u},0$ ] x,x,3/4 [u,u,0]		
6	e	$\bar{1}'$	1/2,0,0 [0,0,0] 0,1/2,1/2 [0,0,0]	0,1/2,0 [0,0,0] 1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]		
4	d	3..	1/3,2/3,z [0,0,w]	2/3,1/3, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	1/3,2/3,z+1/2 [0,0,w]	
4	c	3..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]	
2	b	$\bar{3}'..$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]			
2	a	32.	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p6m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

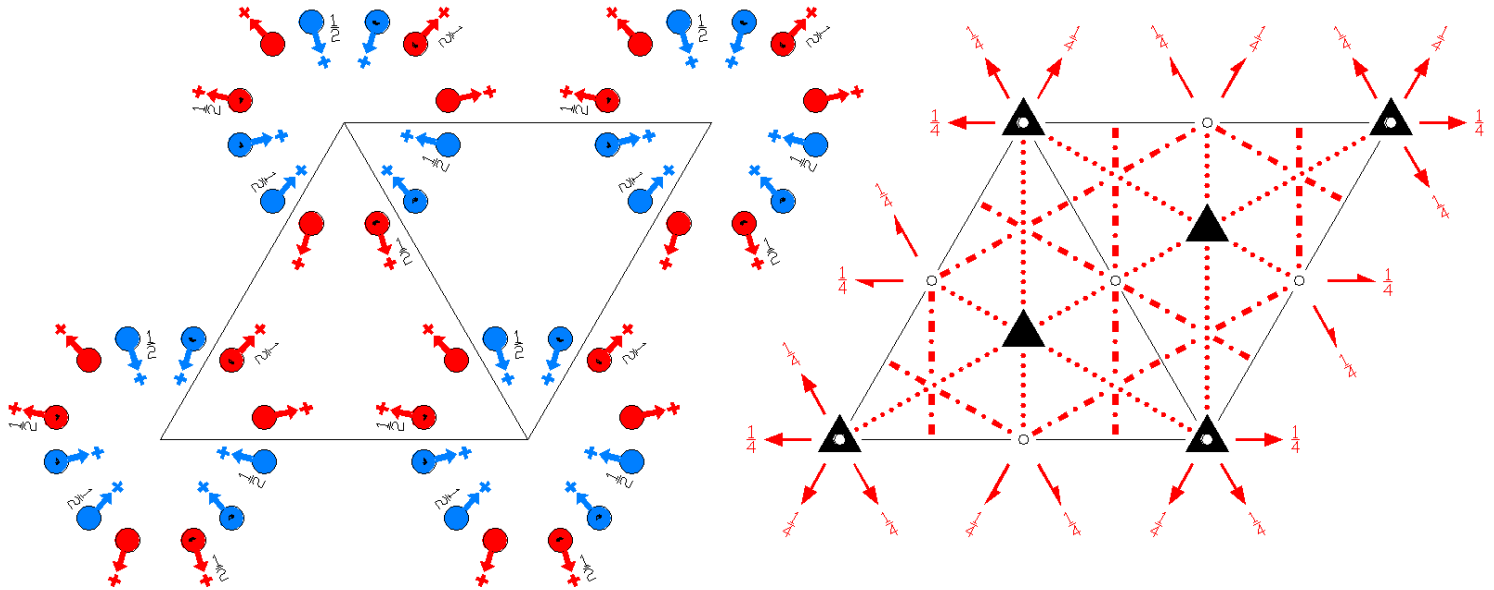
Along [2,1,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P\bar{3}c'1$   
165.5.1326

$\bar{3}m'1$   
 $P\bar{3}2'/c'1$

Trigonal



Origin on center ( $\bar{3}$ ) at  $\bar{3}c'1$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

### Symmetry Operations

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) $2'$ x,x,1/4<br>( $2_{xy}$  0,0,1/2)'                    | (5) $2'$ x,0,1/4<br>( $2_x$  0,0,1/2)'                | (6) $2'$ 0,y,1/4<br>( $2_y$  0,0,1/2)'                     |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)                         | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) $c'$ (0,0,1/2) x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,1/2)' | (11) $c'$ (0,0,1/2) x,2x,z<br>( $m_x$  0,0,1/2)'      | (12) $c'$ (0,0,1/2) 2x,x,z<br>( $m_y$  0,0,1/2)'           |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
12	g	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]	
			(4) y,x, $\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(5) x-y, $\bar{y},\bar{z}+1/2$ [ $\bar{u}+v,v,w$ ]	(6) $\bar{x},\bar{x}+y,\bar{z}+1/2$ [u,u-v,w]	
			(7) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(8) y, $\bar{x}+y,\bar{z}$ [ $\bar{v},u-v,w$ ]	(9) x-y,x, $\bar{z}$ [ $\bar{u}+v,\bar{u},w$ ]	
			(10) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(11) $\bar{x}+y,y,z+1/2$ [ $\bar{u}+v,v,w$ ]	(12) x,x-y,z+1/2 [u,u-v,w]	
6	f	.2'	x,0,1/4 [u,2u,w]	0,x,1/4 [2 $\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},1/4$ [u, $\bar{u},w$ ]	
			$\bar{x},0,3/4$ [u,2u,w]	0, $\bar{x},3/4$ [2 $\bar{u},\bar{u},w$ ]	x,x,3/4 [u, $\bar{u},w$ ]	
6	e	$\bar{1}$	1/2,0,0 [u,v,w]	0,1/2,0 [ $\bar{v},u-v,w$ ]	1/2,1/2,0 [ $\bar{u}+v,\bar{u},w$ ]	
			0,1/2,1/2 [ $\bar{v},\bar{u},w$ ]	1/2,0,1/2 [ $\bar{u}+v,v,w$ ]	1/2,1/2,1/2 [u,u-v,w]	
4	d	3..	1/3,2/3,z [0,0,w]	2/3,1/3, $\bar{z}+1/2$ [0,0,w]	2/3,1/3, $\bar{z}$ [0,0,w]	1/3,2/3,z+1/2 [0,0,w]
4	c	3..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0,w]
2	b	$\bar{3}$ ..	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]		
2	a	32'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		

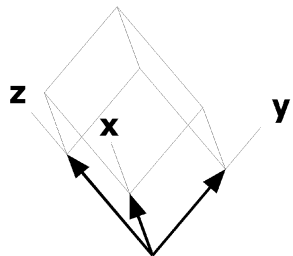
**Symmetry of Special Projections**

Along [0,0,1] p6'm'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'11  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2'mg'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0

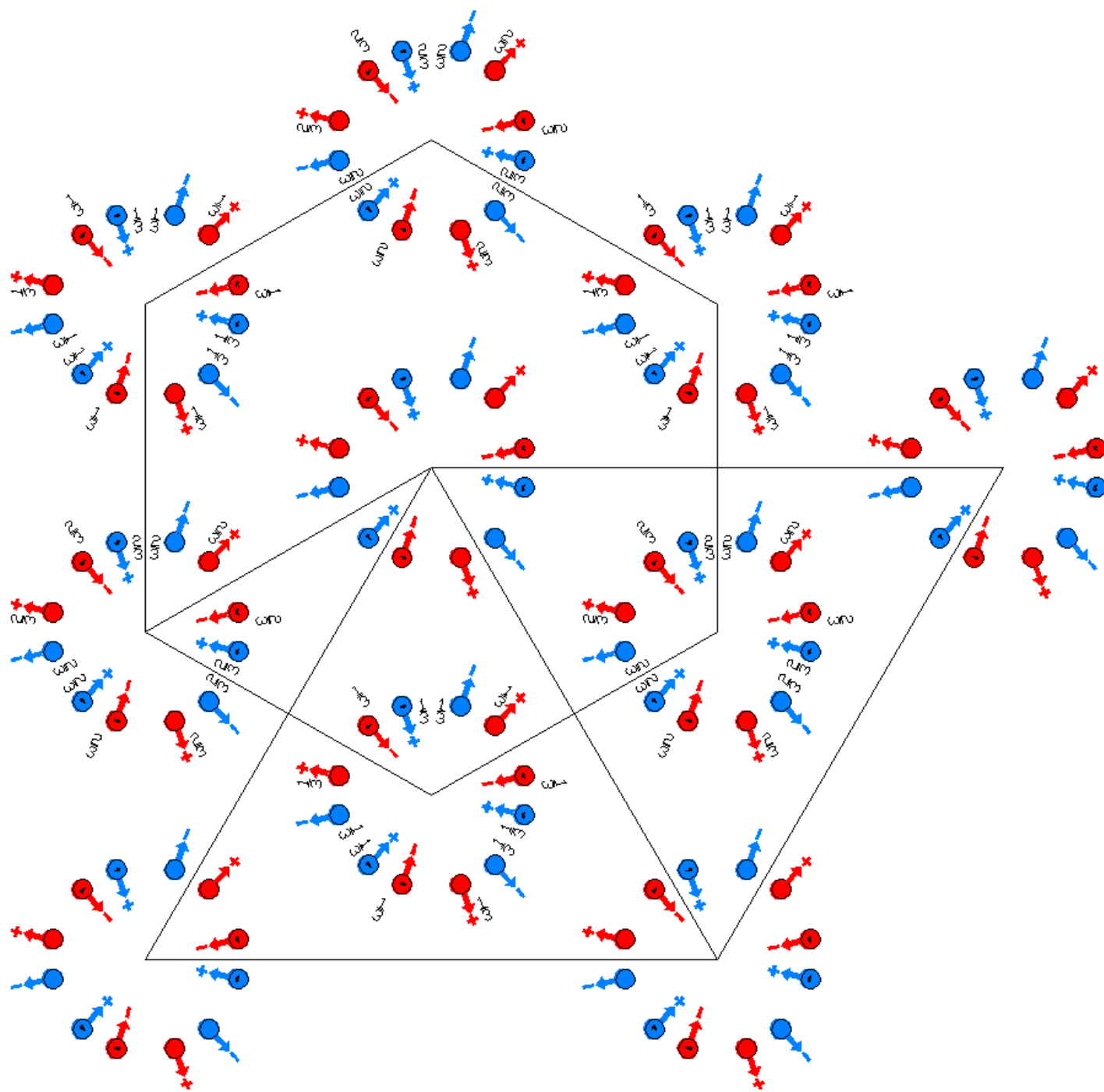


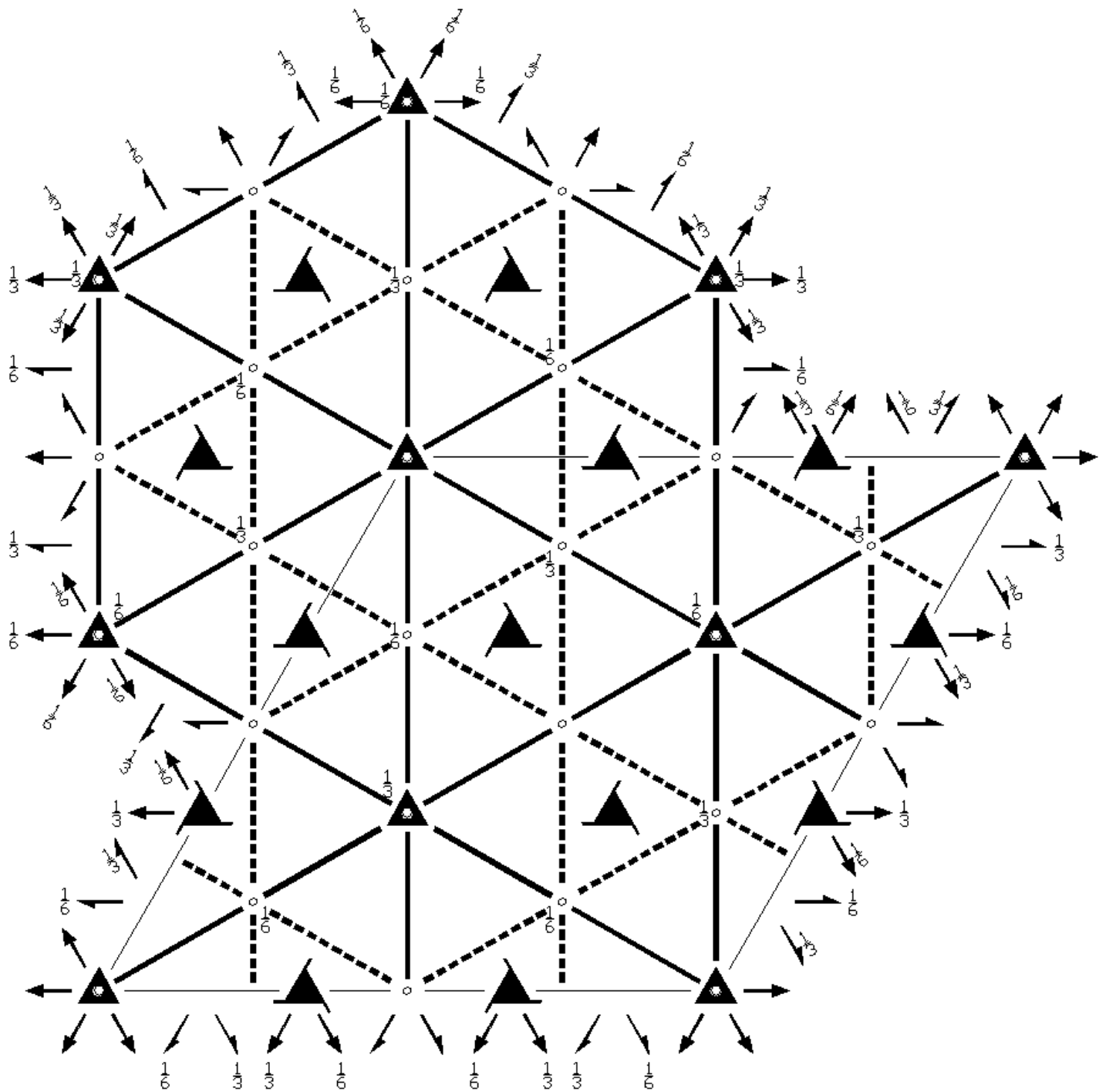


$R\bar{3}m$   
166.1.1327

$\bar{3}m$   
 $R\bar{3}2/m$

Trigonal





Origin on center ( $\bar{3}m$ )

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $0 \leq z \leq 1/6$ ;  $x \leq y/2$ ;  $y \leq \min(1-x, 2x)$

Vertices	0,0,0	2/3,1/3,0	1/3,2/3,0
	0,0,1/6	2/3,1/3,1/6	1/3,2/3,1/6

**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)     | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)            | (5) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                  | (6) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                            |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)               | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z^+$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^-$  0,0,0)           |
| (10) m x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0) | (11) m x,2x,z<br>(m <sub>x</sub>  0,0,0)                | (12) m 2x,x,z<br>(m <sub>y</sub>  0,0,0)                          |

For (2/3,1/3,1/3) + set

- |   |   |   |
|---|---|---|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)                                      | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3)   | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3) |
| (4) 2 (1/2,1/2,0) x,x-1/6,1/6<br>(2 <sub>xy</sub>  2/3,1/3,1/3)             | (5) 2 (1/2,0,0) x,1/6,1/6<br>(2 <sub>x</sub>  2/3,1/3,1/3)                | (6) 2 1/3,y,1/6<br>(2 <sub>y</sub>  2/3,1/3,1/3)                                    |
| (7) $\bar{1}$ 1/3,1/6,1/6<br>( $\bar{1}$  2/3,1/3,1/3)                      | (8) $\bar{3}^+$ 1/3,-1/3,z; 1/3,-1/3,1/6<br>( $\bar{3}_z^+$  2/3,1/3,1/3) | (9) $\bar{3}^-$ 1/3,2/3,z; 1/3,2/3,1/6<br>( $\bar{3}_z^-$  2/3,1/3,1/3)             |
| (10) g (1/6,-1/6,1/3) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  2/3,1/3,1/3) | (11) g (1/6,1/3,1/3) x,2x-1/2,z<br>(m <sub>x</sub>  2/3,1/3,1/3)          | (12) g (2/3,1/3,1/3) 2x,x,z<br>(m <sub>y</sub>  2/3,1/3,1/3)                        |

For (1/3,2/3,2/3) + set

- |   |   |   |
|---|---|---|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)                                      | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3)   | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3) |
| (4) 2 (1/2,1/2,0) x,x+1/6,1/3<br>(2 <sub>xy</sub>  1/3,2/3,2/3)             | (5) 2 x,1/3,1/3<br>(2 <sub>x</sub>  1/3,2/3,2/3)                        | (6) 2 (0,1/2,0) 1/6,y,1/3<br>(2 <sub>y</sub>  1/3,2/3,2/3)                            |
| (4) $\bar{1}$ 1/6,1/3,1/3<br>( $\bar{1}$  1/3,2/3,2/3)                      | (5) $\bar{3}^+$ 2/3,1/3,z; 2/3,1/3,1/3<br>( $\bar{3}_z^+$  1/3,2/3,2/3) | (6) $\bar{3}^-$ -1/3,1/3,z; -1/3,1/3,1/3<br>( $\bar{3}_z^-$  1/3,2/3,2/3)             |
| (10) g (-1/6,1/6,2/3) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/3,2/3,2/3) | (11) g (1/3,2/3,2/3) x,2x,z<br>(m <sub>x</sub>  1/3,2/3,2/3)            | (12) g (1/3,1/6,2/3) 2x-1/2,x,z<br>(m <sub>y</sub>  1/3,2/3,2/3)                      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4); (7).**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (2/3,1/3,1/3) + (1/3,2/3,2/3) +

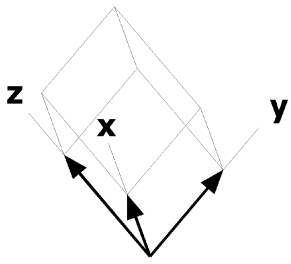
36	i	1	(1) $x,y,z [u,v,w]$ (4) $y,x,\bar{z} [v,u,\bar{w}]$ (7) $\bar{x},\bar{y},\bar{z} [u,v,w]$ (10) $\bar{y},\bar{x},z [v,u,\bar{w}]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$ (5) $x-y,\bar{y},\bar{z} [u-v,\bar{v},\bar{w}]$ (8) $y,\bar{x}+y,\bar{z} [\bar{v},u-v,w]$ (11) $\bar{x}+y,y,z [u-v,\bar{v},\bar{w}]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$ (6) $\bar{x},\bar{x}+y,\bar{z} [\bar{u},\bar{u}+v,\bar{w}]$ (9) $x-y,x,\bar{z} [\bar{u}+v,\bar{u},w]$ (12) $x,x-y,z [\bar{u},\bar{u}+v,\bar{w}]$
18	h	.m	$x,\bar{x},z [u,u,0]$ $\bar{x},x,\bar{z} [u,u,0]$	$x,2x,z [\bar{u},0,0]$ $2x,x,\bar{z} [0,\bar{u},0]$	$2\bar{x},\bar{x},z [0,\bar{u},0]$ $\bar{x},2\bar{x},\bar{z} [\bar{u},0,0]$
18	g	.2	$x,0,1/2 [u,0,0]$ $\bar{x},0,1/2 [u,0,0]$	$0,x,1/2 [0,u,0]$ $0,\bar{x},1/2 [0,u,0]$	$\bar{x},\bar{x},1/2 [\bar{u},\bar{u},0]$ $x,x,1/2 [\bar{u},\bar{u},0]$
18	f	.2	$x,0,0 [u,0,0]$ $\bar{x},0,0 [u,0,0]$	$0,x,0 [0,u,0]$ $0,\bar{x},0 [0,u,0]$	$\bar{x},\bar{x},0 [\bar{u},\bar{u},0]$ $x,x,0 [\bar{u},\bar{u},0]$
9	e	.2/m	$1/2,0,0 [u,0,0]$	$0,1/2,0 [0,u,0]$	$1/2,1/2,0 [\bar{u},\bar{u},0]$
9	d	.2/m	$1/2,0,1/2 [u,0,0]$	$0,1/2,1/2 [0,u,0]$	$1/2,1/2,1/2 [\bar{u},\bar{u},0]$
6	c	3m	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$	
3	b	$\bar{3}m$	$0,0,1/2 [0,0,0]$		
3	a	$\bar{3}m$	$0,0,0 [0,0,0]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p6'mm'$   
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2111'$   
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

Along  $[2,1,0]$   $p2'mm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/3$   
 Origin at  $x,x/2,0$



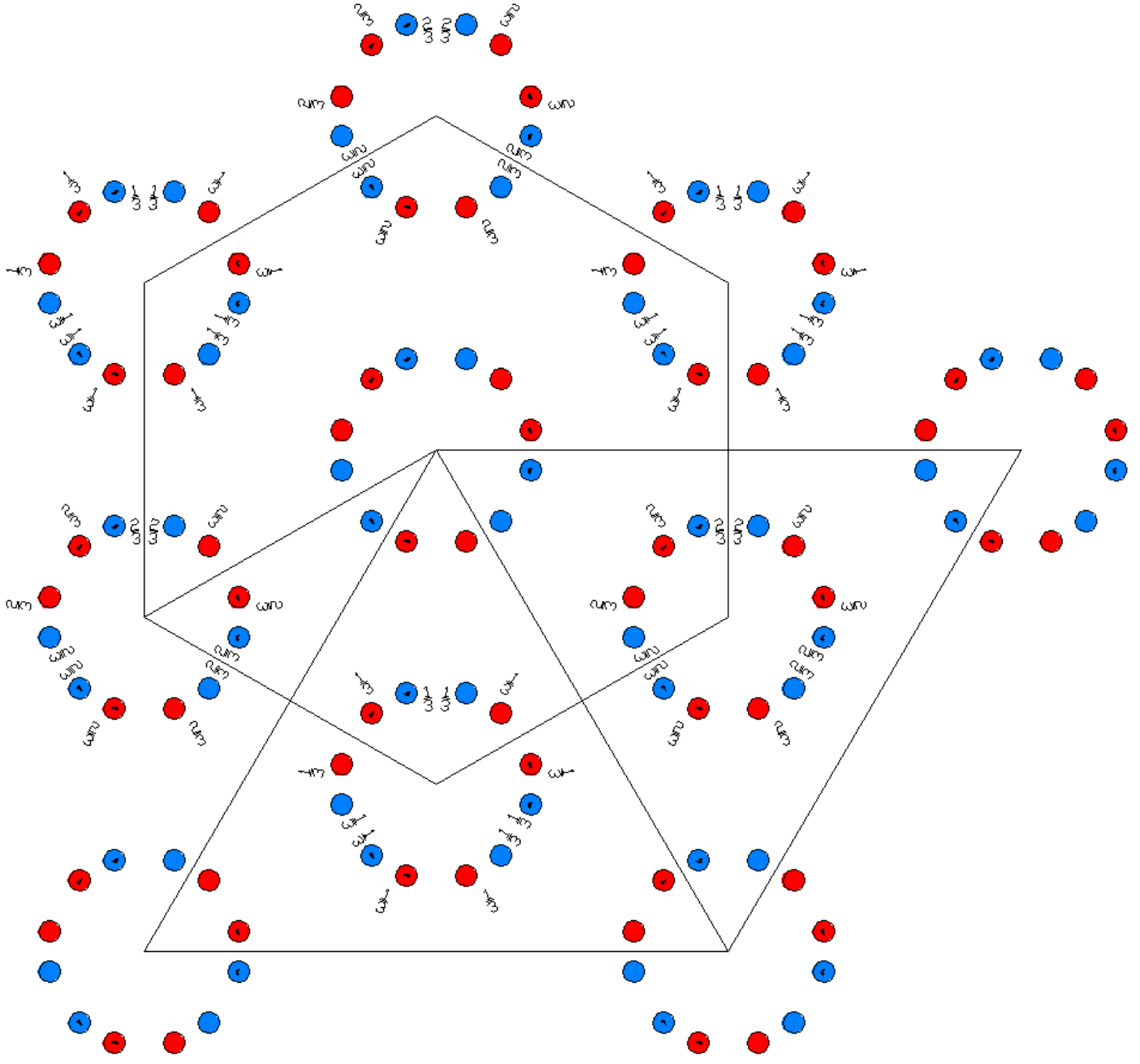
$R\bar{3}m1'$

166.2.1328

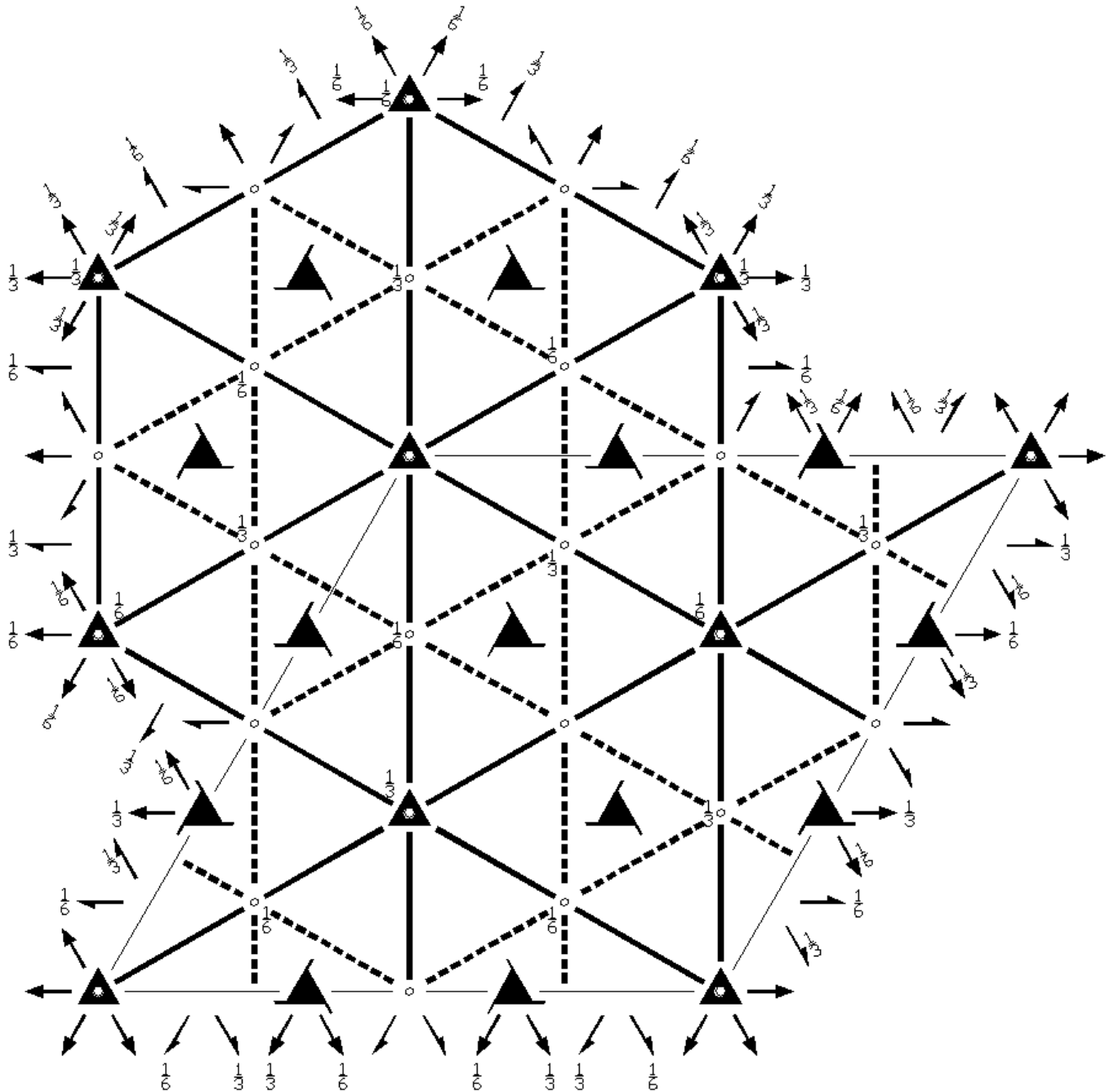
$\bar{3}m1'$

$R\bar{3}2/m1'$

Trigonal



1'



**Origin** on center ( $\bar{3}m1'$ )

**Asymmetric unit**  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $0 \leq z \leq 1/6$ ;  $x \leq y/2$ ;  $y \leq \min(1-x, 2x)$

**Vertices**  $0,0,0$   $2/3,1/3,0$   $1/3,2/3,0$   
 $0,0,1/6$   $2/3,1/3,1/6$   $1/3,2/3,1/6$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)     | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)            | (5) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                  | (6) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                            |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)               | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z^+$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^-$  0,0,0)           |
| (10) m x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0) | (11) m x,2x,z<br>(m <sub>x</sub>  0,0,0)                | (12) m 2x,x,z<br>(m <sub>y</sub>  0,0,0)                          |

For (2/3,1/3,1/3) + set

- |   |   |   |
|---|---|---|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)                                      | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3)   | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3) |
| (4) 2 (1/2,1/2,0) x,x-1/6,1/6<br>(2 <sub>xy</sub>  2/3,1/3,1/3)             | (5) 2 (1/2,0,0) x,1/6,1/6<br>(2 <sub>x</sub>  2/3,1/3,1/3)                | (6) 2 1/3,y,1/6<br>(2 <sub>y</sub>  2/3,1/3,1/3)                                    |
| (7) $\bar{1}$ 1/3,1/6,1/6<br>( $\bar{1}$  2/3,1/3,1/3)                      | (8) $\bar{3}^+$ 1/3,-1/3,z; 1/3,-1/3,1/6<br>( $\bar{3}_z^+$  2/3,1/3,1/3) | (9) $\bar{3}^-$ 1/3,2/3,z; 1/3,2/3,1/6<br>( $\bar{3}_z^-$  2/3,1/3,1/3)             |
| (10) g (1/6,-1/6,1/3) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  2/3,1/3,1/3) | (11) g (1/6,1/3,1/3) x,2x-1/2,z<br>(m <sub>x</sub>  2/3,1/3,1/3)          | (12) g (2/3,1/3,1/3) 2x,x,z<br>(m <sub>y</sub>  2/3,1/3,1/3)                        |

For (1/3,2/3,2/3) + set

- |   |   |   |
|---|---|---|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)                                      | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3)   | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3) |
| (4) 2 (1/2,1/2,0) x,x+1/6,1/3<br>(2 <sub>xy</sub>  1/3,2/3,2/3)             | (5) 2 x,1/3,1/3<br>(2 <sub>x</sub>  1/3,2/3,2/3)                        | (6) 2 (0,1/2,0) 1/6,y,1/3<br>(2 <sub>y</sub>  1/3,2/3,2/3)                            |
| (4) $\bar{1}$ 1/6,1/3,1/3<br>( $\bar{1}$  1/3,2/3,2/3)                      | (5) $\bar{3}^+$ 2/3,1/3,z; 2/3,1/3,1/3<br>( $\bar{3}_z^+$  1/3,2/3,2/3) | (6) $\bar{3}^-$ -1/3,1/3,z; -1/3,1/3,1/3<br>( $\bar{3}_z^-$  1/3,2/3,2/3)             |
| (10) g (-1/6,1/6,2/3) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/3,2/3,2/3) | (11) g (1/3,2/3,2/3) x,2x,z<br>(m <sub>x</sub>  1/3,2/3,2/3)            | (12) g (1/3,1/6,2/3) 2x-1/2,x,z<br>(m <sub>y</sub>  1/3,2/3,2/3)                      |

For (0,0,0)' + set

- |  |  |  |
|--|--|--|
| (1) 1'<br>(1 0,0,0)'                                 | (2) 3 <sup>+</sup> ' 0,0,z<br>(3 <sub>z</sub>  0,0,0)'     | (3) 3 <sup>-</sup> ' 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (4) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'            | (5) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                   | (6) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                             |
| (7) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)'              | (8) $\bar{3}^+$ ' 0,0,z; 0,0,0<br>( $\bar{3}_z^+$  0,0,0)' | (9) $\bar{3}^-$ ' 0,0,z; 0,0,0<br>( $\bar{3}_z^-$  0,0,0)'           |
| (10) m' x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)' | (11) m' x,2x,z<br>(m <sub>x</sub>  0,0,0)'                 | (12) m' 2x,x,z<br>(m <sub>y</sub>  0,0,0)'                           |

## For (2/3,1/3,1/3)' + set

- |   |  |   |
|---|--|---|
| (1) $t' (2/3, 1/3, 1/3)$<br>(1   2/3, 1/3, 1/3)'                                      | (2) $3^{+'} (0, 0, 1/3)$ 1/3, 1/3, z<br>(3 <sub>z</sub>   2/3, 1/3, 1/3)'            | (3) $3^{-'} (0, 0, 1/3)$ 1/3, 0, z<br>(3 <sub>z</sub> <sup>-1</sup>   2/3, 1/3, 1/3)'   |
| (4) $2' (1/2, 1/2, 0)$ x, x-1/6, 1/6<br>(2 <sub>xy</sub>   2/3, 1/3, 1/3)'            | (5) $2' (1/2, 0, 0)$ x, 1/6, 1/6<br>(2 <sub>x</sub>   2/3, 1/3, 1/3)'                | (6) $2' (1/3, y, 1/6)$<br>(2 <sub>y</sub>   2/3, 1/3, 1/3)'                             |
| (7) $\bar{1}' (1/3, 1/6, 1/6)$<br>( $\bar{1}$   2/3, 1/3, 1/3)'                       | (8) $\bar{3}^{+'} (1/3, -1/3, z; 1/3, -1/3, 1/6)$<br>( $\bar{3}_z$   2/3, 1/3, 1/3)' | (9) $\bar{3}^{-'} (1/3, 2/3, z; 1/3, 2/3, 1/6)$<br>( $\bar{3}_z^{-1}$   2/3, 1/3, 1/3)' |
| (10) $g' (1/6, -1/6, 1/3)$ x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>   2/3, 1/3, 1/3)' | (11) $g' (1/6, 1/3, 1/3)$ x, 2x-1/2, z<br>(m <sub>x</sub>   2/3, 1/3, 1/3)'          | (12) $g' (2/3, 1/3, 1/3)$ 2x, x, z<br>(m <sub>y</sub>   2/3, 1/3, 1/3)'                 |

## For (1/3,2/3,2/3)' + set

- |   |  |   |
|---|--|---|
| (1) $t' (1/3, 2/3, 2/3)$<br>(1   1/3, 2/3, 2/3)'                                      | (2) $3^{+'} (0, 0, 2/3)$ 0, 1/3, z<br>(3 <sub>z</sub>   1/3, 2/3, 2/3)'            | (3) $3^{-'} (0, 0, 2/3)$ 1/3, 1/3, z<br>(3 <sub>z</sub> <sup>-1</sup>   1/3, 2/3, 2/3)'   |
| (4) $2' (1/2, 1/2, 0)$ x, x+1/6, 1/3<br>(2 <sub>xy</sub>   1/3, 2/3, 2/3)'            | (5) $2' (x, 1/3, 1/3)$<br>(2 <sub>x</sub>   1/3, 2/3, 2/3)'                        | (6) $2' (0, 1/2, 0)$ 1/6, y, 1/3<br>(2 <sub>y</sub>   1/3, 2/3, 2/3)'                     |
| (4) $\bar{1}' (1/6, 1/3, 1/3)$<br>( $\bar{1}$   1/3, 2/3, 2/3)'                       | (5) $\bar{3}^{+'} (2/3, 1/3, z; 2/3, 1/3, 1/3)$<br>( $\bar{3}_z$   1/3, 2/3, 2/3)' | (6) $\bar{3}^{-'} (-1/3, 1/3, z; -1/3, 1/3, 1/3)$<br>( $\bar{3}_z^{-1}$   1/3, 2/3, 2/3)' |
| (10) $g' (-1/6, 1/6, 2/3)$ x+1/2, $\bar{x}$ , z<br>(m <sub>xy</sub>   1/3, 2/3, 2/3)' | (11) $g' (1/3, 2/3, 2/3)$ x, 2x, z<br>(m <sub>x</sub>   1/3, 2/3, 2/3)'            | (12) $g' (1/3, 1/6, 2/3)$ 2x-1/2, x, z<br>(m <sub>y</sub>   1/3, 2/3, 2/3)'               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4); (7); 1'.

**Positions**

			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.					
			(0,0,0) + (0,0,0)'	(2/3,1/3,1/3) + (2/3,1/3,1/3)'	(1/3,2/3,2/3) + (1/3,2/3,2/3)'
36	i	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ , x-y, z [0,0,0]	(3) $\bar{x}+y$ , $\bar{x}$ , z [0,0,0]
			(4) y, x, $\bar{z}$ [0,0,0]	(5) x-y, $\bar{y}$ , $\bar{z}$ [0,0,0]	(6) $\bar{x}$ , $\bar{x}+y$ , $\bar{z}$ [0,0,0]
			(7) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [0,0,0]	(8) y, $\bar{x}+y$ , $\bar{z}$ [0,0,0]	(9) x-y, x, $\bar{z}$ [0,0,0]
			(10) $\bar{y}$ , $\bar{x}$ , z [0,0,0]	(11) $\bar{x}+y$ , y, z [0,0,0]	(12) x, x-y, z [0,0,0]
18	h	.m1'	x, $\bar{x}$ , z [0,0,0]	x, 2x, z [0,0,0]	2 $\bar{x}$ , $\bar{x}$ , z [0,0,0]
			$\bar{x}$ , x, $\bar{z}$ [0,0,0]	2x, x, $\bar{z}$ [0,0,0]	$\bar{x}$ , 2 $\bar{x}$ , $\bar{z}$ [0,0,0]
18	g	.21'	x, 0, 1/2 [0,0,0]	0, x, 1/2 [0,0,0]	$\bar{x}$ , $\bar{x}$ , 1/2 [0,0,0]
			$\bar{x}$ , 0, 1/2 [0,0,0]	0, $\bar{x}$ , 1/2 [0,0,0]	x, x, 1/2 [0,0,0]



Continued

166.2.1328

 $R\bar{3}m1'$ 

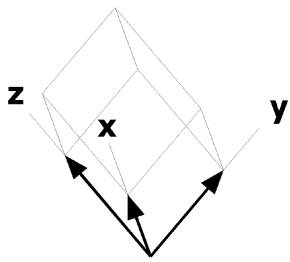
18	f	.21'	x,0,0 [0,0,0]	0,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]
			$\bar{x},0,0$ [0,0,0]	$0,\bar{x},0$ [0,0,0]	x,x,0 [0,0,0]
9	e	.2/m1'	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]
9	d	.2/m1'	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]
6	c	3m1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	
3	b	$\bar{3}m1'$	0,0,1/2 [0,0,0]		
3	a	$\bar{3}m1'$	0,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at 0,0,z

Along [1,0,0] p2111'  
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

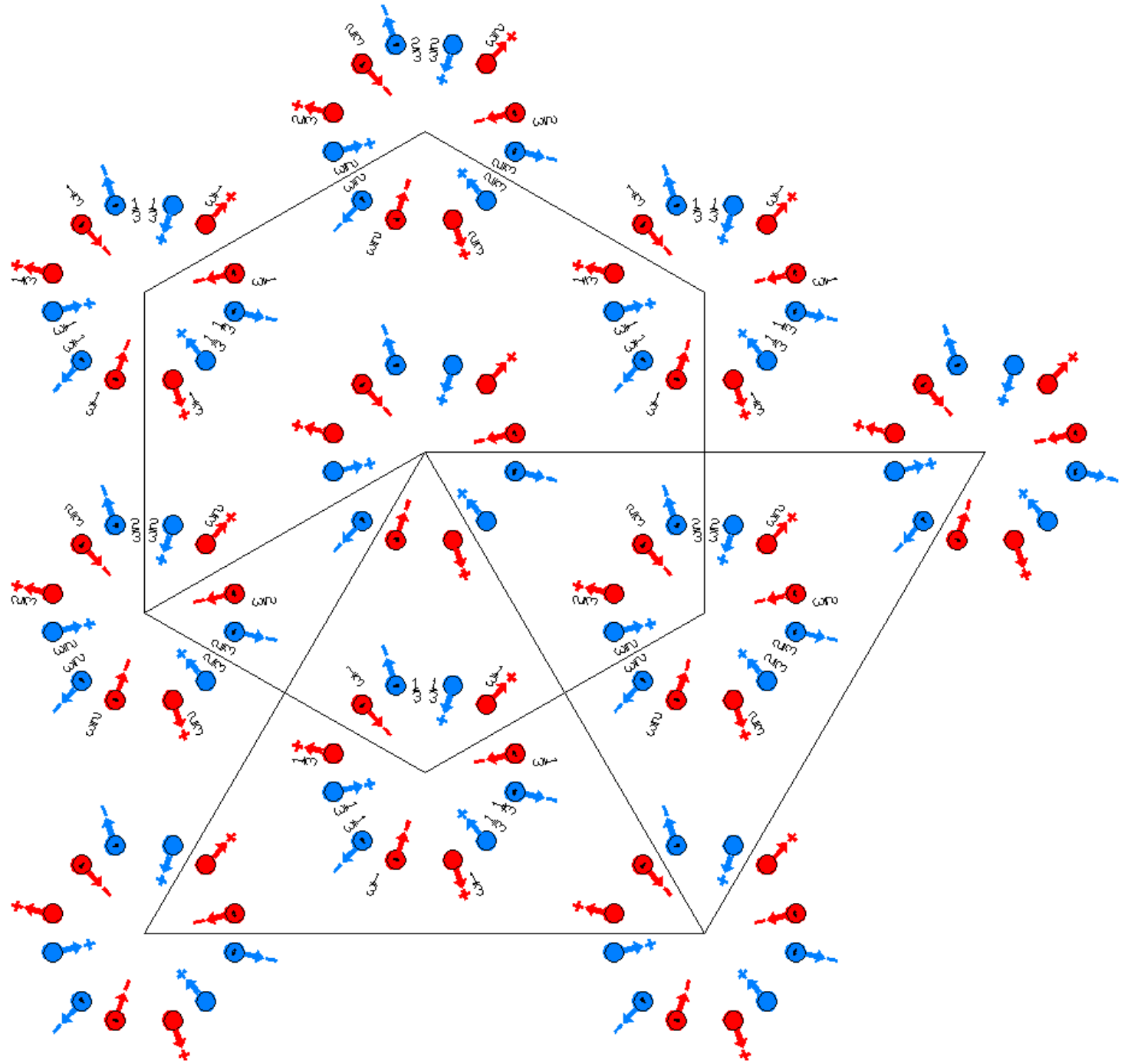
Along [2,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/3$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0

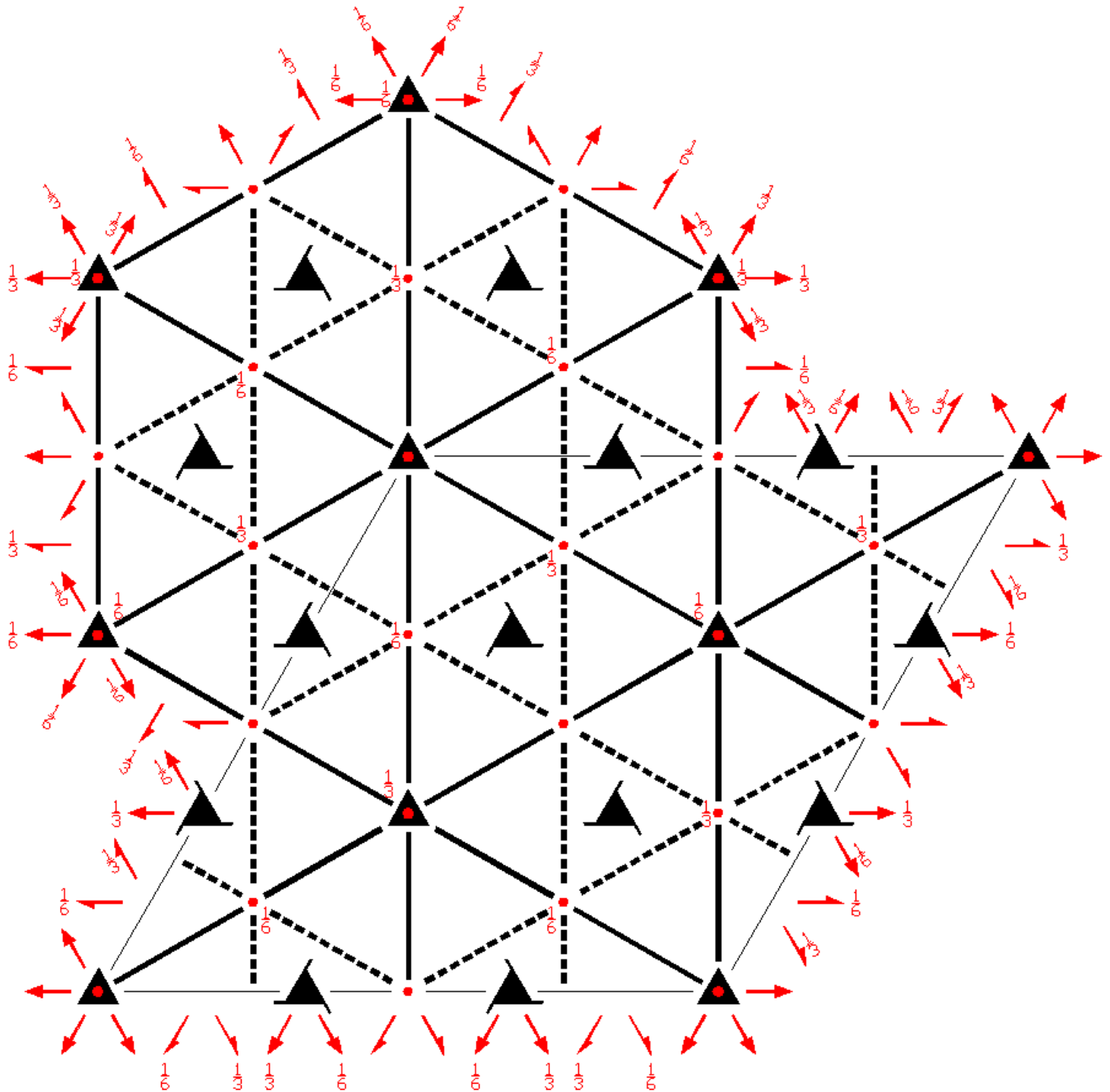


$R\bar{3}m$   
166.3.1329

$\bar{3}m$   
 $R\bar{3}2/m$

Trigonal





Origin on center ( $\bar{3}m$ )

**Asymmetric unit**  $0 \leq x \leq 2/3;$   $0 \leq y \leq 2/3;$   $0 \leq z \leq 1/6;$   $x \leq y/2;$   $y \leq \min(1-x, 2x)$

Vertices	0,0,0	$2/3, 1/3, 0$	$1/3, 2/3, 0$
	0,0,1/6	$2/3, 1/3, 1/6$	$1/3, 2/3, 1/6$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |
|--|--|--|
| (1) 1<br>(1 0,0,0)                                 | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)                            | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)                            |
| (4) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'          | (5) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                                       | (6) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'   |
| (7) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)'            | (8) $\bar{3}$ <sup>+</sup> ' 0,0,z; 0,0,0<br>( $\bar{3}$ <sub>z</sub>  0,0,0)' | (9) $\bar{3}$ <sup>-</sup> ' 0,0,z; 0,0,0<br>( $\bar{3}$ <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (10) m x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0) | (11) m x,2x,z<br>(m <sub>x</sub>  0,0,0)                                       | (12) m 2x,x,z<br>(m <sub>y</sub>  0,0,0)   |

For (2/3,1/3,1/3) + set

- |   |  |  |
|---|--|--|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)                                      | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3)                          | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3)                          |
| (4) 2' (1/2,1/2,0) x,x-1/6,1/6<br>(2 <sub>xy</sub>  2/3,1/3,1/3)'           | (5) 2' (1/2,0,0) x,1/6,1/6<br>(2 <sub>x</sub>  2/3,1/3,1/3)'                                     | (6) 2' 1/3,y,1/6<br>(2 <sub>y</sub>  2/3,1/3,1/3)'   |
| (7) $\bar{1}$ ' 1/3,1/6,1/6<br>( $\bar{1}$  2/3,1/3,1/3)'                   | (8) $\bar{3}$ <sup>+</sup> ' 1/3,-1/3,z; 1/3,-1/3,1/6<br>( $\bar{3}$ <sub>z</sub>  2/3,1/3,1/3)' | (9) $\bar{3}$ <sup>-</sup> ' 1/3,2/3,z; 1/3,2/3,1/6<br>( $\bar{3}$ <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3)' |
| (10) g (1/6,-1/6,1/3) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  2/3,1/3,1/3) | (11) g (1/6,1/3,1/3) x,2x-1/2,z<br>(m <sub>x</sub>  2/3,1/3,1/3)                                 | (12) g (2/3,1/3,1/3) 2x,x,z<br>(m <sub>y</sub>  2/3,1/3,1/3)   |

For (1/3,2/3,2/3) + set

- |   |  |  |
|---|--|--|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)                                      | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3)                          | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3)                          |
| (4) 2' (1/2,1/2,0) x,x+1/6,1/3<br>(2 <sub>xy</sub>  1/3,2/3,2/3)'           | (5) 2' x,1/3,1/3<br>(2 <sub>x</sub>  1/3,2/3,2/3)'   | (6) 2' (0,1/2,0) 1/6,y,1/3<br>(2 <sub>y</sub>  1/3,2/3,2/3)'   |
| (4) $\bar{1}$ ' 1/6,1/3,1/3<br>( $\bar{1}$  1/3,2/3,2/3)'                   | (5) $\bar{3}$ <sup>+</sup> ' 2/3,1/3,z; 2/3,1/3,1/3<br>( $\bar{3}$ <sub>z</sub>  1/3,2/3,2/3)' | (6) $\bar{3}$ <sup>-</sup> ' -1/3,1/3,z; -1/3,1/3,1/3<br>( $\bar{3}$ <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3)' |
| (10) g (-1/6,1/6,2/3) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/3,2/3,2/3) | (11) g (1/3,2/3,2/3) x,2x,z<br>(m <sub>x</sub>  1/3,2/3,2/3)                                   | (12) g (1/3,1/6,2/3) 2x-1/2,x,z<br>(m <sub>y</sub>  1/3,2/3,2/3)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4); (7).**Positions**Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (2/3,1/3,1/3) + (1/3,2/3,2/3) +

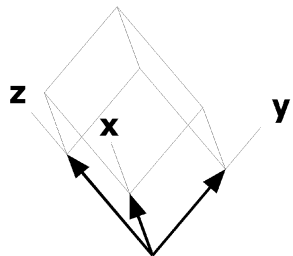
36	i	1	(1) $x,y,z$ [ $u,v,w$ ] (4) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ] (7) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (10) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $x-y,\bar{y},\bar{z}$ [ $\bar{u}+v,v,w$ ] (8) $y,\bar{x}+y,\bar{z}$ [ $v,\bar{u}+v,\bar{w}$ ] (11) $\bar{x}+y,y,z$ [ $u-v,\bar{v},\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x},\bar{x}+y,\bar{z}$ [ $u,u-v,w$ ] (9) $x-y,x,\bar{z}$ [ $u-v,u,\bar{w}$ ] (12) $x,x-y,z$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
18	h	.m	$x,\bar{x},z$ [ $u,u,0$ ] $\bar{x},x,\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$x,2x,z$ [ $\bar{u},0,0$ ] $2x,x,\bar{z}$ [ $0,u,0$ ]	$2\bar{x},\bar{x},z$ [ $0,\bar{u},0$ ] $\bar{x},2\bar{x},\bar{z}$ [ $u,0,0$ ]
18	g	.2'	$x,0,1/2$ [ $u,2u,w$ ] $\bar{x},0,1/2$ [ $\bar{u},2\bar{u},\bar{w}$ ]	$0,x,1/2$ [ $2\bar{u},\bar{u},w$ ] $0,\bar{x},1/2$ [ $2u,u,\bar{w}$ ]	$\bar{x},\bar{x},1/2$ [ $u,\bar{u},w$ ] $x,x,1/2$ [ $\bar{u},u,\bar{w}$ ]
18	f	.2'	$x,0,0$ [ $u,2u,w$ ] $\bar{x},0,0$ [ $\bar{u},2\bar{u},\bar{w}$ ]	$0,x,0$ [ $2\bar{u},\bar{u},w$ ] $0,\bar{x},0$ [ $2u,u,\bar{w}$ ]	$\bar{x},\bar{x},0$ [ $u,\bar{u},w$ ] $x,x,0$ [ $\bar{u},u,\bar{w}$ ]
9	e	.2'/m	$1/2,0,0$ [ $0,0,0$ ]	$0,1/2,0$ [ $0,0,0$ ]	$1/2,1/2,0$ [ $0,0,0$ ]
9	d	.2'/m	$1/2,0,1/2$ [ $0,0,0$ ]	$0,1/2,1/2$ [ $0,0,0$ ]	$1/2,1/2,1/2$ [ $0,0,0$ ]
6	c	3m.	$0,0,z$ [ $0,0,0$ ]	$0,0,\bar{z}$ [ $0,0,0$ ]	
3	b	$\bar{3}$ 'm	$0,0,1/2$ [ $0,0,0$ ]		
3	a	$\bar{3}$ 'm	$0,0,0$ [ $0,0,0$ ]		

### Symmetry of Special Projections

Along  $[0,0,1]$  p6mm  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p2'11  
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

Along  $[2,1,0]$  p2m'm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/3$   
 Origin at  $x,x/2,0$



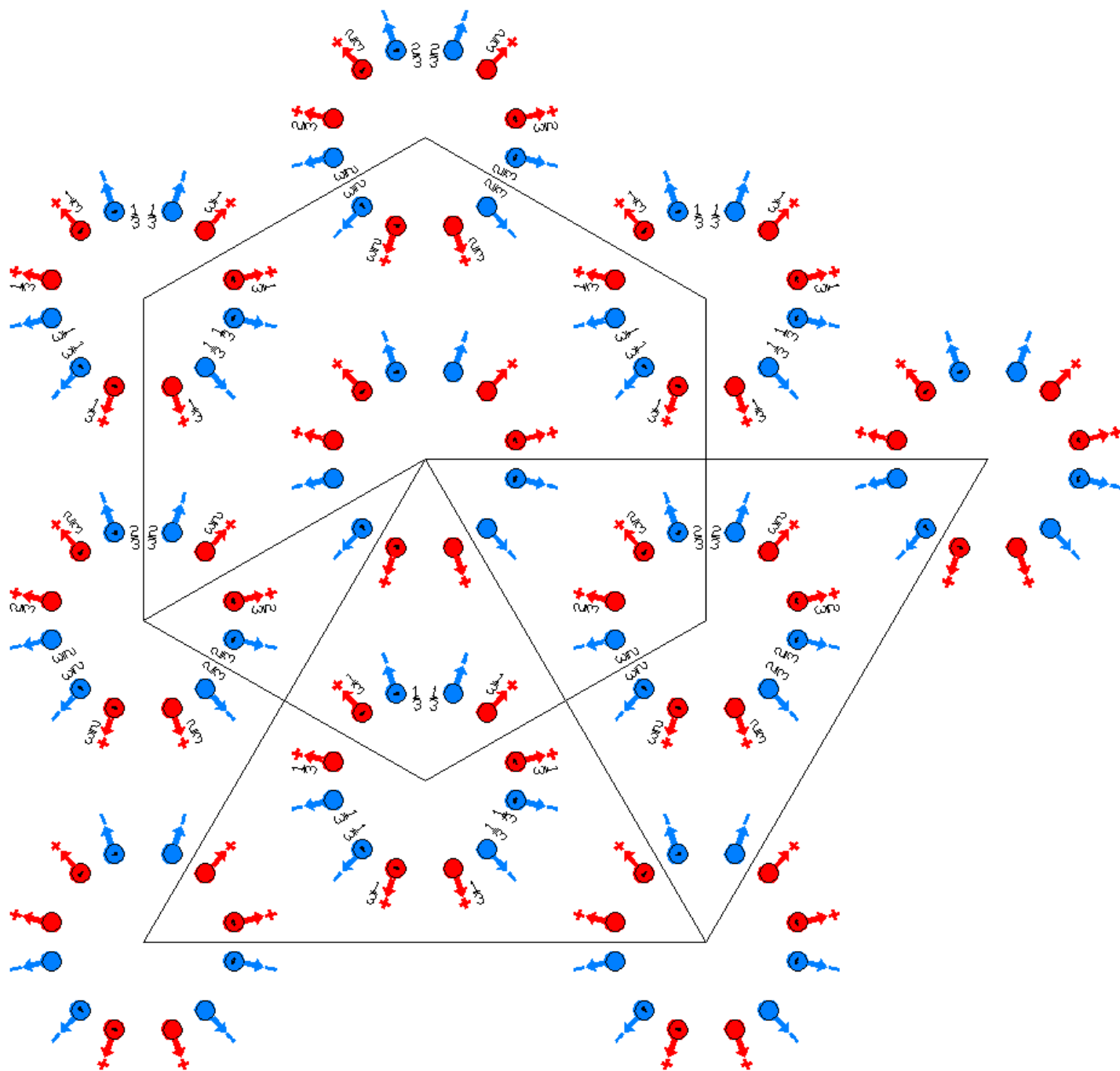
$R\bar{3}'m'$

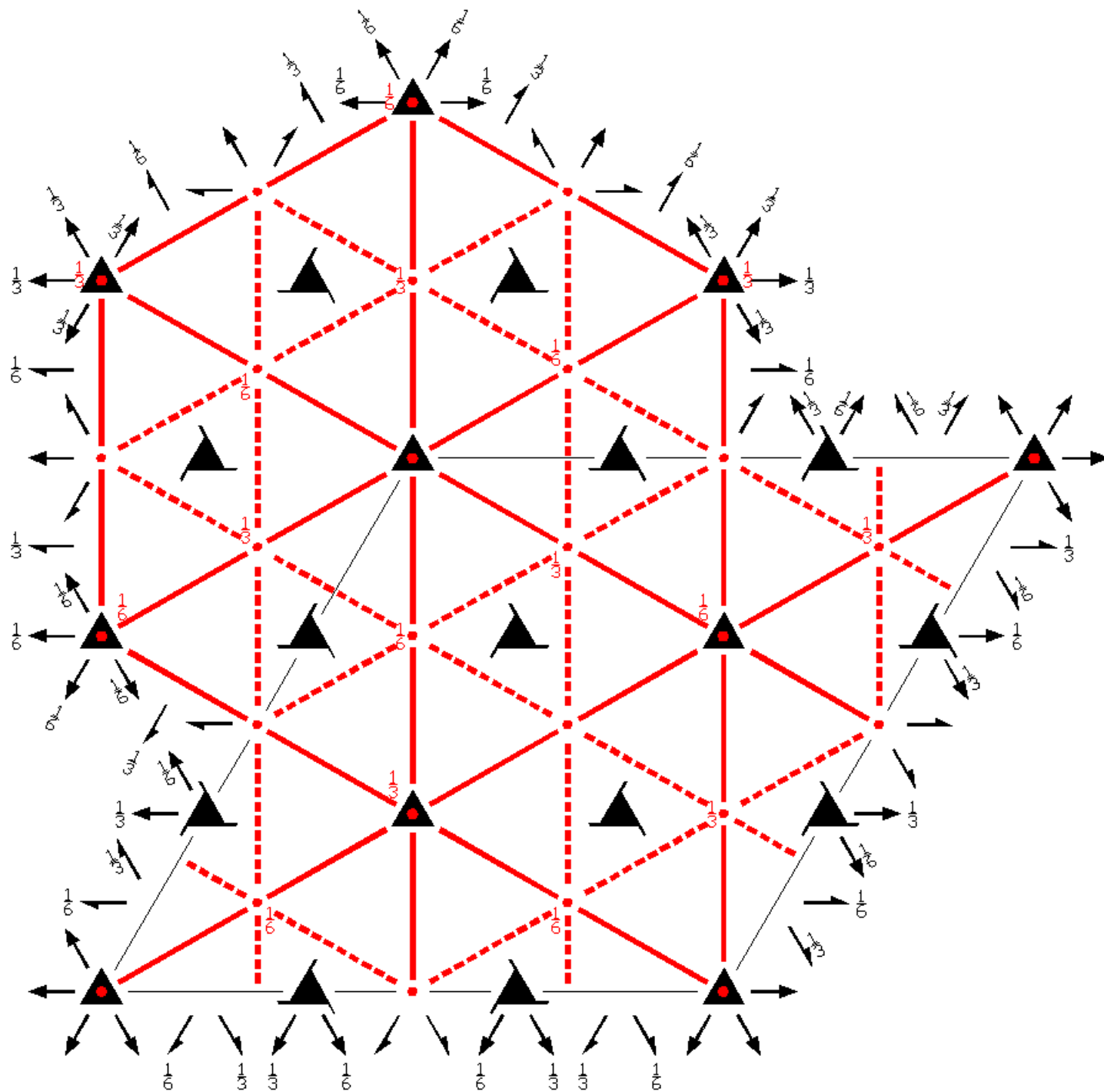
166.4.1330

$\bar{3}'m'$

$R\bar{3}'2/m'$

Trigonal





**Origin** on center ( $\bar{3}'m'$ )

**Asymmetric unit**  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $0 \leq z \leq 1/6$ ;  $x \leq y/2$ ;  $y \leq \min(1-x, 2x)$

**Vertices**  $0,0,0$   $2/3,1/3,0$   $1/3,2/3,0$   
 $0,0,1/6$   $2/3,1/3,1/6$   $1/3,2/3,1/6$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |
|--|--|--|
| (1) 1<br>(1 0,0,0)                                   | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)                            | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)                            |
| (4) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)              | (5) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   | (6) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   |
| (7) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)'              | (8) $\bar{3}$ <sup>+</sup> ' 0,0,z; 0,0,0<br>( $\bar{3}$ <sub>z</sub>  0,0,0)' | (9) $\bar{3}$ <sup>-</sup> ' 0,0,z; 0,0,0<br>( $\bar{3}$ <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (10) m' x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)' | (11) m' x,2x,z<br>(m <sub>x</sub>  0,0,0)'                                     | (12) m' 2x,x,z<br>(m <sub>y</sub>  0,0,0)'   |

For (2/3,1/3,1/3) + set

- |   |  |  |
|---|--|--|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)  | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3)                          | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3)                          |
| (4) 2 (1/2,1/2,0) x,x-1/6,1/6<br>(2 <sub>xy</sub>  2/3,1/3,1/3)               | (5) 2 (1/2,0,0) x,1/6,1/6<br>(2 <sub>x</sub>  2/3,1/3,1/3)                                       | (6) 2 1/3,y,1/6<br>(2 <sub>y</sub>  2/3,1/3,1/3)   |
| (7) $\bar{1}$ ' 1/3,1/6,1/6<br>( $\bar{1}$  2/3,1/3,1/3)'                     | (8) $\bar{3}$ <sup>+</sup> ' 1/3,-1/3,z; 1/3,-1/3,1/6<br>( $\bar{3}$ <sub>z</sub>  2/3,1/3,1/3)' | (9) $\bar{3}$ <sup>-</sup> ' 1/3,2/3,z; 1/3,2/3,1/6<br>( $\bar{3}$ <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3)' |
| (10) g' (1/6,-1/6,1/3) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  2/3,1/3,1/3)' | (11) g' (1/6,1/3,1/3) x,2x-1/2,z<br>(m <sub>x</sub>  2/3,1/3,1/3)'                               | (12) g' (2/3,1/3,1/3) 2x,x,z<br>(m <sub>y</sub>  2/3,1/3,1/3)'   |

For (1/3,2/3,2/3) + set

- |   |  |  |
|---|--|--|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)  | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3)                          | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3)                          |
| (4) 2 (1/2,1/2,0) x,x+1/6,1/3<br>(2 <sub>xy</sub>  1/3,2/3,2/3)               | (5) 2 x,1/3,1/3<br>(2 <sub>x</sub>  1/3,2/3,2/3)   | (6) 2 (0,1/2,0) 1/6,y,1/3<br>(2 <sub>y</sub>  1/3,2/3,2/3)   |
| (4) $\bar{1}$ ' 1/6,1/3,1/3<br>( $\bar{1}$  1/3,2/3,2/3)'                     | (5) $\bar{3}$ <sup>+</sup> ' 2/3,1/3,z; 2/3,1/3,1/3<br>( $\bar{3}$ <sub>z</sub>  1/3,2/3,2/3)' | (6) $\bar{3}$ <sup>-</sup> ' -1/3,1/3,z; -1/3,1/3,1/3<br>( $\bar{3}$ <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3)' |
| (10) g' (-1/6,1/6,2/3) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/3,2/3,2/3)' | (11) g' (1/3,2/3,2/3) x,2x,z<br>(m <sub>x</sub>  1/3,2/3,2/3)'                                 | (12) g' (1/3,1/6,2/3) 2x-1/2,x,z<br>(m <sub>y</sub>  1/3,2/3,2/3)'   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4); (7).**Positions**Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (2/3,1/3,1/3) + (1/3,2/3,2/3) +



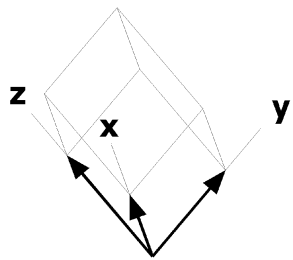
36	i	1	(1) $x,y,z [u,v,w]$ (4) $y,x,\bar{z} [v,u,\bar{w}]$ (7) $\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$ (10) $\bar{y},\bar{x},z [\bar{v},\bar{u},w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$ (5) $x-y,\bar{y},\bar{z} [u-v,\bar{v},\bar{w}]$ (8) $y,\bar{x}+y,\bar{z} [v,\bar{u}+v,\bar{w}]$ (11) $\bar{x}+y,y,z [\bar{u}+v,v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$ (6) $\bar{x},\bar{x}+y,\bar{z} [\bar{u},\bar{u}+v,\bar{w}]$ (9) $x-y,x,\bar{z} [u-v,u,\bar{w}]$ (12) $x,x-y,z [u,u-v,w]$
18	h	.m'	$x,\bar{x},z [u,\bar{u},w]$ $\bar{x},x,\bar{z} [\bar{u},u,\bar{w}]$	$x,2x,z [u,2u,w]$ $2x,x,\bar{z} [2u,u,\bar{w}]$	$2\bar{x},\bar{x},z [2\bar{u},\bar{u},w]$ $\bar{x},2\bar{x},\bar{z} [\bar{u},2\bar{u},\bar{w}]$
18	g	.2	$x,0,1/2 [u,0,0]$ $\bar{x},0,1/2 [\bar{u},0,0]$	$0,x,1/2 [0,u,0]$ $0,\bar{x},1/2 [0,\bar{u},0]$	$\bar{x},\bar{x},1/2 [\bar{u},\bar{u},0]$ $x,x,1/2 [u,u,0]$
18	f	.2	$x,0,0 [u,0,0]$ $\bar{x},0,0 [\bar{u},0,0]$	$0,x,0 [0,u,0]$ $0,\bar{x},0 [0,\bar{u},0]$	$\bar{x},\bar{x},0 [\bar{u},\bar{u},0]$ $x,x,0 [u,u,0]$
9	e	.2/m'	$1/2,0,0 [0,0,0]$	$0,1/2,0 [0,0,0]$	$1/2,1/2,0 [0,0,0]$
9	d	.2/m'	$1/2,0,1/2 [0,0,0]$	$0,1/2,1/2 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$
6	c	3m'	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,\bar{w}]$	
3	b	$\bar{3}$ 'm'	$0,0,1/2 [0,0,0]$		
3	a	$\bar{3}$ 'm'	$0,0,0 [0,0,0]$		

### Symmetry of Special Projections

Along  $[0,0,1]$  p6m'm'  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p211  
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

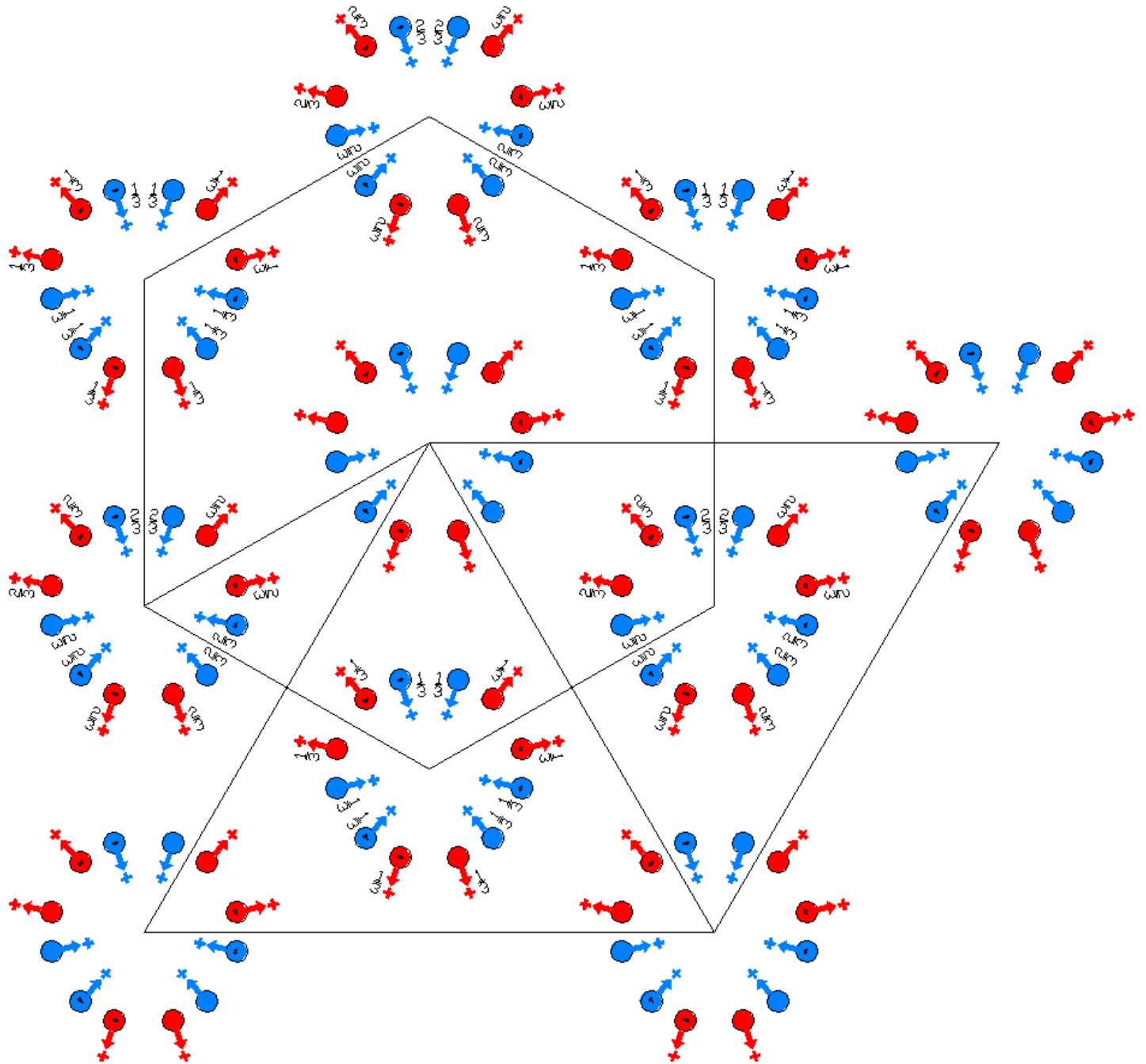
Along  $[2,1,0]$  p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/3$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,0$

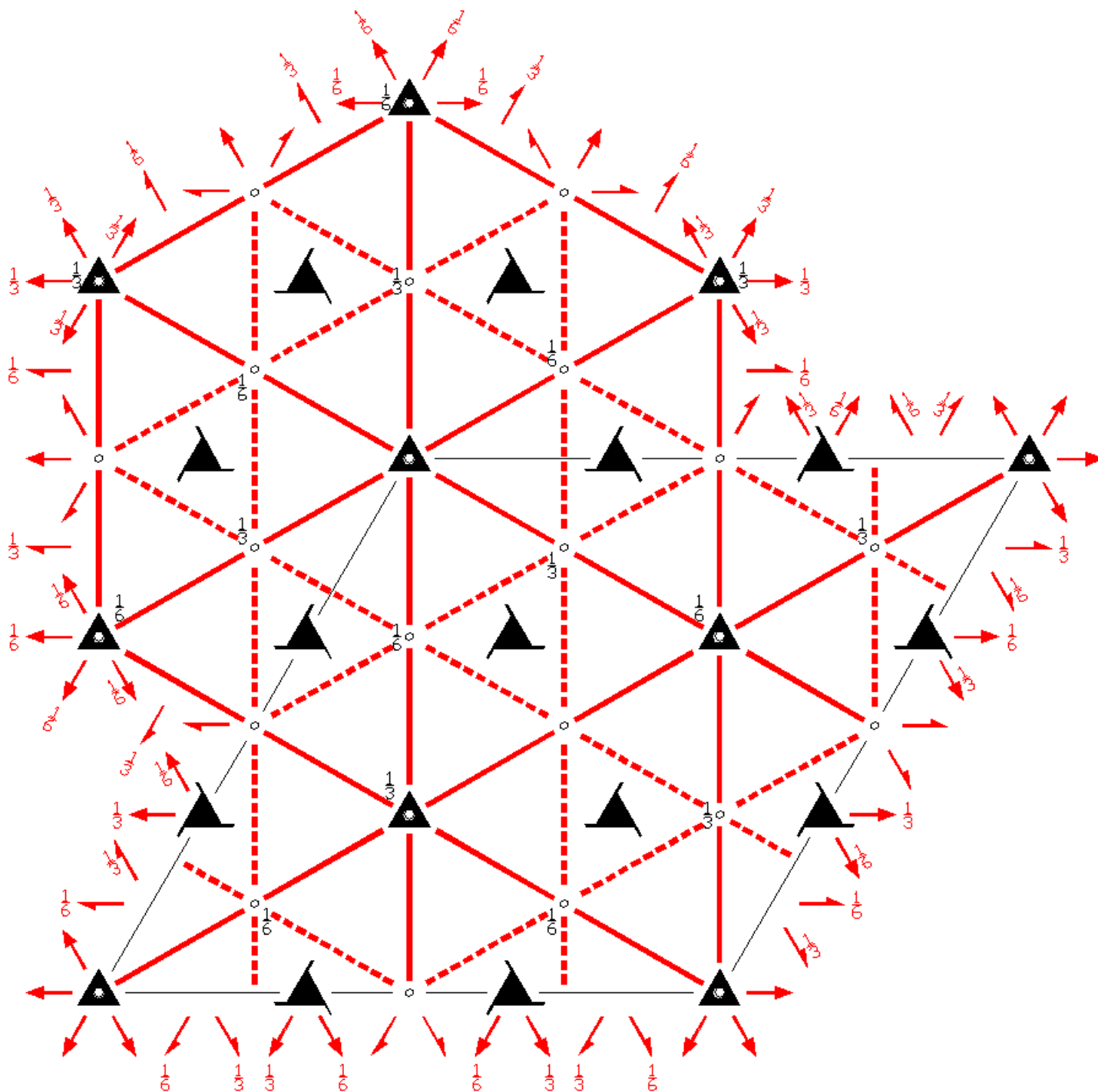


$R\bar{3}m'$   
166.5.1331

$\bar{3}m'$   
 $R\bar{3}2'/m'$

Trigonal





Origin on center ( $\bar{3}m'$ )

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $0 \leq z \leq 1/6$ ;  $x \leq y/2$ ;  $y \leq \min(1-x, 2x)$

Vertices	0,0,0	$2/3, 1/3, 0$	$1/3, 2/3, 0$
	0,0,1/6	$2/3, 1/3, 1/6$	$1/3, 2/3, 1/6$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                   | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)   | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'            | (5) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'              | (6) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                          |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)                 | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)        |
| (10) m' x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)' | (11) m' x,2x,z<br>(m <sub>x</sub>  0,0,0)'            | (12) m' 2x,x,z<br>(m <sub>y</sub>  0,0,0)'                        |

For (2/3,1/3,1/3) + set

- |   |   |   |
|---|---|---|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)  | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3) | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3) |
| (4) 2' (1/2,1/2,0) x,x-1/6,1/6<br>(2 <sub>xy</sub>  2/3,1/3,1/3)'             | (5) 2' (1/2,0,0) x,1/6,1/6<br>(2 <sub>x</sub>  2/3,1/3,1/3)'            | (6) 2' 1/3,y,1/6<br>(2 <sub>y</sub>  2/3,1/3,1/3)'                                  |
| (7) $\bar{1}$ 1/3,1/6,1/6<br>( $\bar{1}$  2/3,1/3,1/3)                        | (8) $\bar{3}^+$ 1/3,-1/3,z; 1/3,-1/3,1/6<br>( $\bar{3}_z$  2/3,1/3,1/3) | (9) $\bar{3}^-$ 1/3,2/3,z; 1/3,2/3,1/6<br>( $\bar{3}_z^{-1}$  2/3,1/3,1/3)          |
| (10) g' (1/6,-1/6,1/3) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  2/3,1/3,1/3)' | (11) g' (1/6,1/3,1/3) x,2x-1/2,z<br>(m <sub>x</sub>  2/3,1/3,1/3)'      | (12) g' (2/3,1/3,1/3) 2x,x,z<br>(m <sub>y</sub>  2/3,1/3,1/3)'                      |

For (1/3,2/3,2/3) + set

- |   |   |   |
|---|---|---|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)  | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3) | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3) |
| (4) 2' (1/2,1/2,0) x,x+1/6,1/3<br>(2 <sub>xy</sub>  1/3,2/3,2/3)'             | (5) 2' x,1/3,1/3<br>(2 <sub>x</sub>  1/3,2/3,2/3)'                    | (6) 2' (0,1/2,0) 1/6,y,1/3<br>(2 <sub>y</sub>  1/3,2/3,2/3)'                          |
| (4) $\bar{1}$ 1/6,1/3,1/3<br>( $\bar{1}$  1/3,2/3,2/3)                        | (5) $\bar{3}^+$ 2/3,1/3,z; 2/3,1/3,1/3<br>( $\bar{3}_z$  1/3,2/3,2/3) | (6) $\bar{3}^-$ -1/3,1/3,z; -1/3,1/3,1/3<br>( $\bar{3}_z^{-1}$  1/3,2/3,2/3)          |
| (10) g' (-1/6,1/6,2/3) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/3,2/3,2/3)' | (11) g' (1/3,2/3,2/3) x,2x,z<br>(m <sub>x</sub>  1/3,2/3,2/3)'        | (12) g' (1/3,1/6,2/3) 2x-1/2,x,z<br>(m <sub>y</sub>  1/3,2/3,2/3)'                    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4); (7).**Positions**Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (2/3,1/3,1/3) + (1/3,2/3,2/3) +

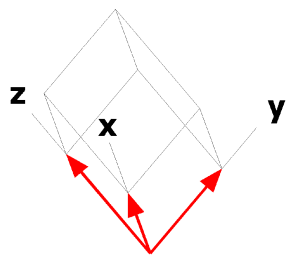
36	i	1	(1) $x,y,z [u,v,w]$ (4) $y,x,\bar{z} [\bar{v},\bar{u},w]$ (7) $\bar{x},\bar{y},\bar{z} [u,v,w]$ (10) $\bar{y},\bar{x},z [\bar{v},\bar{u},w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$ (5) $x-y,\bar{y},\bar{z} [\bar{u}+v,v,w]$ (8) $y,\bar{x}+y,\bar{z} [\bar{v},u-v,w]$ (11) $\bar{x}+y,y,z [\bar{u}+v,v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$ (6) $\bar{x},\bar{x}+y,\bar{z} [u,u-v,w]$ (9) $x-y,x,\bar{z} [\bar{u}+v,\bar{u},w]$ (12) $x,x-y,z [u,u-v,w]$
18	h	.m'	$x,\bar{x},z [u,\bar{u},w]$ $\bar{x},x,\bar{z} [u,\bar{u},w]$	$x,2x,z [u,2u,w]$ $2x,x,\bar{z} [2\bar{u},\bar{u},w]$	$2\bar{x},\bar{x},z [2\bar{u},\bar{u},w]$ $\bar{x},2\bar{x},\bar{z} [u,2u,w]$
18	g	.2'	$x,0,1/2 [u,2u,w]$ $\bar{x},0,1/2 [u,2u,w]$	$0,x,1/2 [2\bar{u},\bar{u},w]$ $0,\bar{x},1/2 [2\bar{u},\bar{u},w]$	$\bar{x},\bar{x},1/2 [u,\bar{u},w]$ $x,x,1/2 [u,\bar{u},w]$
18	f	.2'	$x,0,0 [u,2u,w]$ $\bar{x},0,0 [u,2u,w]$	$0,x,0 [2\bar{u},\bar{u},w]$ $0,\bar{x},0 [2\bar{u},\bar{u},w]$	$\bar{x},\bar{x},0 [u,\bar{u},w]$ $x,x,0 [u,\bar{u},w]$
9	e	.2'/m'	$1/2,0,0 [u,2u,w]$	$0,1/2,0 [2\bar{u},\bar{u},w]$	$1/2,1/2,0 [u,\bar{u},w]$
9	d	.2'/m'	$1/2,0,1/2 [u,2u,w]$	$0,1/2,1/2 [2\bar{u},\bar{u},w]$	$1/2,1/2,1/2 [u,\bar{u},w]$
6	c	3m'	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,w]$	
3	b	$\bar{3}m'$	$0,0,1/2 [0,0,w]$		
3	a	$\bar{3}m'$	$0,0,0 [0,0,w]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p6'm'm$   
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2'11$   
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

Along  $[2,1,0]$   $p2'mm'$   
 $\mathbf{a}^* = \mathbf{c}/3$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,0$



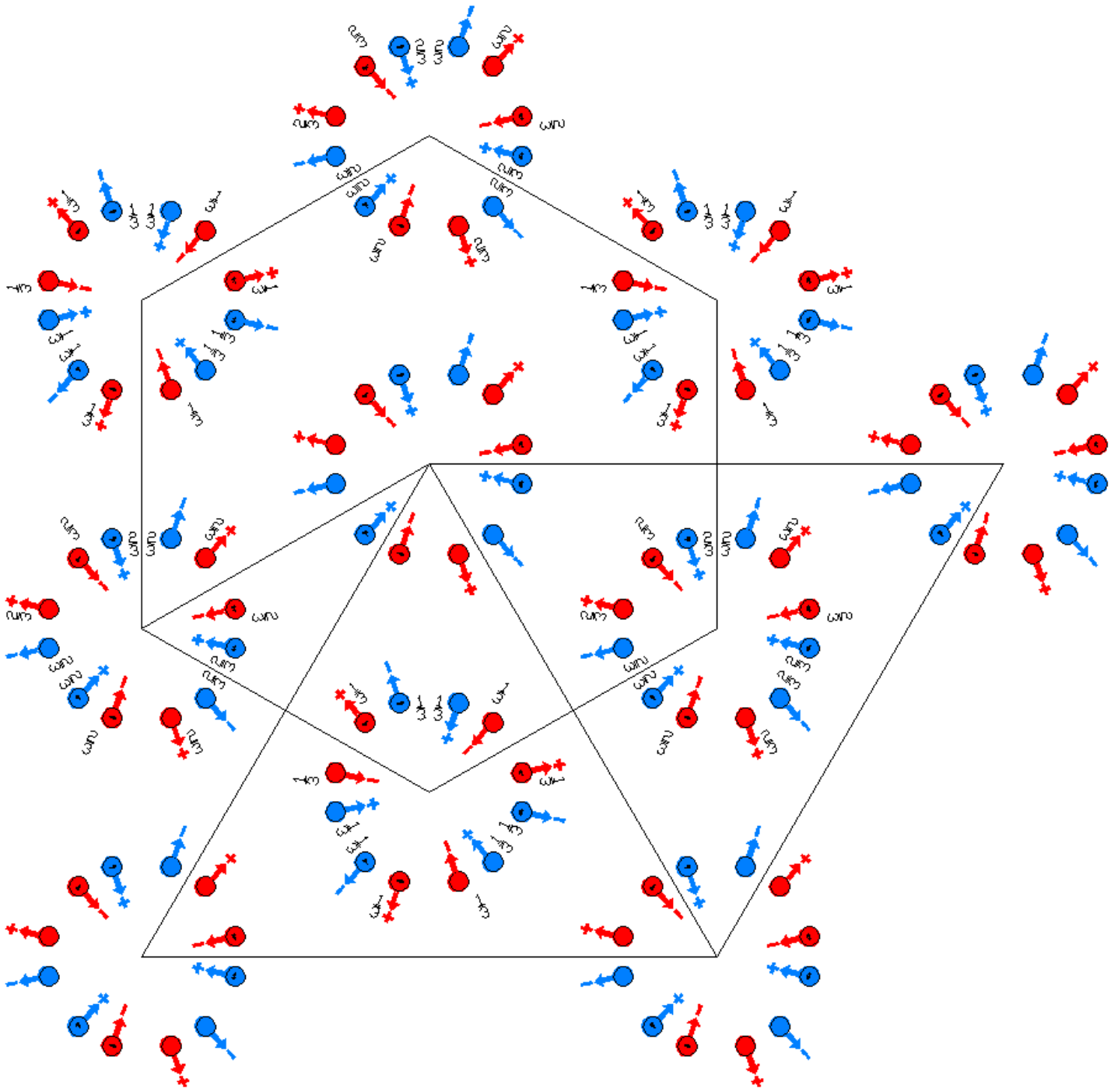
$R_R \bar{3}m$

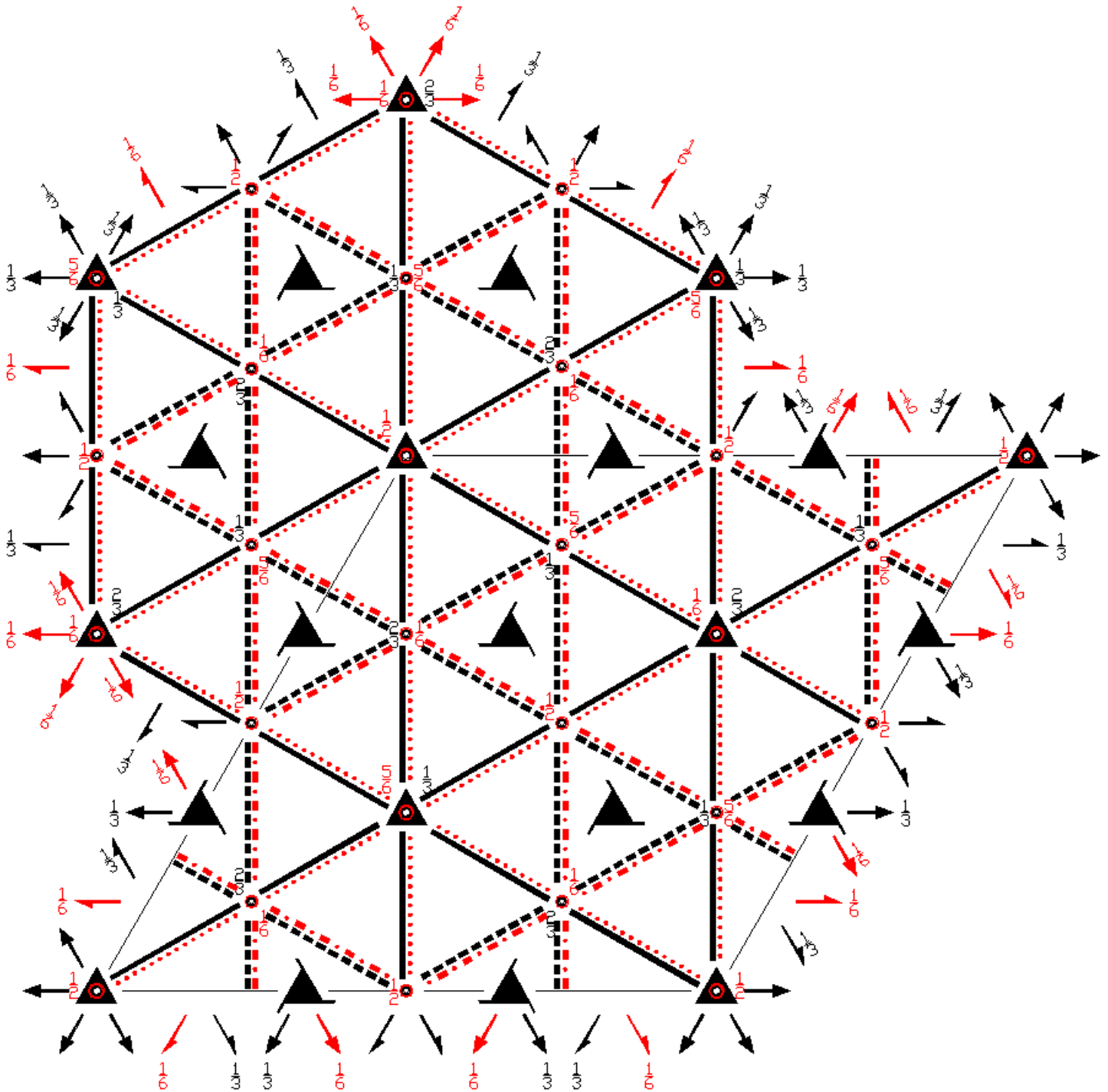
166.6.1332

$\bar{3}m1'$

$R_R \bar{3}2/m$

Trigonal





Origin on center ( $\bar{3}m$ )

**Asymmetric unit**  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $0 \leq z \leq 1/6$ ;  $x \leq y/2$ ;  $y \leq \min(1-x, 2x)$

Vertices  $0,0,0$   $2/3,1/3,0$   $1/3,2/3,0$   
 $0,0,1/6$   $2/3,1/3,1/6$   $1/3,2/3,1/6$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                           | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) 2 x,x,0<br>( $2_{xy}$  0,0,0)            | (5) 2 x,0,0<br>( $2_x$  0,0,0)                        | (6) 2 0,y,0<br>( $2_y$  0,0,0)                             |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)         | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) m x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0) | (11) m x,2x,z<br>( $m_x$  0,0,0)                      | (12) m 2x,x,z<br>( $m_y$  0,0,0)                           |

For (2/3,1/3,1/3)' + set

- |   |   |  |
|---|---|--|
| (1) t' (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)'                                | (2) $3^{+'}$ (0,0,1/3) 1/3,1/3,z<br>( $3_z$  2/3,1/3,1/3)'                  | (3) $3^{-'}$ (0,0,1/3) 1/3,0,z<br>( $3_z^{-1}$  2/3,1/3,1/3)'                  |
| (4) 2' (1/2,1/2,0) x,x-1/6,1/6<br>( $2_{xy}$  2/3,1/3,1/3)'             | (5) 2' (1/2,0,0) x,1/6,1/6<br>( $2_x$  2/3,1/3,1/3)'                        | (6) 2' 1/3,y,1/6<br>( $2_y$  2/3,1/3,1/3)'                                     |
| (7) $\bar{1}'$ 1/3,1/6,1/6<br>( $\bar{1}$  2/3,1/3,1/3)'                | (8) $\bar{3}^{+'}$ 1/3,-1/3,z; 1/3,-1/3,1/6<br>( $\bar{3}_z$  2/3,1/3,1/3)' | (9) $\bar{3}^{-'}$ 1/3,2/3,z; 1/3,2/3,1/6<br>( $\bar{3}_z^{-1}$  2/3,1/3,1/3)' |
| (10) g' (1/6,-1/6,1/3) x+1/2, $\bar{x}$ ,z<br>( $m_{xy}$  2/3,1/3,1/3)' | (11) g' (1/6,1/3,1/3) x,2x-1/2,z<br>( $m_x$  2/3,1/3,1/3)'                  | (12) g' (2/3,1/3,1/3) 2x,x,z<br>( $m_y$  2/3,1/3,1/3)'                         |

For (1/3,2/3,2/3) + set

- |   |   |  |
|---|---|--|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)                                | (2) $3^+$ (0,0,2/3) 0,1/3,z<br>( $3_z$  1/3,2/3,2/3)                  | (3) $3^-$ (0,0,2/3) 1/3,1/3,z<br>( $3_z^{-1}$  1/3,2/3,2/3)                  |
| (4) 2 (1/2,1/2,0) x,x+1/6,1/3<br>( $2_{xy}$  1/3,2/3,2/3)             | (5) 2 x,1/3,1/3<br>( $2_x$  1/3,2/3,2/3)                              | (6) 2 (0,1/2,0) 1/6,y,1/3<br>( $2_y$  1/3,2/3,2/3)                           |
| (7) $\bar{1}$ 1/6,1/3,1/3<br>( $\bar{1}$  1/3,2/3,2/3)                | (8) $\bar{3}^+$ 2/3,1/3,z; 2/3,1/3,1/3<br>( $\bar{3}_z$  1/3,2/3,2/3) | (9) $\bar{3}^-$ -1/3,1/3,z; -1/3,1/3,1/3<br>( $\bar{3}_z^{-1}$  1/3,2/3,2/3) |
| (10) g (-1/6,1/6,2/3) x+1/2, $\bar{x}$ ,z<br>( $m_{xy}$  1/3,2/3,2/3) | (11) g (1/3,2/3,2/3) x,2x,z<br>( $m_x$  1/3,2/3,2/3)                  | (12) g (1/3,1/6,2/3) 2x-1/2,x,z<br>( $m_y$  1/3,2/3,2/3)                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); t'(2/3,1/3,1/3); (2); (4); (7).**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (2/3,1/3,1/3)' + (1/3,2/3,2/3) +



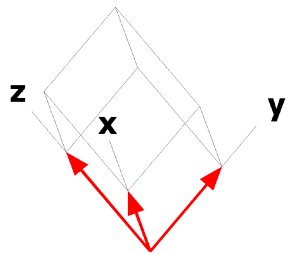
36	i	1	(1) $x,y,z [u,v,w]$ (4) $y,x,\bar{z} [v,u,\bar{w}]$ (7) $\bar{x},\bar{y},\bar{z} [u,v,w]$ (10) $\bar{y},\bar{x},z [v,u,\bar{w}]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$ (5) $x-y,\bar{y},\bar{z} [u-v,\bar{v},\bar{w}]$ (8) $y,\bar{x}+y,\bar{z} [\bar{v},u-v,w]$ (11) $\bar{x}+y,y,z [u-v,\bar{v},\bar{w}]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$ (6) $\bar{x},\bar{x}+y,\bar{z} [\bar{u},\bar{u}+v,\bar{w}]$ (9) $x-y,x,\bar{z} [\bar{u}+v,\bar{u},w]$ (12) $x,x-y,z [\bar{u},\bar{u}+v,\bar{w}]$
18	h	.m	$x,\bar{x},z [u,u,0]$ $\bar{x},x,\bar{z} [u,u,0]$	$x,2x,z [\bar{u},0,0]$ $2x,x,\bar{z} [0,\bar{u},0]$	$2\bar{x},\bar{x},z [0,\bar{u},0]$ $\bar{x},2\bar{x},\bar{z} [\bar{u},0,0]$
18	g	.2'	$x,0,1/2 [u,2u,w]$ $\bar{x},0,1/2 [\bar{u},2\bar{u},\bar{w}]$	$0,x,1/2 [2\bar{u},\bar{u},w]$ $0,\bar{x},1/2 [2u,u,\bar{w}]$	$\bar{x},\bar{x},1/2 [u,\bar{u},w]$ $x,x,1/2 [\bar{u},u,\bar{w}]$
18	f	.2	$x,0,0 [u,0,0]$ $\bar{x},0,0 [u,0,0]$	$0,x,0 [0,u,0]$ $0,\bar{x},0 [0,u,0]$	$\bar{x},\bar{x},0 [\bar{u},\bar{u},0]$ $x,x,0 [\bar{u},\bar{u},0]$
9	e	.2/m	$1/2,0,0 [u,0,0]$	$0,1/2,0 [0,u,0]$	$1/2,1/2,0 [\bar{u},\bar{u},0]$
9	d	.2'/m	$1/2,0,1/2 [0,0,0]$	$0,1/2,1/2 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$
6	c	3m	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$	
3	b	$\bar{3}m$	$0,0,1/2 [0,0,0]$		
3	a	$\bar{3}m$	$0,0,0 [0,0,0]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6mm1'$   
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2111'$   
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

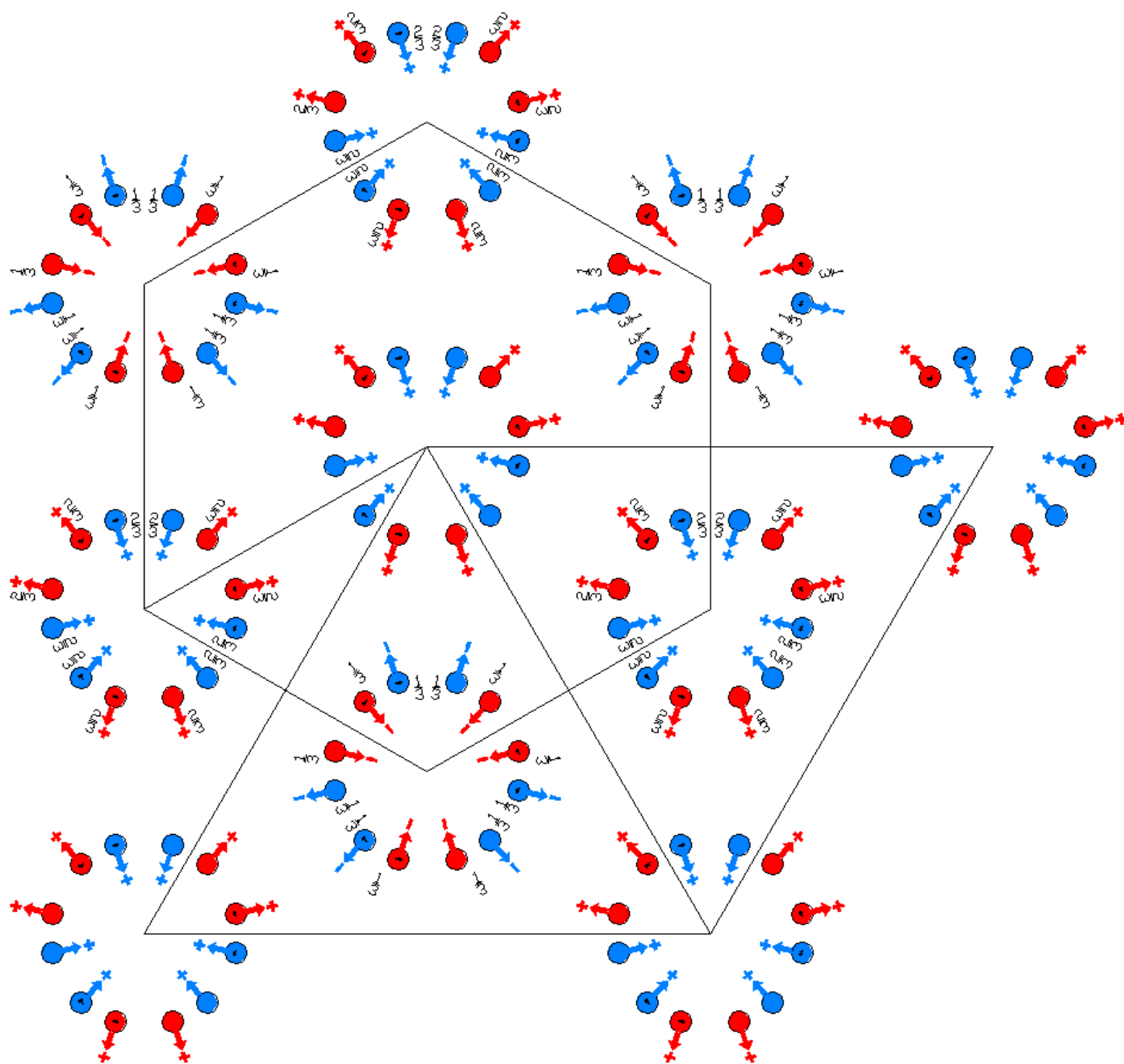
Along  $[2,1,0]$   $p_{2a}2mm$   
 $\mathbf{a}^* = \mathbf{c}/3$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,1/6$

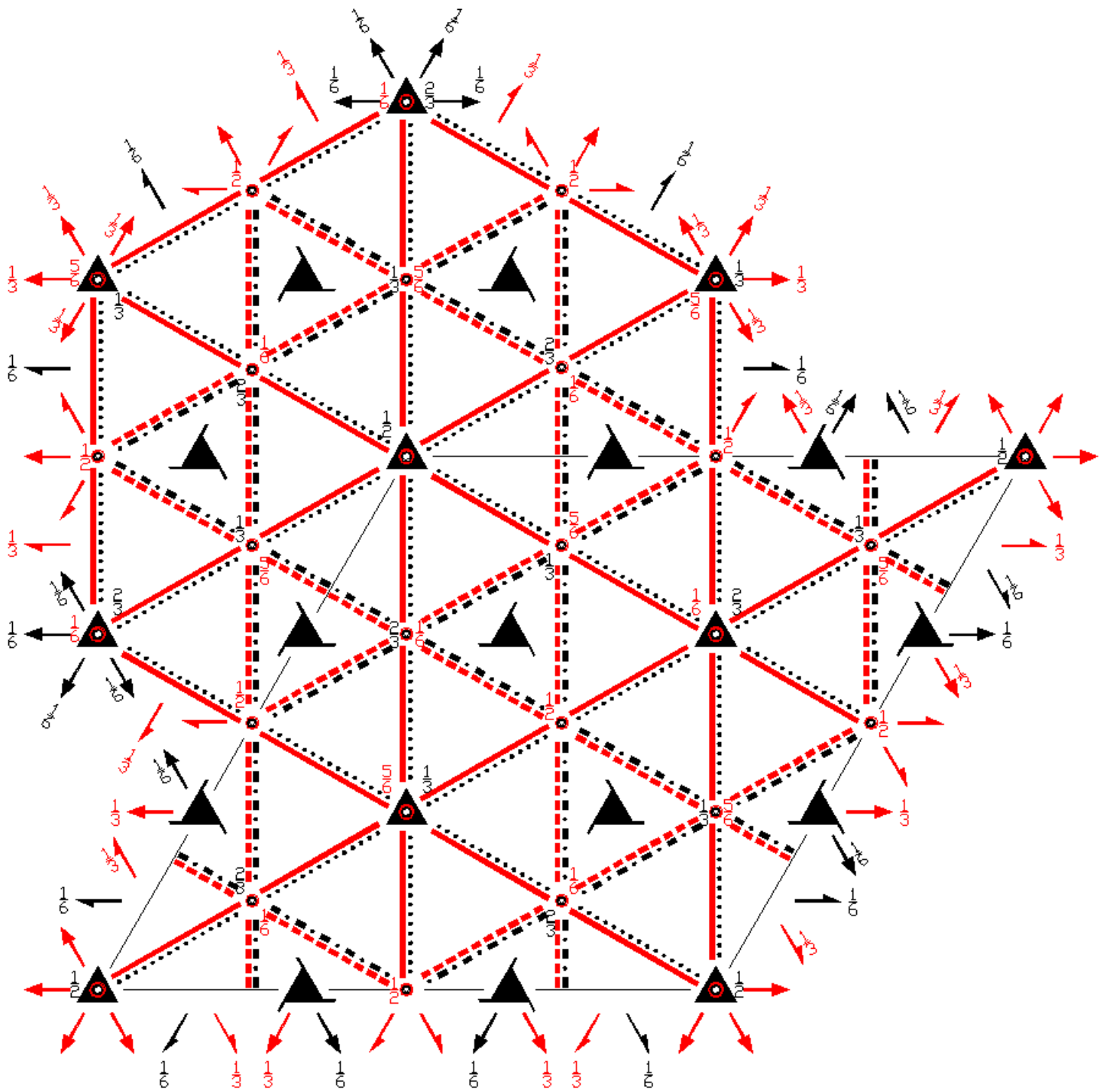


$R_R \bar{3}m'$   
166.7.1333

$\bar{3}m1'$   
 $R_R \bar{3}2/m'$

Trigonal





Origin on center ( $\bar{3}m'$ )

Asymmetric unit  $0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/6; \quad x \leq y/2; \quad y \leq \min(1-x, 2x)$

Vertices  $0,0,0 \quad 2/3,1/3,0 \quad 1/3,2/3,0$   
 $0,0,1/6 \quad 2/3,1/3,1/6 \quad 1/3,2/3,1/6$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                               | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)'            | (5) $2'$ x,0,0<br>( $2_x$  0,0,0)'                    | (6) $2'$ 0,y,0<br>( $2_y$  0,0,0)'                         |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)             | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) $m'$ x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0)' | (11) $m'$ x,2x,z<br>( $m_x$  0,0,0)'                  | (12) $m'$ 2x,x,z<br>( $m_y$  0,0,0)'                       |

For (2/3,1/3,1/3)' + set

- |   |   |  |
|---|---|--|
| (1) $t'$ (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)'                              | (2) $3^{+'}$ (0,0,1/3) 1/3,1/3,z<br>( $3_z$  2/3,1/3,1/3)'                  | (3) $3^{-'}$ (0,0,1/3) 1/3,0,z<br>( $3_z^{-1}$  2/3,1/3,1/3)'                  |
| (4) $2$ (1/2,1/2,0) x,x-1/6,1/6<br>( $2_{xy}$  2/3,1/3,1/3)             | (5) $2$ (1/2,0,0) x,1/6,1/6<br>( $2_x$  2/3,1/3,1/3)                        | (6) $2$ 1/3,y,1/6<br>( $2_y$  2/3,1/3,1/3)                                     |
| (7) $\bar{1}'$ 1/3,1/6,1/6<br>( $\bar{1}$  2/3,1/3,1/3)'                | (8) $\bar{3}^{+'}$ 1/3,-1/3,z; 1/3,-1/3,1/6<br>( $\bar{3}_z$  2/3,1/3,1/3)' | (9) $\bar{3}^{-'}$ 1/3,2/3,z; 1/3,2/3,1/6<br>( $\bar{3}_z^{-1}$  2/3,1/3,1/3)' |
| (10) $g$ (1/6,-1/6,1/3) x+1/2, $\bar{x}$ ,z<br>( $m_{xy}$  2/3,1/3,1/3) | (11) $g$ (1/6,1/3,1/3) x,2x-1/2,z<br>( $m_x$  2/3,1/3,1/3)                  | (12) $g$ (2/3,1/3,1/3) 2x,x,z<br>( $m_y$  2/3,1/3,1/3)                         |

For (1/3,2/3,2/3) + set

- |   |   |  |
|---|---|--|
| (1) $t$ (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)                                  | (2) $3^+$ (0,0,2/3) 0,1/3,z<br>( $3_z$  1/3,2/3,2/3)                  | (3) $3^-$ (0,0,2/3) 1/3,1/3,z<br>( $3_z^{-1}$  1/3,2/3,2/3)                  |
| (4) $2'$ (1/2,1/2,0) x,x+1/6,1/3<br>( $2_{xy}$  1/3,2/3,2/3)'             | (5) $2'$ x,1/3,1/3<br>( $2_x$  1/3,2/3,2/3)'                          | (6) $2'$ (0,1/2,0) 1/6,y,1/3<br>( $2_y$  1/3,2/3,2/3)'                       |
| (7) $\bar{1}$ 1/6,1/3,1/3<br>( $\bar{1}$  1/3,2/3,2/3)                    | (8) $\bar{3}^+$ 2/3,1/3,z; 2/3,1/3,1/3<br>( $\bar{3}_z$  1/3,2/3,2/3) | (9) $\bar{3}^-$ -1/3,1/3,z; -1/3,1/3,1/3<br>( $\bar{3}_z^{-1}$  1/3,2/3,2/3) |
| (10) $g'$ (-1/6,1/6,2/3) x+1/2, $\bar{x}$ ,z<br>( $m_{xy}$  1/3,2/3,2/3)' | (11) $g'$ (1/3,2/3,2/3) x,2x,z<br>( $m_x$  1/3,2/3,2/3)'              | (12) $g'$ (1/3,1/6,2/3) 2x-1/2,x,z<br>( $m_y$  1/3,2/3,2/3)'                 |

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(2/3,1/3,1/3)$ ; (2); (4); (7).**Positions**Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (2/3,1/3,1/3)' + (1/3,2/3,2/3) +

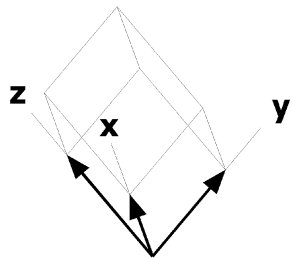
36	i	1	(1) $x,y,z [u,v,w]$ (4) $y,x,\bar{z} [\bar{v},\bar{u},w]$ (7) $\bar{x},\bar{y},\bar{z} [u,v,w]$ (10) $\bar{y},\bar{x},z [\bar{v},\bar{u},w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$ (5) $x-y,\bar{y},\bar{z} [\bar{u}+v,v,w]$ (8) $y,\bar{x}+y,\bar{z} [\bar{v},u-v,w]$ (11) $\bar{x}+y,y,z [\bar{u}+v,v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$ (6) $\bar{x},\bar{x}+y,\bar{z} [u,u-v,w]$ (9) $x-y,x,\bar{z} [\bar{u}+v,\bar{u},w]$ (12) $x,x-y,z [u,u-v,w]$
18	h	.m'	$x,\bar{x},z [u,\bar{u},w]$ $\bar{x},x,\bar{z} [u,\bar{u},w]$	$x,2x,z [u,2u,w]$ $2x,x,\bar{z} [2\bar{u},\bar{u},w]$	$2\bar{x},\bar{x},z [2\bar{u},\bar{u},w]$ $\bar{x},2\bar{x},\bar{z} [u,2u,w]$
18	g	.2	$x,0,1/2 [u,0,0]$ $\bar{x},0,1/2 [\bar{u},0,0]$	$0,x,1/2 [0,u,0]$ $0,\bar{x},1/2 [0,\bar{u},0]$	$\bar{x},\bar{x},1/2 [\bar{u},\bar{u},0]$ $x,x,1/2 [u,u,0]$
18	f	.2'	$x,0,0 [u,2u,w]$ $\bar{x},0,0 [u,2u,w]$	$0,x,0 [2\bar{u},\bar{u},w]$ $0,\bar{x},0 [2\bar{u},\bar{u},w]$	$\bar{x},\bar{x},0 [u,\bar{u},w]$ $x,x,0 [u,\bar{u},w]$
9	e	.2'/m'	$1/2,0,0 [u,2u,w]$	$0,1/2,0 [2\bar{u},\bar{u},w]$	$1/2,1/2,0 [u,\bar{u},w]$
9	d	.2'/m'	$1/2,0,1/2 [0,0,0]$	$0,1/2,1/2 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$
6	c	3m'	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,w]$	
3	b	$\bar{3}m'$	$0,0,1/2 [0,0,w]$		
3	a	$\bar{3}m'$	$0,0,0 [0,0,w]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6mm1'$   
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a}211$   
 $\mathbf{a}^* = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x-1/6, -1/3, 1/6$

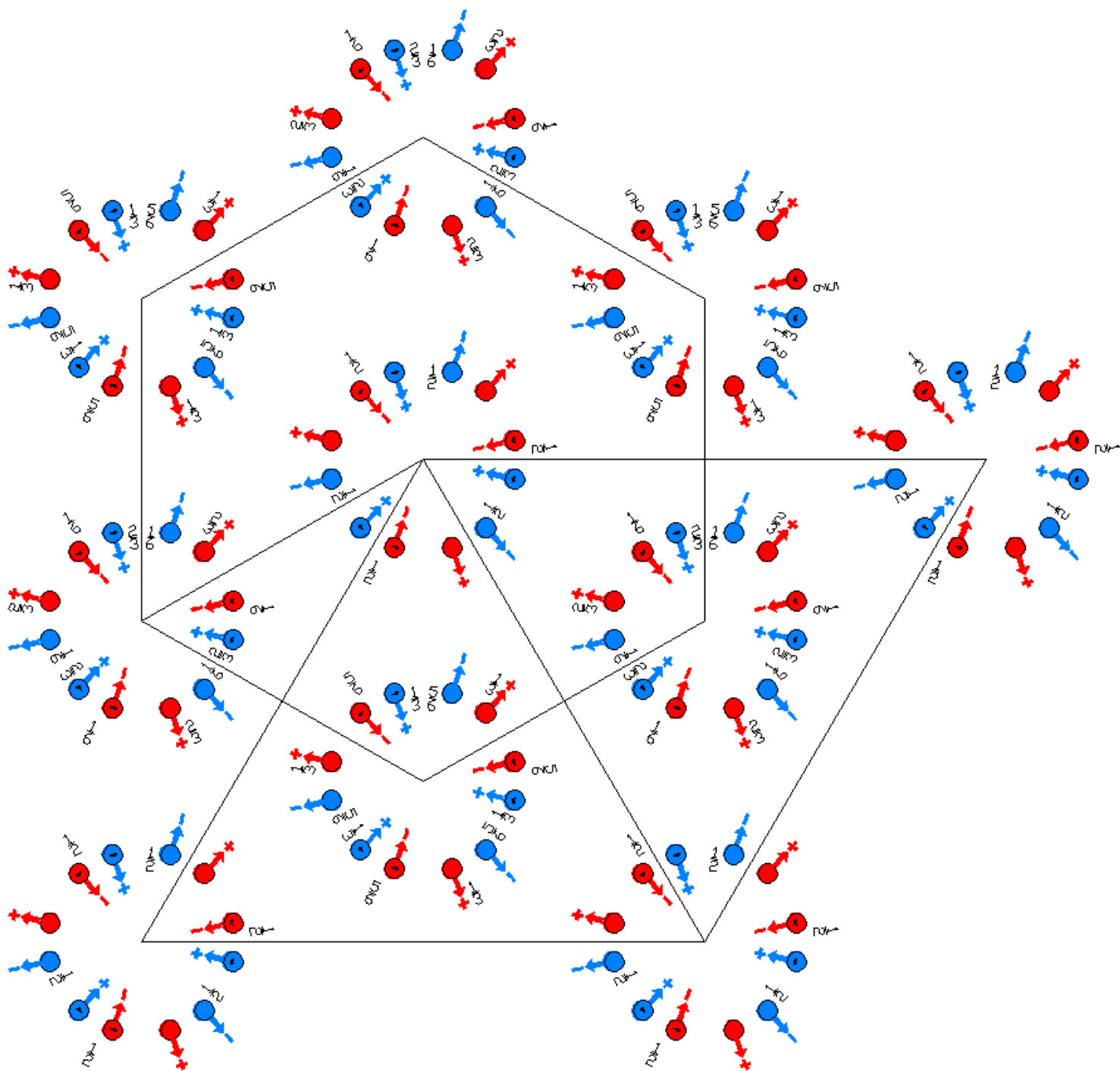
Along  $[2,1,0]$   $p_{2a}2m'm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/3$   
 Origin at  $x,x/2, 1/6$

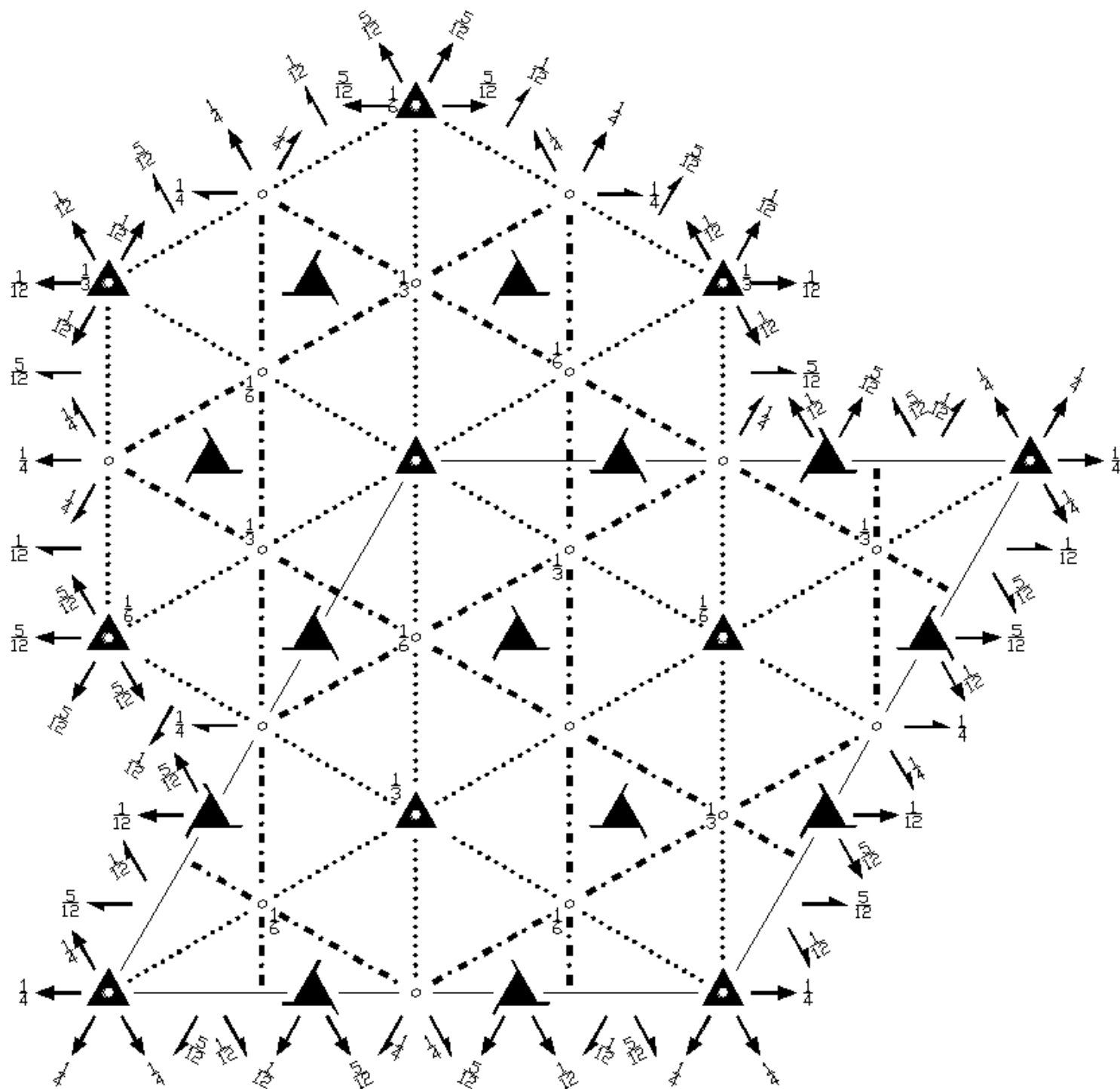


$R\bar{3}c$   
167.1.1334

$\bar{3}m$   
 $R\bar{3}2/c$

Trigonal





Origin on  $(\bar{3})$  at  $\bar{3}c$

**Asymmetric unit**  $0 \leq x \leq 2/3;$   $0 \leq y \leq 2/3;$   $0 \leq z \leq 1/12;$   $x \leq (1+y)/2;$   $y \leq \min(1-x, (1+x)/2)$

Vertices  $0,0,0$   $1/2,0,0$   $2/3,1/3,0$   $1/3,2/3,0$   $0,1/2,0$   
 $0,0,1/12$   $1/2,0,1/12$   $2/3,1/3,1/12$   $1/3,2/3,1/12$   $0,1/2,1/12$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)   | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                    | (5) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)            | (6) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)                        |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)                           | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)        |
| (10) c (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2) | (11) c (0,0,1/2) x,2x,z<br>(m <sub>x</sub>  0,0,1/2)  | (12) c (0,0,1/2) 2x,x,z<br>(m <sub>y</sub>  0,0,1/2)              |

For (2/3,1/3,1/3) + set

- |   |   |   |
|---|---|---|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)                                      | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3) | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3) |
| (4) 2(1/2,1/2,0) x,x-1/6,5/12<br>(2 <sub>xy</sub>  2/3,1/3,5/6)             | (5) 2 (1/2,0,0) x,1/6,5/12<br>(2 <sub>x</sub>  2/3,1/3,5/6)             | (6) 2 1/3,y,5/12<br>(2 <sub>y</sub>  2/3,1/3,5/6)                                   |
| (7) $\bar{1}$ 1/3,1/6,1/6<br>( $\bar{1}$  2/3,1/3,1/3)                      | (8) $\bar{3}^+$ 1/3,-1/3,z; 1/3,-1/3,1/6<br>( $\bar{3}_z$  2/3,1/3,1/3) | (9) $\bar{3}^-$ 1/3,2/3,z; 1/3,2/3,1/6<br>( $\bar{3}_z^{-1}$  2/3,1/3,1/3)          |
| (10) g (1/6,-1/6,5/6) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  2/3,1/3,5/6) | (11) g (1/6,1/3,5/6) x,2x-1/2,z<br>(m <sub>x</sub>  2/3,1/3,5/6)        | (12) g (2/3,1/3,5/6) 2x,x,z<br>(m <sub>y</sub>  2/3,1/3,5/6)                        |

For (1/3,2/3,2/3) + set

- |   |   |   |
|---|---|---|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)                                      | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3) | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3) |
| (4) 2(1/2,1/2,0) x,x+1/6,1/12<br>(2 <sub>xy</sub>  1/3,2/3,1/6)             | (5) 2 x,1/3,1/12<br>(2 <sub>x</sub>  1/3,2/3,1/6)                     | (6) 2 (0,1/2,0) 1/6,y,1/12<br>(2 <sub>y</sub>  1/3,2/3,1/6)                           |
| (7) $\bar{1}$ 1/6,1/3,1/3<br>( $\bar{1}$  1/3,2/3,2/3)                      | (8) $\bar{3}^+$ 2/3,1/3,z; 2/3,1/3,1/3<br>( $\bar{3}_z$  1/3,2/3,2/3) | (9) $\bar{3}^-$ -1/3,1/3,z; -1/3,1/3,1/3<br>( $\bar{3}_z^{-1}$  1/3,2/3,2/3)          |
| (10) g (-1/6,1/6,1/6) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/3,2/3,1/6) | (11) g (1/3,2/3,1/6) x,2x,z<br>(m <sub>x</sub>  1/3,2/3,1/6)          | (12) g (1/3,1/6,1/6) 2x-1/2,x,z<br>(m <sub>y</sub>  1/3,2/3,1/6)                      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4); (7).**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (2/3,1/3,1/3) + (1/3,2/3,2/3) +



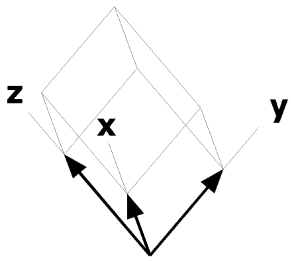
36	f	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$
			(4) $y,x,\bar{z}+1/2 [v,u,\bar{w}]$	(5) $x-y,\bar{y},\bar{z}+1/2 [u-v,\bar{v},\bar{w}]$	(6) $\bar{x},\bar{x}+y,\bar{z}+1/2 [\bar{u},\bar{u}+v,\bar{w}]$
			(7) $\bar{x},\bar{y},\bar{z} [u,v,w]$	(8) $y,\bar{x}+y,\bar{z} [\bar{v},u-v,w]$	(9) $x-y,x,\bar{z} [\bar{u}+v,\bar{u},w]$
			(10) $\bar{y},\bar{x},z+1/2 [v,u,\bar{w}]$	(11) $\bar{x}+y,y,z+1/2 [u-v,\bar{v},\bar{w}]$	(12) $x,x-y,z+1/2 [\bar{u},\bar{u}+v,\bar{w}]$
18	e	.2	$x,0,1/4 [u,0,0]$	$0,x,1/4 [0,u,0]$	$\bar{x},\bar{x},1/4 [\bar{u},\bar{u},0]$
			$\bar{x},0,3/4 [u,0,0]$	$0,\bar{x},3/4 [0,u,0]$	$x,x,3/4 [\bar{u},\bar{u},0]$
18	d	$\bar{1}$	$1/2,0,0 [u,v,w]$	$0,1/2,0 [\bar{v},u-v,w]$	$1/2,1/2,0 [\bar{u}+v,\bar{u},w]$
			$0,1/2,1/2 [v,u,\bar{w}]$	$1/2,0,1/2 [u-v,\bar{v},\bar{w}]$	$1/2,1/2,1/2 [\bar{u},\bar{u}+v,\bar{w}]$
12	c	3.	$0,0,z [0,0,w]$	$0,0,\bar{z}+1/2 [0,0,\bar{w}]$	$0,0,\bar{z} [0,0,w]$
					$0,0,z+1/2 [0,0,\bar{w}]$
6	b	$\bar{3}$ .	$0,0,0 [0,0,w]$	$0,0,1/2 [0,0,\bar{w}]$	
6	a	32	$0,0,1/4 [0,0,0]$	$0,0,3/4 [0,0,0]$	

### Symmetry of Special Projections

Along  $[0,0,1]$   $p6'mm'$   
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a}211$   
 $\mathbf{a}^* = (2\mathbf{a} + 4\mathbf{b} + \mathbf{c})/6$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,1/4$

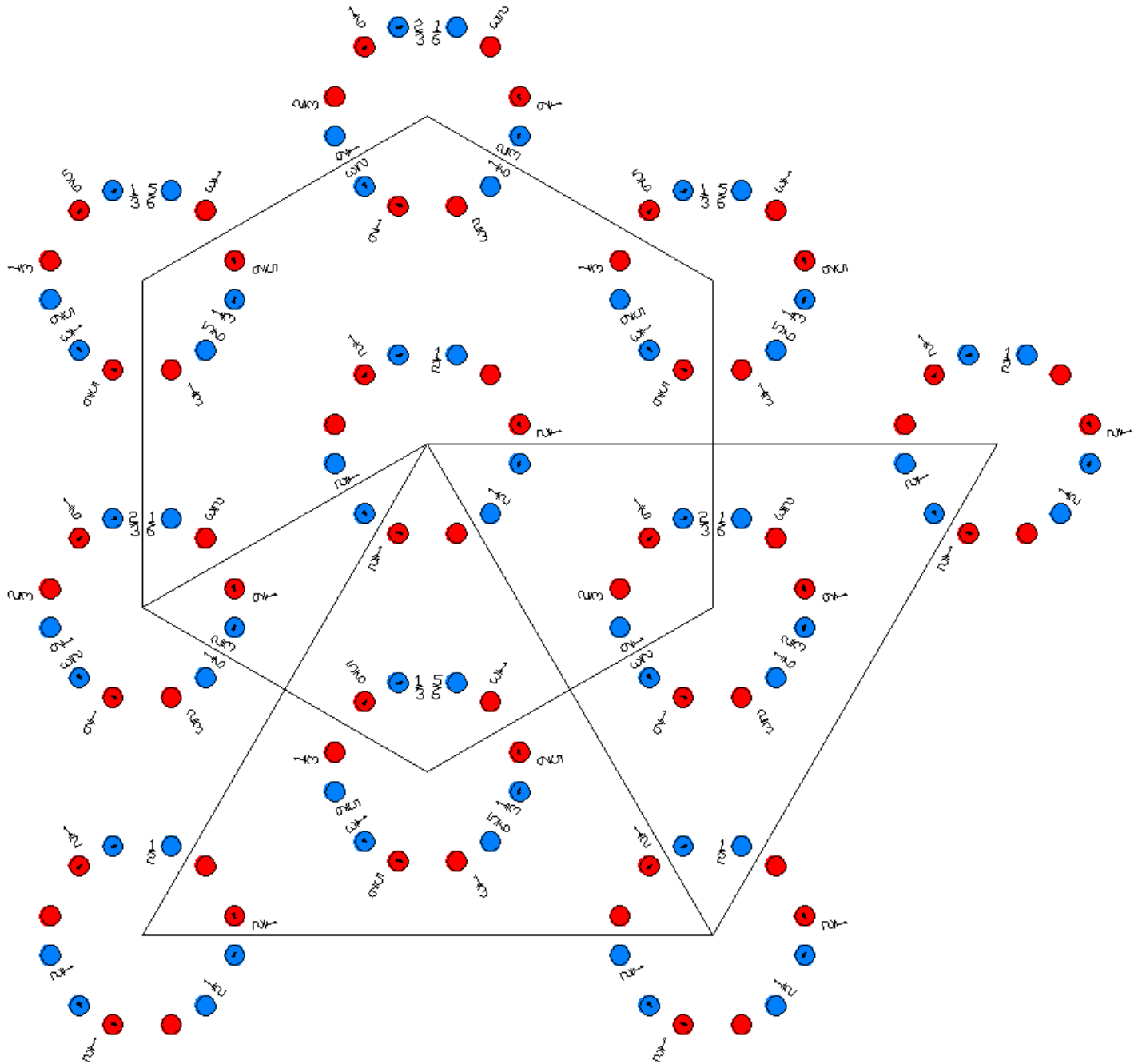
Along  $[2,1,0]$   $p2'm'g$   
 $\mathbf{a}^* = \mathbf{c}/3$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,0$



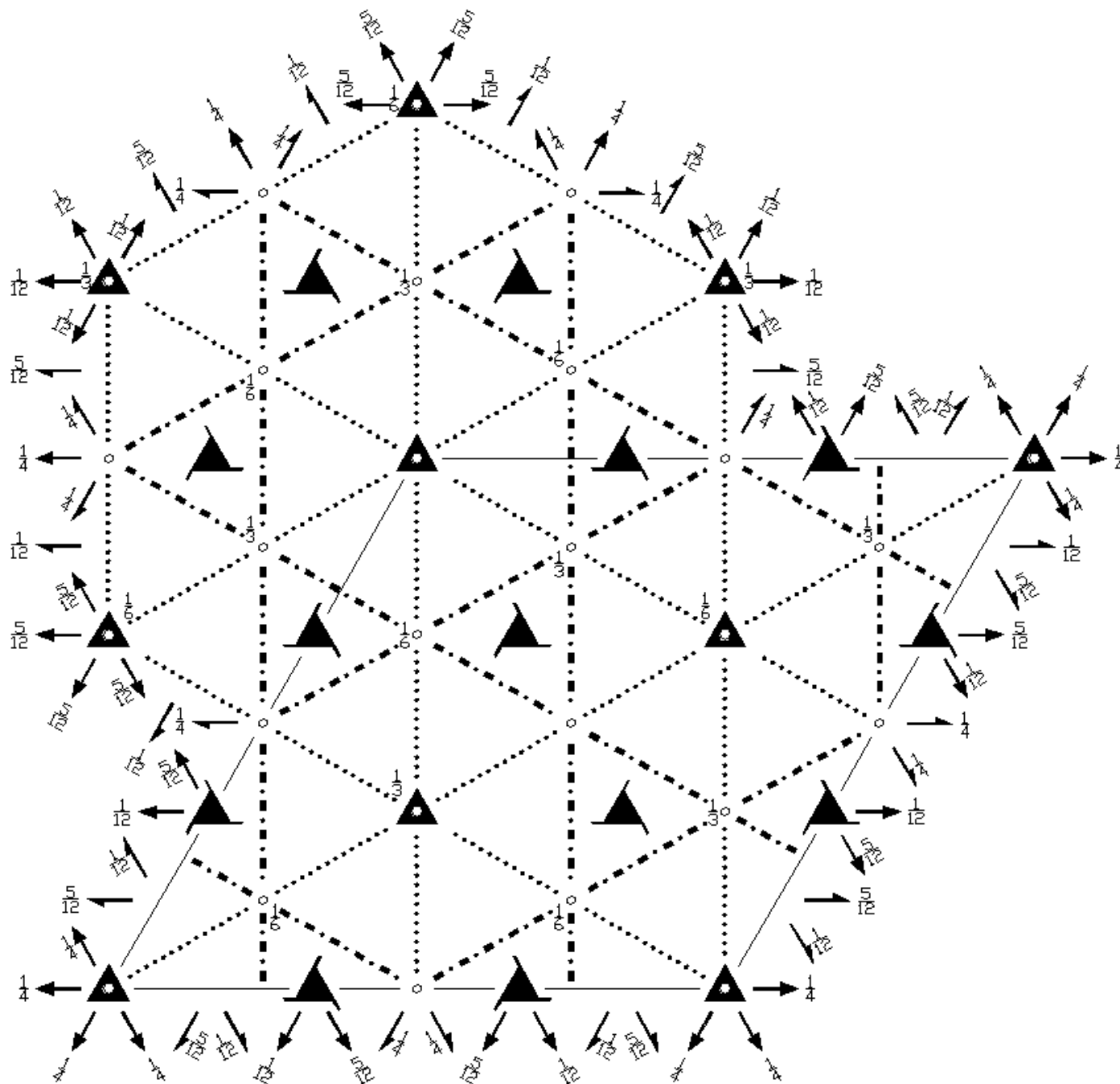
$R\bar{3}c1'$   
167.2.1335

$\bar{3}m1'$   
 $R\bar{3}2/c1'$

Trigonal



1'



Origin on ( $\bar{3}1'$ ) at  $\bar{3}c1'$

**Asymmetric unit**  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $0 \leq z \leq 1/12$ ;  $x \leq (1+y)/2$ ;  $y \leq \min(1-x, (1+x)/2)$

**Vertices**  $0,0,0$   $1/2,0,0$   $2/3,1/3,0$   $1/3,2/3,0$   $0,1/2,0$   
 $0,0,1/12$   $1/2,0,1/12$   $2/3,1/3,1/12$   $1/3,2/3,1/12$   $0,1/2,1/12$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |  |
|--|---|--|
| (1) $1$<br>( $1 0,0,0$ )                                 | (2) $3^+$ 0,0,z<br>( $3_z 0,0,0$ )                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1} 0,0,0$ )                    |
| (4) $2$ x,x,1/4<br>( $2_{xy} 0,0,1/2$ )                  | (5) $2$ x,0,1/4<br>( $2_x 0,0,1/2$ )                  | (6) $2$ 0,y,1/4<br>( $2_y 0,0,1/2$ )                       |
| (7) $\bar{1}$<br>( $\bar{1} 0,0,0$ )                     | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z 0,0,0$ ) | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1} 0,0,0$ ) |
| (10) c (0,0,1/2) x, $\bar{x}$ ,z<br>( $m_{xy} 0,0,1/2$ ) | (11) c (0,0,1/2) x,2x,z<br>( $m_x 0,0,1/2$ )          | (12) c (0,0,1/2) 2x,x,z<br>( $m_y 0,0,1/2$ )               |

For (2/3,1/3,1/3) + set

- |   |   |  |
|---|---|--|
| (1) t (2/3,1/3,1/3)<br>( $1 2/3,1/3,1/3$ )                            | (2) $3^+$ (0,0,1/3) 1/3,1/3,z<br>( $3_z 2/3,1/3,1/3$ )                  | (3) $3^-$ (0,0,1/3) 1/3,0,z<br>( $3_z^{-1} 2/3,1/3,1/3$ )                  |
| (4) $2$ (1/2,1/2,0) x,x-1/6,5/12<br>( $2_{xy} 2/3,1/3,5/6$ )          | (5) $2$ (1/2,0,0) x,1/6,5/12<br>( $2_x 2/3,1/3,5/6$ )                   | (6) $2$ 1/3,y,5/12<br>( $2_y 2/3,1/3,5/6$ )                                |
| (7) $\bar{1}$ 1/3,1/6,1/6<br>( $\bar{1} 2/3,1/3,1/3$ )                | (8) $\bar{3}^+$ 1/3,-1/3,z; 1/3,-1/3,1/6<br>( $\bar{3}_z 2/3,1/3,1/3$ ) | (9) $\bar{3}^-$ 1/3,2/3,z; 1/3,2/3,1/6<br>( $\bar{3}_z^{-1} 2/3,1/3,1/3$ ) |
| (10) g (1/6,-1/6,5/6) x+1/2, $\bar{x}$ ,z<br>( $m_{xy} 2/3,1/3,5/6$ ) | (11) g (1/6,1/3,5/6) x,2x-1/2,z<br>( $m_x 2/3,1/3,5/6$ )                | (12) g (2/3,1/3,5/6) 2x,x,z<br>( $m_y 2/3,1/3,5/6$ )                       |

For (1/3,2/3,2/3) + set

- |   |   |  |
|---|---|--|
| (1) t (1/3,2/3,2/3)<br>( $1 1/3,2/3,2/3$ )                            | (2) $3^+$ (0,0,2/3) 0,1/3,z<br>( $3_z 1/3,2/3,2/3$ )                  | (3) $3^-$ (0,0,2/3) 1/3,1/3,z<br>( $3_z^{-1} 1/3,2/3,2/3$ )                  |
| (4) $2$ (1/2,1/2,0) x,x+1/6,1/12<br>( $2_{xy} 1/3,2/3,1/6$ )          | (5) $2$ x,1/3,1/12<br>( $2_x 1/3,2/3,1/6$ )                           | (6) $2$ (0,1/2,0) 1/6,y,1/12<br>( $2_y 1/3,2/3,1/6$ )                        |
| (7) $\bar{1}$ 1/6,1/3,1/3<br>( $\bar{1} 1/3,2/3,2/3$ )                | (8) $\bar{3}^+$ 2/3,1/3,z; 2/3,1/3,1/3<br>( $\bar{3}_z 1/3,2/3,2/3$ ) | (9) $\bar{3}^-$ -1/3,1/3,z; -1/3,1/3,1/3<br>( $\bar{3}_z^{-1} 1/3,2/3,2/3$ ) |
| (10) g (-1/6,1/6,1/6) x+1/2, $\bar{x}$ ,z<br>( $m_{xy} 1/3,2/3,1/6$ ) | (11) g (1/3,2/3,1/6) x,2x,z<br>( $m_x 1/3,2/3,1/6$ )                  | (12) g (1/3,1/6,1/6) 2x-1/2,x,z<br>( $m_y 1/3,2/3,1/6$ )                     |

For (0,0,0)' + set

- |  |   |  |
|--|---|--|
| (1) $1'$<br>( $1 0,0,0$ )'                                 | (2) $3^{+'}$ 0,0,z<br>( $3_z 0,0,0$ )'                    | (3) $3^{-'}$ 0,0,z<br>( $3_z^{-1} 0,0,0$ )'                    |
| (4) $2'$ x,x,1/4<br>( $2_{xy} 0,0,1/2$ )'                  | (5) $2'$ x,0,1/4<br>( $2_x 0,0,1/2$ )'                    | (6) $2'$ 0,y,1/4<br>( $2_y 0,0,1/2$ )'                         |
| (7) $\bar{1}'$<br>( $\bar{1} 0,0,0$ )'                     | (8) $\bar{3}^{+'}$ 0,0,z; 0,0,0<br>( $\bar{3}_z 0,0,0$ )' | (9) $\bar{3}^{-'}$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1} 0,0,0$ )' |
| (10) c' (0,0,1/2) x, $\bar{x}$ ,z<br>( $m_{xy} 0,0,1/2$ )' | (11) c' (0,0,1/2) x,2x,z<br>( $m_x 0,0,1/2$ )'            | (12) c' (0,0,1/2) 2x,x,z<br>( $m_y 0,0,1/2$ )'                 |

## For (2/3,1/3,1/3)' + set

- |  |   |  |
|--|---|--|
| (1) $t' (2/3, 1/3, 1/3)$<br>(1   2/3, 1/3, 1/3)'                               | (2) $3^+ ' (0, 0, 1/3) \ 1/3, 1/3, z$<br>( $3_z$   2/3, 1/3, 1/3)'                    | (3) $3^- ' (0, 0, 1/3) \ 1/3, 0, z$<br>( $3_z^{-1}$   2/3, 1/3, 1/3)'                    |
| (4) $2' (1/2, 1/2, 0) \ x, x-1/6, 5/12$<br>( $2_{xy}$   2/3, 1/3, 5/6)'        | (5) $2' (1/2, 0, 0) \ x, 1/6, 5/12$<br>( $2_x$   2/3, 1/3, 5/6)'                      | (6) $2' \ 1/3, y, 5/12$<br>( $2_y$   2/3, 1/3, 5/6)'                                     |
| (7) $\bar{1}' \ 1/3, 1/6, 1/6$<br>( $\bar{1}$   2/3, 1/3, 1/3)'                | (8) $\bar{3}^+ ' \ 1/3, -1/3, z; \ 1/3, -1/3, 1/6$<br>( $\bar{3}_z$   2/3, 1/3, 1/3)' | (9) $\bar{3}^- ' \ 1/3, 2/3, z; \ 1/3, 2/3, 1/6$<br>( $\bar{3}_z^{-1}$   2/3, 1/3, 1/3)' |
| (10) $g' (1/6, -1/6, 5/6) \ x+1/2, \bar{x}, z$<br>( $m_{xy}$   2/3, 1/3, 5/6)' | (11) $g' (1/6, 1/3, 5/6) \ x, 2x-1/2, z$<br>( $m_x$   2/3, 1/3, 5/6)'                 | (12) $g' (2/3, 1/3, 5/6) \ 2x, x, z$<br>( $m_y$   2/3, 1/3, 5/6)'                        |

## For (1/3,2/3,2/3)' + set

- |  |   |  |
|--|---|--|
| (1) $t' (1/3, 2/3, 2/3)$<br>(1   1/3, 2/3, 2/3)'                               | (2) $3^+ ' (0, 0, 2/3) \ 0, 1/3, z$<br>( $3_z$   1/3, 2/3, 2/3)'                    | (3) $3^- ' (0, 0, 2/3) \ 1/3, 1/3, z$<br>( $3_z^{-1}$   1/3, 2/3, 2/3)'                    |
| (4) $2' (1/2, 1/2, 0) \ x, x+1/6, 1/12$<br>( $2_{xy}$   1/3, 2/3, 1/6)'        | (5) $2' \ x, 1/3, 1/12$<br>( $2_x$   1/3, 2/3, 1/6)'                                | (6) $2' (0, 1/2, 0) \ 1/6, y, 1/12$<br>( $2_y$   1/3, 2/3, 1/6)'                           |
| (7) $\bar{1}' \ 1/6, 1/3, 1/3$<br>( $\bar{1}$   1/3, 2/3, 2/3)'                | (8) $\bar{3}^+ ' \ 2/3, 1/3, z; \ 2/3, 1/3, 1/3$<br>( $\bar{3}_z$   1/3, 2/3, 2/3)' | (9) $\bar{3}^- ' \ -1/3, 1/3, z; \ -1/3, 1/3, 1/3$<br>( $\bar{3}_z^{-1}$   1/3, 2/3, 2/3)' |
| (10) $g' (-1/6, 1/6, 1/6) \ x+1/2, \bar{x}, z$<br>( $m_{xy}$   1/3, 2/3, 1/6)' | (11) $g' (1/3, 2/3, 1/6) \ x, 2x, z$<br>( $m_x$   1/3, 2/3, 1/6)'                   | (12) $g' (1/3, 1/6, 1/6) \ 2x-1/2, x, z$<br>( $m_y$   1/3, 2/3, 1/6)'                      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4); (7); 1'.

**Positions**

			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) + (0,0,0)' +	(2/3,1/3,1/3) + (2/3,1/3,1/3)' +	(1/3,2/3,2/3) + (1/3,2/3,2/3)' +
36	f	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}, x-y, z$ [0,0,0]	(3) $\bar{x}+y, \bar{x}, z$ [0,0,0]
			(4) y,x, $\bar{z}+1/2$ [0,0,0]	(5) x-y, $\bar{y}, \bar{z}+1/2$ [0,0,0]	(6) $\bar{x}, \bar{x}+y, \bar{z}+1/2$ [0,0,0]
			(7) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]	(8) y, $\bar{x}+y, \bar{z}$ [0,0,0]	(9) x-y,x, $\bar{z}$ [0,0,0]
			(10) $\bar{y}, \bar{x}, z+1/2$ [0,0,0]	(11) $\bar{x}+y, y, z+1/2$ [0,0,0]	(12) x,x-y,z+1/2 [0,0,0]
18	e	.21'	x,0,1/4 [0,0,0]	0,x,1/4 [0,0,0]	$\bar{x}, \bar{x}, 1/4$ [0,0,0]
			$\bar{x}, 0, 3/4$ [0,0,0]	0, $\bar{x}, 3/4$ [0,0,0]	x,x,3/4 [0,0,0]
18	d	$\bar{1}1'$	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]
			0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]
12	c	3.1'	0,0,z [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]
					0,0,z+1/2 [0,0,0]

Continued

167.2.1335

$\overline{R3c1'}$

6      b       $\overline{3.1'}$       0,0,0 [0,0,0]      0,0,1/2 [0,0,0]

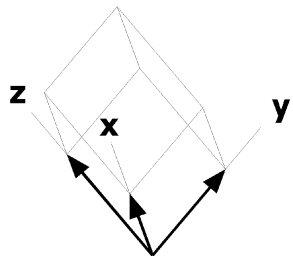
6      a      321'      0,0,1/4 [0,0,0]      0,0,3/4 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]      p6mm1'  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$        $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
Origin at 0,0,z

Along [1,0,0]      p2111'  
 $\mathbf{a}^* = (2\mathbf{a} + 4\mathbf{b} + \mathbf{c})/6$        $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,0

Along [2,1,0]      p2mg1'  
 $\mathbf{a}^* = \mathbf{c}/3$        $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,x/2,0



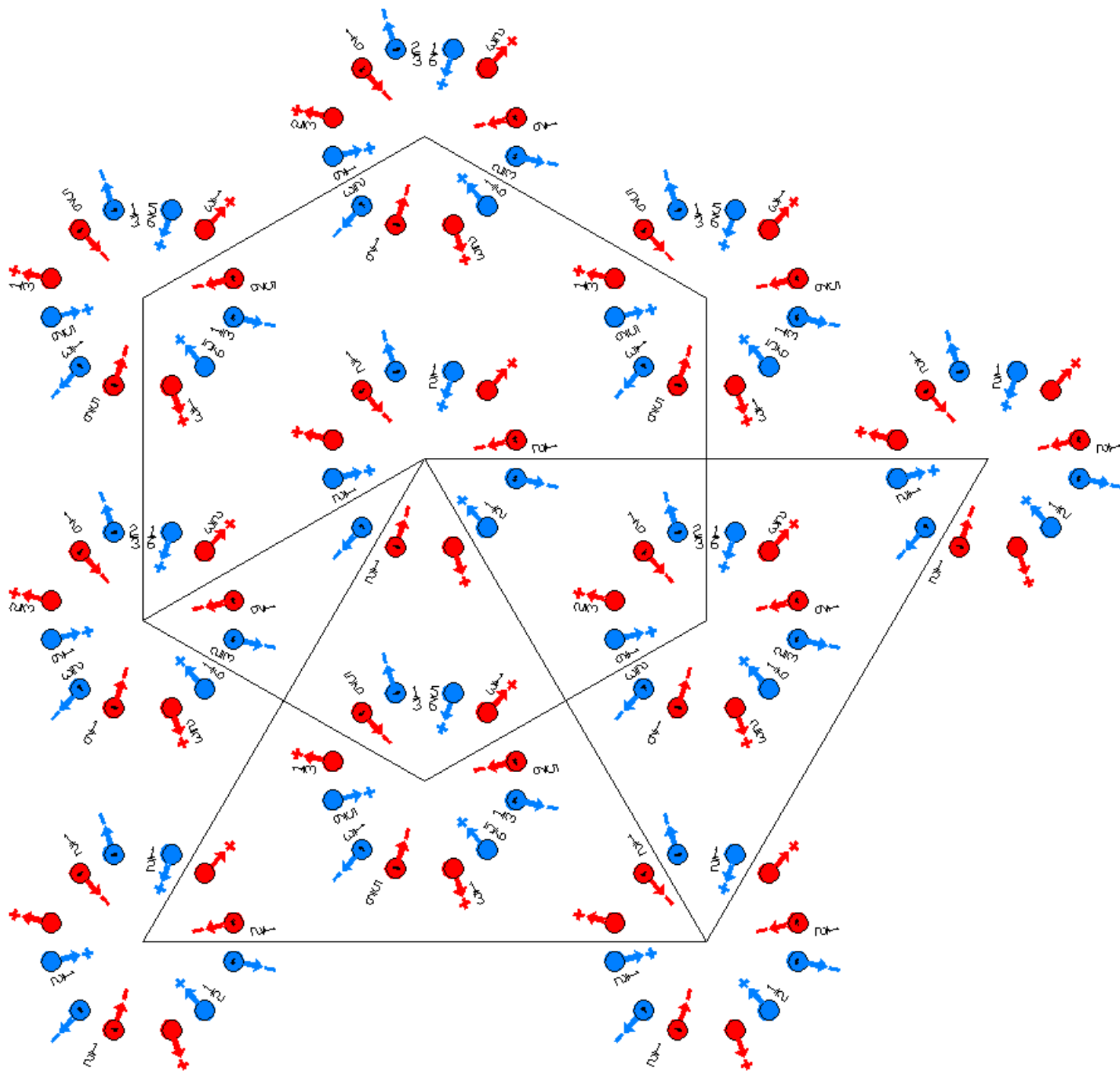
$R\bar{3}c$

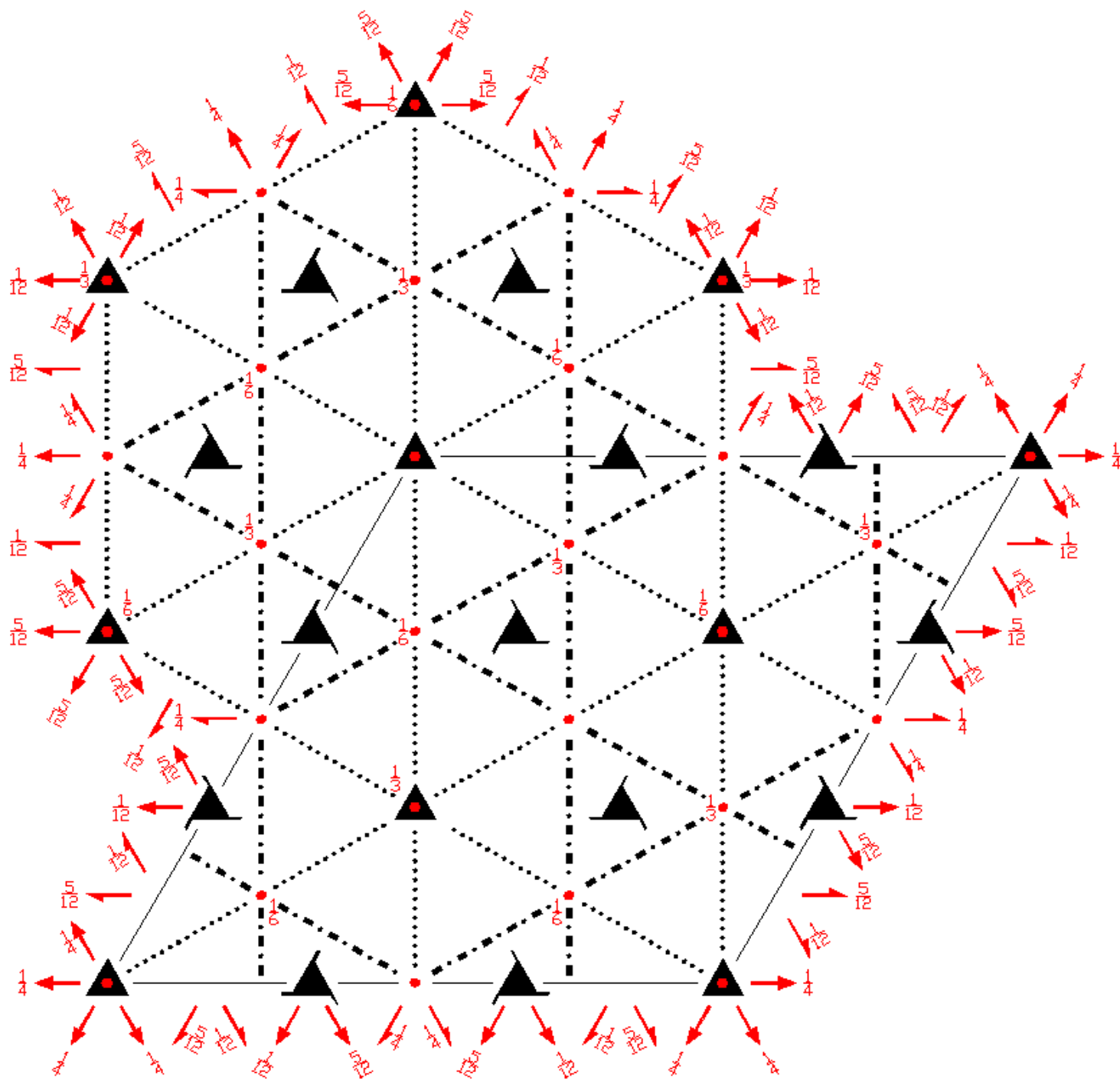
167.3.1336

$\bar{3}m$

$R\bar{3}2'/c$

Trigonal





Origin on ( $\bar{3}$ ') at  $\bar{3}$ 'c

**Asymmetric unit**  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $0 \leq z \leq 1/12$ ;  $x \leq (1+y)/2$ ;  $y \leq \min(1-x, (1+x)/2)$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/12	1/2,0,1/12	2/3,1/3,1/12	1/3,2/3,1/12	0,1/2,1/12



**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |
|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)                            | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)                            |
| (4) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                  | (5) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'                                   | (6) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'   |
| (7) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)'                        | (8) $\bar{3}$ <sup>+</sup> ' 0,0,z; 0,0,0<br>( $\bar{3}$ <sub>z</sub>  0,0,0)' | (9) $\bar{3}$ <sup>-</sup> ' 0,0,z; 0,0,0<br>( $\bar{3}$ <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (10) c (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2) | (11) c (0,0,1/2) x,2x,z<br>(m <sub>x</sub>  0,0,1/2)                           | (12) c (0,0,1/2) 2x,x,z<br>(m <sub>y</sub>  0,0,1/2)   |

For (2/3,1/3,1/3) + set

- |   |  |  |
|---|--|--|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)                                      | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3)                          | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3)                          |
| (4) 2'(1/2,1/2,0) x,x-1/6,5/12<br>(2 <sub>xy</sub>  2/3,1/3,5/6)'           | (5) 2' (1/2,0,0) x,1/6,5/12<br>(2 <sub>x</sub>  2/3,1/3,5/6)'                                    | (6) 2' 1/3,y,5/12<br>(2 <sub>y</sub>  2/3,1/3,5/6)'  |
| (7) $\bar{1}$ ' 1/3,1/6,1/6<br>( $\bar{1}$  2/3,1/3,1/3)'                   | (8) $\bar{3}$ <sup>+</sup> ' 1/3,-1/3,z; 1/3,-1/3,1/6<br>( $\bar{3}$ <sub>z</sub>  2/3,1/3,1/3)' | (9) $\bar{3}$ <sup>-</sup> ' 1/3,2/3,z; 1/3,2/3,1/6<br>( $\bar{3}$ <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3)' |
| (10) g (1/6,-1/6,5/6) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  2/3,1/3,5/6) | (11) g (1/6,1/3,5/6) x,2x-1/2,z<br>(m <sub>x</sub>  2/3,1/3,5/6)                                 | (12) g (2/3,1/3,5/6) 2x,x,z<br>(m <sub>y</sub>  2/3,1/3,5/6)   |

For (1/3,2/3,2/3) + set

- |   |  |  |
|---|--|--|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)                                      | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3)                          | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3)                          |
| (4) 2'(1/2,1/2,0) x,x+1/6,1/12<br>(2 <sub>xy</sub>  1/3,2/3,1/6)'           | (5) 2' x,1/3,1/12<br>(2 <sub>x</sub>  1/3,2/3,1/6)'  | (6) 2' (0,1/2,0) 1/6,y,1/12<br>(2 <sub>y</sub>  1/3,2/3,1/6)'  |
| (7) $\bar{1}$ ' 1/6,1/3,1/3<br>( $\bar{1}$  1/3,2/3,2/3)'                   | (8) $\bar{3}$ <sup>+</sup> ' 2/3,1/3,z; 2/3,1/3,1/3<br>( $\bar{3}$ <sub>z</sub>  1/3,2/3,2/3)' | (9) $\bar{3}$ <sup>-</sup> ' -1/3,1/3,z; -1/3,1/3,1/3<br>( $\bar{3}$ <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3)' |
| (10) g (-1/6,1/6,1/6) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/3,2/3,1/6) | (11) g (1/3,2/3,1/6) x,2x,z<br>(m <sub>x</sub>  1/3,2/3,1/6)                                   | (12) g (1/3,1/6,1/6) 2x-1/2,x,z<br>(m <sub>y</sub>  1/3,2/3,1/6)   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4); (7).**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (2/3,1/3,1/3) + (1/3,2/3,2/3) +

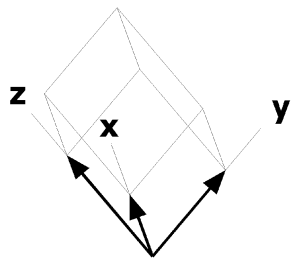
36	f	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$
			(4) $y,x,\bar{z}+1/2 [\bar{v},\bar{u},w]$	(5) $x-y,\bar{y},\bar{z}+1/2 [\bar{u}+v,v,w]$	(6) $\bar{x},\bar{x}+y,\bar{z}+1/2 [u,u-v,w]$
			(7) $\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$	(8) $y,\bar{x}+y,\bar{z} [v,\bar{u}+v,\bar{w}]$	(9) $x-y,x,\bar{z} [u-v,u,\bar{w}]$
			(10) $\bar{y},\bar{x},z+1/2 [v,u,\bar{w}]$	(11) $\bar{x}+y,y,z+1/2 [u-v,\bar{v},\bar{w}]$	(12) $x,x-y,z+1/2 [\bar{u},\bar{u}+v,\bar{w}]$
18	e	.2'	$x,0,1/4 [u,2u,w]$	$0,x,1/4 [2\bar{u},\bar{u},w]$	$\bar{x},\bar{x},1/4 [u,\bar{u},w]$
			$\bar{x},0,3/4 [\bar{u},2\bar{u},\bar{w}]$	$0,\bar{x},3/4 [2u,u,\bar{w}]$	$x,x,3/4 [\bar{u},u,\bar{w}]$
18	d	$\bar{1}'$	$1/2,0,0 [0,0,0]$	$0,1/2,0 [0,0,0]$	$1/2,1/2,0 [0,0,0]$
			$0,1/2,1/2 [0,0,0]$	$1/2,0,1/2 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$
12	c	3.	$0,0,z [0,0,w]$	$0,0,\bar{z}+1/2 [0,0,w]$	$0,0,\bar{z} [0,0,\bar{w}]$
					$0,0,z+1/2 [0,0,\bar{w}]$
6	b	$\bar{3}'$ .	$0,0,0 [0,0,0]$	$0,0,1/2 [0,0,0]$	
6	a	32'	$0,0,1/4 [0,0,w]$	$0,0,3/4 [0,0,\bar{w}]$	

### Symmetry of Special Projections

Along  $[0,0,1]$  p6mm  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p2111'  
 $\mathbf{a}^* = (2\mathbf{a} + 4\mathbf{b} + \mathbf{c})/6$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

Along  $[2,1,0]$  p2mg  
 $\mathbf{a}^* = \mathbf{c}/3$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,0$



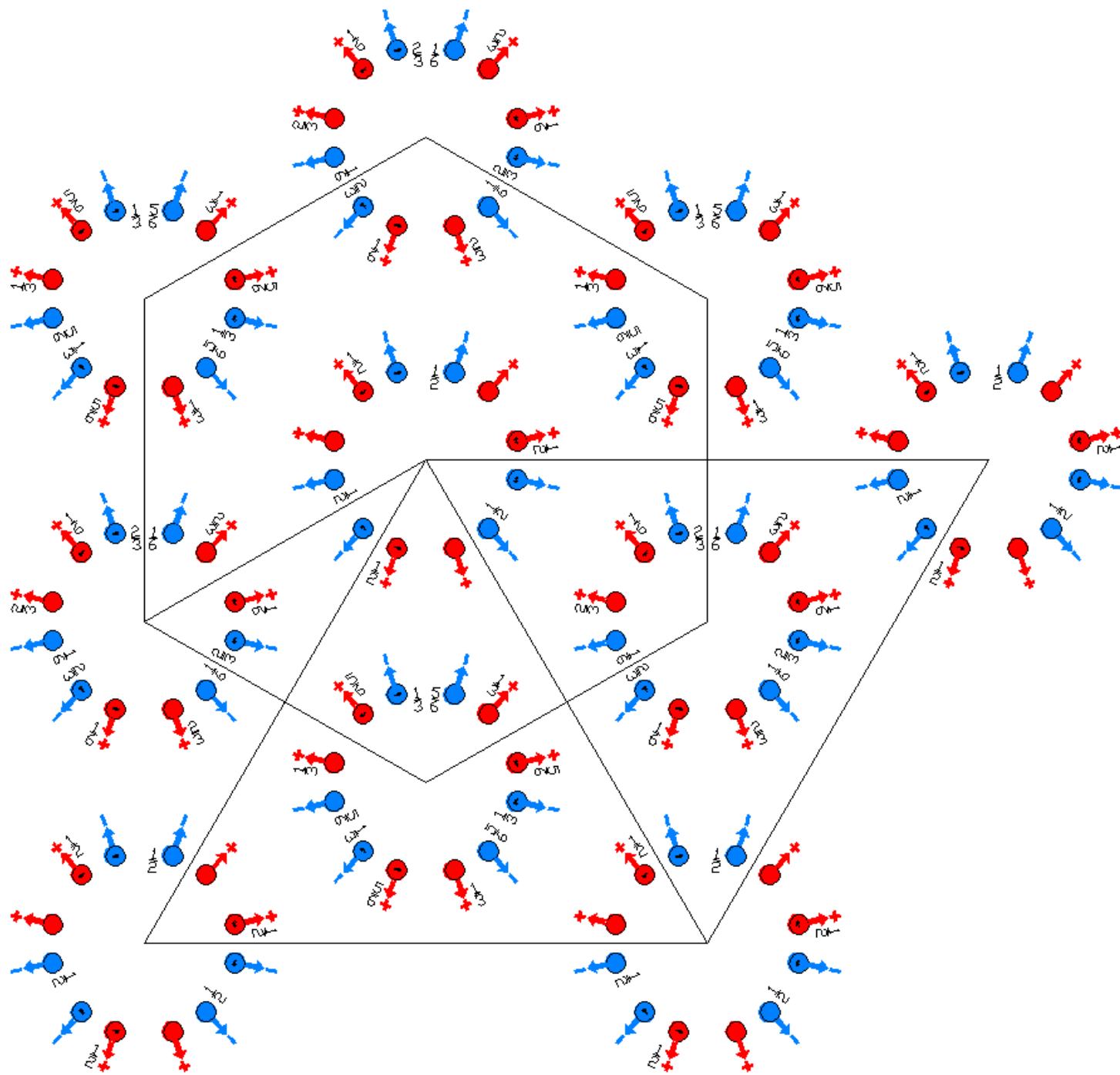
$R\bar{3}'c'$

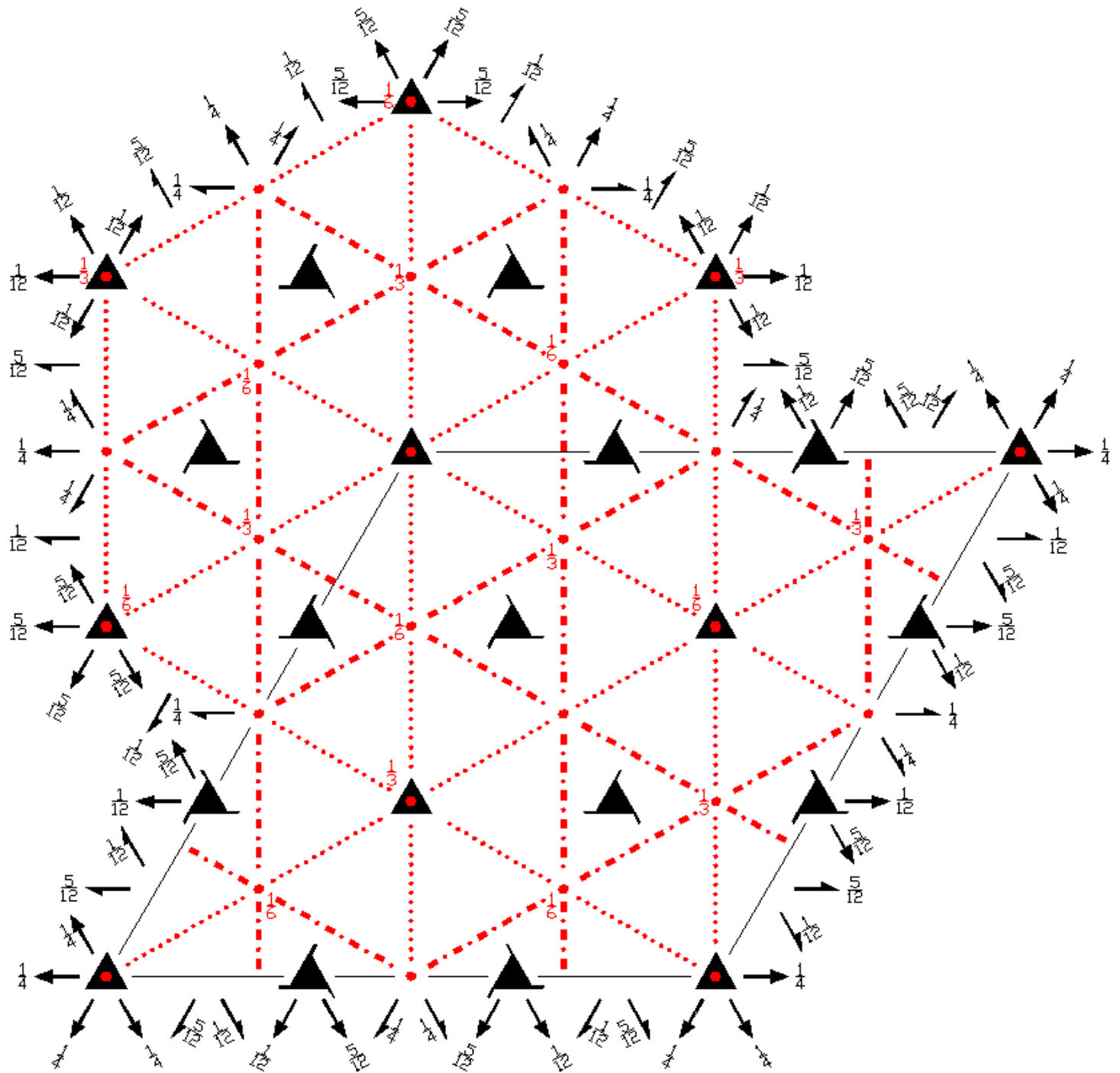
167.4.1337

$\bar{3}'m'$

$R\bar{3}'2/c'$

Trigonal





Origin on ( $\bar{3}'$ ) at  $\bar{3}'c'$

**Asymmetric unit**  $0 \leq x \leq 2/3;$   $0 \leq y \leq 2/3;$   $0 \leq z \leq 1/12;$   $x \leq (1+y)/2;$   $y \leq \min(1-x, (1+x)/2)$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/12	1/2,0,1/12	2/3,1/3,1/12	1/3,2/3,1/12	0,1/2,1/12

**Symmetry Operations**

For (0,0,0) + set

- |  |  |  |
|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)                            | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)                            |
| (4) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)                      | (5) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)                                     | (6) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)   |
| (7) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)'                          | (8) $\bar{3}$ <sup>+</sup> ' 0,0,z; 0,0,0<br>( $\bar{3}$ <sub>z</sub>  0,0,0)' | (9) $\bar{3}$ <sup>-</sup> ' 0,0,z; 0,0,0<br>( $\bar{3}$ <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (10) c' (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2)' | (11) c' (0,0,1/2) x,2x,z<br>(m <sub>x</sub>  0,0,1/2)'                         | (12) c' (0,0,1/2) 2x,x,z<br>(m <sub>y</sub>  0,0,1/2)'                                       |

For (2/3,1/3,1/3) + set

- |   |  |  |
|---|--|--|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)  | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3)                          | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3)                          |
| (4) 2(1/2,1/2,0) x,x-1/6,5/12<br>(2 <sub>xy</sub>  2/3,1/3,5/6)               | (5) 2 (1/2,0,0) x,1/6,5/12<br>(2 <sub>x</sub>  2/3,1/3,5/6)                                      | (6) 2 1/3,y,5/12<br>(2 <sub>y</sub>  2/3,1/3,5/6)  |
| (7) $\bar{1}$ ' 1/3,1/6,1/6<br>( $\bar{1}$  2/3,1/3,1/3)'                     | (8) $\bar{3}$ <sup>+</sup> ' 1/3,-1/3,z; 1/3,-1/3,1/6<br>( $\bar{3}$ <sub>z</sub>  2/3,1/3,1/3)' | (9) $\bar{3}$ <sup>-</sup> ' 1/3,2/3,z; 1/3,2/3,1/6<br>( $\bar{3}$ <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3)' |
| (10) g' (1/6,-1/6,5/6) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  2/3,1/3,5/6)' | (11) g' (1/6,1/3,5/6) x,2x-1/2,z<br>(m <sub>x</sub>  2/3,1/3,5/6)'                               | (12) g' (2/3,1/3,5/6) 2x,x,z<br>(m <sub>y</sub>  2/3,1/3,5/6)'   |

For (1/3,2/3,2/3) + set

- |   |  |  |
|---|--|--|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)  | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3)                          | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3)                          |
| (4) 2(1/2,1/2,0) x,x+1/6,1/12<br>(2 <sub>xy</sub>  1/3,2/3,1/6)               | (5) 2 x,1/3,1/12<br>(2 <sub>x</sub>  1/3,2/3,1/6)  | (6) 2 (0,1/2,0) 1/6,y,1/12<br>(2 <sub>y</sub>  1/3,2/3,1/6)  |
| (7) $\bar{1}$ ' 1/6,1/3,1/3<br>( $\bar{1}$  1/3,2/3,2/3)'                     | (8) $\bar{3}$ <sup>+</sup> ' 2/3,1/3,z; 2/3,1/3,1/3<br>( $\bar{3}$ <sub>z</sub>  1/3,2/3,2/3)' | (9) $\bar{3}$ <sup>-</sup> ' -1/3,1/3,z; -1/3,1/3,1/3<br>( $\bar{3}$ <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3)' |
| (10) g' (-1/6,1/6,1/6) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/3,2/3,1/6)' | (11) g' (1/3,2/3,1/6) x,2x,z<br>(m <sub>x</sub>  1/3,2/3,1/6)'                                 | (12) g' (1/3,1/6,1/6) 2x-1/2,x,z<br>(m <sub>y</sub>  1/3,2/3,1/6)'   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4); (7).**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (2/3,1/3,1/3) + (1/3,2/3,2/3) +

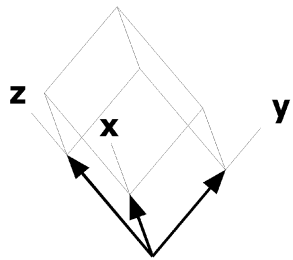
36	f	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$
			(4) $y,x,\bar{z}+1/2 [v,u,\bar{w}]$	(5) $x-y,\bar{y},\bar{z}+1/2 [u-v,\bar{v},\bar{w}]$	(6) $\bar{x},\bar{x}+y,\bar{z}+1/2 [\bar{u},\bar{u}+v,\bar{w}]$
			(7) $\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$	(8) $y,\bar{x}+y,\bar{z} [v,\bar{u}+v,\bar{w}]$	(9) $x-y,x,\bar{z} [u-v,u,\bar{w}]$
			(10) $\bar{y},\bar{x},\bar{z}+1/2 [\bar{v},\bar{u},w]$	(11) $\bar{x}+y,y,\bar{z}+1/2 [\bar{u}+v,v,w]$	(12) $x,x-y,\bar{z}+1/2 [u,u-v,w]$
18	e	.2	$x,0,1/4 [u,0,0]$	$0,x,1/4 [0,u,0]$	$\bar{x},\bar{x},1/4 [\bar{u},\bar{u},0]$
			$\bar{x},0,3/4 [\bar{u},0,0]$	$0,\bar{x},3/4 [0,\bar{u},0]$	$x,x,3/4 [u,u,0]$
18	d	$\bar{1}'$	$1/2,0,0 [0,0,0]$	$0,1/2,0 [0,0,0]$	$1/2,1/2,0 [0,0,0]$
			$0,1/2,1/2 [0,0,0]$	$1/2,0,1/2 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$
12	c	3.	$0,0,z [0,0,w]$	$0,0,\bar{z}+1/2 [0,0,\bar{w}]$	$0,0,\bar{z} [0,0,\bar{w}]$
					$0,0,z+1/2 [0,0,w]$
6	b	$\bar{3}'$ .	$0,0,0 [0,0,0]$	$0,0,1/2 [0,0,0]$	
6	a	32	$0,0,1/4 [0,0,0]$	$0,0,3/4 [0,0,0]$	

### Symmetry of Special Projections

Along  $[0,0,1]$  p6m'm'  
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p211  
 $\mathbf{a}^* = (2\mathbf{a} + 4\mathbf{b} + \mathbf{c})/6$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

Along  $[2,1,0]$  p2m'g'  
 $\mathbf{a}^* = \mathbf{c}/3$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,0$



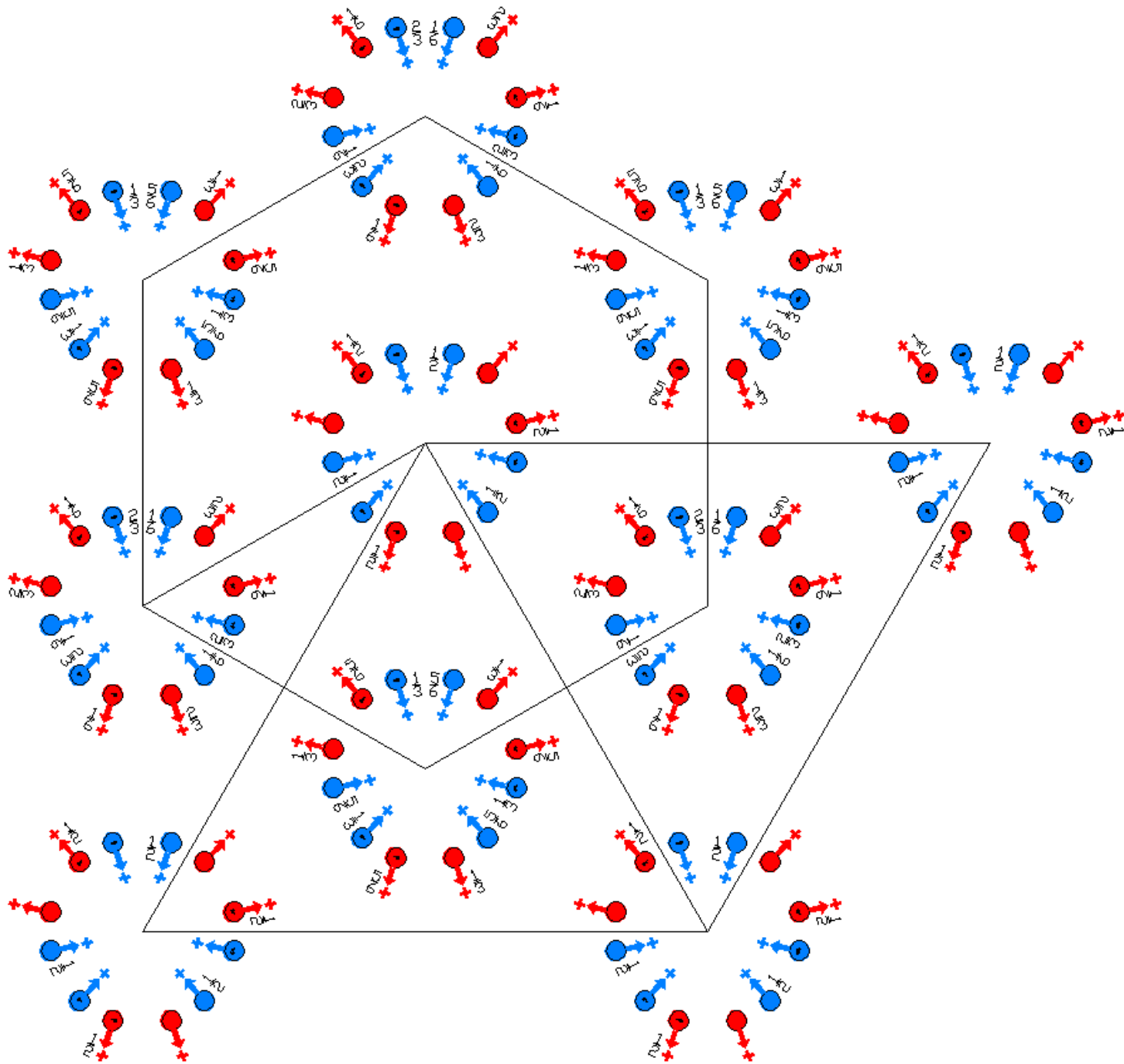
$R\bar{3}c'$

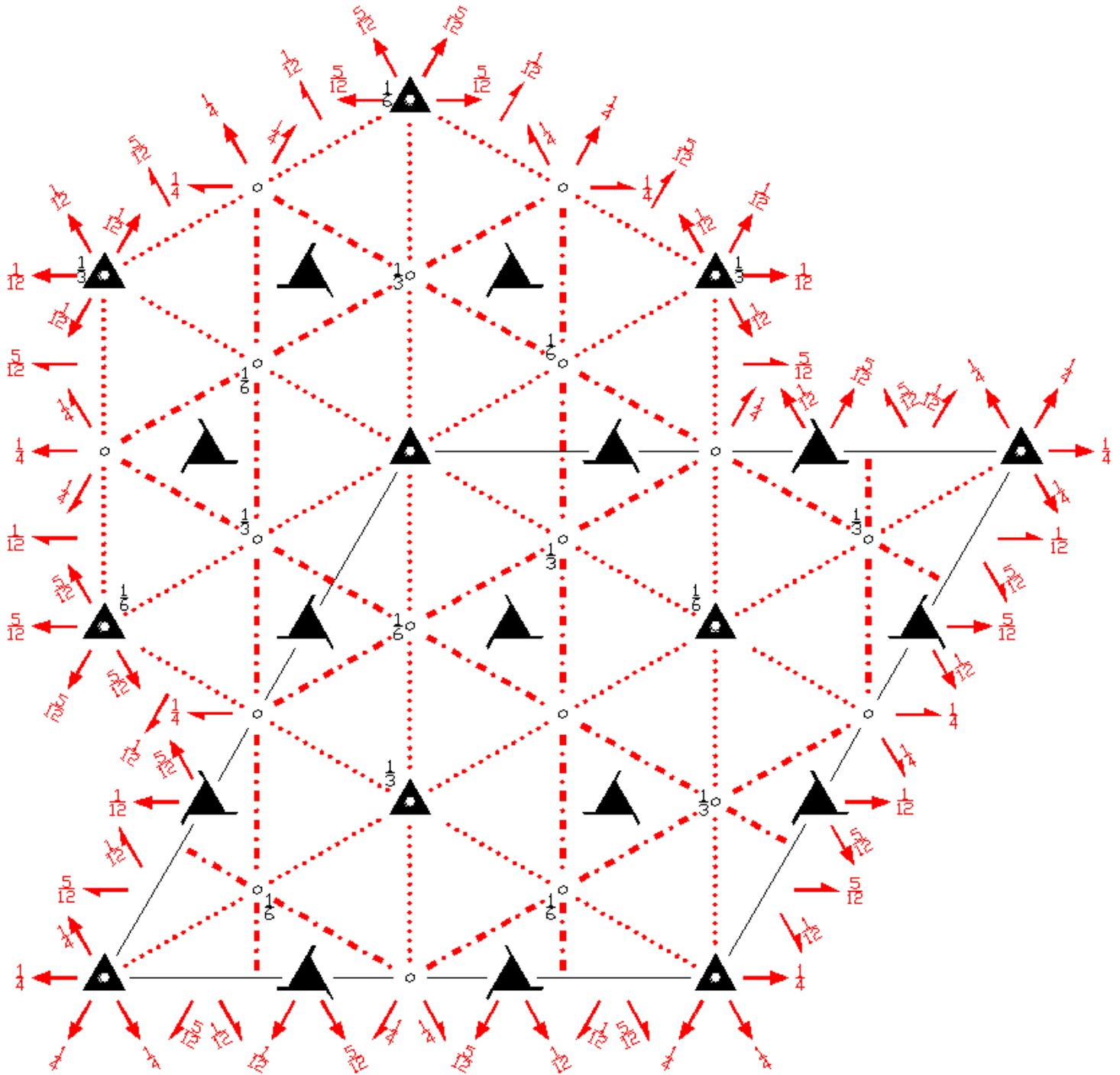
167.5.1338

$\bar{3}m'$

$R\bar{3}2'/c'$

Trigonal





Origin on  $(\bar{3})$  at  $\bar{3}c'$

**Asymmetric unit**  $0 \leq x \leq 2/3;$   $0 \leq y \leq 2/3;$   $0 \leq z \leq 1/12;$   $x \leq (1+y)/2;$   $y \leq \min(1-x, (1+x)/2)$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/12	1/2,0,1/12	2/3,1/3,1/12	1/3,2/3,1/12	0,1/2,1/12



**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)   | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)    | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'                    | (5) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'           | (6) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'                      |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)                             | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)  | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)        |
| (10) c' (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1/2)' | (11) c' (0,0,1/2) x,2x,z<br>(m <sub>x</sub>  0,0,1/2)' | (12) c' (0,0,1/2) 2x,x,z<br>(m <sub>y</sub>  0,0,1/2)'            |

For (2/3,1/3,1/3) + set

- |   |   |   |
|---|---|---|
| (1) t (2/3,1/3,1/3)<br>(1 2/3,1/3,1/3)  | (2) 3 <sup>+</sup> (0,0,1/3) 1/3,1/3,z<br>(3 <sub>z</sub>  2/3,1/3,1/3) | (3) 3 <sup>-</sup> (0,0,1/3) 1/3,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  2/3,1/3,1/3) |
| (4) 2'(1/2,1/2,0) x,x-1/6,5/12<br>(2 <sub>xy</sub>  2/3,1/3,5/6)'             | (5) 2' (1/2,0,0) x,1/6,5/12<br>(2 <sub>x</sub>  2/3,1/3,5/6)'           | (6) 2' 1/3,y,5/12<br>(2 <sub>y</sub>  2/3,1/3,5/6)'                                 |
| (7) $\bar{1}$ 1/3,1/6,1/6<br>( $\bar{1}$  2/3,1/3,1/3)                        | (8) $\bar{3}^+$ 1/3,-1/3,z; 1/3,-1/3,1/6<br>( $\bar{3}_z$  2/3,1/3,1/3) | (9) $\bar{3}^-$ 1/3,2/3,z; 1/3,2/3,1/6<br>( $\bar{3}_z^{-1}$  2/3,1/3,1/3)          |
| (10) g' (1/6,-1/6,5/6) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  2/3,1/3,5/6)' | (11) g' (1/6,1/3,5/6) x,2x-1/2,z<br>(m <sub>x</sub>  2/3,1/3,5/6)'      | (12) g' (2/3,1/3,5/6) 2x,x,z<br>(m <sub>y</sub>  2/3,1/3,5/6)'                      |

For (1/3,2/3,2/3) + set

- |   |   |   |
|---|---|---|
| (1) t (1/3,2/3,2/3)<br>(1 1/3,2/3,2/3)  | (2) 3 <sup>+</sup> (0,0,2/3) 0,1/3,z<br>(3 <sub>z</sub>  1/3,2/3,2/3) | (3) 3 <sup>-</sup> (0,0,2/3) 1/3,1/3,z<br>(3 <sub>z</sub> <sup>-1</sup>  1/3,2/3,2/3) |
| (4) 2'(1/2,1/2,0) x,x+1/6,1/12<br>(2 <sub>xy</sub>  1/3,2/3,1/6)'             | (5) 2' x,1/3,1/12<br>(2 <sub>x</sub>  1/3,2/3,1/6)'                   | (6) 2' (0,1/2,0) 1/6,y,1/12<br>(2 <sub>y</sub>  1/3,2/3,1/6)'                         |
| (7) $\bar{1}$ 1/6,1/3,1/3<br>( $\bar{1}$  1/3,2/3,2/3)                        | (8) $\bar{3}^+$ 2/3,1/3,z; 2/3,1/3,1/3<br>( $\bar{3}_z$  1/3,2/3,2/3) | (9) $\bar{3}^-$ -1/3,1/3,z; -1/3,1/3,1/3<br>( $\bar{3}_z^{-1}$  1/3,2/3,2/3)          |
| (10) g' (-1/6,1/6,1/6) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/3,2/3,1/6)' | (11) g' (1/3,2/3,1/6) x,2x,z<br>(m <sub>x</sub>  1/3,2/3,1/6)'        | (12) g' (1/3,1/6,1/6) 2x-1/2,x,z<br>(m <sub>y</sub>  1/3,2/3,1/6)'                    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4); (7).**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (2/3,1/3,1/3) + (1/3,2/3,2/3) +

Continued

167.5.1338

R $\bar{3}c'$ 

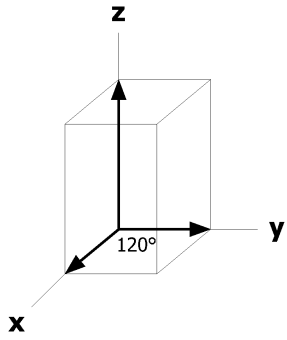
36	f	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$
			(4) $y,x,\bar{z}+1/2 [\bar{v},\bar{u},w]$	(5) $x-y,\bar{y},\bar{z}+1/2 [\bar{u}+v,v,w]$	(6) $\bar{x},\bar{x}+y,\bar{z}+1/2 [u,u-v,w]$
			(7) $\bar{x},\bar{y},\bar{z} [u,v,w]$	(8) $y,\bar{x}+y,\bar{z} [\bar{v},u-v,w]$	(9) $x-y,x,\bar{z} [\bar{u}+v,\bar{u},w]$
			(10) $\bar{y},\bar{x},\bar{z}+1/2 [\bar{v},\bar{u},w]$	(11) $\bar{x}+y,y,\bar{z}+1/2 [\bar{u}+v,v,w]$	(12) $x,x-y,\bar{z}+1/2 [u,u-v,w]$
18	e	.2'	$x,0,1/4 [u,2u,w]$	$0,x,1/4 [2\bar{u},\bar{u},w]$	$\bar{x},\bar{x},1/4 [u,\bar{u},w]$
			$\bar{x},0,3/4 [u,2u,w]$	$0,\bar{x},3/4 [2\bar{u},\bar{u},w]$	$x,x,3/4 [u,\bar{u},w]$
18	d	$\bar{1}$	$1/2,0,0 [u,v,w]$	$0,1/2,0 [\bar{v},u-v,w]$	$1/2,1/2,0 [\bar{u}+v,\bar{u},w]$
			$0,1/2,1/2 [\bar{v},\bar{u},w]$	$1/2,0,1/2 [\bar{u}+v,v,w]$	$1/2,1/2,1/2 [u,u-v,w]$
12	c	3.	$0,0,z [0,0,w]$	$0,0,\bar{z}+1/2 [0,0,w]$	$0,0,\bar{z} [0,0,w]$
					$0,0,z+1/2 [0,0,w]$
6	b	$\bar{3}$ .	$0,0,0 [0,0,w]$	$0,0,1/2 [0,0,w]$	
6	a	32'	$0,0,1/4 [0,0,w]$	$0,0,3/4 [0,0,w]$	

### Symmetry of Special Projections

Along  $[0,0,1]$   $p6'm'm$   
 $\mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3$   $\mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2'11$   
 $\mathbf{a}^* = (2\mathbf{a} + 4\mathbf{b} + \mathbf{c})/6$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

Along  $[2,1,0]$   $p2'mg'$   
 $\mathbf{a}^* = \mathbf{c}/3$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,0$



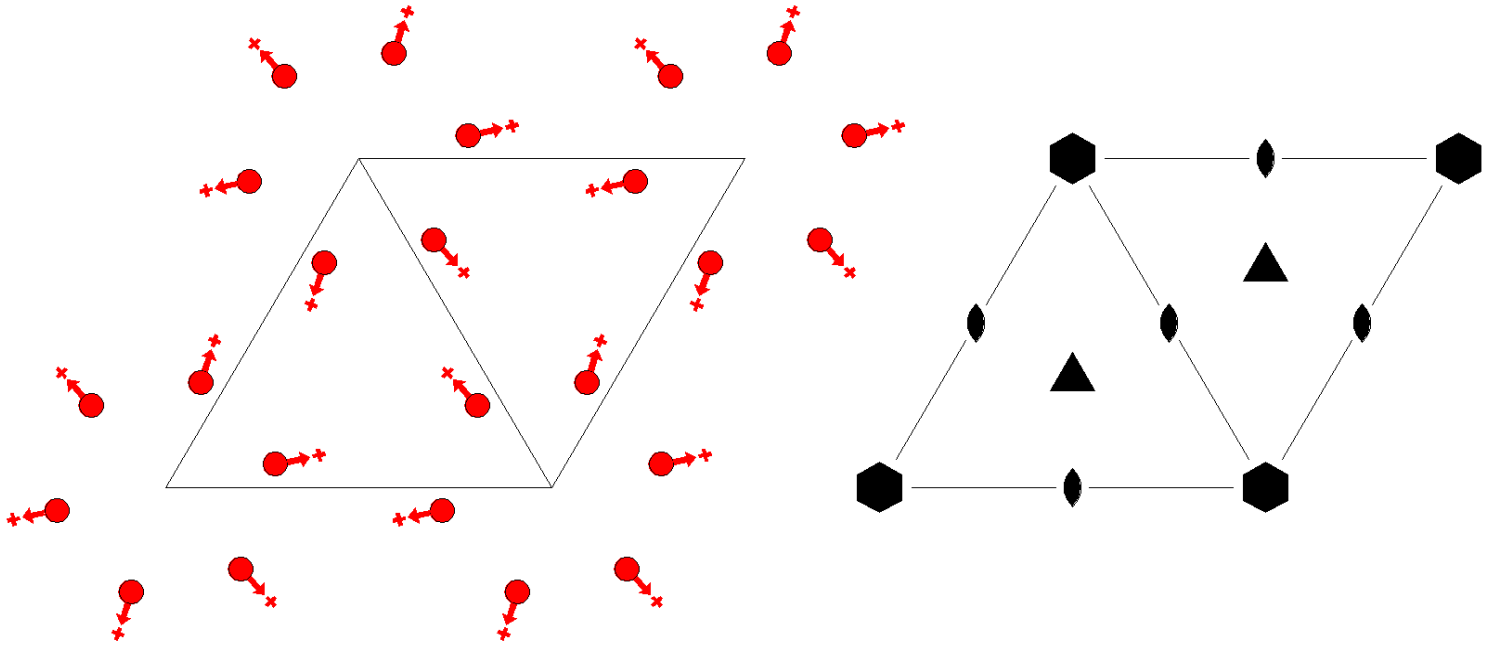
P6

168.1.1339

6

P6

Hexagonal



Origin on 6

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1	1/2,0,1	2/3,1/3,1	1/2,1/2,1	

**Symmetry Operations**

- |  |  |  |
|--|--|--|
| (1) 1<br>(1 0,0,0)                     | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub> <sup>+</sup>  0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub> <sup>+</sup>  0,0,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

### Positions

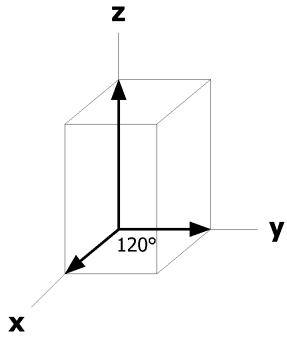
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	d	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$
			(4) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(5) $y,\bar{x}+y,z [v,\bar{u}+v,w]$	(6) $x-y,x,z [u-v,u,w]$
3	c	2..	$1/2,0,z [0,0,w]$	$0,1/2,z [0,0,w]$	$1/2,1/2,z [0,0,w]$
2	b	3..	$1/3,2/3,z [0,0,w]$	$2/3,1/3,z [0,0,w]$	
1	a	6..	$0,0,z [0,0,w]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p6$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p1m'1$   
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

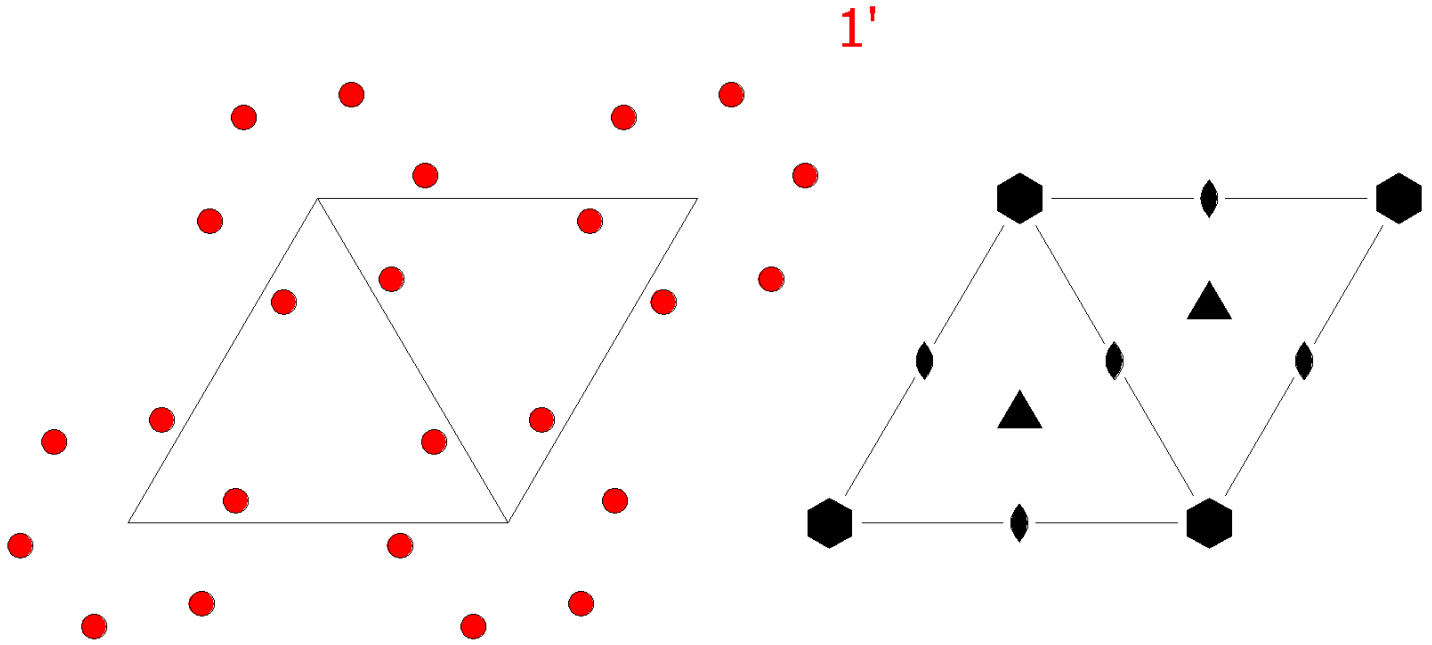
Along  $[2,1,0]$   $p1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x/2,0$



P61'  
168.2.1340

61'  
P61'

Hexagonal



Origin on 61'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1	1/2,1/2,0 1/2,1/2,1	

**Symmetry Operations**

For 1 + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |

For 1' + set

- |  |  |  |
|--|--|--|
| (1) 1'<br>(1 0,0,0)'                     | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)'               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (4) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)'               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

### Positions

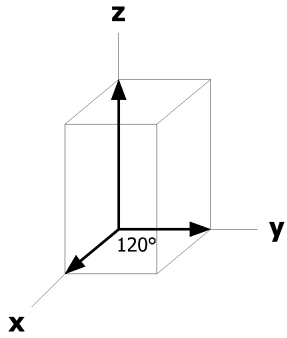
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			1 +	1' +	
6 d 11'	(1)	x,y,z [0,0,0]	(2)	$\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x}$ ,z [0,0,0]
	(4)	$\bar{x},\bar{y}$ ,z [0,0,0]	(5)	y, $\bar{x}+y$ ,z [0,0,0]	(6) x-y,x,z [0,0,0]
3 c 2..1'		1/2,0,z [0,0,0]		0,1/2,z [0,0,0]	1/2,1/2,z [0,0,0]
2 b 3..1'		1/3,2/3,z [0,0,0]		2/3,1/3,z [0,0,0]	
1 a 6..1'		0,0,z [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

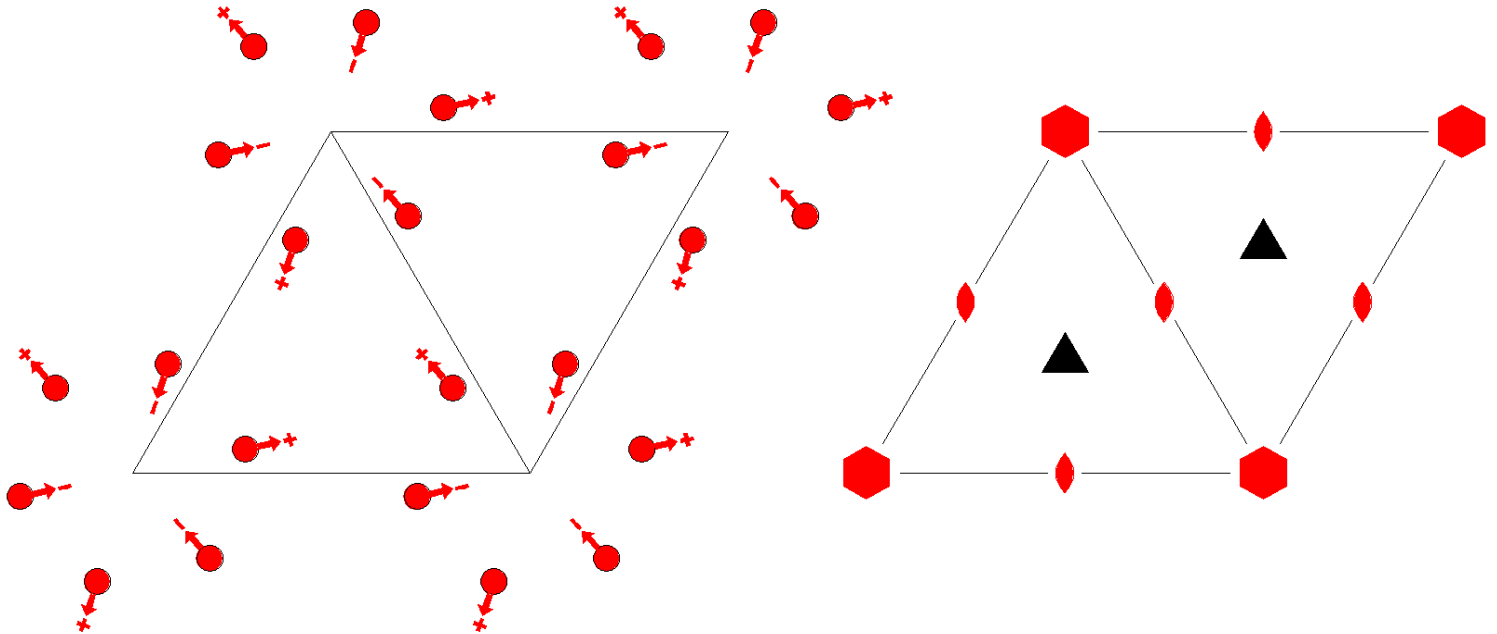
Along [2,1,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



P6'  
168.3.1341

6'  
P6'

Hexagonal



Origin on 6'

Asymmetric unit	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1	1/2,1/2,0 1/2,1/2,1	

### Symmetry Operations

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                       | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)                | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)'              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	d	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$
			(4) $\bar{x},\bar{y},z [u,v,\bar{w}]$	(5) $y,\bar{x}+y,z [\bar{v},u-v,\bar{w}]$	(6) $x-y,x,z [\bar{u}+v,\bar{u},\bar{w}]$
3	c	2'..	$1/2,0,z [u,v,0]$	$0,1/2,z [\bar{v},u-v,0]$	$1/2,1/2,z [\bar{u}+v,\bar{u},0]$
2	b	3..	$1/3,2/3,z [0,0,w]$	$2/3,1/3,z [0,0,\bar{w}]$	
1	a	6'..	$0,0,z [0,0,0]$		

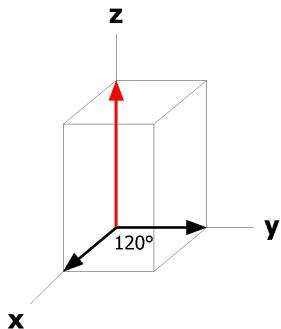
**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p1m1$   
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[2,1,0]$   $p1m1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x/2,0$





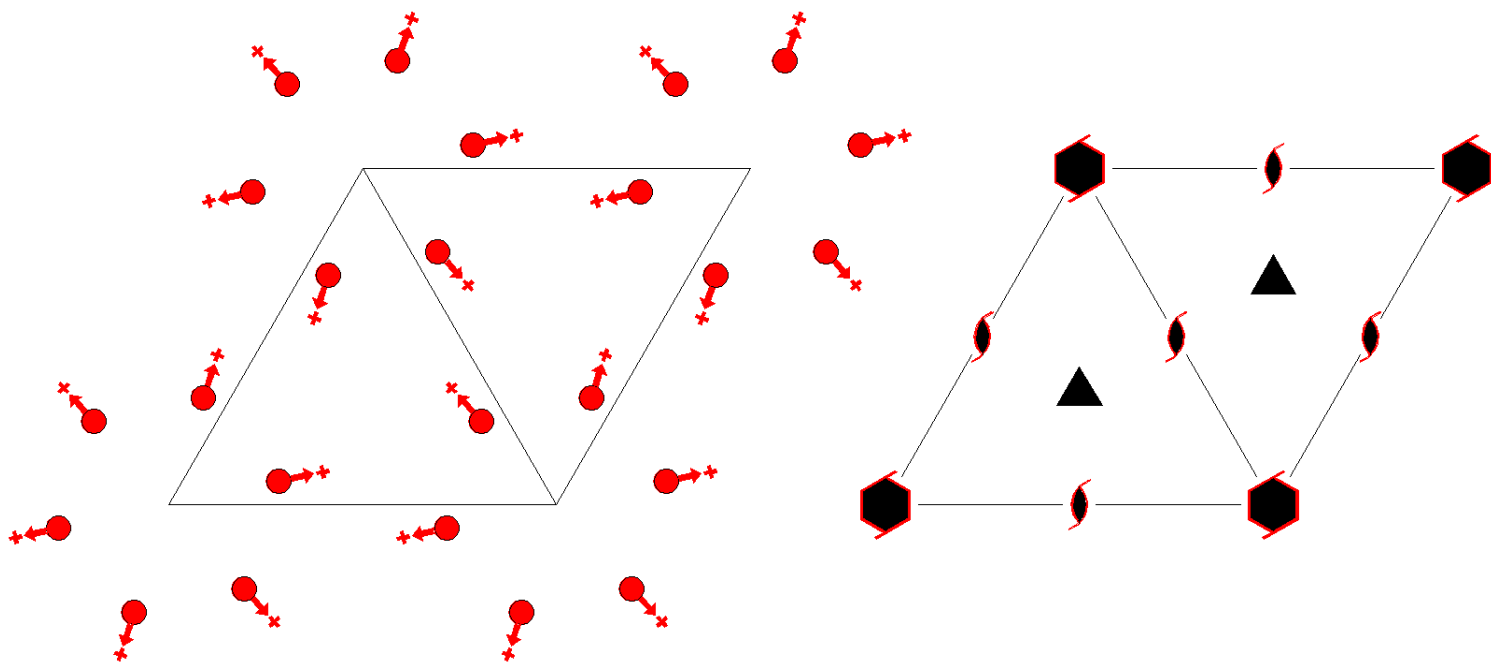
$P_{2c}6$

168.4.1342

$61'$

$P_{2c}6$

Hexagonal



Origin on 6

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1	1/2,0,1	2/3,1/3,1	1/2,1/2,1	

**Symmetry Operations**

For (0,0,0) + set

- |                                |   |   |
|--------------------------------|---|---|
| (1) 1<br>(1 0,0,0)             | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)      | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) 2 0,0,z<br>( $2_z$  0,0,0) | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0) | (6) $6^+$ 0,0,z<br>( $6_z$  0,0,0)      |

For (0,0,1)' + set

- |  |   |   |
|--|---|---|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'             | (2) $3^+'$ (0,0,1) 0,0,z<br>( $3_z$  0,0,1)'      | (3) $3^-'$ (0,0,1) 0,0,z<br>( $3_z^{-1}$  0,0,1)' |
| (4) $2'$ (0,0,1) 0,0,z<br>( $2_z$  0,0,1)' | (5) $6^-'$ (0,0,1) 0,0,z<br>( $6_z^{-1}$  0,0,1)' | (6) $6^+'$ (0,0,1) 0,0,z<br>( $6_z$  0,0,1)'      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

### Positions

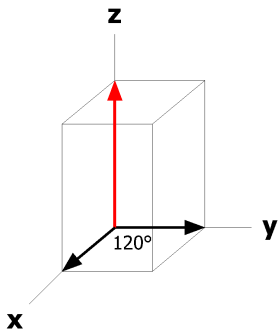
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			(0,0,0) +	(0,0,1)' +	
12	d	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z$ [ $\bar{u}+v, \bar{u}, w$ ]
			(4) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(5) $y, \bar{x}+y, z$ [ $v, \bar{u}+v, w$ ]	(6) x-y,x,z [u-v,u,w]
6	c	2..	1/2,0,z [0,0,w]	0,1/2,z [0,0,w]	1/2,1/2,z [0,0,w]
4	b	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0,w]	
2	a	6..	0,0,z [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>·1m'1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

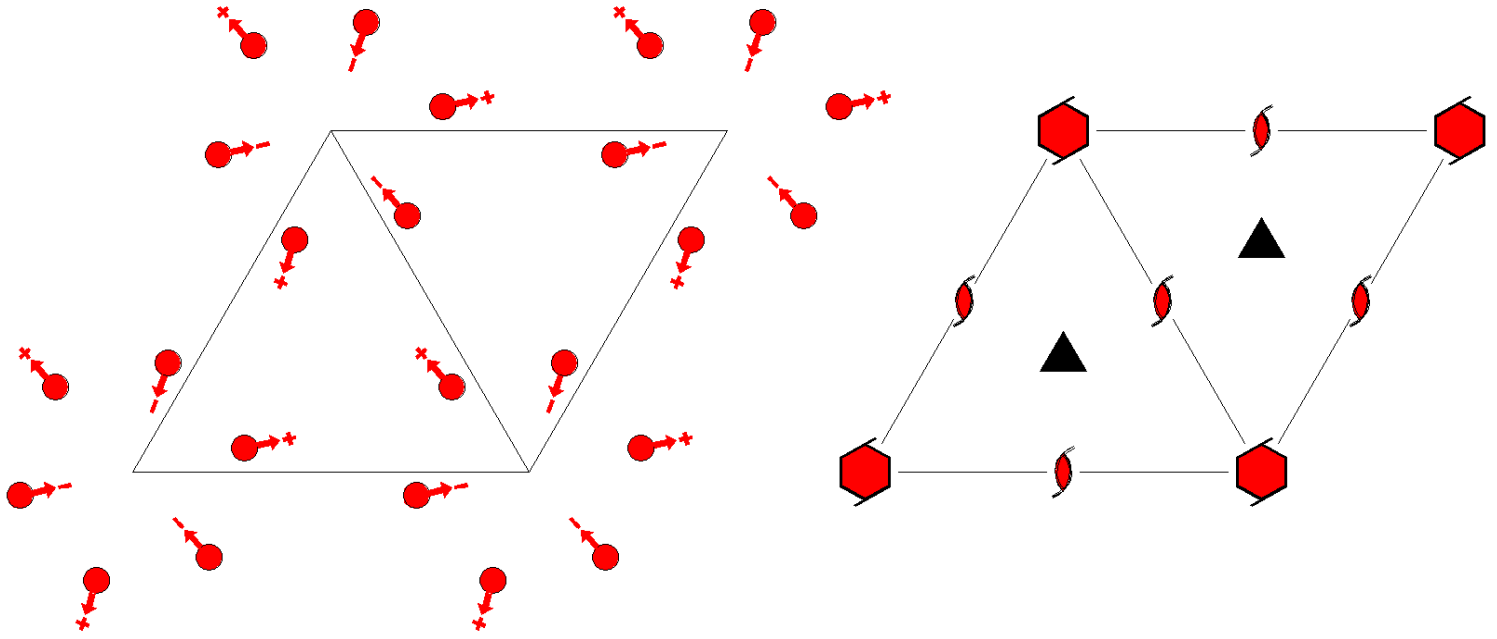
Along [2,1,0] p<sub>2b</sub>·1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$P_{2c}6'$   
168.5.1343

$61'$   
 $P_{2c}6'$

Hexagonal



Origin on  $6'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1	1/2,0,1	2/3,1/3,1	1/2,1/2,1	

**Symmetry Operations**

For (0,0,0) + set

- |                                    |  |   |
|------------------------------------|--|---|
| (1) 1<br>(1 0,0,0)                 | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)       | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0)' | (6) $6^+$ 0,0,z<br>( $6_z$  0,0,0)'     |

For (0,0,1)' + set

- |  |   |  |
|--|---|--|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'         | (2) $3^+$ (0,0,1) 0,0,z<br>( $3_z$  0,0,1)'     | (3) $3^-$ (0,0,1) 0,0,z<br>( $3_z^{-1}$  0,0,1)' |
| (4) 2 (0,0,1) 0,0,z<br>( $2_z$  0,0,1) | (5) $6^-$ (0,0,1) 0,0,z<br>( $6_z^{-1}$  0,0,1) | (6) $6^+$ (0,0,1) 0,0,z<br>( $6_z$  0,0,1)       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

### Positions

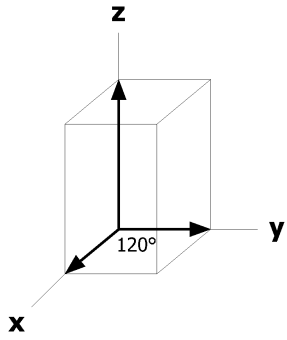
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			(0,0,0) +	(0,0,1)' +	
12	d	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y,\bar{x}$ ,z [ $\bar{u}+v,\bar{u}$ ,w]
			(4) $\bar{x},\bar{y}$ ,z [u,v, $\bar{w}$ ]	(5) y, $\bar{x}+y$ ,z [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) x-y,x,z [u-v,u,w]
6	c	2'..	1/2,0,z [u,v,0]	0,1/2,z [ $\bar{v}$ ,u-v,0]	1/2,1/2,z [ $\bar{u}+v,\bar{u}$ ,0]
4	b	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0, $\bar{w}$ ]	
2	a	6'..	0,0,z [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>·1m1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

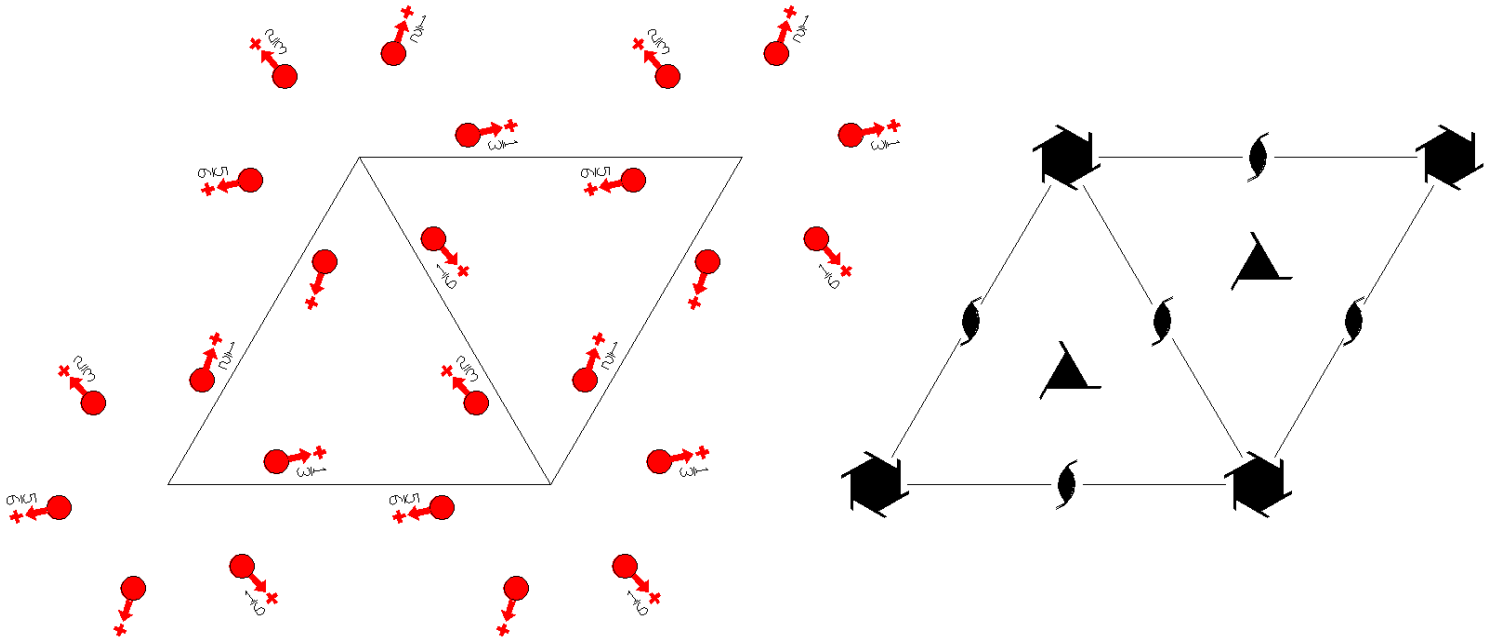
Along [2,1,0] p<sub>2b</sub>·1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$P6_1$   
169.1.1344

6  
 $P6_1$

Hexagonal



Origin on  $6_1$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

### Symmetry Operations

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                         | (2) $3^+$ (0,0,1/3) 0,0,z<br>( $3_z$  0,0,1/3)      | (3) $3^-$ (0,0,2/3) 0,0,z<br>( $3_z^{-1}$  0,0,2/3) |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2) | (5) $6^-$ (0,0,5/6) 0,0,z<br>( $6_z^{-1}$  0,0,5/6) | (6) $6^+$ (0,0,1/6) 0,0,z<br>( $6_z$  0,0,1/6)      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

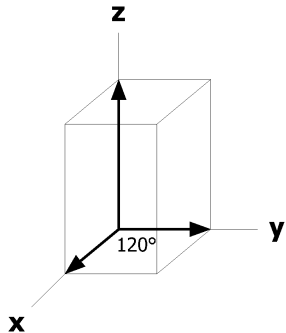
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.					
6	a	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z+1/3$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z+2/3$ [ $\bar{u}+v, \bar{u}, w$ ]
			(4) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(5) $y, \bar{x}+y, z+5/6$ [ $v, \bar{u}+v, w$ ]	(6) x-y,x,z+1/6 [u-v,u,w]

**Symmetry of Special Projections**

Along [0,0,1] p6  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g'1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

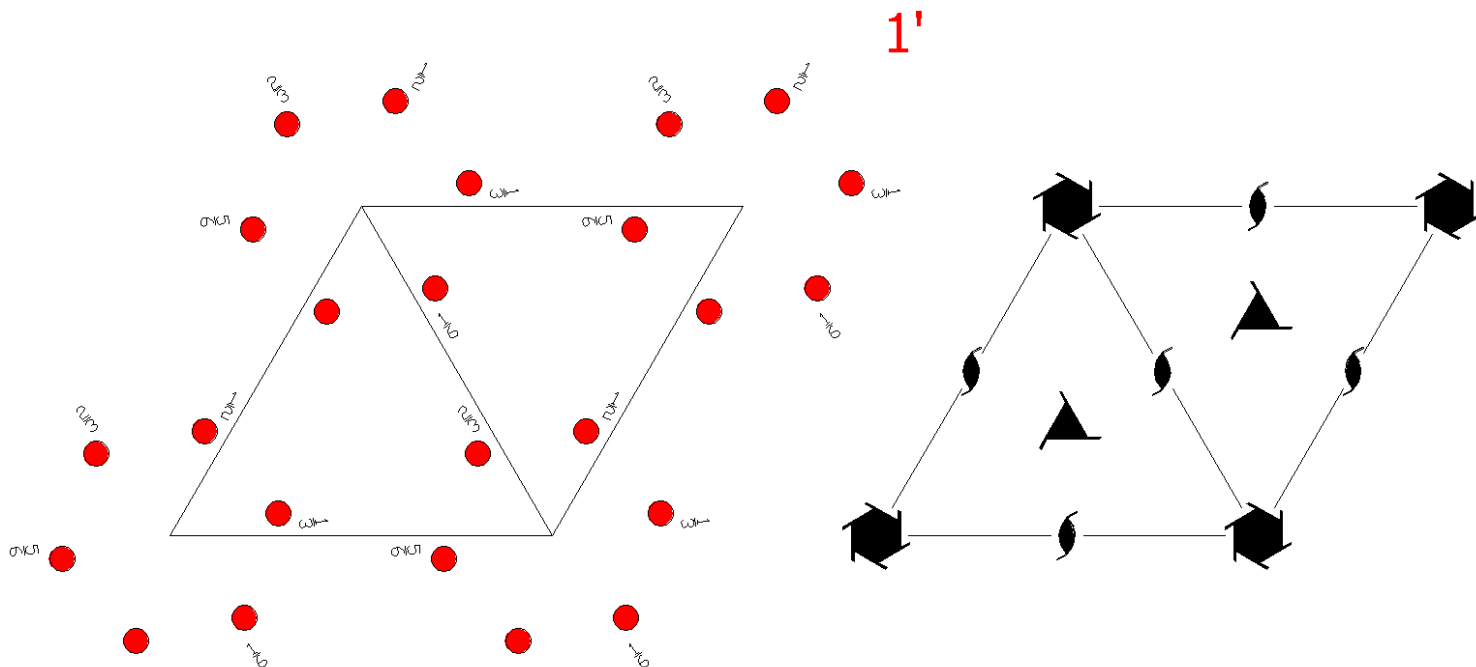
Along [2,1,0] p1g'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



P6<sub>1</sub>1'  
169.2.1345

61'  
P6<sub>1</sub>1'

Hexagonal



Origin on 6<sub>1</sub>1'

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

### Symmetry Operations

For 1 + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 3 <sup>+</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub>  0,0,1/3)               | (3) 3 <sup>-</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,2/3) |
| (4) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (5) 6 <sup>-</sup> (0,0,5/6) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,5/6) | (6) 6 <sup>+</sup> (0,0,1/6) 0,0,z<br>(6 <sub>z</sub>  0,0,1/6)               |

For 1' + set

- |  |  |  |
|--|--|--|
| (1) 1'<br>(1 0,0,0)'                                 | (2) 3 <sup>+</sup> ' (0,0,1/3) 0,0,z<br>(3 <sub>z</sub>  0,0,1/3)'               | (3) 3 <sup>-</sup> ' (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,2/3)' |
| (4) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)' | (5) 6 <sup>-</sup> ' (0,0,5/6) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,5/6)' | (6) 6 <sup>+</sup> ' (0,0,1/6) 0,0,z<br>(6 <sub>z</sub>  0,0,1/6)'               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			1 +	1' +	
6	a	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z+1/3 [0,0,0]	(3) $\bar{x}+y,\bar{x},z+2/3$ [0,0,0]
			(4) $\bar{x},\bar{y},z+1/2$ [0,0,0]	(5) y, $\bar{x}+y,z+5/6$ [0,0,0]	(6) x-y,x,z+1/6 [0,0,0]

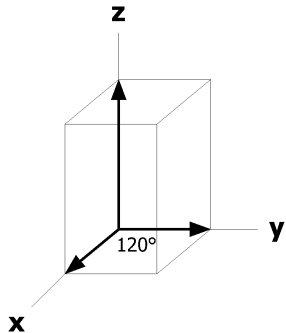
**Symmetry of Special Projections**

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [2,1,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0

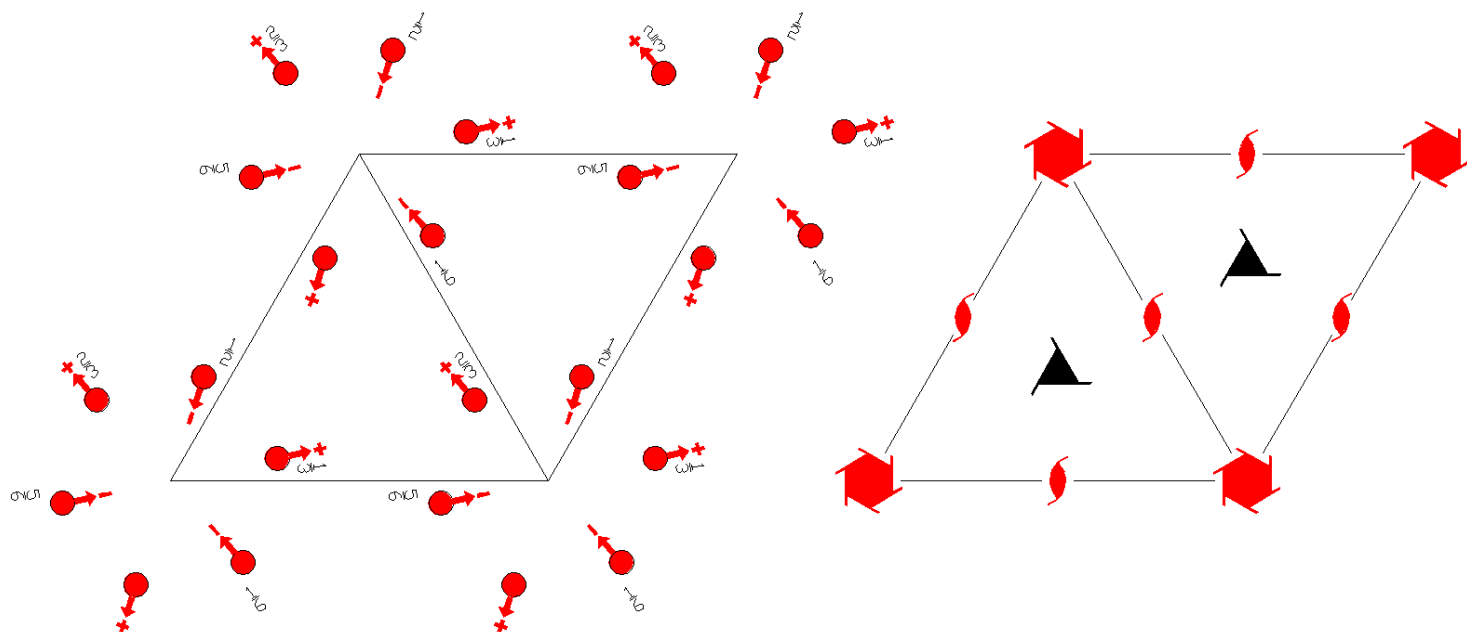




$P6_1'$   
169.3.1346

$6'$   
 $P6_1'$

Hexagonal



Origin on  $6_1'$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

**Symmetry Operations**

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                             | (2) $3^+$ (0,0,1/3) 0,0,z<br>( $3_z$  0,0,1/3)       | (3) $3^-$ (0,0,2/3) 0,0,z<br>( $3_z^{-1}$  0,0,2/3) |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)' | (5) $6^-$ (0,0,5/6) 0,0,z<br>( $6_z^{-1}$  0,0,5/6)' | (6) $6^+$ (0,0,1/6) 0,0,z<br>( $6_z$  0,0,1/6)'     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

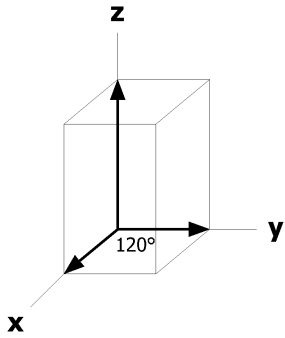
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.					
6	a	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z+1/3$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z+2/3$ [ $\bar{u}+v, \bar{u}, w$ ]
			(4) $\bar{x}, \bar{y}, z+1/2$ [ $u, v, \bar{w}$ ]	(5) $y, \bar{x}+y, z+5/6$ [ $\bar{v}, u-v, \bar{w}$ ]	(6) $x-y, x, z+1/6$ [ $\bar{u}+v, \bar{u}, \bar{w}$ ]

**Symmetry of Special Projections**

Along [0,0,1] p6'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

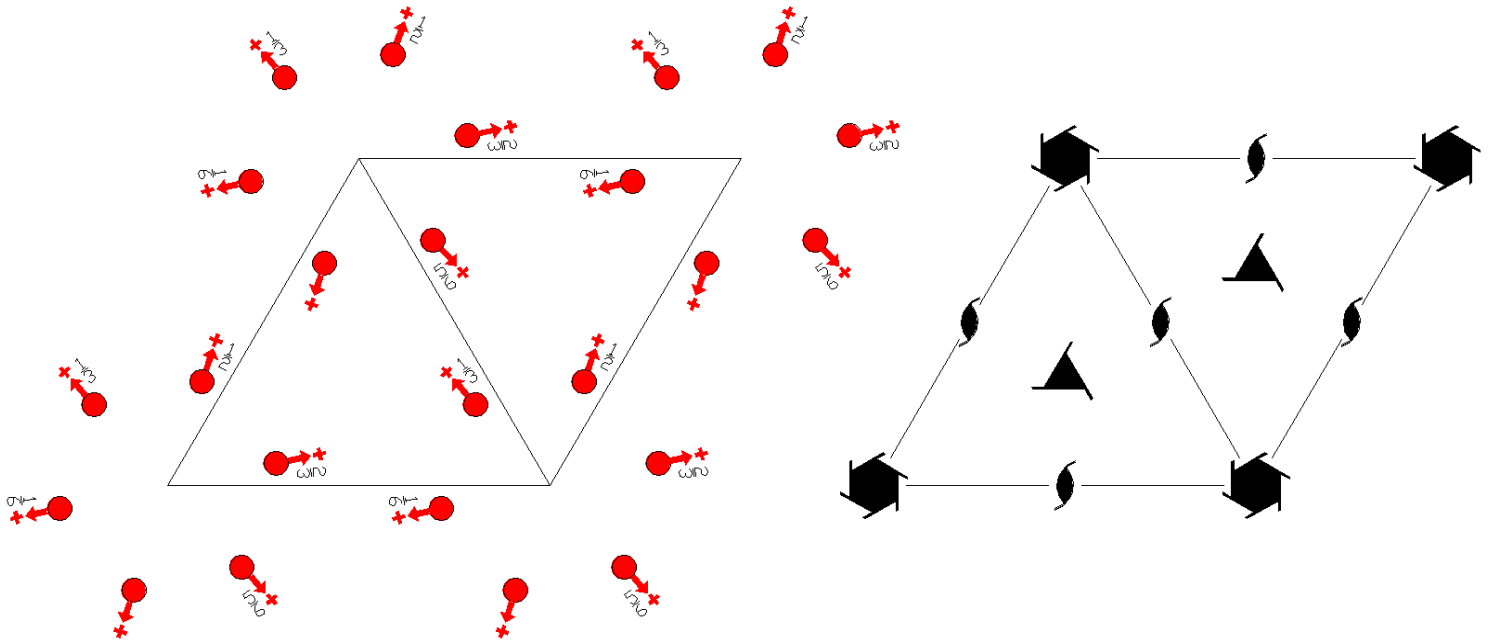
Along [2,1,0] p1g1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$P6_5$   
170.1.1347

6  
 $P6_5$

Hexagonal



Origin on  $6_5$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

**Symmetry Operations**

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                         | (2) $3^+$ (0,0,2/3) 0,0,z<br>( $3_z$  0,0,2/3)      | (3) $3^-$ (0,0,1/3) 0,0,z<br>( $3_z^{-1}$  0,0,1/3) |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2) | (5) $6^-$ (0,0,1/6) 0,0,z<br>( $6_z^{-1}$  0,0,1/6) | (6) $6^+$ (0,0,5/6) 0,0,z<br>( $6_z$  0,0,5/6)      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

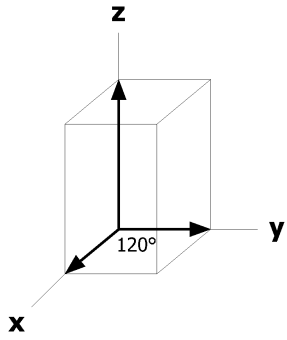
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.					
6	a	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z+2/3$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z+1/3$ [ $\bar{u}+v, \bar{u}, w$ ]
			(4) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(5) $y, \bar{x}+y, z+1/6$ [ $v, \bar{u}+v, w$ ]	(6) $x-y, x, z+5/6$ [ $u-v, u, w$ ]

**Symmetry of Special Projections**

Along [0,0,1] p6  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g'1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

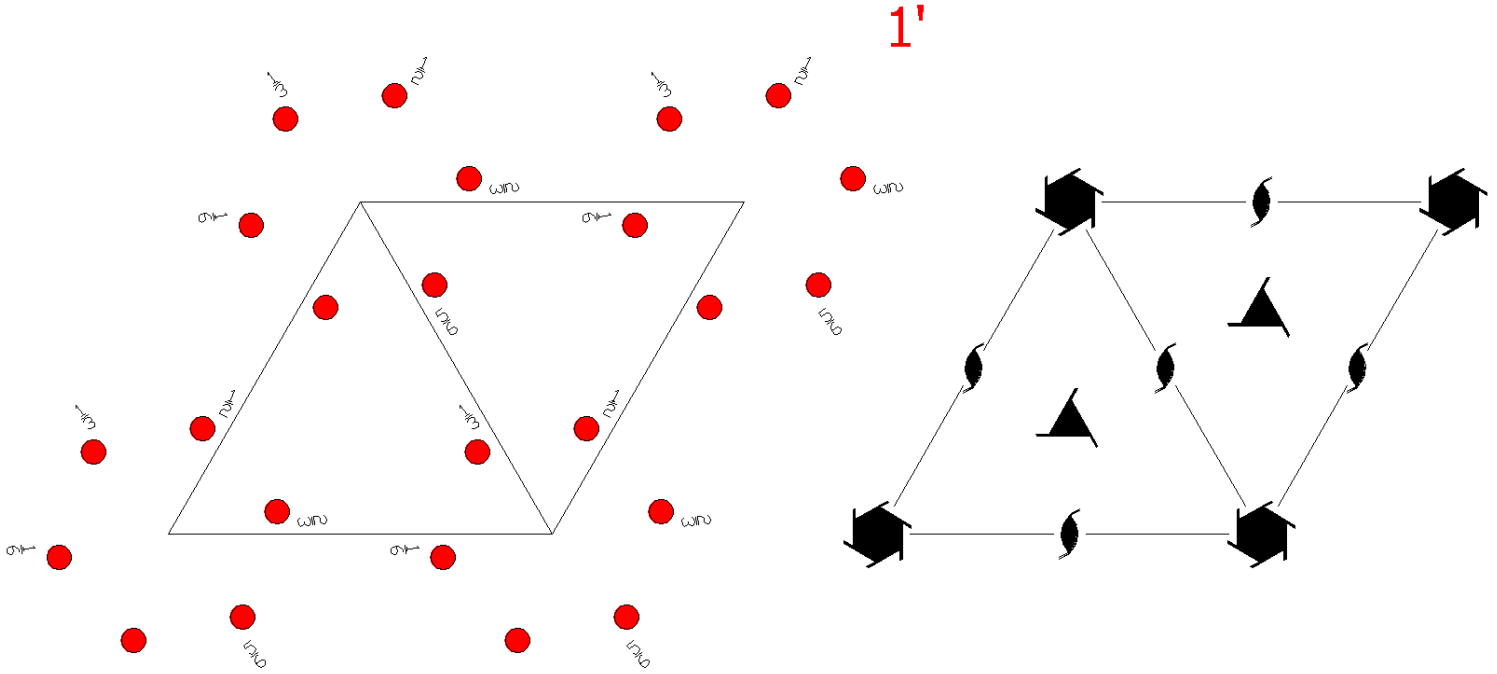
Along [2,1,0] p1g'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$P6_51'$   
170.2.1348

$61'$   
 $P6_51'$

Hexagonal



Origin on  $6_51'$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

### Symmetry Operations

For 1 + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                         | (2) $3^+$ (0,0,2/3) 0,0,z<br>( $3_z$  0,0,2/3)      | (3) $3^-$ (0,0,1/3) 0,0,z<br>( $3_z^{-1}$  0,0,1/3) |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2) | (5) $6^-$ (0,0,1/6) 0,0,z<br>( $6_z^{-1}$  0,0,1/6) | (6) $6^+$ (0,0,5/6) 0,0,z<br>( $6_z$  0,0,5/6)      |

For  $1'$  + set

- |  |   |   |
|--|---|---|
| (1) $1'$<br>(1 0,0,0)'                         | (2) $3^{+'}$ (0,0,2/3) 0,0,z<br>( $3_z$  0,0,2/3)'      | (3) $3^{-'}$ (0,0,1/3) 0,0,z<br>( $3_z^{-1}$  0,0,1/3)' |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)' | (5) $6^{-'}$ (0,0,1/6) 0,0,z<br>( $6_z^{-1}$  0,0,1/6)' | (6) $6^{+'}$ (0,0,5/6) 0,0,z<br>( $6_z$  0,0,5/6)'      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

**Positions**

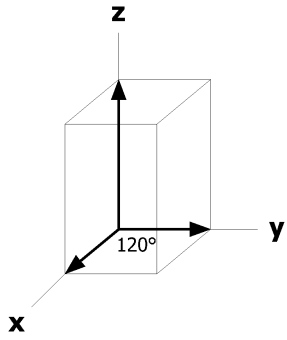
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.					
6	a	11'	(1) x,y,z [0,0,0]	(2) $\bar{y},x-y,z+2/3$ [0,0,0]	(3) $\bar{x}+y,\bar{x},z+1/3$ [0,0,0]
			(4) $\bar{x},\bar{y},z+1/2$ [0,0,0]	(5) $y,\bar{x}+y,z+1/6$ [0,0,0]	(6) x-y,x,z+5/6 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

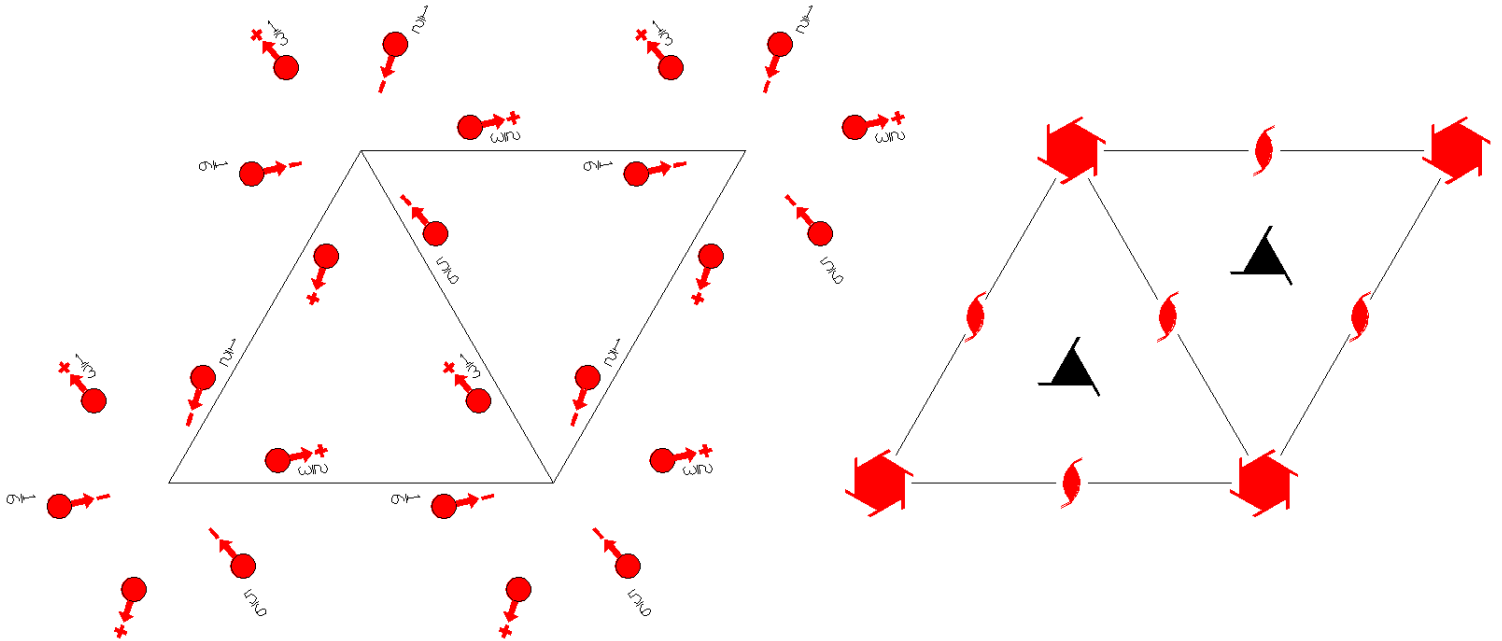
Along [2,1,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$P6_5'$   
170.3.1349

$6'$   
 $P6_5'$

Hexagonal



Origin on  $6_5'$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/6	1,0,1/6	1,1,1/6	0,1,1/6

### Symmetry Operations

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                             | (2) $3^+$ (0,0,2/3) 0,0,z<br>( $3_z$  0,0,2/3)        | (3) $3^-$ (0,0,1/3) 0,0,z<br>( $3_z^{-1}$  0,0,1/3) |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)' | (5) $6^-'$ (0,0,1/6) 0,0,z<br>( $6_z^{-1}$  0,0,1/6)' | (6) $6^+'$ (0,0,5/6) 0,0,z<br>( $6_z$  0,0,5/6)'    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.					
6	a	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z+2/3$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z+1/3$ [ $\bar{u}+v, \bar{u}, w$ ]
			(4) $\bar{x}, \bar{y}, z+1/2$ [ $u, v, \bar{w}$ ]	(5) $y, \bar{x}+y, z+1/6$ [ $\bar{v}, u-v, \bar{w}$ ]	(6) $x-y, x, z+5/6$ [ $\bar{u}+v, \bar{u}, \bar{w}$ ]

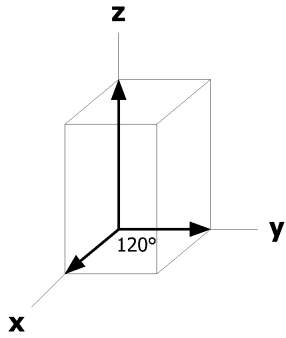
**Symmetry of Special Projections**

Along [0,0,1] p6'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [2,1,0] p1g1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0

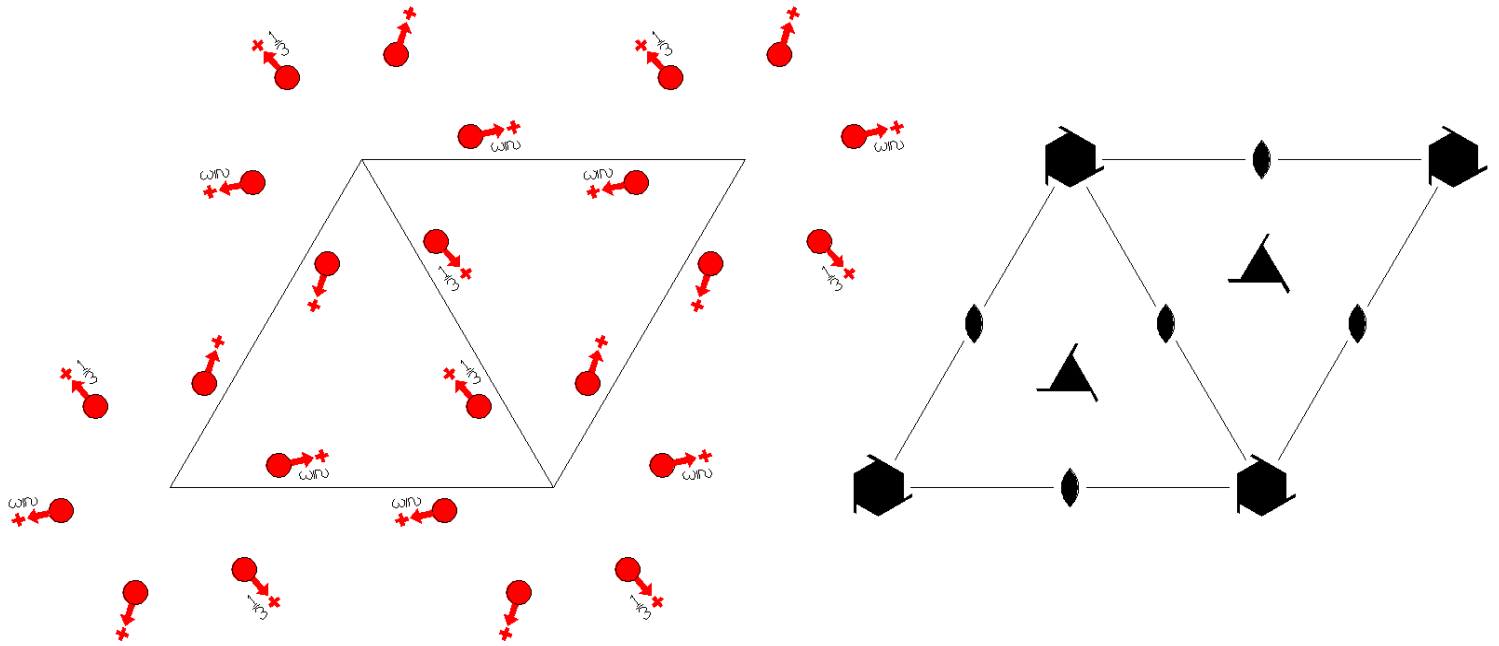




P6<sub>2</sub>  
171.1.1350

6  
P6<sub>2</sub>

Hexagonal



Origin on 2 on 6<sub>2</sub>

**Asymmetric unit**     $0 \leq x \leq 1;$      $0 \leq y \leq 1;$      $0 \leq z \leq 1/3;$      $y \leq x$

**Vertices**             $0,0,0$              $1,0,0$              $1,1,0$   
                            $0,0,1/3$            $1,0,1/3$            $1,1,1/3$

**Symmetry Operations**

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 3 <sup>+</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub>  0,0,2/3)               | (3) 3 <sup>-</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,1/3) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (5) 6 <sup>-</sup> (0,0,2/3) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,2/3) | (6) 6 <sup>+</sup> (0,0,1/3) 0,0,z<br>(6 <sub>z</sub>  0,0,1/3)               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

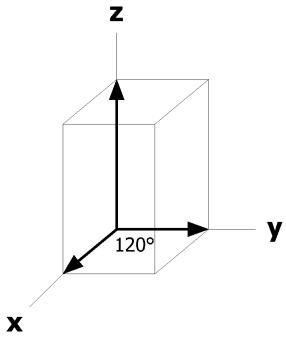
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	c	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z+2/3$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z+1/3$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(5) $y,\bar{x}+y,z+2/3$ [ $v,\bar{u}+v,w$ ]	(6) $x-y,x,z+1/3$ [u-v,u,w]
3	b	2..	$1/2,1/2,z$ [0,0,w]	$1/2,0,z+2/3$ [0,0,w]	$0,1/2,z+1/3$ [0,0,w]
3	a	2..	$0,0,z$ [0,0,w]	$0,0,z+2/3$ [0,0,w]	$0,0,z+1/3$ [0,0,w]

**Symmetry of Special Projections**

Along [0,0,1] p6  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [2,1,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0

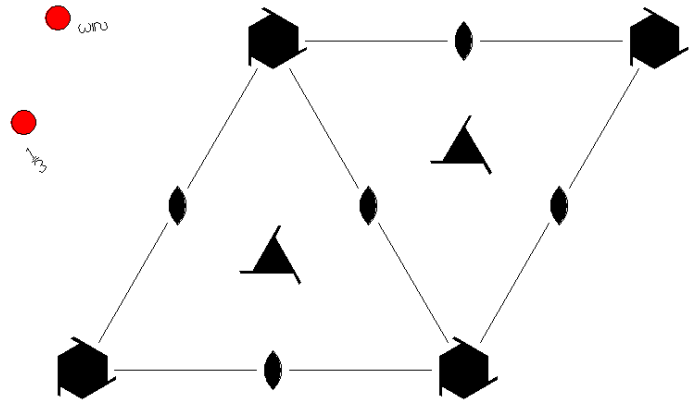
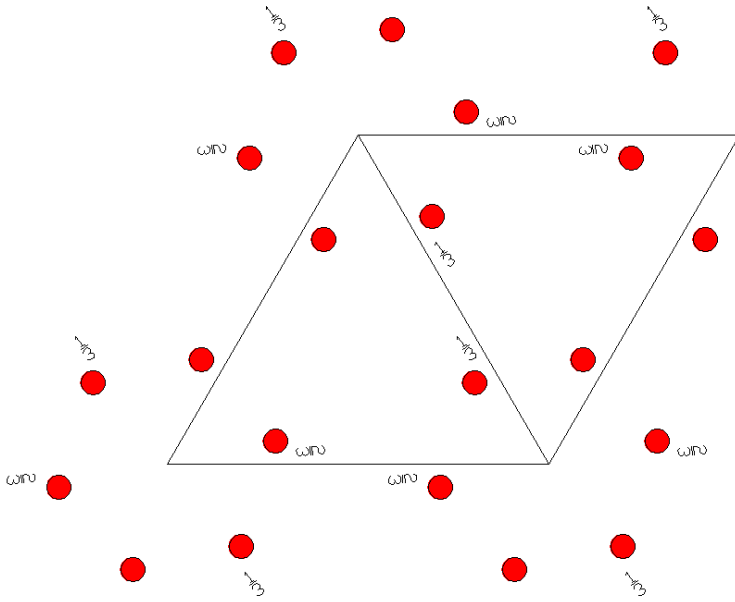


$P6_21'$   
171.2.1351

$61'$   
 $P6_21'$

Hexagonal

$1'$



Origin on  $21'$  on  $6_21'$

Asymmetric unit  $0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/3; \quad y \leq x$

Vertices  $0,0,0 \quad 1,0,0 \quad 1,1,0$   
 $0,0,1/3 \quad 1,0,1/3 \quad 1,1,1/3$

**Symmetry Operations**

For  $1 +$  set

- |                                      |   |   |
|--------------------------------------|---|---|
| (1) $1$<br>$(1 0,0,0)$               | (2) $3^+ (0,0,2/3) \quad 0,0,z$<br>$(3_z 0,0,2/3)$      | (3) $3^- (0,0,1/3) \quad 0,0,z$<br>$(3_z^{-1} 0,0,1/3)$ |
| (4) $2 \quad 0,0,z$<br>$(2_z 0,0,0)$ | (5) $6^- (0,0,2/3) \quad 0,0,z$<br>$(6_z^{-1} 0,0,2/3)$ | (6) $6^+ (0,0,1/3) \quad 0,0,z$<br>$(6_z 0,0,1/3)$      |

For  $1' +$  set

- |                                    |   |   |
|------------------------------------|---|---|
| (1) $1'$<br>$(1 0,0,0)'$           | (2) $3^{+'} (0,0,2/3) \quad 0,0,z$<br>$(3_z 0,0,2/3)'$      | (3) $3^{-'} (0,0,1/3) \quad 0,0,z$<br>$(3_z^{-1} 0,0,1/3)'$ |
| (4) $2'$ $0,0,z$<br>$(2_z 0,0,0)'$ | (5) $6^{-'} (0,0,2/3) \quad 0,0,z$<br>$(6_z^{-1} 0,0,2/3)'$ | (6) $6^{+'} (0,0,1/3) \quad 0,0,z$<br>$(6_z 0,0,1/3)'$      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

### Positions

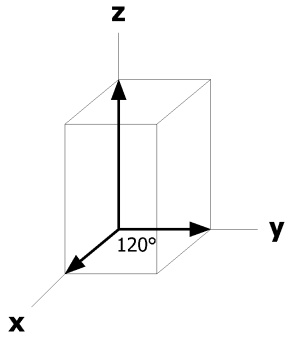
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			1 +	1' +	
6	c	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}, x-y, z+2/3$ [0,0,0]	(3) $\bar{x}+y, \bar{x}, z+1/3$ [0,0,0]
			(4) $\bar{x}, \bar{y}, z$ [0,0,0]	(5) $y, \bar{x}+y, z+2/3$ [0,0,0]	(6) x-y,x,z+1/3 [0,0,0]
3	b	2..1'	1/2,1/2,z [0,0,0]	1/2,0,z+2/3 [0,0,0]	0,1/2,z+1/3 [0,0,0]
3	a	2..1'	0,0,z [0,0,0]	0,0,z+2/3 [0,0,0]	0,0,z+1/3 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

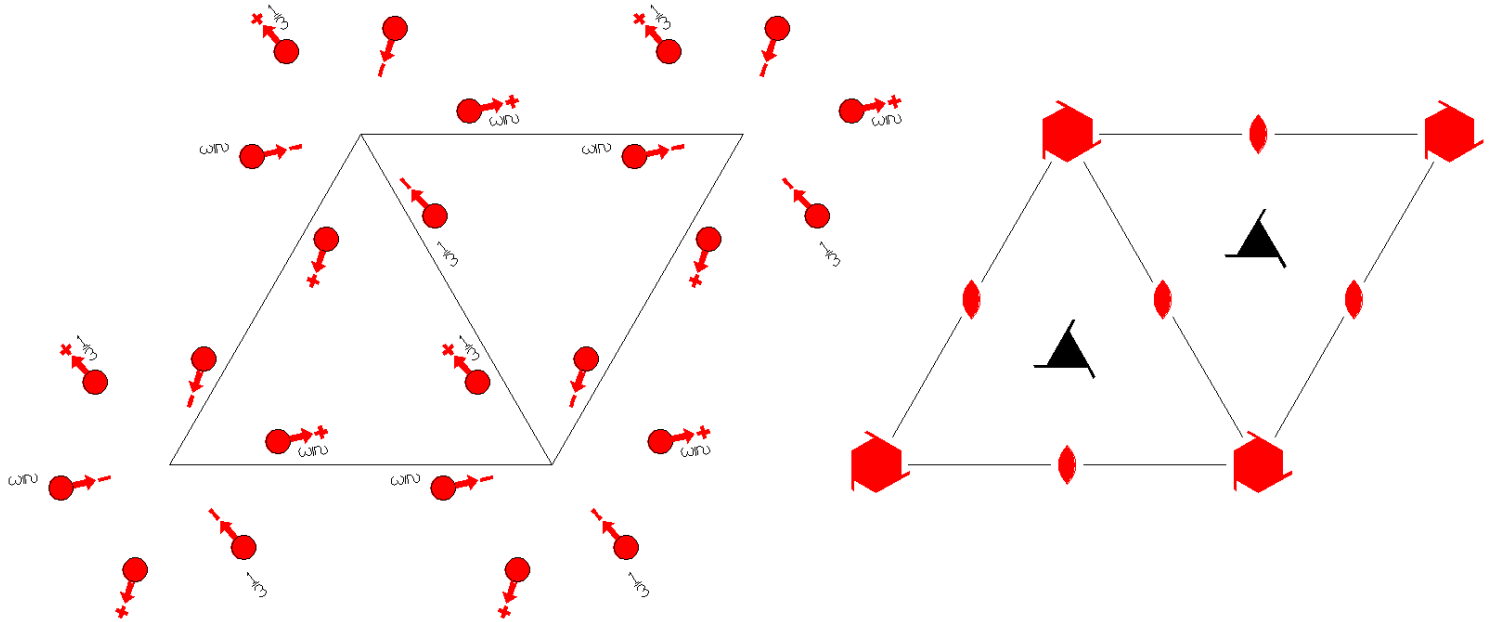
Along [2,1,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$P6_2'$   
171.3.1352

$6'$   
 $P6_2'$

Hexagonal



Origin on  $2'$  on  $6_2'$

**Asymmetric unit**     $0 \leq x \leq 1$ ;     $0 \leq y \leq 1$ ;     $0 \leq z \leq 1/3$ ;     $y \leq x$

Vertices             $0,0,0$              $1,0,0$              $1,1,0$   
                           $0,0,1/3$            $1,0,1/3$            $1,1,1/3$

**Symmetry Operations**

- |                                    |  |   |
|------------------------------------|--|---|
| (1) 1<br>(1 0,0,0)                 | (2) $3^+$ (0,0,2/3) 0,0,z<br>( $3_z$  0,0,2/3)       | (3) $3^-$ (0,0,1/3) 0,0,z<br>( $3_z^{-1}$  0,0,1/3) |
| (4) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (5) $6^-$ (0,0,2/3) 0,0,z<br>( $6_z^{-1}$  0,0,2/3)' | (6) $6^+$ (0,0,1/3) 0,0,z<br>( $6_z$  0,0,1/3)'     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

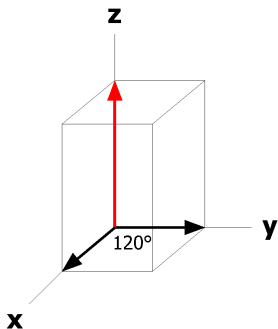
			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
6	c	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z+2/3$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z+1/3$ [ $\bar{u}+v, \bar{u}, w$ ]
			(4) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	(5) $y, \bar{x}+y, z+2/3$ [ $\bar{v}, u-v, \bar{w}$ ]	(6) x-y,x,z+1/3 [ $\bar{u}+v, \bar{u}, \bar{w}$ ]
3	b	2'..	1/2, 1/2, z [u,v,0]	1/2, 0, z+2/3 [ $\bar{v}, u-v, 0$ ]	0, 1/2, z+1/3 [ $\bar{u}+v, \bar{u}, 0$ ]
3	a	2'..	0, 0, z [u,v,0]	0, 0, z+2/3 [ $\bar{v}, u-v, 0$ ]	0, 0, z+1/3 [ $\bar{u}+v, \bar{u}, 0$ ]

**Symmetry of Special Projections**

Along [0,0,1] p6'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

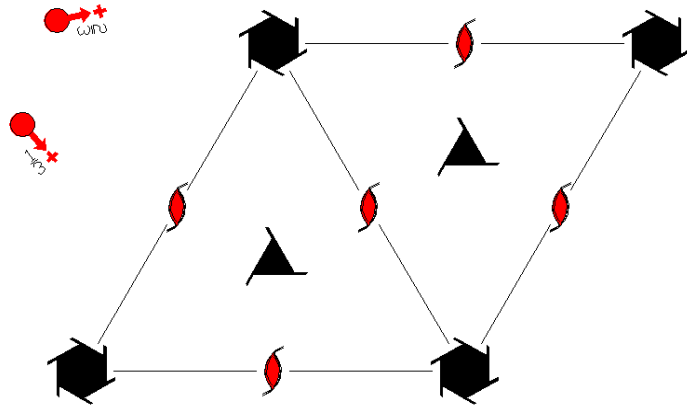
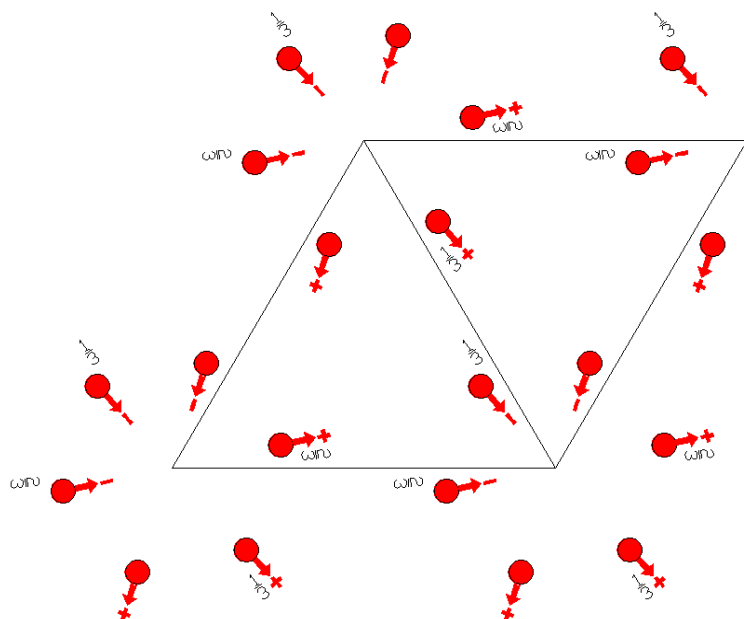
Along [2,1,0] p1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$P_{2c}6_2$   
171.4.1353

61'  
 $P_{2c}6_2$

Hexagonal



Origin on  $2'$  on  $6_2$

Asymmetric unit  $0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/3; \quad y \leq x$

Vertices	0,0,0	1,0,0	1,1,0
	0,0,1/3	1,0,1/3	1,1,1/3

### Symmetry Operations

For (0,0,0) + set

- |                                    |  |  |
|------------------------------------|--|--|
| (1) 1<br>(1 0,0,0)                 | (2) $3^+$ (0,0,2/3) 0,0,z<br>( $3_z$  0,0,2/3)       | (3) $3^-$ (0,0,1/3) 0,0,z<br>( $3_z^{-1}$  0,0,1/3)' |
| (4) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (5) $6^-$ (0,0,2/3) 0,0,z<br>( $6_z^{-1}$  0,0,2/3)' | (6) $6^+$ (0,0,1/3) 0,0,z<br>( $6_z$  0,0,1/3)       |

For (0,0,1)' + set

- |  |   |   |
|--|---|---|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'         | (2) $3^+$ (0,0,5/3) 0,0,z<br>( $3_z$  0,0,5/3)'     | (3) $3^-$ (0,0,4/3) 0,0,z<br>( $3_z^{-1}$  0,0,4/3) |
| (4) 2 (0,0,1) 0,0,z<br>( $2_z$  0,0,1) | (5) $6^-$ (0,0,5/3) 0,0,z<br>( $6_z^{-1}$  0,0,5/3) | (6) $6^+$ (0,0,4/3) 0,0,z<br>( $6_z$  0,0,4/3)'     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			(0,0,0) +	(0,0,1)' +	
12	c	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z+2/3$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z+1/3$ [u-v, u, $\bar{w}$ ]
			(4) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	(5) $y, \bar{x}+y, z+2/3$ [ $\bar{v}, u-v, \bar{w}$ ]	(6) x-y, x, z+1/3 [u-v, u, w]
6	b	2'..	1/2, 1/2, z [u,v,0]	1/2, 0, z+2/3 [ $\bar{v}, u-v, 0$ ]	0, 1/2, z+1/3 [u-v, u, 0]
6	a	2'..	0, 0, z [u,v,0]	0, 0, z+2/3 [ $\bar{v}, u-v, 0$ ]	0, 0, z+1/3 [u-v, u, 0]

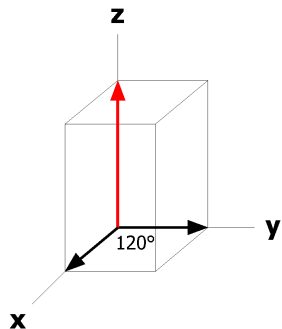
### Symmetry of Special Projections

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>\* 1m'1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [2,1,0] p<sub>2b</sub>\* 1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x, x/2, 0

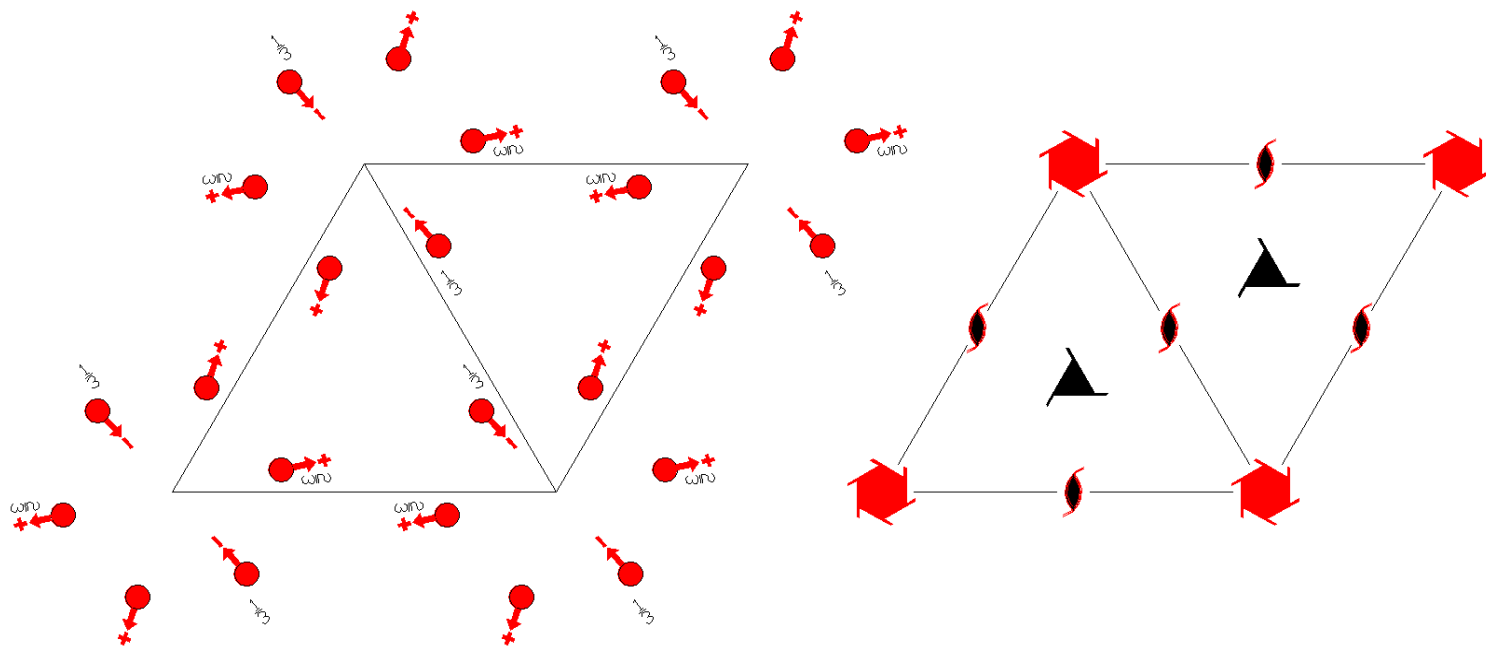




$P_{2c}6_2'$   
171.5.1354

$61'$   
 $P_{2c}6_2'$

Hexagonal



Origin on  $2'$  on  $6_2'$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/3$ ;  $y \leq x$

Vertices	0,0,0	1,0,0	1,1,0
	0,0,1/3	1,0,1/3	1,1,1/3

### Symmetry Operations

For (0,0,0) + set

- |                                |   |  |
|--------------------------------|---|--|
| (1) 1<br>(1 0,0,0)             | (2) $3^+$ (0,0,2/3) 0,0,z<br>( $3_z$  0,0,2/3)      | (3) $3^-$ (0,0,1/3) 0,0,z<br>( $3_z^{-1}$  0,0,1/3)' |
| (4) 2 0,0,z<br>( $2_z$  0,0,0) | (5) $6^-$ (0,0,2/3) 0,0,z<br>( $6_z^{-1}$  0,0,2/3) | (6) $6^+$ (0,0,1/3) 0,0,z<br>( $6_z$  0,0,1/3)'      |

For (0,0,1)' + set

- |  |  |   |
|--|--|---|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'             | (2) $3^+$ (0,0,5/3) 0,0,z<br>( $3_z$  0,0,5/3)'      | (3) $3^-$ (0,0,4/3) 0,0,z<br>( $3_z^{-1}$  0,0,4/3) |
| (4) $2'$ (0,0,1) 0,0,z<br>( $2_z$  0,0,1)' | (5) $6^-$ (0,0,5/3) 0,0,z<br>( $6_z^{-1}$  0,0,5/3)' | (6) $6^+$ (0,0,4/3) 0,0,z<br>( $6_z$  0,0,4/3)      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

### Positions

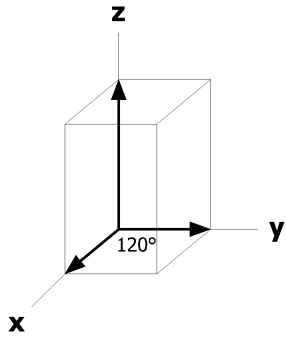
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			(0,0,0)+	(0,0,1)' +	
12	c	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z+2/3$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z+1/3$ [ $u-v, u, \bar{w}$ ]
			(4) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(5) $y, \bar{x}+y, z+2/3$ [ $v, \bar{u}+v, w$ ]	(6) $x-y, x, z+1/3$ [ $\bar{u}+v, \bar{u}, \bar{w}$ ]
6	b	2..	1/2, 1/2, z [0,0,w]	1/2, 0, z+2/3 [0,0,w]	0, 1/2, z+1/3 [0,0, $\bar{w}$ ]
6	a	2..	0,0,z [0,0,w]	0,0,z+2/3 [0,0,w]	0,0,z+1/3 [0,0, $\bar{w}$ ]

### Symmetry of Special Projections

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>\* 1m1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

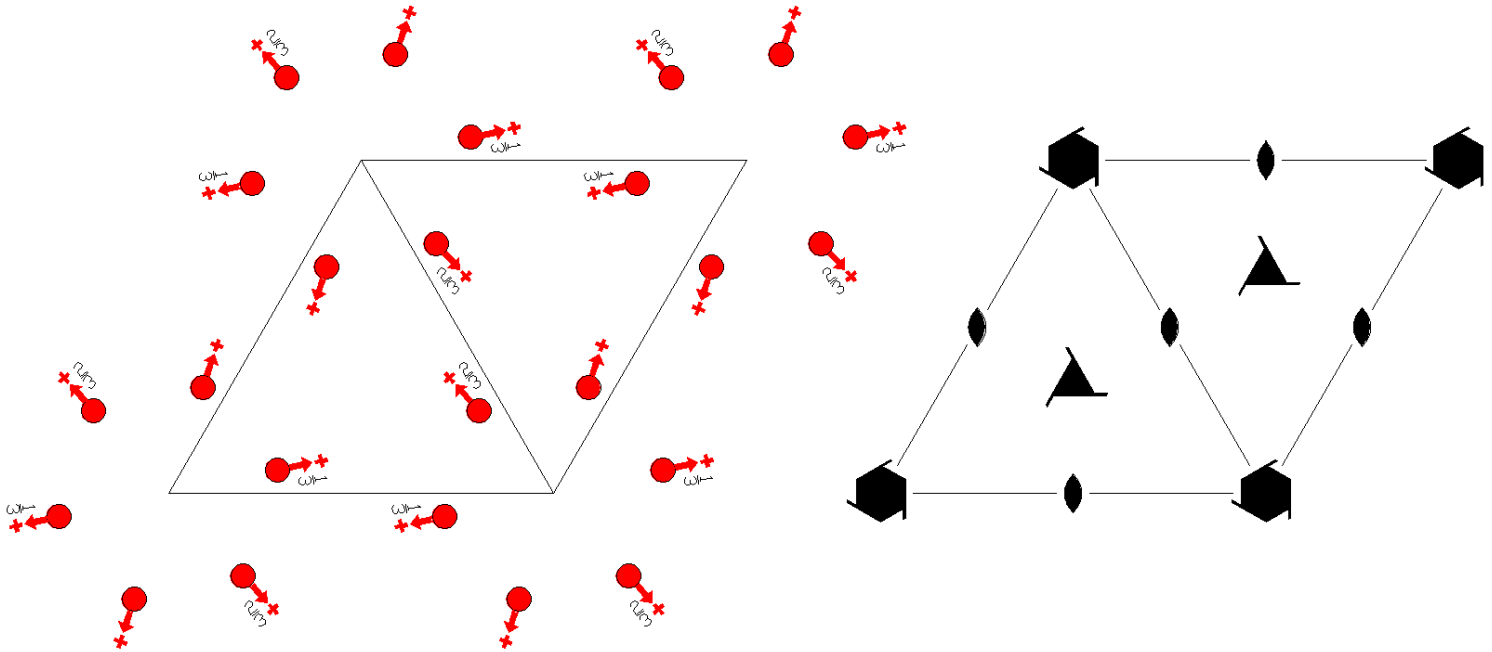
Along [2,1,0] p<sub>2b</sub>\* 1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$P6_4$   
172.1.1355

6  
 $P6_4$

Hexagonal



Origin on 2 on  $6_4$

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/3;$   $y \leq x$

Vertices  $0,0,0$   $1,0,0$   $1,1,0$   
 $0,0,1/3$   $1,0,1/3$   $1,1,1/3$

**Symmetry Operations**

- |                                |   |   |
|--------------------------------|---|---|
| (1) 1<br>(1 0,0,0)             | (2) $3^+$ (0,0,1/3) 0,0,z<br>( $3_z$  0,0,1/3)      | (3) $3^-$ (0,0,2/3) 0,0,z<br>( $3_z^{-1}$  0,0,2/3) |
| (4) 2 0,0,z<br>( $2_z$  0,0,0) | (5) $6^-$ (0,0,1/3) 0,0,z<br>( $6_z^{-1}$  0,0,1/3) | (6) $6^+$ (0,0,2/3) 0,0,z<br>( $6_z$  0,0,2/3)      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

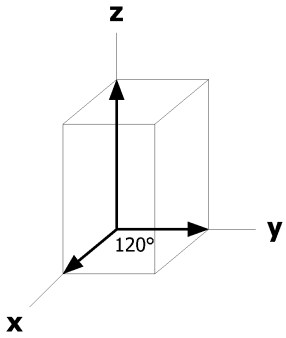
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	c	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z+1/3 [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z+2/3 [\bar{u}+v,\bar{u},w]$
			(4) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(5) $y,\bar{x}+y,z+1/3 [v,\bar{u}+v,w]$	(6) $x-y,x,z+2/3 [u-v,u,w]$
3	b	2..	$1/2,1/2,z [0,0,w]$	$1/2,0,z+1/3 [0,0,w]$	$0,1/2,z+2/3 [0,0,w]$
3	a	2..	$0,0,z [0,0,w]$	$0,0,z+1/3 [0,0,w]$	$0,0,z+2/3 [0,0,w]$

**Symmetry of Special Projections**

Along  $[0,0,1]$  p6  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along  $[1,0,0]$  p1m'1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along  $[2,1,0]$  p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



P6<sub>4</sub>1'

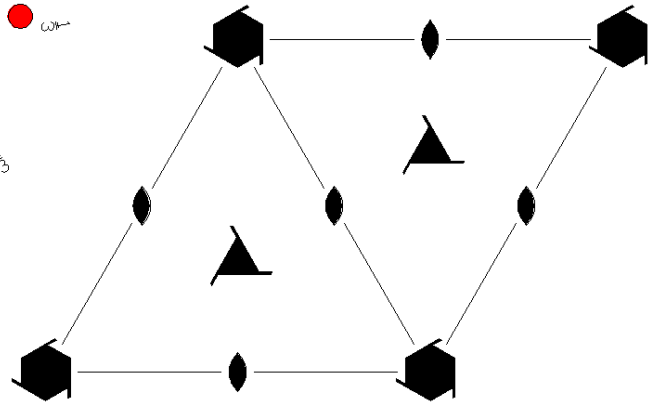
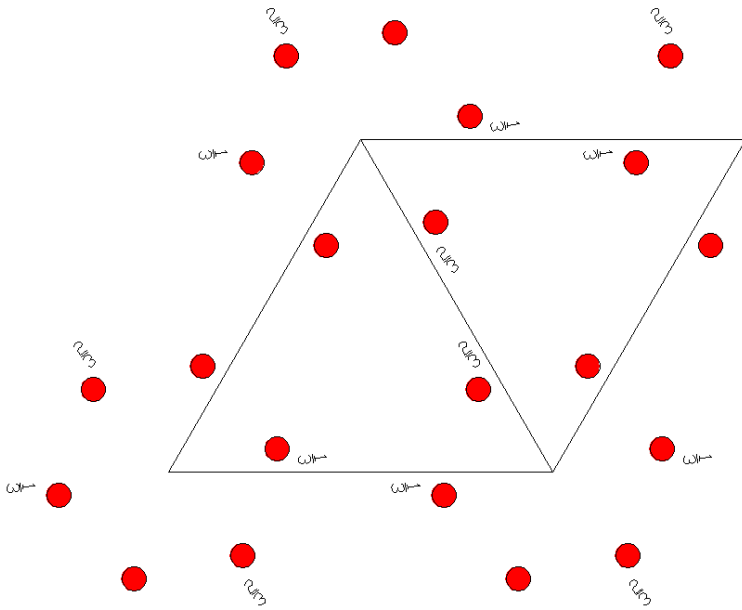
172.2.1356

61'

P6<sub>4</sub>1'

Hexagonal

1'



Origin on 21' on 6<sub>4</sub>1'

Asymmetric unit  $0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/3; \quad y \leq x$

Vertices  $0,0,0 \quad 1,0,0 \quad 1,1,0$   
 $0,0,1/3 \quad 1,0,1/3 \quad 1,1,1/3$

**Symmetry Operations**

For 1 + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) 3 <sup>+</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub>  0,0,1/3)               | (3) 3 <sup>-</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,2/3) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0) | (5) 6 <sup>-</sup> (0,0,1/3) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,1/3) | (6) 6 <sup>+</sup> (0,0,2/3) 0,0,z<br>(6 <sub>z</sub>  0,0,2/3)               |

For 1' + set

- |  |  |  |
|--|--|--|
| (1) 1'<br>(1 0,0,0)'                     | (2) 3 <sup>+</sup> ' (0,0,1/3) 0,0,z<br>(3 <sub>z</sub>  0,0,1/3)'               | (3) 3 <sup>-</sup> ' (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,2/3)' |
| (4) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)' | (5) 6 <sup>-</sup> ' (0,0,1/3) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,1/3)' | (6) 6 <sup>+</sup> ' (0,0,2/3) 0,0,z<br>(6 <sub>z</sub>  0,0,2/3)'               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

### Positions

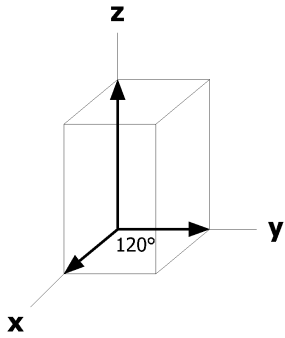
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			1+	1' +	
6	c	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}, x-y, z+1/3$ [0,0,0]	(3) $\bar{x}+y, \bar{x}, z+2/3$ [0,0,0]
			(4) $\bar{x}, \bar{y}, z$ [0,0,0]	(5) $y, \bar{x}+y, z+1/3$ [0,0,0]	(6) x-y,x,z+2/3 [0,0,0]
3	b	2..1'	1/2,1/2,z [0,0,0]	1/2,0,z+1/3 [0,0,0]	0,1/2,z+2/3 [0,0,0]
3	a	2..1'	0,0,z [0,0,0]	0,0,z+1/3 [0,0,0]	0,0,z+2/3 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

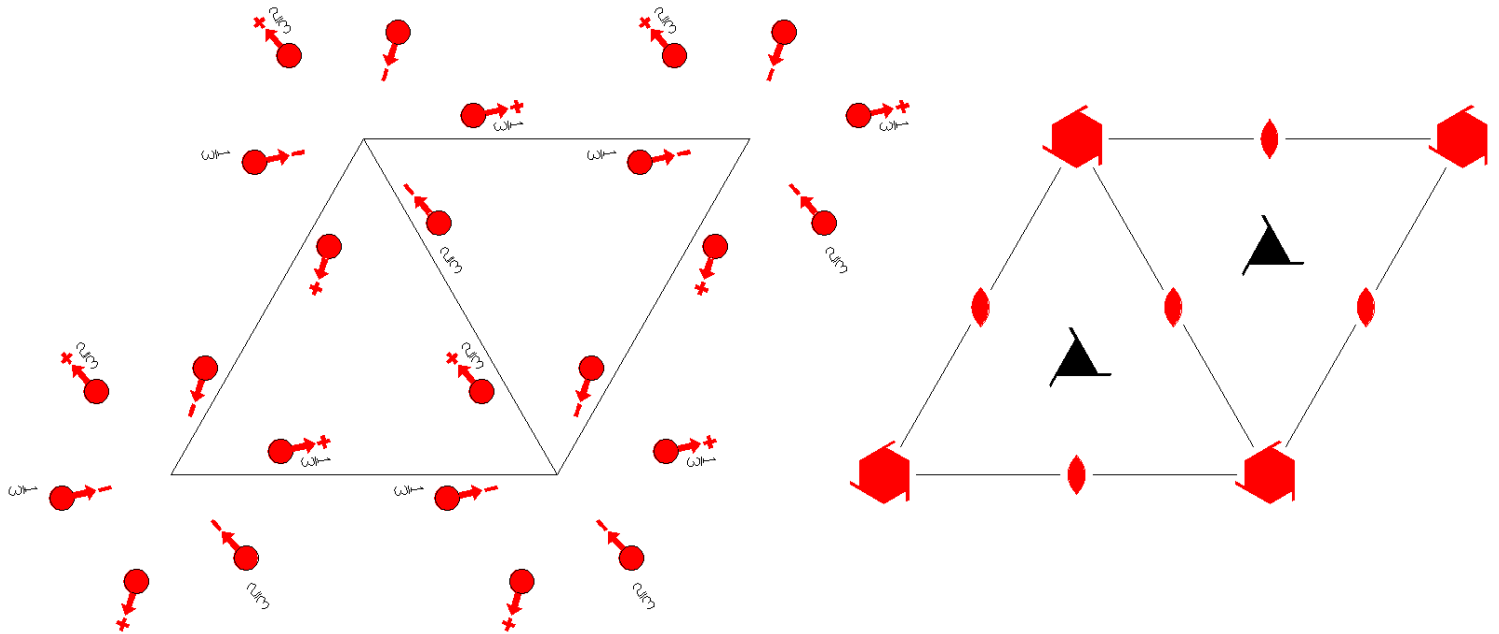
Along [2,1,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$P6_4'$   
172.3.1357

$6'$   
 $P6_4'$

Hexagonal



Origin on  $2'$  on  $6_4'$

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/3;$   $y \leq x$

Vertices  $0,0,0$   $1,0,0$   $1,1,0$   
 $0,0,1/3$   $1,0,1/3$   $1,1,1/3$

### Symmetry Operations

- |                                    |   |   |
|------------------------------------|---|---|
| (1) $1$<br>$(1 0,0,0)$             | (2) $3^+$ $(0,0,1/3)$ $0,0,z$<br>$(3_z 0,0,1/3)$        | (3) $3^-$ $(0,0,2/3)$ $0,0,z$<br>$(3_z^{-1} 0,0,2/3)$ |
| (4) $2'$ $0,0,z$<br>$(2_z 0,0,0)'$ | (5) $6^-'$ $(0,0,1/3)$ $0,0,z$<br>$(6_z^{-1} 0,0,1/3)'$ | (6) $6^+'$ $(0,0,2/3)$ $0,0,z$<br>$(6_z 0,0,2/3)'$    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
6	c	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z+1/3$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z+2/3$ [ $\bar{u}+v, \bar{u}, w$ ]
			(4) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	(5) $y, \bar{x}+y, z+1/3$ [ $\bar{v}, u-v, \bar{w}$ ]	(6) $x-y, x, z+2/3$ [ $\bar{u}+v, \bar{u}, \bar{w}$ ]
3	b	2'..	1/2, 1/2, z [u,v,0]	1/2, 0, z+1/3 [ $\bar{v}, u-v, 0$ ]	0, 1/2, z+2/3 [ $\bar{u}+v, \bar{u}, 0$ ]
3	a	2'..	0, 0, z [u,v,0]	0, 0, z+1/3 [ $\bar{v}, u-v, 0$ ]	0, 0, z+2/3 [ $\bar{u}+v, \bar{u}, 0$ ]

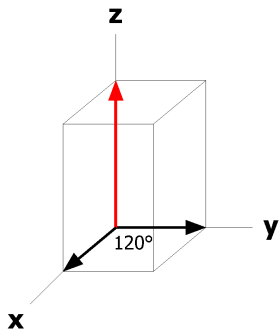
**Symmetry of Special Projections**

Along [0,0,1] p6'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [2,1,0] p1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0

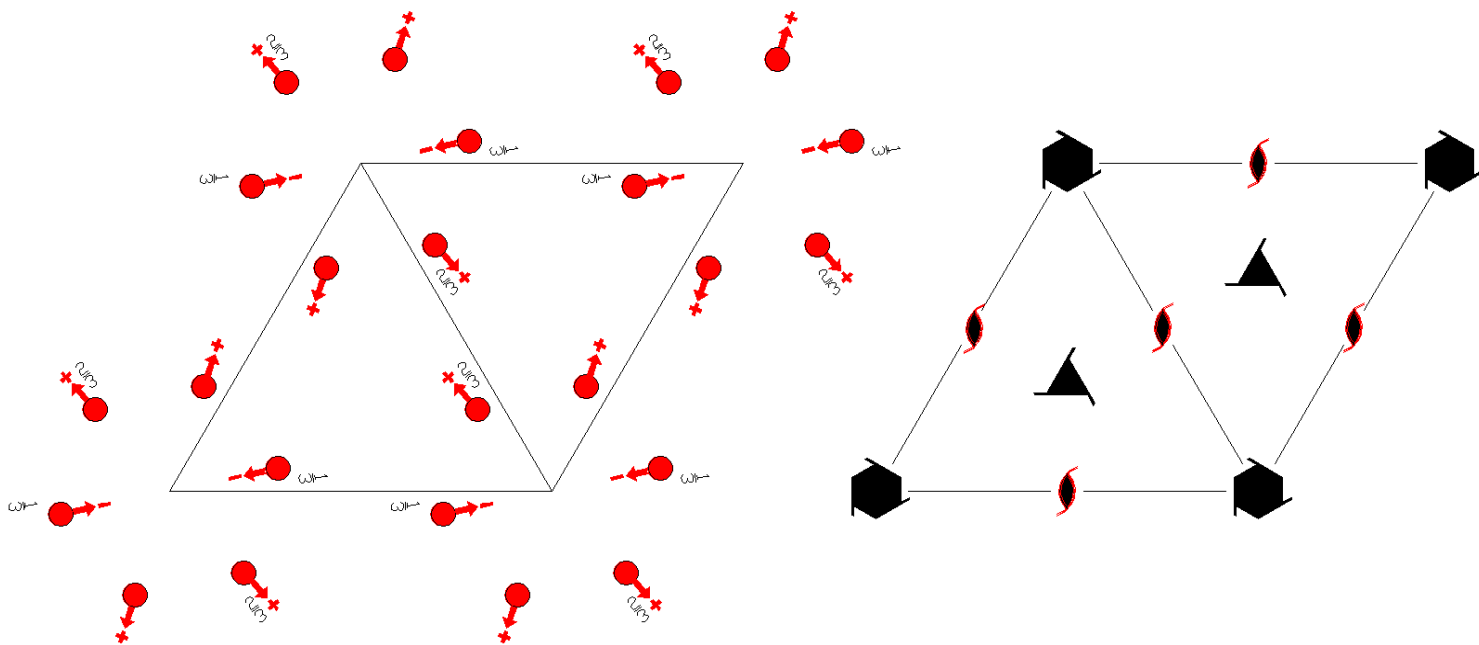




$P_{2c}6_4$   
172.4.1358

$61'$   
 $P_{2c}6_4$

Hexagonal



Origin on 2 on  $6_4'$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/3$ ;  $y \leq x$

Vertices  $0,0,0$   $1,0,0$   $1,1,0$   
 $0,0,1/3$   $1,0,1/3$   $1,1,1/3$

### Symmetry Operations

For  $(0,0,0)$  + set

- |                                |  |   |
|--------------------------------|--|---|
| (1) 1<br>(1 0,0,0)             | (2) $3^+ (0,0,1/3) 0,0,z$<br>( $3_z$  0,0,1/3)'      | (3) $3^- (0,0,2/3) 0,0,z$<br>( $3_z^{-1}$  0,0,2/3) |
| (4) 2 0,0,z<br>( $2_z$  0,0,0) | (5) $6^- (0,0,1/3) 0,0,z$<br>( $6_z^{-1}$  0,0,1/3)' | (6) $6^+ (0,0,2/3) 0,0,z$<br>( $6_z$  0,0,2/3)      |

For  $(0,0,1)'$  + set

- |  |   |  |
|--|---|--|
| (1) $t' (0,0,1)$<br>(1 0,0,1)'             | (2) $3^+ (0,0,4/3) 0,0,z$<br>( $3_z$  0,0,4/3)      | (3) $3^- (0,0,5/3) 0,0,z$<br>( $3_z^{-1}$  0,0,5/3)' |
| (4) $2' (0,0,1) 0,0,z$<br>( $2_z$  0,0,1)' | (5) $6^- (0,0,4/3) 0,0,z$<br>( $6_z^{-1}$  0,0,4/3) | (6) $6^+ (0,0,5/3) 0,0,z$<br>( $6_z$  0,0,5/3)'      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

### Positions

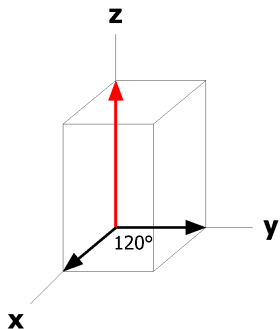
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			(0,0,0) +	(0,0,1)' +	
12	c	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z+1/3$ [ $\bar{v}, \bar{u}+v, \bar{w}$ ]	(3) $\bar{x}+y, \bar{x}, z+2/3$ [ $\bar{u}+v, \bar{u}, w$ ]
			(4) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(5) $y, \bar{x}+y, z+1/3$ [ $\bar{v}, u-v, \bar{w}$ ]	(6) x-y,x,z+2/3 [u-v,u,w]
6	b	2..	1/2,1/2,z [0,0,w]	1/2,0,z+1/3 [0,0, $\bar{w}$ ]	0,1/2,z+2/3 [0,0,w]
6	a	2..	0,0,z [0,0,w]	0,0,z+1/3 [0,0, $\bar{w}$ ]	0,0,z+2/3 [0,0,w]

### Symmetry of Special Projections

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>\* 1m'1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

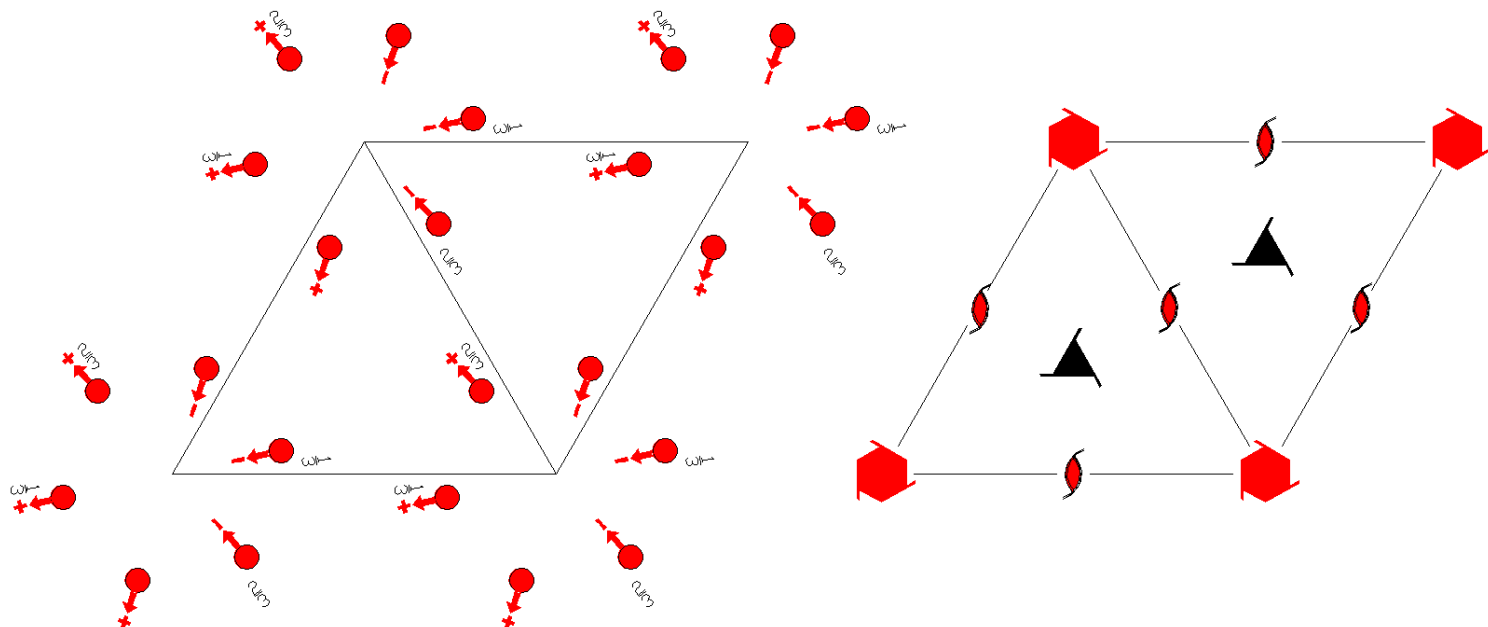
Along [2,1,0] p<sub>2b</sub>\* 1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$P_{2c}6_4'$   
172.5.1359

$61'$   
 $P_{2c}6_4'$

Hexagonal



Origin on  $2'$  on  $6_4'$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/3$ ;  $y \leq x$

Vertices	0,0,0	1,0,0	1,1,0
	0,0,1/3	1,0,1/3	1,1,1/3

### Symmetry Operations

For (0,0,0) + set

- |                                    |   |   |
|------------------------------------|---|---|
| (1) 1<br>(1 0,0,0)                 | (2) $3^+$ (0,0,1/3) 0,0,z<br>( $3_z$  0,0,1/3)'     | (3) $3^-$ (0,0,2/3) 0,0,z<br>( $3_z^{-1}$  0,0,2/3) |
| (4) $2'$ 0,0,z<br>( $2_z$  0,0,0)' | (5) $6^-$ (0,0,1/3) 0,0,z<br>( $6_z^{-1}$  0,0,1/3) | (6) $6^+$ (0,0,2/3) 0,0,z<br>( $6_z$  0,0,2/3)'     |

For (0,0,1)' + set

- |  |  |  |
|--|--|--|
| (1) $t'$ (0,0,1)<br>(1 0,0,1)'         | (2) $3^+$ (0,0,4/3) 0,0,z<br>( $3_z$  0,0,4/3)       | (3) $3^-$ (0,0,5/3) 0,0,z<br>( $3_z^{-1}$  0,0,5/3)' |
| (4) 2 (0,0,1) 0,0,z<br>( $2_z$  0,0,1) | (5) $6^-$ (0,0,4/3) 0,0,z<br>( $6_z^{-1}$  0,0,4/3)' | (6) $6^+$ (0,0,5/3) 0,0,z<br>( $6_z$  0,0,5/3)       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

### Positions

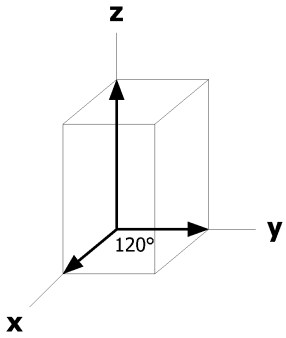
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			(0,0,0) +	(0,0,1)' +	
12	c	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z+1/3$ [v, $\bar{u}+v, \bar{w}$ ]	(3) $\bar{x}+y, \bar{x}, z+2/3$ [ $\bar{u}+v, \bar{u}, w$ ]
			(4) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ]	(5) $y, \bar{x}+y, z+1/3$ [v, $\bar{u}+v, w$ ]	(6) x-y,x,z+2/3 [ $\bar{u}+v, \bar{u}, \bar{w}$ ]
6	b	2'..	1/2,1/2,z [u,v,0]	1/2,0,z+1/3 [v, $\bar{u}+v, 0$ ]	0,1/2,z+2/3 [ $\bar{u}+v, \bar{u}, 0$ ]
6	a	2'..	0,0,z [u,v,0]	0,0,z+1/3 [v, $\bar{u}+v, 0$ ]	0,0,z+2/3 [ $\bar{u}+v, \bar{u}, 0$ ]

### Symmetry of Special Projections

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>\* 1m1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

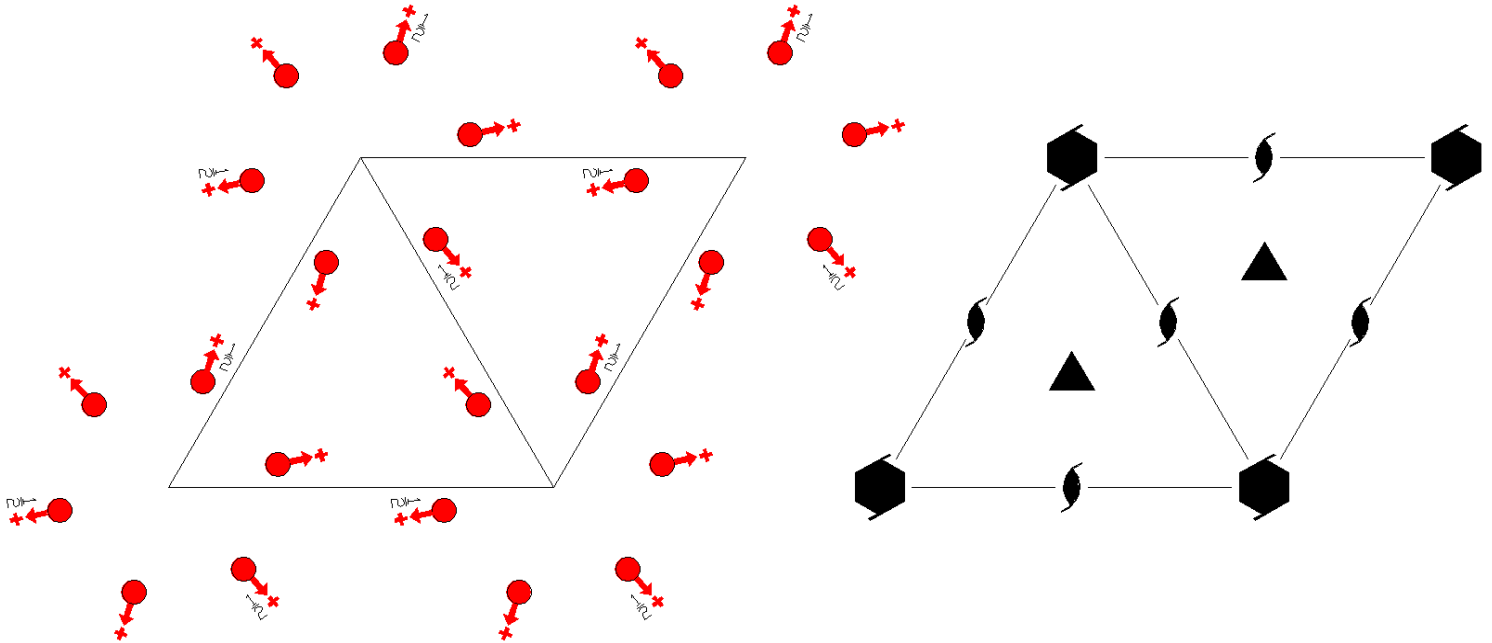
Along [2,1,0] p<sub>2b</sub>\* 1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$P6_3$   
173.1.1360

6  
 $P6_3$

Hexagonal



Origin on 3 on  $6_3$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1 + y)/2;$	$y \leq \min(1 - x, (1 + x)/2)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/3,2/3,0 1/3,2/3,1/2	0,1/2,0 0,1/2,1/2

**Symmetry Operations**

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                         | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)        |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2) | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

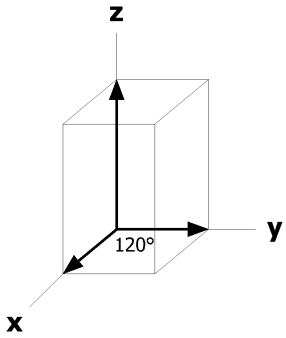
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	c	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(5) $y,\bar{x}+y,z+1/2$ [ $v,\bar{u}+v,w$ ]	(6) x-y,x,z+1/2 [u-v,u,w]
2	b	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z+1/2 [0,0,w]	
2	a	3..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	

**Symmetry of Special Projections**

Along [0,0,1] p6  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g'1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

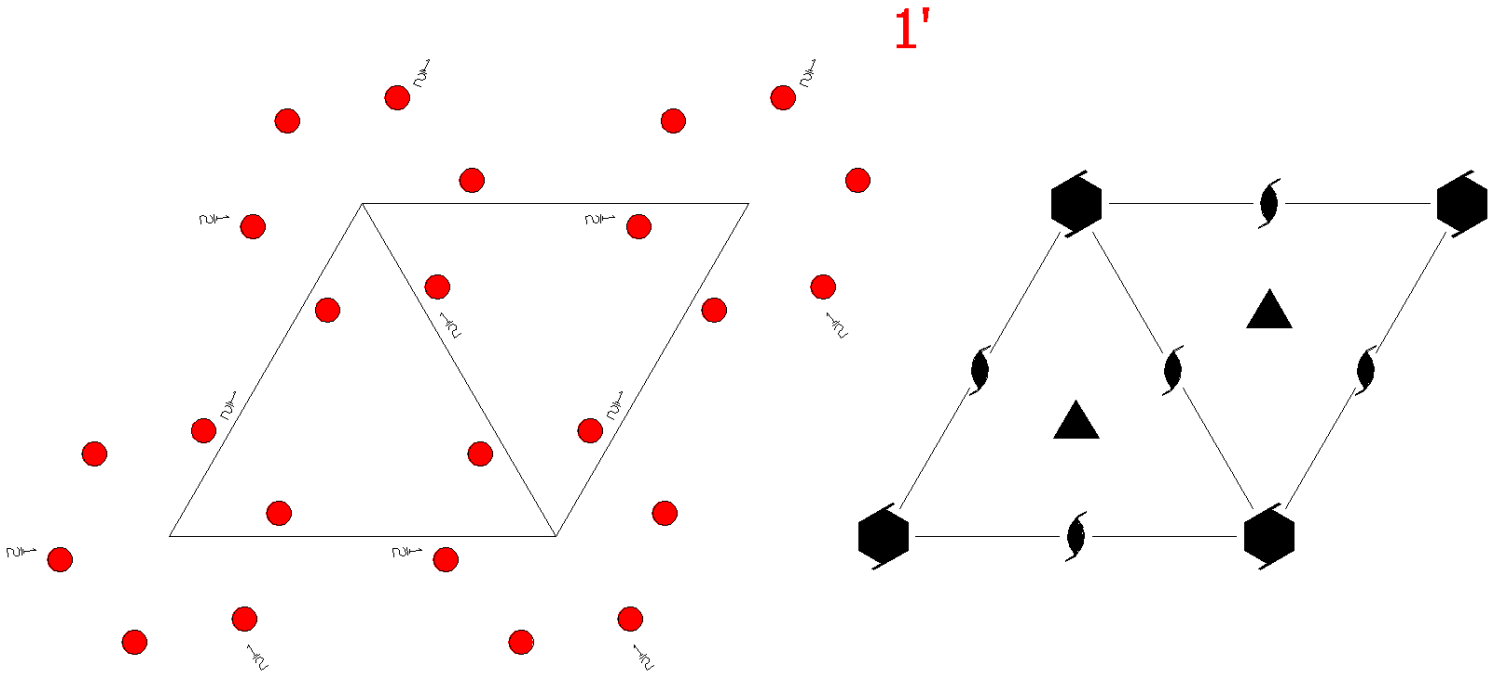
Along [2,1,0] p1g'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$P6_31'$   
173.2.1361

$61'$   
 $P6_31'$

Hexagonal



Origin on  $31'$  on  $6_31'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1 + y)/2;$	$y \leq \min(1 - x, (1 + x)/2)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/3,2/3,0 1/3,2/3,1/2	0,1/2,0 0,1/2,1/2

**Symmetry Operations**

For  $1 +$  set

- |  |   |  |
|--|---|--|
| (1) $1$<br>( $1 0,0,0$ )                       | (2) $3^+$ $0,0,z$<br>( $3_z 0,0,0$ )                  | (3) $3^-$ $0,0,z$<br>( $3_z^{-1} 0,0,0$ )        |
| (4) $2$ $(0,0,1/2) 0,0,z$<br>( $2_z 0,0,1/2$ ) | (5) $6^-$ $(0,0,1/2) 0,0,z$<br>( $6_z^{-1} 0,0,1/2$ ) | (6) $6^+$ $(0,0,1/2) 0,0,z$<br>( $6_z 0,0,1/2$ ) |

For  $1' +$  set

- |  |  |   |
|--|--|---|
| (1) $1'$<br>( $1 0,0,0$ )'                       | (2) $3^{+ '}$ $0,0,z$<br>( $3_z 0,0,0$ )'                  | (3) $3^{- '}$ $0,0,z$<br>( $3_z^{-1} 0,0,0$ )'        |
| (4) $2'$ $(0,0,1/2) 0,0,z$<br>( $2_z 0,0,1/2$ )' | (5) $6^{- '}$ $(0,0,1/2) 0,0,z$<br>( $6_z^{-1} 0,0,1/2$ )' | (6) $6^{+ '}$ $(0,0,1/2) 0,0,z$<br>( $6_z 0,0,1/2$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			1 +	1' +	
6	c	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x}$ ,z [0,0,0]
			(4) $\bar{x},\bar{y}$ ,z+1/2 [0,0,0]	(5) y, $\bar{x}+y$ ,z+1/2 [0,0,0]	(6) x-y,x,z+1/2 [0,0,0]
2	b	3..1'	1/3,2/3,z [0,0,0]	2/3,1/3,z+1/2 [0,0,0]	
2	a	3..1'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	

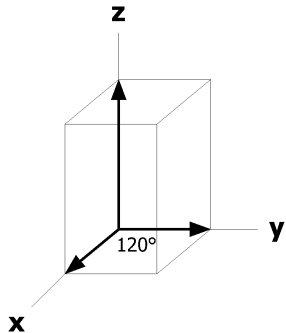
### Symmetry of Special Projections

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [2,1,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0

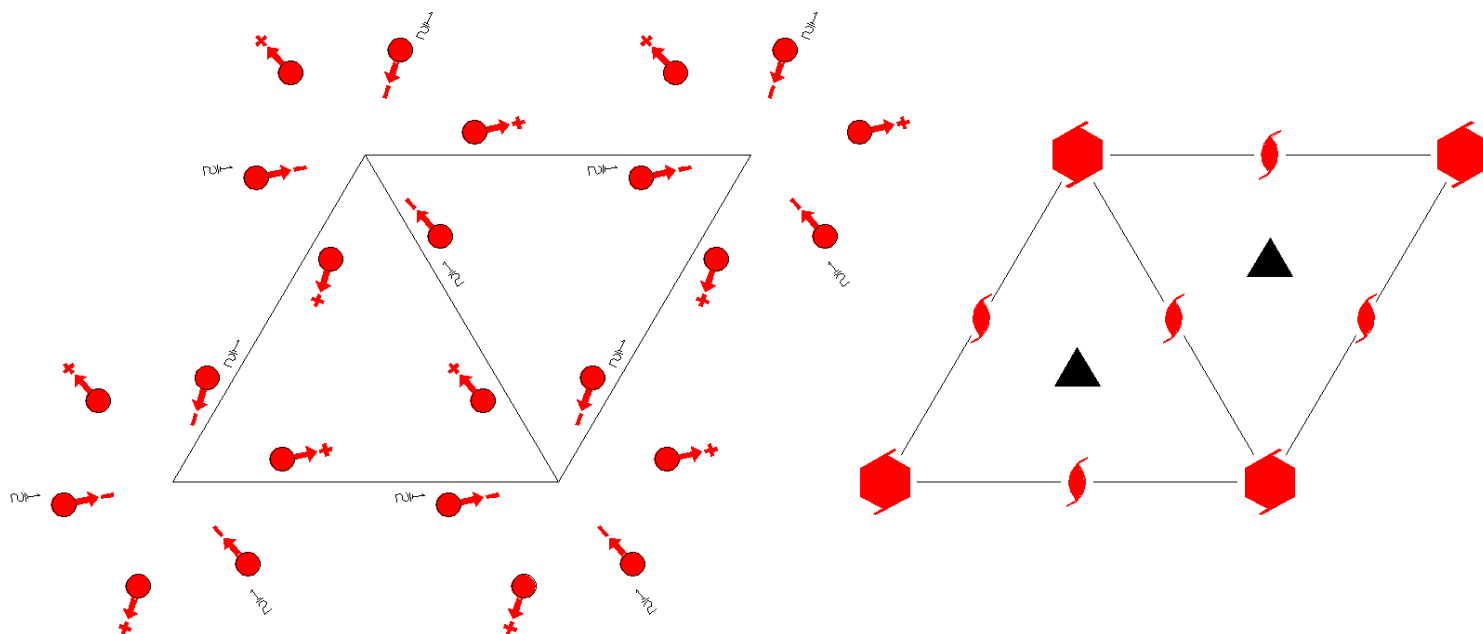




$P6_3'$   
173.3.1362

$6'$   
 $P6_3'$

Hexagonal



Origin on 3 on  $6_3'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1 + y)/2;$	$y \leq \min(1 - x, (1 + x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/3,2/3,1/2	0,1/2,1/2

**Symmetry Operations**

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                             | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)          |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)' | (5) $6^-'$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)' | (6) $6^+'$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

### Positions

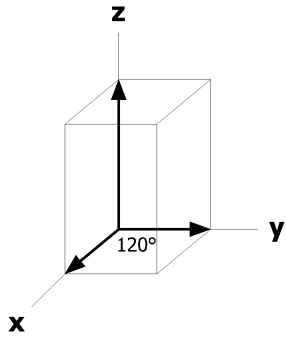
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	c	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(5) $y,\bar{x}+y,z+1/2$ [ $\bar{v},u-v,\bar{w}$ ]	(6) x-y,x,z+1/2 [ $\bar{u}+v,\bar{u},\bar{w}$ ]
2	b	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z+1/2 [0,0, $\bar{w}$ ]	
2	a	3..	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	

### Symmetry of Special Projections

Along [0,0,1] p6'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

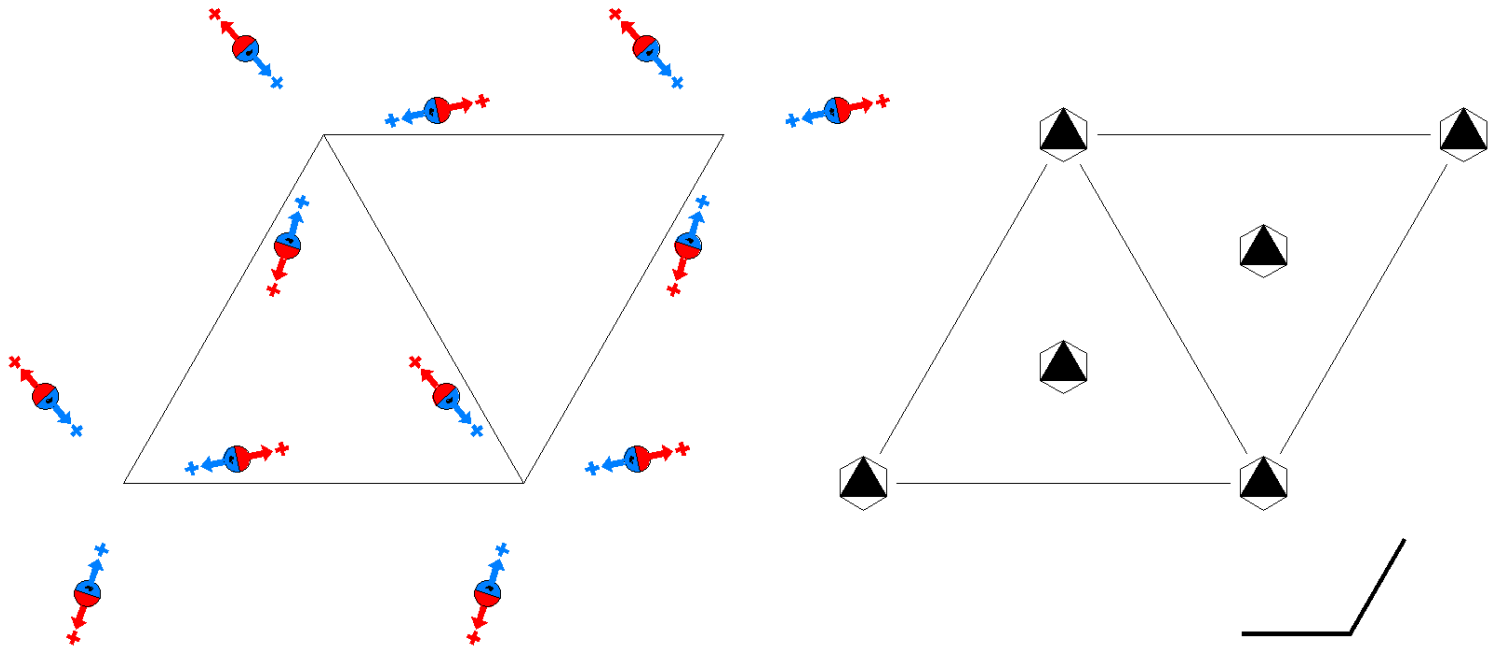
Along [2,1,0] p1g1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$\overline{P6}$   
174.1.1363

$\overline{6}$   
 $\overline{P6}$

Hexagonal



Origin on  $\overline{6}$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/3,2/3,0 1/3,2/3,1/2	0,1/2,0 0,1/2,1/2

**Symmetry Operations**

- |                                |  |   |
|--------------------------------|--|---|
| (1) 1<br>(1 0,0,0)             | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                                   | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                         |
| (4) m x,y,0<br>( $m_z$  0,0,0) | (5) $\overline{6}^-$ 0,0,z; 0,0,0<br>( $\overline{6}_z^{-1}$  0,0,0) | (6) $\overline{6}^+$ 0,0,z; 0,0,0<br>( $\overline{6}_z$  0,0,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

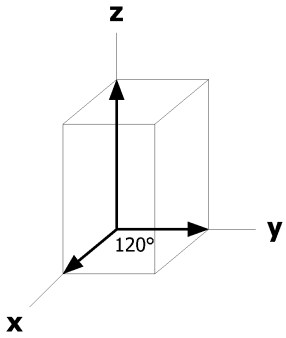
			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
6	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(5) $\bar{y}$ ,x-y, $\bar{z}$ [ $\bar{v},\bar{u}+v,w$ ]	(6) $\bar{x}+y,\bar{x},\bar{z}$ [u-v,u,w]
3	k	m..	x,y,1/2 [0,0,w]	$\bar{y}$ ,x-y,1/2 [0,0,w]	$\bar{x}+y,\bar{x},1/2$ [0,0,w]
3	j	m..	x,y,0 [0,0,w]	$\bar{y}$ ,x-y,0 [0,0,w]	$\bar{x}+y,\bar{x},0$ [0,0,w]
2	i	3..	2/3,1/3,z [0,0,w]	2/3,1/3, $\bar{z}$ [0,0,w]	
2	h	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ [0,0,w]	
2	g	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	
1	f	$\bar{6}$ ..	2/3,1/3,1/2 [0,0,w]		
1	e	$\bar{6}$ ..	2/3,1/3,0 [0,0,w]		
1	d	$\bar{6}$ ..	1/3,2/3,1/2 [0,0,w]		
1	c	$\bar{6}$ ..	1/3,2/3,0 [0,0,w]		
1	b	$\bar{6}$ ..	0,0,1/2 [0,0,w]		
1	a	$\bar{6}$ ..	0,0,0 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p31'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p1m1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0

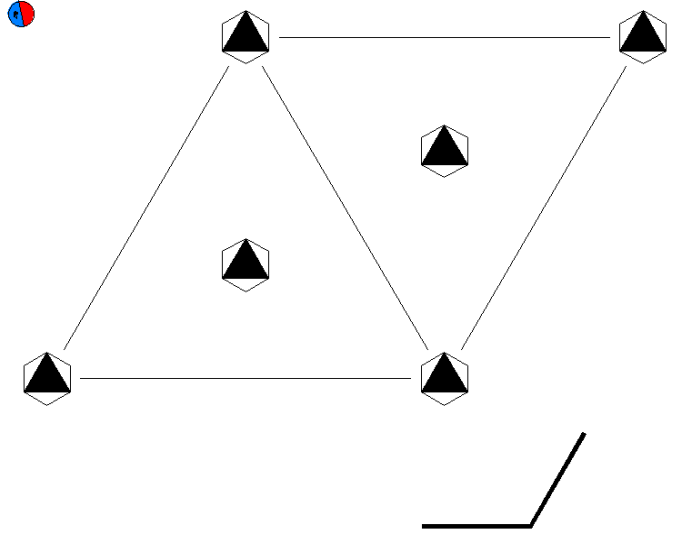
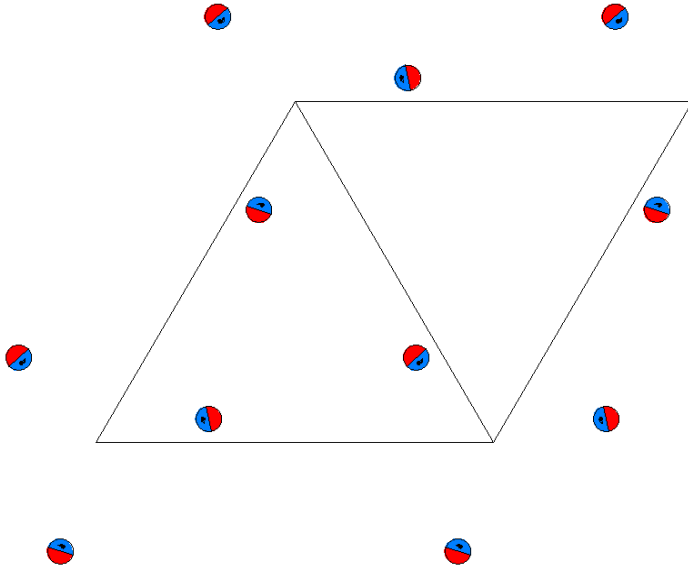


$P\bar{6}1'$   
174.2.1364

$\bar{6}1'$   
 $P\bar{6}1'$

Hexagonal

$1'$



Origin on  $\bar{6}1'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/3,2/3,0 1/3,2/3,1/2	0,1/2,0 0,1/2,1/2

**Symmetry Operations**

For  $1 +$  set

- |                                    |  |   |
|------------------------------------|--|---|
| (1) $1$<br>( $1 0,0,0$ )           | (2) $3^+$ $0,0,z$<br>( $3_z 0,0,0$ )                         | (3) $3^-$ $0,0,z$<br>( $3_z^{-1} 0,0,0$ )               |
| (4) $m$ $x,y,0$<br>( $m_z 0,0,0$ ) | (5) $\bar{6}^-$ $0,0,z; 0,0,0$<br>( $\bar{6}_z^{-1} 0,0,0$ ) | (6) $\bar{6}^+$ $0,0,z; 0,0,0$<br>( $\bar{6}_z 0,0,0$ ) |

For  $1' +$  set

- |                                      |  |   |
|--------------------------------------|--|---|
| (1) $1'$<br>( $1 0,0,0$ )'           | (2) $3^{+'}$ $0,0,z$<br>( $3_z 0,0,0$ )'                         | (3) $3^{-'}$ $0,0,z$<br>( $3_z^{-1} 0,0,0$ )'               |
| (4) $m'$ $x,y,0$<br>( $m_z 0,0,0$ )' | (5) $\bar{6}^{-'}$ $0,0,z; 0,0,0$<br>( $\bar{6}_z^{-1} 0,0,0$ )' | (6) $\bar{6}^{+'}$ $0,0,z; 0,0,0$<br>( $\bar{6}_z 0,0,0$ )' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

**Positions**

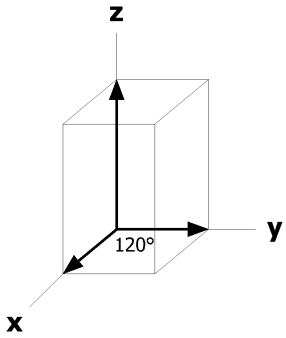
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			1 +		1' +
6	l	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0]
			(4) x,y, $\bar{z}$ [0,0,0]	(5) $\bar{y}$ ,x-y, $\bar{z}$ [0,0,0]	(6) $\bar{x}+y,\bar{x},\bar{z}$ [0,0,0]
3	k	m..1'	x,y,1/2 [0,0,0]	$\bar{y}$ ,x-y,1/2 [0,0,0]	$\bar{x}+y,\bar{x},1/2$ [0,0,0]
3	j	m..1'	x,y,0 [0,0,0]	$\bar{y}$ ,x-y,0 [0,0,0]	$\bar{x}+y,\bar{x},0$ [0,0,0]
2	i	3..1'	2/3,1/3,z [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	
2	h	3..1'	1/3,2/3,z [0,0,0]	1/3,2/3, $\bar{z}$ [0,0,0]	
2	g	3..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	
1	f	$\bar{6}..1'$	2/3,1/3,1/2 [0,0,0]		
1	e	$\bar{6}..1'$	2/3,1/3,0 [0,0,0]		
1	d	$\bar{6}..1'$	1/3,2/3,1/2 [0,0,0]		
1	c	$\bar{6}..1'$	1/3,2/3,0 [0,0,0]		
1	b	$\bar{6}..1'$	0,0,1/2 [0,0,0]		
1	a	$\bar{6}..1'$	0,0,0 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p31'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

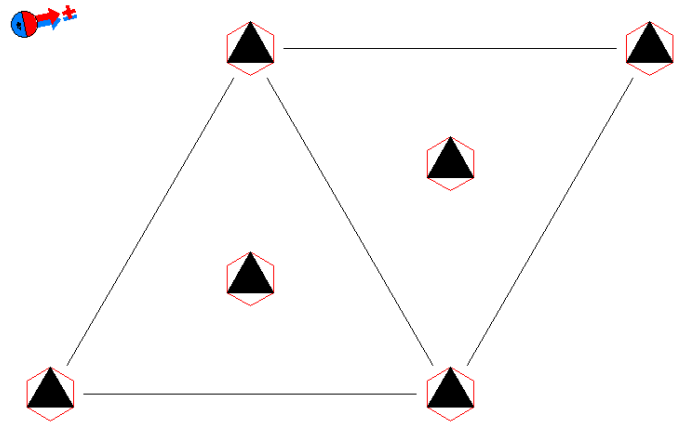
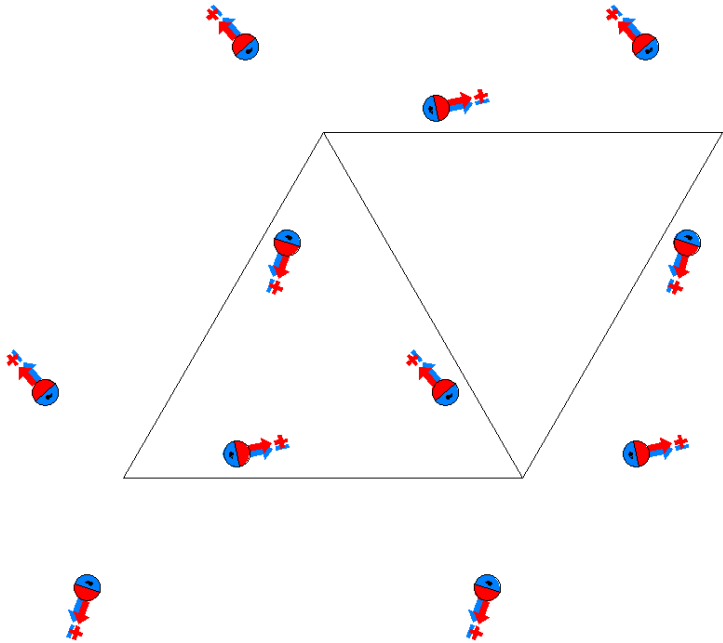
Along [2,1,0] p1m11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P\bar{6}'$   
174.3.1365

$\bar{6}'$   
 $P\bar{6}'$

Hexagonal



Origin on  $\bar{6}'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/3,2/3,1/2	0,1/2,1/2

**Symmetry Operations**

- |                                   |  |   |
|-----------------------------------|--|---|
| (1) 1<br>(1 0,0,0)                | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                         | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)               |
| (4) $m'$ x,y,0<br>( $m_z$  0,0,0) | (5) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (6) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
6	l	1	(1) x,y,z [u,v,w] (4) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w] (5) $\bar{y}$ ,x-y, $\bar{z}$ [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x}+y,\bar{x},\bar{z}$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]
3	k	m'..	x,y,1/2 [u,v,0]	$\bar{y}$ ,x-y,1/2 [ $\bar{v}$ ,u-v,0]	$\bar{x}+y,\bar{x},1/2$ [ $\bar{u}+v,\bar{u},0$ ]
3	j	m'..	x,y,0 [u,v,0]	$\bar{y}$ ,x-y,0 [ $\bar{v}$ ,u-v,0]	$\bar{x}+y,\bar{x},0$ [ $\bar{u}+v,\bar{u},0$ ]
2	i	3..	2/3,1/3,z [0,0,w]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	
2	h	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ [0,0, $\bar{w}$ ]	
2	g	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	
1	f	$\bar{6}'..$	2/3,1/3,1/2 [0,0,0]		
1	e	$\bar{6}'..$	2/3,1/3,0 [0,0,0]		
1	d	$\bar{6}'..$	1/3,2/3,1/2 [0,0,0]		
1	c	$\bar{6}'..$	1/3,2/3,0 [0,0,0]		
1	b	$\bar{6}'..$	0,0,1/2 [0,0,0]		
1	a	$\bar{6}'..$	0,0,0 [0,0,0]		

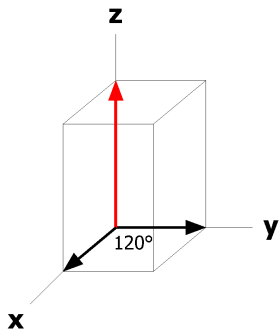
**Symmetry of Special Projections**

Along [0,0,1] p3  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p1m'1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0

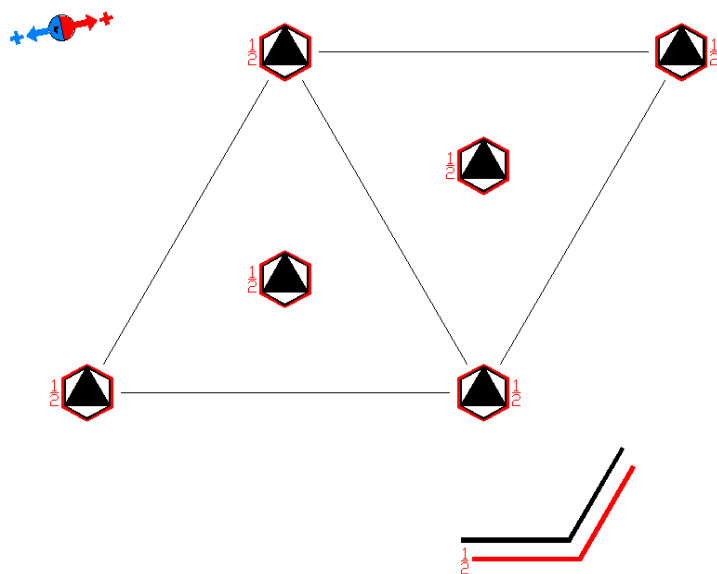
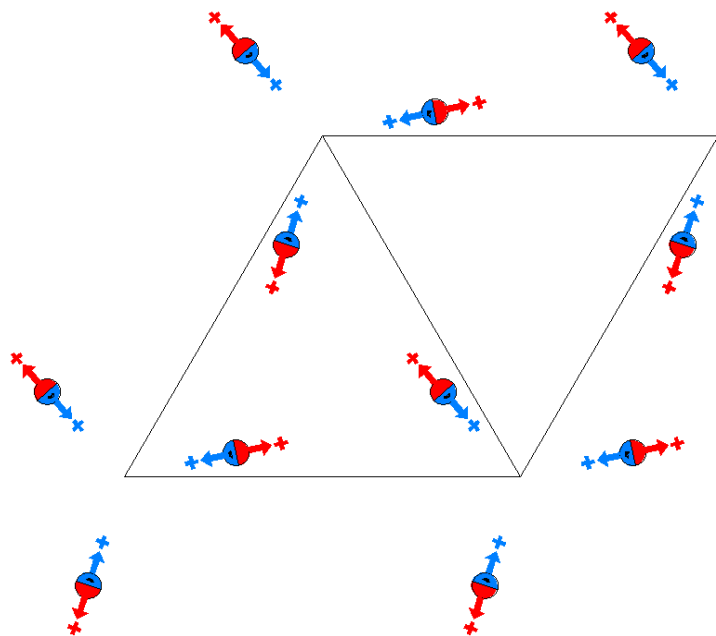




$P_{2c}\bar{6}$   
174.4.1366

$\bar{6}1'$   
 $P_{2c}\bar{6}$

Hexagonal



Origin on  $\bar{6}$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/3,2/3,0 1/3,2/3,1/2	0,1/2,0 0,1/2,1/2

**Symmetry Operations**

For (0,0,0) + set

- |                                |  |   |
|--------------------------------|--|---|
| (1) 1<br>(1 0,0,0)             | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                         | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)               |
| (4) m x,y,0<br>( $m_z$  0,0,0) | (5) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (6) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0) |

For (0,0,1)' + set

- |                                    |   |  |
|------------------------------------|---|--|
| (1) t' (0,0,1)<br>(1 0,0,1)'       | (2) $3^+$ ' (0,0,1) 0,0,z<br>( $3_z$  0,0,1)'                   | (3) $3^-$ ' (0,0,1) 0,0,z<br>( $3_z^{-1}$  0,0,1)'         |
| (4) m' x,y,1/2<br>( $m_z$  0,0,1)' | (5) $\bar{6}^-$ ' 0,0,z; 0,0,1/2<br>( $\bar{6}_z^{-1}$  0,0,1)' | (6) $\bar{6}^+$ ' 0,0,z; 0,0,1/2<br>( $\bar{6}_z$  0,0,1)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

**Positions**

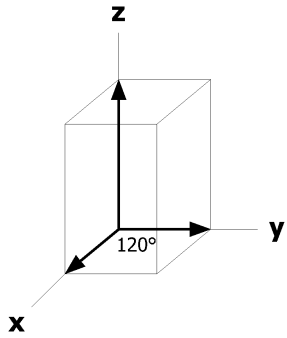
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
			(0,0,0) +	(0,0,1)' +	
12	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(5) $\bar{y}$ ,x-y, $\bar{z}$ [ $\bar{v},\bar{u}+v,w$ ]	(6) $\bar{x}+y,\bar{x},\bar{z}$ [u-v,u,w]
6	k	m'..	x,y,1/2 [u,v,0]	$\bar{y}$ ,x-y,1/2 [ $\bar{v}$ ,u-v,0]	$\bar{x}+y,\bar{x},1/2$ [ $\bar{u}+v,\bar{u},0$ ]
6	j	m..	x,y,0 [0,0,w]	$\bar{y}$ ,x-y,0 [0,0,w]	$\bar{x}+y,\bar{x},0$ [0,0,w]
4	i	3..	2/3,1/3,z [0,0,w]	2/3,1/3, $\bar{z}$ [0,0,w]	
4	h	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ [0,0,w]	
4	g	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]	
2	f	$\bar{6}'..$	2/3,1/3,1/2 [0,0,0]		
2	e	$\bar{6}..$	2/3,1/3,0 [0,0,w]		
2	d	$\bar{6}'..$	1/3,2/3,1/2 [0,0,0]		
2	c	$\bar{6}..$	1/3,2/3,0 [0,0,w]		
2	b	$\bar{6}'..$	0,0,1/2 [0,0,0]		
2	a	$\bar{6}..$	0,0,0 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p31'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>\* 1m1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

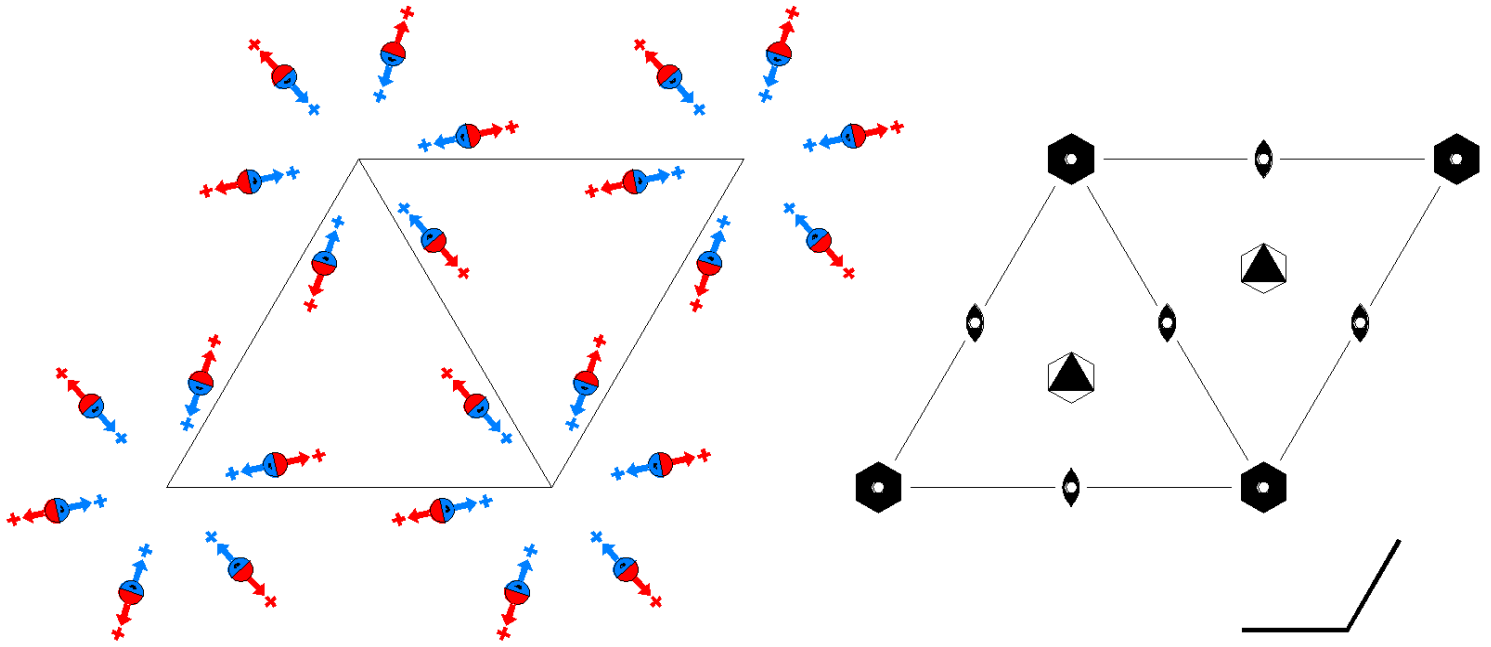
Along [2,1,0] p<sub>2a</sub>\* 1m1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P6/m  
175.1.1367

6/m  
P6/m

Hexagonal



Origin on center (6/m)

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

### Symmetry Operations

- |                                      |   |  |
|--------------------------------------|---|--|
| (1) 1<br>(1 0,0,0)                   | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                          | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) 2 0,0,z<br>( $2_z$  0,0,0)       | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0)                     | (6) $6^+$ 0,0,z<br>( $6_z$  0,0,0)                         |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)       | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) m x,y,0<br>( $m_z$  0,0,0)      | (11) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (12) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0)     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

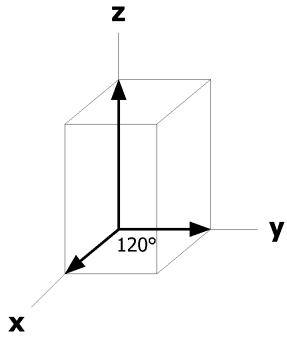
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y,\bar{x}$ ,z [ $\bar{u}+v,\bar{u}$ ,w]	
			(4) $\bar{x},\bar{y}$ ,z [ $\bar{u},\bar{v}$ ,w]	(5) y, $\bar{x}+y$ ,z [v, $\bar{u}+v$ ,w]	(6) x-y,x,z [u-v,u,w]	
			(7) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(8) y, $\bar{x}+y,\bar{z}$ [ $\bar{v}$ ,u-v,w]	(9) x-y,x, $\bar{z}$ [ $\bar{u}+v,\bar{u}$ ,w]	
			(10) x,y, $\bar{z}$ [ $\bar{u},\bar{v}$ ,w]	(11) $\bar{y}$ ,x-y, $\bar{z}$ [v, $\bar{u}+v$ ,w]	(12) $\bar{x}+y,\bar{x},\bar{z}$ [u-v,u,w]	
6	k	m..	x,y,1/2 [0,0,w]	$\bar{y}$ ,x-y,1/2 [0,0,w]	$\bar{x}+y,\bar{x}$ ,1/2 [0,0,w]	
			$\bar{x},\bar{y}$ ,1/2 [0,0,w]	y, $\bar{x}+y$ ,1/2 [0,0,w]	x-y,x,1/2 [0,0,w]	
6	j	m..	x,y,0 [0,0,w]	$\bar{y}$ ,x-y,0 [0,0,w]	$\bar{x}+y,\bar{x}$ ,0 [0,0,w]	
			$\bar{x},\bar{y}$ ,0 [0,0,w]	y, $\bar{x}+y$ ,0 [0,0,w]	x-y,x,0 [0,0,w]	
6	i	2..	1/2,0,z [0,0,w]	0,1/2,z [0,0,w]	1/2,1/2,z [0,0,w]	
			1/2,0, $\bar{z}$ [0,0,w]	0,1/2, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}$ [0,0,w]	
4	h	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0,w]	2/3,1/3, $\bar{z}$ [0,0,w]	1/3,2/3, $\bar{z}$ [0,0,w]
3	g	2/m..	1/2,0,1/2 [0,0,w]	0,1/2,1/2 [0,0,w]	1/2,1/2,1/2 [0,0,w]	
3	f	2/m..	1/2,0,0 [0,0,w]	0,1/2,0 [0,0,w]	1/2,1/2,0 [0,0,w]	
2	e	6..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
2	d	$\bar{6}$ ..	1/3,2/3,1/2 [0,0,w]	2/3,1/3,1/2 [0,0,w]		
2	c	$\bar{6}$ ..	1/3,2/3,0 [0,0,w]	2/3,1/3,0 [0,0,w]		
1	b	6/m..	0,0,1/2 [0,0,w]			
1	a	6/m..	0,0,0 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

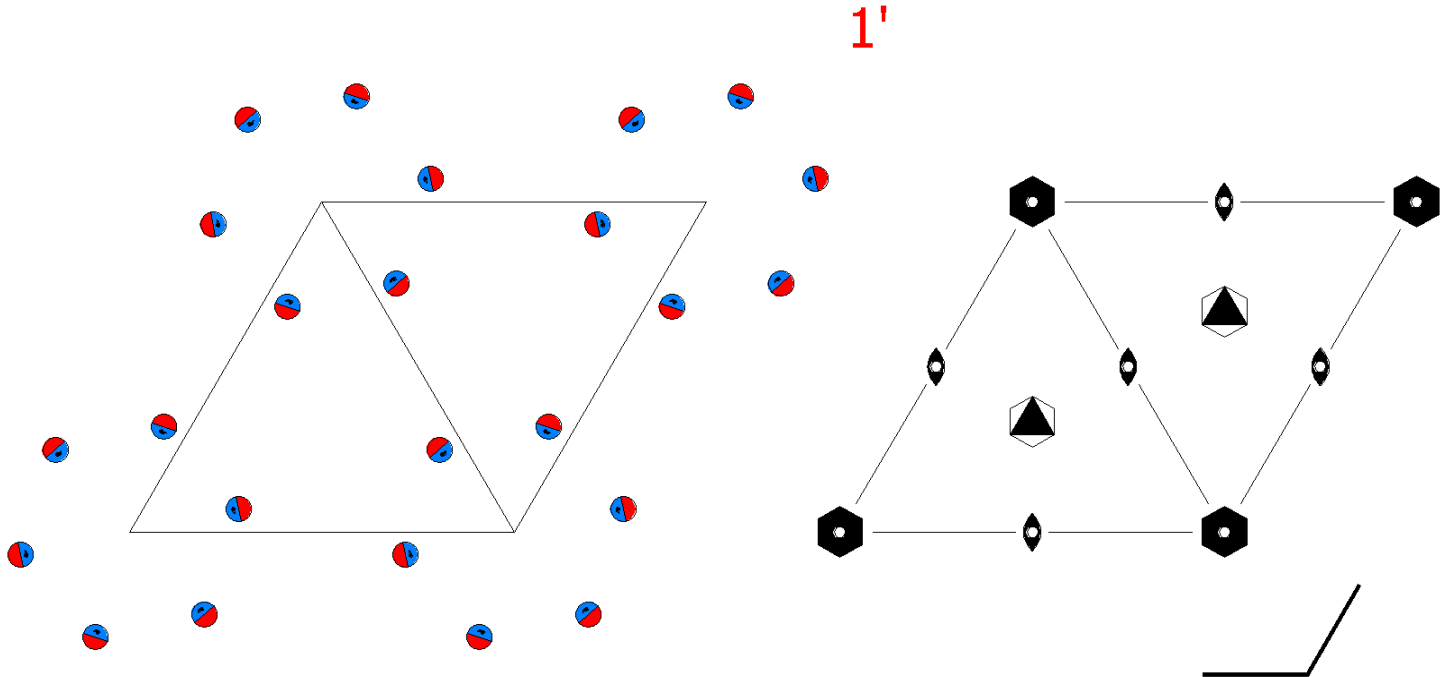
Along [2,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P6/m1'  
175.2.1368

6/m1'  
P6/m1'

Hexagonal



Origin on center (6/m1')

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

**Symmetry Operations**

For 1 + set

- |                                      |   |  |
|--------------------------------------|---|--|
| (1) 1<br>(1 0,0,0)                   | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                          | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) 2 0,0,z<br>( $2_z$  0,0,0)       | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0)                     | (6) $6^+$ 0,0,z<br>( $6_z$  0,0,0)                         |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)       | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) m x,y,0<br>( $m_z$  0,0,0)      | (11) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (12) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0)     |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 3 <sup>+</sup> 0,0,z (3 <sub>z</sub>  0,0,0)'	(3) 3 <sup>-</sup> 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(4) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(5) 6 <sup>-</sup> 0,0,z (6 <sub>z</sub> <sup>-1</sup>  0,0,0)'	(6) 6 <sup>+</sup> 0,0,z (6 <sub>z</sub>  0,0,0)'
(7) 1' (1 0,0,0)'	(8) 3 <sup>+</sup> 0,0,z; 0,0,0 (3 <sub>z</sub>  0,0,0)'	(9) 3 <sup>-</sup> 0,0,z; 0,0,0 (3 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(10) m' x,y,0 (m <sub>z</sub>  0,0,0)'	(11) 6 <sup>-</sup> 0,0,z; 0,0,0 (6 <sub>z</sub> <sup>-1</sup>  0,0,0)'	(12) 6 <sup>+</sup> 0,0,z; 0,0,0 (6 <sub>z</sub>  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

**Positions**

			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			1 +	1' +	
12	l	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0]
			(4) $\bar{x},\bar{y},z$ [0,0,0]	(5) y, $\bar{x}+y,z$ [0,0,0]	(6) x-y,x,z [0,0,0]
			(7) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(8) y, $\bar{x}+\bar{y},\bar{z}$ [0,0,0]	(9) x-y,x, $\bar{z}$ [0,0,0]
			(10) x,y, $\bar{z}$ [0,0,0]	(11) $\bar{y}$ ,x-y, $\bar{z}$ [0,0,0]	(12) $\bar{x}+y,\bar{x},\bar{z}$ [0,0,0]
6	k	m..1'	x,y,1/2 [0,0,0]	$\bar{y}$ ,x-y,1/2 [0,0,0]	$\bar{x}+y,\bar{x},1/2$ [0,0,0]
			$\bar{x},\bar{y},1/2$ [0,0,0]	y, $\bar{x}+y,1/2$ [0,0,0]	x-y,x,1/2 [0,0,0]
6	j	m..1'	x,y,0 [0,0,0]	$\bar{y}$ ,x-y,0 [0,0,0]	$\bar{x}+y,\bar{x},0$ [0,0,0]
			$\bar{x},\bar{y},0$ [0,0,0]	y, $\bar{x}+y,0$ [0,0,0]	x-y,x,0 [0,0,0]
6	i	2..1'	1/2,0,z [0,0,0]	0,1/2,z [0,0,0]	1/2,1/2,z [0,0,0]
			1/2,0, $\bar{z}$ [0,0,0]	0,1/2, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]
4	h	3..1'	1/3,2/3,z [0,0,0]	2/3,1/3,z [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]
					1/3,2/3, $\bar{z}$ [0,0,0]
3	g	2/m..1'	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]
3	f	2/m..1'	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]
2	e	6..1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	
2	d	6 <sup>-</sup> ..1'	1/3,2/3,1/2 [0,0,0]	2/3,1/3,1/2 [0,0,0]	
2	c	6 <sup>-</sup> ..1'	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]	
1	b	6/m..1'	0,0,1/2 [0,0,0]		

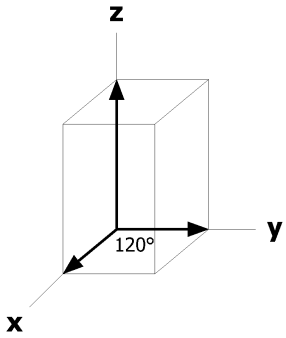
1 a 6/m..1' 0,0,0 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,0

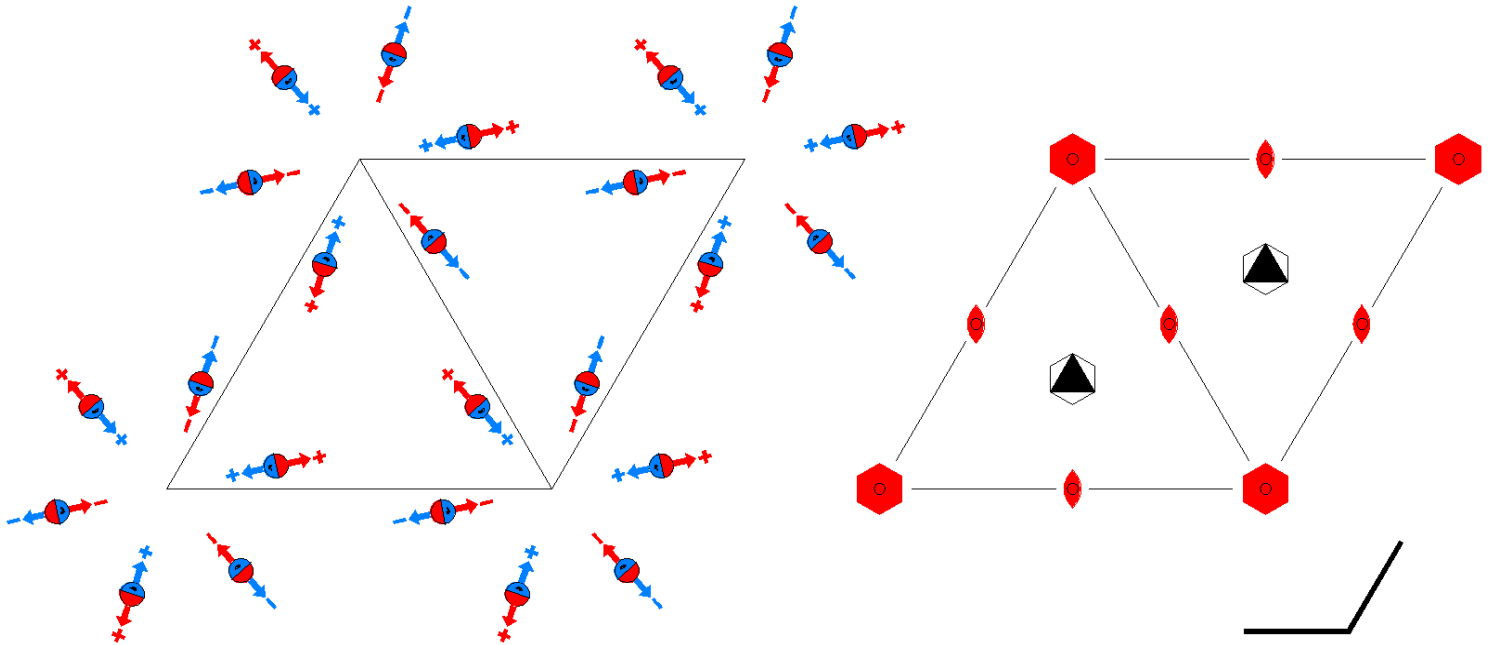
Along [2,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,x/2,0



P6'/m  
175.3.1369

6'/m  
P6'/m

Hexagonal



Origin on center (6'/m)

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

**Symmetry Operations**

- |                                       |   |   |
|---------------------------------------|---|---|
| (1) 1<br>(1 0,0,0)                    | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                          | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                     |
| (4) $2'$ 0,0,z<br>( $2_z$  0,0,0)'    | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0)'                    | (6) $6^+$ 0,0,z<br>( $6_z$  0,0,0)'                         |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)' | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)'      | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)' |
| (10) m x,y,0<br>( $m_z$  0,0,0)       | (11) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (12) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0)      |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

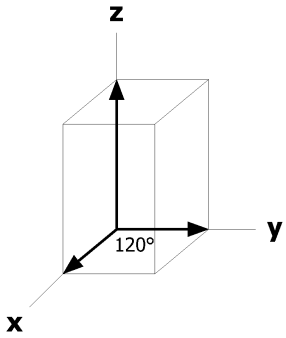
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	l	1	(1) x,y,z [u,v,w] (4) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (7) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) y, $\bar{x}+y,z$ [ $\bar{v},u-v,\bar{w}$ ] (8) y, $\bar{x}+y,\bar{z}$ [ $\bar{v},\bar{u}+v,\bar{w}$ ] (11) $\bar{y},x-y,\bar{z}$ [ $\bar{v},\bar{u}+v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) x-y,x,z [ $\bar{u}+v,\bar{u},\bar{w}$ ] (9) x-y,x, $\bar{z}$ [ $\bar{u}-v,u,\bar{w}$ ] (12) $\bar{x}+y,\bar{x},\bar{z}$ [ $\bar{u}-v,u,w$ ]	
6	k	m..	x,y,1/2 [0,0,w] $\bar{x},\bar{y},1/2$ [0,0, $\bar{w}$ ]	$\bar{y},x-y,1/2$ [0,0,w] y, $\bar{x}+y,1/2$ [0,0, $\bar{w}$ ]	$\bar{x}+y,\bar{x},1/2$ [0,0,w] x-y,x,1/2 [0,0, $\bar{w}$ ]	
6	j	m..	x,y,0 [0,0,w] $\bar{x},\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{y},x-y,0$ [0,0,w] y, $\bar{x}+y,0$ [0,0, $\bar{w}$ ]	$\bar{x}+y,\bar{x},0$ [0,0,w] x-y,x,0 [0,0, $\bar{w}$ ]	
6	i	2'..	1/2,0,z [u,v,0] 1/2,0, $\bar{z}$ [ $\bar{u},\bar{v},0$ ]	0,1/2,z [ $\bar{v},u-v,0$ ] 0,1/2, $\bar{z}$ [ $\bar{v},\bar{u}+v,0$ ]	1/2,1/2,z [ $\bar{u}+v,\bar{u},0$ ] 1/2,1/2, $\bar{z}$ [ $\bar{u}-v,u,0$ ]	
4	h	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	1/3,2/3, $\bar{z}$ [0,0,w]
3	g	2'/m..	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
3	f	2'/m..	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
2	e	6'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	d	$\bar{6}$ ..	1/3,2/3,1/2 [0,0,w]	2/3,1/3,1/2 [0,0, $\bar{w}$ ]		
2	c	$\bar{6}$ ..	1/3,2/3,0 [0,0,w]	2/3,1/3,0 [0,0, $\bar{w}$ ]		
1	b	6'/m..	0,0,1/2 [0,0,0]			
1	a	6'/m..	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

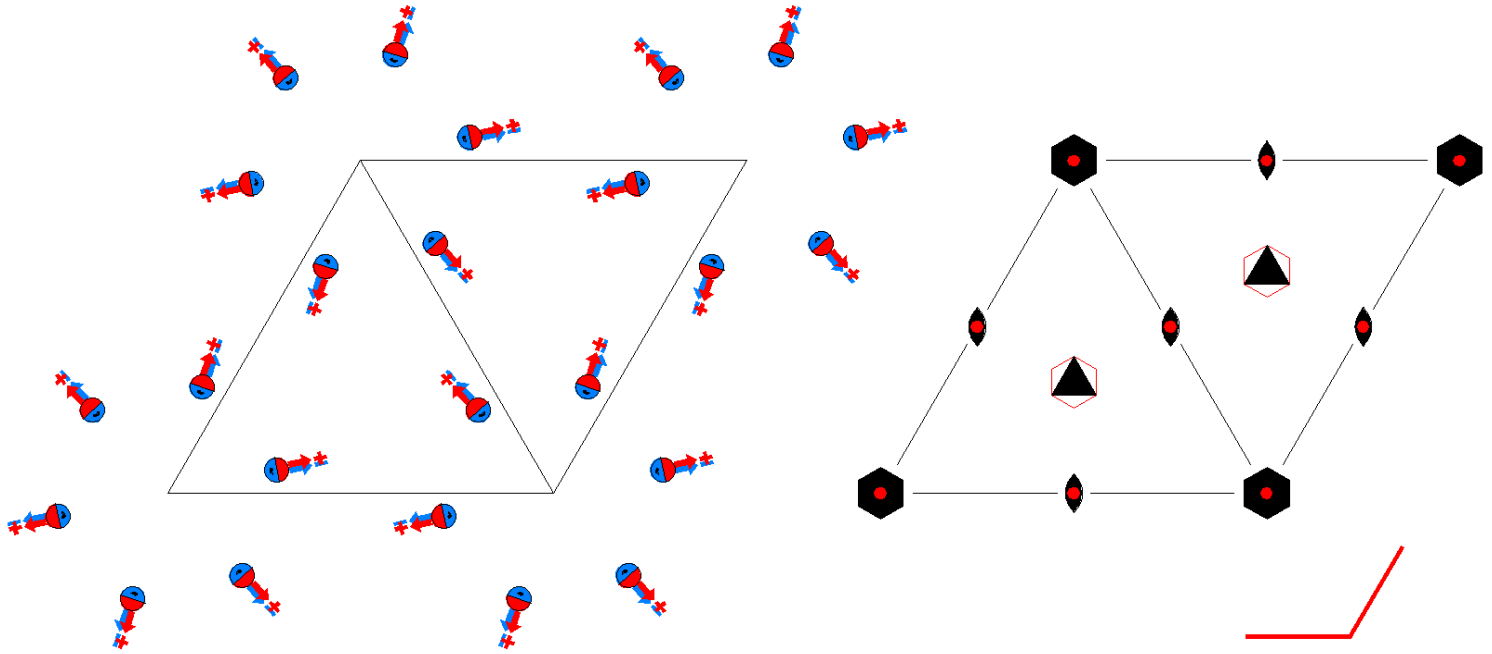
Along [2,1,0] p2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P6/m'  
175.4.1370

6/m'  
P6/m'

Hexagonal



Origin on center (6/m')

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

**Symmetry Operations**

- |                                       |  |   |
|---------------------------------------|--|---|
| (1) 1<br>(1 0,0,0)                    | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                           | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                     |
| (4) 2 0,0,z<br>( $2_z$  0,0,0)        | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0)                      | (6) $6^+$ 0,0,z<br>( $6_z$  0,0,0)                          |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)' | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)'       | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)' |
| (10) $m'$ x,y,0<br>( $m_z$  0,0,0)'   | (11) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0)' | (12) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0)'     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

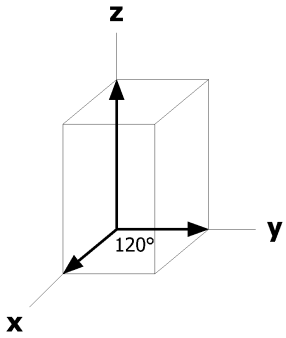
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	l	1	(1) x,y,z [u,v,w] (4) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (7) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (10) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) y, $\bar{x}+y,z$ [v, $\bar{u}+v,w$ ] (8) y, $\bar{x}+y,\bar{z}$ [v, $\bar{u}+v,\bar{w}$ ] (11) $\bar{y},x-y,\bar{z}$ [ $\bar{v},u-v,\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) x-y,x,z [u-v,u,w] (9) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ] (12) $\bar{x}+y,\bar{x},\bar{z}$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]	
6	k	m'..	x,y,1/2 [u,v,0] $\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x-y,1/2$ [ $\bar{v},u-v,0$ ] y, $\bar{x}+y,1/2$ [v, $\bar{u}+v,0$ ]	$\bar{x}+y,\bar{x},1/2$ [ $\bar{u}+v,\bar{u},0$ ] x-y,x,1/2 [u-v,u,0]	
6	j	m'..	x,y,0 [u,v,0] $\bar{x},\bar{y},0$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x-y,0$ [ $\bar{v},u-v,0$ ] y, $\bar{x}+y,0$ [v, $\bar{u}+v,0$ ]	$\bar{x}+y,\bar{x},0$ [ $\bar{u}+v,\bar{u},0$ ] x-y,x,0 [u-v,u,0]	
6	i	2..	1/2,0,z [0,0,w] 1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z [0,0,w] 0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2,z [0,0,w] 1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	
4	h	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0,w]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ] 1/3,2/3, $\bar{z}$ [0,0, $\bar{w}$ ]	
3	g	2/m'..	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
3	f	2/m'..	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
2	e	6..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	d	$\bar{6}'$ ..	1/3,2/3,1/2 [0,0,0]	2/3,1/3,1/2 [0,0,0]		
2	c	$\bar{6}'$ ..	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]		
1	b	6/m'..	0,0,1/2 [0,0,0]			
1	a	6/m'..	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p6'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

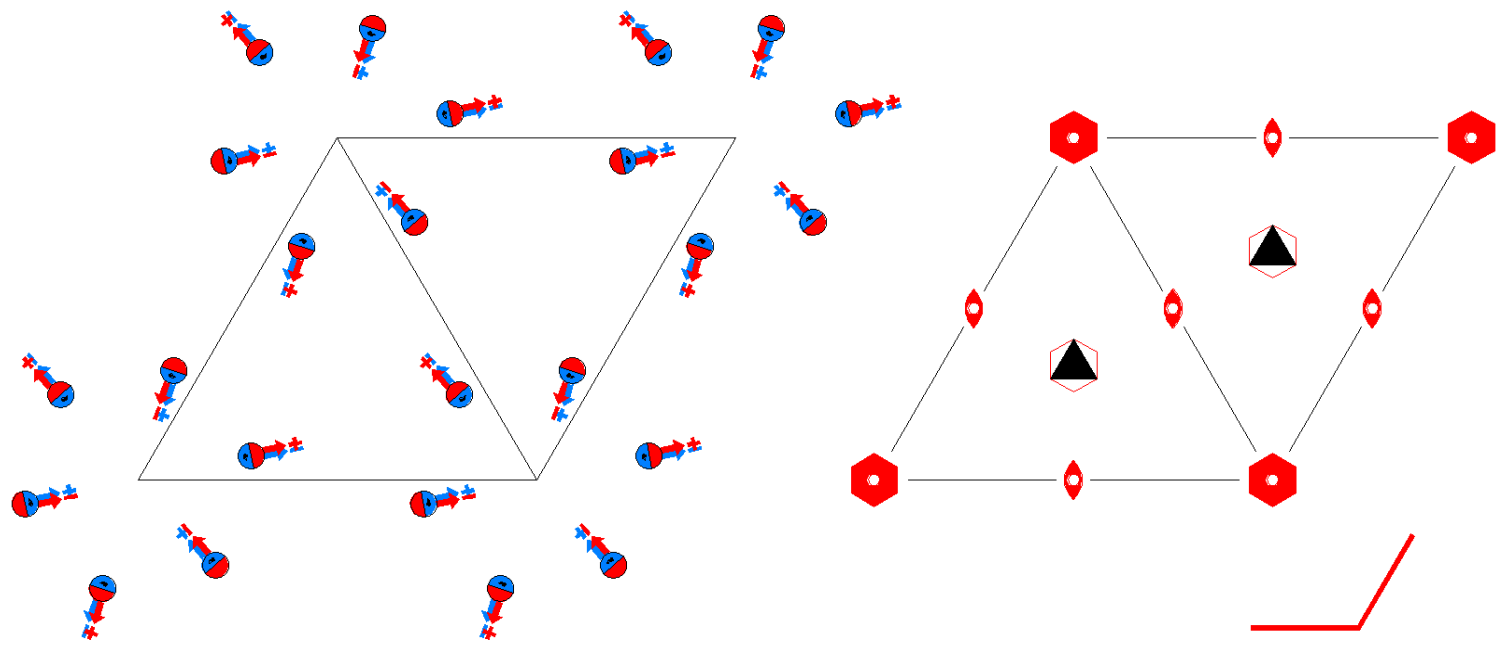
Along [2,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P6'/m'  
175.5.1371

6'/m'  
P6'/m'

Hexagonal



Origin on center (6'/m')

Asymmetric unit  $0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq \min(1-x, x)$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/2,1/2,1/2

**Symmetry Operations**

- (1) 1  
(1|0,0,0)
- (2)  $3^+$  0,0,z  
( $3_z$ |0,0,0)
- (3)  $3^-$  0,0,z  
( $3_z^{-1}$ |0,0,0)
- (4)  $2'$  0,0,z  
( $2_z$ |0,0,0)'
- (5)  $6^-$  0,0,z  
( $6_z^{-1}$ |0,0,0)'
- (6)  $6^+$  0,0,z  
( $6_z$ |0,0,0)'
- (7)  $\bar{1}$   
( $\bar{1}$ |0,0,0)
- (8)  $\bar{3}^+$  0,0,z; 0,0,0  
( $\bar{3}_z$ |0,0,0)
- (9)  $\bar{3}^-$  0,0,z; 0,0,0  
( $\bar{3}_z^{-1}$ |0,0,0)
- (10)  $m'$  x,y,0  
( $m_z$ |0,0,0)'
- (11)  $\bar{6}^-$  0,0,z; 0,0,0  
( $\bar{6}_z^{-1}$ |0,0,0)'
- (12)  $\bar{6}^+$  0,0,z; 0,0,0  
( $\bar{6}_z$ |0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

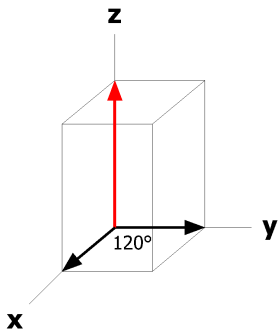
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	l	1	(1) x,y,z [u,v,w] (4) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (7) $\bar{x},\bar{y},\bar{z}$ [u,v,w] (10) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) y, $\bar{x}+y,z$ [ $\bar{v},u-v,\bar{w}$ ] (8) y, $\bar{x}+y,\bar{z}$ [ $\bar{v},u-v,w$ ] (11) $\bar{y},x-y,\bar{z}$ [ $\bar{v},u-v,\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) x-y,x,z [ $\bar{u}+v,\bar{u},\bar{w}$ ] (9) x-y,x, $\bar{z}$ [ $\bar{u}+v,\bar{u},w$ ] (12) $\bar{x}+y,\bar{x},\bar{z}$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]	
6	k	m'..	x,y,1/2 [u,v,0] $\bar{x},\bar{y},1/2$ [u,v,0]	$\bar{y},x-y,1/2$ [ $\bar{v},u-v,0$ ] y, $\bar{x}+y,1/2$ [ $\bar{v},u-v,0$ ]	$\bar{x}+y,\bar{x},1/2$ [ $\bar{u}+v,\bar{u},0$ ] x-y,x,1/2 [ $\bar{u}+v,\bar{u},0$ ]	
6	j	m'..	x,y,0 [u,v,0] $\bar{x},\bar{y},0$ [u,v,0]	$\bar{y},x-y,0$ [ $\bar{v},u-v,0$ ] y, $\bar{x}+y,0$ [ $\bar{v},u-v,0$ ]	$\bar{x}+y,\bar{x},0$ [ $\bar{u}+v,\bar{u},0$ ] x-y,x,0 [ $\bar{u}+v,\bar{u},0$ ]	
6	i	2'..	1/2,0,z [u,v,0] 1/2,0, $\bar{z}$ [u,v,0]	0,1/2,z [ $\bar{v},u-v,0$ ] 0,1/2, $\bar{z}$ [ $\bar{v},u-v,0$ ]	1/2,1/2,z [ $\bar{u}+v,\bar{u},0$ ] 1/2,1/2, $\bar{z}$ [ $\bar{u}+v,\bar{u},0$ ]	
4	h	3..	1/3,2/3,z [0,0,w] 2/3,1/3,z [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0,w] 1/3,2/3, $\bar{z}$ [0,0, $\bar{w}$ ]		
3	g	2'/m'..	1/2,0,1/2 [u,v,0]	0,1/2,1/2 [ $\bar{v},u-v,0$ ]	1/2,1/2,1/2 [ $\bar{u}+v,\bar{u},0$ ]	
3	f	2'/m'..	1/2,0,0 [u,v,0]	0,1/2,0 [ $\bar{v},u-v,0$ ]	1/2,1/2,0 [ $\bar{u}+v,\bar{u},0$ ]	
2	e	6'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	d	$\bar{6}'$ ..	1/3,2/3,1/2 [0,0,0]	2/3,1/3,1/2 [0,0,0]		
2	c	$\bar{6}'$ ..	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]		
1	b	6'/m'..	0,0,1/2 [0,0,0]			
1	a	6'/m'..	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p6'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

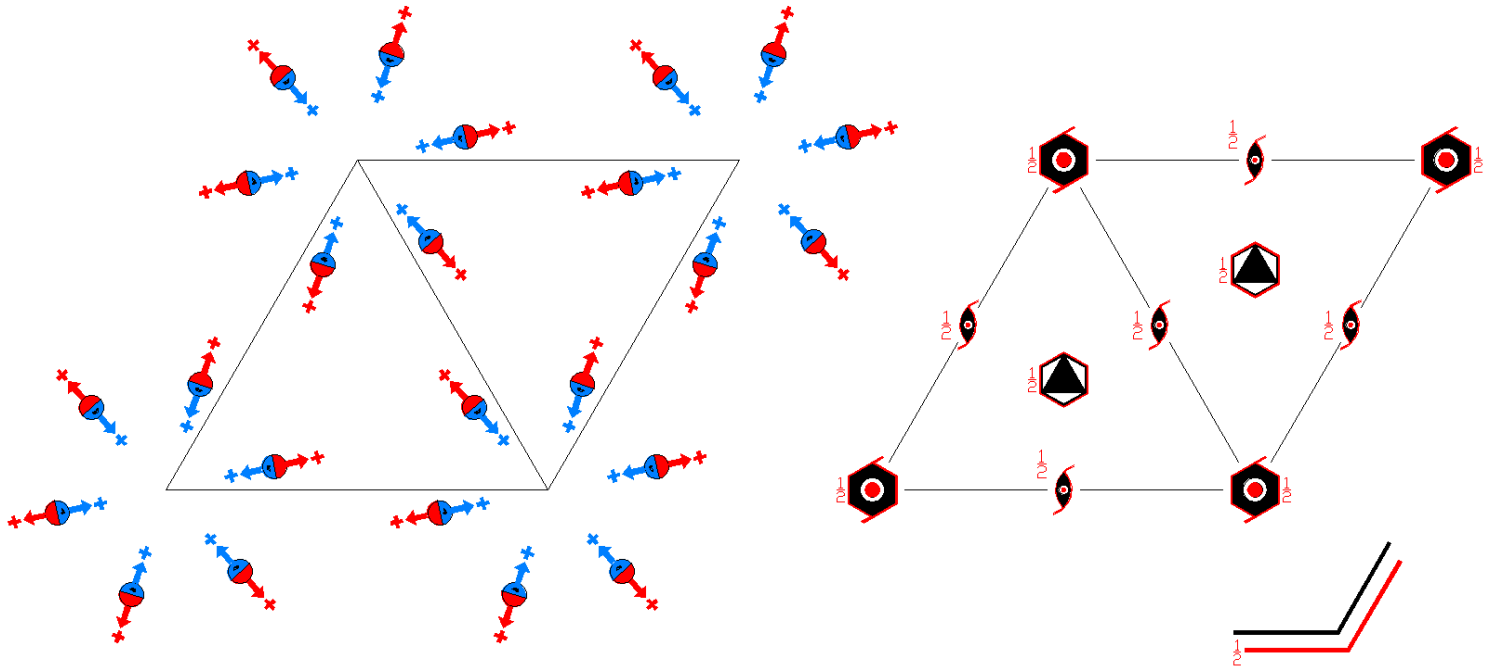
Along [2,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$P_{2c} 6/m$   
175.6.1372

$6/m1'$   
 $P_{2c} 6/m$

Hexagonal



Origin on center (6/m)

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

**Symmetry Operations**

For (0,0,0) + set

- |                                      |   |  |
|--------------------------------------|---|--|
| (1) 1<br>(1 0,0,0)                   | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                          | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) 2 0,0,z<br>( $2_z$  0,0,0)       | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0)                     | (6) $6^+$ 0,0,z<br>( $6_z$  0,0,0)                         |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0) | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)       | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) m x,y,0<br>( $m_z$  0,0,0)      | (11) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (12) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0)     |

## For (0,0,1)' + set

(1) $t' (0,0,1)$ $(1 0,0,1)'$	(2) $3^{+'} (0,0,1)$ 0,0,z $(3_z 0,0,1)'$	(3) $3^{-'} (0,0,1)$ 0,0,z $(3_z^{-1} 0,0,1)'$
(4) $2' (0,0,1)$ 0,0,z $(2_z 0,0,1)'$	(5) $6^{-'} (0,0,1)$ 0,0,z $(6_z^{-1} 0,0,1)'$	(6) $6^{+'} (0,0,1)$ 0,0,z $(6_z 0,0,1)'$
(7) $\bar{1}'$ 0,0,1/2 $(\bar{1} 0,0,1)'$	(8) $\bar{3}^{+'}$ 0,0,z; 0,0,1/2 $(\bar{3}_z 0,0,1)'$	(9) $\bar{3}^{-'}$ 0,0,z; 0,0,1/2 $(\bar{3}_z^{-1} 0,0,1)'$
(10) $m'$ x,y,1/2 $(m_z 0,0,1)'$	(11) $\bar{6}^{-'}$ 0,0,z; 0,0,1/2 $(\bar{6}_z^{-1} 0,0,1)'$	(12) $\bar{6}^{+'}$ 0,0,z; 0,0,1/2 $(\bar{6}_z 0,0,1)'$

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) + (0,0,1)' +			
24	l	1	(1) x,y,z [u,v,w] (4) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (7) $\bar{x},\bar{y},\bar{z}$ [u,v,w] (10) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) y, $\bar{x}+y,z$ [ $\bar{v},\bar{u}+v,w$ ] (8) y, $\bar{x}+y,\bar{z}$ [ $\bar{v},u-v,w$ ] (11) $\bar{y},x-y,\bar{z}$ [ $\bar{v},\bar{u}+v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) x-y,x,z [u-v,u,w] (9) x-y,x, $\bar{z}$ [ $\bar{u}+v,\bar{u},w$ ] (12) $\bar{x}+y,\bar{x},\bar{z}$ [u-v,u,w]	
12	k	m'..	x,y,1/2 [u,v,0] $\bar{x},\bar{y},1/2$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x-y,1/2$ [ $\bar{v},u-v,0$ ] y, $\bar{x}+y,1/2$ [ $\bar{v},\bar{u}+v,0$ ]	$\bar{x}+y,\bar{x},1/2$ [ $\bar{u}+v,\bar{u},0$ ] x-y,x,1/2 [u-v,u,0]	
12	j	m..	x,y,0 [0,0,w] $\bar{x},\bar{y},0$ [0,0,w]	$\bar{y},x-y,0$ [0,0,w] y, $\bar{x}+y,0$ [0,0,w]	$\bar{x}+y,\bar{x},0$ [0,0,w] x-y,x,0 [0,0,w]	
12	i	2..	1/2,0,z [0,0,w] 1/2,0, $\bar{z}$ [0,0,w]	0,1/2,z [0,0,w] 0,1/2, $\bar{z}$ [0,0,w]	1/2,1/2,z [0,0,w] 1/2,1/2, $\bar{z}$ [0,0,w]	
8	h	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0,w]	2/3,1/3, $\bar{z}$ [0,0,w]	
6	g	2'/m'..	1/2,0,1/2 [u,v,0]	0,1/2,1/2 [ $\bar{v},u-v,0$ ]	1/2,1/2,1/2 [ $\bar{u}+v,\bar{u},0$ ]	
6	f	2/m..	1/2,0,0 [0,0,w]	0,1/2,0 [0,0,w]	1/2,1/2,0 [0,0,w]	
4	e	6..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
4	d	$\bar{6}$ ..	1/3,2/3,1/2 [0,0,w]	2/3,1/3,1/2 [0,0,w]		
4	c	$\bar{6}$ ..	1/3,2/3,0 [0,0,w]	2/3,1/3,0 [0,0,w]		
2	b	6/m'..	0,0,1/2 [0,0,0]			

2      a      6/m..    0,0,0 [0,0,w]

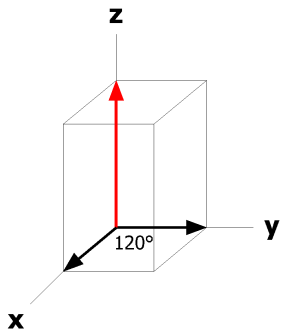
### Symmetry of Special Projections

Along [0,0,1]    p61'  
 $\mathbf{a}^* = \mathbf{a}$     $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]    p<sub>2a</sub>\* 2m'm'  
 $\mathbf{a}^* = \mathbf{c}$     $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/2

Along [2,1,0]    p<sub>2a</sub>\* 2m'm'  
 $\mathbf{a}^* = \mathbf{c}$     $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/2

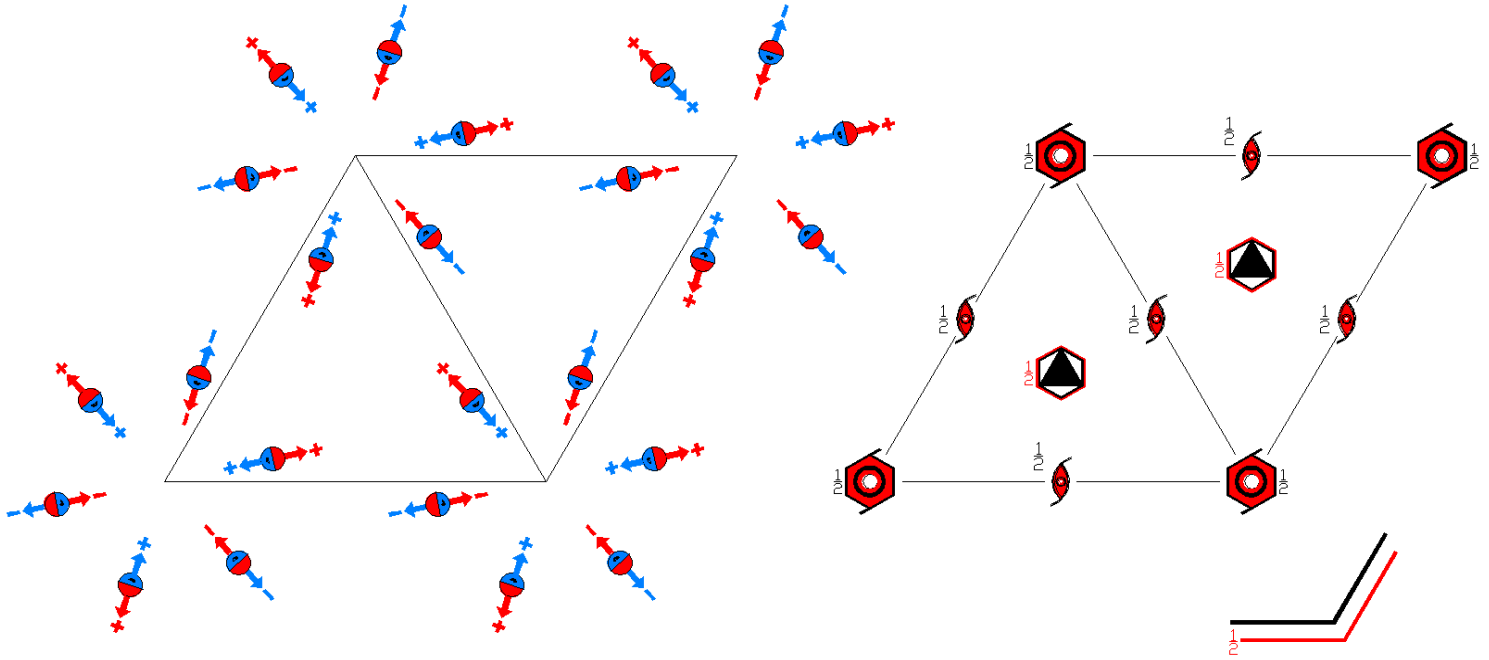




$P_{2c}6'/m$   
175.7.1373

$6/m1'$   
 $P_{2c}6'/m$

Hexagonal



Origin on center ( $6'/m$ )

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$ ;  $x \leq (1+y)/2$ ;  $y \leq \min(1-x, x)$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/2,1/2,1/2

### Symmetry Operations

For (0,0,0) + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                     | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                          | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                     |
| (4) $2'$ 0,0,z<br>( $2_z$  0,0,0)'     | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0)'                    | (6) $6^{+1}$ 0,0,z<br>( $6_z$  0,0,0)'                      |
| (7) $\bar{1}'$<br>( $\bar{1}$  0,0,0)' | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)'      | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)' |
| (10) m x,y,0<br>( $m_z$  0,0,0)        | (11) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (12) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0)      |

## For (0,0,1)' + set

(1) $t' (0,0,1)$ $(1 0,0,1)'$	(2) $3^{+'} (0,0,1) \ 0,0,z$ $(3_z 0,0,1)'$	(3) $3^{-'} (0,0,1) \ 0,0,z$ $(3_z^{-1} 0,0,1)'$
(4) $2 (0,0,1) \ 0,0,z$ $(2_z 0,0,1)$	(5) $6^{-} (0,0,1) \ 0,0,z$ $(6_z^{-1} 0,0,1)$	(6) $6^{+} (0,0,1) \ 0,0,z$ $(6_z 0,0,1)$
(7) $\bar{1} \ 0,0,1/2$ $(\bar{1} 0,0,1)$	(8) $\bar{3}^{+} \ 0,0,z; \ 0,0,1/2$ $(\bar{3}_z 0,0,1)$	(9) $\bar{3}^{-} \ 0,0,z; \ 0,0,1/2$ $(\bar{3}_z^{-1} 0,0,1)$
(10) $m' \ x,y,1/2$ $(m_z 0,0,1)'$	(11) $\bar{6}^{-'} \ 0,0,z; \ 0,0,1/2$ $(\bar{6}_z^{-1} 0,0,1)'$	(12) $\bar{6}^{+'} \ 0,0,z; \ 0,0,1/2$ $(\bar{6}_z 0,0,1)'$

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) + (0,0,1)' +			
24	l	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$	
			(4) $\bar{x},\bar{y},z [u,v,\bar{w}]$	(5) $y,\bar{x}+y,z [\bar{v},u-v,\bar{w}]$	(6) $x-y,x,z [\bar{u}+v,\bar{u},\bar{w}]$	
			(7) $\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$	(8) $y,\bar{x}+y,\bar{z} [v,\bar{u}+v,\bar{w}]$	(9) $x-y,x,\bar{z} [u-v,u,\bar{w}]$	
			(10) $x,y,\bar{z} [\bar{u},\bar{v},w]$	(11) $\bar{y},x-y,\bar{z} [v,\bar{u}+v,w]$	(12) $\bar{x}+y,\bar{x},\bar{z} [u-v,u,w]$	
12	k	m'..	$x,y,1/2 [u,v,0]$	$\bar{y},x-y,1/2 [\bar{v},u-v,0]$	$\bar{x}+y,\bar{x},1/2 [\bar{u}+v,\bar{u},0]$	
			$\bar{x},\bar{y},1/2 [u,v,0]$	$y,\bar{x}+y,1/2 [\bar{v},u-v,0]$	$x-y,x,1/2 [\bar{u}+v,\bar{u},0]$	
12	j	m..	$x,y,0 [0,0,w]$	$\bar{y},x-y,0 [0,0,w]$	$\bar{x}+y,\bar{x},0 [0,0,w]$	
			$\bar{x},\bar{y},0 [0,0,\bar{w}]$	$y,\bar{x}+y,0 [0,0,\bar{w}]$	$x-y,x,0 [0,0,\bar{w}]$	
12	i	2'..	$1/2,0,z [u,v,0]$	$0,1/2,z [\bar{v},u-v,0]$	$1/2,1/2,z [\bar{u}+v,\bar{u},0]$	
			$1/2,0,\bar{z} [\bar{u},\bar{v},0]$	$0,1/2,\bar{z} [v,\bar{u}+v,0]$	$1/2,1/2,\bar{z} [u-v,u,0]$	
8	h	3..	$1/3,2/3,z [0,0,w]$	$2/3,1/3,z [0,0,\bar{w}]$	$2/3,1/3,\bar{z} [0,0,\bar{w}]$	
			$1/3,2/3,\bar{z} [0,0,w]$	$1/3,2/3,z [0,0,\bar{w}]$	$1/3,2/3,\bar{z} [0,0,w]$	
6	g	2/m'..	$1/2,0,1/2 [0,0,0]$	$0,1/2,1/2 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$	
6	f	2'/m..	$1/2,0,0 [0,0,0]$	$0,1/2,0 [0,0,0]$	$1/2,1/2,0 [0,0,0]$	
4	e	6'..	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$		
4	d	$\bar{6}$ ..	$1/3,2/3,1/2 [0,0,w]$	$2/3,1/3,1/2 [0,0,\bar{w}]$		
4	c	$\bar{6}$ ..	$1/3,2/3,0 [0,0,w]$	$2/3,1/3,0 [0,0,\bar{w}]$		
2	b	6'/m'..	$0,0,1/2 [0,0,0]$			

2 a 6/m.. 0,0,0 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p61'

$\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$

Origin at 0,0,z

Along [1,0,0] p<sub>2a\*</sub> 2mm

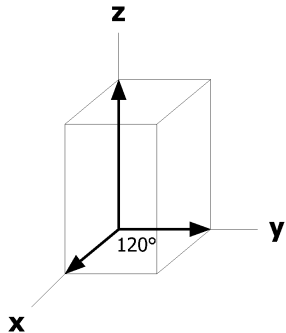
$\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$

Origin at x,0,0

Along [2,1,0] p<sub>2a\*</sub> 2mm

$\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$

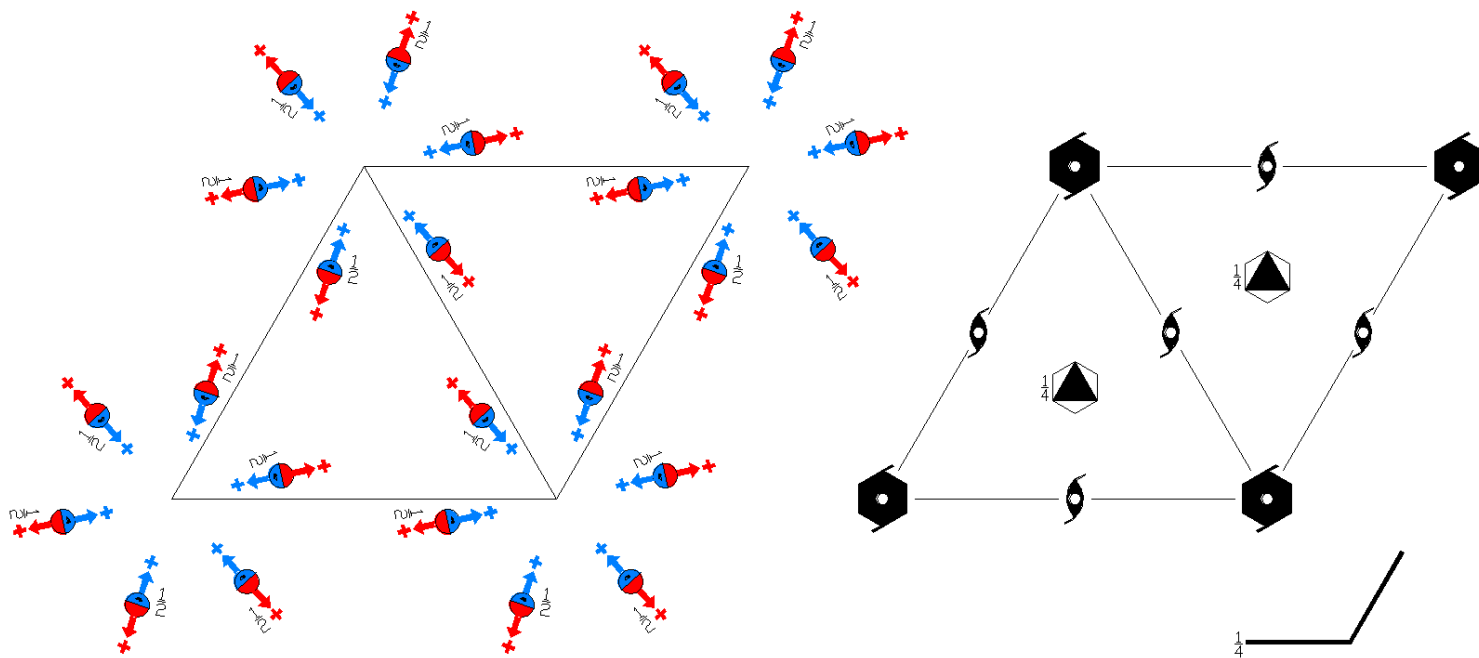
Origin at x,x/2,0



$P6_3/m$   
176.1.1374

$6/m$   
 $P6_3/m$

Hexagonal



Origin at center  $\bar{3}$  on  $6_3$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/4	1/2,0,0 1/2,0,1/4	2/3,1/3,0 2/3,1/3,1/4	1/3,2/3,0 1/3,2/3,1/4	0,1/2,0 0,1/2,1/4

### Symmetry Operations

- |  |   |  |
|--|---|--|
| (1) $1$<br>( $1 0,0,0$ )                         | (2) $3^+$ $0,0,z$<br>( $3_z 0,0,0$ )                              | (3) $3^-$ $0,0,z$<br>( $3_z^{-1} 0,0,0$ )                    |
| (4) $2$ $(0,0,1/2)$ $0,0,z$<br>( $2_z 0,0,1/2$ ) | (5) $6^-$ $(0,0,1/2)$ $0,0,z$<br>( $6_z^{-1} 0,0,1/2$ )           | (6) $6^+$ $(0,0,1/2)$ $0,0,z$<br>( $6_z 0,0,1/2$ )           |
| (7) $\bar{1}$<br>( $\bar{1} 0,0,0$ )             | (8) $\bar{3}^+$ $0,0,z; 0,0,0$<br>( $\bar{3}_z 0,0,0$ )           | (9) $\bar{3}^-$ $0,0,z; 0,0,0$<br>( $\bar{3}_z^{-1} 0,0,0$ ) |
| (10) $m$ $x,y,1/4$<br>( $m_z 0,0,1/2$ )          | (11) $\bar{6}^-$ $0,0,z; 0,0,1/4$<br>( $\bar{6}_z^{-1} 0,0,1/2$ ) | (12) $\bar{6}^+$ $0,0,z; 0,0,1/4$<br>( $\bar{6}_z 0,0,1/2$ ) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

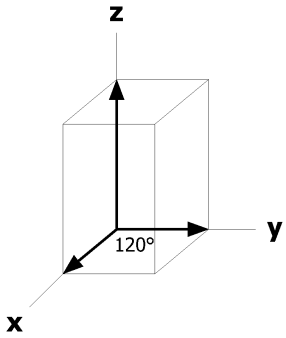
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
12	i	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]	
			(4) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(5) y, $\bar{x}+y,z+1/2$ [v, $\bar{u}+v,w$ ]	(6) x-y,x,z+1/2 [u-v,u,w]	
			(7) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(8) y, $\bar{x}+y,\bar{z}$ [ $\bar{v},u-v,w$ ]	(9) x-y,x, $\bar{z}$ [ $\bar{u}+v,\bar{u},w$ ]	
			(10) x,y, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(11) $\bar{y}$ ,x-y, $\bar{z}+1/2$ [v, $\bar{u}+v,w$ ]	(12) $\bar{x}+y,\bar{x},\bar{z}+1/2$ [u-v,u,w]	
6	h	m..	x,y,1/4 [0,0,w]	$\bar{y}$ ,x-y,1/4 [0,0,w]	$\bar{x}+y,\bar{x},1/4$ [0,0,w]	
			$\bar{x},\bar{y},3/4$ [0,0,w]	y, $\bar{x}+y,3/4$ [0,0,w]	x-y,x,3/4 [0,0,w]	
6	g	$\bar{1}$	1/2,0,0 [u,v,w]	0,1/2,0 [ $\bar{v},u-v,w$ ]	1/2,1/2,0 [ $\bar{u}+v,\bar{u},w$ ]	
			1/2,0,1/2 [ $\bar{u},\bar{v},w$ ]	0,1/2,1/2 [v, $\bar{u}+v,w$ ]	1/2,1/2,1/2 [u-v,u,w]	
4	f	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z+1/2 [0,0,w]	2/3,1/3, $\bar{z}$ [0,0,w]	1/3,2/3, $\bar{z}+1/2$ [0,0,w]
4	e	3..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]
2	d	$\bar{6}..$	2/3,1/3,1/4 [0,0,w]	1/3,2/3,3/4 [0,0,w]		
2	c	$\bar{6}..$	1/3,2/3,1/4 [0,0,w]	2/3,1/3,3/4 [0,0,w]		
2	b	$\bar{3}..$	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]		
2	a	$\bar{6}..$	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p6  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

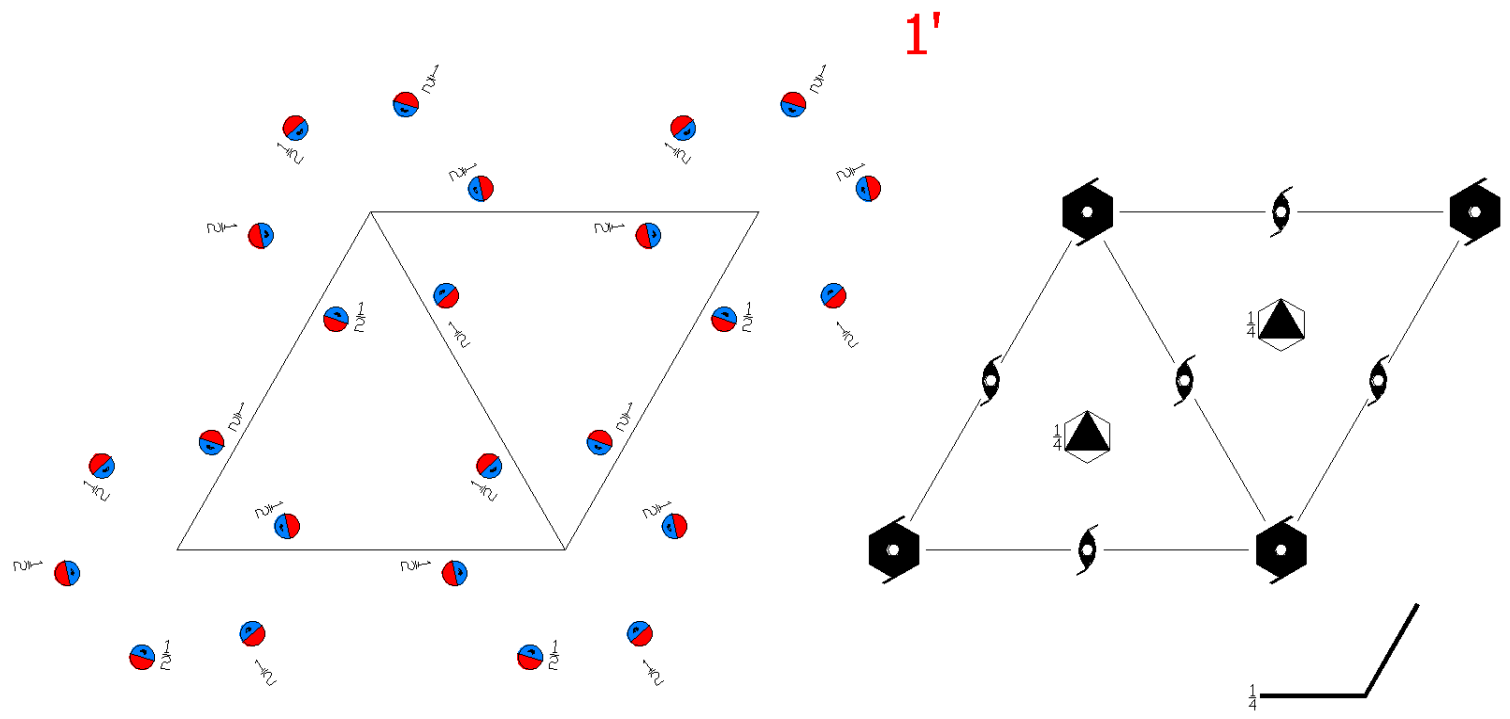
Along [2,1,0] p2'mg'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P6_3/m1'$   
176.2.1375

$6/m1'$   
 $P6_3/m1'$

Hexagonal



Origin at center  $\bar{3}1'$  on  $6_31'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/4	1/2,0,0 1/2,0,1/4	2/3,1/3,0 2/3,1/3,1/4	1/3,2/3,0 1/3,2/3,1/4	0,1/2,0 0,1/2,1/4

**Symmetry Operations**

For 1 + set

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                         | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                              | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2) | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)             | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)             |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)       | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)           | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (10) m x,y,1/4<br>( $m_z$  0,0,1/2)        | (11) $\bar{6}^-$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2) | (12) $\bar{6}^+$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2) |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 3 <sup>+</sup> ' 0,0,z (3 <sub>z</sub>  0,0,0)'	(3) 3 <sup>-</sup> ' 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(4) 2' (0,0,1/2) 0,0,z (2 <sub>z</sub>  0,0,1/2)'	(5) 6 <sup>-</sup> ' (0,0,1/2) 0,0,z (6 <sub>z</sub> <sup>-1</sup>  0,0,1/2)'	(6) 6 <sup>+</sup> ' (0,0,1/2) 0,0,z (6 <sub>z</sub>  0,0,1/2)'
(7) $\bar{1}$ ' ( $\bar{1}$  0,0,0)'	(8) $\bar{3}$ <sup>+</sup> ' 0,0,z; 0,0,0 ( $\bar{3}$ <sub>z</sub>  0,0,0)'	(9) $\bar{3}$ <sup>-</sup> ' 0,0,z; 0,0,0 ( $\bar{3}$ <sub>z</sub> <sup>-1</sup>  0,0,0)'
(10) m' x,y,1/4 (m <sub>z</sub>  0,0,1/2)'	(11) $\bar{6}$ <sup>-</sup> ' 0,0,z; 0,0,1/4 ( $\bar{6}$ <sub>z</sub> <sup>-1</sup>  0,0,1/2)'	(12) $\bar{6}$ <sup>+</sup> ' 0,0,z; 0,0,1/4 ( $\bar{6}$ <sub>z</sub>  0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			1 +		1' +	
12	i	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0]	
			(4) $\bar{x},\bar{y},z+1/2$ [0,0,0]	(5) y, $\bar{x}+y,z+1/2$ [0,0,0]	(6) x-y,x,z+1/2 [0,0,0]	
			(7) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(8) y, $\bar{x}+\bar{y},\bar{z}$ [0,0,0]	(9) x-y,x, $\bar{z}$ [0,0,0]	
			(10) x,y, $\bar{z}+1/2$ [0,0,0]	(11) $\bar{y}$ ,x-y, $\bar{z}+1/2$ [0,0,0]	(12) $\bar{x}+y,\bar{x},\bar{z}+1/2$ [0,0,0]	
6	h	m..1'	x,y,1/4 [0,0,0]	$\bar{y}$ ,x-y,1/4 [0,0,0]	$\bar{x}+y,\bar{x},1/4$ [0,0,0]	
			$\bar{x},\bar{y},3/4$ [0,0,0]	y, $\bar{x}+y,3/4$ [0,0,0]	x-y,x,3/4 [0,0,0]	
6	g	$\bar{1}1'$	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
			1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
4	f	3..1'	1/3,2/3,z [0,0,0]	2/3,1/3,z+1/2 [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	1/3,2/3, $\bar{z}+1/2$ [0,0,0]
4	e	3..1'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]
2	d	$\bar{6}$ ..1'	2/3,1/3,1/4 [0,0,0]	1/3,2/3,3/4 [0,0,0]		
2	c	$\bar{6}$ ..1'	1/3,2/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]		
2	b	$\bar{3}$ ..1'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
2	a	$\bar{6}$ ..1'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

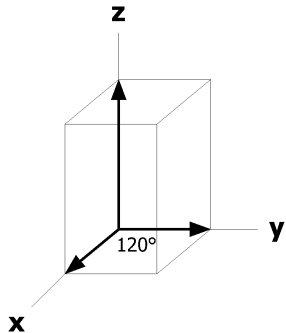
**Symmetry of Special Projections**

Along [0,0,1] p61'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,0

Along [2,1,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,x/2,0

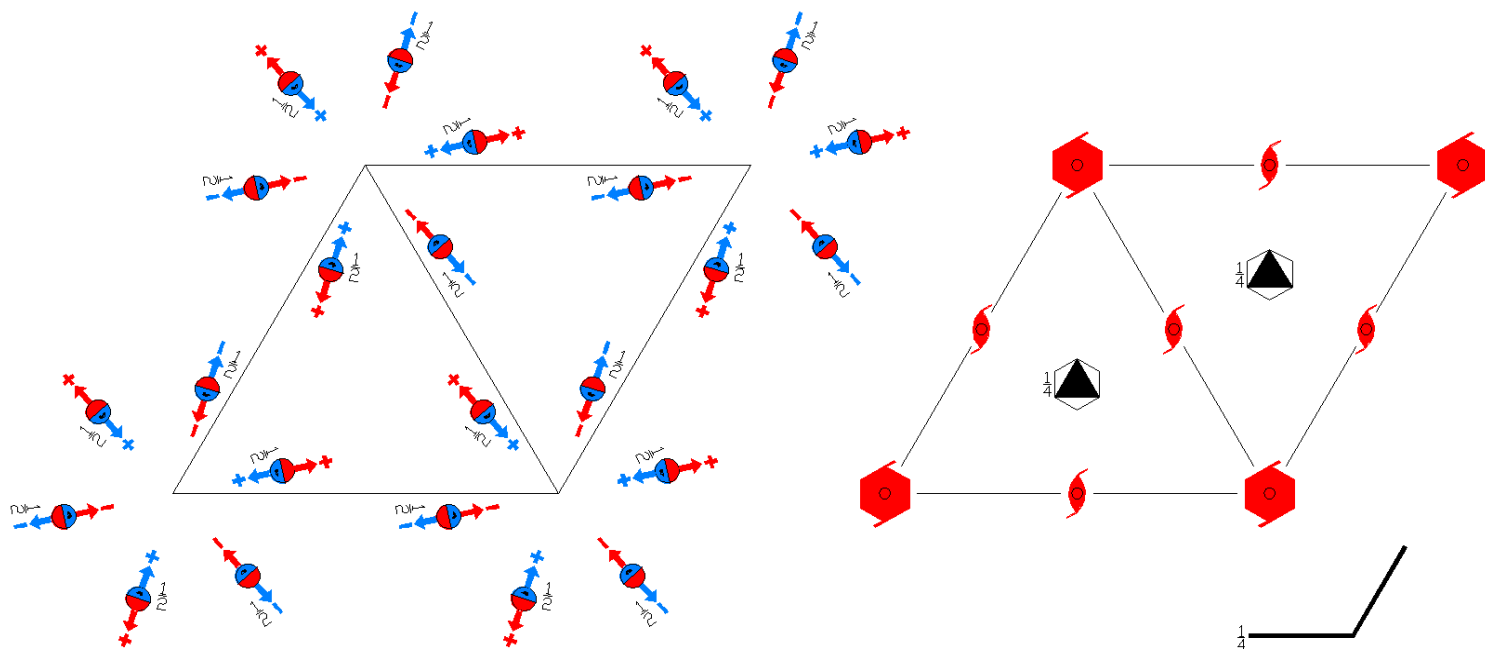




$P6_3'/m$   
176.3.1376

$6'/m$   
 $P6_3'/m$

Hexagonal



Origin at center  $\bar{3}'$  on  $6_3'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

### Symmetry Operations

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                             | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                              | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                     |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)' | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)'            | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)'             |
| (7) $\bar{1}'$<br>( $\bar{1}$  0,0,0)'         | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)'          | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)' |
| (10) m x,y,1/4<br>( $m_z$  0,0,1/2)            | (11) $\bar{6}^-$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2) | (12) $\bar{6}^+$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2)  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

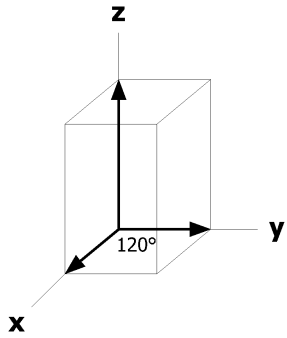
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	i	1	(1) x,y,z [u,v,w] (4) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ] (7) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (10) x,y, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) y, $\bar{x}+y,z+1/2$ [ $\bar{v},u-v,\bar{w}$ ] (8) y, $\bar{x}+y,\bar{z}$ [v, $\bar{u}+v,\bar{w}$ ] (11) $\bar{y},x-y,\bar{z}+1/2$ [v, $\bar{u}+v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) x-y,x,z+1/2 [ $\bar{u}+v,\bar{u},\bar{w}$ ] (9) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ] (12) $\bar{x}+y,\bar{x},\bar{z}+1/2$ [u-v,u,w]	
6	h	m..	x,y,1/4 [0,0,w] $\bar{x},\bar{y},3/4$ [0,0, $\bar{w}$ ]	$\bar{y},x-y,1/4$ [0,0,w] y, $\bar{x}+y,3/4$ [0,0, $\bar{w}$ ]	$\bar{x}+y,\bar{x},1/4$ [0,0,w] x-y,x,3/4 [0,0, $\bar{w}$ ]	
6	g	$\bar{1}'$	1/2,0,0 [0,0,0] 1/2,0,1/2 [0,0,0]	0,1/2,0 [0,0,0] 0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]	
4	f	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z+1/2 [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	1/3,2/3, $\bar{z}+1/2$ [0,0,w]
4	e	3..	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0,w]
2	d	$\bar{6}..$	2/3,1/3,1/4 [0,0,w]	1/3,2/3,3/4 [0,0, $\bar{w}$ ]		
2	c	$\bar{6}..$	1/3,2/3,1/4 [0,0,w]	2/3,1/3,3/4 [0,0, $\bar{w}$ ]		
2	b	$\bar{3}'..$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
2	a	$\bar{6}..$	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p6'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

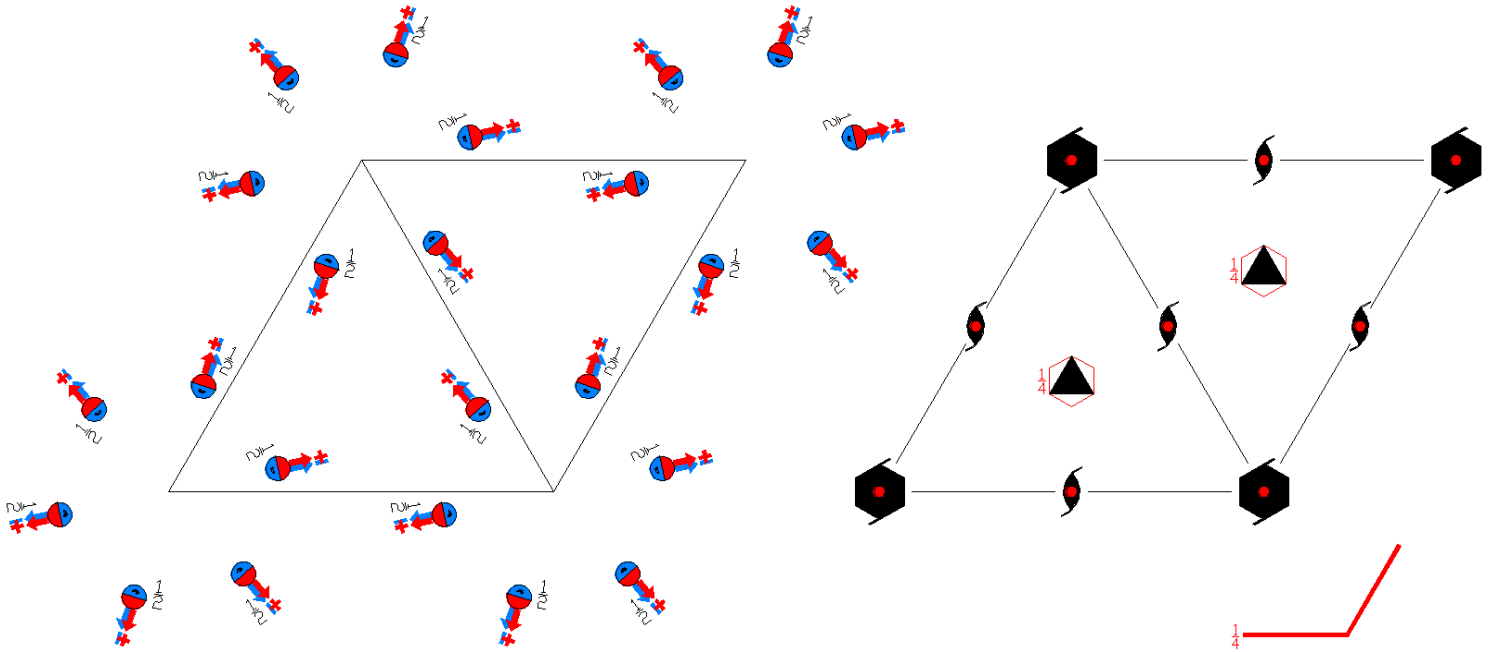
Along [2,1,0] p2mg  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P6_3/m'$   
176.4.1377

$6/m'$   
 $P6_3/m'$

Hexagonal



Origin at center  $\bar{3}'$  on  $6_3$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

### Symmetry Operations

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                         | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                               | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                     |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2) | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)              | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)              |
| (7) $\bar{1}'$<br>( $\bar{1}$  0,0,0)'     | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)'           | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)' |
| (10) $m'$ x,y,1/4<br>( $m_z$  0,0,1/2)'    | (11) $\bar{6}^-$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2)' | (12) $\bar{6}^+$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

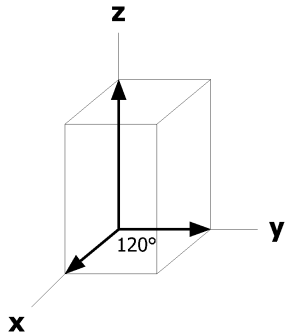
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates				
12	i	1	(1) x,y,z [u,v,w] (4) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ] (7) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ] (10) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) y, $\bar{x}+y,z+1/2$ [v, $\bar{u}+v,w$ ] (8) y, $\bar{x}+y,\bar{z}$ [v, $\bar{u}+v,\bar{w}$ ] (11) $\bar{y},x-y,\bar{z}+1/2$ [ $\bar{v},u-v,\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) x-y,x,z+1/2 [u-v,u,w] (9) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ] (12) $\bar{x}+y,\bar{x},\bar{z}+1/2$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]		
6	h	m'..	x,y,1/4 [u,v,0] $\bar{x},\bar{y},3/4$ [ $\bar{u},\bar{v},0$ ]	$\bar{y},x-y,1/4$ [ $\bar{v},u-v,0$ ] y, $\bar{x}+y,3/4$ [v, $\bar{u}+v,0$ ]	$\bar{x}+y,\bar{x},1/4$ [ $\bar{u}+v,\bar{u},0$ ] x-y,x,3/4 [u-v,u,0]		
6	g	$\bar{1}'$	1/2,0,0 [0,0,0] 1/2,0,1/2 [0,0,0]	0,1/2,0 [0,0,0] 0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]		
4	f	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z+1/2 [0,0,w]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	1/3,2/3, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	
4	e	3..	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	
2	d	$\bar{6}'..$	2/3,1/3,1/4 [0,0,0]	1/3,2/3,3/4 [0,0,0]			
2	c	$\bar{6}'..$	1/3,2/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]			
2	b	$\bar{3}'..$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]			
2	a	$\bar{6}'..$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p6  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

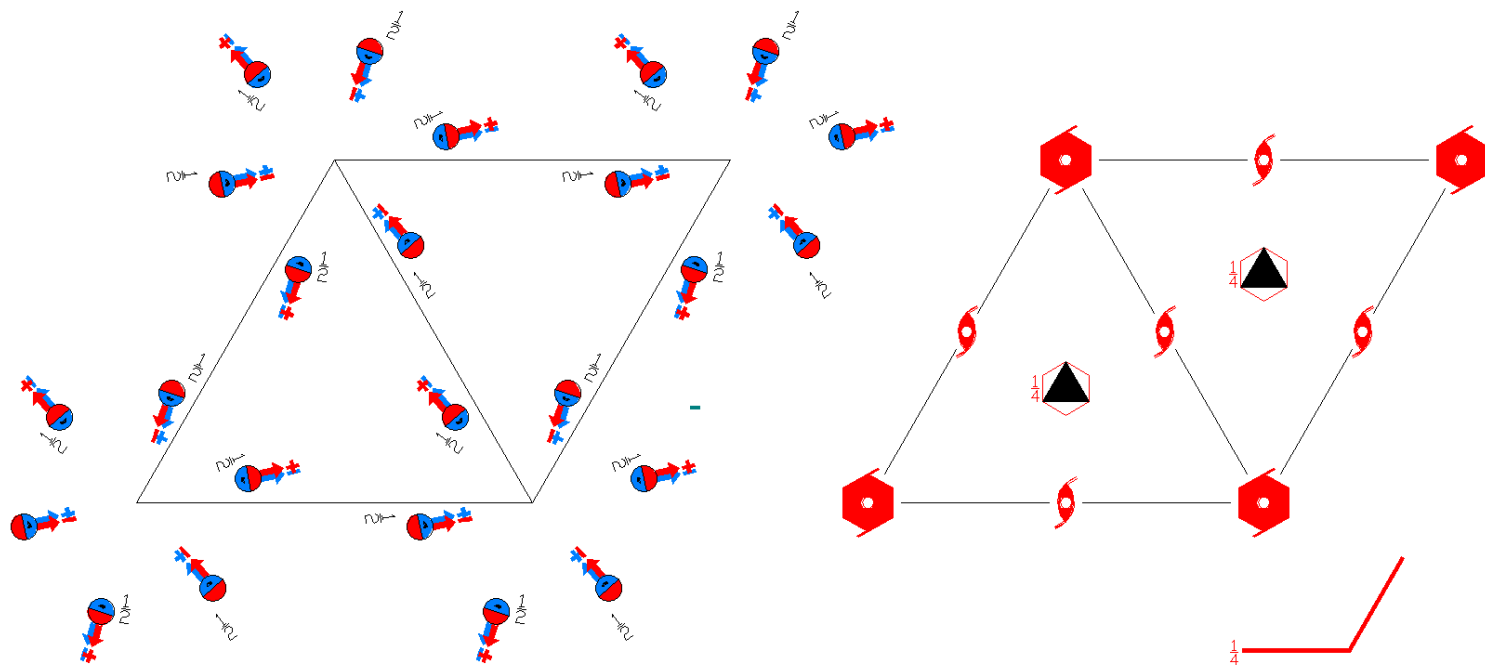
Along [2,1,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P6_3'/m'$   
176.5.1378

$6'/m'$   
 $P6_3'/m'$

Hexagonal



Origin at center  $\bar{3}$  on  $6_3'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

**Symmetry Operations**

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                             | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                               | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                     |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)' | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)'             | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)'             |
| (7) $\bar{1}$<br>( $\bar{1}$  0,0,0)           | (8) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)            | (9) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)  |
| (10) $m'$ x,y,1/4<br>( $m_z$  0,0,1/2)'        | (11) $\bar{6}^-$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2)' | (12) $\bar{6}^+$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

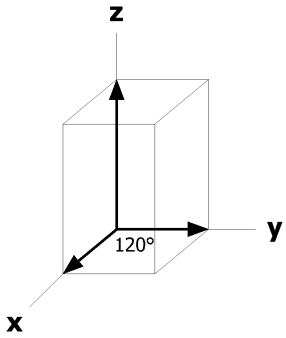
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
12	i	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y,\bar{x}$ ,z [ $\bar{u}+v,\bar{u}$ ,w]	
			(4) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(5) y, $\bar{x}+y,z+1/2$ [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) x-y,x,z+1/2 [ $\bar{u}+v,\bar{u},\bar{w}$ ]	
			(7) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(8) y, $\bar{x}+y,\bar{z}$ [ $\bar{v}$ ,u-v,w]	(9) x-y,x, $\bar{z}$ [ $\bar{u}+v,\bar{u}$ ,w]	
			(10) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(11) $\bar{y}$ ,x-y, $\bar{z}+1/2$ [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(12) $\bar{x}+y,\bar{x},\bar{z}+1/2$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]	
6	h	m'..	x,y,1/4 [u,v,0]	$\bar{y}$ ,x-y,1/4 [ $\bar{v}$ ,u-v,0]	$\bar{x}+y,\bar{x}$ ,1/4 [ $\bar{u}+v,\bar{u}$ ,0]	
			$\bar{x},\bar{y}$ ,3/4 [u,v,0]	y, $\bar{x}+y$ ,3/4 [ $\bar{v}$ ,u-v,0]	x-y,x,3/4 [ $\bar{u}+v,\bar{u}$ ,0]	
6	g	$\bar{1}$	1/2,0,0 [u,v,w]	0,1/2,0 [ $\bar{v}$ ,u-v,w]	1/2,1/2,0 [ $\bar{u}+v,\bar{u}$ ,w]	
			1/2,0,1/2 [u,v, $\bar{w}$ ]	0,1/2,1/2 [ $\bar{v}$ ,u-v, $\bar{w}$ ]	1/2,1/2,1/2 [ $\bar{u}+v,\bar{u},\bar{w}$ ]	
4	f	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z+1/2 [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0,w]	1/3,2/3, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	e	3..	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
2	d	$\bar{6}'$ ..	2/3,1/3,1/4 [0,0,0]	1/3,2/3,3/4 [0,0,0]		
2	c	$\bar{6}'$ ..	1/3,2/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]		
2	b	$\bar{3}$ ..	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		
2	a	$\bar{6}'$ ..	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p6'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

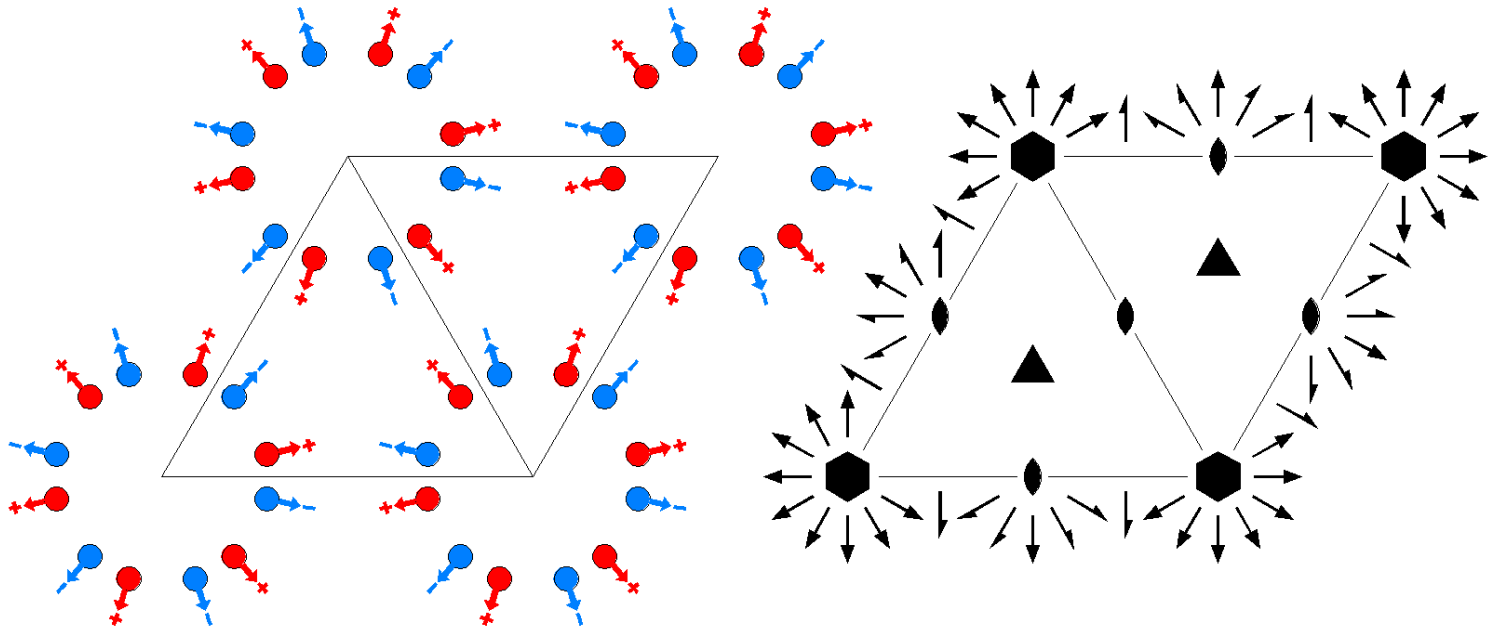
Along [2,1,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P622  
177.1.1379

622  
P622

Hexagonal



**Origin on 622**

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/2,1/2,1/2	

**Symmetry Operations**

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                         | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub> ^+ 0,0,0) | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> ^- 0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub> ^+ 0,0,0)   | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> ^- 0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub> ^+ 0,0,0) |
| (7) 2 x,x,0<br>(2 <sub>xy</sub> ^+ 0,0,0)  | (8) 2 x,0,0<br>(2 <sub>x</sub> ^+ 0,0,0)              | (9) 2 0,y,0<br>(2 <sub>y</sub> ^+ 0,0,0)              |
| (10) 2 x,x̄,0<br>(2 <sub>3</sub> ^+ 0,0,0) | (11) 2 x,2x,0<br>(2 <sub>2</sub> ^+ 0,0,0)            | (12) 2 2x,x,0<br>(2 <sub>1</sub> ^+ 0,0,0)            |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	n	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$	
			(4) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(5) $y,\bar{x}+y,z [v,\bar{u}+v,w]$	(6) $x-y,x,z [u-v,u,w]$	
			(7) $y,x,\bar{z} [v,u,\bar{w}]$	(8) $x-y,\bar{y},\bar{z} [u-v,\bar{v},\bar{w}]$	(9) $\bar{x},\bar{x}+y,\bar{z} [\bar{u},\bar{u}+v,\bar{w}]$	
			(10) $\bar{y},\bar{x},\bar{z} [\bar{v},\bar{u},\bar{w}]$	(11) $\bar{x}+y,y,\bar{z} [\bar{u}+v,v,\bar{w}]$	(12) $x,x-y,\bar{z} [u,u-v,\bar{w}]$	
6	m	..2	$x,\bar{x},1/2 [u,\bar{u},0]$	$x,2x,1/2 [u,2u,0]$	$2\bar{x},\bar{x},1/2 [2\bar{u},\bar{u},0]$	
			$\bar{x},x,1/2 [\bar{u},u,0]$	$\bar{x},2\bar{x},1/2 [\bar{u},2\bar{u},0]$	$2x,x,1/2 [2u,u,0]$	
6	l	..2	$x,\bar{x},0 [u,\bar{u},0]$	$x,2x,0 [u,2u,0]$	$2\bar{x},\bar{x},0 [2\bar{u},\bar{u},0]$	
			$\bar{x},x,0 [\bar{u},u,0]$	$\bar{x},2\bar{x},0 [\bar{u},2\bar{u},0]$	$2x,x,0 [2u,u,0]$	
6	k	.2.	$x,0,1/2 [u,0,0]$	$0,x,1/2 [0,u,0]$	$\bar{x},\bar{x},1/2 [\bar{u},\bar{u},0]$	
			$\bar{x},0,1/2 [\bar{u},0,0]$	$0,\bar{x},1/2 [0,\bar{u},0]$	$x,x,1/2 [u,u,0]$	
6	j	.2.	$x,0,0 [u,0,0]$	$0,x,0 [0,u,0]$	$\bar{x},\bar{x},0 [\bar{u},\bar{u},0]$	
			$\bar{x},0,0 [\bar{u},0,0]$	$0,\bar{x},0 [0,\bar{u},0]$	$x,x,0 [u,u,0]$	
6	i	2..	$1/2,0,z [0,0,w]$	$0,1/2,z [0,0,w]$	$1/2,1/2,z [0,0,w]$	
			$0,1/2,\bar{z} [0,0,\bar{w}]$	$1/2,0,\bar{z} [0,0,\bar{w}]$	$1/2,1/2,\bar{z} [0,0,\bar{w}]$	
4	h	3..	$1/3,2/3,z [0,0,w]$	$2/3,1/3,z [0,0,w]$	$2/3,1/3,\bar{z} [0,0,\bar{w}]$	$1/3,2/3,\bar{z} [0,0,\bar{w}]$
3	g	222	$1/2,0,1/2 [0,0,0]$	$0,1/2,1/2 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$	
3	f	222	$1/2,0,0 [0,0,0]$	$0,1/2,0 [0,0,0]$	$1/2,1/2,0 [0,0,0]$	
2	e	6..	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,\bar{w}]$		
2	d	3.2	$1/3,2/3,1/2 [0,0,0]$	$2/3,1/3,1/2 [0,0,0]$		
2	c	3.2	$1/3,2/3,0 [0,0,0]$	$2/3,1/3,0 [0,0,0]$		
1	b	622	$0,0,1/2 [0,0,0]$			
1	a	622	$0,0,0 [0,0,0]$			

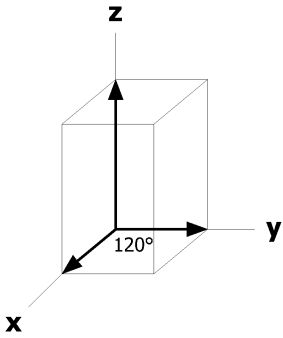


**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at  $x,0,0$

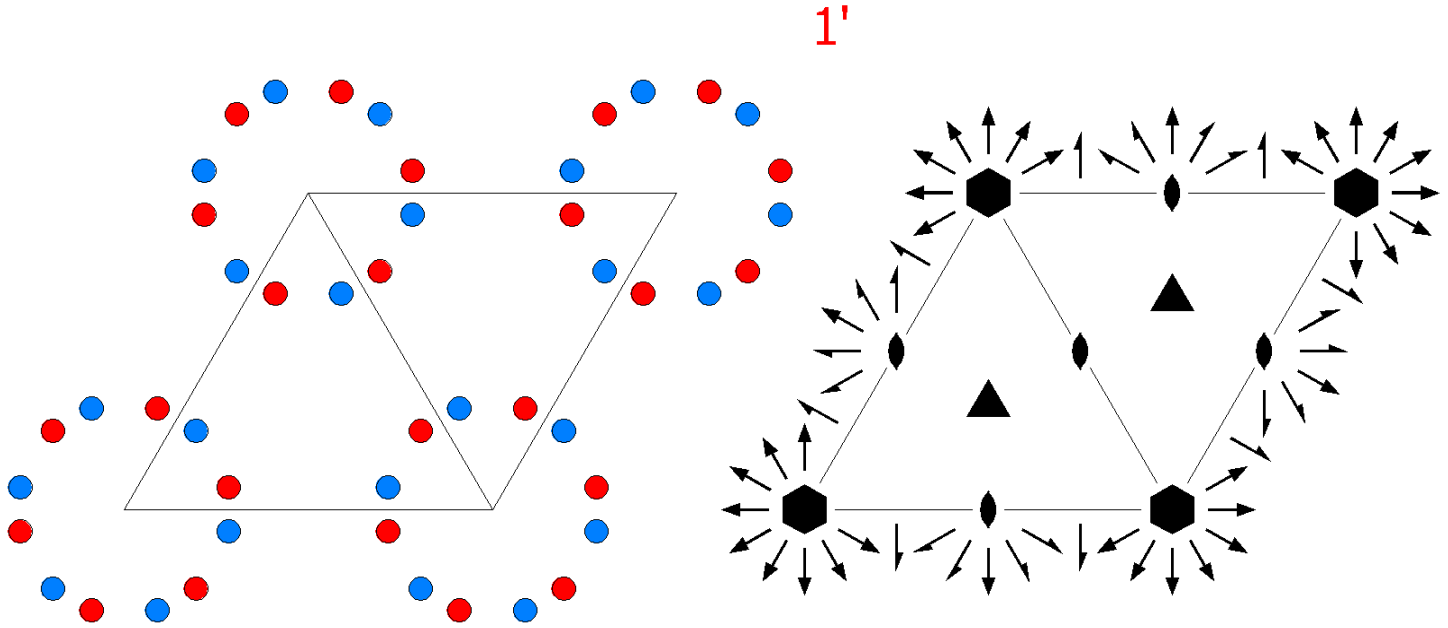
Along  $[2,1,0]$   $p2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $x,x/2,0$



P6221'  
177.2.1380

6221'  
P6221'

Hexagonal



Origin on 6221'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

**Symmetry Operations**

For 1 + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                                | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)            | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)           | (8) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                            | (9) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                            |
| (10) 2 x, $\bar{x}$ ,0<br>(2 <sub>3</sub>  0,0,0) | (11) 2 x,2x,0<br>(2 <sub>2</sub>  0,0,0)                          | (12) 2 2x,x,0<br>(2 <sub>1</sub>  0,0,0)                          |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 3 <sup>+</sup> 0,0,z (3 <sub>z</sub>  0,0,0)'	(3) 3 <sup>-</sup> 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(4) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(5) 6 <sup>-</sup> 0,0,z (6 <sub>z</sub> <sup>-1</sup>  0,0,0)'	(6) 6 <sup>+</sup> 0,0,z (6 <sub>z</sub>  0,0,0)'
(7) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'	(9) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'
(10) 2' x, $\bar{x}$ ,0 (2 <sub>3</sub>  0,0,0)'	(11) 2' x,2x,0 (2 <sub>2</sub>  0,0,0)'	(12) 2' 2x,x,0 (2 <sub>1</sub>  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			1 +	1' +		
12	n	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0]	
			(4) $\bar{x},\bar{y},z$ [0,0,0]	(5) y, $\bar{x}+y,z$ [0,0,0]	(6) x-y,x,z [0,0,0]	
			(7) y,x, $\bar{z}$ [0,0,0]	(8) x-y, $\bar{y},\bar{z}$ [0,0,0]	(9) $\bar{x},\bar{x}+y,\bar{z}$ [0,0,0]	
			(10) $\bar{y},\bar{x},\bar{z}$ [0,0,0]	(11) $\bar{x}+y,y,\bar{z}$ [0,0,0]	(12) x,x-y, $\bar{z}$ [0,0,0]	
6	m	..21'	x, $\bar{x}$ ,1/2 [0,0,0]	x,2x,1/2 [0,0,0]	2 $\bar{x},\bar{x}$ ,1/2 [0,0,0]	
			$\bar{x},x$ ,1/2 [0,0,0]	$\bar{x},2\bar{x}$ ,1/2 [0,0,0]	2x,x,1/2 [0,0,0]	
6	l	..21'	x, $\bar{x}$ ,0 [0,0,0]	x,2x,0 [0,0,0]	2 $\bar{x},\bar{x}$ ,0 [0,0,0]	
			$\bar{x},x$ ,0 [0,0,0]	$\bar{x},2\bar{x}$ ,0 [0,0,0]	2x,x,0 [0,0,0]	
6	k	.2.1'	x,0,1/2 [0,0,0]	0,x,1/2 [0,0,0]	$\bar{x},\bar{x}$ ,1/2 [0,0,0]	
			$\bar{x}$ ,0,1/2 [0,0,0]	0, $\bar{x}$ ,1/2 [0,0,0]	x,x,1/2 [0,0,0]	
6	j	.2.1'	x,0,0 [0,0,0]	0,x,0 [0,0,0]	$\bar{x},\bar{x}$ ,0 [0,0,0]	
			$\bar{x}$ ,0,0 [0,0,0]	0, $\bar{x}$ ,0 [0,0,0]	x,x,0 [0,0,0]	
6	i	2..1'	1/2,0,z [0,0,0]	0,1/2,z [0,0,0]	1/2,1/2,z [0,0,0]	
			0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	
4	h	3..1'	1/3,2/3,z [0,0,0]	2/3,1/3,z [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	1/3,2/3, $\bar{z}$ [0,0,0]
3	g	2221'	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
3	f	2221'	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	

Continued

177.2.1380

P6221'

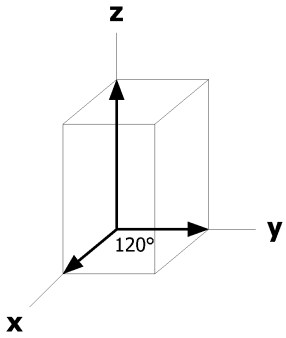
2	e	6..1'	0,0,z [0,0,0]	$0,0,\bar{z}$ [0,0,0]
2	d	3.21'	1/3,2/3,1/2 [0,0,0]	2/3,1/3,1/2 [0,0,0]
2	c	3.21'	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]
1	b	6221'	0,0,1/2 [0,0,0]	
1	a	6221'	0,0,0 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,0

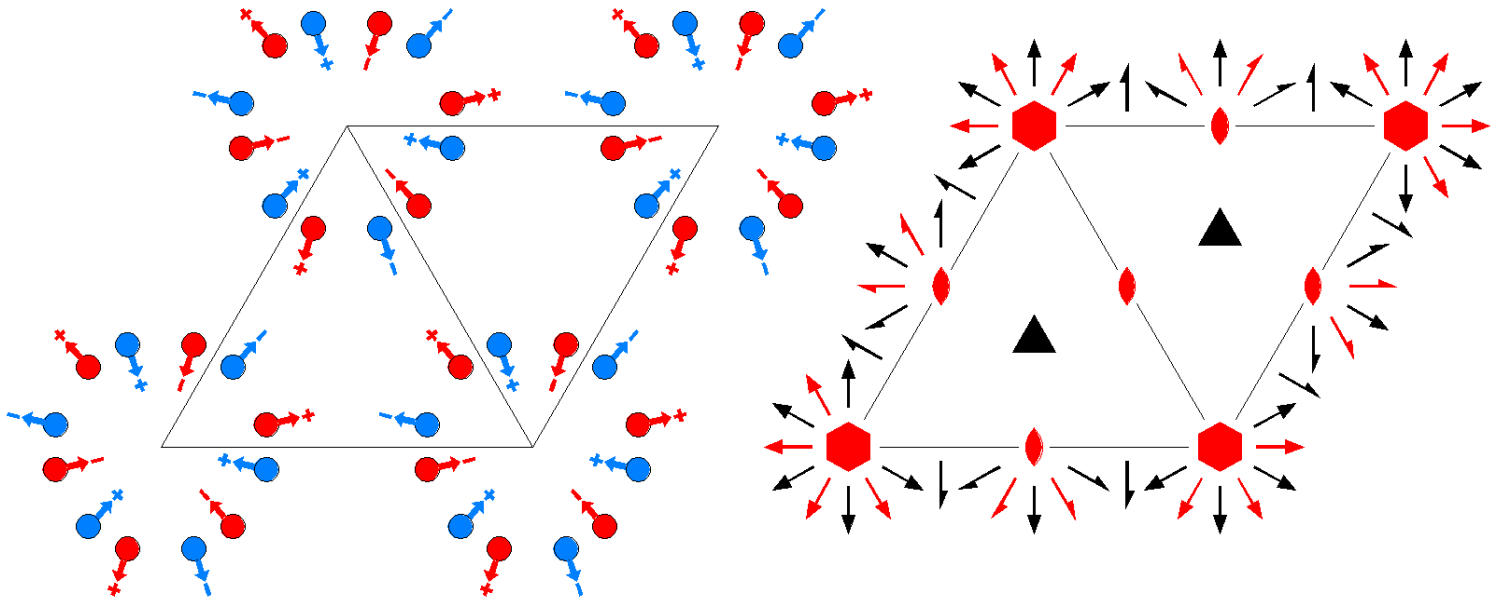
Along [2,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,x/2,0



P6'2'2  
177.3.1381

6'2'2  
P6'2'2

Hexagonal



**Origin on 6'2'2**

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                        | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)                | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'  | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)'              |
| (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)' | (8) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                           | (9) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                          |
| (10) 2 x,x̄,0<br>(2 <sub>3</sub>  0,0,0)  | (11) 2 x,2x,0<br>(2 <sub>2</sub>  0,0,0)                           | (12) 2 2x,x,0<br>(2 <sub>1</sub>  0,0,0)                          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

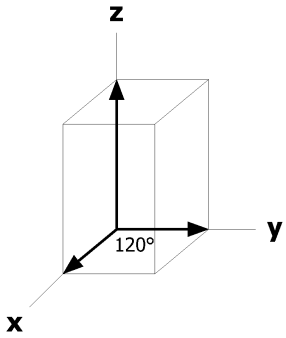
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	n	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$	
			(4) $\bar{x},\bar{y},z [u,v,\bar{w}]$	(5) $y,\bar{x}+y,z [\bar{v},u-v,\bar{w}]$	(6) $x-y,x,z [\bar{u}+v,\bar{u},\bar{w}]$	
			(7) $y,x,\bar{z} [\bar{v},\bar{u},w]$	(8) $x-y,\bar{y},\bar{z} [\bar{u}+v,v,w]$	(9) $\bar{x},\bar{x}+y,\bar{z} [u,u-v,w]$	
			(10) $\bar{y},\bar{x},\bar{z} [\bar{v},\bar{u},\bar{w}]$	(11) $\bar{x}+y,y,\bar{z} [\bar{u}+v,v,\bar{w}]$	(12) $x,x-y,\bar{z} [u,u-v,\bar{w}]$	
6	m	..2	$x,\bar{x},1/2 [u,\bar{u},0]$	$x,2x,1/2 [u,2u,0]$	$2\bar{x},\bar{x},1/2 [2\bar{u},\bar{u},0]$	
			$\bar{x},x,1/2 [u,\bar{u},0]$	$\bar{x},2\bar{x},1/2 [u,2u,0]$	$2x,x,1/2 [2\bar{u},\bar{u},0]$	
6	l	..2	$x,\bar{x},0 [u,\bar{u},0]$	$x,2x,0 [u,2u,0]$	$2\bar{x},\bar{x},0 [2\bar{u},\bar{u},0]$	
			$\bar{x},x,0 [u,\bar{u},0]$	$\bar{x},2\bar{x},0 [u,2u,0]$	$2x,x,0 [2\bar{u},\bar{u},0]$	
6	k	.2'	$x,0,1/2 [u,2u,w]$	$0,x,1/2 [2\bar{u},\bar{u},w]$	$\bar{x},\bar{x},1/2 [u,\bar{u},w]$	
			$\bar{x},0,1/2 [u,2u,\bar{w}]$	$0,\bar{x},1/2 [2\bar{u},\bar{u},\bar{w}]$	$x,x,1/2 [u,\bar{u},\bar{w}]$	
6	j	.2'	$x,0,0 [u,2u,w]$	$0,x,0 [2\bar{u},\bar{u},w]$	$\bar{x},\bar{x},0 [u,\bar{u},w]$	
			$\bar{x},0,0 [u,2u,\bar{w}]$	$0,\bar{x},0 [2\bar{u},\bar{u},\bar{w}]$	$x,x,0 [u,\bar{u},\bar{w}]$	
6	i	2'..	$1/2,0,z [u,v,0]$	$0,1/2,z [\bar{v},u-v,0]$	$1/2,1/2,z [\bar{u}+v,\bar{u},0]$	
			$0,1/2,\bar{z} [\bar{v},\bar{u},0]$	$1/2,0,\bar{z} [\bar{u}+v,v,0]$	$1/2,1/2,\bar{z} [u,u-v,0]$	
4	h	3..	$1/3,2/3,z [0,0,w]$	$2/3,1/3,z [0,0,\bar{w}]$	$2/3,1/3,\bar{z} [0,0,\bar{w}]$	$1/3,2/3,\bar{z} [0,0,w]$
3	g	2'22'	$1/2,0,1/2 [u,2u,0]$	$0,1/2,1/2 [2\bar{u},\bar{u},0]$	$1/2,1/2,1/2 [u,\bar{u},0]$	
3	f	2'22'	$1/2,0,0 [u,2u,0]$	$0,1/2,0 [2\bar{u},\bar{u},0]$	$1/2,1/2,0 [u,\bar{u},0]$	
2	e	6'..	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$		
2	d	3.2	$1/3,2/3,1/2 [0,0,0]$	$2/3,1/3,1/2 [0,0,0]$		
2	c	3.2	$1/3,2/3,0 [0,0,0]$	$2/3,1/3,0 [0,0,0]$		
1	b	6'2'2	$0,0,1/2 [0,0,0]$			
1	a	6'2'2	$0,0,0 [0,0,0]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6'm'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2'mm'$   
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,0,0$

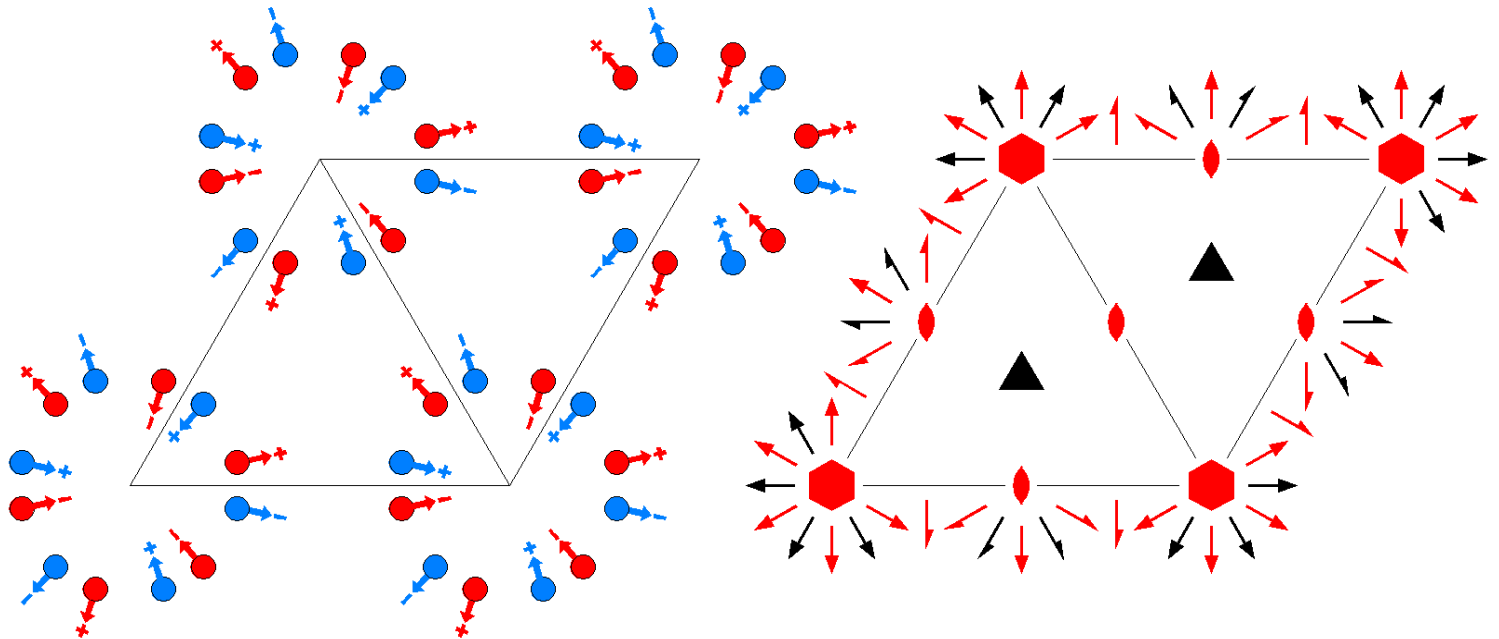
Along  $[2,1,0]$   $p2mm$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $x,x/2,0$



P6'22'  
177.4.1382

6'22'  
P6'22'

Hexagonal



Origin on 6'22'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

**Symmetry Operations**

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                         | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)                | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'   | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)'              |
| (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)    | (8) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                             | (9) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                            |
| (10) 2' x,x̄,0<br>(2 <sub>3</sub>  0,0,0)' | (11) 2' x,2x,0<br>(2 <sub>2</sub>  0,0,0)'                         | (12) 2' 2x,x,0<br>(2 <sub>1</sub>  0,0,0)'                        |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

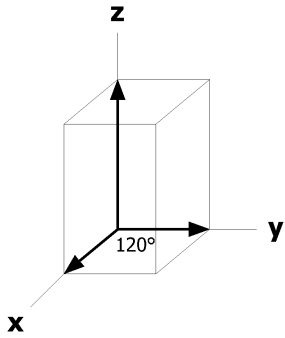
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
12	n	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$	
			(4) $\bar{x},\bar{y},z [u,v,\bar{w}]$	(5) $y,\bar{x}+y,z [\bar{v},u-v,\bar{w}]$	(6) $x-y,x,z [\bar{u}+v,\bar{u},\bar{w}]$	
			(7) $y,x,\bar{z} [v,u,\bar{w}]$	(8) $x-y,\bar{y},\bar{z} [u-v,\bar{v},\bar{w}]$	(9) $\bar{x},\bar{x}+y,\bar{z} [\bar{u},\bar{u}+v,\bar{w}]$	
			(10) $\bar{y},\bar{x},\bar{z} [v,u,w]$	(11) $\bar{x}+y,y,\bar{z} [u-v,\bar{v},w]$	(12) $x,x-y,\bar{z} [\bar{u},\bar{u}+v,w]$	
6	m	..2'	$x,\bar{x},1/2 [u,u,w]$	$x,2x,1/2 [\bar{u},0,w]$	$2\bar{x},\bar{x},1/2 [0,\bar{u},w]$	
			$\bar{x},x,1/2 [u,u,\bar{w}]$	$\bar{x},2\bar{x},1/2 [\bar{u},0,\bar{w}]$	$2x,x,1/2 [0,\bar{u},\bar{w}]$	
6	l	..2'	$x,\bar{x},0 [u,u,w]$	$x,2x,0 [\bar{u},0,w]$	$2\bar{x},\bar{x},0 [0,\bar{u},w]$	
			$\bar{x},x,0 [u,u,\bar{w}]$	$\bar{x},2\bar{x},0 [\bar{u},0,\bar{w}]$	$2x,x,0 [0,\bar{u},\bar{w}]$	
6	k	.2.	$x,0,1/2 [u,0,0]$	$0,x,1/2 [0,u,0]$	$\bar{x},\bar{x},1/2 [\bar{u},\bar{u},0]$	
			$\bar{x},0,1/2 [u,0,0]$	$0,\bar{x},1/2 [0,u,0]$	$x,x,1/2 [\bar{u},\bar{u},0]$	
6	j	.2.	$x,0,0 [u,0,0]$	$0,x,0 [0,u,0]$	$\bar{x},\bar{x},0 [\bar{u},\bar{u},0]$	
			$\bar{x},0,0 [u,0,0]$	$0,\bar{x},0 [0,u,0]$	$x,x,0 [\bar{u},\bar{u},0]$	
6	i	2'..	$1/2,0,z [u,v,0]$	$0,1/2,z [\bar{v},u-v,0]$	$1/2,1/2,z [\bar{u}+v,\bar{u},0]$	
			$0,1/2,\bar{z} [v,u,0]$	$1/2,0,\bar{z} [u-v,\bar{v},0]$	$1/2,1/2,\bar{z} [\bar{u},\bar{u}+v,0]$	
4	h	3..	$1/3,2/3,z [0,0,w]$	$2/3,1/3,z [0,0,\bar{w}]$	$2/3,1/3,\bar{z} [0,0,\bar{w}]$	$1/3,2/3,\bar{z} [0,0,w]$
3	g	22'2'	$1/2,0,1/2 [u,0,0]$	$0,1/2,1/2 [0,u,0]$	$1/2,1/2,1/2 [\bar{u},\bar{u},0]$	
3	f	22'2'	$1/2,0,0 [u,0,0]$	$0,1/2,0 [0,u,0]$	$1/2,1/2,0 [\bar{u},\bar{u},0]$	
2	e	6'..	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$		
2	d	3.2'	$1/3,2/3,1/2 [0,0,w]$	$2/3,1/3,1/2 [0,0,\bar{w}]$		
2	c	3.2'	$1/3,2/3,0 [0,0,w]$	$2/3,1/3,0 [0,0,\bar{w}]$		
1	b	6'22'	$0,0,1/2 [0,0,0]$			
1	a	6'22'	$0,0,0 [0,0,0]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6'mm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mm$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at  $x,0,0$

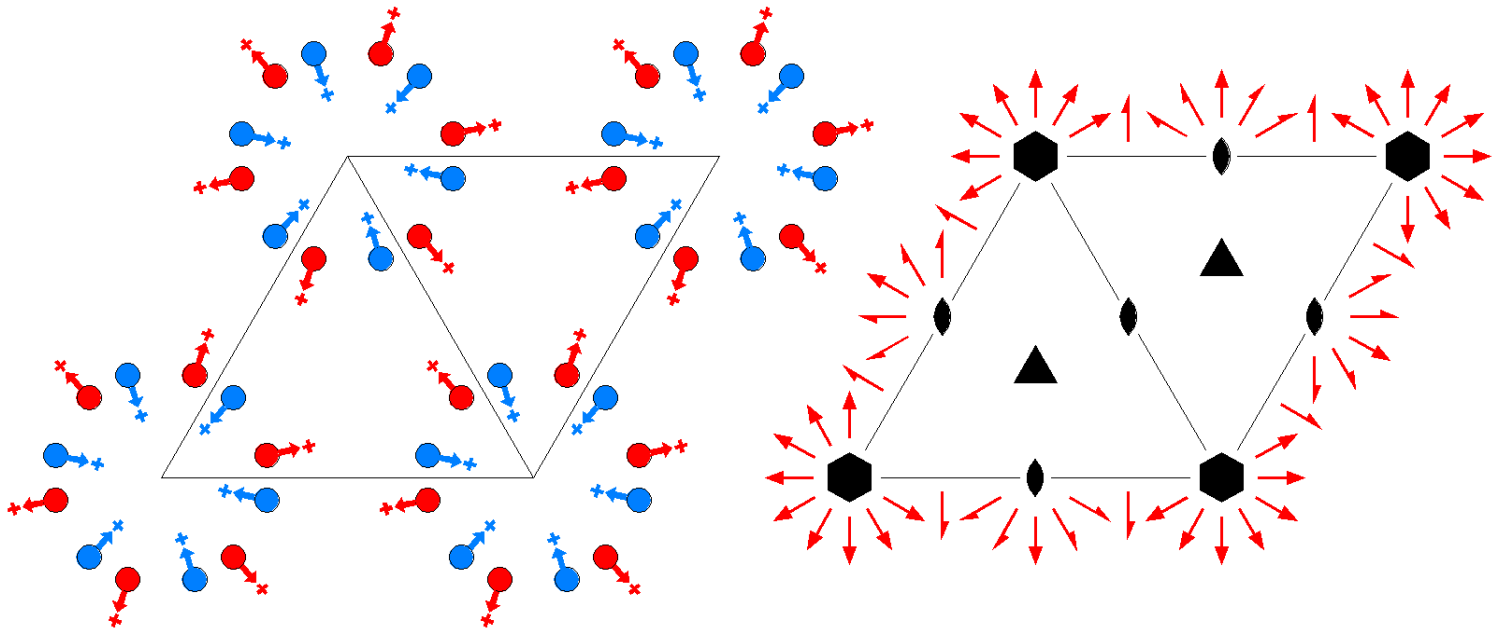
Along  $[2,1,0]$   $p2'mm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,x/2,0$



P62'2'  
177.5.1383

62'2'  
P62'2'

Hexagonal



Origin on 62'2'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/2,1/2,1/2	

**Symmetry Operations**

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                         | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)     | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'  | (8) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                          | (9) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                          |
| (10) 2' x,x̄,0<br>(2 <sub>3</sub>  0,0,0)' | (11) 2' x,2x,0<br>(2 <sub>2</sub>  0,0,0)'                        | (12) 2' 2x,x,0<br>(2 <sub>1</sub>  0,0,0)'                        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

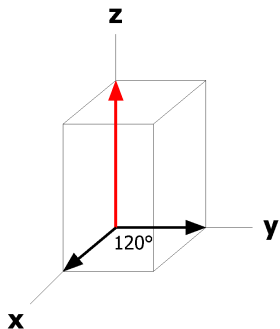
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	n	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$	
			(4) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(5) $y,\bar{x}+y,z [v,\bar{u}+v,w]$	(6) $x-y,x,z [u-v,u,w]$	
			(7) $y,x,\bar{z} [\bar{v},\bar{u},w]$	(8) $x-y,\bar{y},\bar{z} [\bar{u}+v,v,w]$	(9) $\bar{x},\bar{x}+y,\bar{z} [u,u-v,w]$	
			(10) $\bar{y},\bar{x},\bar{z} [v,u,w]$	(11) $\bar{x}+y,y,\bar{z} [u-v,\bar{v},w]$	(12) $x,x-y,\bar{z} [\bar{u},\bar{u}+v,w]$	
6	m	..2'	$x,\bar{x},1/2 [u,u,w]$	$x,2x,1/2 [\bar{u},0,w]$	$2\bar{x},\bar{x},1/2 [0,\bar{u},w]$	
			$\bar{x},x,1/2 [\bar{u},\bar{u},w]$	$\bar{x},2\bar{x},1/2 [u,0,w]$	$2x,x,1/2 [0,u,w]$	
6	l	..2'	$x,\bar{x},0 [u,u,w]$	$x,2x,0 [\bar{u},0,w]$	$2\bar{x},\bar{x},0 [0,\bar{u},w]$	
			$\bar{x},x,0 [\bar{u},\bar{u},w]$	$\bar{x},2\bar{x},0 [u,0,w]$	$2x,x,0 [0,u,w]$	
6	k	.2'	$x,0,1/2 [u,2u,w]$	$0,x,1/2 [2\bar{u},\bar{u},w]$	$\bar{x},\bar{x},1/2 [u,\bar{u},w]$	
			$\bar{x},0,1/2 [\bar{u},2\bar{u},w]$	$0,\bar{x},1/2 [2u,u,w]$	$x,x,1/2 [\bar{u},u,w]$	
6	j	.2'	$x,0,0 [u,2u,w]$	$0,x,0 [2\bar{u},\bar{u},w]$	$\bar{x},\bar{x},0 [u,\bar{u},w]$	
			$\bar{x},0,0 [\bar{u},2\bar{u},w]$	$0,\bar{x},0 [2u,u,w]$	$x,x,0 [\bar{u},u,w]$	
6	i	2..	$1/2,0,z [0,0,w]$	$0,1/2,z [0,0,w]$	$1/2,1/2,z [0,0,w]$	
			$0,1/2,\bar{z} [0,0,w]$	$1/2,0,\bar{z} [0,0,w]$	$1/2,1/2,\bar{z} [0,0,w]$	
4	h	3..	$1/3,2/3,z [0,0,w]$	$2/3,1/3,z [0,0,w]$	$2/3,1/3,\bar{z} [0,0,w]$	$1/3,2/3,\bar{z} [0,0,w]$
3	g	2'2'2	$1/2,0,1/2 [0,0,w]$	$0,1/2,1/2 [0,0,w]$	$1/2,1/2,1/2 [0,0,w]$	
3	f	2'2'2	$1/2,0,0 [0,0,w]$	$0,1/2,0 [0,0,w]$	$1/2,1/2,0 [0,0,w]$	
2	e	6..	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,w]$		
2	d	3.2'	$1/3,2/3,1/2 [0,0,w]$	$2/3,1/3,1/2 [0,0,w]$		
2	c	3.2'	$1/3,2/3,0 [0,0,w]$	$2/3,1/3,0 [0,0,w]$		
1	b	62'2'	$0,0,1/2 [0,0,w]$			
1	a	62'2'	$0,0,0 [0,0,w]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at  $x,0,0$

Along  $[2,1,0]$   $p2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $x,x/2,0$



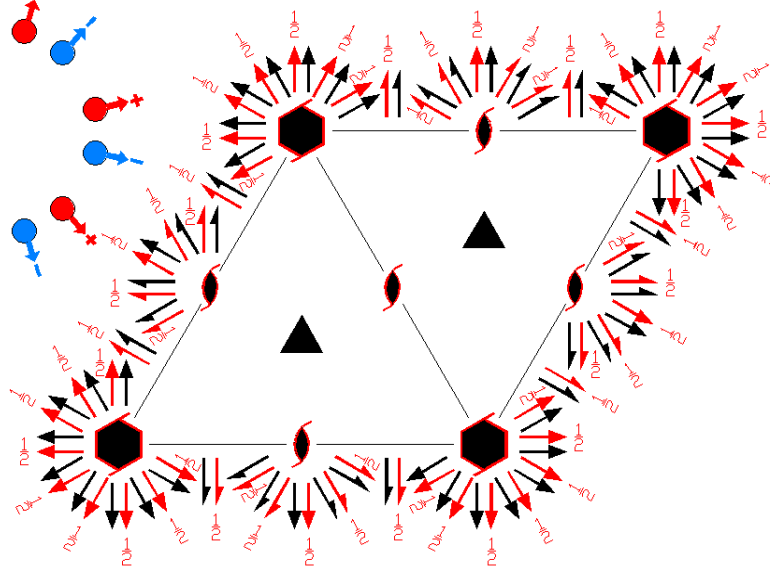
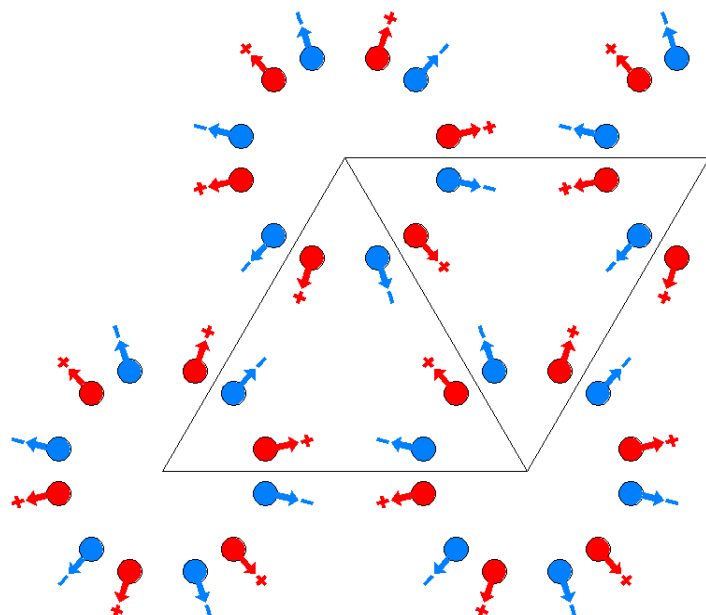
$P_{2c} 622$

177.6.1384

6221'

$P_{2c} 622$

Hexagonal



Origin on 622

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$ ;  $x \leq (1+y)/2$ ;  $y \leq \min(1-x, x)$

Vertices  $0,0,0$   $1/2,0,0$   $2/3,1/3,0$   $1/2,1/2,0$   
 $0,0,1/2$   $1/2,0,1/2$   $2/3,1/3,1/2$   $1/2,1/2,1/2$

Symmetry Operations

For  $(0,0,0)$  + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                        | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)      | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) 2 0,0,z<br>( $2_z$  0,0,0)            | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0) | (6) $6^+$ 0,0,z<br>( $6_z$  0,0,0)      |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0)         | (8) 2 x,0,0<br>( $2_x$  0,0,0)          | (9) 2 0,y,0<br>( $2_y$  0,0,0)          |
| (10) 2 $x, \bar{x}, 0$<br>( $2_3$  0,0,0) | (11) 2 x,2x,0<br>( $2_2$  0,0,0)        | (12) 2 2x,x,0<br>( $2_1$  0,0,0)        |

## For (0,0,1)' + set

(1) $t' (0,0,1)$ $(1 0,0,1)'$	(2) $3^{+'} (0,0,1)$ 0,0,z $(3_z 0,0,1)'$	(3) $3^{-'} (0,0,1)$ 0,0,z $(3_z^{-1} 0,0,1)'$
(4) $2' (0,0,1)$ 0,0,z $(2_z 0,0,1)'$	(5) $6^{-'} (0,0,1)$ 0,0,z $(6_z^{-1} 0,0,1)'$	(6) $6^{+'} (0,0,1)$ 0,0,z $(6_z 0,0,1)'$
(7) $2' x,x,1/2$ $(2_{xy} 0,0,1)'$	(8) $2' x,0,1/2$ $(2_x 0,0,1)'$	(9) $2' 0,y,1/2$ $(2_y 0,0,1)'$
(10) $2' x,\bar{x},1/2$ $(2_3 0,0,1)'$	(11) $2' x,2x,1/2$ $(2_2 0,0,1)'$	(12) $2' 2x,x,1/2$ $(2_1 0,0,1)'$

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

**Positions**

			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(0,0,1)' +	
24	n	1	(1) x,y,z [u,v,w] (4) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ] (10) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) y, $\bar{x}+y,z$ [v, $\bar{u}+v,w$ ] (8) x-y, $\bar{y},\bar{z}$ [u-v, $\bar{v},\bar{w}$ ] (11) $\bar{x}+y,y,\bar{z}$ [ $\bar{u}+v,v,\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) x-y,x,z [u-v,u,w] (9) $\bar{x},\bar{x}+y,\bar{z}$ [ $\bar{u},\bar{u}+v,\bar{w}$ ] (12) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ]
12	m	..2'	x, $\bar{x},1/2$ [u,u,w] $\bar{x},x,1/2$ [ $\bar{u},\bar{u},w$ ]	x,2x,1/2 [ $\bar{u},0,w$ ] $\bar{x},2\bar{x},1/2$ [u,0,w]	2 $\bar{x},\bar{x},1/2$ [0, $\bar{u},w$ ] 2x,x,1/2 [0,u,w]
12	l	..2	x, $\bar{x},0$ [u, $\bar{u},0$ ] $\bar{x},x,0$ [ $\bar{u},u,0$ ]	x,2x,0 [u,2u,0] $\bar{x},2\bar{x},0$ [ $\bar{u},2\bar{u},0$ ]	2 $\bar{x},\bar{x},0$ [2 $\bar{u},\bar{u},0$ ] 2x,x,0 [2u,u,0]
12	k	.2'	x,0,1/2 [u,2u,w] $\bar{x},0,1/2$ [ $\bar{u},2\bar{u},w$ ]	0,x,1/2 [2 $\bar{u},\bar{u},w$ ] 0, $\bar{x},1/2$ [2u,u,w]	$\bar{x},\bar{x},1/2$ [u, $\bar{u},w$ ] x,x,1/2 [ $\bar{u},u,w$ ]
12	j	.2.	x,0,0 [u,0,0] $\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0,u,0] 0, $\bar{x},0$ [0, $\bar{u},0$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ] x,x,0 [u,u,0]
12	i	2..	1/2,0,z [0,0,w] 0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]	0,1/2,z [0,0,w] 1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2,z [0,0,w] 1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ]
8	h	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0,w]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ] 1/3,2/3, $\bar{z}$ [0,0, $\bar{w}$ ]
6	g	2'2'2	1/2,0,1/2 [0,0,w]	0,1/2,1/2 [0,0,w]	1/2,1/2,1/2 [0,0,w]
6	f	222	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]

4	e	6..	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]
4	d	3.2'	1/3,2/3,1/2 [0,0,w]	2/3,1/3,1/2 [0,0,w]
4	c	3.2	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]
2	b	622	0,0,1/2 [0,0,0]	
2	a	622	0,0,0 [0,0,0]	

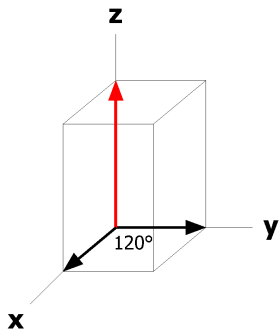
### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0





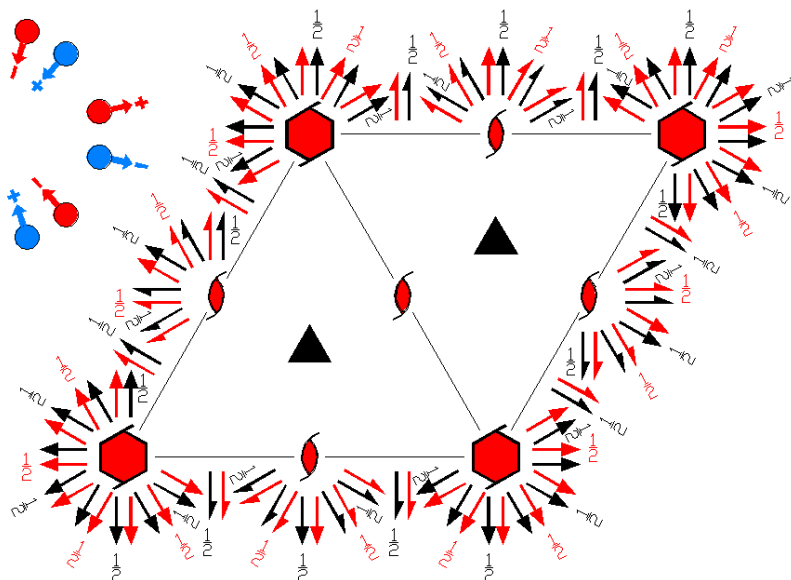
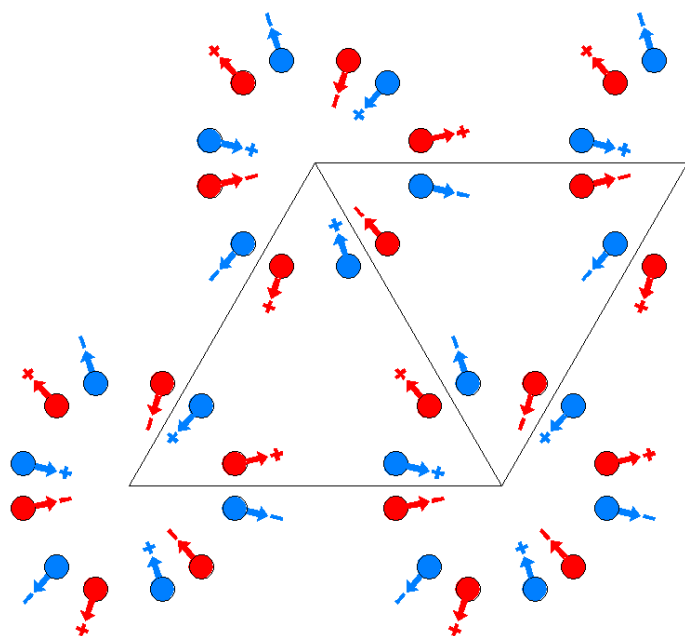
$P_{2c} 6'22'$

177.7.1385

6221'

$P_{2c} 6'22'$

Hexagonal



Origin on  $6'22'$

Asymmetric unit  $0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq \min(1-x, x)$

Vertices  $0,0,0 \quad 1/2,0,0 \quad 2/3,1/3,0 \quad 1/2,1/2,0$   
 $0,0,1/2 \quad 1/2,0,1/2 \quad 2/3,1/3,1/2 \quad 1/2,1/2,1/2$

Symmetry Operations

For  $(0,0,0) + \text{set}$

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                            | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)       | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) $2'$ 0,0,z<br>( $2_z$  0,0,0)'            | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0)' | (6) $6^{+}$ 0,0,z<br>( $6_z$  0,0,0)'   |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0)             | (8) 2 x,0,0<br>( $2_x$  0,0,0)           | (9) 2 0,y,0<br>( $2_y$  0,0,0)          |
| (10) $2'$ x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)' | (11) $2'$ x,2x,0<br>( $2_2$  0,0,0)'     | (12) $2'$ 2x,x,0<br>( $2_1$  0,0,0)'    |

## For (0,0,1)' + set

(1) $t' (0,0,1)$ $(1 0,0,1)'$	(2) $3^{+'} (0,0,1) 0,0,z$ $(3_z 0,0,1)'$	(3) $3^{-'} (0,0,1) 0,0,z$ $(3_z^{-1} 0,0,1)'$
(4) $2 (0,0,1) 0,0,z$ $(2_z 0,0,1)$	(5) $6^{-} (0,0,1) 0,0,z$ $(6_z^{-1} 0,0,1)$	(6) $6^{+} (0,0,1) 0,0,z$ $(6_z 0,0,1)$
(7) $2' x,x,1/2$ $(2_{xy} 0,0,1)'$	(8) $2' x,0,1/2$ $(2_x 0,0,1)'$	(9) $2' 0,y,1/2$ $(2_y 0,0,1)'$
(10) $2 x,\bar{x},1/2$ $(2_3 0,0,1)$	(11) $2 x,2x,1/2$ $(2_2 0,0,1)$	(12) $2 2x,x,1/2$ $(2_1 0,0,1)$

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

**Positions**

			Coordinates			
			(0,0,0) +		(0,0,1)' +	
Multiplicity,	Wyckoff letter,	Site Symmetry.				
24	n	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$	
			(4) $\bar{x},\bar{y},z [u,v,\bar{w}]$	(5) $y,\bar{x}+y,z [\bar{v},u-v,\bar{w}]$	(6) $x-y,x,z [\bar{u}+v,\bar{u},\bar{w}]$	
			(7) $y,x,\bar{z} [v,u,\bar{w}]$	(8) $x-y,\bar{y},\bar{z} [u-v,\bar{v},\bar{w}]$	(9) $\bar{x},\bar{x}+y,\bar{z} [\bar{u},\bar{u}+v,\bar{w}]$	
			(10) $\bar{y},\bar{x},\bar{z} [v,u,w]$	(11) $\bar{x}+y,y,\bar{z} [u-v,\bar{v},w]$	(12) $x,x-y,\bar{z} [\bar{u},\bar{u}+v,w]$	
12	m	..2	$x,\bar{x},1/2 [u,\bar{u},0]$	$x,2x,1/2 [u,2u,0]$	$2\bar{x},\bar{x},1/2 [2\bar{u},\bar{u},0]$	
			$\bar{x},x,1/2 [u,\bar{u},0]$	$\bar{x},2\bar{x},1/2 [u,2u,0]$	$2x,x,1/2 [2\bar{u},\bar{u},0]$	
12	l	..2'	$x,\bar{x},0 [u,u,w]$	$x,2x,0 [\bar{u},0,w]$	$2\bar{x},\bar{x},0 [0,\bar{u},w]$	
			$\bar{x},x,0 [u,u,\bar{w}]$	$\bar{x},2\bar{x},0 [\bar{u},0,\bar{w}]$	$2x,x,0 [0,\bar{u},\bar{w}]$	
12	k	.2'	$x,0,1/2 [u,2u,w]$	$0,x,1/2 [2\bar{u},\bar{u},w]$	$\bar{x},\bar{x},1/2 [u,\bar{u},w]$	
			$\bar{x},0,1/2 [u,2u,\bar{w}]$	$0,\bar{x},1/2 [2\bar{u},\bar{u},\bar{w}]$	$x,x,1/2 [u,\bar{u},\bar{w}]$	
12	j	.2.	$x,0,0 [u,0,0]$	$0,x,0 [0,u,0]$	$\bar{x},\bar{x},0 [\bar{u},\bar{u},0]$	
			$\bar{x},0,0 [u,0,0]$	$0,\bar{x},0 [0,u,0]$	$x,x,0 [\bar{u},\bar{u},0]$	
12	i	2'..	$1/2,0,z [u,v,0]$	$0,1/2,z [\bar{v},u-v,0]$	$1/2,1/2,z [\bar{u}+v,\bar{u},0]$	
			$0,1/2,\bar{z} [v,u,0]$	$1/2,0,\bar{z} [u-v,\bar{v},0]$	$1/2,1/2,\bar{z} [\bar{u},\bar{u}+v,0]$	
8	h	3..	$1/3,2/3,z [0,0,w]$	$2/3,1/3,z [0,0,\bar{w}]$	$2/3,1/3,\bar{z} [0,0,\bar{w}]$	$1/3,2/3,\bar{z} [0,0,w]$
6	g	2'22'	$1/2,0,1/2 [u,2u,0]$	$0,1/2,1/2 [2\bar{u},\bar{u},0]$	$1/2,1/2,1/2 [u,\bar{u},0]$	
6	f	22'2'	$1/2,0,0 [u,0,0]$	$0,1/2,0 [0,u,0]$	$1/2,1/2,0 [\bar{u},\bar{u},0]$	

Continued

177.7.1385

P<sub>2c</sub> 6'22'

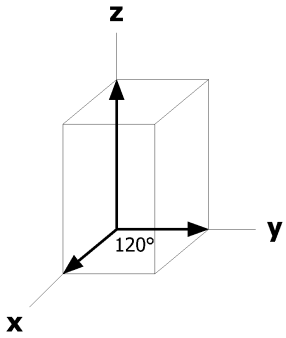
4	e	6'..	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	d	3.2	1/3,2/3,1/2 [0,0,0]	2/3,1/3,1/2 [0,0,0]
4	c	3.2'	1/3,2/3,0 [0,0,w]	2/3,1/3,0 [0,0, $\bar{w}$ ]
2	b	6'22'	0,0,1/2 [0,0,0]	
2	a	6'22'	0,0,0 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub> 2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,0

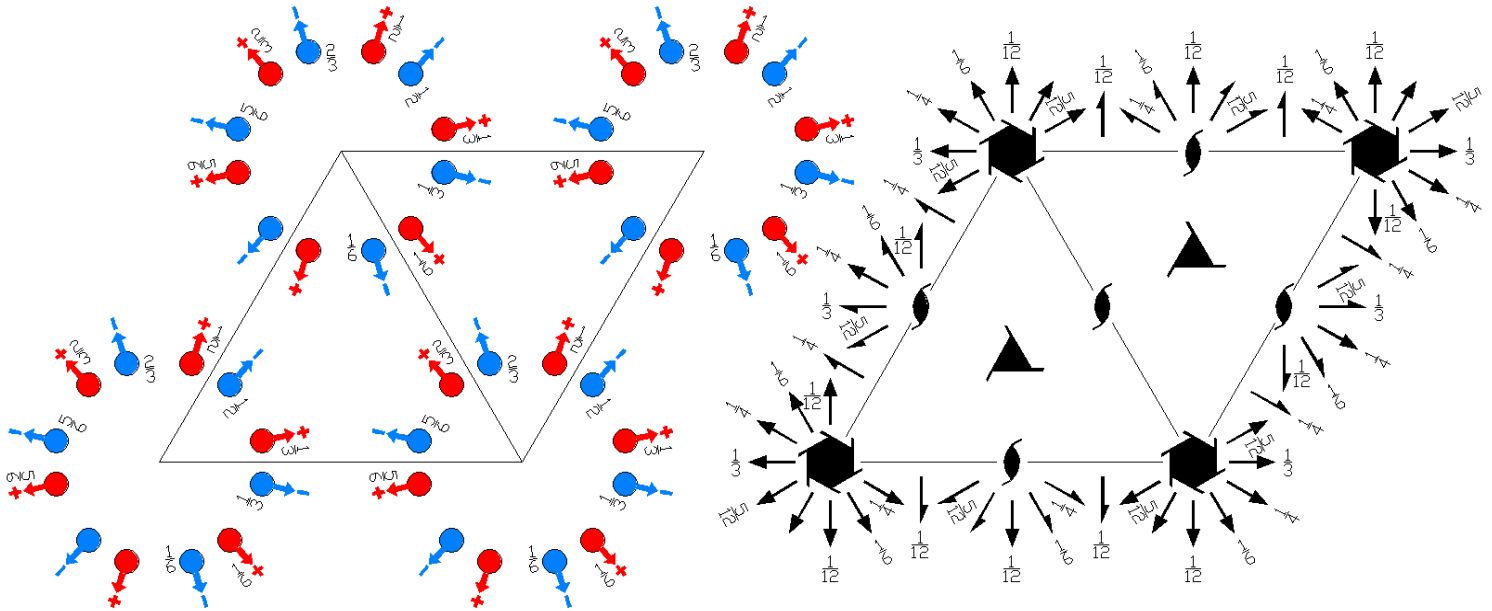
Along [2,1,0] p<sub>2a</sub> 2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,x/2,1/2



P6<sub>1</sub>22  
178.1.1386

622  
P6<sub>1</sub>22

Hexagonal



Origin on 2 [100] at 6<sub>1</sub> (2,1,1) 1

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/12$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/12	1,0,1/12	1,1,1/12	0,1,1/12

### Symmetry Operations

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 3 <sup>+</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub>  0,0,1/3)               | (3) 3 <sup>-</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,2/3) |
| (4) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)     | (5) 6 <sup>-</sup> (0,0,5/6) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,5/6) | (6) 6 <sup>+</sup> (0,0,1/6) 0,0,z<br>(6 <sub>z</sub>  0,0,1/6)               |
| (7) 2 x,x,1/6<br>(2 <sub>xy</sub>  0,0,1/3)            | (8) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (9) 2 0,y,1/3<br>(2 <sub>y</sub>  0,0,2/3)                                    |
| (10) 2 x, $\bar{x}$ ,5/12<br>(2 <sub>3</sub>  0,0,5/6) | (11) 2 x,2x,1/4<br>(2 <sub>2</sub>  0,0,1/2)                                  | (12) 2 2x,x,1/12<br>(2 <sub>1</sub>  0,0,1/6)                                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

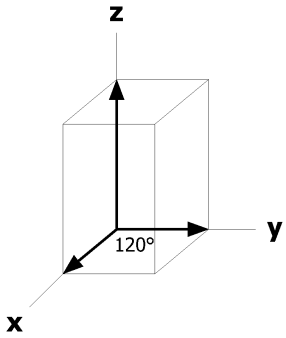
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	c	1	(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{y}, x-y, z+1/3$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z+2/3$ [ $\bar{u}+v, \bar{u}, w$ ]
			(4) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(5) $y, \bar{x}+y, z+5/6$ [ $v, \bar{u}+v, w$ ]	(6) $x-y, x, z+1/6$ [ $u-v, u, w$ ]
			(7) $y, x, \bar{z}+1/3$ [ $v, u, \bar{w}$ ]	(8) $x-y, \bar{y}, \bar{z}$ [ $u-v, \bar{v}, \bar{w}$ ]	(9) $\bar{x}, \bar{x}+y, \bar{z}+2/3$ [ $\bar{u}, \bar{u}+v, \bar{w}$ ]
			(10) $\bar{y}, \bar{x}, \bar{z}+5/6$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(11) $\bar{x}+y, y, \bar{z}+1/2$ [ $\bar{u}+v, v, \bar{w}$ ]	(12) $x, x-y, \bar{z}+1/6$ [ $u, u-v, \bar{w}$ ]
6	b	..2	$x, 2x, 1/4$ [ $u, 2u, 0$ ]	$2\bar{x}, \bar{x}, 7/12$ [ $2\bar{u}, \bar{u}, 0$ ]	$x, \bar{x}, 11/12$ [ $u, \bar{u}, 0$ ]
			$\bar{x}, 2\bar{x}, 3/4$ [ $\bar{u}, 2\bar{u}, 0$ ]	$2x, x, 1/12$ [ $2u, u, 0$ ]	$\bar{x}, x, 5/12$ [ $\bar{u}, u, 0$ ]
6	a	.2.	$x, 0, 0$ [ $u, 0, 0$ ]	$0, x, 1/3$ [ $0, u, 0$ ]	$\bar{x}, \bar{x}, 2/3$ [ $\bar{u}, \bar{u}, 0$ ]
			$\bar{x}, 0, 1/2$ [ $\bar{u}, 0, 0$ ]	$0, \bar{x}, 5/6$ [ $0, \bar{u}, 0$ ]	$x, x, 1/6$ [ $u, u, 0$ ]

**Symmetry of Special Projections**

Along  $[0, 0, 1]$  p6mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$  p2m'g'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x, 0, 0$

Along  $[2, 1, 0]$  p2mg  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x, x/2, 1/12$



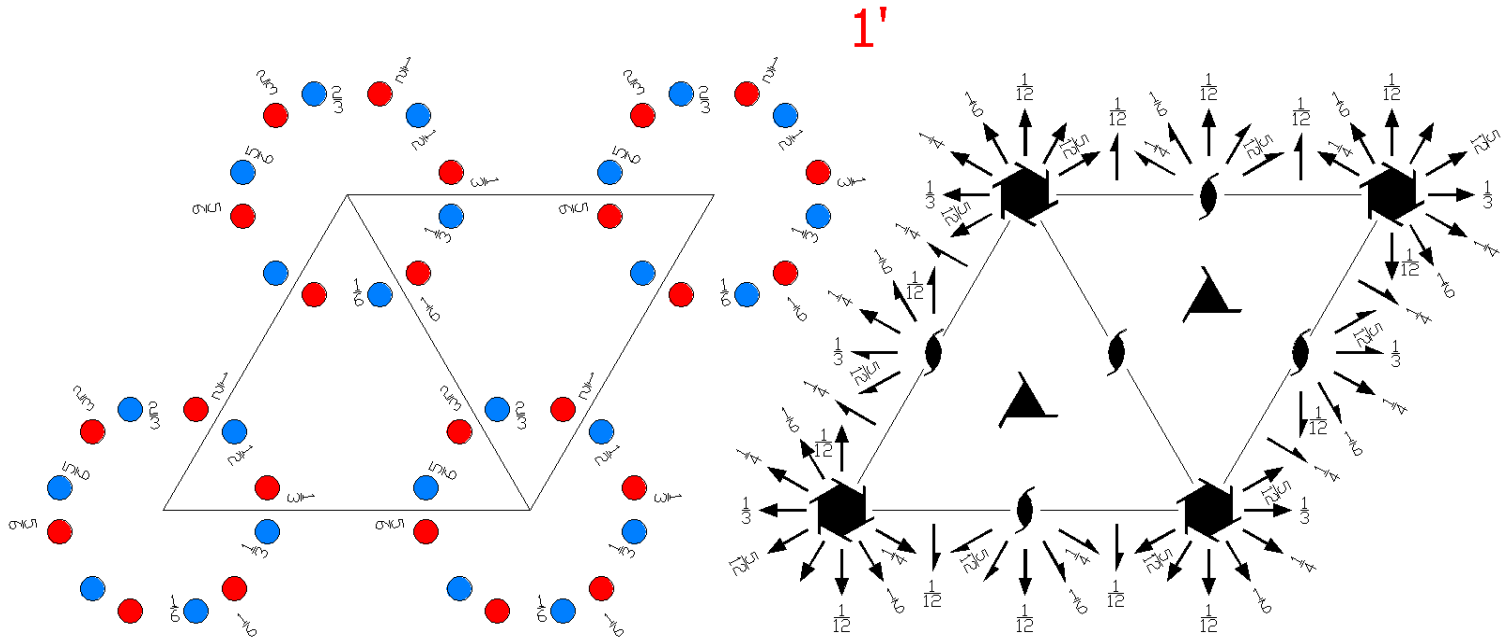
P6<sub>1</sub>221'

178.2.1387

6221'

P6<sub>1</sub>221'

Hexagonal



Origin on 21' [100] at 6<sub>1</sub> (2,1,1) 11'

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/12$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/12	1,0,1/12	1,1,1/12	0,1,1/12

**Symmetry Operations**

For 1 + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 3 <sup>+</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub>  0,0,1/3)               | (3) 3 <sup>-</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,2/3) |
| (4) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (5) 6 <sup>-</sup> (0,0,5/6) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,5/6) | (6) 6 <sup>+</sup> (0,0,1/6) 0,0,z<br>(6 <sub>z</sub>  0,0,1/6)               |
| (7) 2 x,x,1/6<br>(2 <sub>xy</sub>  0,0,1/3)        | (8) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (9) 2 0,y,1/3<br>(2 <sub>y</sub>  0,0,2/3)                                    |
| (10) 2 x,x̄,5/12<br>(2 <sub>3</sub>  0,0,5/6)      | (11) 2 x,2x,1/4<br>(2 <sub>2</sub>  0,0,1/2)                                  | (12) 2 2x,x,1/12<br>(2 <sub>1</sub>  0,0,1/6)                                 |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 3 <sup>+</sup> ' (0,0,1/3) 0,0,z (3 <sub>z</sub>  0,0,1/3)'	(3) 3 <sup>-</sup> ' (0,0,2/3) 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,2/3)'
(4) 2' (0,0,1/2) 0,0,z (2 <sub>z</sub>  0,0,1/2)'	(5) 6 <sup>-</sup> ' (0,0,5/6) 0,0,z (6 <sub>z</sub> <sup>-1</sup>  0,0,5/6)'	(6) 6 <sup>+</sup> ' (0,0,1/6) 0,0,z (6 <sub>z</sub>  0,0,1/6)'
(7) 2' x,x,1/6 (2 <sub>xy</sub>  0,0,1/3)'	(8) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'	(9) 2' 0,y,1/3 (2 <sub>y</sub>  0,0,2/3)'
(10) 2' x, $\bar{x}$ ,5/12 (2 <sub>3</sub>  0,0,5/6)'	(11) 2' x,2x,1/4 (2 <sub>2</sub>  0,0,1/2)'	(12) 2' 2x,x,1/12 (2 <sub>1</sub>  0,0,1/6)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

**Positions**

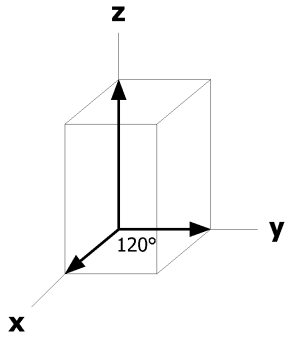
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			1 +	1' +	
12	c	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z+1/3 [0,0,0]	(3) $\bar{x}$ +y, $\bar{x}$ ,z+2/3 [0,0,0]
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [0,0,0]	(5) y, $\bar{x}$ +y,z+5/6 [0,0,0]	(6) x-y,x,z+1/6 [0,0,0]
			(7) y,x, $\bar{z}$ +1/3 [0,0,0]	(8) x-y, $\bar{y}$ , $\bar{z}$ [0,0,0]	(9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ +2/3 [0,0,0]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ +5/6 [0,0,0]	(11) $\bar{x}$ +y,y, $\bar{z}$ +1/2 [0,0,0]	(12) x,x-y, $\bar{z}$ +1/6 [0,0,0]
6	b	..21'	x,2x,1/4 [0,0,0]	2 $\bar{x}$ , $\bar{x}$ ,7/12 [0,0,0]	x, $\bar{x}$ ,11/12 [0,0,0]
			$\bar{x}$ ,2 $\bar{x}$ ,3/4 [0,0,0]	2x,x,1/12 [0,0,0]	$\bar{x}$ ,x,5/12 [0,0,0]
6	a	.2.1'	x,0,0 [0,0,0]	0,x,1/3 [0,0,0]	$\bar{x}$ , $\bar{x}$ ,2/3 [0,0,0]
			$\bar{x}$ ,0,1/2 [0,0,0]	0, $\bar{x}$ ,5/6 [0,0,0]	x,x,1/6 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

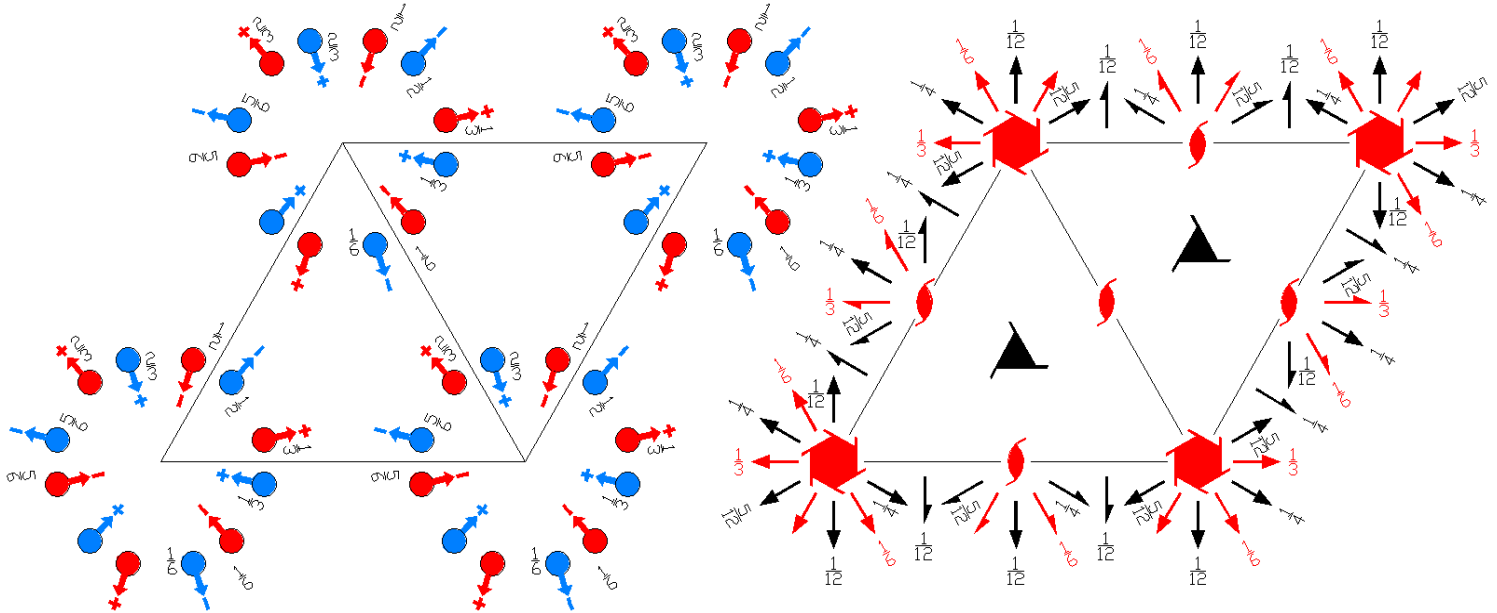
Along [2,1,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/12



$P6_1'2'2$   
178.3.1388

$6'2'2$   
 $P6_1'2'2$

Hexagonal



Origin on  $2'$   $[100]$  at  $6_1'$   $(2',1,1)$   $1$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/12$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/12	1,0,1/12	1,1,1/12	0,1,1/12

### Symmetry Operations

- |  |  |   |
|--|--|---|
| (1) $1$<br>$(1 0,0,0)$                           | (2) $3^+$ $(0,0,1/3)$ $0,0,z$<br>$(3_z 0,0,1/3)$       | (3) $3^-$ $(0,0,2/3)$ $0,0,z$<br>$(3_z^{-1} 0,0,2/3)$ |
| (4) $2'$ $(0,0,1/2)$ $0,0,z$<br>$(2_z 0,0,1/2)'$ | (5) $6^-$ $(0,0,5/6)$ $0,0,z$<br>$(6_z^{-1} 0,0,5/6)'$ | (6) $6^+$ $(0,0,1/6)$ $0,0,z$<br>$(6_z 0,0,1/6)'$     |
| (7) $2'$ $x,x,1/6$<br>$(2_{xy} 0,0,1/3)'$        | (8) $2'$ $x,0,0$<br>$(2_x 0,0,0)'$                     | (9) $2'$ $0,y,1/3$<br>$(2_y 0,0,2/3)'$                |
| (10) $2$ $x,\bar{x},5/12$<br>$(2_3 0,0,5/6)$     | (11) $2$ $x,2x,1/4$<br>$(2_2 0,0,1/2)$                 | (12) $2$ $2x,x,1/12$<br>$(2_1 0,0,1/6)$               |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

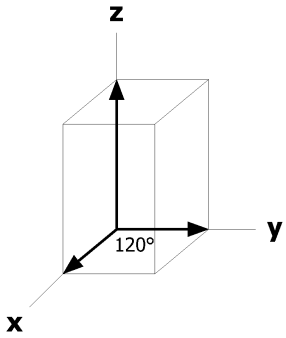
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	c	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{y},x-y,z+1/3$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z+2/3$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z+1/2$ [ $u,v,\bar{w}$ ]	(5) $y,\bar{x}+y,z+5/6$ [ $\bar{v},u-v,\bar{w}$ ]	(6) $x-y,x,z+1/6$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]
			(7) $y,x,\bar{z}+1/3$ [ $\bar{v},\bar{u},w$ ]	(8) $x-y,\bar{y},\bar{z}$ [ $\bar{u}+v,v,w$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}+2/3$ [ $u,u-v,w$ ]
			(10) $\bar{y},\bar{x},\bar{z}+5/6$ [ $\bar{v},\bar{u},\bar{w}$ ]	(11) $\bar{x}+y,y,\bar{z}+1/2$ [ $\bar{u}+v,v,\bar{w}$ ]	(12) $x,x-y,\bar{z}+1/6$ [ $u,u-v,\bar{w}$ ]
6	b	..2	$x,2x,1/4$ [ $u,2u,0$ ]	$2\bar{x},\bar{x},7/12$ [ $2\bar{u},\bar{u},0$ ]	$x,\bar{x},11/12$ [ $u,\bar{u},0$ ]
			$\bar{x},2\bar{x},3/4$ [ $u,2u,0$ ]	$2x,x,1/12$ [ $2\bar{u},\bar{u},0$ ]	$\bar{x},x,5/12$ [ $u,\bar{u},0$ ]
6	a	.2'	$x,0,0$ [ $u,2u,w$ ]	$0,x,1/3$ [ $2\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},2/3$ [ $u,\bar{u},w$ ]
			$\bar{x},0,1/2$ [ $u,2u,\bar{w}$ ]	$0,\bar{x},5/6$ [ $2\bar{u},\bar{u},\bar{w}$ ]	$x,x,1/6$ [ $u,\bar{u},\bar{w}$ ]

**Symmetry of Special Projections**

Along  $[0,0,1]$  p6'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p2'm'g  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

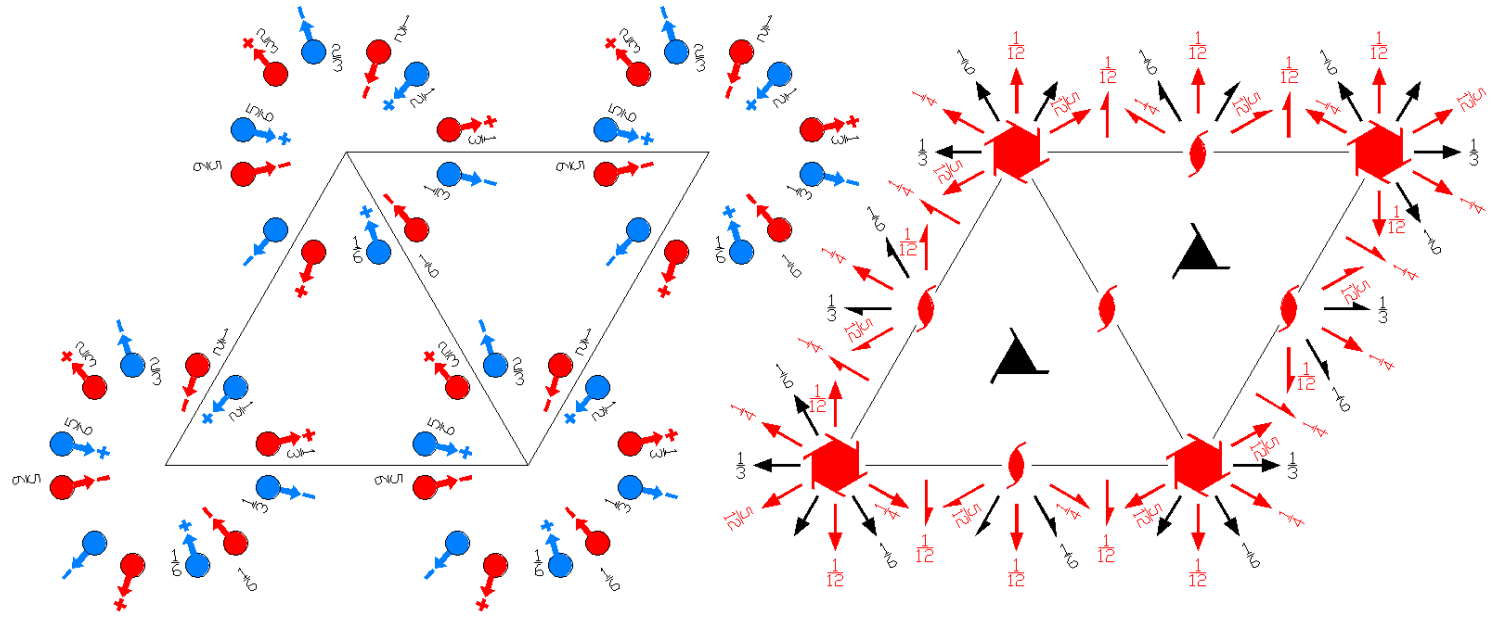
Along  $[2,1,0]$  p2mg  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,1/12$



$P6_1'22'$   
178.4.1389

$6'22'$   
 $P6_1'22'$

Hexagonal



Origin on 2 [100] at  $6_1' (2,1,1) 1$

<b>Asymmetric unit</b>	$0 \leq x \leq 1;$	$0 \leq y \leq 1;$	$0 \leq z \leq 1/12$
Vertices	0,0,0	1,0,0	1,1,0
	0,0,1/12	1,0,1/12	1,1,1/12
			0,1,0
			0,1,1/12

**Symmetry Operations**

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                             | (2) $3^+ (0,0,1/3) 0,0,z$<br>( $3_z$  0,0,1/3)       | (3) $3^- (0,0,2/3) 0,0,z$<br>( $3_z^{-1}$  0,0,2/3) |
| (4) $2' (0,0,1/2) 0,0,z$<br>( $2_z$  0,0,1/2)' | (5) $6^- (0,0,5/6) 0,0,z$<br>( $6_z^{-1}$  0,0,5/6)' | (6) $6^+ (0,0,1/6) 0,0,z$<br>( $6_z$  0,0,1/6)'     |
| (7) 2 $x,x,1/6$<br>( $2_{xy}$  0,0,1/3)        | (8) 2 $x,0,0$<br>( $2_x$  0,0,0)                     | (9) 2 $0,y,1/3$<br>( $2_y$  0,0,2/3)                |
| (10) $2' x,\bar{x},5/12$<br>( $2_3$  0,0,5/6)' | (11) $2' x,2x,1/4$<br>( $2_2$  0,0,1/2)'             | (12) $2' 2x,x,1/12$<br>( $2_1$  0,0,1/6)'           |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

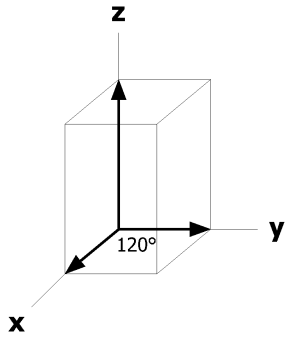
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	c	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z+1/3$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z+2/3$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(5) $y,\bar{x}+y,z+5/6$ [ $\bar{v},u-v,\bar{w}$ ]	(6) $x-y,x,z+1/6$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]
			(7) $y,x,\bar{z}+1/3$ [v,u, $\bar{w}$ ]	(8) $x-y,\bar{y},\bar{z}$ [u-v, $\bar{v},\bar{w}$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}+2/3$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
			(10) $\bar{y},\bar{x},\bar{z}+5/6$ [v,u,w]	(11) $\bar{x}+y,y,\bar{z}+1/2$ [u-v, $\bar{v},w$ ]	(12) $x,x-y,\bar{z}+1/6$ [ $\bar{u},\bar{u}+v,w$ ]
6	b	..2'	$x,2x,1/4$ [u,0,w]	$2\bar{x},\bar{x},7/12$ [0,u,w]	$x,\bar{x},11/12$ [ $\bar{u},\bar{u},w$ ]
			$\bar{x},2\bar{x},3/4$ [u,0, $\bar{w}$ ]	$2x,x,1/12$ [0,u, $\bar{w}$ ]	$\bar{x},x,5/12$ [ $\bar{u},\bar{u},\bar{w}$ ]
6	a	.2.	$x,0,0$ [u,0,0]	$0,x,1/3$ [0,u,0]	$\bar{x},\bar{x},2/3$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},0,1/2$ [u,0,0]	$0,\bar{x},5/6$ [0,u,0]	$x,x,1/6$ [ $\bar{u},\bar{u},0$ ]

**Symmetry of Special Projections**

Along [0,0,1] p6'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/12



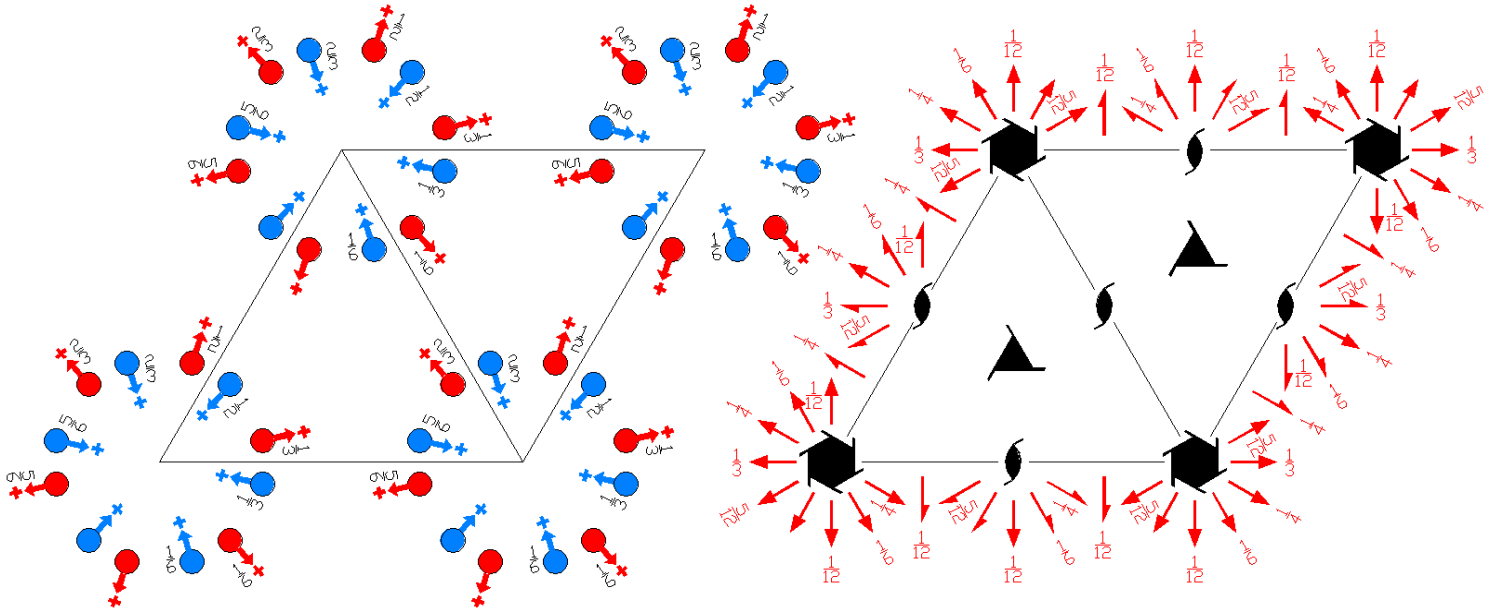
P6<sub>1</sub> 2' 2'

178.5.1390

62' 2'

P6<sub>1</sub> 2' 2'

Hexagonal



Origin on 2' [100] at 6<sub>1</sub> (2', 1, 1) 1

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/12$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/12	1,0,1/12	1,1,1/12	0,1,1/12

### Symmetry Operations

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 3 <sup>+</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub>  0,0,1/3)               | (3) 3 <sup>-</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,2/3) |
| (4) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)        | (5) 6 <sup>-</sup> (0,0,5/6) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,5/6) | (6) 6 <sup>+</sup> (0,0,1/6) 0,0,z<br>(6 <sub>z</sub>  0,0,1/6)               |
| (7) 2' x,x,1/6<br>(2 <sub>xy</sub>  0,0,1/3)'             | (8) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                                      | (9) 2' 0,y,1/3<br>(2 <sub>y</sub>  0,0,2/3)'                                  |
| (10) 2' x, $\bar{x}$ , 5/12<br>(2 <sub>3</sub>  0,0,5/6)' | (11) 2' x, 2x, 1/4<br>(2 <sub>2</sub>  0,0,1/2)'                              | (12) 2' 2x, x, 1/12<br>(2 <sub>1</sub>  0,0,1/6)'                             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

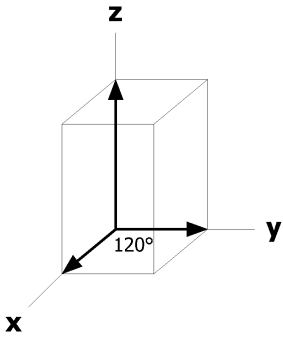
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	c	1	(1) $x,y,z$ [ $u,v,w$ ] (4) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ] (7) $y,x,\bar{z}+1/3$ [ $\bar{v},\bar{u},w$ ] (10) $\bar{y},\bar{x},\bar{z}+5/6$ [ $v,u,w$ ]	(2) $\bar{y},x-y,z+1/3$ [ $\bar{v},u-v,w$ ] (5) $y,\bar{x}+y,z+5/6$ [ $v,\bar{u}+v,w$ ] (8) $x-y,\bar{y},\bar{z}$ [ $\bar{u}+v,v,w$ ] (11) $\bar{x}+y,y,\bar{z}+1/2$ [ $u-v,\bar{v},w$ ]	(3) $\bar{x}+y,\bar{x},z+2/3$ [ $\bar{u}+v,\bar{u},w$ ] (6) $x-y,x,z+1/6$ [ $u-v,u,w$ ] (9) $\bar{x},\bar{x}+y,\bar{z}+2/3$ [ $u,u-v,w$ ] (12) $x,x-y,\bar{z}+1/6$ [ $\bar{u},\bar{u}+v,w$ ]
6	b	..2'	$x,2x,1/4$ [ $u,0,w$ ] $\bar{x},2\bar{x},3/4$ [ $\bar{u},0,w$ ]	$2\bar{x},\bar{x},7/12$ [ $0,u,w$ ] $2x,x,1/12$ [ $0,\bar{u},w$ ]	$x,\bar{x},11/12$ [ $\bar{u},\bar{u},w$ ] $\bar{x},x,5/12$ [ $u,u,w$ ]
6	a	.2'	$x,0,0$ [ $u,2u,w$ ] $\bar{x},0,1/2$ [ $\bar{u},2\bar{u},w$ ]	$0,x,1/3$ [ $2\bar{u},\bar{u},w$ ] $0,\bar{x},5/6$ [ $2u,u,w$ ]	$\bar{x},\bar{x},2/3$ [ $u,\bar{u},w$ ] $x,x,1/6$ [ $\bar{u},u,w$ ]

**Symmetry of Special Projections**

Along  $[0,0,1]$  p6mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p2'mg'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

Along  $[2,1,0]$  p2'mg'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,1/12$



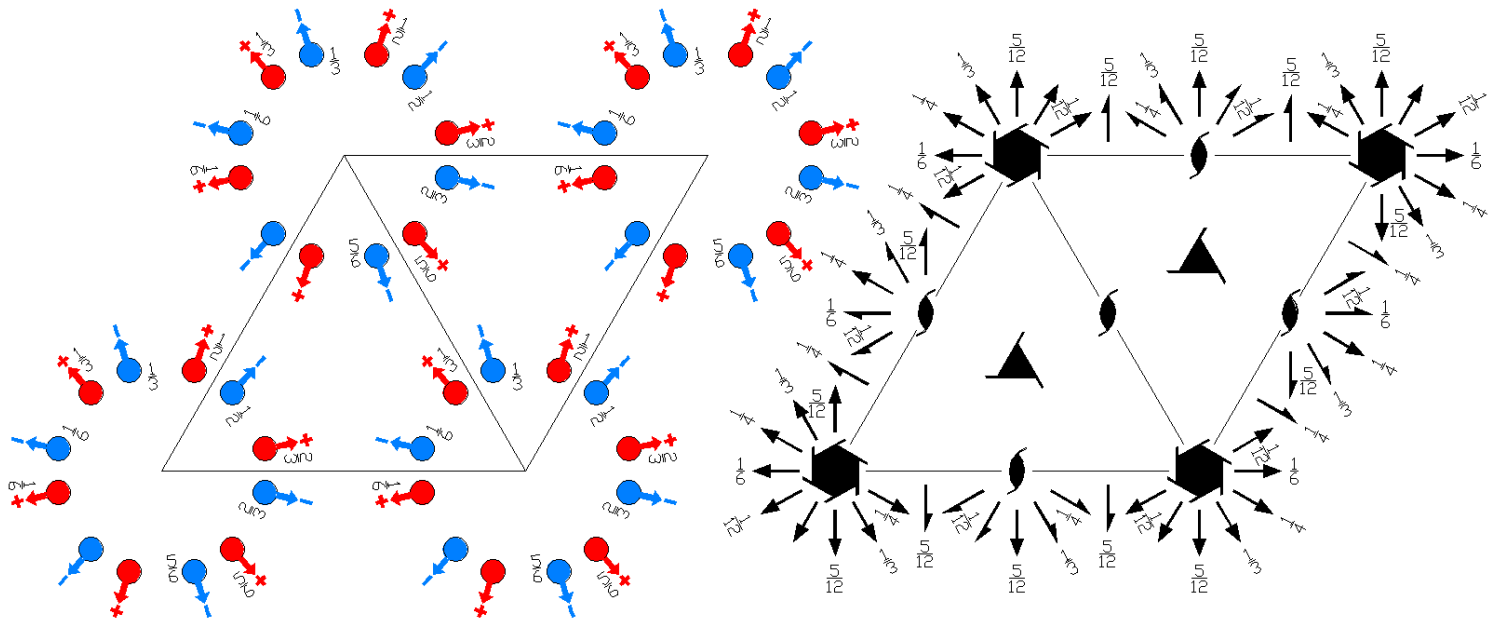
$P6_5 22$

622

Hexagonal

179.1.1391

$P6_5 22$



Origin on 2 [100] at  $6_5 (2,1,1) 1$

Asymmetric unit  $0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/12$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/12	1,0,1/12	1,1,1/12	0,1,1/12

### Symmetry Operations

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                             | (2) $3^+ (0,0,2/3) \quad 0,0,z$<br>( $3_z$  0,0,2/3)      | (3) $3^- (0,0,1/3) \quad 0,0,z$<br>( $3_z^{-1}$  0,0,1/3) |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)     | (5) $6^- (0,0,1/6) \quad 0,0,z$<br>( $6_z^{-1}$  0,0,1/6) | (6) $6^+ (0,0,5/6) \quad 0,0,z$<br>( $6_z$  0,0,5/6)      |
| (7) 2 x,x,1/3<br>( $2_{xy}$  0,0,2/3)          | (8) 2 x,0,0<br>( $2_x$  0,0,0)                            | (9) 2 0,y,1/6<br>( $2_y$  0,0,1/3)                        |
| (10) 2 $x, \bar{x}, 1/12$<br>( $2_3$  0,0,1/6) | (11) 2 x,2x,1/4<br>( $2_2$  0,0,1/2)                      | (12) 2 2x,x,5/12<br>( $2_1$  0,0,5/6)                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

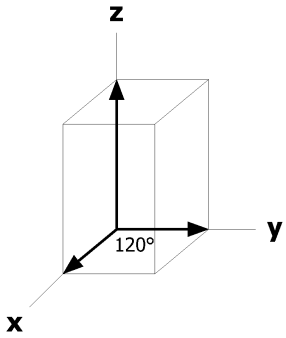
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	c	1	(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{y}, x-y, z+2/3$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z+1/3$ [ $\bar{u}+v, \bar{u}, w$ ]
			(4) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(5) $y, \bar{x}+y, z+1/6$ [ $v, \bar{u}+v, w$ ]	(6) $x-y, x, z+5/6$ [ $u-v, u, w$ ]
			(7) $y, x, \bar{z}+2/3$ [ $v, u, \bar{w}$ ]	(8) $x-y, \bar{y}, \bar{z}$ [ $u-v, \bar{v}, \bar{w}$ ]	(9) $\bar{x}, \bar{x}+y, \bar{z}+1/3$ [ $\bar{u}, \bar{u}+v, \bar{w}$ ]
			(10) $\bar{y}, \bar{x}, \bar{z}+1/6$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(11) $\bar{x}+y, y, \bar{z}+1/2$ [ $\bar{u}+v, v, \bar{w}$ ]	(12) $x, x-y, \bar{z}+5/6$ [ $u, u-v, \bar{w}$ ]
6	b	..2	$x, 2x, 3/4$ [ $u, 2u, 0$ ]	$2\bar{x}, \bar{x}, 5/12$ [ $2\bar{u}, \bar{u}, 0$ ]	$x, \bar{x}, 1/12$ [ $u, \bar{u}, 0$ ]
			$\bar{x}, 2\bar{x}, 1/4$ [ $\bar{u}, 2\bar{u}, 0$ ]	$2x, x, 11/12$ [ $2u, u, 0$ ]	$\bar{x}, x, 7/12$ [ $\bar{u}, u, 0$ ]
6	a	.2.	$x, 0, 0$ [ $u, 0, 0$ ]	$0, x, 2/3$ [ $0, u, 0$ ]	$\bar{x}, \bar{x}, 1/3$ [ $\bar{u}, \bar{u}, 0$ ]
			$\bar{x}, 0, 1/2$ [ $\bar{u}, 0, 0$ ]	$0, \bar{x}, 1/6$ [ $0, \bar{u}, 0$ ]	$x, x, 5/6$ [ $u, u, 0$ ]

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'g'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

Along  $[2,1,0]$   $p2m'g'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x, x/2, 5/12$



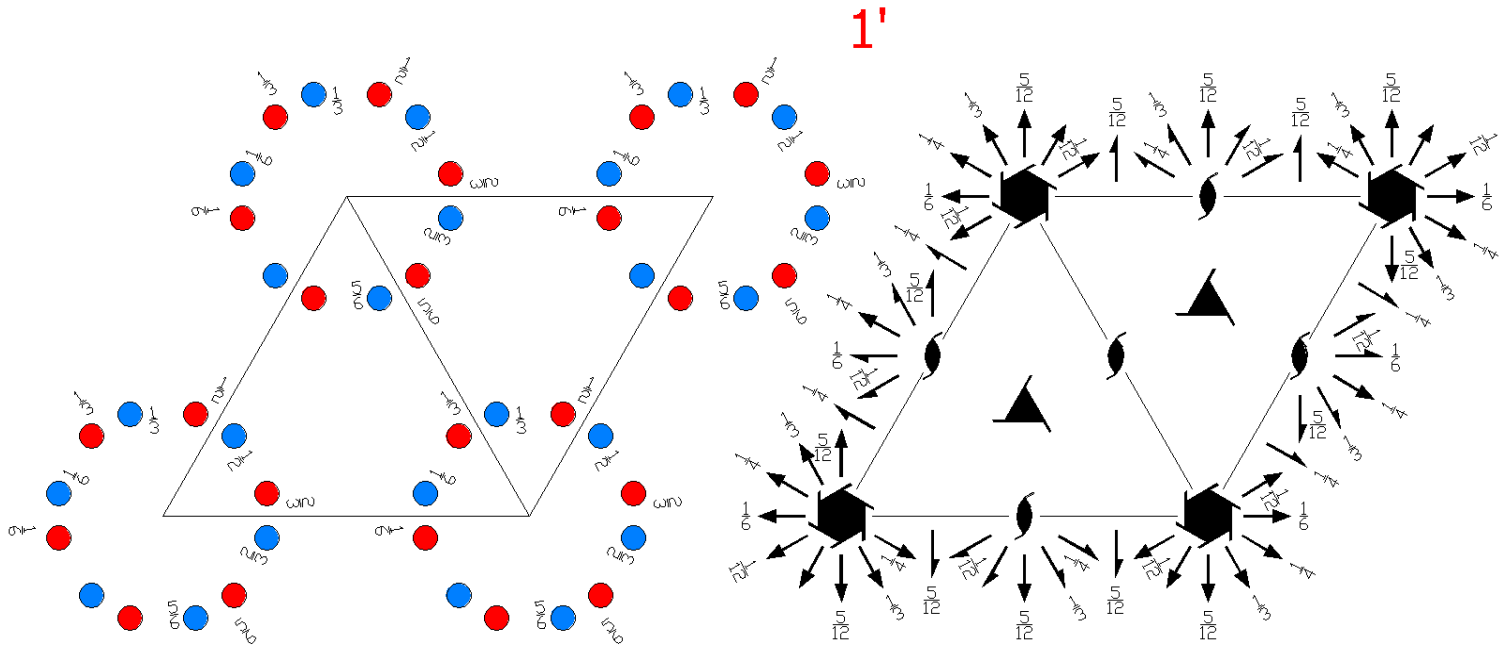
P6<sub>5</sub> 221'

179.2.1392

6221'

P6<sub>5</sub> 221'

Hexagonal



Origin on 21' [100] at 6<sub>5</sub> (2,1,1) 11'

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/12$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/12	1,0,1/12	1,1,1/12	0,1,1/12

**Symmetry Operations**

For 1 + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 3 <sup>+</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub>  0,0,2/3)               | (3) 3 <sup>-</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,1/3) |
| (4) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2) | (5) 6 <sup>-</sup> (0,0,1/6) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,1/6) | (6) 6 <sup>+</sup> (0,0,5/6) 0,0,z<br>(6 <sub>z</sub>  0,0,5/6)               |
| (7) 2 x,x,1/3<br>(2 <sub>xy</sub>  0,0,2/3)        | (8) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (9) 2 0,y,1/6<br>(2 <sub>y</sub>  0,0,1/3)                                    |
| (10) 2 x,x̄,1/12<br>(2 <sub>3</sub>  0,0,1/6)      | (11) 2 x,2x,1/4<br>(2 <sub>2</sub>  0,0,1/2)                                  | (12) 2 2x,x,5/12<br>(2 <sub>1</sub>  0,0,5/6)                                 |



## For 1' + set

(1) 1' (1 0,0,0)'	(2) 3 <sup>+</sup> '(0,0,2/3) 0,0,z (3 <sub>z</sub>  0,0,2/3)'	(3) 3 <sup>-</sup> '(0,0,1/3) 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,1/3)'
(4) 2' (0,0,1/2) 0,0,z (2 <sub>z</sub>  0,0,1/2)'	(5) 6 <sup>-</sup> '(0,0,1/6) 0,0,z (6 <sub>z</sub> <sup>-1</sup>  0,0,1/6)'	(6) 6 <sup>+</sup> '(0,0,5/6) 0,0,z (6 <sub>z</sub>  0,0,5/6)'
(7) 2' x,x,1/3 (2 <sub>xy</sub>  0,0,2/3)'	(8) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'	(9) 2' 0,y,1/6 (2 <sub>y</sub>  0,0,1/3)'
(10) 2' x, $\bar{x}$ ,1/12 (2 <sub>3</sub>  0,0,1/6)'	(11) 2' x,2x,1/4 (2 <sub>2</sub>  0,0,1/2)'	(12) 2' 2x,x,5/12 (2 <sub>1</sub>  0,0,5/6)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

**Positions**

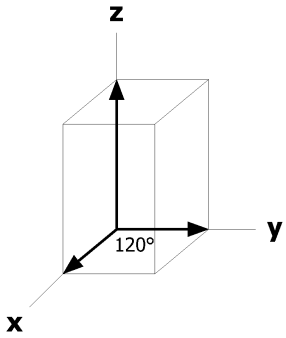
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			1 +	1' +	
12	c	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z+2/3 [0,0,0]	(3) $\bar{x}$ +y, $\bar{x}$ ,z+1/3 [0,0,0]
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [0,0,0]	(5) y, $\bar{x}$ +y,z+1/6 [0,0,0]	(6) x-y,x,z+5/6 [0,0,0]
			(7) y,x, $\bar{z}$ +2/3 [0,0,0]	(8) x-y, $\bar{y}$ , $\bar{z}$ [0,0,0]	(9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ +1/3 [0,0,0]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ +1/6 [0,0,0]	(11) $\bar{x}$ +y,y, $\bar{z}$ +1/2 [0,0,0]	(12) x,x-y, $\bar{z}$ +5/6 [0,0,0]
6	b	..21'	x,2x,3/4 [0,0,0]	2 $\bar{x}$ , $\bar{x}$ ,5/12 [0,0,0]	x, $\bar{x}$ ,1/12 [0,0,0]
			$\bar{x}$ ,2 $\bar{x}$ ,1/4 [0,0,0]	2x,x,11/12 [0,0,0]	$\bar{x}$ ,x,7/12 [0,0,0]
6	a	.2.1'	x,0,0 [0,0,0]	0,x,2/3 [0,0,0]	$\bar{x}$ , $\bar{x}$ ,1/3 [0,0,0]
			$\bar{x}$ ,0,1/2 [0,0,0]	0, $\bar{x}$ ,1/6 [0,0,0]	x,x,5/6 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

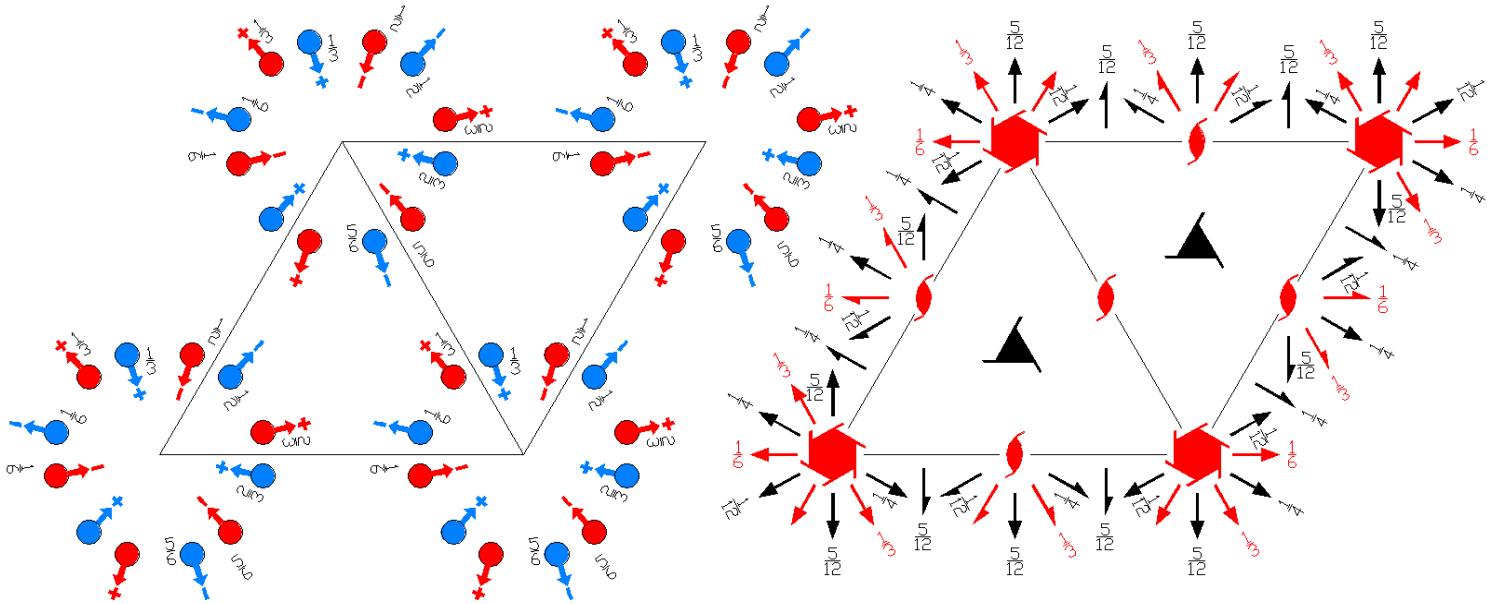
Along [2,1,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,5/12



$P6_5'2'2$   
179.3.1393

$6'2'2$   
 $P6_5'2'2$

Hexagonal



Origin on  $2'$   $[100]$  at  $6_5'$   $(2',1,1)$  1

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/12$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/12	1,0,1/12	1,1,1/12	0,1,1/12

### Symmetry Operations

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                             | (2) $3^+$ (0,0,2/3) 0,0,z<br>( $3_z$  0,0,2/3)       | (3) $3^-$ (0,0,1/3) 0,0,z<br>( $3_z^{-1}$  0,0,1/3) |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)' | (5) $6^-$ (0,0,1/6) 0,0,z<br>( $6_z^{-1}$  0,0,1/6)' | (6) $6^+$ (0,0,5/6) 0,0,z<br>( $6_z$  0,0,5/6)'     |
| (7) $2'$ x,x,1/3<br>( $2_{xy}$  0,0,2/3)'      | (8) $2'$ x,0,0<br>( $2_x$  0,0,0)'                   | (9) $2'$ 0,y,1/6<br>( $2_y$  0,0,1/3)'              |
| (10) 2 x, $\bar{x}$ ,1/12<br>( $2_3$  0,0,1/6) | (11) 2 x,2x,1/4<br>( $2_2$  0,0,1/2)                 | (12) 2 2x,x,5/12<br>( $2_1$  0,0,5/6)               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

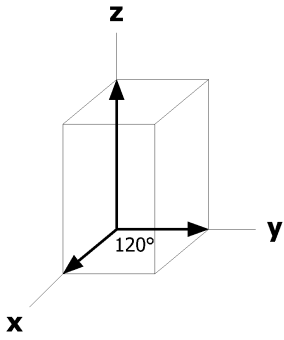
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	c	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{y},x-y,z+2/3$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z+1/3$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z+1/2$ [ $u,v,\bar{w}$ ]	(5) $y,\bar{x}+y,z+1/6$ [ $\bar{v},u-v,\bar{w}$ ]	(6) $x-y,x,z+5/6$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]
			(7) $y,x,\bar{z}+2/3$ [ $\bar{v},\bar{u},w$ ]	(8) $x-y,\bar{y},\bar{z}$ [ $\bar{u}+v,v,w$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}+1/3$ [ $u,u-v,w$ ]
			(10) $\bar{y},\bar{x},\bar{z}+1/6$ [ $\bar{v},\bar{u},\bar{w}$ ]	(11) $\bar{x}+y,y,\bar{z}+1/2$ [ $\bar{u}+v,v,\bar{w}$ ]	(12) $x,x-y,\bar{z}+5/6$ [ $u,u-v,\bar{w}$ ]
6	b	..2	$x,2x,3/4$ [ $u,2u,0$ ]	$2\bar{x},\bar{x},5/12$ [ $2\bar{u},\bar{u},0$ ]	$x,\bar{x},1/12$ [ $u,\bar{u},0$ ]
			$\bar{x},2\bar{x},1/4$ [ $u,2u,0$ ]	$2x,x,11/12$ [ $2\bar{u},\bar{u},0$ ]	$\bar{x},x,7/12$ [ $u,\bar{u},0$ ]
6	a	.2'	$x,0,0$ [ $u,2u,w$ ]	$0,x,2/3$ [ $2\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},1/3$ [ $u,\bar{u},w$ ]
			$\bar{x},0,1/2$ [ $u,2u,\bar{w}$ ]	$0,\bar{x},1/6$ [ $2\bar{u},\bar{u},\bar{w}$ ]	$x,x,5/6$ [ $u,\bar{u},\bar{w}$ ]

**Symmetry of Special Projections**

Along  $[0,0,1]$  p6'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p2'm'g  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

Along  $[2,1,0]$  p2mg  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,5/12$



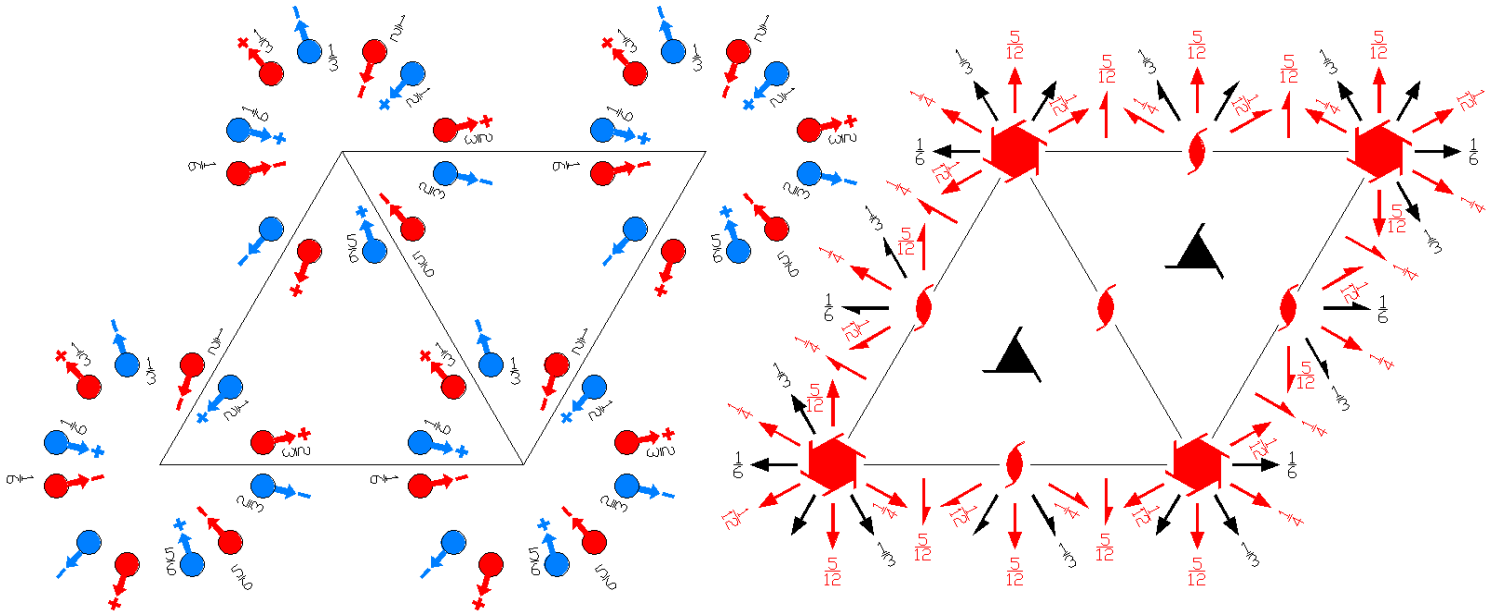
$P6_5'22'$

179.4.1394

$6'22'$

$P6_5'22'$

Hexagonal



Origin on 2 [100] at  $6_5'$  (2,1,1) 1

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/12$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/12	1,0,1/12	1,1,1/12	0,1,1/12

### Symmetry Operations

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                                 | (2) $3^+$ (0,0,2/3) 0,0,z<br>( $3_z$  0,0,2/3)       | (3) $3^-$ (0,0,1/3) 0,0,z<br>( $3_z^{-1}$  0,0,1/3) |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)'     | (5) $6^-$ (0,0,1/6) 0,0,z<br>( $6_z^{-1}$  0,0,1/6)' | (6) $6^+$ (0,0,5/6) 0,0,z<br>( $6_z$  0,0,5/6)'     |
| (7) 2 x,x,1/3<br>( $2_{xy}$  0,0,2/3)              | (8) 2 x,0,0<br>( $2_x$  0,0,0)                       | (9) 2 0,y,1/6<br>( $2_y$  0,0,1/3)                  |
| (10) $2'$ x, $\bar{x}$ ,1/12<br>( $2_3$  0,0,1/6)' | (11) $2'$ x,2x,1/4<br>( $2_2$  0,0,1/2)'             | (12) $2'$ 2x,x,5/12<br>( $2_1$  0,0,5/6)'           |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

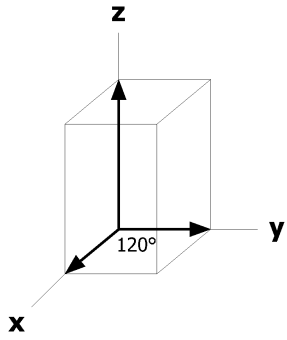
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	c	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z+2/3$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z+1/3$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(5) $y,\bar{x}+y,z+1/6$ [ $\bar{v},u-v,\bar{w}$ ]	(6) $x-y,x,z+5/6$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]
			(7) $y,x,\bar{z}+2/3$ [v,u, $\bar{w}$ ]	(8) $x-y,\bar{y},\bar{z}$ [u-v, $\bar{v},\bar{w}$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}+1/3$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
			(10) $\bar{y},\bar{x},\bar{z}+1/6$ [v,u,w]	(11) $\bar{x}+y,y,\bar{z}+1/2$ [u-v, $\bar{v},w$ ]	(12) $x,x-y,\bar{z}+5/6$ [ $\bar{u},\bar{u}+v,w$ ]
6	b	..2'	$x,2x,3/4$ [u,0,w]	$2\bar{x},\bar{x},5/12$ [0,u,w]	$x,\bar{x},1/12$ [ $\bar{u},\bar{u},w$ ]
			$\bar{x},2\bar{x},1/4$ [u,0, $\bar{w}$ ]	$2x,x,11/12$ [0,u, $\bar{w}$ ]	$\bar{x},x,7/12$ [ $\bar{u},\bar{u},\bar{w}$ ]
6	a	.2.	$x,0,0$ [u,0,0]	$0,x,2/3$ [0,u,0]	$\bar{x},\bar{x},1/3$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},0,1/2$ [u,0,0]	$0,\bar{x},1/6$ [0,u,0]	$x,x,5/6$ [ $\bar{u},\bar{u},0$ ]

**Symmetry of Special Projections**

Along [0,0,1] p6'm'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,5/12



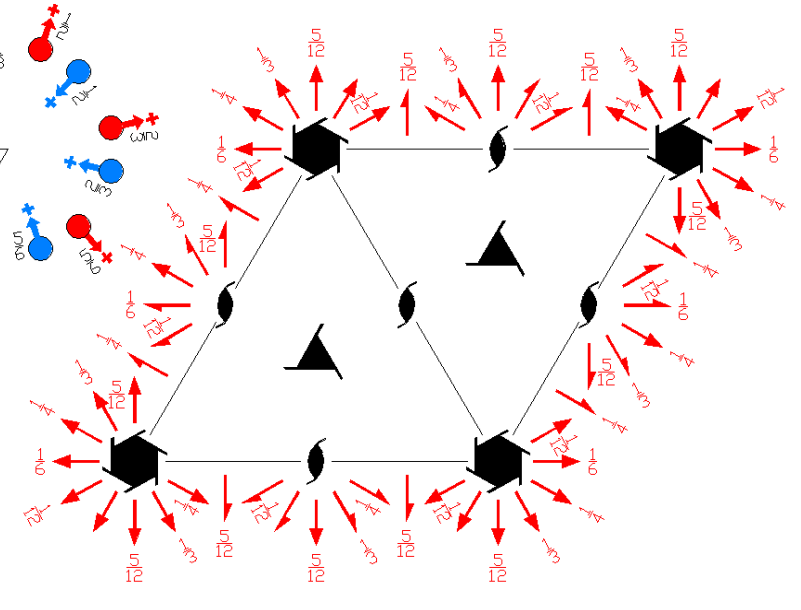
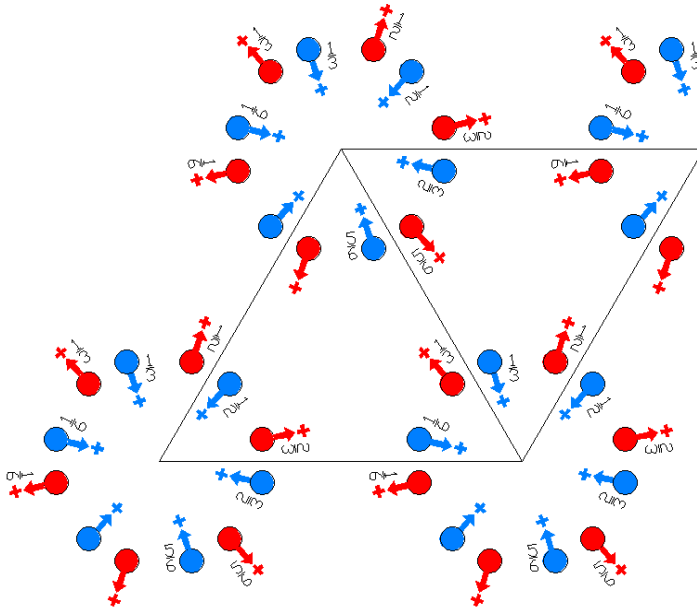
$P6_5 2'2'$

179.5.1395

$62'2'$

$P6_5 2'2'$

Hexagonal



Origin on  $2'$   $[100]$  at  $6_5 (2',1,1) 1$

Asymmetric unit  $0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/12$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,1/12	1,0,1/12	1,1,1/12	0,1,1/12

**Symmetry Operations**

- |  |   |   |
|--|---|---|
| (1) $1$<br>$(1 0,0,0)$                             | (2) $3^+ (0,0,2/3) \quad 0,0,z$<br>$(3_z 0,0,2/3)$      | (3) $3^- (0,0,1/3) \quad 0,0,z$<br>$(3_z^{-1} 0,0,1/3)$ |
| (4) $2 (0,0,1/2) \quad 0,0,z$<br>$(2_z 0,0,1/2)$   | (5) $6^- (0,0,1/6) \quad 0,0,z$<br>$(6_z^{-1} 0,0,1/6)$ | (6) $6^+ (0,0,5/6) \quad 0,0,z$<br>$(6_z 0,0,5/6)$      |
| (7) $2' \quad x,x,1/3$<br>$(2_{xy} 0,0,2/3)'$      | (8) $2' \quad x,0,0$<br>$(2_x 0,0,0)'$                  | (9) $2' \quad 0,y,1/6$<br>$(2_y 0,0,1/3)'$              |
| (10) $2' \quad x,\bar{x},1/12$<br>$(2_3 0,0,1/6)'$ | (11) $2' \quad x,2x,1/4$<br>$(2_2 0,0,1/2)'$            | (12) $2' \quad 2x,x,5/12$<br>$(2_1 0,0,5/6)'$           |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	c	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{y},x-y,z+2/3$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z+1/3$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(5) $y,\bar{x}+y,z+1/6$ [ $v,\bar{u}+v,w$ ]	(6) $x-y,x,z+5/6$ [ $u-v,u,w$ ]
			(7) $y,x,\bar{z}+2/3$ [ $\bar{v},\bar{u},w$ ]	(8) $x-y,\bar{y},\bar{z}$ [ $\bar{u}+v,v,w$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}+1/3$ [ $u,u-v,w$ ]
			(10) $\bar{y},\bar{x},\bar{z}+1/6$ [ $v,u,w$ ]	(11) $\bar{x}+y,y,\bar{z}+1/2$ [ $u-v,\bar{v},w$ ]	(12) $x,x-y,\bar{z}+5/6$ [ $\bar{u},\bar{u}+v,w$ ]
6	b	..2'	$x,2x,3/4$ [ $u,0,w$ ]	$2\bar{x},\bar{x},5/12$ [ $0,u,w$ ]	$x,\bar{x},1/12$ [ $\bar{u},\bar{u},w$ ]
			$\bar{x},2\bar{x},1/4$ [ $\bar{u},0,w$ ]	$2x,x,11/12$ [ $0,\bar{u},w$ ]	$\bar{x},x,7/12$ [ $u,u,w$ ]
6	a	.2'	$x,0,0$ [ $u,2u,w$ ]	$0,x,2/3$ [ $2\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},1/3$ [ $u,\bar{u},w$ ]
			$\bar{x},0,1/2$ [ $\bar{u},2\bar{u},w$ ]	$0,\bar{x},1/6$ [ $2u,u,w$ ]	$x,x,5/6$ [ $\bar{u},u,w$ ]

**Symmetry of Special Projections**

Along  $[0,0,1]$  p6mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p2'mg'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

Along  $[2,1,0]$  p2'mg'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,5/12$

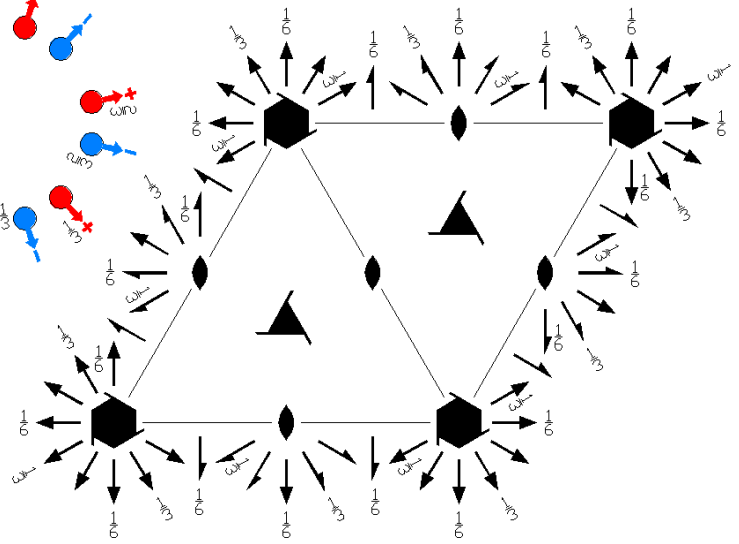
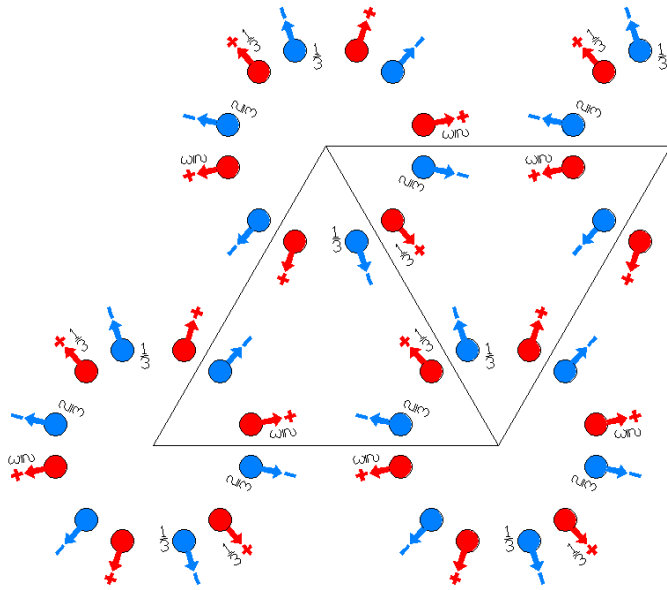
P6<sub>2</sub>22

622

Hexagonal

180.1.1396

P6<sub>2</sub>22



Origin at 222 at 6<sub>2</sub> (2,1,1) (1,2,1)

<b>Asymmetric unit</b>	$0 \leq x \leq 1;$	$0 \leq y \leq 1;$	$0 \leq z \leq 1/6$	$y \leq x$
Vertices	0,0,0 0,0,1/6	1,0,0 1,0,1/6	1,1,0 1,1,1/6	

**Symmetry Operations**

- |   |   |   |
|---|---|---|
| (1) 1<br>(1*0,0,0)                          | (2) 3 <sup>+</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> *0,0,2/3)               | (3) 3 <sup>-</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup> *0,0,1/3) |
| (4) 2 0,0,z<br>(2 <sub>z</sub> *0,0,0)      | (5) 6 <sup>-</sup> (0,0,2/3) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup> *0,0,2/3) | (6) 6 <sup>+</sup> (0,0,1/3) 0,0,z<br>(6 <sub>z</sub> *0,0,1/3)               |
| (7) 2 x,x,1/3<br>(2 <sub>xy</sub> *0,0,2/3) | (8) 2 x,0,0<br>(2 <sub>x</sub> *0,0,0)  | (9) 2 0,y,1/6<br>(2 <sub>y</sub> *0,0,1/3)                                    |
| (10) 2 x,&,1/3<br>(2 <sub>3</sub> *0,0,2/3) | (11) 2 x,2x,0<br>(2 <sub>2</sub> *0,0,0)                                      | (12) 2 2x,x,1/6<br>(2 <sub>1</sub> *0,0,1/3)                                  |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	k	1	(1) $x,y,z$ [u,v,w] (4) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (7) $y,x,\bar{z}+2/3$ [v,u, $\bar{w}$ ] (10) $\bar{y},\bar{x},\bar{z}+2/3$ [ $\bar{v},\bar{u},\bar{w}$ ]	(2) $\bar{y},x-y,z+2/3$ [ $\bar{v},u-v,w$ ] (5) $y,\bar{x}+y,z+2/3$ [v, $\bar{u}+v,w$ ] (8) $x-y,\bar{y},\bar{z}$ [u-v, $\bar{v},\bar{w}$ ] (11) $\bar{x}+y,y,\bar{z}$ [ $\bar{u}+v,v,\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z+1/3$ [ $\bar{u}+v,\bar{u},w$ ] (6) $x-y,x,z+1/3$ [u-v,u,w] (9) $\bar{x},\bar{x}+y,\bar{z}+1/3$ [ $\bar{u},\bar{u}+v,\bar{w}$ ] (12) $x,x-y,\bar{z}+1/3$ [u,u-v, $\bar{w}$ ]
6	j	..2	$x,2x,1/2$ [u,2u,0] $\bar{x},2\bar{x},1/2$ [ $\bar{u},2\bar{u},0$ ]	$2\bar{x},\bar{x},1/6$ [ $2\bar{u},\bar{u},0$ ] $2x,x,1/6$ [2u,u,0]	$x,\bar{x},5/6$ [u, $\bar{u},0$ ] $\bar{x},x,5/6$ [ $\bar{u},u,0$ ]
6	i	..2	$x,2x,0$ [u,2u,0] $\bar{x},2\bar{x},0$ [ $\bar{u},2\bar{u},0$ ]	$2\bar{x},\bar{x},2/3$ [ $2\bar{u},\bar{u},0$ ] $2x,x,2/3$ [2u,u,0]	$x,\bar{x},1/3$ [u, $\bar{u},0$ ] $\bar{x},x,1/3$ [ $\bar{u},u,0$ ]
6	h	.2.	$x,0,1/2$ [u,0,0] $\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	$0,x,1/6$ [0,u,0] $0,\bar{x},1/6$ [0, $\bar{u},0$ ]	$\bar{x},\bar{x},5/6$ [ $\bar{u},\bar{u},0$ ] $x,x,5/6$ [u,u,0]
6	g	.2.	$x,0,0$ [u,0,0] $\bar{x},0,0$ [ $\bar{u},0,0$ ]	$0,x,2/3$ [0,u,0] $0,\bar{x},2/3$ [0, $\bar{u},0$ ]	$\bar{x},\bar{x},1/3$ [ $\bar{u},\bar{u},0$ ] $x,x,1/3$ [u,u,0]
6	f	2..	$1/2,0,z$ [0,0,w] $0,1/2,\bar{z}+2/3$ [0,0, $\bar{w}$ ]	$0,1/2,z+2/3$ [0,0,w] $1/2,0,\bar{z}$ [0,0, $\bar{w}$ ]	$1/2,1/2,z+1/3$ [0,0,w] $1/2,1/2,\bar{z}+1/3$ [0,0, $\bar{w}$ ]
6	e	2..	$0,0,z$ [0,0,w] $0,0,\bar{z}+2/3$ [0,0, $\bar{w}$ ]	$0,0,z+2/3$ [0,0,w] $0,0,\bar{z}$ [0,0, $\bar{w}$ ]	$0,0,z+1/3$ [0,0,w] $0,0,\bar{z}+1/3$ [0,0, $\bar{w}$ ]
3	d	222	$1/2,0,1/2$ [0,0,0]	$0,1/2,1/6$ [0,0,0]	$1/2,1/2,5/6$ [0,0,0]
3	c	222	$1/2,0,0$ [0,0,0]	$0,1/2,2/3$ [0,0,0]	$1/2,1/2,1/3$ [0,0,0]
3	b	222	$0,0,1/2$ [0,0,0]	$0,0,1/6$ [0,0,0]	$0,0,5/6$ [0,0,0]
3	a	222	$0,0,0$ [0,0,0]	$0,0,2/3$ [0,0,0]	$0,0,1/3$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p6m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/6

P6<sub>2</sub>221'

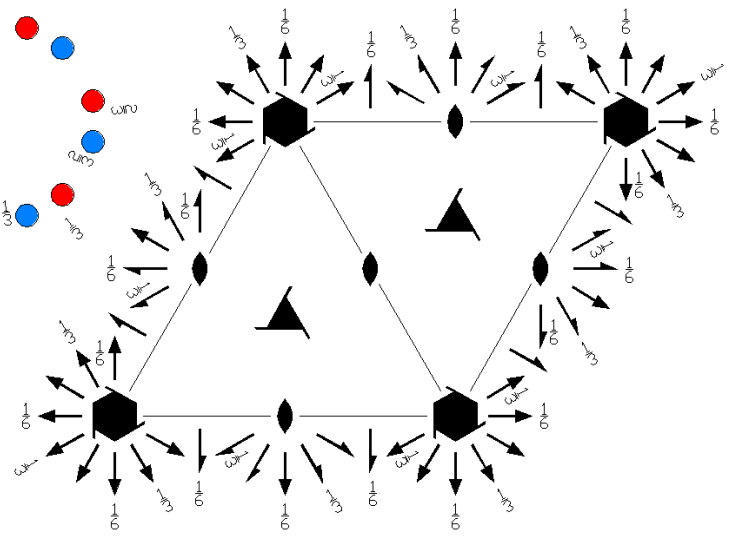
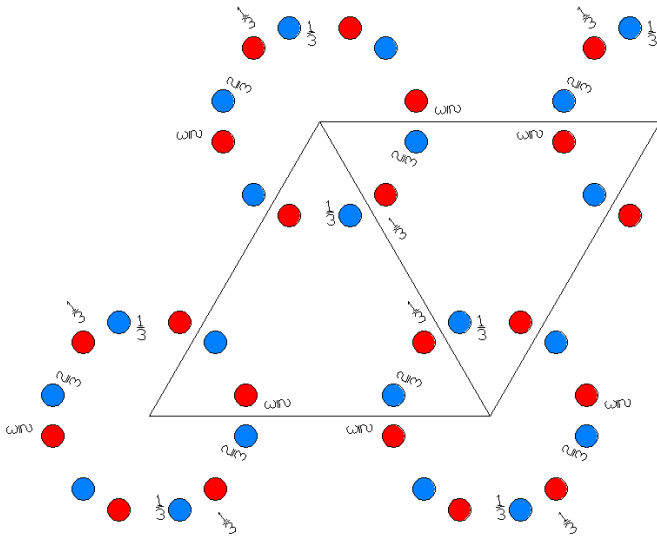
6221'

Hexagonal

180.2.1397

P6<sub>2</sub>221'

1'



Origin at 2221' at 6<sub>2</sub> (2,1,1) (1,2,1)1'

<b>Asymmetric unit</b>	$0 \leq x \leq 1;$	$0 \leq y \leq 1;$	$0 \leq z \leq 1/6$	$y \leq x$
Vertices	0,0,0 0,0,1/6	1,0,0 1,0,1/6	1,1,0 1,1,1/6	

**Symmetry Operations**

For 1 + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1*0,0,0)                          | (2) 3 <sup>+</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> *0,0,2/3)               | (3) 3 <sup>-</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup> *0,0,1/3) |
| (4) 2 0,0,z<br>(2 <sub>z</sub> *0,0,0)      | (5) 6 <sup>-</sup> (0,0,2/3) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup> *0,0,2/3) | (6) 6 <sup>+</sup> (0,0,1/3) 0,0,z<br>(6 <sub>z</sub> *0,0,1/3)               |
| (7) 2 x,x,1/3<br>(2 <sub>xy</sub> *0,0,2/3) | (8) 2 x,0,0<br>(2 <sub>x</sub> *0,0,0)  | (9) 2 0,y,1/6<br>(2 <sub>y</sub> *0,0,1/3)                                    |
| (10) 2 x,&,1/3<br>(2 <sub>3</sub> *0,0,2/3) | (11) 2 x,2x,0<br>(2 <sub>2</sub> *0,0,0)                                      | (12) 2 2x,x,1/6<br>(2 <sub>1</sub> *0,0,1/3)                                  |

For 1' + set

- |   |  |  |
|---|--|--|
| (1) 1'<br>(1*0,0,0)'                          | (2) 3 <sup>+</sup> ' (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> *0,0,2/3)'               | (3) 3 <sup>-</sup> ' (0,0,1/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup> *0,0,1/3)' |
| (4) 2' 0,0,z<br>(2 <sub>z</sub> *0,0,0)'      | (5) 6 <sup>-</sup> ' (0,0,2/3) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup> *0,0,2/3)' | (6) 6 <sup>+</sup> ' (0,0,1/3) 0,0,z<br>(6 <sub>z</sub> *0,0,1/3)'               |
| (7) 2' x,x,1/3<br>(2 <sub>xy</sub> *0,0,2/3)' | (8) 2' x,0,0<br>(2 <sub>x</sub> *0,0,0)'   | (9) 2' 0,y,1/6<br>(2 <sub>y</sub> *0,0,1/3)'                                     |
| (10) 2' x,&,1/3<br>(2 <sub>3</sub> *0,0,2/3)' | (11) 2' x,2x,0<br>(2 <sub>2</sub> *0,0,0)'                                       | (12) 2' 2x,x,1/6<br>(2 <sub>1</sub> *0,0,1/3)'                                   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates		
		1 +	1' +
12 k 11'	(1) x,y,z [0,0,0] (4) $\bar{x},\bar{y},z$ [0,0,0] (7) y,x, $\bar{z}+2/3$ [0,0,0] (10) $\bar{y},\bar{x},\bar{z}+2/3$ [0,0,0]	(2) $\bar{y},x-y,z+2/3$ [0,0,0] (5) y, $\bar{x}+y,z+2/3$ [0,0,0] (8) x-y, $\bar{y},\bar{z}$ [0,0,0] (11) $\bar{x}+y,y,\bar{z}$ [0,0,0]	(3) $\bar{x}+y,\bar{x},z+1/3$ [0,0,0] (6) x-y,x,z+1/3 [0,0,0] (9) $\bar{x},\bar{x}+y,\bar{z}+1/3$ [0,0,0] (12) x,x-y, $\bar{z}+1/3$ [0,0,0]
6 j ..21'	x,2x,1/2 [0,0,0] $\bar{x},2\bar{x},1/2$ [0,0,0]	$2\bar{x},\bar{x},1/6$ [0,0,0] 2x,x,1/6 [0,0,0]	x, $\bar{x},5/6$ [0,0,0] $\bar{x},x,5/6$ [0,0,0]
6 i ..21'	x,2x,0 [0,0,0] $\bar{x},2\bar{x},0$ [0,0,0]	$2\bar{x},\bar{x},2/3$ [0,0,0] 2x,x,2/3 [0,0,0]	x, $\bar{x},1/3$ [0,0,0] $\bar{x},x,1/3$ [0,0,0]
6 h .2.1'	x,0,1/2 [0,0,0] $\bar{x},0,1/2$ [0,0,0]	0,x,1/6 [0,0,0] 0, $\bar{x},1/6$ [0,0,0]	$\bar{x},\bar{x},5/6$ [0,0,0] x,x,5/6 [0,0,0]
6 g .2.1'	x,0,0 [0,0,0] $\bar{x},0,0$ [0,0,0]	0,x,2/3 [0,0,0] 0, $\bar{x},2/3$ [0,0,0]	$\bar{x},\bar{x},1/3$ [0,0,0] x,x,1/3 [0,0,0]
6 f 2..1'	1/2,0,z [0,0,0] 0,1/2, $\bar{z}+2/3$ [0,0,0]	0,1/2,z+2/3 [0,0,0] 1/2,0, $\bar{z}$ [0,0,0]	1/2,1/2,z+1/3 [0,0,0] 1/2,1/2, $\bar{z}+1/3$ [0,0,0]
6 e 2..1'	0,0,z [0,0,0] 0,0, $\bar{z}+2/3$ [0,0,0]	0,0,z+2/3 [0,0,0] 0,0, $\bar{z}$ [0,0,0]	0,0,z+1/3 [0,0,0] 0,0, $\bar{z}+1/3$ [0,0,0]
3 d 2221'	1/2,0,1/2 [0,0,0]	0,1/2,1/6 [0,0,0]	1/2,1/2,5/6 [0,0,0]
3 c 2221'	1/2,0,0 [0,0,0]	0,1/2,2/3 [0,0,0]	1/2,1/2,1/3 [0,0,0]
3 b 2221'	0,0,1/2 [0,0,0]	0,0,1/6 [0,0,0]	0,0,5/6 [0,0,0]
3 a 2221'	0,0,0 [0,0,0]	0,0,2/3 [0,0,0]	0,0,1/3 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/6

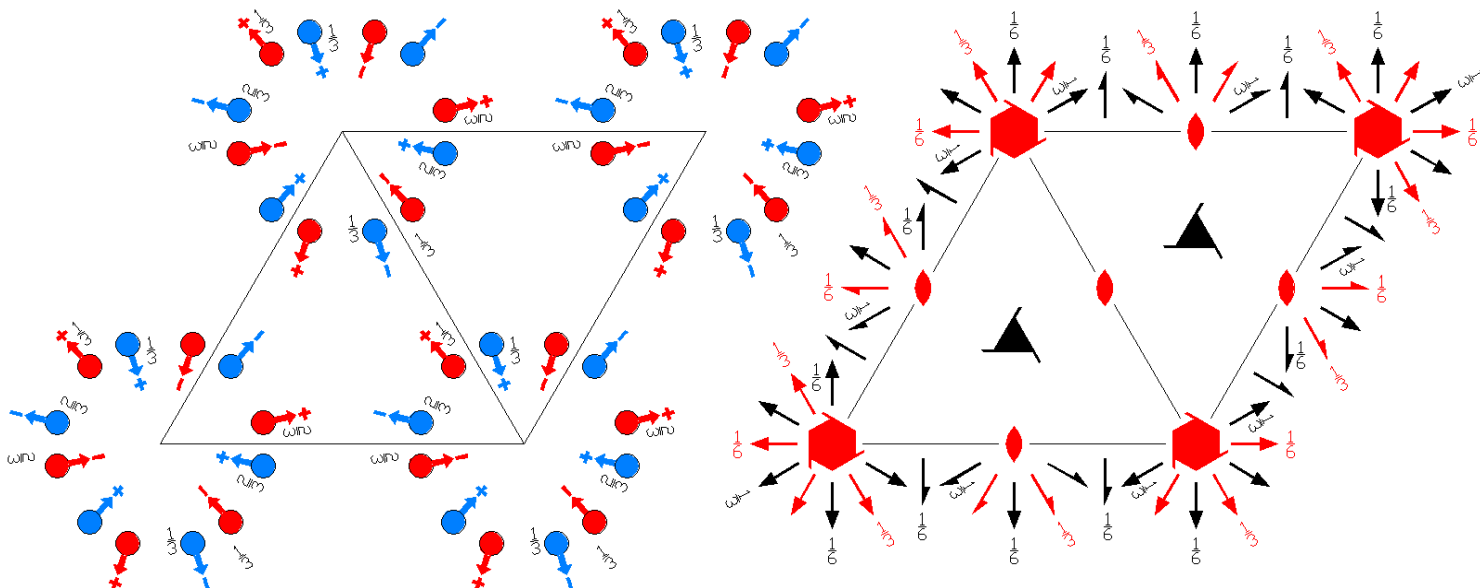
P6<sub>2</sub>'2'2

6'2'2

Hexagonal

180.3.1398

P6<sub>2</sub>'2'2



Origin at 2'22' at 6<sub>2</sub>' (2',1,1) (1,2',1)

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/6$   $y \leq x$

Vertices  $0,0,0$   $1,0,0$   $1,1,0$   
 $0,0,1/6$   $1,0,1/6$   $1,1,1/6$

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1*0,0,0)                            | (2) 3 <sup>+</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> *0,0,2/3)                | (3) 3 <sup>-</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup> *0,0,1/3) |
| (4) 2' 0,0,z<br>(2 <sub>z</sub> *0,0,0)'      | (5) 6 <sup>-</sup> (0,0,2/3) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup> *0,0,2/3)' | (6) 6 <sup>+</sup> (0,0,1/3) 0,0,z<br>(6 <sub>z</sub> *0,0,1/3)'              |
| (7) 2' x,x,1/3<br>(2 <sub>xy</sub> *0,0,2/3)' | (8) 2' x,0,0<br>(2 <sub>x</sub> *0,0,0)'                                       | (9) 2' 0,y,1/6<br>(2 <sub>y</sub> *0,0,1/3)'                                  |
| (10) 2 x,&,1/3<br>(2 <sub>3</sub> *0,0,2/3)   | (11) 2 x,2x,0<br>(2 <sub>2</sub> *0,0,0)                                       | (12) 2 2x,x,1/6<br>(2 <sub>1</sub> *0,0,1/3)                                  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	k	1	(1) x,y,z [u,v,w] (4) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (7) y,x, $\bar{z}+2/3$ [ $\bar{v},\bar{u},w$ ] (10) $\bar{y},\bar{x},\bar{z}+2/3$ [ $\bar{v},\bar{u},\bar{w}$ ]	(2) $\bar{y},x-y,z+2/3$ [ $\bar{v},u-v,w$ ] (5) y, $\bar{x}+y,z+2/3$ [ $\bar{v},u-v,\bar{w}$ ] (8) x-y, $\bar{y},\bar{z}$ [ $\bar{u}+v,v,w$ ] (11) $\bar{x}+y,y,\bar{z}$ [ $\bar{u}+v,v,\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z+1/3$ [ $\bar{u}+v,\bar{u},w$ ] (6) x-y,x,z+1/3 [ $\bar{u}+v,\bar{u},\bar{w}$ ] (9) $\bar{x},\bar{x}+y,\bar{z}+1/3$ [u,u-v,w] (12) x,x-y, $\bar{z}+1/3$ [u,u-v, $\bar{w}$ ]
6	j	..2	x,2x,1/2 [u,2u,0] $\bar{x},2\bar{x},1/2$ [u,2u,0]]	$2\bar{x},\bar{x},1/6$ [ $2\bar{u},\bar{u},0$ ] 2x,x,1/6 [ $2\bar{u},\bar{u},0$ ]	x, $\bar{x},5/6$ [u, $\bar{u},0$ ] $\bar{x},x,5/6$ [u, $\bar{u},0$ ]
6	i	..2	x,2x,0 [u,2u,0] $\bar{x},2\bar{x},0$ [u,2u,0]	$2\bar{x},\bar{x},2/3$ [ $2\bar{u},\bar{u},0$ ] 2x,x,2/3 [ $2\bar{u},\bar{u},0$ ]	x, $\bar{x},1/3$ [u, $\bar{u},0$ ] $\bar{x},x,1/3$ [u, $\bar{u},0$ ]
6	h	.2'	x,0,1/2 [u,2u,w] $\bar{x},0,1/2$ [u,2u, $\bar{w}$ ]	0,x,1/6 [ $2\bar{u},\bar{u},w$ ] 0, $\bar{x},1/6$ [ $2\bar{u},\bar{u},\bar{w}$ ]	$\bar{x},\bar{x},5/6$ [u, $\bar{u},w$ ] x,x,5/6 [u, $\bar{u},\bar{w}$ ]
6	g	.2'	x,0,0 [u,2u,w] $\bar{x},0,0$ [u,2u, $\bar{w}$ ]	0,x,2/3 [ $2\bar{u},\bar{u},w$ ] 0, $\bar{x},2/3$ [ $2\bar{u},\bar{u},\bar{w}$ ]	$\bar{x},\bar{x},1/3$ [u, $\bar{u},w$ ] x,x,1/3 [u, $\bar{u},\bar{w}$ ]
6	f	2'..	1/2,0,z [u,v,0] 0,1/2, $\bar{z}+2/3$ [ $\bar{v},\bar{u},0$ ]	0,1/2,z+2/3 [ $\bar{v},u-v,0$ ] 1/2,0, $\bar{z}$ [ $\bar{u}+v,v,0$ ]	1/2,1/2,z+1/3 [ $\bar{u}+v,\bar{u},0$ ] 1/2,1/2, $\bar{z}+1/3$ [u,u-v,0]
6	e	2'..	0,0,z [u,v,0] 0,0, $\bar{z}+2/3$ [ $\bar{v},\bar{u},0$ ]	0,0,z+2/3 [ $\bar{v},u-v,0$ ] 0,0, $\bar{z}$ [ $\bar{u}+v,v,0$ ]	0,0,z+1/3 [ $\bar{u}+v,\bar{u},0$ ] 0,0, $\bar{z}+1/3$ [u,u-v,0]
3	d	2'22'	1/2,0,1/2 [u,2u,0]	0,1/2,1/6 [ $2\bar{u},\bar{u},0$ ]	1/2,1/2,5/6 [u, $\bar{u},0$ ]
3	c	2'22'	1/2,0,0 [u,2u,0]	0,1/2,2/3 [ $2\bar{u},\bar{u},0$ ]	1/2,1/2,1/3 [u, $\bar{u},0$ ]
3	b	2'22'	0,0,1/2 [u,2u,0]	0,0,1/6 [ $2\bar{u},\bar{u},0$ ]	0,0,5/6 [u, $\bar{u},0$ ]
3	a	2'22'	0,0,0 [u,2u,0]	0,0,2/3 [ $2\bar{u},\bar{u},0$ ]	0,0,1/3 [u, $\bar{u},0$ ]

**Symmetry of Special Projections**

Along [0,0,1] p6'm'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [2,1,0] p2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/6

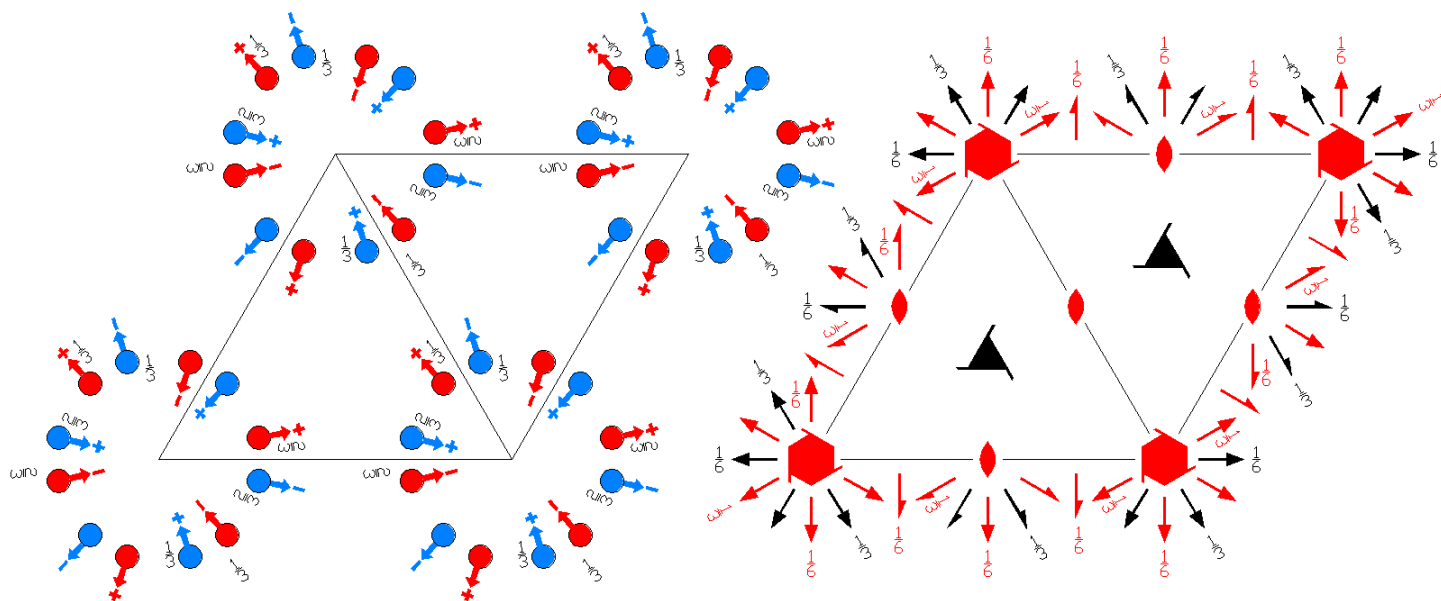
P6<sub>2</sub>'22'

6'22'

Hexagonal

180.4.1399

P6<sub>2</sub>'22'



Origin at 22'2' at 6<sub>2</sub>' (2,1,1) (1,2',1)

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/6$   $y \leq x$

Vertices  $0,0,0$   $1,0,0$   $1,1,0$   
 $0,0,1/6$   $1,0,1/6$   $1,1,1/6$

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1*0,0,0)                            | (2) 3 <sup>+</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> *0,0,2/3)                  | (3) 3 <sup>-</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup> *0,0,1/3) |
| (4) 2' 0,0,z<br>(2 <sub>z</sub> *0,0,0)'      | (5) 6 <sup>-</sup> ' (0,0,2/3) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup> *0,0,2/3)' | (6) 6 <sup>+</sup> ' (0,0,1/3) 0,0,z<br>(6 <sub>z</sub> *0,0,1/3)'            |
| (7) 2 x,x,1/3<br>(2 <sub>xy</sub> *0,0,2/3)   | (8) 2 x,0,0<br>(2 <sub>x</sub> *0,0,0)   | (9) 2 0,y,1/6<br>(2 <sub>y</sub> *0,0,1/3)                                    |
| (10) 2' x,&,1/3<br>(2 <sub>3</sub> *0,0,2/3)' | (11) 2' x,2x,0<br>(2 <sub>2</sub> *0,0,0)'                                       | (12) 2' 2x,x,1/6<br>(2 <sub>1</sub> *0,0,1/3)'                                |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
12	k	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z+2/3$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z+1/3$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(5) $y,\bar{x}+y,z+2/3$ [ $\bar{v},u-v,\bar{w}$ ]	(6) $x-y,x,z+1/3$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]
			(7) $y,x,\bar{z}+2/3$ [v,u, $\bar{w}$ ]	(8) $x-y,\bar{y},\bar{z}$ [u-v, $\bar{v},\bar{w}$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}+1/3$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
			(10) $\bar{y},\bar{x},\bar{z}+2/3$ [v,u,w]	(11) $\bar{x}+y,y,\bar{z}$ [u-v, $\bar{v},w$ ]	(12) $x,x-y,\bar{z}+1/3$ [ $\bar{u},\bar{u}+v,w$ ]
6	j	..2'	$x,2x,1/2$ [u,0,w]	$2\bar{x},\bar{x},1/6$ [0,u,w]	$x,\bar{x},5/6$ [ $\bar{u},\bar{u},w$ ]
			$\bar{x},2\bar{x},1/2$ [u,0, $\bar{w}$ ]	$2x,x,1/6$ [0,u, $\bar{w}$ ]	$\bar{x},x,5/6$ [ $\bar{u},\bar{u},\bar{w}$ ]
6	i	..2'	$x,2x,0$ [u,0,w]	$2\bar{x},\bar{x},2/3$ [0,u,w]	$x,\bar{x},1/3$ [ $\bar{u},\bar{u},w$ ]
			$\bar{x},2\bar{x},0$ [u,0, $\bar{w}$ ]	$2x,x,2/3$ [0,u, $\bar{w}$ ]	$\bar{x},x,1/3$ [ $\bar{u},\bar{u},\bar{w}$ ]
6	h	.2.	$x,0,1/2$ [u,0,0]	$0,x,1/6$ [0,u,0]	$\bar{x},\bar{x},5/6$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},0,1/2$ [u,0,0]	$0,\bar{x},1/6$ [0,u,0]	$x,x,5/6$ [ $\bar{u},\bar{u},0$ ]
6	g	.2.	$x,0,0$ [u,0,0]	$0,x,2/3$ [0,u,0]	$\bar{x},\bar{x},1/3$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},0,0$ [u,0,0]	$0,\bar{x},2/3$ [0,u,0]	$x,x,1/3$ [ $\bar{u},\bar{u},0$ ]
6	f	2'..	$1/2,0,z$ [u,v,0]	$0,1/2,z+2/3$ [ $\bar{v},u-v,0$ ]	$1/2,1/2,z+1/3$ [ $\bar{u}+v,\bar{u},0$ ]
			$0,1/2,\bar{z}+2/3$ [v,u,0]	$1/2,0,\bar{z}$ [u-v, $\bar{v},0$ ]	$1/2,1/2,\bar{z}+1/3$ [ $\bar{u},\bar{u}+v,0$ ]
6	e	2'..	$0,0,z$ [u,v,0]	$0,0,z+2/3$ [ $\bar{v},u-v,0$ ]	$0,0,z+1/3$ [ $\bar{u}+v,\bar{u},0$ ]
			$0,0,\bar{z}+2/3$ [v,u,0]	$0,0,\bar{z}$ [u-v, $\bar{v},0$ ]	$0,0,\bar{z}+1/3$ [ $\bar{u},\bar{u}+v,0$ ]
3	d	22'2'	$1/2,0,1/2$ [u,0,0]	$0,1/2,1/6$ [0,u,0]	$1/2,1/2,5/6$ [ $\bar{u},\bar{u},0$ ]
3	c	22'2'	$1/2,0,0$ [u,0,0]	$0,1/2,2/3$ [0,u,0]	$1/2,1/2,1/3$ [ $\bar{u},\bar{u},0$ ]
3	b	22'2'	$0,0,1/2$ [u,0,0]	$0,0,1/6$ [0,u,0]	$0,0,5/6$ [ $\bar{u},\bar{u},0$ ]
3	a	22'2'	$0,0,0$ [u,0,0]	$0,0,2/3$ [0,u,0]	$0,0,1/3$ [ $\bar{u},\bar{u},0$ ]

### Symmetry of Special Projections

Along [0,0,1] p6'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,1/6

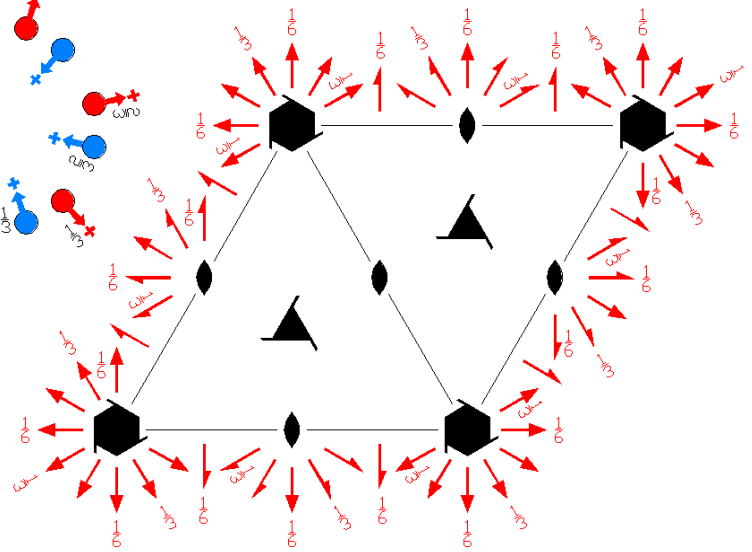
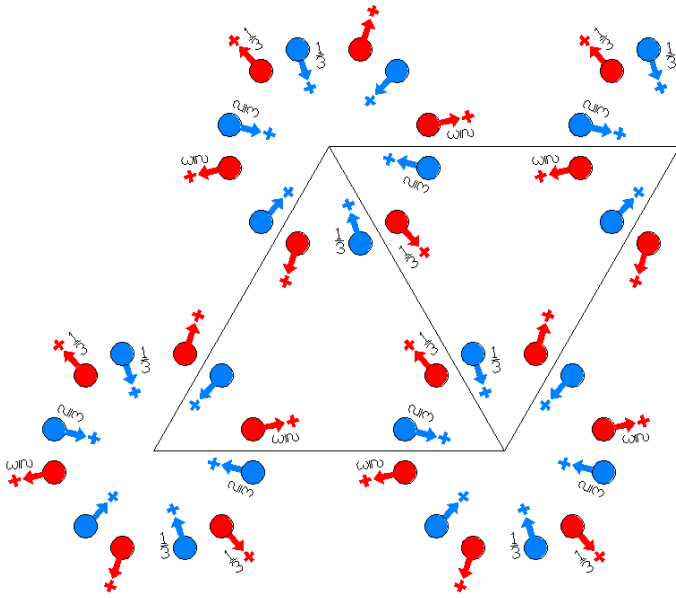
P6<sub>2</sub>2'2'

180.5.1400

62'2'

P6<sub>2</sub>2'2'

Hexagonal



Origin at 2'2'2' at 6<sub>2</sub> (2',1,1) (1,2',1)

<b>Asymmetric unit</b>	$0 \leq x \leq 1;$	$0 \leq y \leq 1;$	$0 \leq z \leq 1/6$	$y \leq x$
Vertices	0,0,0	1,0,0	1,1,0	
	0,0,1/6	1,0,1/6	1,1,1/6	

**Symmetry Operations**

- |   |   |   |
|---|---|---|
| (1) 1<br>(1*0,0,0)                            | (2) 3 <sup>+</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> *0,0,2/3)               | (3) 3 <sup>-</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup> *0,0,1/3) |
| (4) 2 0,0,z<br>(2 <sub>z</sub> *0,0,0)        | (5) 6 <sup>-</sup> (0,0,2/3) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup> *0,0,2/3) | (6) 6 <sup>+</sup> (0,0,1/3) 0,0,z<br>(6 <sub>z</sub> *0,0,1/3)               |
| (7) 2' x,x,1/3<br>(2 <sub>xy</sub> *0,0,2/3)' | (8) 2' x,0,0<br>(2 <sub>x</sub> *0,0,0)'                                      | (9) 2' 0,y,1/6<br>(2 <sub>y</sub> *0,0,1/3)'                                  |
| (10) 2' x,&,1/3<br>(2 <sub>3</sub> *0,0,2/3)' | (11) 2' x,2x,0<br>(2 <sub>2</sub> *0,0,0)'                                    | (12) 2' 2x,x,1/6<br>(2 <sub>1</sub> *0,0,1/3)'                                |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
12	k	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z+2/3$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z+1/3$ [ $\bar{u}+v, \bar{u}, w$ ]
			(4) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(5) $y, \bar{x}+y, z+2/3$ [ $v, \bar{u}+v, w$ ]	(6) $x-y, x, z+1/3$ [ $u-v, u, w$ ]
			(7) $y, x, \bar{z}+2/3$ [ $\bar{v}, \bar{u}, w$ ]	(8) $x-y, \bar{y}, \bar{z}$ [ $\bar{u}+v, v, w$ ]	(9) $\bar{x}, \bar{x}+y, \bar{z}+1/3$ [ $u, u-v, w$ ]
			(10) $\bar{y}, \bar{x}, \bar{z}+2/3$ [ $v, u, w$ ]	(11) $\bar{x}+y, y, \bar{z}$ [ $u-v, \bar{v}, w$ ]	(12) $x, x-y, \bar{z}+1/3$ [ $\bar{u}, \bar{u}+v, w$ ]
6	j	..2'	x, 2x, 1/2 [u, 0, w]	$2\bar{x}, \bar{x}, 1/6$ [0, u, w]	$x, \bar{x}, 5/6$ [ $\bar{u}, \bar{u}, w$ ]
			$\bar{x}, 2\bar{x}, 1/2$ [ $\bar{u}, 0, w$ ]	$2x, x, 1/6$ [0, $\bar{u}, w$ ]	$\bar{x}, x, 5/6$ [u, u, w]
6	i	..2'	x, 2x, 0 [u, 0, w]	$2\bar{x}, \bar{x}, 2/3$ [0, u, w]	$x, \bar{x}, 1/3$ [ $\bar{u}, \bar{u}, w$ ]
			$\bar{x}, 2\bar{x}, 0$ [ $\bar{u}, 0, w$ ]	$2x, x, 2/3$ [0, $\bar{u}, w$ ]	$\bar{x}, x, 1/3$ [u, u, w]
6	h	.2'	x, 0, 1/2 [u, 2u, w]	$0, x, 1/6$ [ $2\bar{u}, \bar{u}, w$ ]	$\bar{x}, \bar{x}, 5/6$ [u, $\bar{u}, w$ ]
			$\bar{x}, 0, 1/2$ [ $\bar{u}, 2\bar{u}, w$ ]	$0, \bar{x}, 1/6$ [2u, u, w]	$x, x, 5/6$ [ $\bar{u}, u, w$ ]
6	g	.2'	x, 0, 0 [u, 2u, w]	$0, x, 2/3$ [ $2\bar{u}, \bar{u}, w$ ]	$\bar{x}, \bar{x}, 1/3$ [u, $\bar{u}, w$ ]
			$\bar{x}, 0, 0$ [ $\bar{u}, 2\bar{u}, w$ ]	$0, \bar{x}, 2/3$ [2u, u, w]	$x, x, 1/3$ [ $\bar{u}, u, w$ ]
6	f	2..	1/2, 0, z [0, 0, w]	$0, 1/2, z+2/3$ [0, 0, w]	$1/2, 1/2, z+1/3$ [0, 0, w]
			$0, 1/2, \bar{z}+2/3$ [0, 0, w]	$1/2, 0, \bar{z}$ [0, 0, w]	$1/2, 1/2, \bar{z}+1/3$ [0, 0, w]
6	e	2..	0, 0, z [0, 0, w]	$0, 0, z+2/3$ [0, 0, w]	$0, 0, z+1/3$ [0, 0, w]
			$0, 0, \bar{z}+2/3$ [0, 0, w]	$0, 0, \bar{z}$ [0, 0, w]	$0, 0, \bar{z}+1/3$ [0, 0, w]
3	d	2'2'2	1/2, 0, 1/2 [0, 0, w]	$0, 1/2, 1/6$ [0, 0, w]	$1/2, 1/2, 5/6$ [0, 0, w]
3	c	2'2'2	1/2, 0, 0 [0, 0, w]	$0, 1/2, 2/3$ [0, 0, w]	$1/2, 1/2, 1/3$ [0, 0, w]
3	b	2'2'2	0, 0, 1/2 [0, 0, w]	$0, 0, 1/6$ [0, 0, w]	$0, 0, 5/6$ [0, 0, w]
3	a	2'2'2	0, 0, 0 [0, 0, w]	$0, 0, 2/3$ [0, 0, w]	$0, 0, 1/3$ [0, 0, w]

### Symmetry of Special Projections

Along [0,0,1] p6mm  
 $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/6

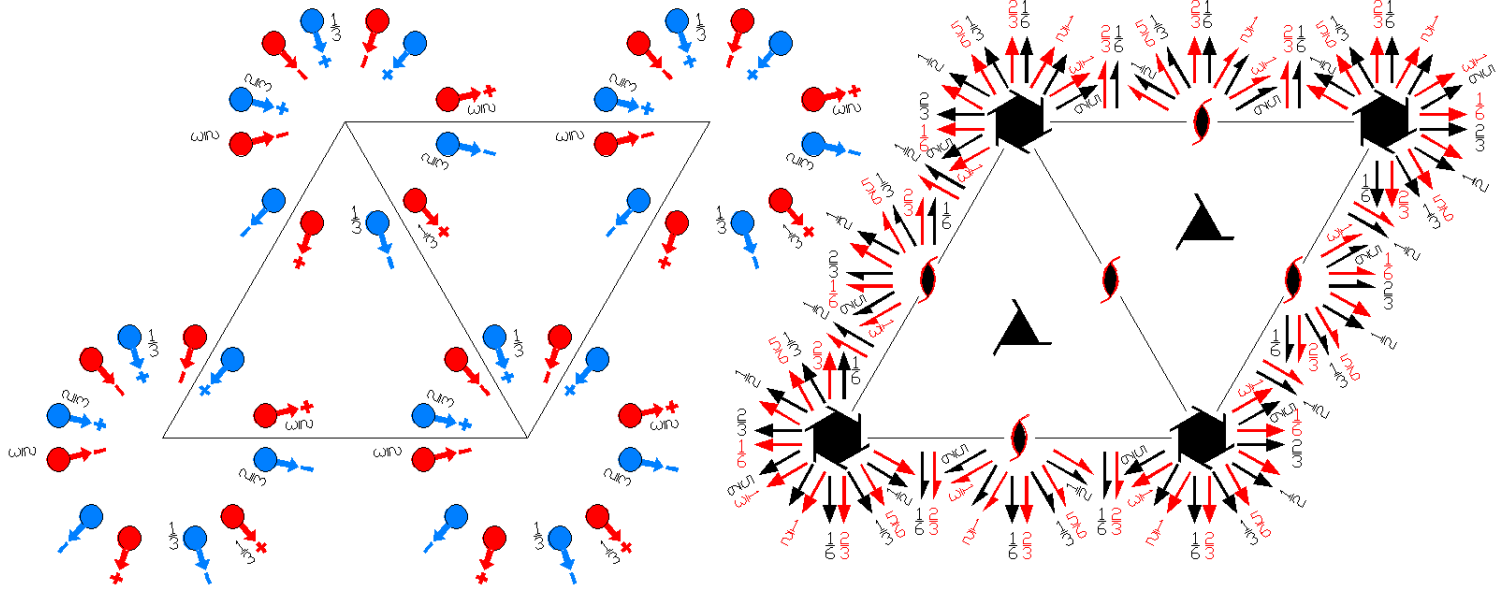
P<sub>2c</sub>6<sub>2</sub>22

6221'

Hexagonal

180.6.1401

P<sub>2c</sub>6<sub>2</sub>22



Origin at 22'2' at 6<sub>2</sub> (2,1,1) (1,2,1)

<b>Asymmetric unit</b>	$0 \leq x \leq 1;$	$0 \leq y \leq 1;$	$0 \leq z \leq 1/6$	$y \leq x$
Vertices	0,0,0 0,0,1/6	1,0,0 1,0,1/6	1,1,0 1,1,1/6	

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |
|---|--|--|
| (1) 1<br>(1*0,0,0)                            | (2) 3 <sup>+</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> *0,0,2/3)                | (3) 3 <sup>-</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup> *0,0,1/3)' |
| (4) 2' 0,0,z<br>(2 <sub>z</sub> *0,0,0)'      | (5) 6 <sup>-</sup> (0,0,2/3) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup> *0,0,2/3)' | (6) 6 <sup>+</sup> (0,0,1/3) 0,0,z<br>(6 <sub>z</sub> *0,0,1/3)                |
| (7) 2 x,x,1/3<br>(2 <sub>xy</sub> *0,0,2/3)   | (8) 2 x,0,0<br>(2 <sub>x</sub> *0,0,0)   | (9) 2' 0,y,1/6<br>(2 <sub>y</sub> *0,0,1/3)'                                   |
| (10) 2' x,&,1/3<br>(2 <sub>3</sub> *0,0,2/3)' | (11) 2' x,2x,0<br>(2 <sub>2</sub> *0,0,0)'                                     | (12) 2 2x,x,1/6<br>(2 <sub>1</sub> *0,0,1/3)                                   |

For (0,0,1)' + set

- |  |   |   |
|--|---|---|
| (1) t' (0,0,1)<br>(1*0,0,0)'                   | (2) 3 <sup>+</sup> (0,0,5/3) 0,0,z<br>(3 <sub>z</sub> *0,0,5/3)'              | (3) 3 <sup>-</sup> (0,0,4/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup> *0,0,4/3) |
| (4) 2 (0,0,1) 0,0,z<br>(2 <sub>z</sub> *0,0,1) | (5) 6 <sup>-</sup> (0,0,5/3) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup> *0,0,5/3) | (6) 6 <sup>+</sup> (0,0,4/3) 0,0,z<br>(6 <sub>z</sub> *0,0,4/3)'              |
| (7) 2' x,x,5/6<br>(2 <sub>xy</sub> *0,0,5/3)'  | (8) 2' x,0,1/2<br>(2 <sub>x</sub> *0,0,1)'                                    | (9) 2 0,y,2/3<br>(2 <sub>y</sub> *0,0,4/3)                                    |
| (10) 2 x,&,5/6<br>(2 <sub>3</sub> *0,0,5/3)    | (11) 2 x,2x,1/2<br>(2 <sub>2</sub> *0,0,1)                                    | (12) 2' 2x,x,2/3<br>(2 <sub>1</sub> *0,0,4/3)'                                |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates		
		(0,0,0) +	(0,0,1)' +
24 k 1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z+2/3$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z+1/3$ [u-v,u, $\bar{w}$ ]
	(4) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(5) $y,\bar{x}+y,z+2/3$ [ $\bar{v},u-v,\bar{w}$ ]	(6) x-y,x,z+1/3 [u-v,u,w]
	(7) $y,x,\bar{z}+2/3$ [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y},\bar{z}$ [u-v, $\bar{v},\bar{w}$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}+1/3$ [u,u-v,w]
	(10) $\bar{y},\bar{x},\bar{z}+2/3$ [v,u,w]	(11) $\bar{x}+y,y,\bar{z}$ [u-v, $\bar{v},w$ ]	(12) x,x-y, $\bar{z}+1/3$ [u,u-v, $\bar{w}$ ]
12 j ..2	x,2x,1/2 [u,2u,0]	$2\bar{x},\bar{x},1/6$ [2u,u,0]	x, $\bar{x},5/6$ [u, $\bar{u},0$ ]
	$\bar{x},2\bar{x},1/2$ [u,2u,0]	2x,x,1/6 [2u,u,0]	$\bar{x},x,5/6$ [u, $\bar{u},0$ ]
12 i ..2'	x,2x,0 [u,0,w]	$2\bar{x},\bar{x},2/3$ [0,u,w]	x, $\bar{x},1/3$ [u,u, $\bar{w}$ ]
	$\bar{x},2\bar{x},0$ [u,0, $\bar{w}$ ]	2x,x,2/3 [0,u, $\bar{w}$ ]	$\bar{x},x,1/3$ [u,u,w]
12 h .2'	x,0,1/2 [u,2u,w]	0,x,1/6 [2u,u, $\bar{w}$ ]	$\bar{x},\bar{x},5/6$ [u,u,w]
	$\bar{x},0,1/2$ [u,2u, $\bar{w}$ ]	0, $\bar{x},1/6$ [2u,u,w]	x,x,5/6 [u,u, $\bar{w}$ ]
12 g .2.	x,0,0 [u,0,0]	0,x,2/3 [0,u,0]	$\bar{x},\bar{x},1/3$ [u,u,0]
	$\bar{x},0,0$ [u,0,0]	0, $\bar{x},2/3$ [0,u,0]	x,x,1/3 [u,u,0]
12 f 2'..	1/2,0,z [u,v,0]	0,1/2,z+2/3 [ $\bar{v},u-v,0$ ]	1/2,1/2,z+1/3 [u-v,u,0]
	0,1/2, $\bar{z}+2/3$ [v,u,0]	1/2,0, $\bar{z}$ [u-v, $\bar{v},0$ ]	1/2,1/2, $\bar{z}+1/3$ [u,u-v,0]
12 e 2'..	0,0,z [u,v,0]	0,0,z+2/3 [ $\bar{v},u-v,0$ ]	0,0,z+1/3 [u-v,u,0]
	0,0, $\bar{z}+2/3$ [v,u,0]	0,0, $\bar{z}$ [u-v, $\bar{v},0$ ]	0,0, $\bar{z}+1/3$ [u,u-v,0]
6 d 2'22'	1/2,0,1/2 [u,2u,0]	0,1/2,1/6 [2 $\bar{u},\bar{u},0$ ]	1/2,1/2,5/6 [u, $\bar{u},0$ ]
6 c 22'2'	1/2,0,0 [u,0,0]	0,1/2,2/3 [0,u,0]	1/2,1/2,1/3 [u,u,0]
6 b 2'22'	0,0,1/2 [u,2u,0]	0,0,1/6 [2 $\bar{u},\bar{u},0$ ]	0,0,5/6 [u, $\bar{u},0$ ]
6 a 22'2'	0,0,0 [u,0,0]	0,0,2/3 [0,u,0]	0,0,1/3 [u,u,0]

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/6

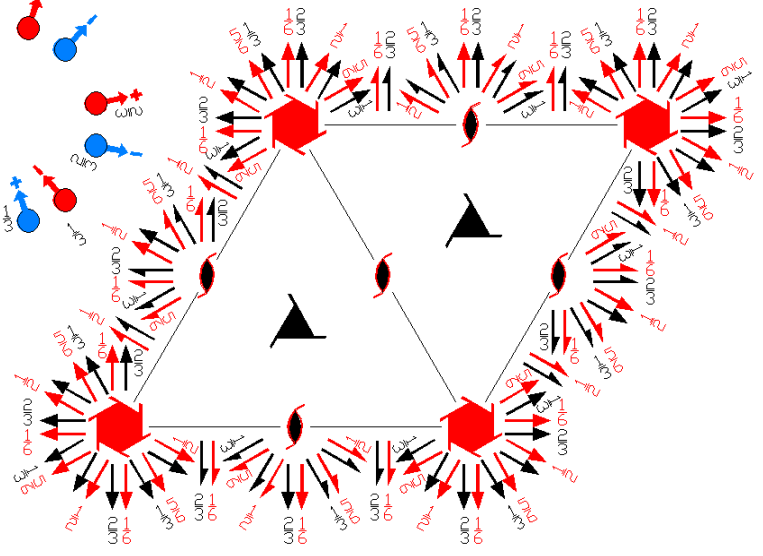
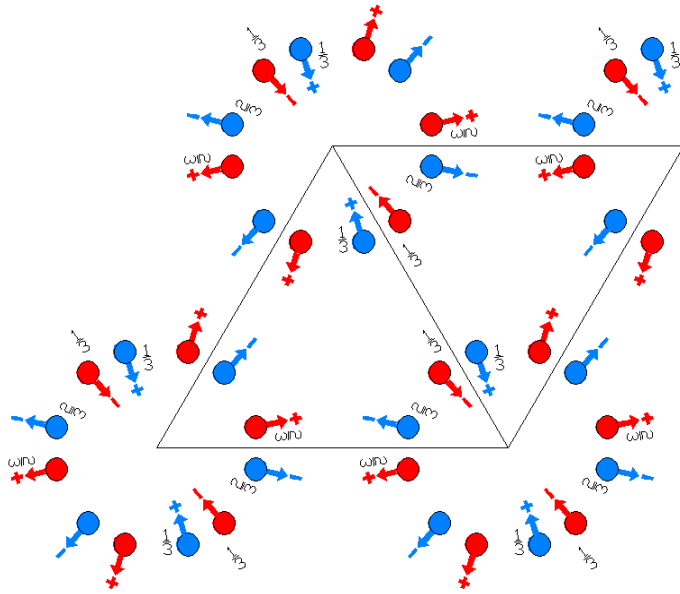
$P_{2c}6_2'22'$

180.7.1402

6221'

$P_{2c}6_2'22'$

Hexagonal



Origin at 222 at  $6_2'$  (2,1,1) (1,2,1)

<b>Asymmetric unit</b>	$0 \leq x \leq 1;$	$0 \leq y \leq 1;$	$0 \leq z \leq 1/6$	$y \leq x$
Vertices	0,0,0 0,0,1/6	1,0,0 1,0,1/6	1,1,0 1,1,1/6	

**Symmetry Operations**

For (0,0,0) + set

- |  |   |  |
|--|---|--|
| (1) 1<br>(1*0,0,0)                     | (2) $3^+$ (0,0,2/3) 0,0,z<br>( $3_z^*$ 0,0,2/3)     | (3) $3^-$ (0,0,1/3) 0,0,z<br>( $3_z^{-1}$ *0,0,1/3)' |
| (4) 2 0,0,z<br>( $2_z^*$ 0,0,0)        | (5) $6^-$ (0,0,2/3) 0,0,z<br>( $6_z^{-1}$ *0,0,2/3) | (6) $6^+$ (0,0,1/3) 0,0,z<br>( $6_z^*$ 0,0,1/3)'     |
| (7) 2 x,x,1/3<br>( $2_{xy}^*$ 0,0,2/3) | (8) 2 x,0,0<br>( $2_x^*$ 0,0,0)                     | (9) $2'$ 0,y,1/6<br>( $2_y^*$ 0,0,1/3)'              |
| (10) 2 x,&,1/3<br>( $2_3^*$ 0,0,2/3)   | (11) 2 x,2x,0<br>( $2_2^*$ 0,0,0)                   | (12) $2'$ 2x,x,1/6<br>( $2_1^*$ 0,0,1/3)'            |

For (0,0,1)' + set

- |   |  |   |
|---|--|---|
| (1) $t'$ (0,0,1)<br>(1*0,0,0)'              | (2) $3^+$ (0,0,5/3) 0,0,z<br>( $3_z^*$ 0,0,5/3)'     | (3) $3^-$ (0,0,4/3) 0,0,z<br>( $3_z^{-1}$ *0,0,4/3) |
| (4) $2'$ (0,0,1) 0,0,z<br>( $2_z^*$ 0,0,1)' | (5) $6^-$ (0,0,5/3) 0,0,z<br>( $6_z^{-1}$ *0,0,5/3)' | (6) $6^+$ (0,0,4/3) 0,0,z<br>( $6_z^*$ 0,0,4/3)     |
| (7) $2'$ x,x,5/6<br>( $2_{xy}^*$ 0,0,5/3)'  | (8) $2'$ x,0,1/2<br>( $2_x^*$ 0,0,1)'                | (9) 2 0,y,2/3<br>( $2_y^*$ 0,0,4/3)                 |
| (10) $2'$ x,&,5/6<br>( $2_3^*$ 0,0,5/3)'    | (11) $2'$ x,2x,1/2<br>( $2_2^*$ 0,0,1)'              | (12) 2 2x,x,2/3<br>( $2_1^*$ 0,0,4/3)               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

**Positions**

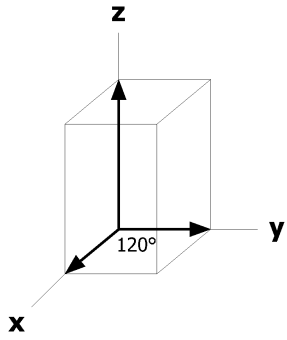
Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates		
		(0,0,0) +	(0,0,1)' +
24 k 1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z+2/3$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z+1/3$ [u-v,u, $\bar{w}$ ]
	(4) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(5) $y,\bar{x}+y,z+2/3$ [v, $\bar{u}+v,w$ ]	(6) x-y,x,z+1/3 [ $\bar{u}+v,\bar{u},\bar{w}$ ]
	(7) $y,x,\bar{z}+2/3$ [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y},\bar{z}$ [u-v, $\bar{v},\bar{w}$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}+1/3$ [u,u-v,w]
	(10) $\bar{y},\bar{x},\bar{z}+2/3$ [ $\bar{v},\bar{u},\bar{w}$ ]	(11) $\bar{x}+y,y,\bar{z}$ [ $\bar{u}+v,v,\bar{w}$ ]	(12) x,x-y, $\bar{z}+1/3$ [ $\bar{u},\bar{u}+v,w$ ]
12 j ..2'	x,2x,1/2 [u,0,w]	$2\bar{x},\bar{x},1/6$ [0, $\bar{u},\bar{w}$ ]	x, $\bar{x},5/6$ [ $\bar{u},\bar{u},w$ ]
	$\bar{x},2\bar{x},1/2$ [ $\bar{u},0,w$ ]	2x,x,1/6 [0,u, $\bar{w}$ ]	$\bar{x},x,5/6$ [u,u,w]
12 i ..2	x,2x,0 [u,2u,0]	$2\bar{x},\bar{x},2/3$ [2 $\bar{u},\bar{u},0$ ]	x, $\bar{x},1/3$ [ $\bar{u},u,0$ ]
	$\bar{x},2\bar{x},0$ [ $\bar{u},2\bar{u},0$ ]	2x,x,2/3 [2u,u,0]	$\bar{x},x,1/3$ [u, $\bar{u},0$ ]
12 h .2'	x,0,1/2 [u,2u,w]	0,x,1/6 [2u,u, $\bar{w}$ ]	$\bar{x},\bar{x},5/6$ [u, $\bar{u},w$ ]
	$\bar{x},0,1/2$ [ $\bar{u},2\bar{u},w$ ]	0, $\bar{x},1/6$ [2 $\bar{u},\bar{u},w$ ]	x,x,5/6 [ $\bar{u},u,w$ ]
12 g .2.	x,0,0 [u,0,0]	0,x,2/3 [0,u,0]	$\bar{x},\bar{x},1/3$ [u,u,0]
	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0, $\bar{x},2/3$ [0, $\bar{u},0$ ]	x,x,1/3 [ $\bar{u},\bar{u},0$ ]
12 f 2..	1/2,0,z [0,0,w]	0,1/2,z+2/3 [0,0,w]	1/2,1/2,z+1/3 [0,0, $\bar{w}$ ]
	0,1/2, $\bar{z}+2/3$ [0,0,w]	1/2,0, $\bar{z}$ [0,0,w]	1/2,1/2, $\bar{z}+1/3$ [0,0, $\bar{w}$ ]
12 e 2..	0,0,z [0,0,w]	0,0,z+2/3 [0,0,w]	0,0,z+1/3 [0,0, $\bar{w}$ ]
	0,0, $\bar{z}+2/3$ [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/3$ [0,0, $\bar{w}$ ]
6 d 2'2'2	1/2,0,1/2 [0,0,w]	0,1/2,1/6 [0,0, $\bar{w}$ ]	1/2,1/2,5/6 [0,0,w]
6 c 222	1/2,0,0 [0,0,0]	0,1/2,2/3 [0,0,0]	1/2,1/2,1/3 [0,0,0]
6 b 2'2'2	0,0,1/2 [0,0,w]	0,0,1/6 [0,0, $\bar{w}$ ]	0,0,5/6 [0,0,w]
6 a 222	0,0,0 [0,0,0]	0,0,2/3 [0,0,0]	0,0,1/3 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,2/3



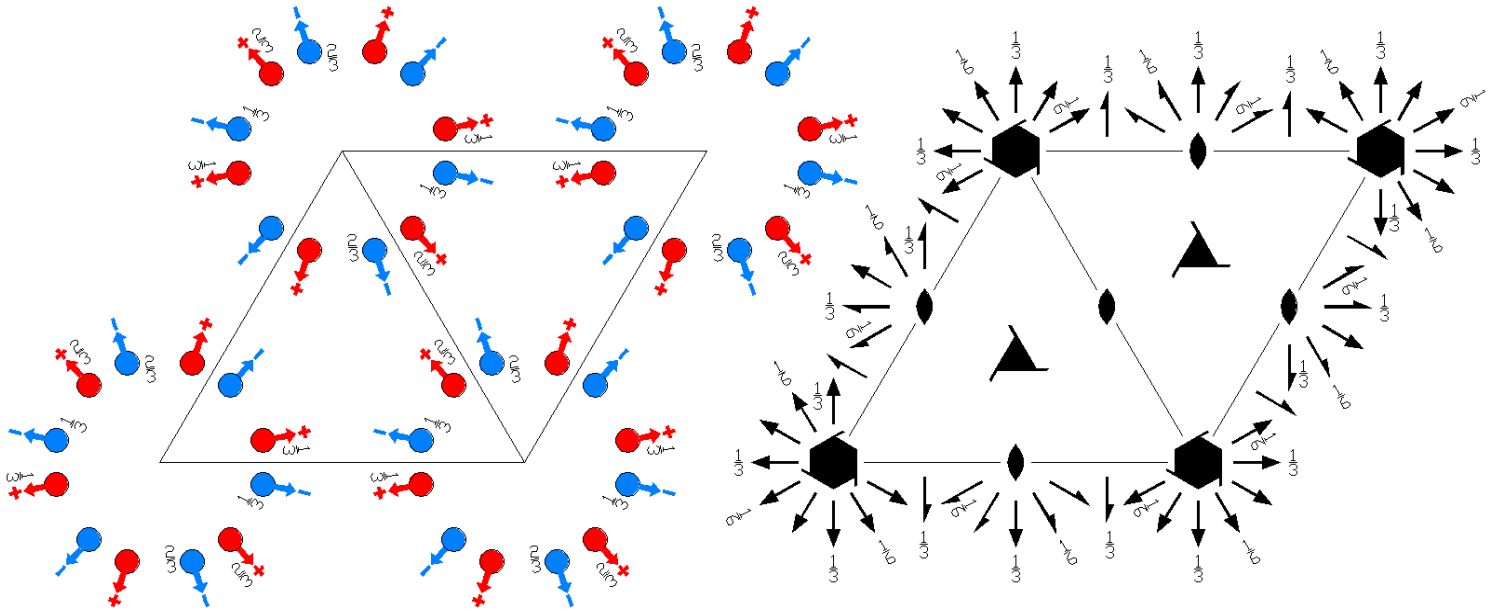
P6<sub>4</sub>22

622

Hexagonal

181.1.1403

P6<sub>4</sub>22



Origin at 222 at 6<sub>4</sub> (2,1,1) (1,2,1)

**Asymmetric unit**     $0 \leq x \leq 1$ ;     $0 \leq y \leq 1$ ;     $0 \leq z \leq 1/6$      $y \leq x$

Vertices             $0,0,0$              $1,0,0$              $1,1,0$   
                           $0,0,1/6$            $1,0,1/6$            $1,1,1/6$

**Symmetry Operations**

- |  |  |  |
|--|--|--|
| (1) 1<br>(1 0,0,0)                           | (2) 3 <sup>+</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub> <sup>+</sup>  0,0,1/3) | (3) 3 <sup>-</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> <sup>-</sup>  0,0,2/3) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)       | (5) 6 <sup>-</sup> (0,0,1/3) 0,0,z<br>(6 <sub>z</sub> <sup>-</sup>  0,0,1/3) | (6) 6 <sup>+</sup> (0,0,2/3) 0,0,z<br>(6 <sub>z</sub> <sup>+</sup>  0,0,2/3) |
| (7) 2 x,x,1/6<br>(2 <sub>xy</sub>  0,0,1/3)  | (8) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                                       | (9) 2 0,y,1/3<br>(2 <sub>y</sub>  0,0,2/3)                                   |
| (10) 2 x,x̄,1/6<br>(2 <sub>3</sub>  0,0,1/3) | (11) 2 x,2x,0<br>(2 <sub>2</sub>  0,0,0)                                     | (12) 2 2x,x,1/3<br>(2 <sub>1</sub>  0,0,2/3)                                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

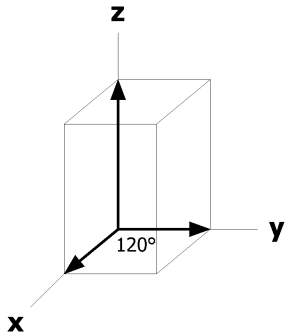
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	k	1	(1) x,y,z [u,v,w] (4) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (7) y,x, $\bar{z}+1/3$ [v,u, $\bar{w}$ ] (10) $\bar{y},\bar{x},\bar{z}+1/3$ [ $\bar{v},\bar{u},\bar{w}$ ]	(2) $\bar{y},x-y,z+1/3$ [ $\bar{v},u-v,w$ ] (5) y, $\bar{x}+y,z+1/3$ [v, $\bar{u}+v,w$ ] (8) x-y, $\bar{y},\bar{z}$ [u-v, $\bar{v},\bar{w}$ ] (11) $\bar{x}+y,y,\bar{z}$ [ $\bar{u}+v,v,\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z+2/3$ [ $\bar{u}+v,\bar{u},w$ ] (6) x-y,x,z+2/3 [u-v,u,w] (9) $\bar{x},\bar{x}+y,\bar{z}+2/3$ [ $\bar{u},\bar{u}+v,\bar{w}$ ] (12) x,x-y, $\bar{z}+2/3$ [u,u-v, $\bar{w}$ ]
6	j	..2	x,2x,1/2 [u,2u,0] $\bar{x},2\bar{x},1/2$ [ $\bar{u},2\bar{u},0$ ]	$2\bar{x},\bar{x},5/6$ [ $2\bar{u},\bar{u},0$ ] 2x,x,5/6 [2u,u,0]	x, $\bar{x},1/6$ [u, $\bar{u},0$ ] $\bar{x},x,1/6$ [ $\bar{u},u,0$ ]
6	i	..2	x,2x,0 [u,2u,0] $\bar{x},2\bar{x},0$ [ $\bar{u},2\bar{u},0$ ]	$2\bar{x},\bar{x},1/3$ [ $2\bar{u},\bar{u},0$ ] 2x,x,1/3 [2u,u,0]	x, $\bar{x},2/3$ [u, $\bar{u},0$ ] $\bar{x},x,2/3$ [ $\bar{u},u,0$ ]
6	h	.2.	x,0,1/2 [u,0,0] $\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	0,x,5/6 [0,u,0] 0, $\bar{x},5/6$ [0, $\bar{u},0$ ]	$\bar{x},x,1/6$ [ $\bar{u},\bar{u},0$ ] x,x,1/6 [u,u,0]
6	g	.2.	x,0,0 [u,0,0] $\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,1/3 [0,u,0] 0, $\bar{x},1/3$ [0, $\bar{u},0$ ]	$\bar{x},x,2/3$ [ $\bar{u},\bar{u},0$ ] x,x,2/3 [u,u,0]
6	f	2..	1/2,0,z [0,0,w] 0,1/2, $\bar{z}+1/3$ [0,0, $\bar{w}$ ]	0,1/2,z+1/3 [0,0,w] 1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ]	1/2,1/2,z+2/3 [0,0,w] 1/2,1/2, $\bar{z}+2/3$ [0,0, $\bar{w}$ ]
6	e	2..	0,0,z [0,0,w] 0,0, $\bar{z}+1/3$ [0,0, $\bar{w}$ ]	0,0,z+1/3 [0,0,w] 0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+2/3 [0,0,w] 0,0, $\bar{z}+2/3$ [0,0, $\bar{w}$ ]
3	d	222	1/2,0,1/2 [0,0,0]	0,1/2,5/6 [0,0,0]	1/2,1/2,1/6 [0,0,0]
3	c	222	1/2,0,0 [0,0,0]	0,1/2,1/3 [0,0,0]	1/2,1/2,2/3 [0,0,0]
3	b	222	0,0,1/2 [0,0,0]	0,0,5/6 [0,0,0]	0,0,1/6 [0,0,0]
3	a	222	0,0,0 [0,0,0]	0,0,1/3 [0,0,0]	0,0,2/3 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p6m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/3



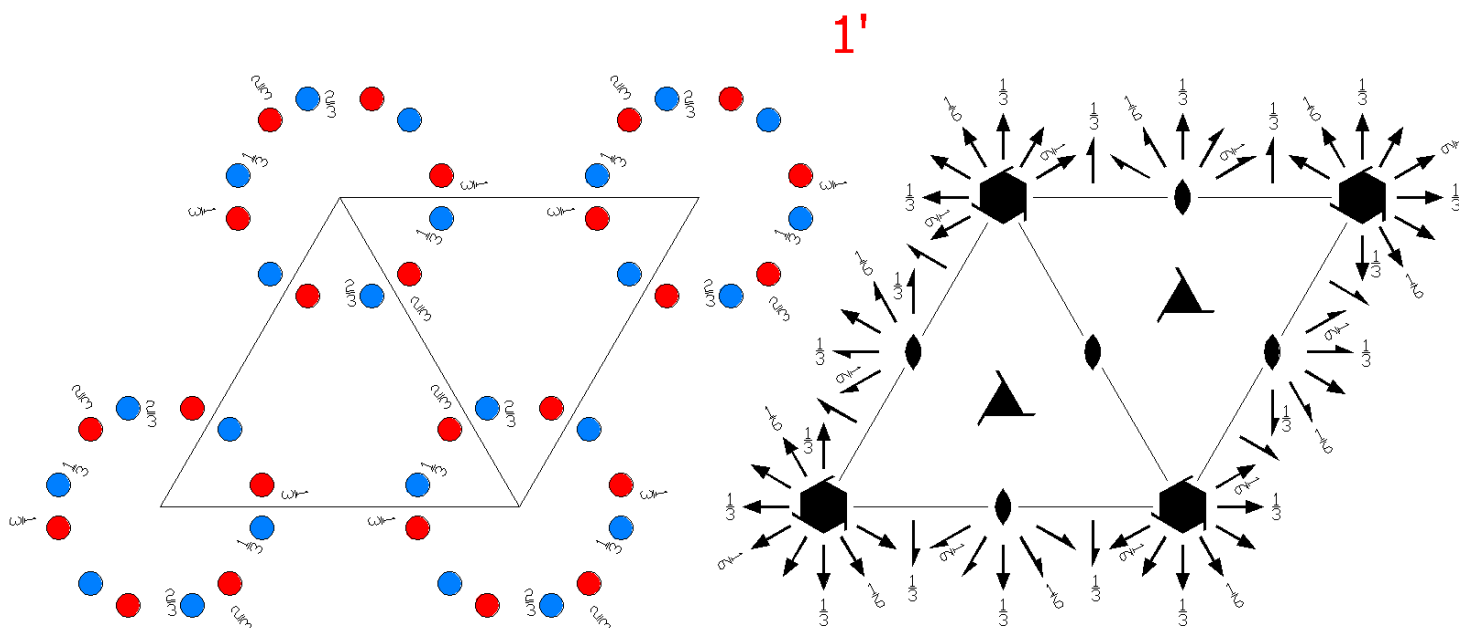
$P6_4 221'$

181.2.1404

$6221'$

$P6_4 221'$

Hexagonal



Origin at  $2221'$  at  $6_4 (2,1,1) (1,2,1)1'$

Asymmetric unit  $0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/6 \quad y \leq x$

Vertices	0,0,0	1,0,0	1,1,0
	0,0,1/6	1,0,1/6	1,1,1/6

**Symmetry Operations**

For 1 + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                          | (2) $3^+ (0,0,1/3) \ 0,0,z$<br>( $3_z$  0,0,1/3)      | (3) $3^- (0,0,2/3) \ 0,0,z$<br>( $3_z^{-1}$  0,0,2/3) |
| (4) 2 $0,0,z$<br>( $2_z$  0,0,0)            | (5) $6^- (0,0,1/3) \ 0,0,z$<br>( $6_z^{-1}$  0,0,1/3) | (6) $6^+ (0,0,2/3) \ 0,0,z$<br>( $6_z$  0,0,2/3)      |
| (7) 2 $x,x,1/6$<br>( $2_{xy}$  0,0,1/3)     | (8) 2 $x,0,0$<br>( $2_x$  0,0,0)                      | (9) 2 $0,y,1/3$<br>( $2_y$  0,0,2/3)                  |
| (10) 2 $x,\bar{x},1/6$<br>( $2_3$  0,0,1/3) | (11) 2 $x,2x,0$<br>( $2_2$  0,0,0)                    | (12) 2 $2x,x,1/3$<br>( $2_1$  0,0,2/3)                |



## For 1' + set

(1) 1' (1 0,0,0)'	(2) 3 <sup>+</sup> ' (0,0,1/3) 0,0,z (3 <sub>z</sub>  0,0,1/3)'	(3) 3 <sup>-</sup> ' (0,0,2/3) 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,2/3)'
(4) 2' (2 <sub>z</sub>  0,0,0)'	(5) 6 <sup>-</sup> ' (0,0,1/3) 0,0,z (6 <sub>z</sub> <sup>-1</sup>  0,0,1/3)'	(6) 6 <sup>+</sup> ' (0,0,2/3) 0,0,z (6 <sub>z</sub>  0,0,2/3)'
(7) 2' (2 <sub>xy</sub>  0,0,1/3)'	(8) 2' (2 <sub>x</sub>  0,0,0)'	(9) 2' (2 <sub>y</sub>  0,0,2/3)'
(10) 2' (2 <sub>3</sub>  0,0,1/3)'	(11) 2' (2 <sub>2</sub>  0,0,0)'	(12) 2' (2 <sub>1</sub>  0,0,2/3)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

**Positions**

			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			1 +	1' +	
12	k	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z+1/3 [0,0,0]	(3) $\bar{x}+y$ , $\bar{x}$ ,z+2/3 [0,0,0]
			(4) $\bar{x}$ , $\bar{y}$ ,z [0,0,0]	(5) y, $\bar{x}+y$ ,z+1/3 [0,0,0]	(6) x-y,x,z+2/3 [0,0,0]
			(7) y,x, $\bar{z}+1/3$ [0,0,0]	(8) x-y, $\bar{y}$ , $\bar{z}$ [0,0,0]	(9) $\bar{x}$ , $\bar{x}+y$ , $\bar{z}+2/3$ [0,0,0]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}+1/3$ [0,0,0]	(11) $\bar{x}+y$ ,y, $\bar{z}$ [0,0,0]	(12) x,x-y, $\bar{z}+2/3$ [0,0,0]
6	j	..21'	x,2x,1/2 [0,0,0]	2 $\bar{x}$ , $\bar{x}$ ,5/6 [0,0,0]	x, $\bar{x}$ ,1/6 [0,0,0]
			$\bar{x}$ ,2 $\bar{x}$ ,1/2 [0,0,0]	2x,x,5/6 [0,0,0]	$\bar{x}$ ,x,1/6 [0,0,0]
6	i	..21'	x,2x,0 [0,0,0]	2 $\bar{x}$ , $\bar{x}$ ,1/3 [0,0,0]	x, $\bar{x}$ ,2/3 [0,0,0]
			$\bar{x}$ ,2 $\bar{x}$ ,0 [0,0,0]	2x,x,1/3 [0,0,0]	$\bar{x}$ ,x,2/3 [0,0,0]
6	h	.2.1'	x,0,1/2 [0,0,0]	0,x,5/6 [0,0,0]	$\bar{x}$ , $\bar{x}$ ,1/6 [0,0,0]
			$\bar{x}$ ,0,1/2 [0,0,0]	0, $\bar{x}$ ,5/6 [0,0,0]	x,x,1/6 [0,0,0]
6	g	.2.1'	x,0,0 [0,0,0]	0,x,1/3 [0,0,0]	$\bar{x}$ , $\bar{x}$ ,2/3 [0,0,0]
			$\bar{x}$ ,0,0 [0,0,0]	0, $\bar{x}$ ,1/3 [0,0,0]	x,x,2/3 [0,0,0]
6	f	2..1'	1/2,0,z [0,0,0]	0,1/2,z+1/3 [0,0,0]	1/2,1/2,z+2/3 [0,0,0]
			0,1/2, $\bar{z}+1/3$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}+2/3$ [0,0,0]
6	e	2..1'	0,0,z [0,0,0]	0,0,z+1/3 [0,0,0]	0,0,z+2/3 [0,0,0]
			0,0, $\bar{z}+1/3$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0, $\bar{z}+2/3$ [0,0,0]
3	d	2221'	1/2,0,1/2 [0,0,0]	0,1/2,5/6 [0,0,0]	1/2,1/2,1/6 [0,0,0]

Continued

181.2.1404

P6<sub>4</sub>221'

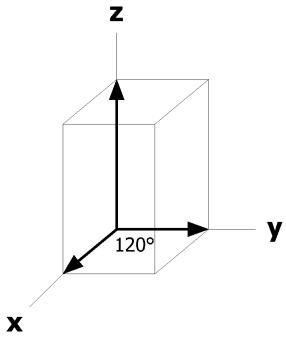
3	c	2221'	1/2,0,0 [0,0,0]	0,1/2,1/3 [0,0,0]	1/2,1/2,2/3 [0,0,0]
3	b	2221'	0,0,1/2 [0,0,0]	0,0,5/6 [0,0,0]	0,0,1/6 [0,0,0]
3	a	2221'	0,0,0 [0,0,0]	0,0,1/3 [0,0,0]	0,0,2/3 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,0

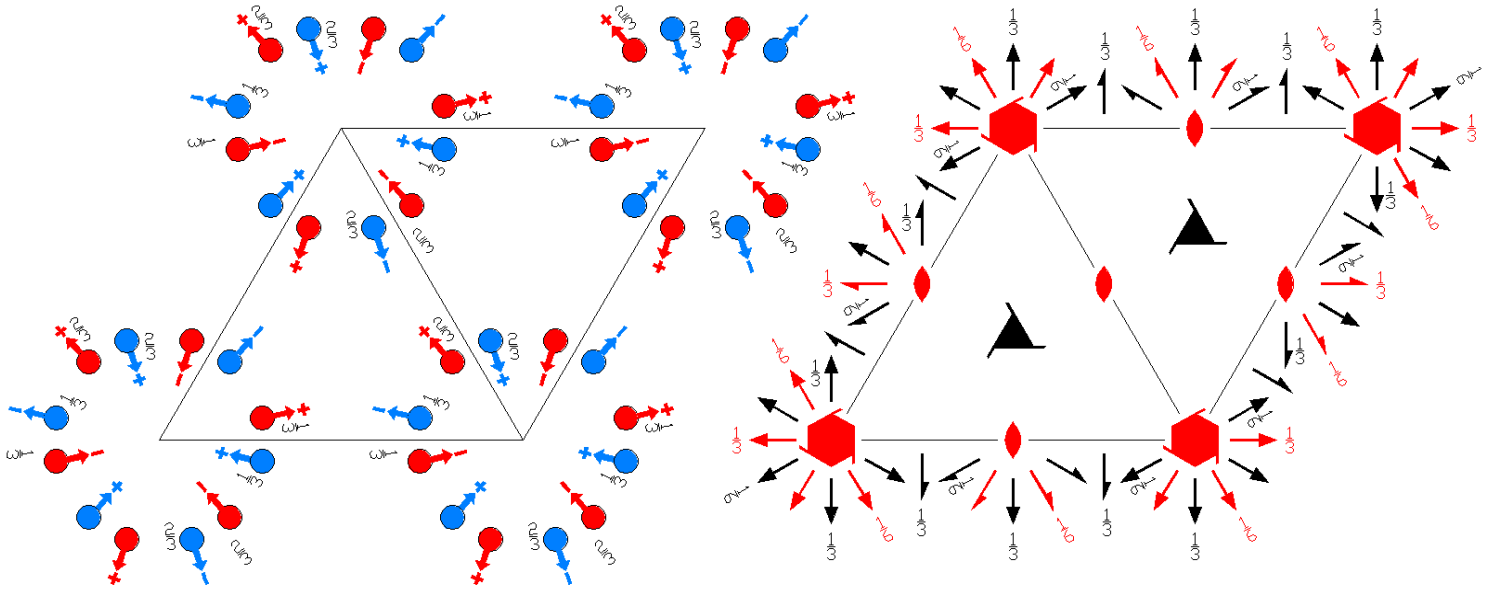
Along [2,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,x/2,1/3



$P6_4'2'2'$   
181.3.1405

$6'2'2'$   
 $P6_4'2'2'$

Hexagonal



Origin at  $2'2'2'$  at  $6_4'$  ( $2',1,1$ ) ( $1,2,1$ )

**Asymmetric unit**  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$   $y \leq x$

Vertices  $0,0,0$   $1,0,0$   $1,1,0$   
 $0,0,1/6$   $1,0,1/6$   $1,1,1/6$

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                              | (2) $3^+$ (0,0,1/3) 0,0,z<br>( $3_z$  0,0,1/3)       | (3) $3^-$ (0,0,2/3) 0,0,z<br>( $3_z^{-1}$  0,0,2/3) |
| (4) $2'$ 0,0,z<br>( $2_z$  0,0,0)'              | (5) $6^-$ (0,0,1/3) 0,0,z<br>( $6_z^{-1}$  0,0,1/3)' | (6) $6^+$ (0,0,2/3) 0,0,z<br>( $6_z$  0,0,2/3)'     |
| (7) $2'$ x,x,1/6<br>( $2_{xy}$  0,0,1/3)'       | (8) $2'$ x,0,0<br>( $2_x$  0,0,0)'                   | (9) $2'$ 0,y,1/3<br>( $2_y$  0,0,2/3)'              |
| (10) $2$ x, $\bar{x}$ ,1/6<br>( $2_3$  0,0,1/3) | (11) $2$ x,2x,0<br>( $2_2$  0,0,0)                   | (12) $2$ 2x,x,1/3<br>( $2_1$  0,0,2/3)              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

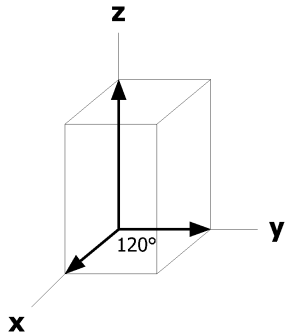
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	k	1	(1) x,y,z [u,v,w] (4) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (7) y,x, $\bar{z}+1/3$ [ $\bar{v},\bar{u},w$ ] (10) $\bar{y},\bar{x},\bar{z}+1/3$ [ $\bar{v},\bar{u},\bar{w}$ ]	(2) $\bar{y},x-y,z+1/3$ [ $\bar{v},u-v,w$ ] (5) y, $\bar{x}+y,z+1/3$ [ $\bar{v},u-v,\bar{w}$ ] (8) x-y, $\bar{y},\bar{z}$ [ $\bar{u}+v,v,w$ ] (11) $\bar{x}+y,y,\bar{z}$ [ $\bar{u}+v,v,\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z+2/3$ [ $\bar{u}+v,\bar{u},w$ ] (6) x-y,x,z+2/3 [ $\bar{u}+v,\bar{u},\bar{w}$ ] (9) $\bar{x},\bar{x}+y,\bar{z}+2/3$ [u,u-v,w] (12) x,x-y, $\bar{z}+2/3$ [u,u-v, $\bar{w}$ ]
6	j	..2	x,2x,1/2 [u,2u,0] $\bar{x},2\bar{x},1/2$ [u,2u,0]	$2\bar{x},\bar{x},5/6$ [ $2\bar{u},\bar{u},0$ ] 2x,x,5/6 [ $2\bar{u},\bar{u},0$ ]	x, $\bar{x},1/6$ [u, $\bar{u},0$ ] $\bar{x},x,1/6$ [u, $\bar{u},0$ ]
6	i	..2	x,2x,0 [u,2u,0] $\bar{x},2\bar{x},0$ [u,2u,0]	$2\bar{x},\bar{x},1/3$ [ $2\bar{u},\bar{u},0$ ] 2x,x,1/3 [ $2\bar{u},\bar{u},0$ ]	x, $\bar{x},2/3$ [u, $\bar{u},0$ ] $\bar{x},x,2/3$ [u, $\bar{u},0$ ]
6	h	.2'	x,0,1/2 [u,2u,w] $\bar{x},0,1/2$ [u,2u, $\bar{w}$ ]	0,x,5/6 [ $2\bar{u},\bar{u},w$ ] 0, $\bar{x},5/6$ [ $2\bar{u},\bar{u},\bar{w}$ ]	$\bar{x},\bar{x},1/6$ [u, $\bar{u},w$ ] x,x,1/6 [u, $\bar{u},\bar{w}$ ]
6	g	.2'	x,0,0 [u,2u,w] $\bar{x},0,0$ [u,2u, $\bar{w}$ ]	0,x,1/3 [ $2\bar{u},\bar{u},w$ ] 0, $\bar{x},1/3$ [ $2\bar{u},\bar{u},\bar{w}$ ]	$\bar{x},\bar{x},2/3$ [u, $\bar{u},w$ ] x,x,2/3 [u, $\bar{u},\bar{w}$ ]
6	f	2'..	1/2,0,z [u,v,0] 0,1/2, $\bar{z}+1/3$ [ $\bar{v},\bar{u},0$ ]	0,1/2,z+1/3 [ $\bar{v},u-v,0$ ] 1/2,0, $\bar{z}$ [ $\bar{u}+v,v,0$ ]	1/2,1/2,z+2/3 [ $\bar{u}+v,\bar{u},0$ ] 1/2,1/2, $\bar{z}+2/3$ [u,u-v,0]
6	e	2'..	0,0,z [u,v,0] 0,0, $\bar{z}+1/3$ [ $\bar{v},\bar{u},0$ ]	0,0,z+1/3 [ $\bar{v},u-v,0$ ] 0,0, $\bar{z}$ [ $\bar{u}+v,v,0$ ]	0,0,z+2/3 [ $\bar{u}+v,\bar{u},0$ ] 0,0, $\bar{z}+2/3$ [u,u-v,0]
3	d	2'2'2	1/2,0,1/2 [u,2u,0]	0,1/2,5/6 [ $2\bar{u},\bar{u},0$ ]	1/2,1/2,1/6 [u, $\bar{u},0$ ]
3	c	2'2'2	1/2,0,0 [u,2u,0]	0,1/2,1/3 [ $2\bar{u},\bar{u},0$ ]	1/2,1/2,2/3 [u, $\bar{u},0$ ]
3	b	2'2'2	0,0,1/2 [u,2u,0]	0,0,5/6 [ $2\bar{u},\bar{u},0$ ]	0,0,1/6 [u, $\bar{u},0$ ]
3	a	2'2'2	0,0,0 [u,2u,0]	0,0,1/3 [ $2\bar{u},\bar{u},0$ ]	0,0,2/3 [u, $\bar{u},0$ ]

**Symmetry of Special Projections**

Along [0,0,1] p6m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/3



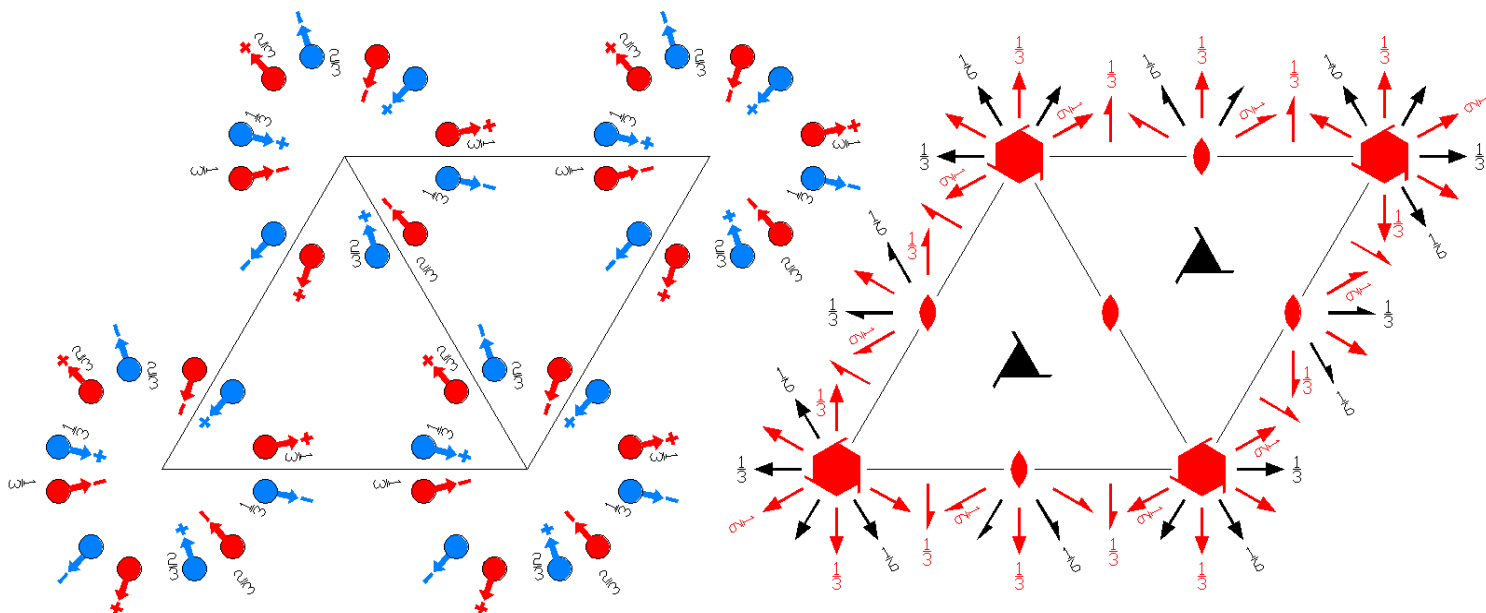
$P6_4'22'$

181.4.1406

$6'22'$

$P6_4'22'$

Hexagonal



Origin at  $22'2'$  at  $6_4'$   $(2,1,1)$   $(1,2',1)$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$   $y \leq x$

Vertices	$0,0,0$	$1,0,0$	$1,1,0$
	$0,0,1/6$	$1,0,1/6$	$1,1,1/6$

### Symmetry Operations

- |   |   |  |
|---|---|--|
| (1) 1<br>$(1 0,0,0)$                          | (2) $3^+(0,0,1/3)$ $0,0,z$<br>$(3_z 0,0,1/3)$           | (3) $3^-(0,0,2/3)$ $0,0,z$<br>$(3_z^{-1} 0,0,2/3)$ |
| (4) $2'$ $0,0,z$<br>$(2_z 0,0,0)'$            | (5) $6^-'$ $(0,0,1/3)$ $0,0,z$<br>$(6_z^{-1} 0,0,1/3)'$ | (6) $6^+'$ $(0,0,2/3)$ $0,0,z$<br>$(6_z 0,0,2/3)'$ |
| (7) $2$ $x,x,1/6$<br>$(2_{xy} 0,0,1/3)$       | (8) $2$ $x,0,0$<br>$(2_x 0,0,0)$                        | (9) $2$ $0,y,1/3$<br>$(2_y 0,0,2/3)$               |
| (10) $2'$ $x,\bar{x},1/6$<br>$(2_3 0,0,1/3)'$ | (11) $2'$ $x,2x,0$<br>$(2_2 0,0,0)'$                    | (12) $2'$ $2x,x,1/3$<br>$(2_1 0,0,2/3)'$           |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

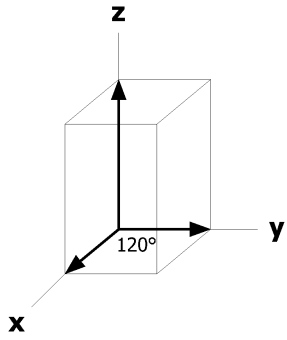
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	k	1	(1) x,y,z [u,v,w] (4) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ] (7) y,x, $\bar{z}+1/3$ [v,u, $\bar{w}$ ] (10) $\bar{y},\bar{x},\bar{z}+1/3$ [v,u,w]	(2) $\bar{y},x-y,z+1/3$ [ $\bar{v},u-v,w$ ] (5) y, $\bar{x}+y,z+1/3$ [ $\bar{v},u-v,\bar{w}$ ] (8) x-y, $\bar{y},\bar{z}$ [u-v, $\bar{v},\bar{w}$ ] (11) $\bar{x}+y,y,\bar{z}$ [u-v, $\bar{v},w$ ]	(3) $\bar{x}+y,\bar{x},z+2/3$ [ $\bar{u}+v,\bar{u},w$ ] (6) x-y,x,z+2/3 [ $\bar{u}+v,\bar{u},\bar{w}$ ] (9) $\bar{x},\bar{x}+y,\bar{z}+2/3$ [ $\bar{u},\bar{u}+v,\bar{w}$ ] (12) x,x-y, $\bar{z}+2/3$ [ $\bar{u},\bar{u}+v,w$ ]
6	j	..2'	x,2x,1/2 [u,0,w] $\bar{x},2\bar{x},1/2$ [u,0, $\bar{w}$ ]	$2\bar{x},\bar{x},5/6$ [0,u,w] 2x,x,5/6 [0,u, $\bar{w}$ ]	x, $\bar{x},1/6$ [ $\bar{u},\bar{u},w$ ] $\bar{x},x,1/6$ [ $\bar{u},\bar{u},\bar{w}$ ]
6	i	..2'	x,2x,0 [u,0,w] $\bar{x},2\bar{x},0$ [u,0, $\bar{w}$ ]	$2\bar{x},\bar{x},1/3$ [0,u,w] 2x,x,1/3 [0,u, $\bar{w}$ ]	x, $\bar{x},2/3$ [ $\bar{u},\bar{u},w$ ] $\bar{x},x,2/3$ [ $\bar{u},\bar{u},\bar{w}$ ]
6	h	.2.	x,0,1/2 [u,0,0] $\bar{x},0,1/2$ [u,0,0]	0,x,5/6 [0,u,0] 0, $\bar{x},5/6$ [0,u,0]	$\bar{x},x,1/6$ [ $\bar{u},\bar{u},0$ ] x,x,1/6 [ $\bar{u},\bar{u},0$ ]
6	g	.2.	x,0,0 [u,0,0] $\bar{x},0,0$ [u,0,0]	0,x,1/3 [0,u,0] 0, $\bar{x},1/3$ [0,u,0]	$\bar{x},x,2/3$ [ $\bar{u},\bar{u},0$ ] x,x,2/3 [ $\bar{u},\bar{u},0$ ]
6	f	2'..	1/2,0,z [u,v,0] 0,1/2, $\bar{z}+1/3$ [v,u,0]	0,1/2,z+1/3 [ $\bar{v},u-v,0$ ] 1/2,0, $\bar{z}$ [u-v, $\bar{v},0$ ]	1/2,1/2,z+2/3 [ $\bar{u}+v,\bar{u},0$ ] 1/2,1/2, $\bar{z}+2/3$ [ $\bar{u},\bar{u}+v,0$ ]
6	e	2'..	0,0,z [u,v,0] 0,0, $\bar{z}+1/3$ [v,u,0]	0,0,z+1/3 [ $\bar{v},u-v,0$ ] 0,0, $\bar{z}$ [u-v, $\bar{v},0$ ]	0,0,z+2/3 [ $\bar{u}+v,\bar{u},0$ ] 0,0, $\bar{z}+2/3$ [ $\bar{u},\bar{u}+v,0$ ]
3	d	2'22'	1/2,0,1/2 [u,0,0]	0,1/2,5/6 [0,u,0]	1/2,1/2,1/6 [ $\bar{u},\bar{u},0$ ]
3	c	2'22'	1/2,0,0 [u,0,0]	0,1/2,1/3 [0,u,0]	1/2,1/2,2/3 [ $\bar{u},\bar{u},0$ ]
3	b	2'22'	0,0,1/2 [u,0,0]	0,0,5/6 [0,u,0]	0,0,1/6 [ $\bar{u},\bar{u},0$ ]
3	a	2'22'	0,0,0 [u,0,0]	0,0,1/3 [0,u,0]	0,0,2/3 [ $\bar{u},\bar{u},0$ ]

**Symmetry of Special Projections**

Along [0,0,1] p6'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,1/3



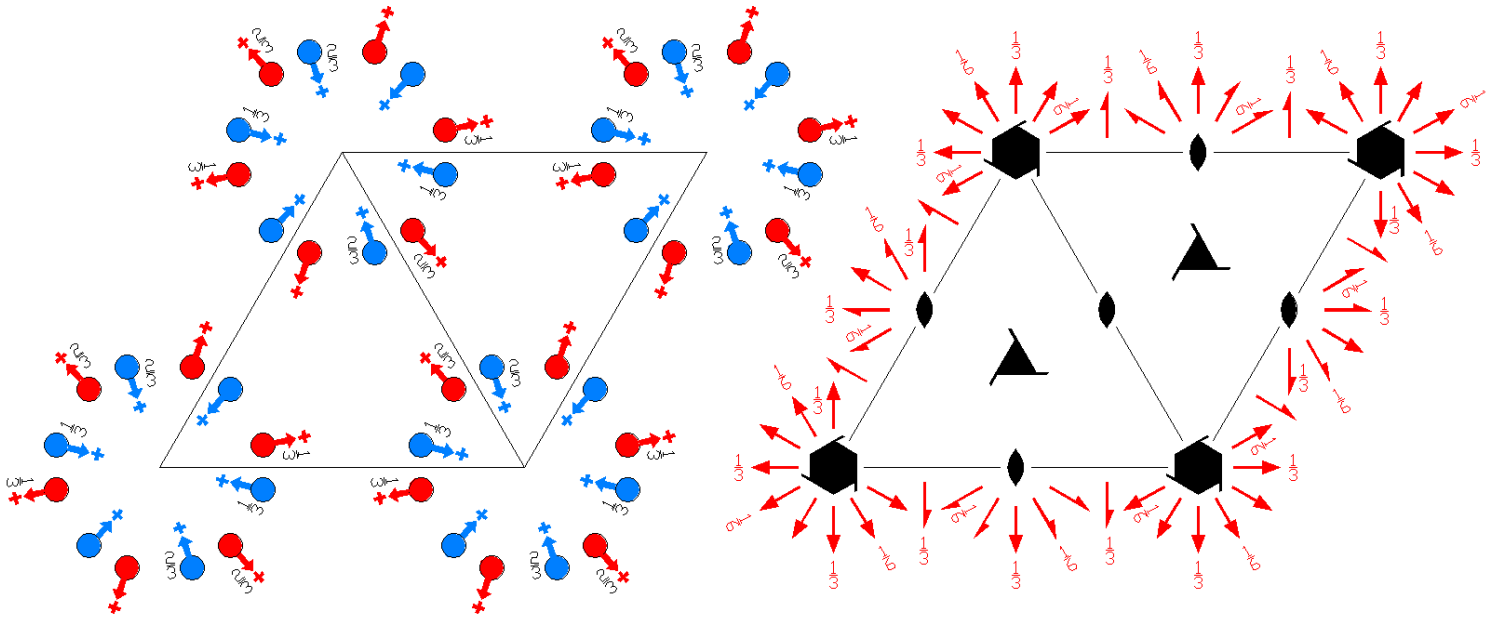
P6<sub>4</sub>2'2'

181.5.1407

62'2'

P6<sub>4</sub>2'2'

Hexagonal



Origin at 2'2'2' at 6<sub>4</sub> (2',1,1) (1,2',1)

<b>Asymmetric unit</b>	$0 \leq x \leq 1;$	$0 \leq y \leq 1;$	$0 \leq z \leq 1/6$	$y \leq x$
Vertices	0,0,0	1,0,0	1,1,0	
	0,0,1/6	1,0,1/6	1,1,1/6	

**Symmetry Operations**

- |   |  |  |
|---|--|--|
| (1) 1<br>(1 0,0,0)                                | (2) 3 <sup>+</sup> (0,0,1/3) 0,0,z<br>(3 <sub>z</sub>   0,0,1/3)               | (3) 3 <sup>-</sup> (0,0,2/3) 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>   0,0,2/3) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>   0,0,0)           | (5) 6 <sup>-</sup> (0,0,1/3) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>   0,0,1/3) | (6) 6 <sup>+</sup> (0,0,2/3) 0,0,z<br>(6 <sub>z</sub>   0,0,2/3)               |
| (7) 2' x,x,1/6<br>(2 <sub>xy</sub>   0,0,1/3)'    | (8) 2' x,0,0<br>(2 <sub>x</sub>   0,0,0)'                                      | (9) 2' 0,y,1/3<br>(2 <sub>y</sub>   0,0,2/3)'                                  |
| (10) 2' x, x̄, 1/6<br>(2 <sub>3</sub>   0,0,1/3)' | (11) 2' x,2x,0<br>(2 <sub>2</sub>   0,0,0)'                                    | (12) 2' 2x,x,1/3<br>(2 <sub>1</sub>   0,0,2/3)'                                |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	k	1	(1) x,y,z [u,v,w] (4) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ] (7) y,x, $\bar{z}+1/3$ [ $\bar{v},\bar{u},w$ ] (10) $\bar{y},\bar{x},\bar{z}+1/3$ [v,u,w]	(2) $\bar{y},x-y,z+1/3$ [ $\bar{v},u-v,w$ ] (5) y, $\bar{x}+y,z+1/3$ [v, $\bar{u}+v,w$ ] (8) x-y, $\bar{y},\bar{z}$ [ $\bar{u}+v,v,w$ ] (11) $\bar{x}+y,y,\bar{z}$ [u-v, $\bar{v},w$ ]	(3) $\bar{x}+y,\bar{x},z+2/3$ [ $\bar{u}+v,\bar{u},w$ ] (6) x-y,x,z+2/3 [u-v,u,w] (9) $\bar{x},\bar{x}+y,\bar{z}+2/3$ [u,u-v,w] (12) x,x-y, $\bar{z}+2/3$ [ $\bar{u},\bar{u}+v,w$ ]
6	j	..2'	x,2x,1/2 [u,0,w] $\bar{x},2\bar{x},1/2$ [ $\bar{u},0,w$ ]	$2\bar{x},\bar{x},5/6$ [0,u,w] 2x,x,5/6 [0, $\bar{u},w$ ]	x, $\bar{x},1/6$ [ $\bar{u},\bar{u},w$ ] $\bar{x},x,1/6$ [u,u,w]
6	i	..2'	x,2x,0 [u,0,w] $\bar{x},2\bar{x},0$ [ $\bar{u},0,w$ ]	$2\bar{x},\bar{x},1/3$ [0,u,w] 2x,x,1/3 [0, $\bar{u},w$ ]	x, $\bar{x},2/3$ [ $\bar{u},\bar{u},w$ ] $\bar{x},x,2/3$ [u,u,w]
6	h	.2'	x,0,1/2 [u,2u,w] $\bar{x},0,1/2$ [ $\bar{u},2\bar{u},w$ ]	0,x,5/6 [2 $\bar{u},\bar{u},w$ ] 0, $\bar{x},5/6$ [2u,u,w]	$\bar{x},\bar{x},1/6$ [u, $\bar{u},w$ ] x,x,1/6 [ $\bar{u},u,w$ ]
6	g	.2'	x,0,0 [u,2u,w] $\bar{x},0,0$ [ $\bar{u},2\bar{u},w$ ]	0,x,1/3 [2 $\bar{u},\bar{u},w$ ] 0, $\bar{x},1/3$ [2u,u,w]	$\bar{x},\bar{x},2/3$ [u, $\bar{u},w$ ] x,x,2/3 [ $\bar{u},u,w$ ]
6	f	2..	1/2,0,z [0,0,w] 0,1/2, $\bar{z}+1/3$ [0,0,w]	0,1/2,z+1/3 [0,0,w] 1/2,0, $\bar{z}$ [0,0,w]	1/2,1/2,z+2/3 [0,0,w] 1/2,1/2, $\bar{z}+2/3$ [0,0,w]
6	e	2..	0,0,z [0,0,w] 0,0, $\bar{z}+1/3$ [0,0,w]	0,0,z+1/3 [0,0,w] 0,0, $\bar{z}$ [0,0,w]	0,0,z+2/3 [0,0,w] 0,0, $\bar{z}+2/3$ [0,0,w]
3	d	22'2'	1/2,0,1/2 [0,0,w]	0,1/2,5/6 [0,0,w]	1/2,1/2,1/6 [0,0,w]
3	c	22'2'	1/2,0,0 [0,0,w]	0,1/2,1/3 [0,0,w]	1/2,1/2,2/3 [0,0,w]
3	b	22'2'	0,0,1/2 [0,0,w]	0,0,5/6 [0,0,w]	0,0,1/6 [0,0,w]
3	a	22'2'	0,0,0 [0,0,w]	0,0,1/3 [0,0,w]	0,0,2/3 [0,0,w]

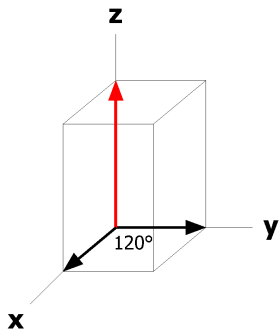
**Symmetry of Special Projections**

Along [0,0,1] p6mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/3





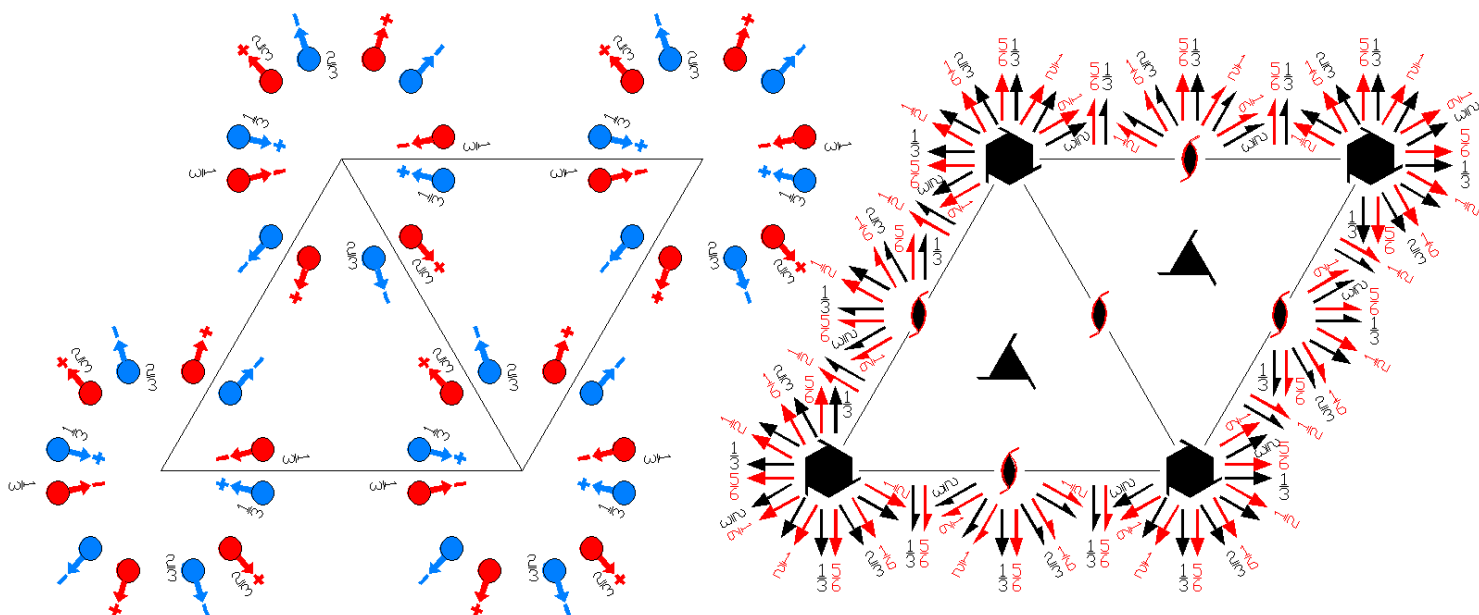
$P_{2c} 6_4 22$

181.6.1408

6221'

$P_{2c} 6_4 22$

Hexagonal



Origin at 222 at  $6_4 (2,1,1) (1,2,1)$

Asymmetric unit  $0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/6 \quad y \leq x$

Vertices  $0,0,0 \quad 1,0,0 \quad 1,1,0$   
 $0,0,1/6 \quad 1,0,1/6 \quad 1,1,1/6$

### Symmetry Operations

For  $(0,0,0) +$  set

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                                    | (2) $3^+ (0,0,1/3) \quad 0,0,z$<br>( $3_z   0,0,1/3$ )'      | (3) $3^- (0,0,2/3) \quad 0,0,z$<br>( $3_z^{-1}   0,0,2/3$ ) |
| (4) 2 $0,0,z$<br>( $2_z   0,0,0$ )                    | (5) $6^- (0,0,1/3) \quad 0,0,z$<br>( $6_z^{-1}   0,0,1/3$ )' | (6) $6^+ (0,0,2/3) \quad 0,0,z$<br>( $6_z   0,0,2/3$ )      |
| (7) $2' \quad x,x,1/6$<br>( $2_{xy}   0,0,1/3$ )'     | (8) 2 $x,0,0$<br>( $2_x   0,0,0$ )                           | (9) 2 $0,y,1/3$<br>( $2_y   0,0,2/3$ )                      |
| (10) $2' \quad x,\bar{x},1/6$<br>( $2_3   0,0,1/3$ )' | (11) 2 $x,2x,0$<br>( $2_2   0,0,0$ )                         | (12) 2 $2x,x,1/3$<br>( $2_1   0,0,2/3$ )                    |

## For (0,0,1)' + set

(1) $t' (0,0,1)$ $(1 0,0,1)'$	(2) $3^+ (0,0,4/3) 0,0,z$ $(3_z 0,0,4/3)$	(3) $3^- (0,0,5/3) 0,0,z$ $(3_z^{-1} 0,0,5/3)'$
(4) $2' (0,0,1) 0,0,z$ $(2_z 0,0,1)'$	(5) $6^- (0,0,4/3) 0,0,z$ $(6_z^{-1} 0,0,4/3)$	(6) $6^+ (0,0,5/3) 0,0,z$ $(6_z 0,0,5/3)'$
(7) $2 x,x,2/3$ $(2_{xy} 0,0,4/3)$	(8) $2' x,0,1/2$ $(2_x 0,0,1)'$	(9) $2' 0,y,5/6$ $(2_y 0,0,5/3)'$
(10) $2 x,\bar{x},2/3$ $(2_3 0,0,4/3)$	(11) $2' x,2x,1/2$ $(2_2 0,0,1)'$	(12) $2' 2x,x,5/6$ $(2_1 0,0,5/3)'$

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

**Positions**

			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) + (0,0,1)' +		
24	k	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z+1/3 [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z+2/3 [\bar{u}+v,\bar{u},w]$
			(4) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(5) $y,\bar{x}+y,z+1/3 [v,\bar{u}+v,w]$	(6) $x-y,x,z+2/3 [u-v,u,w]$
			(7) $y,x,\bar{z}+1/3 [v,u,\bar{w}]$	(8) $x-y,\bar{y},\bar{z} [u-v,\bar{v},\bar{w}]$	(9) $\bar{x},\bar{x}+y,\bar{z}+2/3 [\bar{u},\bar{u}+v,\bar{w}]$
			(10) $\bar{y},\bar{x},\bar{z}+1/3 [\bar{v},\bar{u},\bar{w}]$	(11) $\bar{x}+y,y,\bar{z} [\bar{u}+v,v,\bar{w}]$	(12) $x,x-y,\bar{z}+2/3 [u,u-v,\bar{w}]$
12	j	..2'	$x,2x,1/2 [u,0,w]$	$2\bar{x},\bar{x},5/6 [0,u,w]$	$x,\bar{x},1/6 [u,u,\bar{w}]$
			$\bar{x},2\bar{x},1/2 [\bar{u},0,w]$	$2x,x,5/6 [0,\bar{u},w]$	$\bar{x},x,1/6 [\bar{u},\bar{u},\bar{w}]$
12	i	..2	$x,2x,0 [u,2u,0]$	$2\bar{x},\bar{x},1/3 [2\bar{u},\bar{u},0]$	$x,\bar{x},2/3 [u,\bar{u},0]$
			$\bar{x},2\bar{x},0 [\bar{u},2\bar{u},0]$	$2x,x,1/3 [2u,u,0]$	$\bar{x},x,2/3 [\bar{u},u,0]$
12	h	.2'	$x,0,1/2 [u,2u,w]$	$0,x,5/6 [2\bar{u},\bar{u},w]$	$\bar{x},\bar{x},1/6 [\bar{u},u,\bar{w}]$
			$\bar{x},0,1/2 [\bar{u},2\bar{u},w]$	$0,\bar{x},5/6 [2u,u,w]$	$x,x,1/6 [u,\bar{u},\bar{w}]$
12	g	.2.	$x,0,0 [u,0,0]$	$0,x,1/3 [0,u,0]$	$\bar{x},\bar{x},2/3 [\bar{u},\bar{u},0]$
			$\bar{x},0,0 [\bar{u},0,0]$	$0,\bar{x},1/3 [0,\bar{u},0]$	$x,x,2/3 [u,u,0]$
12	f	2..	$1/2,0,z [0,0,w]$	$0,1/2,z+1/3 [0,0,w]$	$1/2,1/2,z+2/3 [0,0,w]$
			$0,1/2,\bar{z}+1/3 [0,0,\bar{w}]$	$1/2,0,\bar{z} [0,0,\bar{w}]$	$1/2,1/2,\bar{z}+2/3 [0,0,\bar{w}]$
12	e	2..	$0,0,z [0,0,w]$	$0,0,z+1/3 [0,0,w]$	$0,0,z+2/3 [0,0,w]$
			$0,0,\bar{z}+1/3 [0,0,\bar{w}]$	$0,0,\bar{z} [0,0,\bar{w}]$	$0,0,\bar{z}+2/3 [0,0,\bar{w}]$
6	d	22'2'	$1/2,0,1/2 [u,2u,0]$	$0,1/2,5/6 [2\bar{u},\bar{u},0]$	$1/2,1/2,1/6 [\bar{u},u,0]$

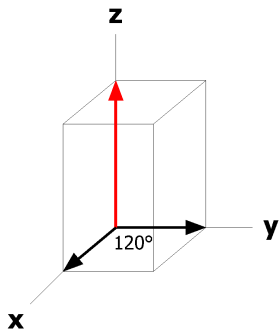
6	c	222	1/2,0,0 [0,0,0]	0,1/2,1/3 [0,0,0]	1/2,1/2,2/3 [0,0,0]
6	b	22'2'	0,0,1/2 [u,2u,0]	0,0,5/6 [2 $\bar{u}$ , $\bar{u}$ ,0]	0,0,1/6 [ $\bar{u}$ ,u,0]
6	a	222	0,0,0 [0,0,0]	0,0,1/3 [0,0,0]	0,0,2/3 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>\*2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p<sub>2a</sub>\*2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/3



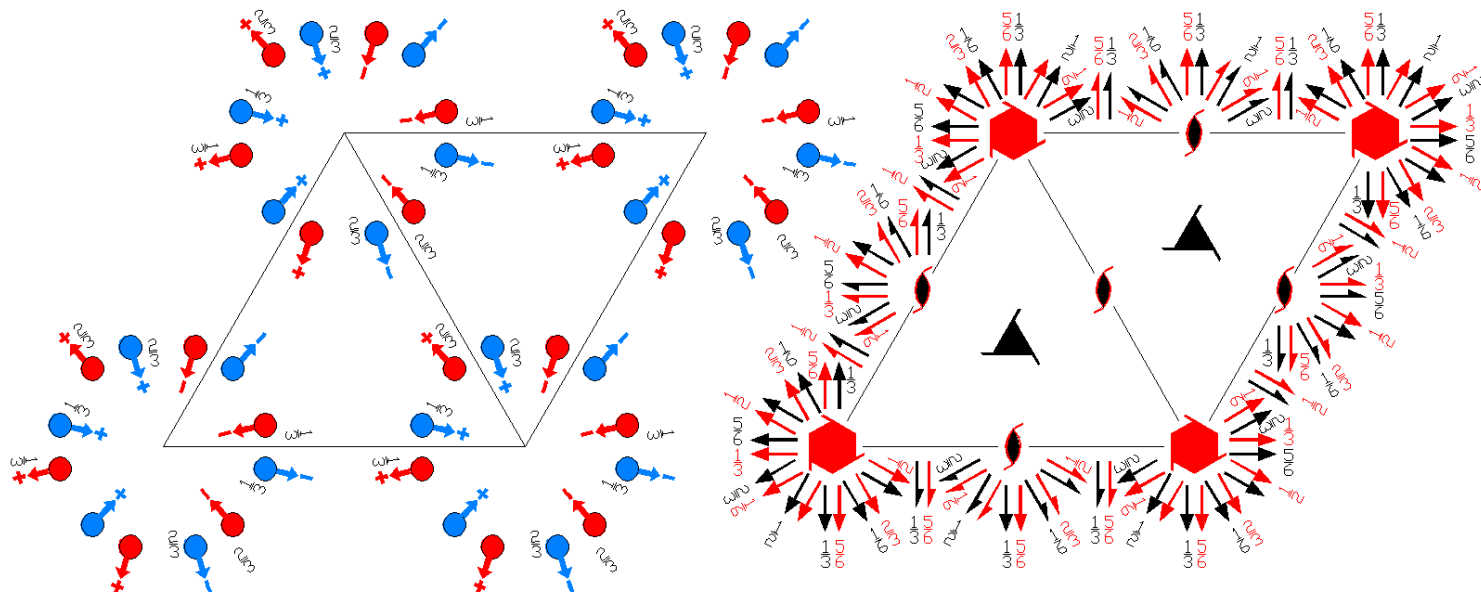
$P_{2c}6_4'2'2'$

181.7.1409

6221'

$P_{2c}6_4'2'2'$

Hexagonal



Origin at  $2'2'2'$  at  $6_4'$   $(2',1,1)$   $(1,2,1)$

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/6$   $y \leq x$

Vertices	0,0,0	1,0,0	1,1,0
	0,0,1/6	1,0,1/6	1,1,1/6

### Symmetry Operations

For  $(0,0,0)$  + set

- |   |  |   |
|---|--|---|
| (1) 1<br>$(1 0,0,0)$                          | (2) $3^+$ $(0,0,1/3)$ $0,0,z$<br>$(3_z 0,0,1/3)'$      | (3) $3^-$ $(0,0,2/3)$ $0,0,z$<br>$(3_z^{-1} 0,0,2/3)$ |
| (4) $2'$ $0,0,z$<br>$(2_z 0,0,0)'$            | (5) $6^-$ $(0,0,1/3)$ $0,0,z$<br>$(6_z^{-1} 0,0,1/3)'$ | (6) $6^+$ $(0,0,2/3)$ $0,0,z$<br>$(6_z 0,0,2/3)'$     |
| (7) $2$ $x,x,1/6$<br>$(2_{xy} 0,0,1/3)$       | (8) $2'$ $x,0,0$<br>$(2_x 0,0,0)'$                     | (9) $2'$ $0,y,1/3$<br>$(2_y 0,0,2/3)'$                |
| (10) $2'$ $x,\bar{x},1/6$<br>$(2_3 0,0,1/3)'$ | (11) $2$ $x,2x,0$<br>$(2_2 0,0,0)$                     | (12) $2$ $2x,x,1/3$<br>$(2_1 0,0,2/3)$                |

## For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 3 <sup>+</sup> (0,0,4/3) 0,0,z (3 <sub>z</sub>  0,0,4/3)	(3) 3 <sup>-</sup> (0,0,5/3) 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,5/3)'
(4) 2 (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)	(5) 6 <sup>-</sup> (0,0,4/3) 0,0,z (6 <sub>z</sub> <sup>-1</sup>  0,0,4/3)'	(6) 6 <sup>+</sup> (0,0,5/3) 0,0,z (6 <sub>z</sub>  0,0,5/3)
(7) 2' x,x,2/3 (2 <sub>xy</sub>  0,0,4/3)'	(8) 2 x,0,1/2 (2 <sub>x</sub>  0,0,1)	(9) 2 0,y,5/6 (2 <sub>y</sub>  0,0,5/3)
(10) 2 x,x̄,2/3 (2 <sub>3</sub>  0,0,4/3)	(11) 2' x,2x,1/2 (2 <sub>2</sub>  0,0,1)'	(12) 2' 2x,x,5/6 (2 <sub>1</sub>  0,0,5/3)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

**Positions**

			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(0,0,1)' +	
24	k	1	(1) x,y,z [u,v,w] (4) x̄,ȳ,z [u,v,w̄] (7) y,x,z̄+1/3 [v̄,u,w] (10) ȳ,x̄,z̄+1/3 [v̄,u,w̄]	(2) ȳ,x-y,z+1/3 [v̄,u-v,w] (5) y,x̄+y,z+1/3 [v̄,u-v,w̄] (8) x-y,ȳ,z̄ [u+v,v,w] (11) x̄+y,ȳ,z̄ [u+v,v,w̄]	(3) x̄+y,x̄,z+2/3 [u+v,u,w] (6) x-y,x,z+2/3 [u+v,u,w̄] (9) x̄,x̄+y,z̄+2/3 [u,u-v,w] (12) x,x-y,z̄+2/3 [u,u-v,w̄]
12	j	..2'	x,2x,1/2 [u,0,w] x̄,2x̄,1/2 [u,0,w̄]	2x̄,x̄,5/6 [0,u,w] 2x,x,5/6 [0,u,w̄]	x,x̄,1/6 [u,u,w̄] x̄,x,1/6 [u,u,w]
12	i	..2	x,2x,0 [u,2u,0] x̄,2x̄,0 [u,2u,0]	2x̄,x̄,1/3 [2ū,u,0] 2x,x,1/3 [2ū,u,0]	x,x̄,2/3 [u,u,0] x̄,x,2/3 [u,u,0]
12	h	.2.	x,0,1/2 [u,0,0] x̄,0,1/2 [u,0,0]	0,x,5/6 [0,u,0] 0,x̄,5/6 [0,u,0]	x̄,x̄,1/6 [u,u,0] x,x,1/6 [u,u,0]
12	g	..2'	x,0,0 [u,2u,w] x̄,0,0 [u,2u,w̄]	0,x,1/3 [2ū,u,w] 0,x̄,1/3 [2ū,u,w̄]	x̄,x̄,2/3 [u,u,w] x,x,2/3 [u,u,w̄]
12	f	2'..	1/2,0,z [u,v,0] 0,1/2,z̄+1/3 [v̄,u,0]	0,1/2,z+1/3 [v̄,u-v,0] 1/2,0,z̄ [u+v,v,0]	1/2,1/2,z+2/3 [u+v,u,0] 1/2,1/2,z̄+2/3 [u,u-v,0]
12	e	2'..	0,0,z [u,v,0] 0,0,z̄+1/3 [v̄,u,0]	0,0,z+1/3 [v̄,u-v,0] 0,0,z̄ [u+v,v,0]	0,0,z+2/3 [u+v,u,0] 0,0,z̄+2/3 [u,u-v,0]
6	d	2'22'	1/2,0,1/2 [u,0,0]	0,1/2,5/6 [0,u,0]	1/2,1/2,1/6 [u,u,0]

Continued

181.7.1409

$P_{2c} 6_4' 2'2$

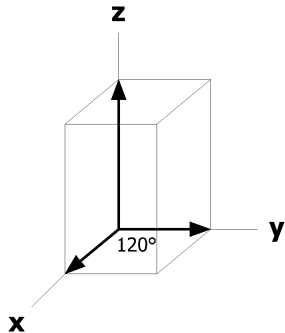
6	c	2'2'2	1/2,0,0 [u,2u,0]	0,1/2,1/3 [ $2\bar{u}, \bar{u}, 0$ ]	1/2,1/2,2/3 [u, $\bar{u}, 0$ ]
6	b	2'2'2'	0,0,1/2 [u,0,0]	0,0,5/6 [0,u,0]	0,0,1/6 [u,u,0]
6	a	2'2'2	0,0,0 [u,2u,0]	0,0,1/3 [ $2\bar{u}, \bar{u}, 0$ ]	0,0,2/3 [u, $\bar{u}, 0$ ]

### Symmetry of Special Projections

Along [0,0,1]  $p6mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0]  $p_{2a} 2mm$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,1/2

Along [2,1,0]  $p_{2a} 2mm$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,x/2,1/3



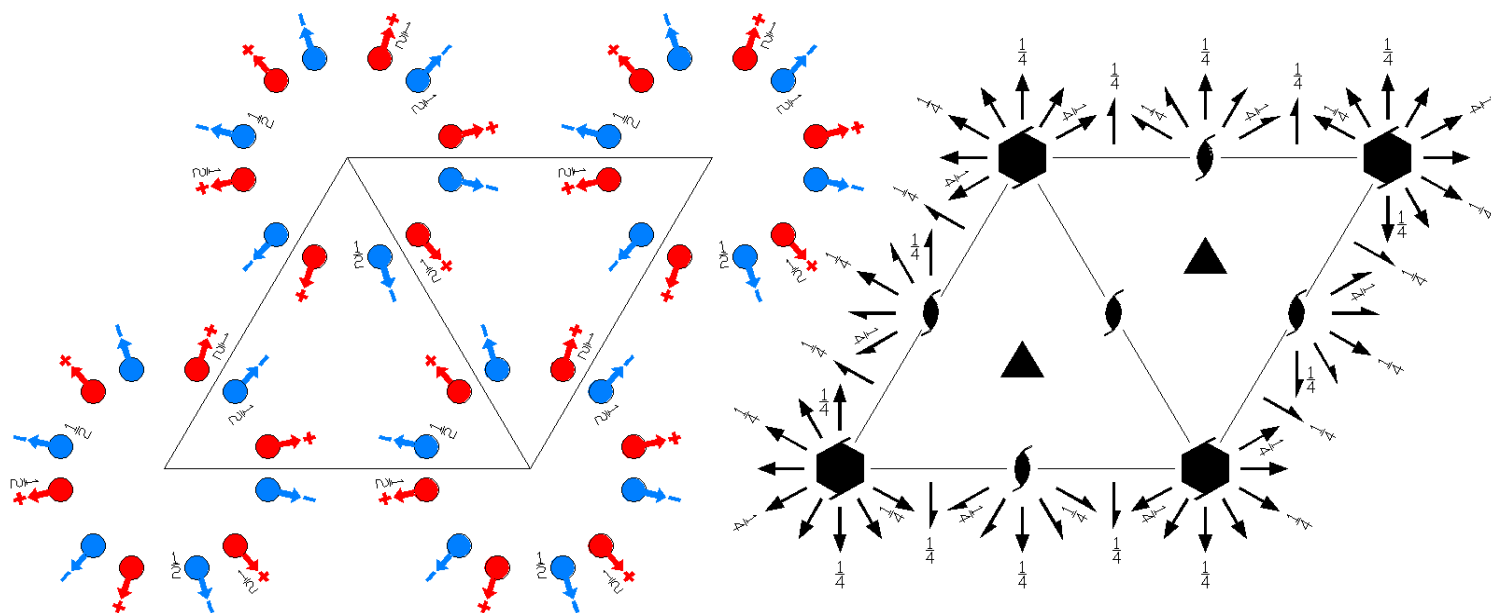
P6<sub>3</sub>22

622

Hexagonal

182.1.1410

P6<sub>3</sub>22



Origin at 321 at 6<sub>3</sub>21

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

**Symmetry Operations**

- |   |  |  |
|---|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub> <sup>+</sup>  0,0,0)             | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-</sup>  0,0,0)             |
| (4) 2 (0,0,1/2) 0,0,z<br>(2 <sub>z</sub> <sup>+</sup>  0,0,1/2) | (5) 6 <sup>-</sup> (0,0,1/2) 0,0,z<br>(6 <sub>z</sub> <sup>-</sup>  0,0,1/2) | (6) 6 <sup>+</sup> (0,0,1/2) 0,0,z<br>(6 <sub>z</sub> <sup>+</sup>  0,0,1/2) |
| (7) 2 x,x,0<br>(2 <sub>xy</sub> <sup>+</sup>  0,0,0)            | (8) 2 x,0,0<br>(2 <sub>x</sub> <sup>+</sup>  0,0,0)                          | (9) 2 0,y,0<br>(2 <sub>y</sub> <sup>+</sup>  0,0,0)                          |
| (10) 2 x,x̄,1/4<br>(2 <sub>3</sub> <sup>+</sup>  0,0,1/2)       | (11) 2 x,2x,1/4<br>(2 <sub>2</sub> <sup>+</sup>  0,0,1/2)                    | (12) 2 2x,x,1/4<br>(2 <sub>1</sub> <sup>+</sup>  0,0,1/2)                    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	i	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$	
			(4) $\bar{x},\bar{y},z+1/2 [\bar{u},\bar{v},w]$	(5) $y,\bar{x}+y,z+1/2 [v,\bar{u}+v,w]$	(6) $x-y,x,z+1/2 [u-v,u,w]$	
			(7) $y,x,\bar{z} [v,u,\bar{w}]$	(8) $x-y,\bar{y},\bar{z} [u-v,\bar{v},\bar{w}]$	(9) $\bar{x},\bar{x}+y,\bar{z} [\bar{u},\bar{u}+v,\bar{w}]$	
			(10) $\bar{y},\bar{x},\bar{z}+1/2 [\bar{v},\bar{u},\bar{w}]$	(11) $\bar{x}+y,y,\bar{z}+1/2 [\bar{u}+v,v,\bar{w}]$	(12) $x,x-y,\bar{z}+1/2 [u,u-v,\bar{w}]$	
6	h	..2	$x,2x,1/4 [u,2u,0]$	$2\bar{x},\bar{x},1/4 [2\bar{u},\bar{u},0]$	$x,\bar{x},1/4 [u,\bar{u},0]$	
			$\bar{x},2\bar{x},3/4 [\bar{u},2\bar{u},0]$	$2x,x,3/4 [2u,u,0]$	$\bar{x},x,3/4 [\bar{u},u,0]$	
6	g	.2.	$x,0,0 [u,0,0]$	$0,x,0 [0,u,0]$	$\bar{x},\bar{x},0 [\bar{u},\bar{u},0]$	
			$\bar{x},0,1/2 [\bar{u},0,0]$	$0,\bar{x},1/2 [0,\bar{u},0]$	$x,x,1/2 [u,u,0]$	
4	f	3..	$1/3,2/3,z [0,0,w]$	$2/3,1/3,z+1/2 [0,0,w]$	$2/3,1/3,\bar{z} [0,0,\bar{w}]$	$1/3,2/3,\bar{z}+1/2 [0,0,\bar{w}]$
4	e	3..	$0,0,z [0,0,w]$	$0,0,z+1/2 [0,0,w]$	$0,0,\bar{z} [0,0,\bar{w}]$	$0,0,\bar{z}+1/2 [0,0,\bar{w}]$
2	d	3.2	$1/3,2/3,3/4 [0,0,0]$	$2/3,1/3,1/4 [0,0,0]$		
2	c	3.2	$1/3,2/3,1/4 [0,0,0]$	$2/3,1/3,3/4 [0,0,0]$		
2	b	3.2	$0,0,1/4 [0,0,0]$	$0,0,3/4 [0,0,0]$		
2	a	32.	$0,0,0 [0,0,0]$	$0,0,1/2 [0,0,0]$		

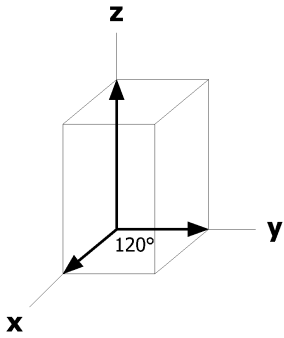
**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p2m'g'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

Along  $[2,1,0]$   $p2m'g'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,1/4$





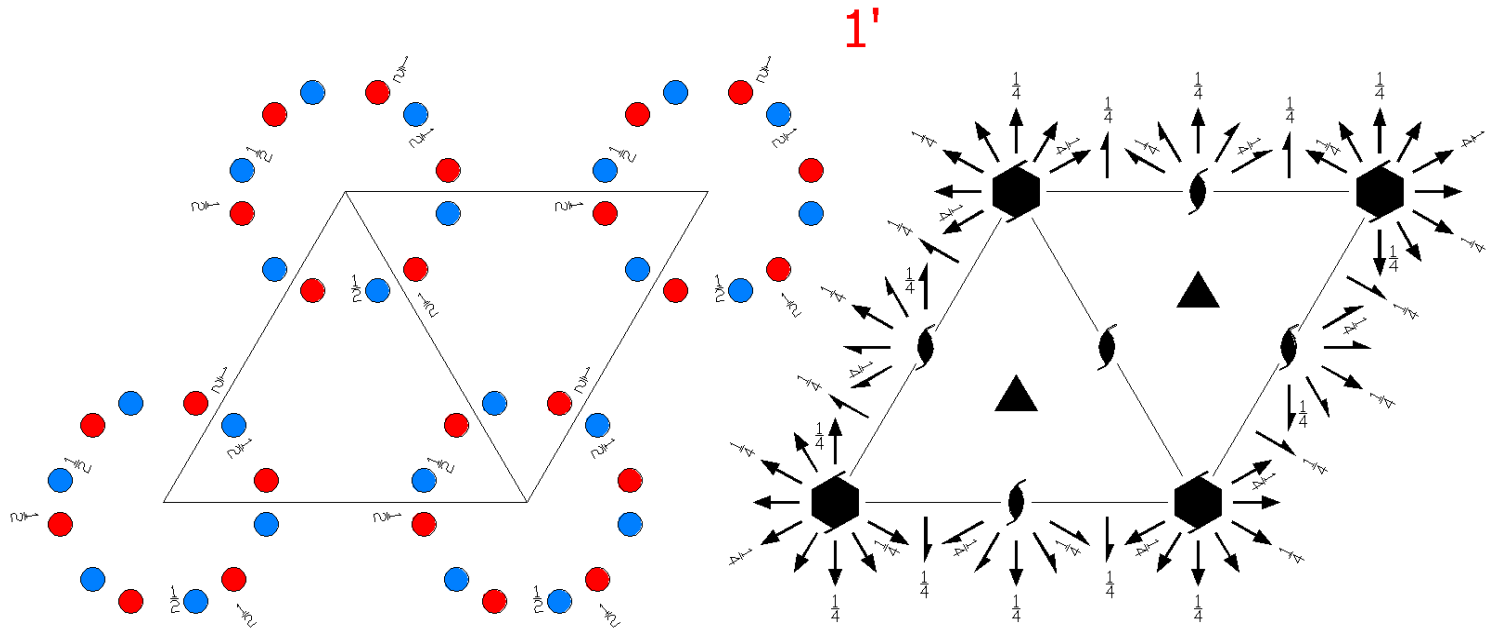
$P6_3 221'$

182.2.1411

$6221'$

$P6_3 221'$

Hexagonal



Origin at  $3211'$  at  $6_3 221'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

**Symmetry Operations**

For 1 + set

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                            | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)        |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)    | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2) |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0)             | (8) 2 x,0,0<br>( $2_x$  0,0,0)                      | (9) 2 0,y,0<br>( $2_y$  0,0,0)                 |
| (10) 2 $x, \bar{x}, 1/4$<br>( $2_3$  0,0,1/2) | (11) 2 x,2x,1/4<br>( $2_2$  0,0,1/2)                | (12) 2 2x,x,1/4<br>( $2_1$  0,0,1/2)           |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 3 <sup>+</sup> 0,0,z (3 <sub>z</sub>  0,0,0)'	(3) 3 <sup>-</sup> 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(4) 2' (0,0,1/2) 0,0,z (2 <sub>z</sub>  0,0,1/2)'	(5) 6 <sup>-</sup> (0,0,1/2) 0,0,z (6 <sub>z</sub> <sup>-1</sup>  0,0,1/2)'	(6) 6 <sup>+</sup> (0,0,1/2) 0,0,z (6 <sub>z</sub>  0,0,1/2)'
(7) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(8) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'	(9) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'
(10) 2' x, $\bar{x}$ ,1/4 (2 <sub>3</sub>  0,0,1/2)'	(11) 2' x,2x,1/4 (2 <sub>2</sub>  0,0,1/2)'	(12) 2' 2x,x,1/4 (2 <sub>1</sub>  0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

**Positions**

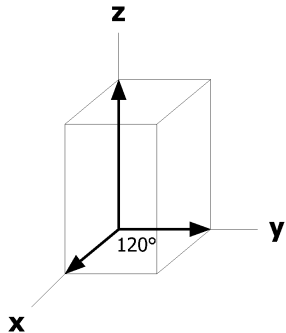
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			1 +	1' +		
12	i	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0]	
			(4) $\bar{x},\bar{y},z+1/2$ [0,0,0]	(5) y, $\bar{x}+y,z+1/2$ [0,0,0]	(6) x-y,x,z+1/2 [0,0,0]	
			(7) y,x, $\bar{z}$ [0,0,0]	(8) x-y, $\bar{y},\bar{z}$ [0,0,0]	(9) $\bar{x},\bar{x}+y,\bar{z}$ [0,0,0]	
			(10) $\bar{y},\bar{x},\bar{z}+1/2$ [0,0,0]	(11) $\bar{x}+y,y,\bar{z}+1/2$ [0,0,0]	(12) x,x-y, $\bar{z}+1/2$ [0,0,0]	
6	h	..21'	x,2x,1/4 [0,0,0]	2 $\bar{x},\bar{x},1/4$ [0,0,0]	x, $\bar{x},1/4$ [0,0,0]	
			$\bar{x},2\bar{x},3/4$ [0,0,0]	2x,x,3/4 [0,0,0]	$\bar{x},x,3/4$ [0,0,0]	
6	g	.2.1'	x,0,0 [0,0,0]	0,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	
			$\bar{x},0,1/2$ [0,0,0]	0, $\bar{x},1/2$ [0,0,0]	x,x,1/2 [0,0,0]	
4	f	3..1'	1/3,2/3,z [0,0,0]	2/3,1/3,z+1/2 [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	1/3,2/3, $\bar{z}+1/2$ [0,0,0]
4	e	3..1'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]
2	d	3.21'	1/3,2/3,3/4 [0,0,0]	2/3,1/3,1/4 [0,0,0]		
2	c	3.21'	1/3,2/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]		
2	b	3.21'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	a	32.1'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,0

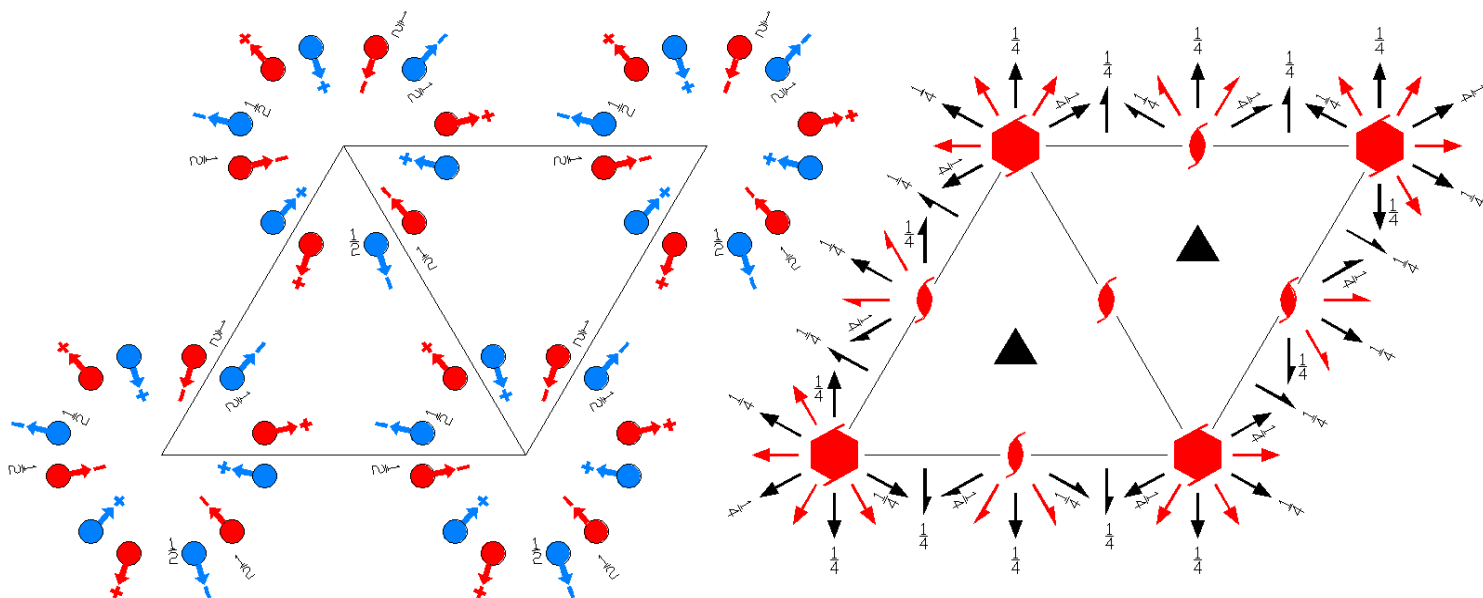
Along [2,1,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,x/2,1/4



$P6_3'2'2'$   
182.3.1412

$6'2'2'$   
 $P6_3'2'2'$

Hexagonal



Origin at  $32'1$  at  $6_3'2'1$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

### Symmetry Operations

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                              | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                   | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)         |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)'  | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)' | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)' |
| (7) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)'           | (8) $2'$ x,0,0<br>( $2_x$  0,0,0)'                   | (9) $2'$ 0,y,0<br>( $2_y$  0,0,0)'              |
| (10) $2$ x, $\bar{x}$ ,1/4<br>( $2_3$  0,0,1/2) | (11) $2$ x,2x,1/4<br>( $2_2$  0,0,1/2)               | (12) $2$ 2x,x,1/4<br>( $2_1$  0,0,1/2)          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

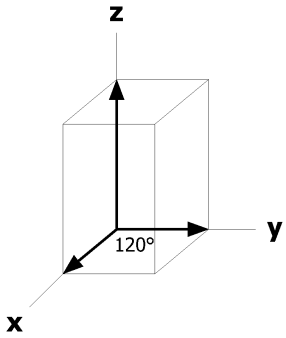
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	i	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]	
			(4) $\bar{x},\bar{y},z+1/2$ [ $u,v,\bar{w}$ ]	(5) $y,\bar{x}+y,z+1/2$ [ $\bar{v},u-v,\bar{w}$ ]	(6) $x-y,x,z+1/2$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]	
			(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $x-y,\bar{y},\bar{z}$ [ $\bar{u}+v,v,w$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}$ [ $u,u-v,w$ ]	
			(10) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(11) $\bar{x}+y,y,\bar{z}+1/2$ [ $\bar{u}+v,v,\bar{w}$ ]	(12) $x,x-y,\bar{z}+1/2$ [ $u,u-v,\bar{w}$ ]	
6	h	..2	$x,2x,1/4$ [ $u,2u,0$ ]	$2\bar{x},\bar{x},1/4$ [ $2\bar{u},\bar{u},0$ ]	$x,\bar{x},1/4$ [ $u,\bar{u},0$ ]	
			$\bar{x},2\bar{x},3/4$ [ $u,2u,0$ ]	$2x,x,3/4$ [ $2\bar{u},\bar{u},0$ ]	$\bar{x},x,3/4$ [ $u,\bar{u},0$ ]	
6	g	.2'	$x,0,0$ [ $u,2u,w$ ]	$0,x,0$ [ $2\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},0$ [ $u,\bar{u},w$ ]	
			$\bar{x},0,1/2$ [ $u,2u,\bar{w}$ ]	$0,\bar{x},1/2$ [ $2\bar{u},\bar{u},\bar{w}$ ]	$x,x,1/2$ [ $u,\bar{u},\bar{w}$ ]	
4	f	3..	$1/3,2/3,z$ [ $0,0,w$ ]	$2/3,1/3,z+1/2$ [ $0,0,\bar{w}$ ]	$2/3,1/3,\bar{z}$ [ $0,0,w$ ]	$1/3,2/3,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]
4	e	3..	$0,0,z$ [ $0,0,w$ ]	$0,0,z+1/2$ [ $0,0,\bar{w}$ ]	$0,0,\bar{z}$ [ $0,0,w$ ]	$0,0,\bar{z}+1/2$ [ $0,0,\bar{w}$ ]
2	d	3.2	$1/3,2/3,3/4$ [ $0,0,0$ ]	$2/3,1/3,1/4$ [ $0,0,0$ ]		
2	c	3.2	$1/3,2/3,1/4$ [ $0,0,0$ ]	$2/3,1/3,3/4$ [ $0,0,0$ ]		
2	b	3.2	$0,0,1/4$ [ $0,0,0$ ]	$0,0,3/4$ [ $0,0,0$ ]		
2	a	32'	$0,0,0$ [ $0,0,w$ ]	$0,0,1/2$ [ $0,0,\bar{w}$ ]		

**Symmetry of Special Projections**

Along  $[0,0,1]$  p6'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p2'm'g  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

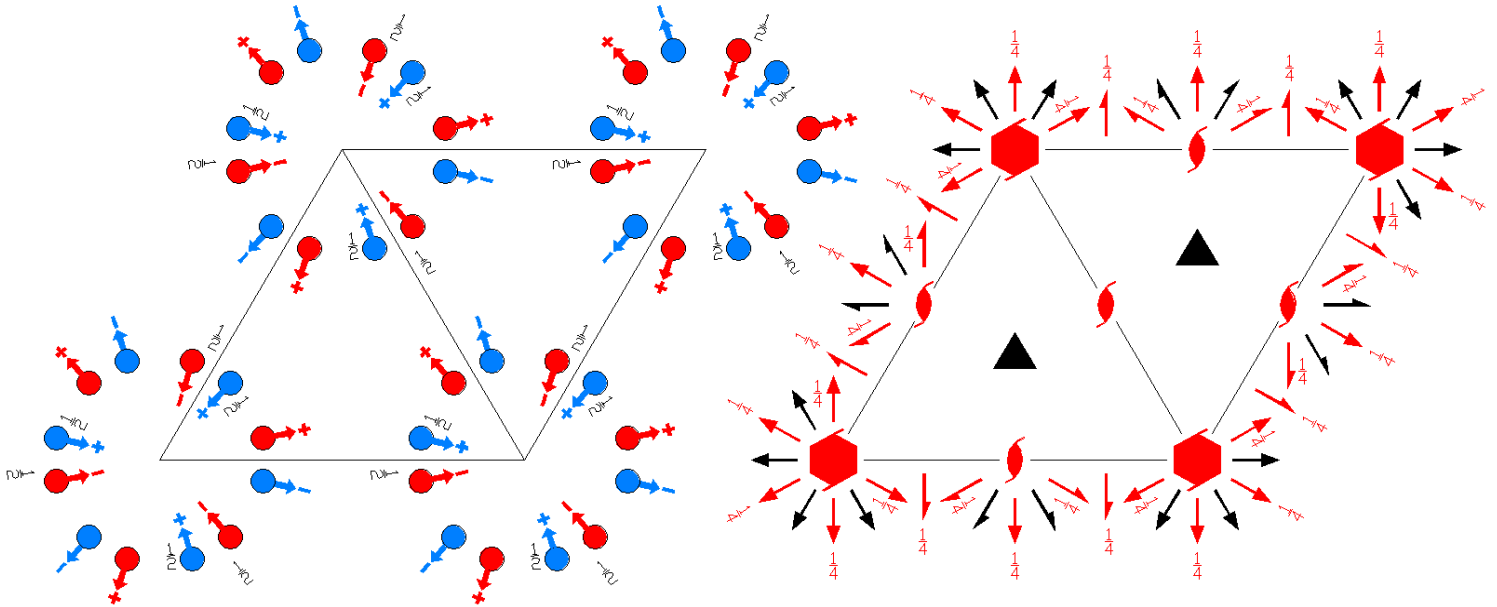
Along  $[2,1,0]$  p2mg  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,1/4$



$P6_3'22'$   
182.4.1413

$6'22'$   
 $P6_3'22'$

Hexagonal



Origin at 321 at  $6_3'21$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                                | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                   | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)         |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)'    | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)' | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)' |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0)                 | (8) 2 x,0,0<br>( $2_x$  0,0,0)                       | (9) 2 0,y,0<br>( $2_y$  0,0,0)                  |
| (10) $2'$ x, $\bar{x}$ ,1/4<br>( $2_3$  0,0,1/2)' | (11) $2'$ x,2x,1/4<br>( $2_2$  0,0,1/2)'             | (12) $2'$ 2x,x,1/4<br>( $2_1$  0,0,1/2)'        |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

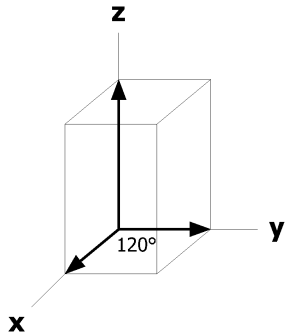
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	i	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]	
			(4) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(5) $y,\bar{x}+y,z+1/2$ [ $\bar{v},u-v,\bar{w}$ ]	(6) $x-y,x,z+1/2$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]	
			(7) $y,x,\bar{z}$ [v,u, $\bar{w}$ ]	(8) $x-y,\bar{y},\bar{z}$ [u-v, $\bar{v},\bar{w}$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]	
			(10) $\bar{y},\bar{x},\bar{z}+1/2$ [v,u,w]	(11) $\bar{x}+y,y,\bar{z}+1/2$ [u-v, $\bar{v},w$ ]	(12) $x,x-y,\bar{z}+1/2$ [ $\bar{u},\bar{u}+v,w$ ]	
6	h	..2'	$x,2x,1/4$ [u,0,w]	$2\bar{x},\bar{x},1/4$ [0,u,w]	$x,\bar{x},1/4$ [ $\bar{u},\bar{u},w$ ]	
			$\bar{x},2\bar{x},3/4$ [u,0, $\bar{w}$ ]	$2x,x,3/4$ [0,u, $\bar{w}$ ]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},\bar{w}$ ]	
6	g	.2.	$x,0,0$ [u,0,0]	$0,x,0$ [0,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	
			$\bar{x},0,1/2$ [u,0,0]	$0,\bar{x},1/2$ [0,u,0]	$x,x,1/2$ [ $\bar{u},\bar{u},0$ ]	
4	f	3..	$1/3,2/3,z$ [0,0,w]	$2/3,1/3,z+1/2$ [0,0, $\bar{w}$ ]	$2/3,1/3,\bar{z}$ [0,0, $\bar{w}$ ]	$1/3,2/3,\bar{z}+1/2$ [0,0,w]
4	e	3..	$0,0,z$ [0,0,w]	$0,0,z+1/2$ [0,0, $\bar{w}$ ]	$0,0,\bar{z}$ [0,0, $\bar{w}$ ]	$0,0,\bar{z}+1/2$ [0,0,w]
2	d	3.2'	$1/3,2/3,3/4$ [0,0,w]	$2/3,1/3,1/4$ [0,0, $\bar{w}$ ]		
2	c	3.2'	$1/3,2/3,1/4$ [0,0,w]	$2/3,1/3,3/4$ [0,0, $\bar{w}$ ]		
2	b	3.2'	$0,0,1/4$ [0,0,w]	$0,0,3/4$ [0,0, $\bar{w}$ ]		
2	a	32.	$0,0,0$ [0,0,0]	$0,0,1/2$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p6'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

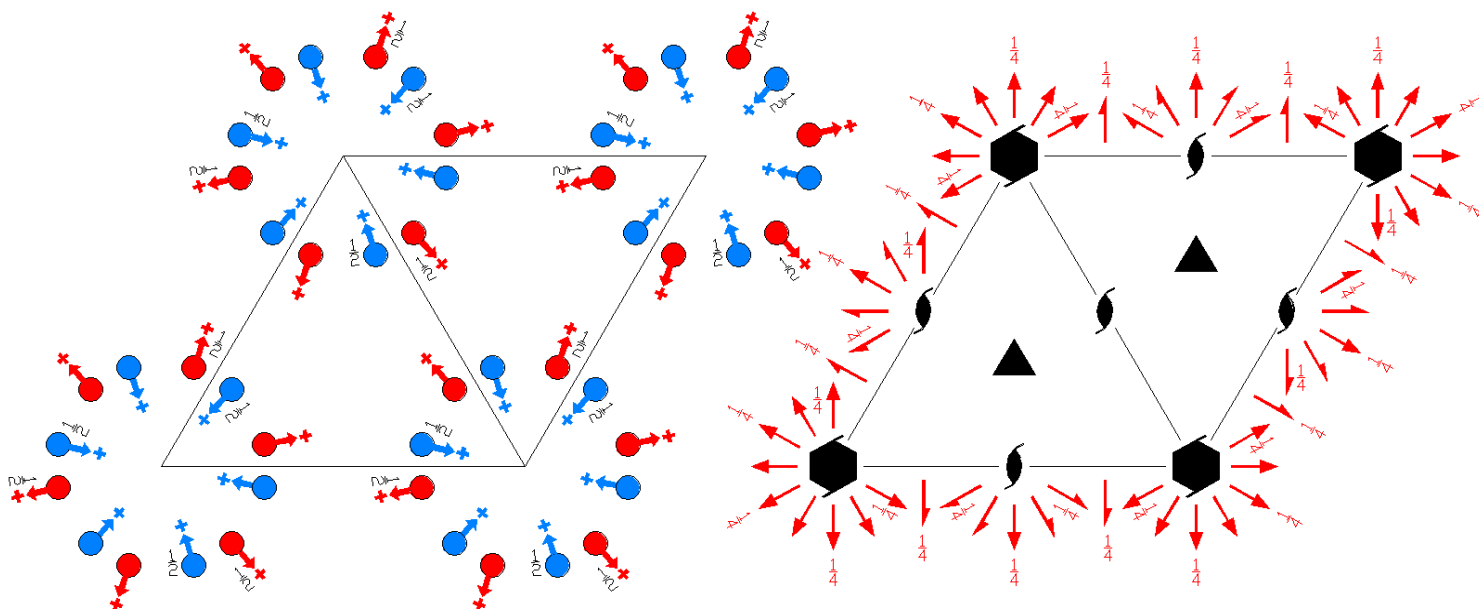
Along [2,1,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/4



$P6_3 2' 2'$   
182.5.1414

$62' 2'$   
 $P6_3 2' 2'$

Hexagonal



Origin at  $32' 1$  at  $6_3 2' 1$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0 0,0,1/4	1/2,0,0 1/2,0,1/4	2/3,1/3,0 2/3,1/3,1/4	1/3,2/3,0 1/3,2/3,1/4	0,1/2,0 0,1/2,1/4

### Symmetry Operations

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                                | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)        |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)        | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2) |
| (7) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)'             | (8) $2'$ x,0,0<br>( $2_x$  0,0,0)'                  | (9) $2'$ 0,y,0<br>( $2_y$  0,0,0)'             |
| (10) $2'$ x, $\bar{x}$ ,1/4<br>( $2_3$  0,0,1/2)' | (11) $2'$ x,2x,1/4<br>( $2_2$  0,0,1/2)'            | (12) $2'$ 2x,x,1/4<br>( $2_1$  0,0,1/2)'       |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

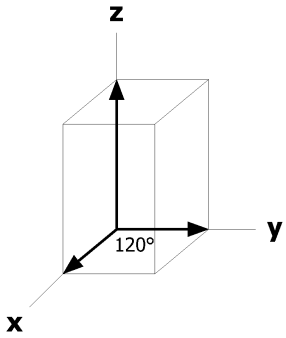
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	i	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]	
			(4) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(5) $y,\bar{x}+y,z+1/2$ [ $v,\bar{u}+v,w$ ]	(6) $x-y,x,z+1/2$ [ $u-v,u,w$ ]	
			(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $x-y,\bar{y},\bar{z}$ [ $\bar{u}+v,v,w$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}$ [ $u,u-v,w$ ]	
			(10) $\bar{y},\bar{x},\bar{z}+1/2$ [ $v,u,w$ ]	(11) $\bar{x}+y,y,\bar{z}+1/2$ [ $u-v,\bar{v},w$ ]	(12) $x,x-y,\bar{z}+1/2$ [ $\bar{u},\bar{u}+v,w$ ]	
6	h	..2'	$x,2x,1/4$ [ $u,0,w$ ]	$2\bar{x},\bar{x},1/4$ [ $0,u,w$ ]	$x,\bar{x},1/4$ [ $\bar{u},\bar{u},w$ ]	
			$\bar{x},2\bar{x},3/4$ [ $\bar{u},0,w$ ]	$2x,x,3/4$ [ $0,\bar{u},w$ ]	$\bar{x},x,3/4$ [ $u,\bar{u},w$ ]	
6	g	.2'	$x,0,0$ [ $u,2u,w$ ]	$0,x,0$ [ $2\bar{u},\bar{u},w$ ]	$\bar{x},\bar{x},0$ [ $u,\bar{u},w$ ]	
			$\bar{x},0,1/2$ [ $\bar{u},2\bar{u},w$ ]	$0,\bar{x},1/2$ [ $2u,u,w$ ]	$x,x,1/2$ [ $\bar{u},u,w$ ]	
4	f	3..	$1/3,2/3,z$ [ $0,0,w$ ]	$2/3,1/3,z+1/2$ [ $0,0,w$ ]	$2/3,1/3,\bar{z}$ [ $0,0,w$ ]	$1/3,2/3,\bar{z}+1/2$ [ $0,0,w$ ]
4	e	3..	$0,0,z$ [ $0,0,w$ ]	$0,0,z+1/2$ [ $0,0,w$ ]	$0,0,\bar{z}$ [ $0,0,w$ ]	$0,0,\bar{z}+1/2$ [ $0,0,w$ ]
2	d	3.2'	$1/3,2/3,3/4$ [ $0,0,w$ ]	$2/3,1/3,1/4$ [ $0,0,w$ ]		
2	c	3.2'	$1/3,2/3,1/4$ [ $0,0,w$ ]	$2/3,1/3,3/4$ [ $0,0,w$ ]		
2	b	3.2'	$0,0,1/4$ [ $0,0,w$ ]	$0,0,3/4$ [ $0,0,w$ ]		
2	a	32'	$0,0,0$ [ $0,0,w$ ]	$0,0,1/2$ [ $0,0,w$ ]		

**Symmetry of Special Projections**

Along  $[0,0,1]$  p6mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p2'mg'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

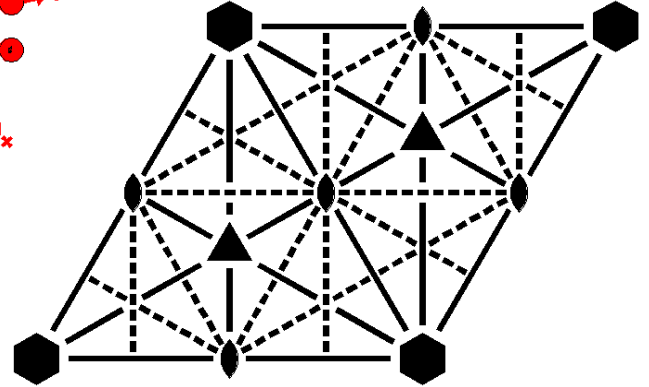
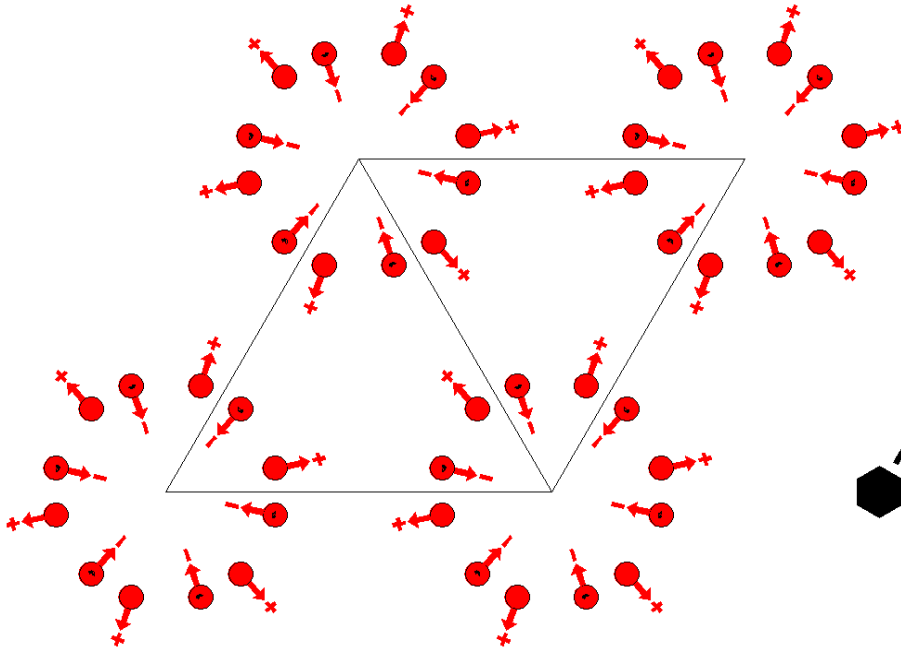
Along  $[2,1,0]$  p2'mg'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,1/4$



P6mm  
183.1.1415

6mm  
P6mm

Hexagonal



Origin on 6mm

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1		

**Symmetry Operations**

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                 | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)             | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) m x, $\bar{x}$ , z<br>(m <sub>xy</sub>  0,0,0) | (8) m x, 2x, z<br>(m <sub>x</sub>  0,0,0)                         | (9) m 2x, x, z<br>(m <sub>y</sub>  0,0,0)                         |
| (10) m x, x, z<br>(m <sub>3</sub>  0,0,0)          | (11) m x, 0, z<br>(m <sub>2</sub>  0,0,0)                         | (12) m 0, y, z<br>(m <sub>1</sub>  0,0,0)                         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

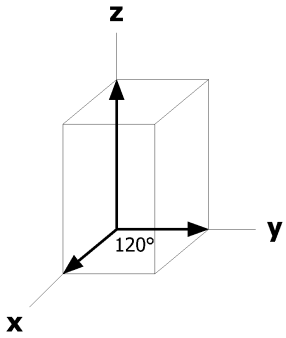
			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
12	f	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(5) $y,\bar{x}+y,z$ [ $v,\bar{u}+v,w$ ]	(6) $x-y,x,z$ [ $u-v,u,w$ ]
			(7) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(8) $\bar{x}+y,y,z$ [ $u-v,\bar{v},\bar{w}$ ]	(9) $x,x-y,z$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
			(10) $y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(11) $x-y,\bar{y},z$ [ $\bar{u}+v,v,\bar{w}$ ]	(12) $\bar{x},\bar{x}+y,z$ [ $u,u-v,\bar{w}$ ]
6	e	.m.	$x,\bar{x},z$ [ $u,u,0$ ]	$x,2x,z$ [ $\bar{u},0,0$ ]	$2\bar{x},\bar{x},z$ [ $0,\bar{u},0$ ]
			$\bar{x},x,z$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},2\bar{x},z$ [ $u,0,0$ ]	$2x,x,z$ [ $0,u,0$ ]
6	d	..m	$x,0,z$ [ $u,2u,0$ ]	$0,x,z$ [ $2\bar{u},\bar{u},0$ ]	$\bar{x},\bar{x},z$ [ $u,\bar{u},0$ ]
			$\bar{x},0,z$ [ $\bar{u},2\bar{u},0$ ]	$0,\bar{x},z$ [ $2u,u,0$ ]	$x,x,z$ [ $\bar{u},u,0$ ]
3	c	2mm	$1/2,0,z$ [ $0,0,0$ ]	$0,1/2,z$ [ $0,0,0$ ]	$1/2,1/2,z$ [ $0,0,0$ ]
2	b	3m.	$1/3,2/3,z$ [ $0,0,0$ ]	$2/3,1/3,z$ [ $0,0,0$ ]	
1	a	6mm	$0,0,z$ [ $0,0,0$ ]		

**Symmetry of Special Projections**

Along  $[0,0,1]$  p6mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p1m11'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[2,1,0]$  p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x/2,0$

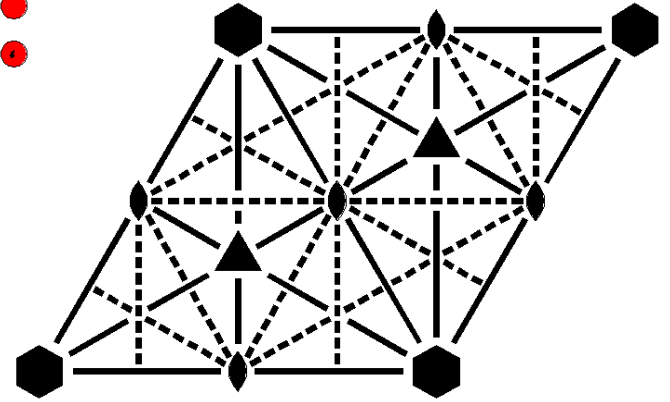
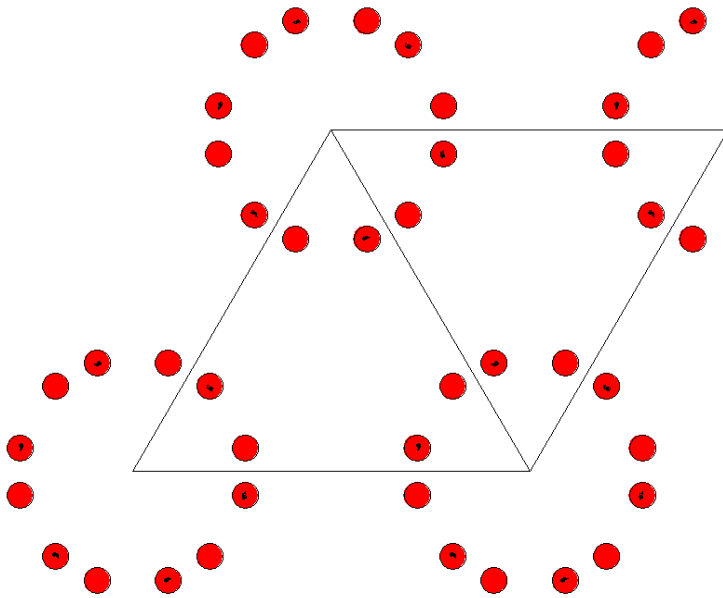


P6mm1'  
183.2.1416

6mm1'  
P6mm1'

Hexagonal

1'



Origin on 6mm1'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1		

**Symmetry Operations**

For 1 + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                         | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)     | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) m x, x̄, z<br>(m <sub>xy</sub>  0,0,0) | (8) m x, 2x, z<br>(m <sub>x</sub>  0,0,0)                         | (9) m 2x, x, z<br>(m <sub>y</sub>  0,0,0)                         |
| (10) m x, x, z<br>(m <sub>3</sub>  0,0,0)  | (11) m x, 0, z<br>(m <sub>2</sub>  0,0,0)                         | (12) m 0, y, z<br>(m <sub>1</sub>  0,0,0)                         |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 3 <sup>+</sup> 0,0,z (3 <sub>z</sub>  0,0,0)'	(3) 3 <sup>-</sup> 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(4) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(5) 6 <sup>-</sup> 0,0,z (6 <sub>z</sub> <sup>-1</sup>  0,0,0)'	(6) 6 <sup>+</sup> 0,0,z (6 <sub>z</sub>  0,0,0)'
(7) m' x, $\bar{x}$ , z (m <sub>xy</sub>  0,0,0)'	(8) m' x, 2x, z (m <sub>x</sub>  0,0,0)'	(9) m' 2x, x, z (m <sub>y</sub>  0,0,0)'
(10) m' x, x, z (m <sub>3</sub>  0,0,0)'	(11) m' x, 0, z (m <sub>2</sub>  0,0,0)'	(12) m' 0, y, z (m <sub>1</sub>  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

**Positions**

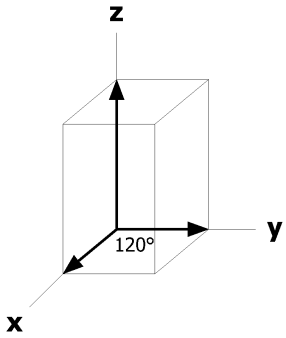
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			1 +	1' +	
12	f	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0]
			(4) $\bar{x},\bar{y},z$ [0,0,0]	(5) y, $\bar{x}+y,z$ [0,0,0]	(6) x-y,x,z [0,0,0]
			(7) $\bar{y},\bar{x},z$ [0,0,0]	(8) $\bar{x}+y,y,z$ [0,0,0]	(9) x,x-y,z [0,0,0]
			(10) y,x,z [0,0,0]	(11) x-y, $\bar{y},z$ [0,0,0]	(12) $\bar{x},\bar{x}+y,z$ [0,0,0]
6	e	.m.1'	x, $\bar{x},z$ [0,0,0]	x,2x,z [0,0,0]	2 $\bar{x},\bar{x},z$ [0,0,0]
			$\bar{x},x,z$ [0,0,0]	$\bar{x},2\bar{x},z$ [0,0,0]	2x,x,z [0,0,0]
6	d	..m1'	x,0,z [0,0,0]	0,x,z [0,0,0]	$\bar{x},\bar{x},z$ [0,0,0]
			$\bar{x},0,z$ [0,0,0]	0, $\bar{x},z$ [0,0,0]	x,x,z [0,0,0]
3	c	2mm1'	1/2,0,z [0,0,0]	0,1/2,z [0,0,0]	1/2,1/2,z [0,0,0]
2	b	3m.1'	1/3,2/3,z [0,0,0]	2/3,1/3,z [0,0,0]	
1	a	6mm1'	0,0,z [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

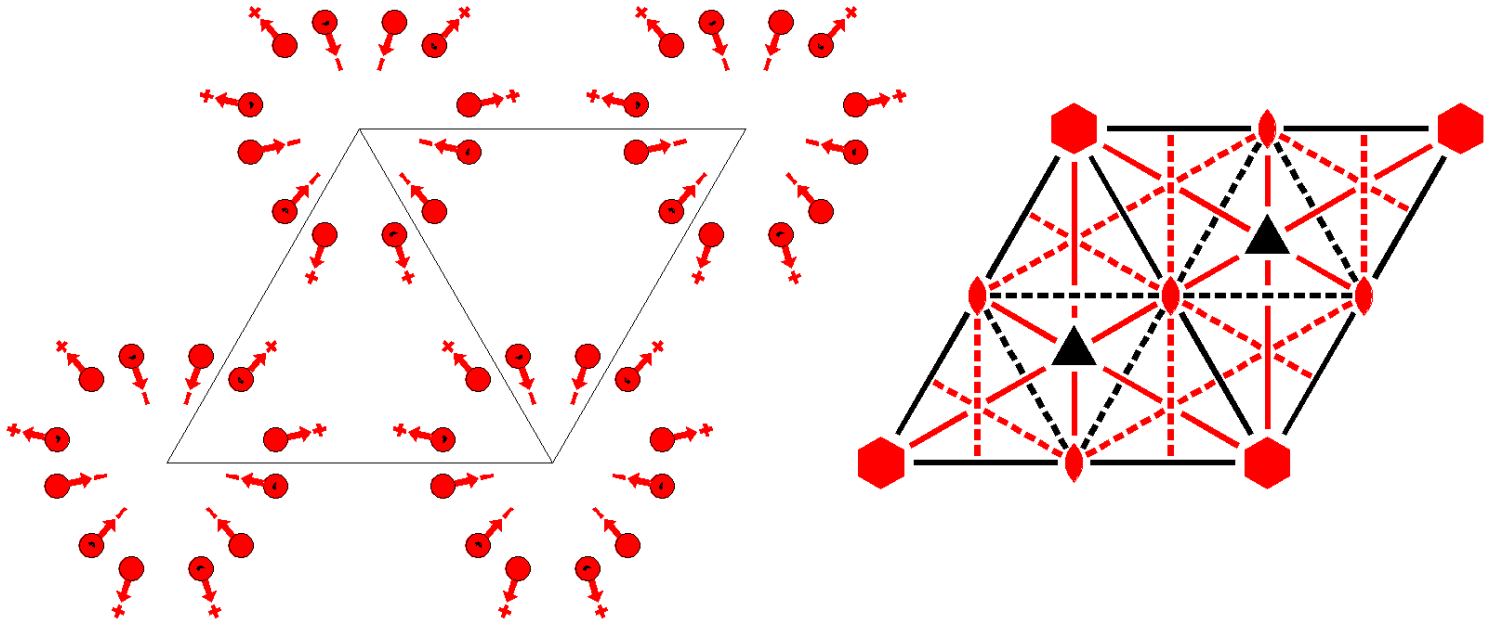
Along [2,1,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



P6'm'm  
183.3.1417

6'm'm  
P6'm'm

Hexagonal



Origin on 6'm'm

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1		

**Symmetry Operations**

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                           | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)                | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'     | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)'              |
| (7) m' x, x̄, z<br>(m <sub>xy</sub>  0,0,0)' | (8) m' x, 2x, z<br>(m <sub>x</sub>  0,0,0)'                        | (9) m' 2x, x, z<br>(m <sub>y</sub>  0,0,0)'                       |
| (10) m x, x, z<br>(m <sub>3</sub>  0,0,0)    | (11) m x, 0, z<br>(m <sub>2</sub>  0,0,0)                          | (12) m 0, y, z<br>(m <sub>1</sub>  0,0,0)                         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

### Positions

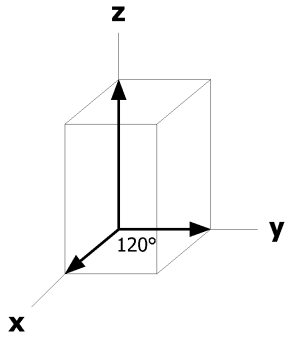
			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
12	f	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$
			(4) $\bar{x},\bar{y},z [u,v,\bar{w}]$	(5) $y,\bar{x}+y,z [\bar{v},u-v,\bar{w}]$	(6) $x-y,x,z [\bar{u}+v,\bar{u},\bar{w}]$
			(7) $\bar{y},\bar{x},z [\bar{v},\bar{u},w]$	(8) $\bar{x}+y,y,z [\bar{u}+v,v,w]$	(9) $x,x-y,z [u,u-v,w]$
			(10) $y,x,z [\bar{v},\bar{u},\bar{w}]$	(11) $x-y,\bar{y},z [\bar{u}+v,v,\bar{w}]$	(12) $\bar{x},\bar{x}+y,z [u,u-v,\bar{w}]$
6	e	.m'	$x,\bar{x},z [u,\bar{u},w]$	$x,2x,z [u,2u,w]$	$2\bar{x},\bar{x},z [2\bar{u},\bar{u},w]$
			$\bar{x},x,z [u,\bar{u},\bar{w}]$	$\bar{x},2\bar{x},z [u,2u,\bar{w}]$	$2x,x,z [2\bar{u},\bar{u},\bar{w}]$
6	d	..m	$x,0,z [u,2u,0]$	$0,x,z [2\bar{u},\bar{u},0]$	$\bar{x},\bar{x},z [u,\bar{u},0]$
			$\bar{x},0,z [u,2u,0]$	$0,\bar{x},z [2\bar{u},\bar{u},0]$	$x,x,z [u,\bar{u},0]$
3	c	2'm'm	$1/2,0,z [u,2u,0]$	$0,1/2,z [2\bar{u},\bar{u},0]$	$1/2,1/2,z [u,\bar{u},0]$
2	b	3m'	$1/3,2/3,z [0,0,w]$	$2/3,1/3,z [0,0,\bar{w}]$	
1	a	6'm'm	$0,0,z [0,0,0]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p6'm'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p1m1$   
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

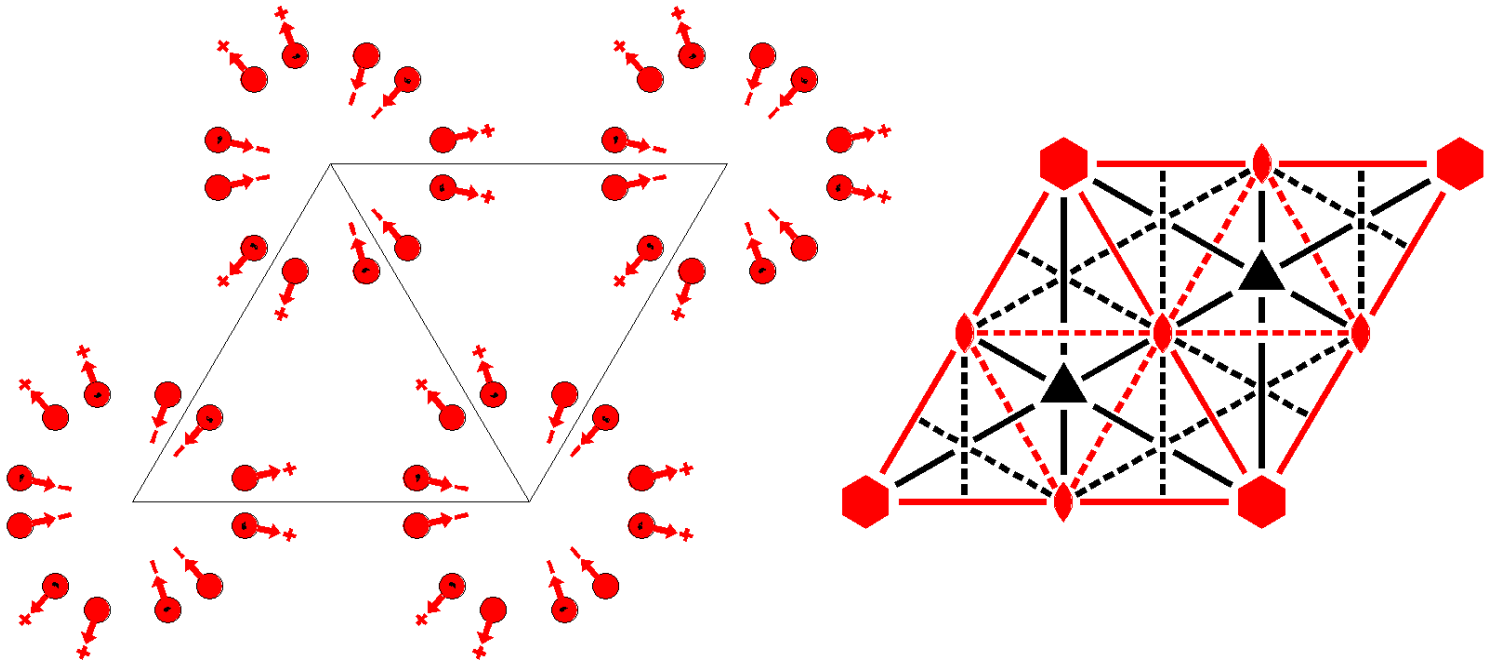
Along  $[2,1,0]$   $p1m11'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x/2,0$



P6'mm'  
183.4.1418

6'mm'  
P6'mm'

Hexagonal



Origin on 6'mm'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1		

**Symmetry Operations**

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                         | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)                | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'   | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)'              |
| (7) m x, x̄,z<br>(m <sub>xy</sub>  0,0,0)  | (8) m x, 2x,z<br>(m <sub>x</sub>  0,0,0)                           | (9) m 2x, x,z<br>(m <sub>y</sub>  0,0,0)                          |
| (10) m' x, x,z<br>(m <sub>3</sub>  0,0,0)' | (11) m' x, 0,z<br>(m <sub>2</sub>  0,0,0)'                         | (12) m' 0, y,z<br>(m <sub>1</sub>  0,0,0)'                        |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

### Positions

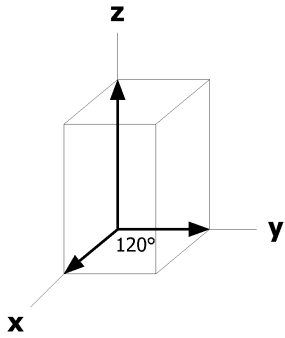
			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
12	f	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(5) $y,\bar{x}+y,z$ [ $\bar{v},u-v,\bar{w}$ ]	(6) $x-y,x,z$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]
			(7) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ]	(8) $\bar{x}+y,y,z$ [u-v, $\bar{v},\bar{w}$ ]	(9) $x,x-y,z$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
			(10) $y,x,z$ [v,u,w]	(11) $x-y,\bar{y},z$ [u-v, $\bar{v},w$ ]	(12) $\bar{x},\bar{x}+y,z$ [ $\bar{u},\bar{u}+v,w$ ]
6	e	.m.	$x,\bar{x},z$ [u,u,0]	$x,2x,z$ [ $\bar{u},0,0$ ]	$2\bar{x},\bar{x},z$ [0, $\bar{u},0$ ]
			$\bar{x},x,z$ [u,u,0]	$\bar{x},2\bar{x},z$ [ $\bar{u},0,0$ ]	$2x,x,z$ [0, $\bar{u},0$ ]
6	d	..m'	$x,0,z$ [u,0,w]	$0,x,z$ [0,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]
			$\bar{x},0,z$ [u,0, $\bar{w}$ ]	$0,\bar{x},z$ [0,u, $\bar{w}$ ]	$x,x,z$ [ $\bar{u},\bar{u},\bar{w}$ ]
3	c	2'mm'	$1/2,0,z$ [u,0,0]	$0,1/2,z$ [0,u,0]	$1/2,1/2,z$ [ $\bar{u},\bar{u},0$ ]
2	b	3m.	$1/3,2/3,z$ [0,0,0]	$2/3,1/3,z$ [0,0,0]	
1	a	6'mm'	$0,0,z$ [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p6'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

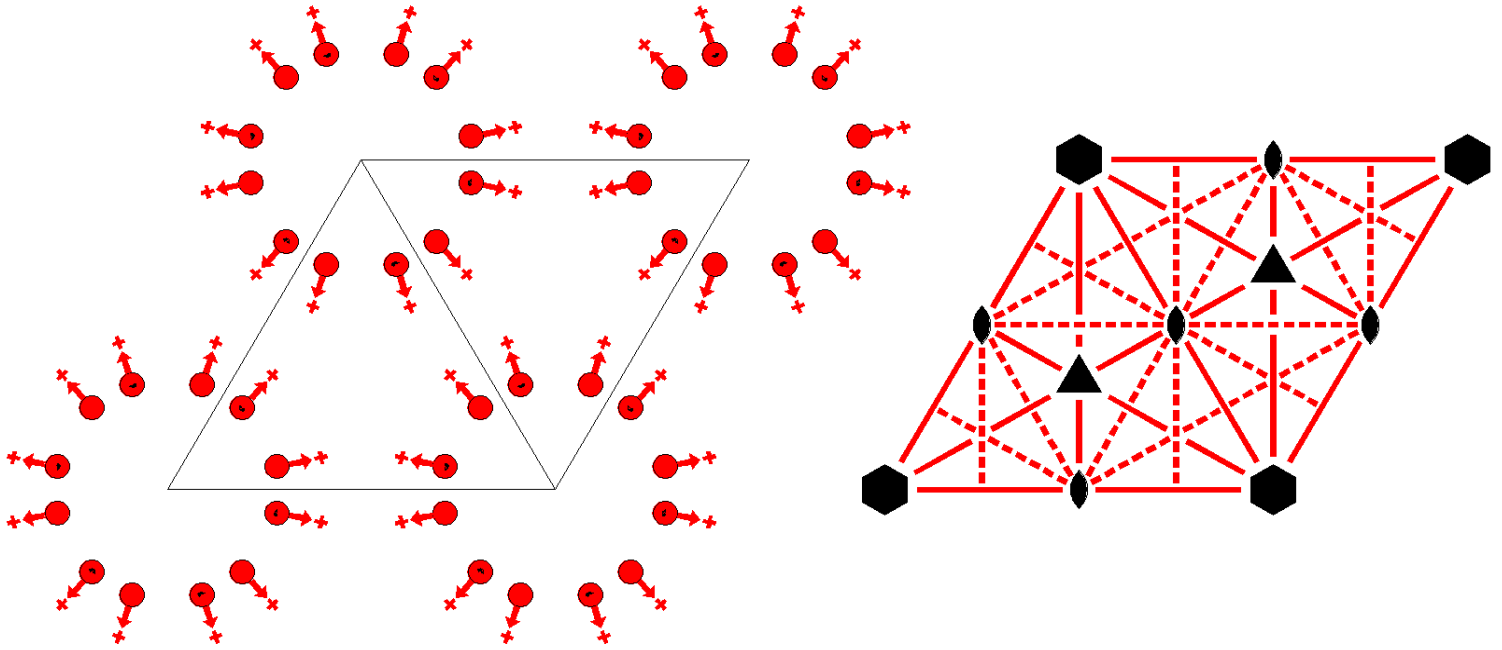
Along [2,1,0] p1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



P6m'm'  
183.5.1419

6m'm'  
P6m'm'

Hexagonal



Origin on 6m'm'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1		

**Symmetry Operations**

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                           | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)       | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) m' x, x̄, z<br>(m <sub>xy</sub>  0,0,0)' | (8) m' x, 2x, z<br>(m <sub>x</sub>  0,0,0)'                       | (9) m' 2x, x, z<br>(m <sub>y</sub>  0,0,0)'                       |
| (10) m' x, x, z<br>(m <sub>3</sub>  0,0,0)'  | (11) m' x, 0, z<br>(m <sub>2</sub>  0,0,0)'                       | (12) m' 0, y, z<br>(m <sub>1</sub>  0,0,0)'                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

### Positions

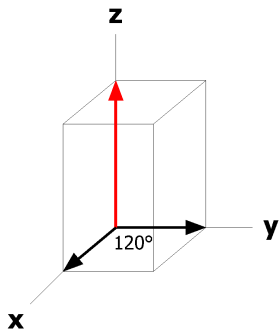
			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
12	f	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(5) $y,\bar{x}+y,z$ [ $v,\bar{u}+v,w$ ]	(6) $x-y,x,z$ [u-v,u,w]
			(7) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{x}+y,y,z$ [ $\bar{u}+v,v,w$ ]	(9) $x,x-y,z$ [u,u-v,w]
			(10) $y,x,z$ [v,u,w]	(11) $x-y,\bar{y},z$ [u-v, $\bar{v},w$ ]	(12) $\bar{x},\bar{x}+y,z$ [ $\bar{u},\bar{u}+v,w$ ]
6	e	.m'	$x,\bar{x},z$ [u, $\bar{u},w$ ]	$x,2x,z$ [u,2u,w]	$2\bar{x},\bar{x},z$ [2 $\bar{u},\bar{u},w$ ]
			$\bar{x},x,z$ [ $\bar{u},u,w$ ]	$\bar{x},2\bar{x},z$ [ $\bar{u},2\bar{u},w$ ]	$2x,x,z$ [2u,u,w]
6	d	..m'	$x,0,z$ [u,0,w]	$0,x,z$ [0,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]
			$\bar{x},0,z$ [ $\bar{u},0,w$ ]	$0,\bar{x},z$ [0, $\bar{u},w$ ]	$x,x,z$ [u,u,w]
3	c	2m'm'	$1/2,0,z$ [0,0,w]	$0,1/2,z$ [0,0,w]	$1/2,1/2,z$ [0,0,w]
2	b	3m'	$1/3,2/3,z$ [0,0,w]	$2/3,1/3,z$ [0,0,w]	
1	a	6m'm'	$0,0,z$ [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] p6m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

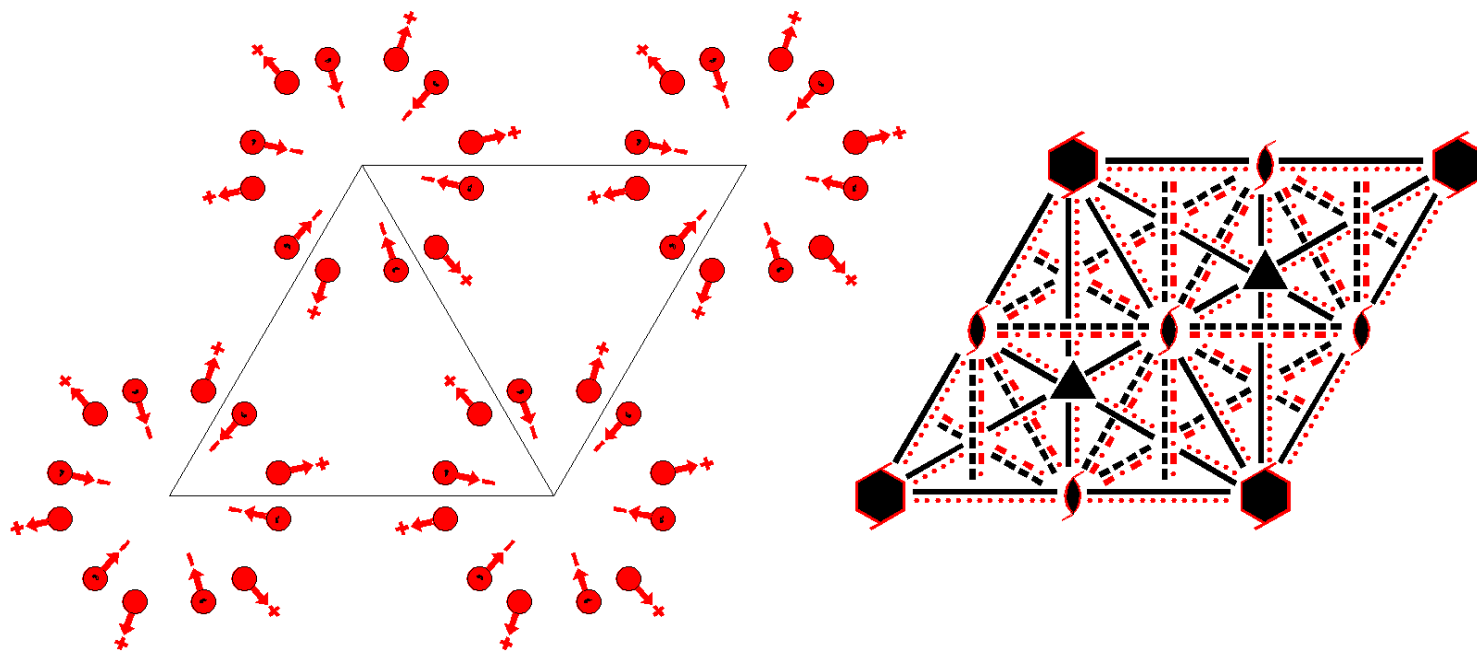
Along [2,1,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$P_{2c} 6mm$   
183.6.1420

$6mm1'$   
 $P_{2c} 6mm$

Hexagonal



Origin on 6mm

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1		

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                          | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)      | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) 2 0,0,z<br>( $2_z$  0,0,0)              | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0) | (6) $6^+$ 0,0,z<br>( $6_z$  0,0,0)      |
| (7) m $x, \bar{x}, z$<br>( $m_{xy}$  0,0,0) | (8) m $x, 2x, z$<br>( $m_x$  0,0,0)     | (9) m $2x, x, z$<br>( $m_y$  0,0,0)     |
| (10) m $x, x, z$<br>( $m_3$  0,0,0)         | (11) m $x, 0, z$<br>( $m_2$  0,0,0)     | (12) m $0, y, z$<br>( $m_1$  0,0,0)     |

## For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 3 <sup>+</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub>  0,0,1)'	(3) 3 <sup>-</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,1)'
(4) 2' (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)'	(5) 6 <sup>-</sup> ' (0,0,1) 0,0,z (6 <sub>z</sub> <sup>-1</sup>  0,0,1)'	(6) 6 <sup>+</sup> ' (0,0,1) 0,0,z (6 <sub>z</sub>  0,0,1)'
(7) c' (0,0,1) x, $\bar{x}$ , z (m <sub>xy</sub>  0,0,1)'	(8) c' (0,0,1) x, 2x, z (m <sub>x</sub>  0,0,1)'	(9) c' (0,0,1) 2x, x, z (m <sub>y</sub>  0,0,1)'
(10) c' (0,0,1) x, x, z (m <sub>3</sub>  0,0,1)'	(11) c' (0,0,1) x, 0, z (m <sub>2</sub>  0,0,1)'	(12) c' (0,0,1) 0, y, z (m <sub>1</sub>  0,0,1)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

**Positions**

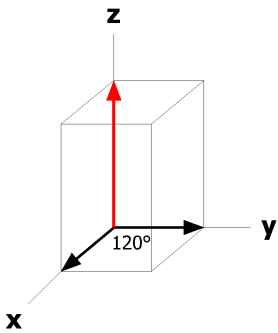
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) + (0,0,1)' +		
24	f	1	(1) x,y,z [u,v,w] (4) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ] (7) $\bar{y}, \bar{x}, z$ [v,u, $\bar{w}$ ] (10) y,x,z [ $\bar{v}, \bar{u}, \bar{w}$ ]	(2) $\bar{y}, x-y, z$ [ $\bar{v}, u-v, w$ ] (5) y, $\bar{x}+y, z$ [v, $\bar{u}+v, w$ ] (8) $\bar{x}+y, y, z$ [u-v, $\bar{v}, \bar{w}$ ] (11) x-y, $\bar{y}, z$ [ $\bar{u}+v, v, \bar{w}$ ]	(3) $\bar{x}+y, \bar{x}, z$ [ $\bar{u}+v, \bar{u}, w$ ] (6) x-y, x, z [u-v, u, w] (9) x, x-y, z [ $\bar{u}, \bar{u}+v, \bar{w}$ ] (12) $\bar{x}, \bar{x}+y, z$ [u, u-v, $\bar{w}$ ]
12	e	.m.	x, $\bar{x}, z$ [u, u, 0] $\bar{x}, x, z$ [ $\bar{u}, \bar{u}, 0$ ]	x, 2x, z [ $\bar{u}, 0, 0$ ] $\bar{x}, 2\bar{x}, z$ [u, 0, 0]	2 $\bar{x}, \bar{x}, z$ [0, $\bar{u}, 0$ ] 2x, x, z [0, u, 0]
12	d	..m	x, 0, z [u, 2u, 0] $\bar{x}, 0, z$ [ $\bar{u}, 2\bar{u}, 0$ ]	0, x, z [2 $\bar{u}, \bar{u}, 0$ ] 0, $\bar{x}, z$ [2u, u, 0]	$\bar{x}, \bar{x}, z$ [u, $\bar{u}, 0$ ] x, x, z [ $\bar{u}, u, 0$ ]
6	c	2mm	1/2, 0, z [0, 0, 0]	0, 1/2, z [0, 0, 0]	1/2, 1/2, z [0, 0, 0]
4	b	3m.	1/3, 2/3, z [0, 0, 0]	2/3, 1/3, z [0, 0, 0]	
2	a	6mm	0, 0, z [0, 0, 0]		

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

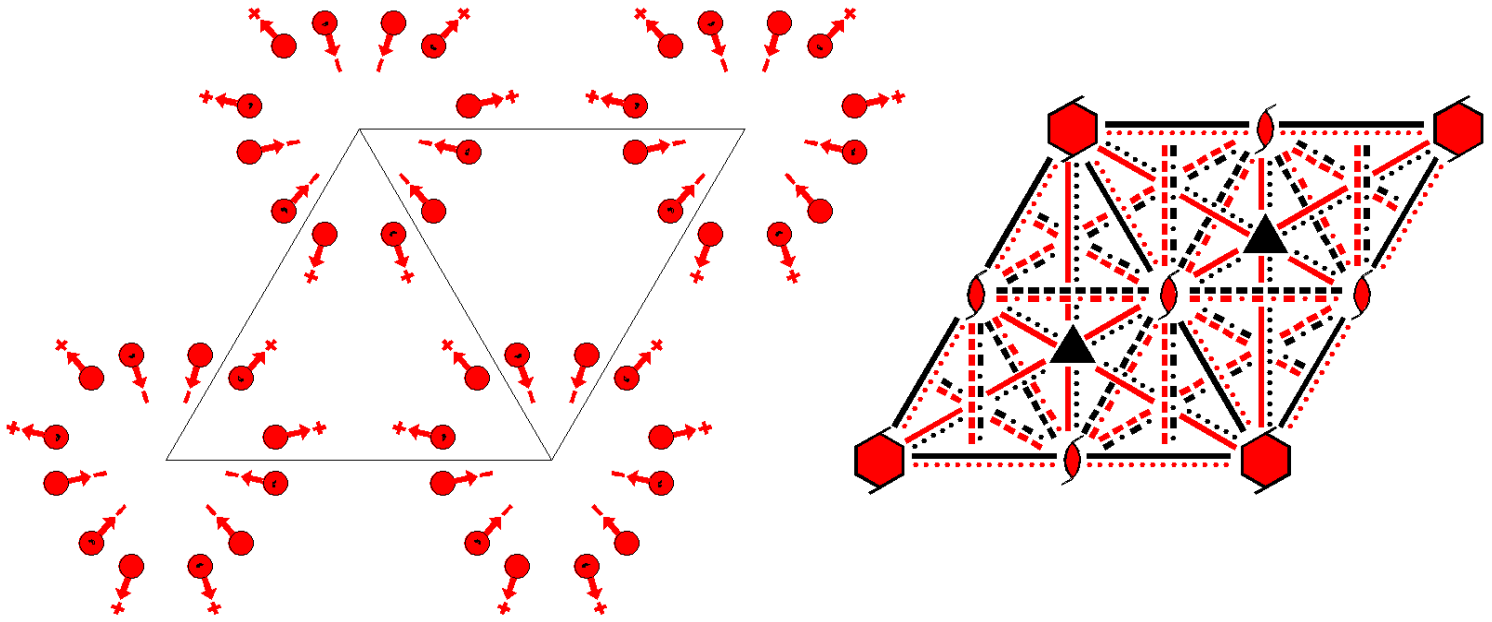
Along [2,1,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x, x/2, 0



$P_{2c} 6'm'm$   
183.7.1421

$6mm1'$   
 $P_{2c} 6'm'm$

Hexagonal



Origin on  $6'm'm$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1		

**Symmetry Operations**

For (0,0,0) + set

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                              | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)       | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) $2'$ 0,0,z<br>( $2_z$  0,0,0)'              | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0)' | (6) $6^+$ 0,0,z<br>( $6_z$  0,0,0)'     |
| (7) $m'$ $x, \bar{x}, z$<br>( $m_{xy}$  0,0,0)' | (8) $m'$ $x, 2x, z$<br>( $m_x$  0,0,0)'  | (9) $m'$ $2x, x, z$<br>( $m_y$  0,0,0)' |
| (10) $m$ $x, x, z$<br>( $m_3$  0,0,0)           | (11) $m$ $x, 0, z$<br>( $m_2$  0,0,0)    | (12) $m$ $0, y, z$<br>( $m_1$  0,0,0)   |

## For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 3 <sup>+</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub>  0,0,1)'	(3) 3 <sup>-</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,1)'
(4) 2 (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)	(5) 6 <sup>-</sup> (0,0,1) 0,0,z (6 <sub>z</sub> <sup>-1</sup>  0,0,1)	(6) 6 <sup>+</sup> (0,0,1) 0,0,z (6 <sub>z</sub>  0,0,1)
(7) c (0,0,1) x, $\bar{x}$ , z (m <sub>xy</sub>  0,0,1)	(8) c (0,0,1) x, 2x, z (m <sub>x</sub>  0,0,1)	(9) c (0,0,1) 2x, x, z (m <sub>y</sub>  0,0,1)
(10) c' (0,0,1) x, x, z (m <sub>3</sub>  0,0,1)'	(11) c' (0,0,1) x, 0, z (m <sub>2</sub>  0,0,1)'	(12) c' (0,0,1) 0, y, z (m <sub>1</sub>  0,0,1)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

**Positions**

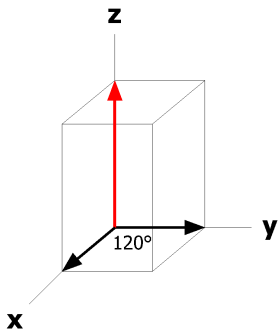
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) + (0,0,1)' +		
24	f	1	(1) x,y,z [u,v,w] (4) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ] (7) $\bar{y}, \bar{x}, z$ [ $\bar{v}, \bar{u}, w$ ] (10) y,x,z [ $\bar{v}, \bar{u}, \bar{w}$ ]	(2) $\bar{y}, x-y, z$ [ $\bar{v}, u-v, w$ ] (5) y, $\bar{x}+y, z$ [ $\bar{v}, u-v, \bar{w}$ ] (8) $\bar{x}+y, y, z$ [ $\bar{u}+v, v, w$ ] (11) x-y, $\bar{y}, z$ [ $\bar{u}+v, v, \bar{w}$ ]	(3) $\bar{x}+y, \bar{x}, z$ [ $\bar{u}+v, \bar{u}, w$ ] (6) x-y, x, z [ $\bar{u}+v, \bar{u}, \bar{w}$ ] (9) x, x-y, z [u, u-v, w] (12) $\bar{x}, \bar{x}+y, z$ [u, u-v, $\bar{w}$ ]
12	e	.m'	x, $\bar{x}, z$ [u, $\bar{u}, w$ ] $\bar{x}, x, z$ [u, $\bar{u}, \bar{w}$ ]	x, 2x, z [u, 2u, w] $\bar{x}, 2\bar{x}, z$ [u, 2u, $\bar{w}$ ]	2 $\bar{x}, \bar{x}, z$ [2 $\bar{u}, \bar{u}, w$ ] 2x, x, z [2 $\bar{u}, \bar{u}, \bar{w}$ ]
12	d	..m	x, 0, z [u, 2u, 0] $\bar{x}, 0, z$ [u, 2u, 0]	0, x, z [2 $\bar{u}, \bar{u}, 0$ ] 0, $\bar{x}, z$ [2 $\bar{u}, \bar{u}, 0$ ]	$\bar{x}, \bar{x}, z$ [u, $\bar{u}, 0$ ] x, x, z [u, $\bar{u}, 0$ ]
6	c	2'm'm	1/2, 0, z [u, 2u, 0]	0, 1/2, z [2 $\bar{u}, \bar{u}, 0$ ]	1/2, 1/2, z [u, $\bar{u}, 0$ ]
4	b	3m'	1/3, 2/3, z [0, 0, w]	2/3, 1/3, z [0, 0, $\bar{w}$ ]	
2	a	6'm'm	0, 0, z [0, 0, 0]		

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>1m1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [2,1,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x, x/2, 0



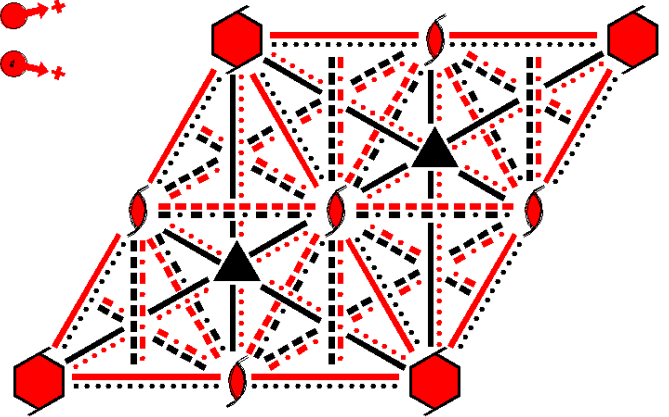
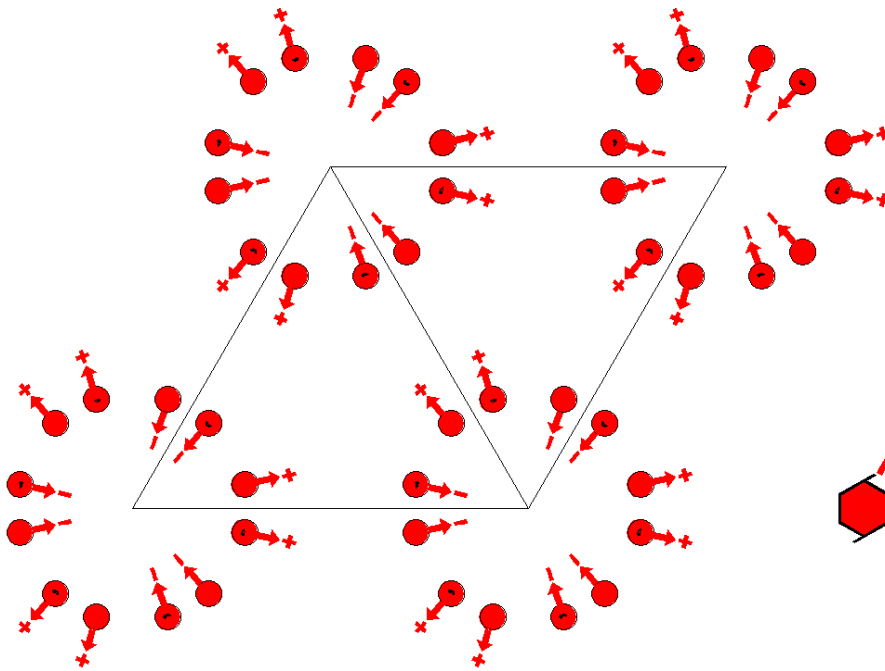
$P_{2c} 6'mm'$

183.8.1422

$6mm1'$

$P_{2c} 6'mm'$

Hexagonal



Origin on  $6'mm'$

Asymmetric unit  $0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/3; \quad 0 \leq z \leq 1; \quad x \leq (1+y)/2; \quad y \leq x/2$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0
	0,0,1	1/2,0,1	2/3,1/3,1

**Symmetry Operations**

For (0,0,0) + set

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                          | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)       | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) $2'$ 0,0,z<br>( $2_z$  0,0,0)'          | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0)' | (6) $6^{+1}$ 0,0,z<br>( $6_z$  0,0,0)'  |
| (7) m $x, \bar{x}, z$<br>( $m_{xy}$  0,0,0) | (8) m $x, 2x, z$<br>( $m_x$  0,0,0)      | (9) m $2x, x, z$<br>( $m_y$  0,0,0)     |
| (10) $m'$ $x, x, z$<br>( $m_3$  0,0,0)'     | (11) $m'$ $x, 0, z$<br>( $m_2$  0,0,0)'  | (12) $m'$ $0, y, z$<br>( $m_1$  0,0,0)' |



## For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 3 <sup>+</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub>  0,0,1)'	(3) 3 <sup>-</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,1)'
(4) 2 (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)	(5) 6 <sup>-</sup> ' (0,0,1) 0,0,z (6 <sub>z</sub> <sup>-1</sup>  0,0,1)	(6) 6 <sup>+</sup> ' (0,0,1) 0,0,z (6 <sub>z</sub>  0,0,1)
(7) c' (0,0,1) x, $\bar{x}$ , z (m <sub>xy</sub>  0,0,1)'	(8) c' (0,0,1) x, 2x, z (m <sub>x</sub>  0,0,1)'	(9) c' (0,0,1) 2x, x, z (m <sub>y</sub>  0,0,1)'
(10) c (0,0,1) x, x, z (m <sub>3</sub>  0,0,1)	(11) c (0,0,1) x, 0, z (m <sub>2</sub>  0,0,1)	(12) c (0,0,1) 0, y, z (m <sub>1</sub>  0,0,1)

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

**Positions**

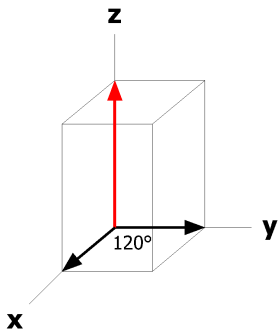
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) + (0,0,1)' +		
24	f	1	(1) x,y,z [u,v,w] (4) $\bar{x}, \bar{y}, z$ [u,v, $\bar{w}$ ] (7) $\bar{y}, \bar{x}, z$ [v,u, $\bar{w}$ ] (10) y,x,z [v,u,w]	(2) $\bar{y}, x-y, z$ [ $\bar{v}, u-v, w$ ] (5) y, $\bar{x}+y, z$ [ $\bar{v}, u-v, \bar{w}$ ] (8) $\bar{x}+y, y, z$ [u-v, $\bar{v}, \bar{w}$ ] (11) x-y, $\bar{y}, z$ [u-v, $\bar{v}, w$ ]	(3) $\bar{x}+y, \bar{x}, z$ [ $\bar{u}+v, \bar{u}, w$ ] (6) x-y, x, z [ $\bar{u}+v, \bar{u}, \bar{w}$ ] (9) x, x-y, z [ $\bar{u}, \bar{u}+v, \bar{w}$ ] (12) $\bar{x}, \bar{x}+y, z$ [ $\bar{u}, \bar{u}+v, w$ ]
12	e	.m.	x, $\bar{x}, z$ [u,u,0] $\bar{x}, x, z$ [u,u,0]	x, 2x, z [ $\bar{u}, 0, 0$ ] $\bar{x}, 2\bar{x}, z$ [ $\bar{u}, 0, 0$ ]	2 $\bar{x}, \bar{x}, z$ [0, $\bar{u}, 0$ ] 2x, x, z [0, $\bar{u}, 0$ ]
12	d	..m'	x, 0, z [u, 0, w] $\bar{x}, 0, z$ [u, 0, $\bar{w}$ ]	0, x, z [0, u, w] 0, $\bar{x}, z$ [0, u, $\bar{w}$ ]	$\bar{x}, \bar{x}, z$ [ $\bar{u}, \bar{u}, w$ ] x, x, z [ $\bar{u}, \bar{u}, \bar{w}$ ]
6	c	2'mm'	1/2, 0, z [u, 0, 0]	0, 1/2, z [0, u, 0]	1/2, 1/2, z [ $\bar{u}, \bar{u}, 0$ ]
4	b	3m.	1/3, 2/3, z [0, 0, 0]	2/3, 1/3, z [0, 0, 0]	
2	a	6'mm'	0, 0, z [0, 0, 0]		

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

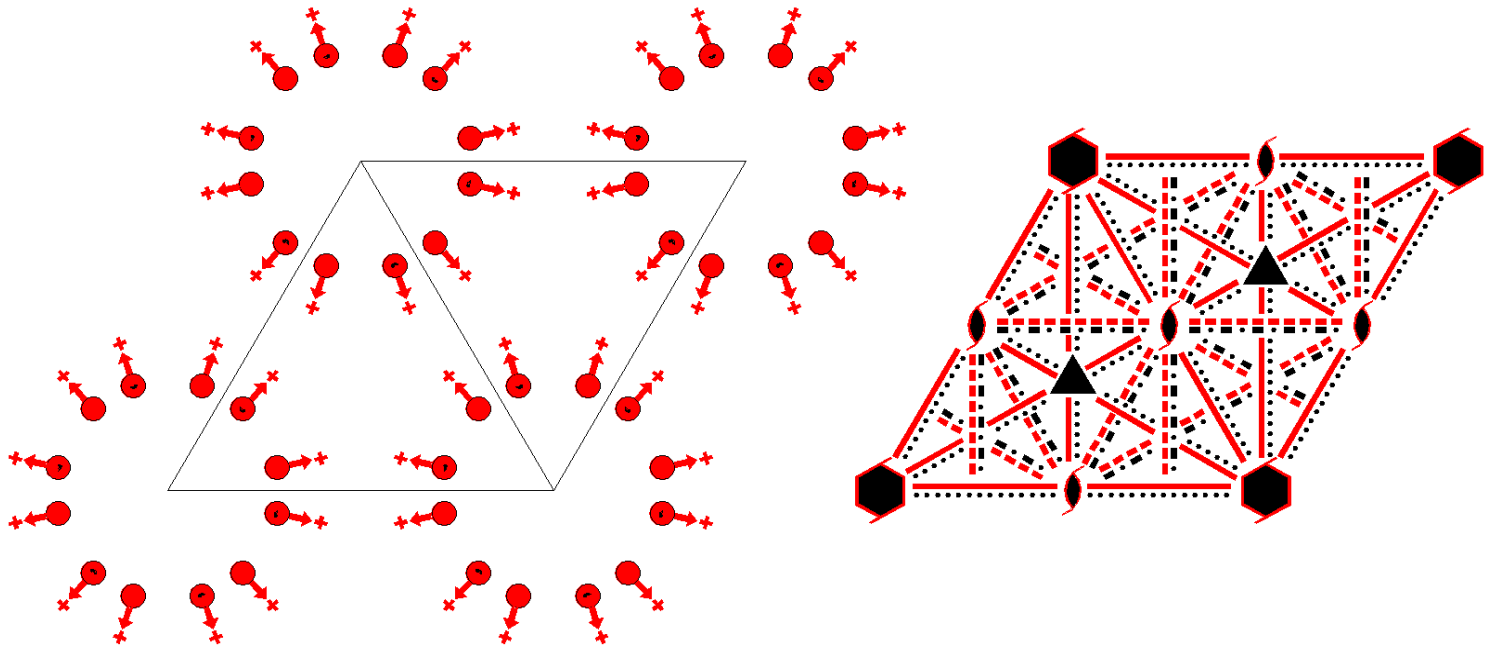
Along [2,1,0] p<sub>2b</sub>1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$P_{2c} 6m'm'$   
183.9.1423

$6mm1'$   
 $P_{2c} 6m'm'$

Hexagonal



Origin on  $6m'm'$

**Asymmetric unit**  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/3$ ;  $0 \leq z \leq 1$ ;  $x \leq (1+y)/2$ ;  $y \leq x/2$

Vertices  $0,0,0$   $1/2,0,0$   $2/3,1/3,0$   
 $0,0,1$   $1/2,0,1$   $2/3,1/3,1$

**Symmetry Operations**

For  $(0,0,0) + \text{set}$

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                              | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)      | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) 2 0,0,z<br>( $2_z$  0,0,0)                  | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0) | (6) $6^+$ 0,0,z<br>( $6_z$  0,0,0)      |
| (7) $m'$ $x, \bar{x}, z$<br>( $m_{xy}$  0,0,0)' | (8) $m'$ $x, 2x, z$<br>( $m_x$  0,0,0)' | (9) $m'$ $2x, x, z$<br>( $m_y$  0,0,0)' |
| (10) $m'$ $x, x, z$<br>( $m_3$  0,0,0)'         | (11) $m'$ $x, 0, z$<br>( $m_2$  0,0,0)' | (12) $m'$ $0, y, z$<br>( $m_1$  0,0,0)' |

## For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 3 <sup>+</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub>  0,0,1)'	(3) 3 <sup>-</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,1)'
(4) 2' (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)'	(5) 6 <sup>-</sup> ' (0,0,1) 0,0,z (6 <sub>z</sub> <sup>-1</sup>  0,0,1)'	(6) 6 <sup>+</sup> ' (0,0,1) 0,0,z (6 <sub>z</sub>  0,0,1)'
(7) c (0,0,1) x, $\bar{x}$ , z (m <sub>xy</sub>  0,0,1)	(8) c (0,0,1) x, 2x, z (m <sub>x</sub>  0,0,1)	(9) c (0,0,1) 2x, x, z (m <sub>y</sub>  0,0,1)
(10) c (0,0,1) x, x, z (m <sub>3</sub>  0,0,1)	(11) c (0,0,1) x, 0, z (m <sub>2</sub>  0,0,1)	(12) c (0,0,1) 0, y, z (m <sub>1</sub>  0,0,1)

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

**Positions**

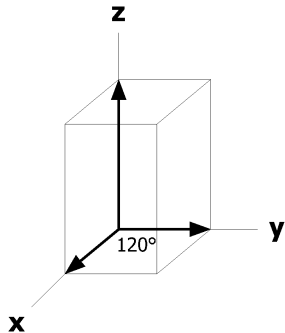
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) + (0,0,1)' +		
24	f	1	(1) x,y,z [u,v,w] (4) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ] (7) $\bar{y}, \bar{x}, z$ [ $\bar{v}, \bar{u}, w$ ] (10) y,x,z [v,u,w]	(2) $\bar{y}, x-y, z$ [ $\bar{v}, u-v, w$ ] (5) y, $\bar{x}+y, z$ [v, $\bar{u}+v, w$ ] (8) $\bar{x}+y, y, z$ [ $\bar{u}+v, v, w$ ] (11) x-y, $\bar{y}, z$ [u-v, $\bar{v}, w$ ]	(3) $\bar{x}+y, \bar{x}, z$ [ $\bar{u}+v, \bar{u}, w$ ] (6) x-y, x, z [u-v, u, w] (9) x, x-y, z [u, u-v, w] (12) $\bar{x}, \bar{x}+y, z$ [ $\bar{u}, \bar{u}+v, w$ ]
12	e	.m'	x, $\bar{x}, z$ [u, $\bar{u}, w$ ] $\bar{x}, x, z$ [ $\bar{u}, u, w$ ]	x, 2x, z [u, 2u, w] $\bar{x}, 2\bar{x}, z$ [ $\bar{u}, 2\bar{u}, w$ ]	2 $\bar{x}, \bar{x}, z$ [2 $\bar{u}, \bar{u}, w$ ] 2x, x, z [2u, u, w]
12	d	..m'	x, 0, z [u, 0, w] $\bar{x}, 0, z$ [ $\bar{u}, 0, w$ ]	0, x, z [0, u, w] 0, $\bar{x}, z$ [0, $\bar{u}, w$ ]	$\bar{x}, \bar{x}, z$ [ $\bar{u}, \bar{u}, w$ ] x, x, z [u, u, w]
6	c	2m'm'	1/2, 0, z [0, 0, w]	0, 1/2, z [0, 0, w]	1/2, 1/2, z [0, 0, w]
4	b	3m'	1/3, 2/3, z [0, 0, w]	2/3, 1/3, z [0, 0, w]	
2	a	6m'm'	0, 0, z [0, 0, w]		

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>1m'1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

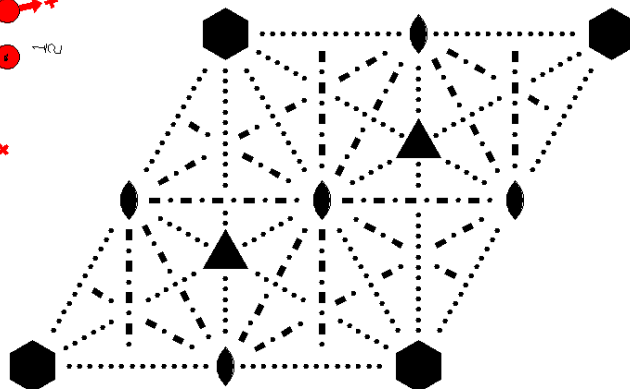
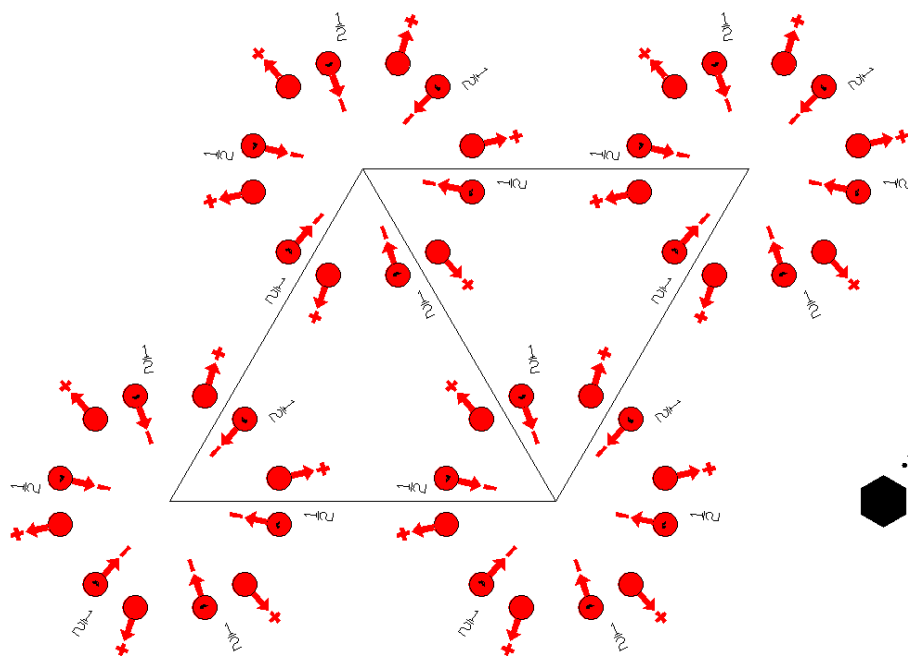
Along [2,1,0] p<sub>2b</sub>1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x, x/2, 0



P6cc  
184.1.1424

6cc  
P6cc

Hexagonal



Origin on 6cc

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

**Symmetry Operations**

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) c (0,0,1/2) x, x̄, z<br>(m <sub>xy</sub>  0,0,1/2) | (8) c (0,0,1/2) x, 2x, z<br>(m <sub>x</sub>  0,0,1/2)             | (9) c (0,0,1/2) 2x, x, z<br>(m <sub>y</sub>  0,0,1/2)             |
| (10) c (0,0,1/2) x, x, z<br>(m <sub>3</sub>  0,0,1/2)  | (11) c (0,0,1/2) x, 0, z<br>(m <sub>2</sub>  0,0,1/2)             | (12) c (0,0,1/2) 0, y, z<br>(m <sub>1</sub>  0,0,1/2)             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

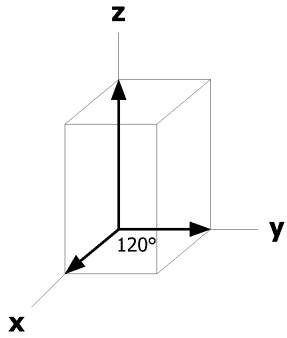
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates											
12	d	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$	(4) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(5) $y,\bar{x}+y,z [v,\bar{u}+v,w]$	(6) $x-y,x,z [u-v,u,w]$	(7) $\bar{y},\bar{x},z+1/2 [v,u,\bar{w}]$	(8) $\bar{x}+y,y,z+1/2 [u-v,\bar{v},\bar{w}]$	(9) $x,x-y,z+1/2 [\bar{u},\bar{u}+v,\bar{w}]$	(10) $y,x,z+1/2 [\bar{v},\bar{u},\bar{w}]$	(11) $x-y,\bar{y},z+1/2 [\bar{u}+v,v,\bar{w}]$	(12) $\bar{x},\bar{x}+y,z+1/2 [u,u-v,\bar{w}]$
6	c	2..	$1/2,0,z [0,0,w]$	$0,1/2,z [0,0,w]$	$1/2,1/2,z [0,0,w]$	$0,1/2,z+1/2 [0,0,\bar{w}]$	$1/2,0,z+1/2 [0,0,\bar{w}]$	$1/2,1/2,z+1/2 [0,0,\bar{w}]$						
4	b	3..	$1/3,2/3,z [0,0,w]$	$2/3,1/3,z [0,0,w]$	$1/3,2/3,z+1/2 [0,0,\bar{w}]$	$2/3,1/3,z+1/2 [0,0,\bar{w}]$								
2	a	6..	$0,0,z [0,0,w]$	$0,0,z+1/2 [0,0,\bar{w}]$										

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2b}1m'1$   
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,0,0$

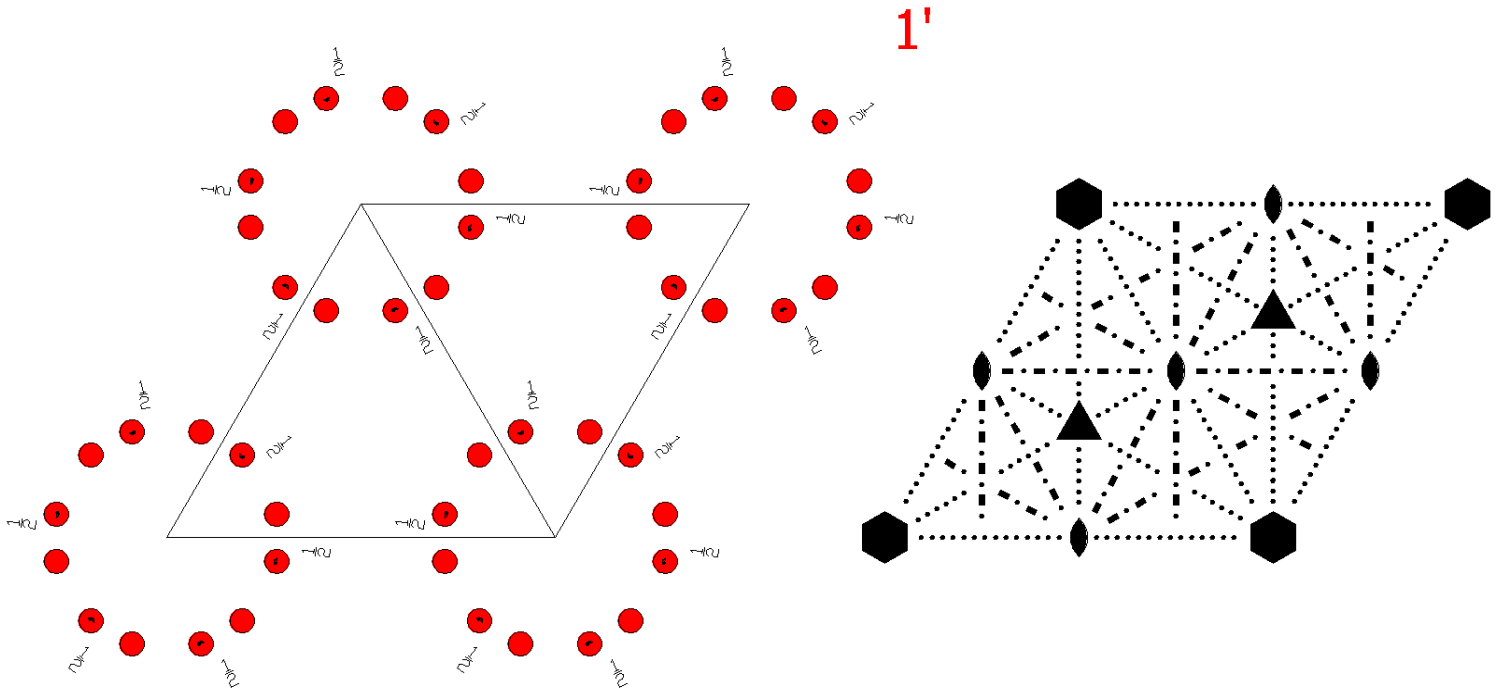
Along  $[2,1,0]$   $p_{2b}1m'1$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x/2,0$



P6cc1'  
184.2.1425

6cc1'  
P6cc1'

Hexagonal



Origin on 6cc1'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

**Symmetry Operations**

For 1 + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                     | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                 | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) c (0,0,1/2) x, x̄, z<br>(m <sub>xy</sub>  0,0,1/2) | (8) c (0,0,1/2) x, 2x, z<br>(m <sub>x</sub>  0,0,1/2)             | (9) c (0,0,1/2) 2x, x, z<br>(m <sub>y</sub>  0,0,1/2)             |
| (10) c (0,0,1/2) x, x, z<br>(m <sub>3</sub>  0,0,1/2)  | (11) c (0,0,1/2) x, 0, z<br>(m <sub>2</sub>  0,0,1/2)             | (12) c (0,0,1/2) 0, y, z<br>(m <sub>1</sub>  0,0,1/2)             |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 3 <sup>+</sup> 1' 0,0,z (3 <sub>z</sub>  0,0,0)'	(3) 3 <sup>-</sup> 1' 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(4) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(5) 6 <sup>-</sup> 1' 0,0,z (6 <sub>z</sub> <sup>-1</sup>  0,0,0)'	(6) 6 <sup>+</sup> 1' 0,0,z (6 <sub>z</sub>  0,0,0)'
(7) c' (0,0,1/2) x, $\bar{x}$ , z (m <sub>xy</sub>  0,0,1/2)'	(8) c' (0,0,1/2) x, 2x, z (m <sub>x</sub>  0,0,1/2)'	(9) c' (0,0,1/2) 2x, x, z (m <sub>y</sub>  0,0,1/2)'
(10) c' (0,0,1/2) x, x, z (m <sub>3</sub>  0,0,1/2)'	(11) c' (0,0,1/2) x, 0, z (m <sub>2</sub>  0,0,1/2)'	(12) c' (0,0,1/2) 0, y, z (m <sub>1</sub>  0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

**Positions**

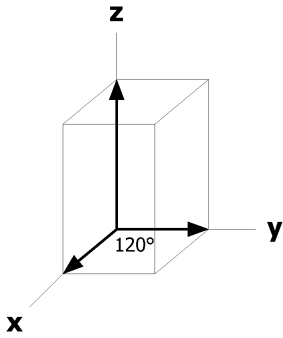
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			1 +		1' +	
12	d	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y, \bar{x}, z$ [0,0,0]	
			(4) $\bar{x}, \bar{y}, z$ [0,0,0]	(5) y, $\bar{x}+y, z$ [0,0,0]	(6) x-y,x,z [0,0,0]	
			(7) $\bar{y}, \bar{x}, z+1/2$ [0,0,0]	(8) $\bar{x}+y, y, z+1/2$ [0,0,0]	(9) x,x-y,z+1/2 [0,0,0]	
			(10) y,x,z+1/2 [0,0,0]	(11) x-y, $\bar{y}, z+1/2$ [0,0,0]	(12) $\bar{x}, \bar{x}+y, z+1/2$ [0,0,0]	
6	c	2..1'	1/2,0,z [0,0,0]	0,1/2,z [0,0,0]	1/2,1/2,z [0,0,0]	
			0,1/2,z+1/2 [0,0,0]	1/2,0,z+1/2 [0,0,0]	1/2,1/2,z+1/2 [0,0,0]	
4	b	3..1'	1/3,2/3,z [0,0,0]	2/3,1/3,z [0,0,0]	1/3,2/3,z+1/2 [0,0,0]	2/3,1/3,z+1/2 [0,0,0]
2	a	6..1'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

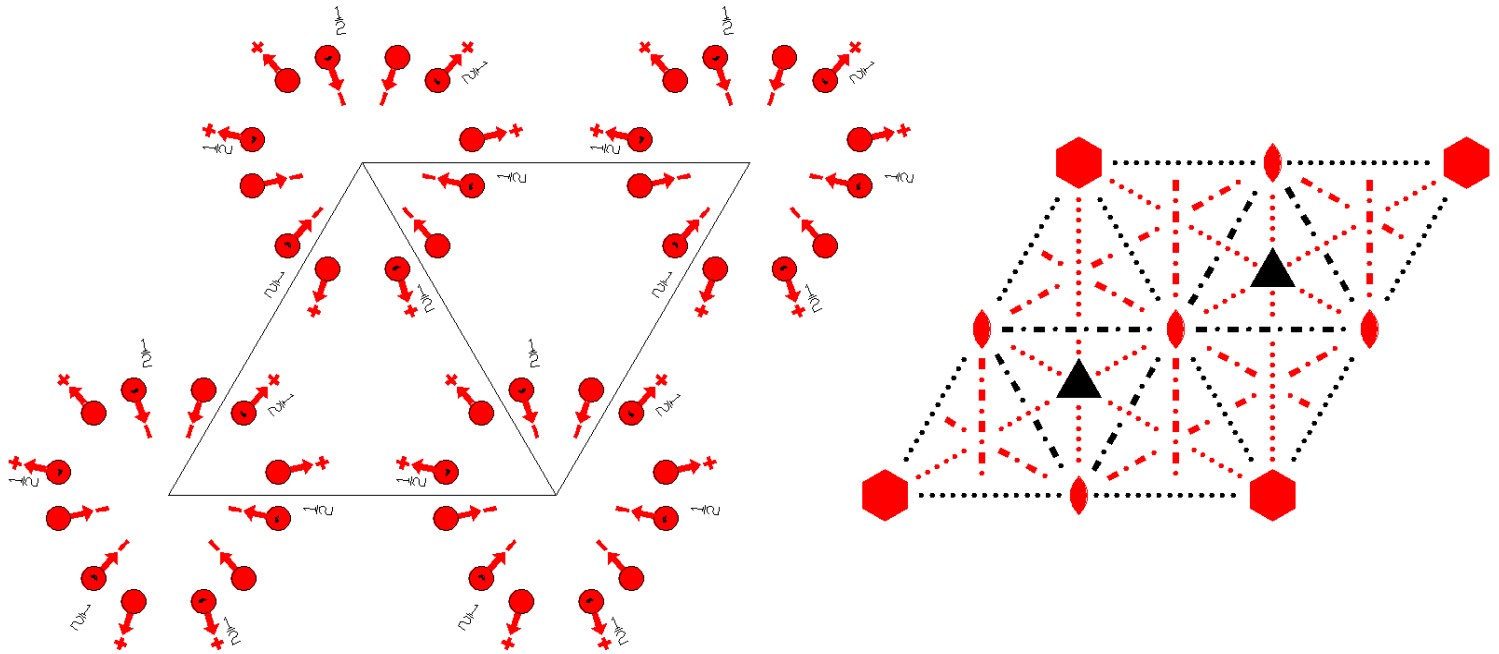
Along [2,1,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x/2,0



P6'c'c  
184.3.1426

6'c'c  
P6'c'c

Hexagonal



Origin on 6'c'c

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/2,1/2,1/2	

**Symmetry Operations**

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)                | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                 | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)'              |
| (7) c' (0,0,1/2) x, x̄, z<br>(m <sub>xy</sub>  0,0,1/2)' | (8) c' (0,0,1/2) x, 2x, z<br>(m <sub>x</sub>  0,0,1/2)'            | (9) c' (0,0,1/2) 2x, x, z<br>(m <sub>y</sub>  0,0,1/2)'           |
| (10) c (0,0,1/2) x, x, z<br>(m <sub>3</sub>  0,0,1/2)    | (11) c (0,0,1/2) x, 0, z<br>(m <sub>2</sub>  0,0,1/2)              | (12) c (0,0,1/2) 0, y, z<br>(m <sub>1</sub>  0,0,1/2)             |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

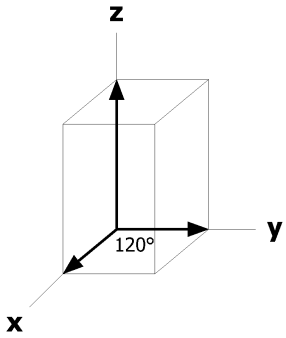
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates					
12	d	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]	(4) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(5) $y,\bar{x}+y,z$ [ $\bar{v},u-v,\bar{w}$ ]	(6) $x-y,x,z$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]
			(7) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{x}+y,y,z+1/2$ [ $\bar{u}+v,v,w$ ]	(9) $x,x-y,z+1/2$ [u,u-v,w]	(10) $y,x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(11) $x-y,\bar{y},z+1/2$ [ $\bar{u}+v,v,\bar{w}$ ]	(12) $\bar{x},\bar{x}+y,z+1/2$ [u,u-v, $\bar{w}$ ]
6	c	2'..	1/2,0,z [u,v,0]	0,1/2,z [ $\bar{v},u-v,0$ ]	1/2,1/2,z [ $\bar{u}+v,\bar{u},0$ ]	0,1/2,z+1/2 [ $\bar{v},\bar{u},0$ ]	1/2,0,z+1/2 [ $\bar{u}+v,v,0$ ]	1/2,1/2,z+1/2 [u,u-v,0]
4	b	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0, $\bar{w}$ ]	1/3,2/3,z+1/2 [0,0,w]	2/3,1/3,z+1/2 [0,0, $\bar{w}$ ]		
2	a	6'..	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]				

**Symmetry of Special Projections**

Along [0,0,1] p6'm'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

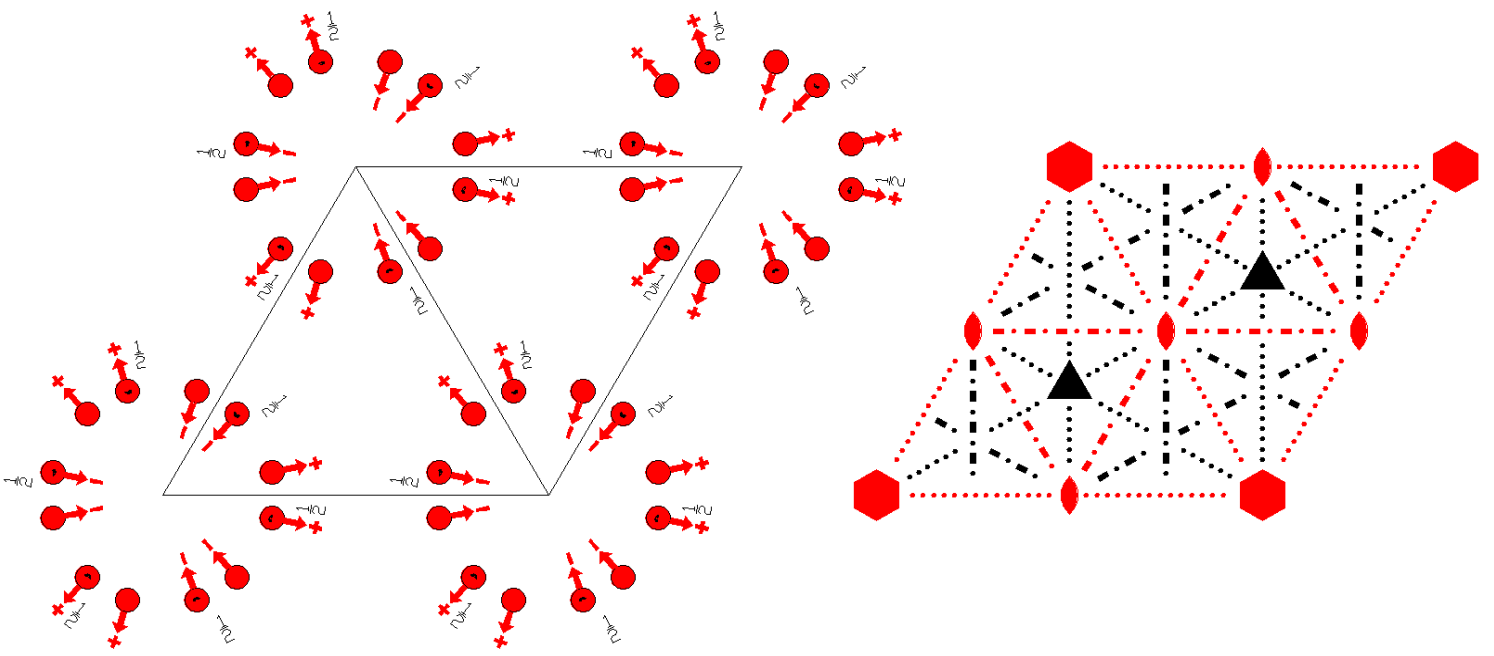
Along [2,1,0] p<sub>2b</sub>'1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x/2,0



P6'cc'  
184.4.1427

6'cc'  
P6'cc'

Hexagonal



Origin on 6'cc'

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$ ;  $x \leq (1+y)/2$ ;  $y \leq \min(1-x, x)$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/2,1/2,1/2

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)                | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                      | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)'              |
| (7) c (0,0,1/2) $x, \bar{x}, z$<br>(m <sub>xy</sub>  0,0,1/2) | (8) c (0,0,1/2) $x, 2x, z$<br>(m <sub>x</sub>  0,0,1/2)            | (9) c (0,0,1/2) $2x, x, z$<br>(m <sub>y</sub>  0,0,1/2)           |
| (10) c' (0,0,1/2) $x, x, z$<br>(m <sub>3</sub>  0,0,1/2)'     | (11) c' (0,0,1/2) $x, 0, z$<br>(m <sub>2</sub>  0,0,1/2)'          | (12) c' (0,0,1/2) $0, y, z$<br>(m <sub>1</sub>  0,0,1/2)'         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

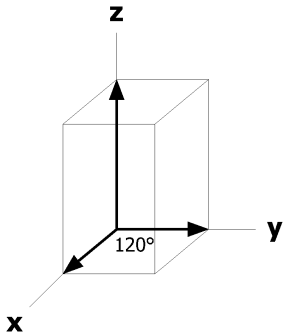
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	d	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]	
			(4) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(5) $y,\bar{x}+y,z$ [ $\bar{v},u-v,\bar{w}$ ]	(6) $x-y,x,z$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]	
			(7) $\bar{y},\bar{x},z+1/2$ [v,u, $\bar{w}$ ]	(8) $\bar{x}+y,y,z+1/2$ [u-v, $\bar{v},\bar{w}$ ]	(9) $x,x-y,z+1/2$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]	
			(10) $y,x,z+1/2$ [v,u,w]	(11) $x-y,\bar{y},z+1/2$ [u-v, $\bar{v},w$ ]	(12) $\bar{x},\bar{x}+y,z+1/2$ [ $\bar{u},\bar{u}+v,w$ ]	
6	c	2'..	1/2,0,z [u,v,0]	0,1/2,z [ $\bar{v},u-v,0$ ]	1/2,1/2,z [ $\bar{u}+v,\bar{u},0$ ]	
			0,1/2,z+1/2 [v,u,0]	1/2,0,z+1/2 [u-v, $\bar{v},0$ ]	1/2,1/2,z+1/2 [ $\bar{u},\bar{u}+v,0$ ]	
4	b	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0, $\bar{w}$ ]	1/3,2/3,z+1/2 [0,0, $\bar{w}$ ]	2/3,1/3,z+1/2 [0,0,w]
2	a	6'..	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p6'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2b}1m1$   
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

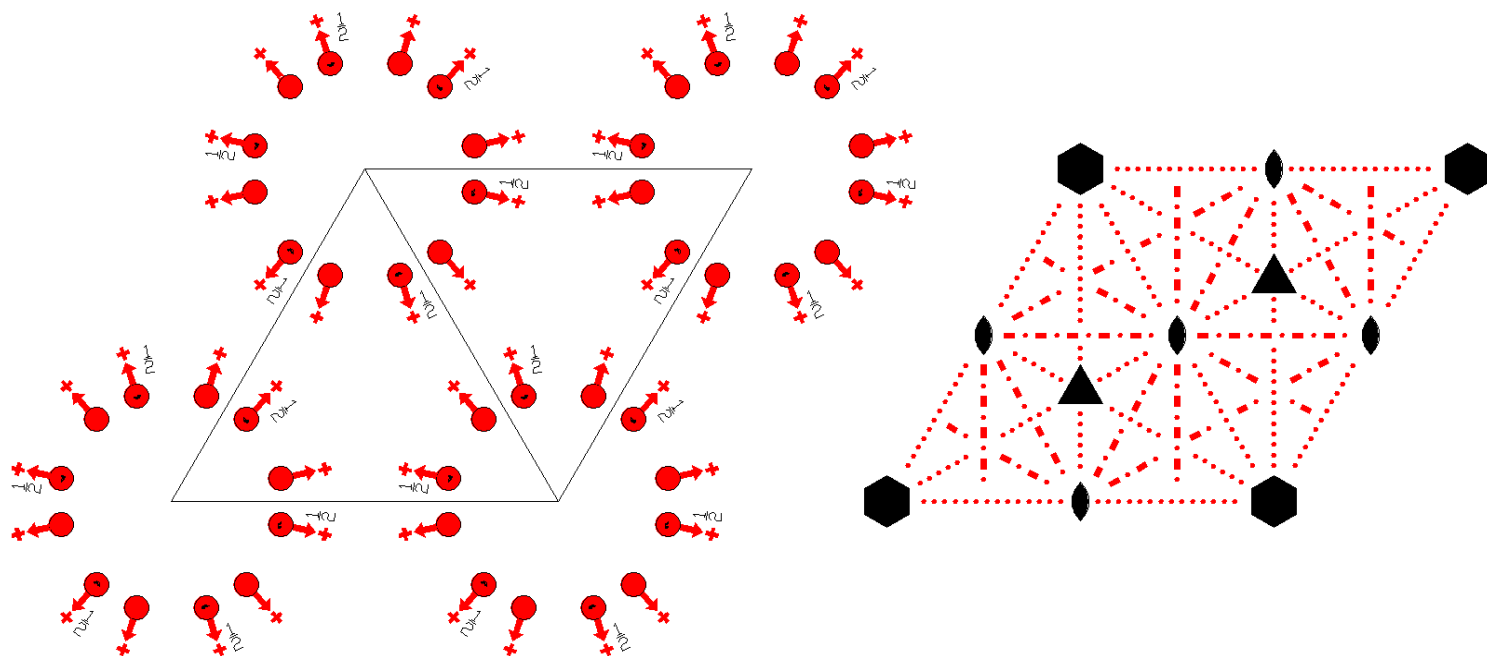
Along [2,1,0] p1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x/2,0



P6c'c'  
184.5.1428

6c'c'  
P6c'c'

Hexagonal



Origin on 6c'c'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/2,1/2,1/2	

**Symmetry Operations**

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                   | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) c' (0,0,1/2) x, x̄, z<br>(m <sub>xy</sub>  0,0,1/2)' | (8) c' (0,0,1/2) x, 2x, z<br>(m <sub>x</sub>  0,0,1/2)'           | (9) c' (0,0,1/2) 2x, x, z<br>(m <sub>y</sub>  0,0,1/2)'           |
| (10) c' (0,0,1/2) x, x, z<br>(m <sub>3</sub>  0,0,1/2)'  | (11) c' (0,0,1/2) x, 0, z<br>(m <sub>2</sub>  0,0,1/2)'           | (12) c' (0,0,1/2) 0, y, z<br>(m <sub>1</sub>  0,0,1/2)'           |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

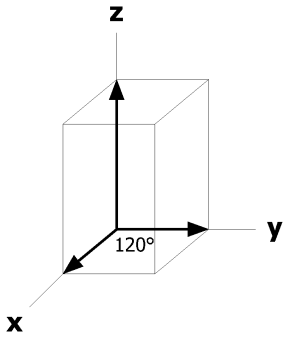
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates				
12	d	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]		
			(4) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(5) $y,\bar{x}+y,z$ [ $v,\bar{u}+v,w$ ]	(6) $x-y,x,z$ [u-v,u,w]		
			(7) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{x}+y,y,z+1/2$ [ $\bar{u}+v,v,w$ ]	(9) $x,x-y,z+1/2$ [u,u-v,w]		
			(10) $y,x,z+1/2$ [v,u,w]	(11) $x-y,\bar{y},z+1/2$ [u-v, $\bar{v},w$ ]	(12) $\bar{x},\bar{x}+y,z+1/2$ [ $\bar{u},\bar{u}+v,w$ ]		
6	c	2..	$1/2,0,z$ [0,0,w]	$0,1/2,z$ [0,0,w]	$1/2,1/2,z$ [0,0,w]		
			$0,1/2,z+1/2$ [0,0,w]	$1/2,0,z+1/2$ [0,0,w]	$1/2,1/2,z+1/2$ [0,0,w]		
4	b	3..	$1/3,2/3,z$ [0,0,w]	$2/3,1/3,z$ [0,0,w]	$1/3,2/3,z+1/2$ [0,0,w]	$2/3,1/3,z+1/2$ [0,0,w]	
2	a	6..	$0,0,z$ [0,0,w]	$0,0,z+1/2$ [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] p6m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [2,1,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x/2,0



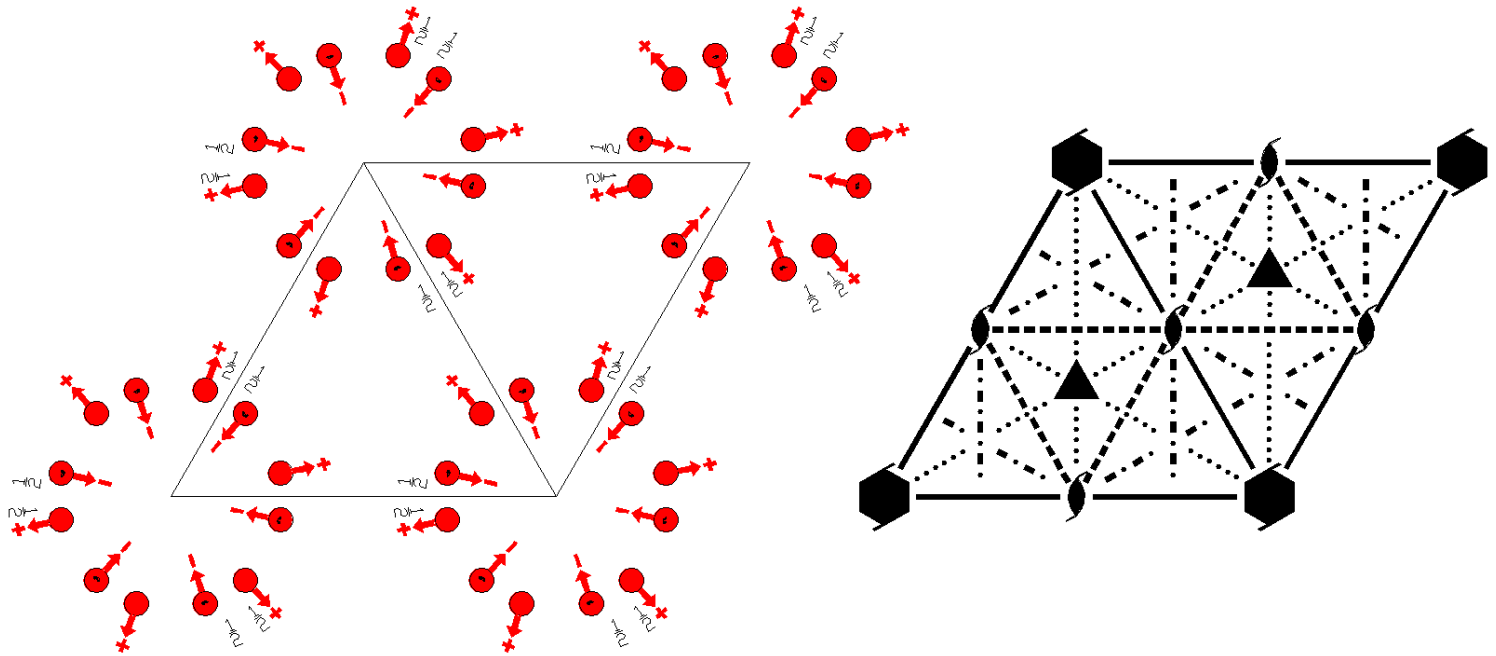
$P6_3 cm$

6mm

Hexagonal

185.1.1429

$P6_3 cm$



Origin on  $31m$  at  $6_3 cm$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/2,1/2,1/2	

**Symmetry Operations**

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                                      | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)         |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)              | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)  |
| (7) c (0,0,1/2) $x, \bar{x}, z$<br>( $m_{xy}$  0,0,1/2) | (8) c (0,0,1/2) $x, 2x, z$<br>( $m_x$  0,0,1/2)     | (9) c (0,0,1/2) $2x, x, z$<br>( $m_y$  0,0,1/2) |
| (10) m $x, x, z$<br>( $m_3$  0,0,0)                     | (11) m $x, 0, z$<br>( $m_2$  0,0,0)                 | (12) m $0, y, z$<br>( $m_1$  0,0,0)             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

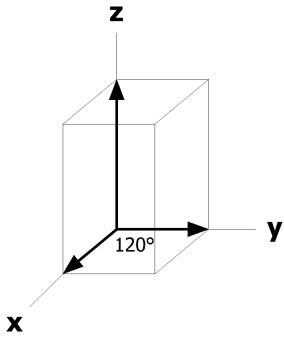
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	d	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y$ , $\bar{x}$ ,z [ $\bar{u}+v$ , $\bar{u}$ ,w]	
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(5) y, $\bar{x}+y$ ,z+1/2 [v, $\bar{u}+v$ ,w]	(6) x-y,x,z+1/2 [u-v,u,w]	
			(7) $\bar{y}$ , $\bar{x}$ ,z+1/2 [v,u, $\bar{w}$ ]	(8) $\bar{x}+y$ ,y,z+1/2 [u-v, $\bar{v}$ , $\bar{w}$ ]	(9) x,x-y,z+1/2 [ $\bar{u}$ , $\bar{u}+v$ , $\bar{w}$ ]	
			(10) y,x,z [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(11) x-y, $\bar{y}$ ,z [ $\bar{u}+v$ ,v, $\bar{w}$ ]	(12) $\bar{x}$ , $\bar{x}+y$ ,z [u,u-v, $\bar{w}$ ]	
6	c	..m	x,0,z [u,2u,0]	0,x,z [2 $\bar{u}$ , $\bar{u}$ ,0]	$\bar{x}$ , $\bar{x}$ ,z [u, $\bar{u}$ ,0]	
			$\bar{x}$ ,0,z+1/2 [ $\bar{u}$ ,2 $\bar{u}$ ,0]	0, $\bar{x}$ ,z+1/2 [2u,u,0]	x,x,z+1/2 [ $\bar{u}$ ,u,0]	
4	b	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z+1/2 [0,0,w]	1/3,2/3,z+1/2 [0,0, $\bar{w}$ ]	2/3,1/3,z [0,0, $\bar{w}$ ]
2	a	3.m	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p6mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>\* 1m1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [2,1,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



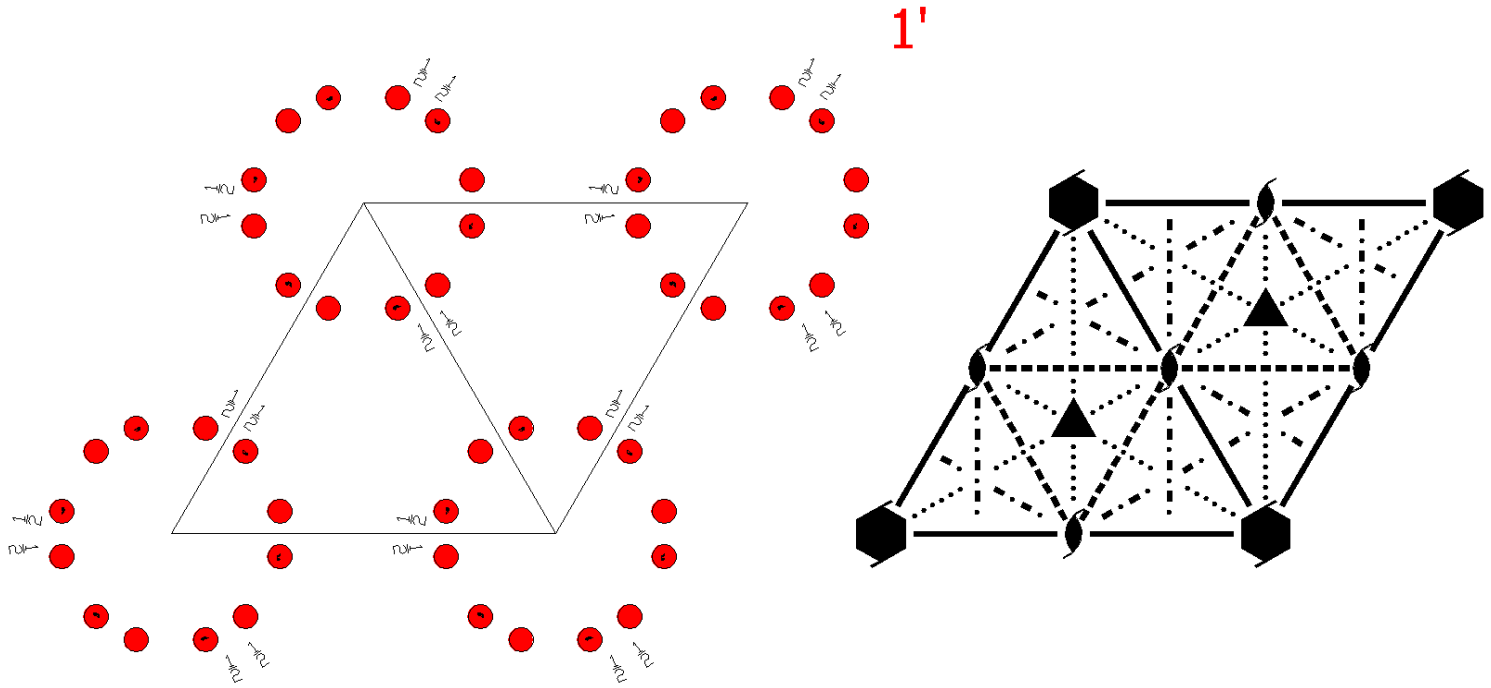
$P6_3 cm1'$

185.2.1430

$6mm1'$

$P6_3 cm1'$

Hexagonal



Origin on  $31m1'$  at  $6_3cm1'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/2,1/2,1/2	

**Symmetry Operations**

For 1 + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                                      | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)         |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)              | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)  |
| (7) c (0,0,1/2) $x, \bar{x}, z$<br>( $m_{xy}$  0,0,1/2) | (8) c (0,0,1/2) $x, 2x, z$<br>( $m_x$  0,0,1/2)     | (9) c (0,0,1/2) $2x, x, z$<br>( $m_y$  0,0,1/2) |
| (10) m $x, x, z$<br>( $m_3$  0,0,0)                     | (11) m $x, 0, z$<br>( $m_2$  0,0,0)                 | (12) m $0, y, z$<br>( $m_1$  0,0,0)             |



## For 1' + set

(1) 1' (1 0,0,0)'	(2) 3 <sup>+</sup> 0,0,z (3 <sub>z</sub>  0,0,0)'	(3) 3 <sup>-</sup> 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(4) 2' (0,0,1/2) 0,0,z (2 <sub>z</sub>  0,0,1/2)'	(5) 6 <sup>-</sup> (0,0,1/2) 0,0,z (6 <sub>z</sub> <sup>-1</sup>  0,0,1/2)'	(6) 6 <sup>+</sup> (0,0,1/2) 0,0,z (6 <sub>z</sub>  0,0,1/2)'
(7) c' (0,0,1/2) x, $\bar{x}$ , z (m <sub>xy</sub>  0,0,1/2)'	(8) c' (0,0,1/2) x, 2x, z (m <sub>x</sub>  0,0,1/2)'	(9) c' (0,0,1/2) 2x, x, z (m <sub>y</sub>  0,0,1/2)'
(10) m' x, x, z (m <sub>3</sub>  0,0,0)'	(11) m' x, 0, z (m <sub>2</sub>  0,0,0)'	(12) m' 0, y, z (m <sub>1</sub>  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

**Positions**

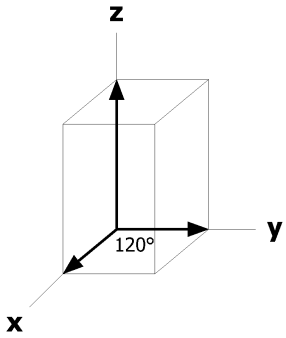
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			1 +		1' +	
12	d	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y, \bar{x}, z$ [0,0,0]	
			(4) $\bar{x}, \bar{y}, z+1/2$ [0,0,0]	(5) y, $\bar{x}+y, z+1/2$ [0,0,0]	(6) x-y,x,z+1/2 [0,0,0]	
			(7) $\bar{y}, \bar{x}, z+1/2$ [0,0,0]	(8) $\bar{x}+y, y, z+1/2$ [0,0,0]	(9) x,x-y,z+1/2 [0,0,0]	
			(10) y,x,z [0,0,0]	(11) x-y, $\bar{y}, z$ [0,0,0]	(12) $\bar{x}, \bar{x}+y, z$ [0,0,0]	
6	c	..m1'	x,0,z [0,0,0]	0,x,z [0,0,0]	$\bar{x}, \bar{x}, z$ [0,0,0]	
			$\bar{x}, 0, z+1/2$ [0,0,0]	0, $\bar{x}, z+1/2$ [0,0,0]	x,x,z+1/2 [0,0,0]	
4	b	3..1'	1/3, 2/3, z [0,0,0]	2/3, 1/3, z+1/2 [0,0,0]	1/3, 2/3, z+1/2 [0,0,0]	2/3, 1/3, z [0,0,0]
2	a	3.m1'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

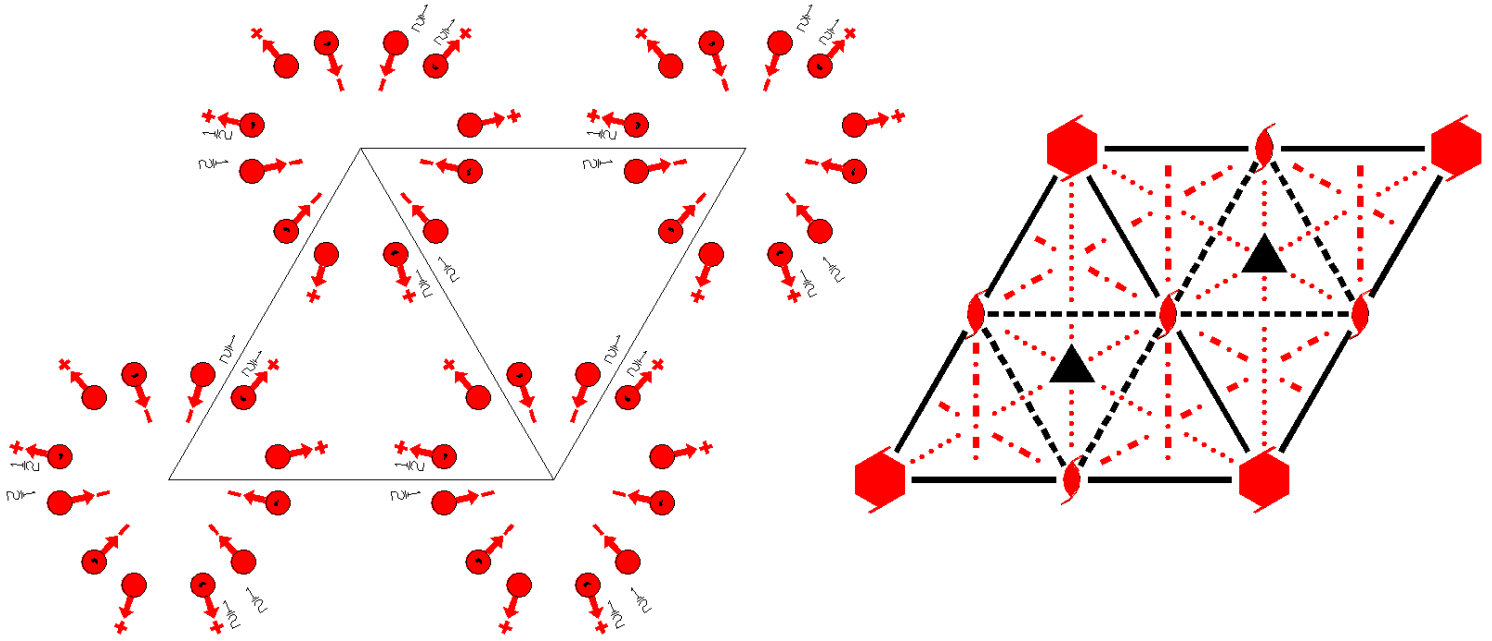
Along [2,1,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



$P6_3'c'm$   
185.3.1431

$6'm'm$   
 $P6_3'c'm$

Hexagonal



Origin on  $31m$  at  $6_3'c'm$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/2,1/2,1/2	

**Symmetry Operations**

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                    | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)             |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)'              | (5) $6^-'$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)' | (6) $6^+'$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)'    |
| (7) $c'$ (0,0,1/2) $x, \bar{x}, z$<br>( $m_{xy}$  0,0,1/2)' | (8) $c'$ (0,0,1/2) $x, 2x, z$<br>( $m_x$  0,0,1/2)'   | (9) $c'$ (0,0,1/2) $2x, x, z$<br>( $m_y$  0,0,1/2)' |
| (10) $m$ $x, x, z$<br>( $m_3$  0,0,0)                       | (11) $m$ $x, 0, z$<br>( $m_2$  0,0,0)                 | (12) $m$ $0, y, z$<br>( $m_1$  0,0,0)               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

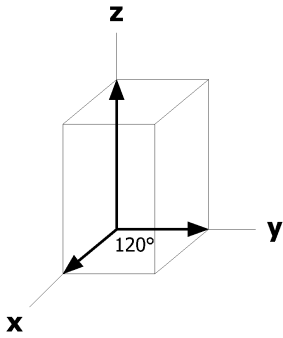
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	d	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]	
			(4) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(5) $y,\bar{x}+y,z+1/2$ [ $\bar{v},u-v,\bar{w}$ ]	(6) x-y,x,z+1/2 [ $\bar{u}+v,\bar{u},\bar{w}$ ]	
			(7) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{x}+y,y,z+1/2$ [ $\bar{u}+v,v,w$ ]	(9) x,x-y,z+1/2 [u,u-v,w]	
			(10) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]	(11) x-y, $\bar{y},z$ [ $\bar{u}+v,v,\bar{w}$ ]	(12) $\bar{x},\bar{x}+y,z$ [u,u-v, $\bar{w}$ ]	
6	c	..m	x,0,z [u,2u,0]	0,x,z [2 $\bar{u},\bar{u},0$ ]	$\bar{x},\bar{x},z$ [u, $\bar{u},0$ ]	
			$\bar{x},0,z+1/2$ [u,2u,0]	0, $\bar{x},z+1/2$ [2 $\bar{u},\bar{u},0$ ]	x,x,z+1/2 [u, $\bar{u},0$ ]	
4	b	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z+1/2 [0,0, $\bar{w}$ ]	1/3,2/3,z+1/2 [0,0,w]	2/3,1/3,z [0,0, $\bar{w}$ ]
2	a	3.m	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p6'm'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [2,1,0] p1g11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



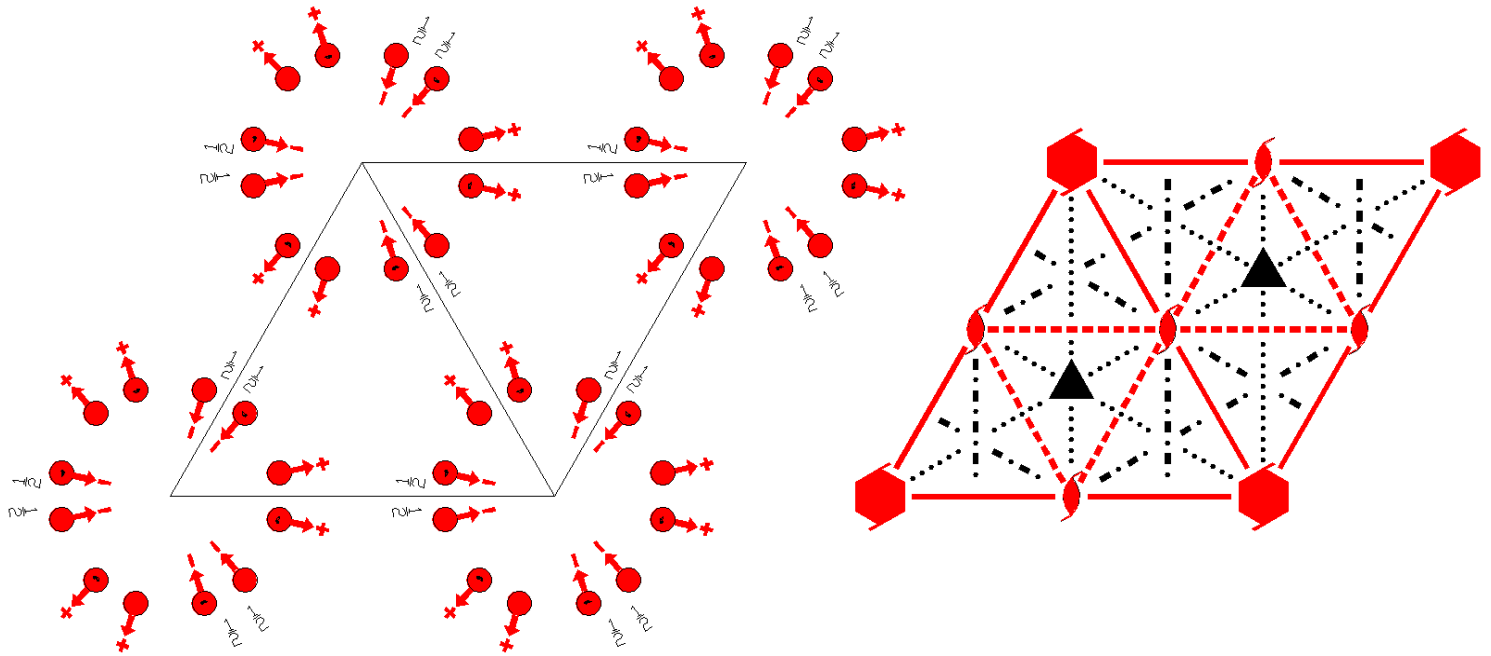
$P6_3'$ 'cm'

185.4.1432

6'mm'

$P6_3'$ 'cm'

Hexagonal



Origin on  $31m'$  at  $6_3'$ 'cm'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/2,1/2,1/2	

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                                      | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                   | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)         |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)'          | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)' | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)' |
| (7) c (0,0,1/2) $x, \bar{x}, z$<br>( $m_{xy}$  0,0,1/2) | (8) c (0,0,1/2) $x, 2x, z$<br>( $m_x$  0,0,1/2)      | (9) c (0,0,1/2) $2x, x, z$<br>( $m_y$  0,0,1/2) |
| (10) $m'$ $x, x, z$<br>( $m_3$  0,0,0)'                 | (11) $m'$ $x, 0, z$<br>( $m_2$  0,0,0)'              | (12) $m'$ $0, y, z$<br>( $m_1$  0,0,0)'         |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

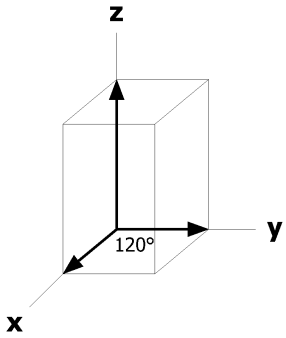
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	d	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]	
			(4) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(5) $y,\bar{x}+y,z+1/2$ [ $\bar{v},u-v,\bar{w}$ ]	(6) x-y,x,z+1/2 [ $\bar{u}+v,\bar{u},\bar{w}$ ]	
			(7) $\bar{y},\bar{x},z+1/2$ [v,u, $\bar{w}$ ]	(8) $\bar{x}+y,y,z+1/2$ [u-v, $\bar{v},\bar{w}$ ]	(9) x,x-y,z+1/2 [ $\bar{u},\bar{u}+v,\bar{w}$ ]	
			(10) y,x,z [v,u,w]	(11) x-y, $\bar{y},z$ [u-v, $\bar{v},w$ ]	(12) $\bar{x},\bar{x}+y,z$ [ $\bar{u},\bar{u}+v,w$ ]	
6	c	..m'	x,0,z [u,0,w]	0,x,z [0,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	
			$\bar{x},0,z+1/2$ [u,0, $\bar{w}$ ]	0, $\bar{x},z+1/2$ [0,u, $\bar{w}$ ]	x,x,z+1/2 [ $\bar{u},\bar{u},\bar{w}$ ]	
4	b	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z+1/2 [0,0, $\bar{w}$ ]	1/3,2/3,z+1/2 [0,0, $\bar{w}$ ]	2/3,1/3,z [0,0,w]
2	a	3.m'	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p6'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2b</sub>\* 1m'1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [2,1,0] p1g1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



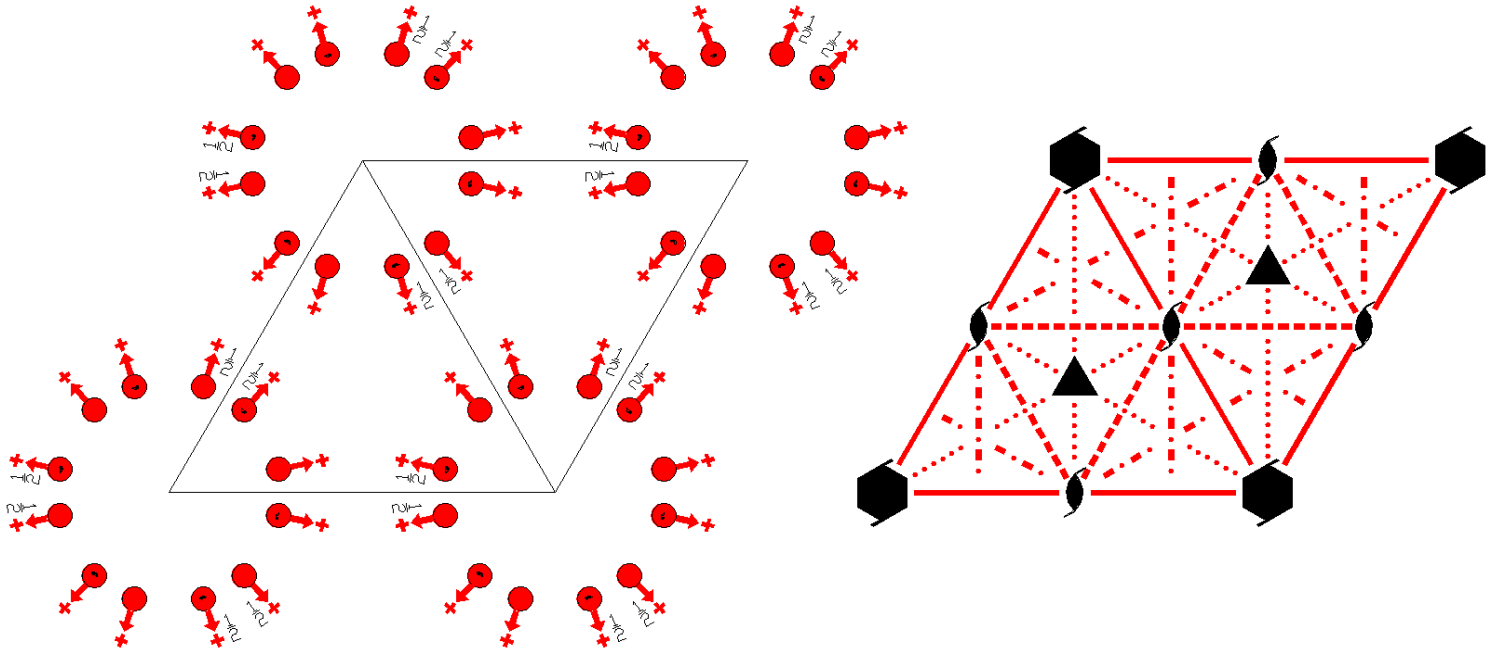
$P6_3 c'm'$

185.5.1433

$6m'm'$

$P6_3 c'm'$

Hexagonal



Origin on  $31m'$  at  $6_3 c'm'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2	1/2,1/2,1/2	

**Symmetry Operations**

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)             |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)                  | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)      |
| (7) $c'$ (0,0,1/2) $x, \bar{x}, z$<br>( $m_{xy}$  0,0,1/2)' | (8) $c'$ (0,0,1/2) $x, 2x, z$<br>( $m_x$  0,0,1/2)' | (9) $c'$ (0,0,1/2) $2x, x, z$<br>( $m_y$  0,0,1/2)' |
| (10) $m'$ $x, x, z$<br>( $m_3$  0,0,0)'                     | (11) $m'$ $x, 0, z$<br>( $m_2$  0,0,0)'             | (12) $m'$ $0, y, z$<br>( $m_1$  0,0,0)'             |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

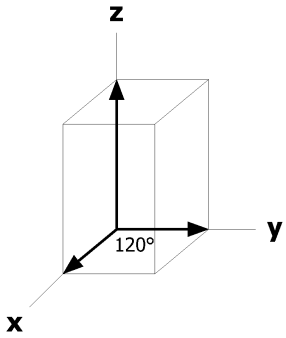
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	d	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]	
			(4) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(5) $y,\bar{x}+y,z+1/2$ [ $v,\bar{u}+v,w$ ]	(6) $x-y,x,z+1/2$ [ $u-v,u,w$ ]	
			(7) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $\bar{x}+y,y,z+1/2$ [ $\bar{u}+v,v,w$ ]	(9) $x,x-y,z+1/2$ [ $u,u-v,w$ ]	
			(10) y,x,z [v,u,w]	(11) $x-y,\bar{y},z$ [ $u-v,\bar{v},w$ ]	(12) $\bar{x},\bar{x}+y,z$ [ $\bar{u},\bar{u}+v,w$ ]	
6	c	..m'	x,0,z [u,0,w]	0,x,z [0,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ]	
			$\bar{x},0,z+1/2$ [ $\bar{u},0,w$ ]	$0,\bar{x},z+1/2$ [ $0,\bar{u},w$ ]	$x,x,z+1/2$ [ $u,u,w$ ]	
4	b	3..	$1/3,2/3,z$ [0,0,w]	$2/3,1/3,z+1/2$ [0,0,w]	$1/3,2/3,z+1/2$ [0,0,w]	$2/3,1/3,z$ [0,0,w]
2	a	3.m'	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p6m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m'1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [2,1,0] p1g'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



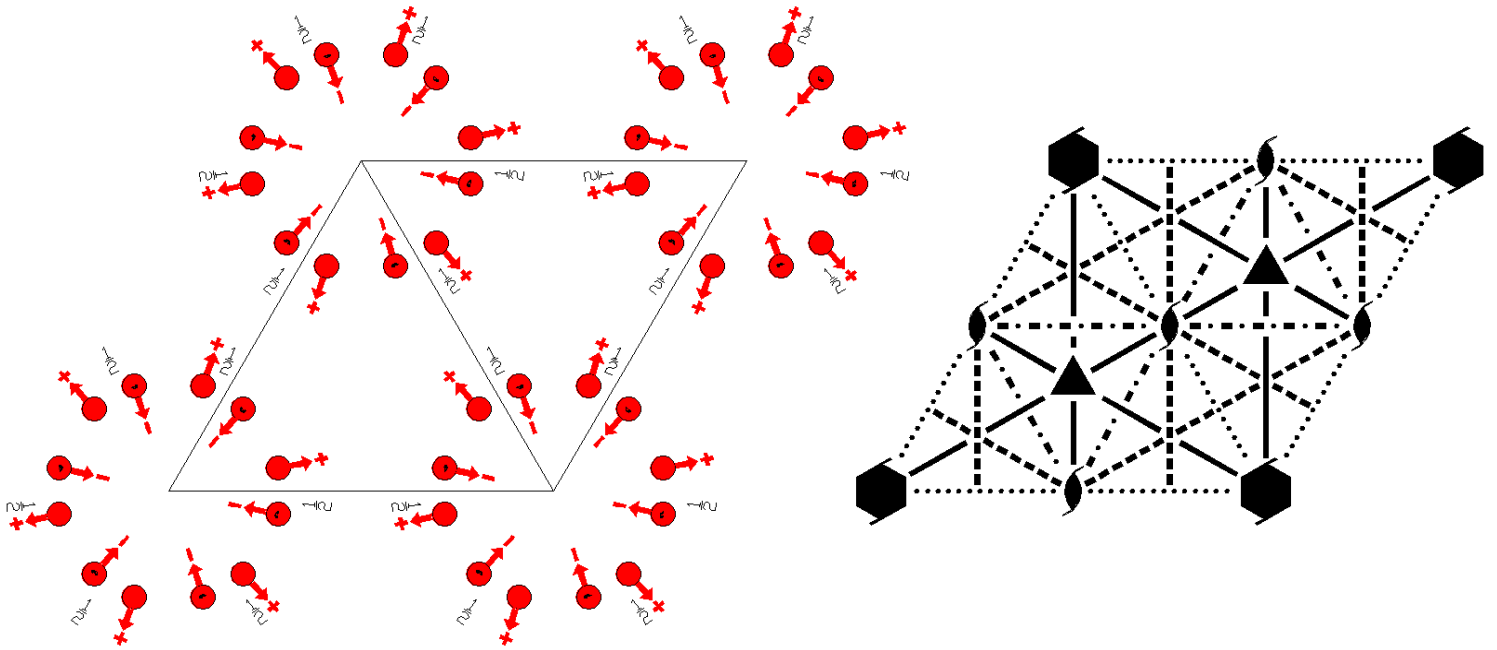
$P6_3 mc$

186.1.1434

6mm

$P6_3 mc$

Hexagonal



Origin on  $3m1$  at  $6_3 mc$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0		
	0,0,1	1/2,0,1	2/3,1/3,1		

**Symmetry Operations**

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                              | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)         |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)      | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)  |
| (7) m $x, \bar{x}, z$<br>( $m_{xy}$  0,0,0)     | (8) m $x, 2x, z$<br>( $m_x$  0,0,0)                 | (9) m $2x, x, z$<br>( $m_y$  0,0,0)             |
| (10) c (0,0,1/2) $x, x, z$<br>( $m_3$  0,0,1/2) | (11) c (0,0,1/2) $x, 0, z$<br>( $m_2$  0,0,1/2)     | (12) c (0,0,1/2) $0, y, z$<br>( $m_1$  0,0,1/2) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

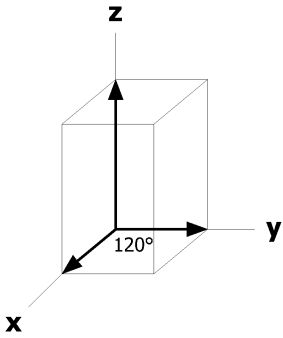
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	d	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(5) $y,\bar{x}+y,z+1/2$ [ $v,\bar{u}+v,w$ ]	(6) $x-y,x,z+1/2$ [ $u-v,u,w$ ]
			(7) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(8) $\bar{x}+y,y,z$ [ $u-v,\bar{v},\bar{w}$ ]	(9) $x,x-y,z$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
			(10) $y,x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(11) $x-y,\bar{y},z+1/2$ [ $\bar{u}+v,v,\bar{w}$ ]	(12) $\bar{x},\bar{x}+y,z+1/2$ [ $u,u-v,\bar{w}$ ]
6	c	.m.	$x,\bar{x},z$ [ $u,u,0$ ]	$x,2x,z$ [ $\bar{u},0,0$ ]	$2\bar{x},\bar{x},z$ [ $0,\bar{u},0$ ]
			$\bar{x},x,z+1/2$ [ $\bar{u},\bar{u},0$ ]	$\bar{x},2\bar{x},z+1/2$ [ $u,0,0$ ]	$2x,x,z+1/2$ [ $0,u,0$ ]
2	b	3m.	$1/3,2/3,z$ [ $0,0,0$ ]	$2/3,1/3,z+1/2$ [ $0,0,0$ ]	
2	a	3m.	$0,0,z$ [ $0,0,0$ ]	$0,0,z+1/2$ [ $0,0,0$ ]	

**Symmetry of Special Projections**

Along  $[0,0,1]$  p6mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$  p1g11'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,0,0$

Along  $[2,1,0]$  p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x/2,0$



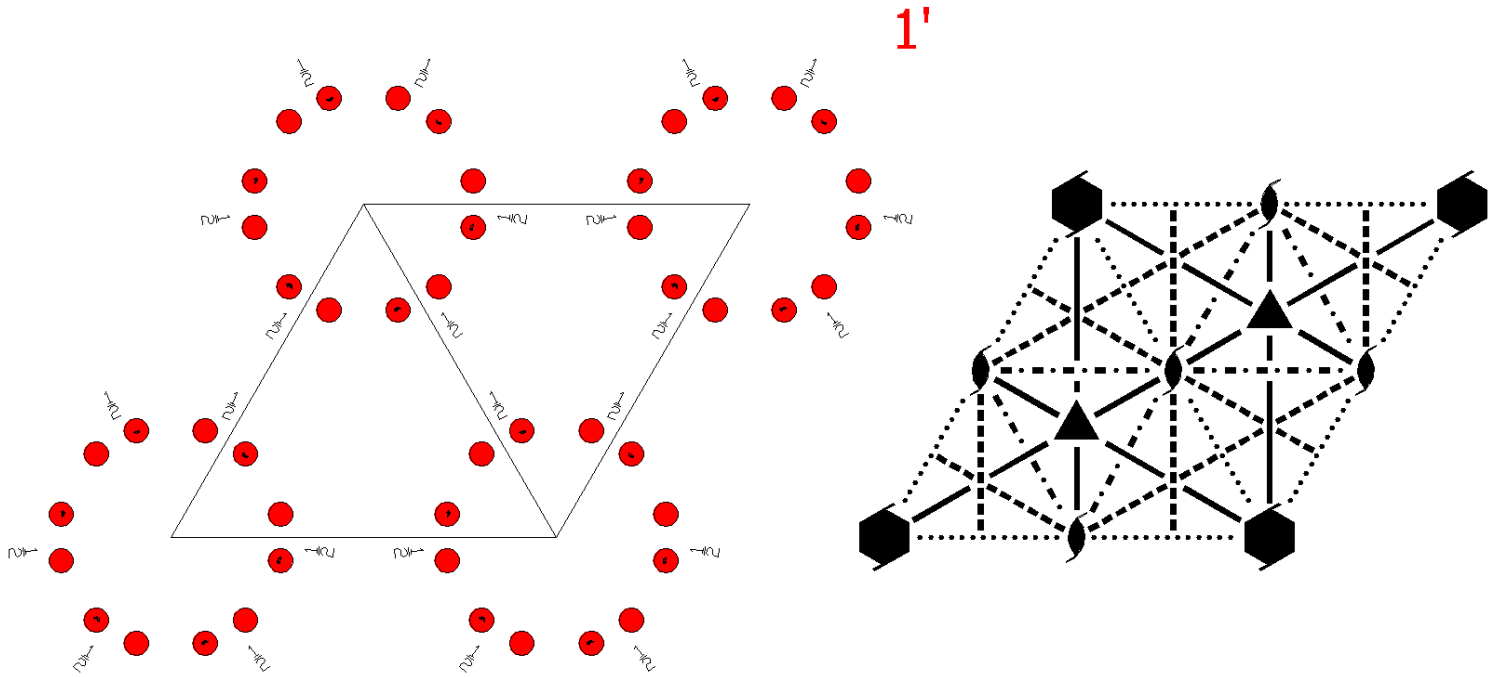
$P6_3 mc1'$

186.2.1435

$6mm1'$

$P6_3 mc1'$

Hexagonal



Origin on  $3m11'$  at  $6_3 mc1'$

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/3$ ;  $0 \leq z \leq 1$ ;  $x \leq (1+y)/2$ ;  $y \leq x/2$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0
	0,0,1	1/2,0,1	2/3,1/3,1

**Symmetry Operations**

For 1 + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                              | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)         |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)      | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)  |
| (7) m $x, \bar{x}, z$<br>( $m_{xy}$  0,0,0)     | (8) m $x, 2x, z$<br>( $m_x$  0,0,0)                 | (9) m $2x, x, z$<br>( $m_y$  0,0,0)             |
| (10) c (0,0,1/2) $x, x, z$<br>( $m_3$  0,0,1/2) | (11) c (0,0,1/2) $x, 0, z$<br>( $m_2$  0,0,1/2)     | (12) c (0,0,1/2) $0, y, z$<br>( $m_1$  0,0,1/2) |

## For 1' + set

- |   |   |   |
|---|---|---|
| (1) 1'<br>(1 0,0,0)'                                    | (2) 3 <sup>+</sup> 1' 0,0,z<br>(3 <sub>z</sub>  0,0,0)'                           | (3) 3 <sup>-</sup> 1' 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (4) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)'    | (5) 6 <sup>-</sup> 1' (0,0,1/2) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' | (6) 6 <sup>+</sup> 1' (0,0,1/2) 0,0,z<br>(6 <sub>z</sub>  0,0,1/2)'   |
| (7) m' x, $\bar{x}$ , z<br>(m <sub>xy</sub>  0,0,0)'    | (8) m' x, 2x, z<br>(m <sub>x</sub>  0,0,0)'                                       | (9) m' 2x, x, z<br>(m <sub>y</sub>  0,0,0)'                           |
| (10) c' (0,0,1/2) x, x, z<br>(m <sub>3</sub>  0,0,1/2)' | (11) c' (0,0,1/2) x, 0, z<br>(m <sub>2</sub>  0,0,1/2)'                           | (12) c' (0,0,1/2) 0, y, z<br>(m <sub>1</sub>  0,0,1/2)'               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

**Positions**

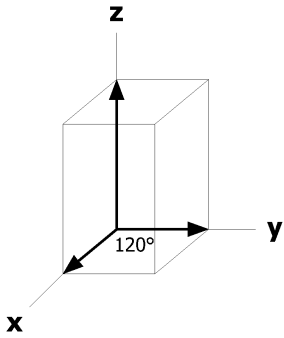
			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			1 +	1' +	
12	d	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y$ , $\bar{x}$ ,z [0,0,0]
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [0,0,0]	(5) y, $\bar{x}+y$ ,z+1/2 [0,0,0]	(6) x-y,x,z+1/2 [0,0,0]
			(7) $\bar{y}$ , $\bar{x}$ ,z [0,0,0]	(8) $\bar{x}+y$ ,y,z [0,0,0]	(9) x,x-y,z [0,0,0]
			(10) y,x,z+1/2 [0,0,0]	(11) x-y, $\bar{y}$ ,z+1/2 [0,0,0]	(12) $\bar{x}$ , $\bar{x}+y$ ,z+1/2 [0,0,0]
6	c	.m.1'	x, $\bar{x}$ ,z [0,0,0]	x,2x,z [0,0,0]	2 $\bar{x}$ , $\bar{x}$ ,z [0,0,0]
			$\bar{x}$ ,x,z+1/2 [0,0,0]	$\bar{x}$ ,2 $\bar{x}$ ,z+1/2 [0,0,0]	2x,x,z+1/2 [0,0,0]
2	b	3m.1'	1/3,2/3,z [0,0,0]	2/3,1/3,z+1/2 [0,0,0]	
2	a	3m.1'	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [2,1,0] p1m11'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x/2,0



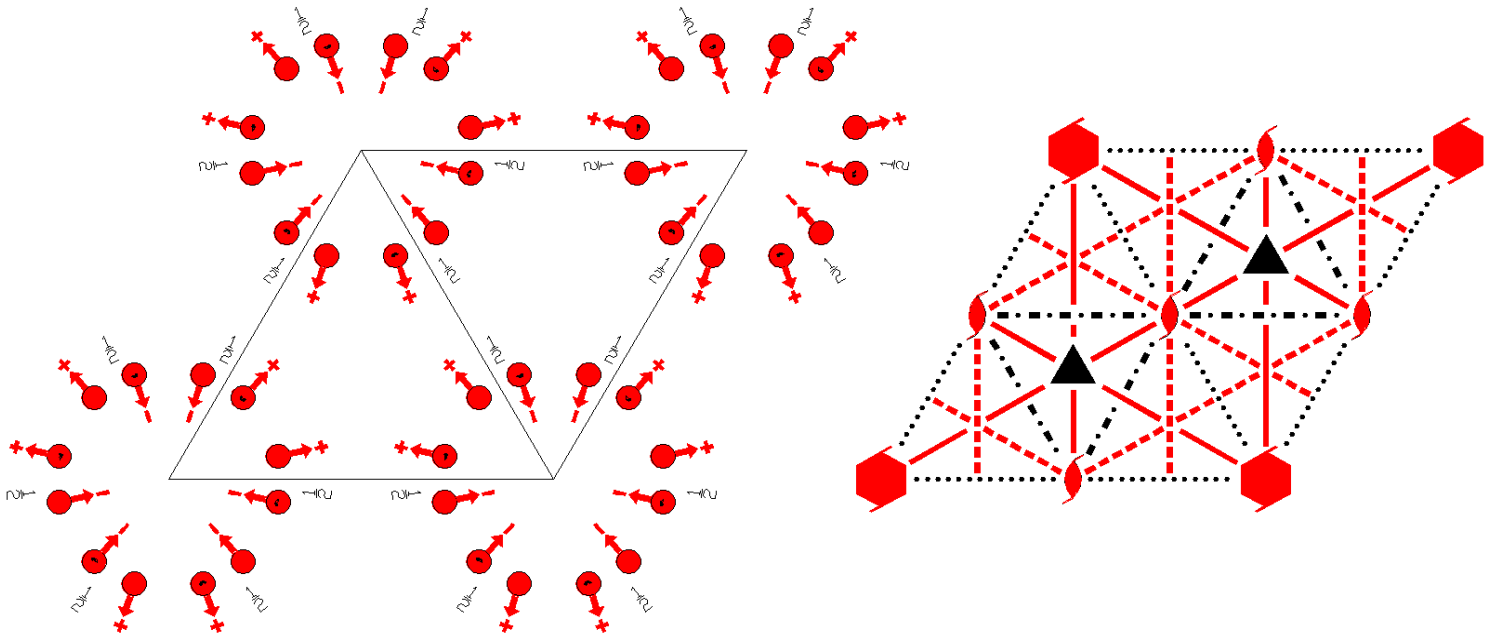
$P6_3'm'c$

186.3.1436

$6'm'm$

$P6_3'm'c$

Hexagonal



Origin on  $3m'1$  at  $6_3'm'c$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0 0,0,1	1/2,0,0 1/2,0,1	2/3,1/3,0 2/3,1/3,1		

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                              | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                   | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)         |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)'  | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)' | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)' |
| (7) $m'$ $x, \bar{x}, z$<br>( $m_{xy}$  0,0,0)' | (8) $m'$ $x, 2x, z$<br>( $m_x$  0,0,0)'              | (9) $m'$ $2x, x, z$<br>( $m_y$  0,0,0)'         |
| (10) c (0,0,1/2) $x, x, z$<br>( $m_3$  0,0,1/2) | (11) c (0,0,1/2) $x, 0, z$<br>( $m_2$  0,0,1/2)      | (12) c (0,0,1/2) $0, y, z$<br>( $m_1$  0,0,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

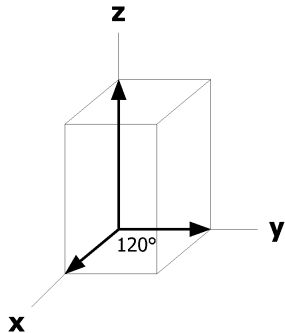
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	d	1	(1) x,y,z [u,v,w] (4) $\bar{x}, \bar{y}, z+1/2$ [u,v, $\bar{w}$ ] (7) $\bar{y}, \bar{x}, z$ [ $\bar{v}, \bar{u}, w$ ] (10) y,x,z+1/2 [ $\bar{v}, \bar{u}, \bar{w}$ ]	(2) $\bar{y}, x-y, z$ [ $\bar{v}, u-v, w$ ] (5) y, $\bar{x}+y, z+1/2$ [ $\bar{v}, u-v, \bar{w}$ ] (8) $\bar{x}+y, y, z$ [ $\bar{u}+v, v, w$ ] (11) x-y, $\bar{y}, z+1/2$ [ $\bar{u}+v, v, \bar{w}$ ]	(3) $\bar{x}+y, \bar{x}, z$ [ $\bar{u}+v, \bar{u}, w$ ] (6) x-y,x,z+1/2 [ $\bar{u}+v, \bar{u}, \bar{w}$ ] (9) x,x-y,z [u,u-v,w] (12) $\bar{x}, \bar{x}+y, z+1/2$ [u,u-v, $\bar{w}$ ]
6	c	.m'	x, $\bar{x}, z$ [u, $\bar{u}, w$ ] $\bar{x}, x, z+1/2$ [u, $\bar{u}, \bar{w}$ ]	x,2x,z [u,2u,w] $\bar{x}, 2\bar{x}, z+1/2$ [u,2u, $\bar{w}$ ]	2 $\bar{x}, \bar{x}, z$ [2 $\bar{u}, \bar{u}, w$ ] 2x,x,z+1/2 [2 $\bar{u}, \bar{u}, \bar{w}$ ]
2	b	3m'	1/3,2/3,z [0,0,w]	2/3,1/3,z+1/2 [0,0, $\bar{w}$ ]	
2	a	3m'	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	

**Symmetry of Special Projections**

Along [0,0,1] p6'm'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [2,1,0] p<sub>2b</sub>'1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x/2,0



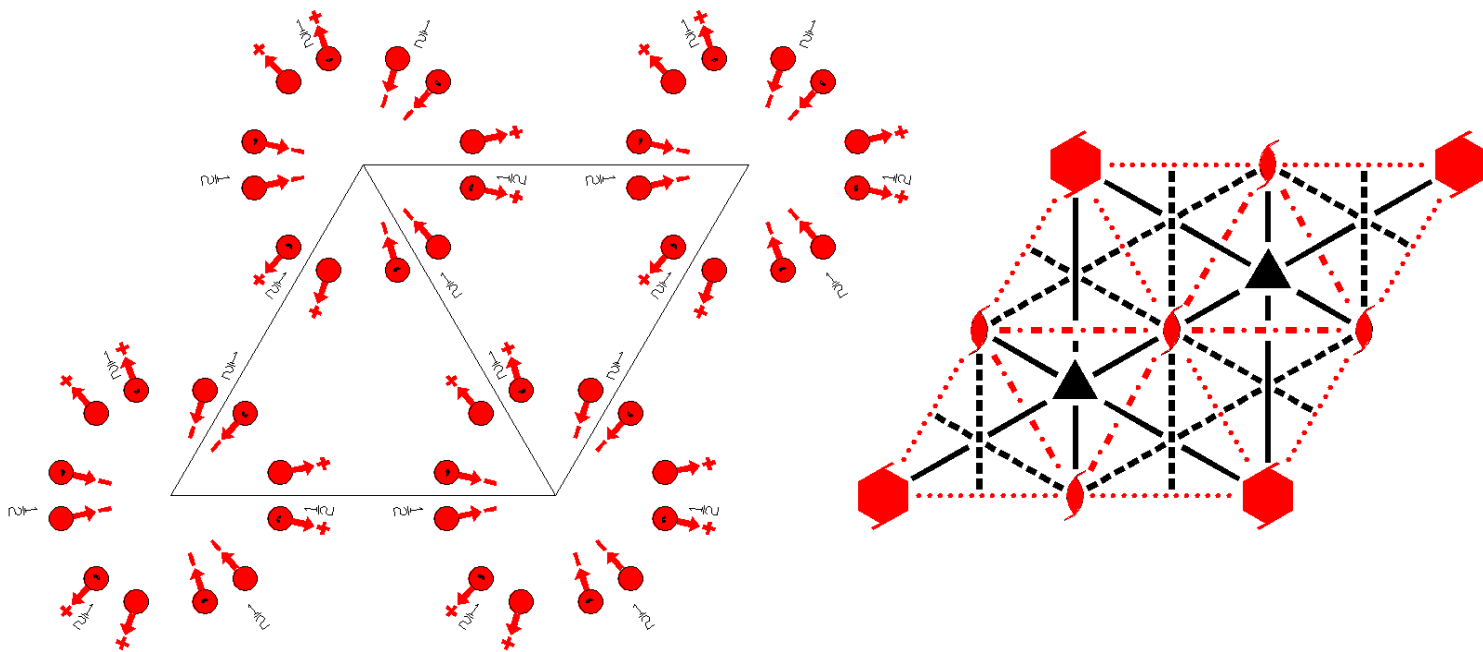
$P6_3'mc'$

186.4.1437

$6'mm'$

$P6_3'mc'$

Hexagonal



Origin on  $3m1$  at  $6_3'mc'$

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/3$ ;  $0 \leq z \leq 1$ ;  $x \leq (1+y)/2$ ;  $y \leq x/2$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0
	0,0,1	1/2,0,1	2/3,1/3,1

### Symmetry Operations

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                                  | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                   | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)             |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)'      | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)' | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)'     |
| (7) m $x, \bar{x}, z$<br>( $m_{xy}$  0,0,0)         | (8) m $x, 2x, z$<br>( $m_x$  0,0,0)                  | (9) m $2x, x, z$<br>( $m_y$  0,0,0)                 |
| (10) $c'$ (0,0,1/2) $x, x, z$<br>( $m_3$  0,0,1/2)' | (11) $c'$ (0,0,1/2) $x, 0, z$<br>( $m_2$  0,0,1/2)'  | (12) $c'$ (0,0,1/2) $0, y, z$<br>( $m_1$  0,0,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

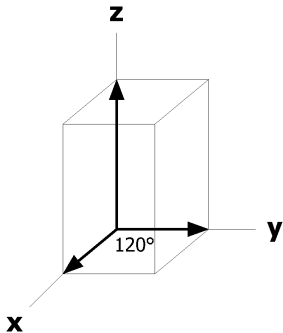
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	d	1	(1) x,y,z [u,v,w] (4) $\bar{x}, \bar{y}, z+1/2$ [u,v, $\bar{w}$ ] (7) $\bar{y}, \bar{x}, z$ [v,u, $\bar{w}$ ] (10) y,x,z+1/2 [v,u,w]	(2) $\bar{y}, x-y, z$ [ $\bar{v}, u-v, w$ ] (5) y, $\bar{x}+y, z+1/2$ [ $\bar{v}, u-v, \bar{w}$ ] (8) $\bar{x}+y, y, z$ [u-v, $\bar{v}, \bar{w}$ ] (11) x-y, $\bar{y}, z+1/2$ [u-v, $\bar{v}, w$ ]	(3) $\bar{x}+y, \bar{x}, z$ [ $\bar{u}+v, \bar{u}, w$ ] (6) x-y,x,z+1/2 [ $\bar{u}+v, \bar{u}, \bar{w}$ ] (9) x,x-y,z [ $\bar{u}, \bar{u}+v, \bar{w}$ ] (12) $\bar{x}, \bar{x}+y, z+1/2$ [ $\bar{u}, \bar{u}+v, w$ ]
6	c	.m.	x, $\bar{x}, z$ [u,u,0] $\bar{x}, x, z+1/2$ [u,u,0]	x,2x,z [ $\bar{u}, 0, 0$ ] $\bar{x}, 2\bar{x}, z+1/2$ [ $\bar{u}, 0, 0$ ]	2 $\bar{x}, \bar{x}, z$ [0, $\bar{u}, 0$ ] 2x,x,z+1/2 [0, $\bar{u}, 0$ ]
2	b	3m.	1/3,2/3,z [0,0,0]	2/3,1/3,z+1/2 [0,0,0]	
2	a	3m.	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	

**Symmetry of Special Projections**

Along [0,0,1] p6'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g11'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

Along [2,1,0] p1m1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x/2,0



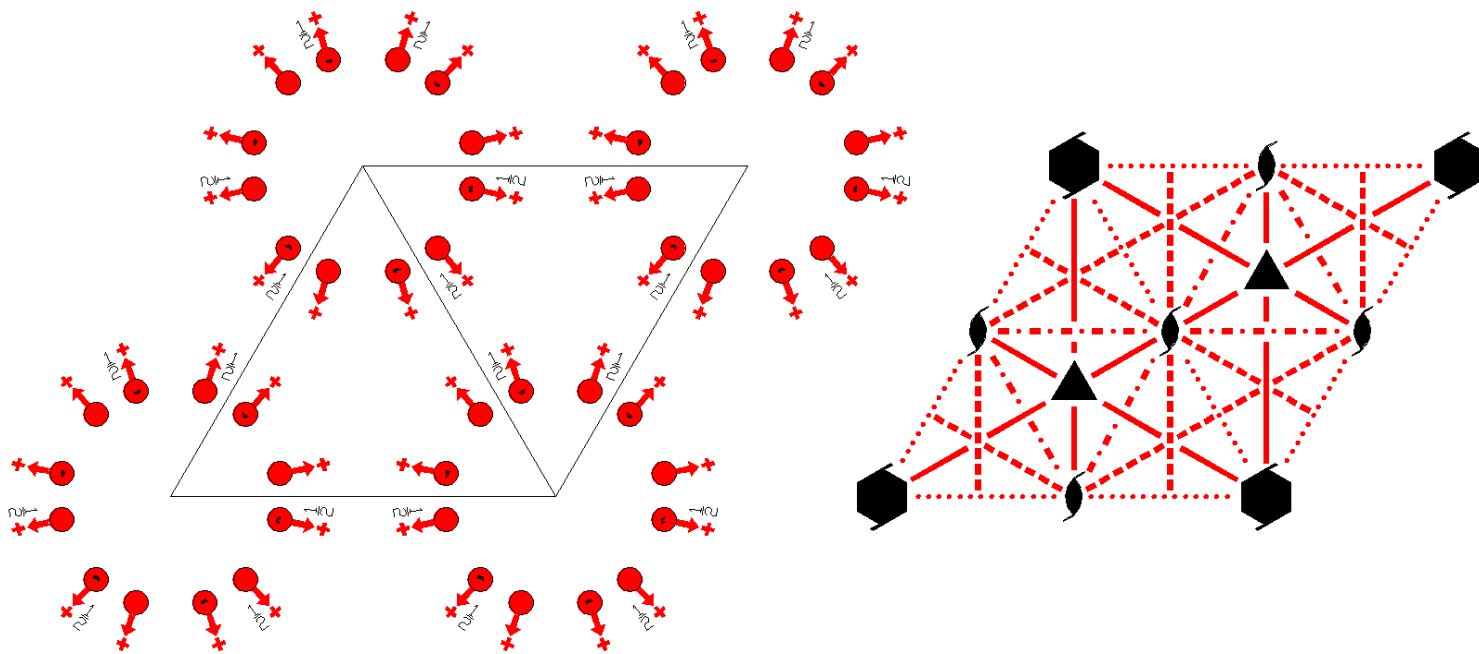
$P6_3 m'c'$

186.5.1438

$6m'm'$

$P6_3 m'c'$

Hexagonal



Origin on  $3m'1$  at  $6_3 m'c'$

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/3$ ;  $0 \leq z \leq 1$ ;  $x \leq (1+y)/2$ ;  $y \leq x/2$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0
	0,0,1	1/2,0,1	2/3,1/3,1

### Symmetry Operations

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                                  | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)             |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)          | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)      |
| (7) $m'$ $x, \bar{x}, z$<br>( $m_{xy}$  0,0,0)'     | (8) $m'$ $x, 2x, z$<br>( $m_x$  0,0,0)'             | (9) $m'$ $2x, x, z$<br>( $m_y$  0,0,0)'             |
| (10) $c'$ (0,0,1/2) $x, x, z$<br>( $m_3$  0,0,1/2)' | (11) $c'$ (0,0,1/2) $x, 0, z$<br>( $m_2$  0,0,1/2)' | (12) $c'$ (0,0,1/2) $0, y, z$<br>( $m_1$  0,0,1/2)' |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

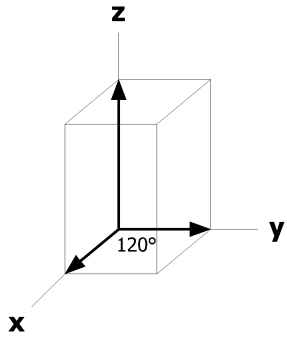
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	d	1	(1) x,y,z [u,v,w] (4) $\bar{x}, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ] (7) $\bar{y}, \bar{x}, z$ [ $\bar{v}, \bar{u}, w$ ] (10) y,x,z+1/2 [v,u,w]	(2) $\bar{y}, x-y, z$ [ $\bar{v}, u-v, w$ ] (5) y, $\bar{x}+y, z+1/2$ [v, $\bar{u}+v, w$ ] (8) $\bar{x}+y, y, z$ [ $\bar{u}+v, v, w$ ] (11) x-y, $\bar{y}, z+1/2$ [u-v, $\bar{v}, w$ ]	(3) $\bar{x}+y, \bar{x}, z$ [ $\bar{u}+v, \bar{u}, w$ ] (6) x-y,x,z+1/2 [u-v,u,w] (9) x,x-y,z [u,u-v,w] (12) $\bar{x}, \bar{x}+y, z+1/2$ [ $\bar{u}, \bar{u}+v, w$ ]
6	c	.m'	x, $\bar{x}, z$ [u, $\bar{u}, w$ ] $\bar{x}, x, z+1/2$ [ $\bar{u}, u, w$ ]	x, 2x, z [u, 2u, w] $\bar{x}, 2\bar{x}, z+1/2$ [ $\bar{u}, 2\bar{u}, w$ ]	2 $\bar{x}, \bar{x}, z$ [2 $\bar{u}, \bar{u}, w$ ] 2x, x, z+1/2 [2u, u, w]
2	b	3m'	1/3, 2/3, z [0, 0, w]	2/3, 1/3, z+1/2 [0, 0, w]	
2	a	3m'	0, 0, z [0, 0, w]	0, 0, z+1/2 [0, 0, w]	

**Symmetry of Special Projections**

Along [0,0,1] p6m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1g'1  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

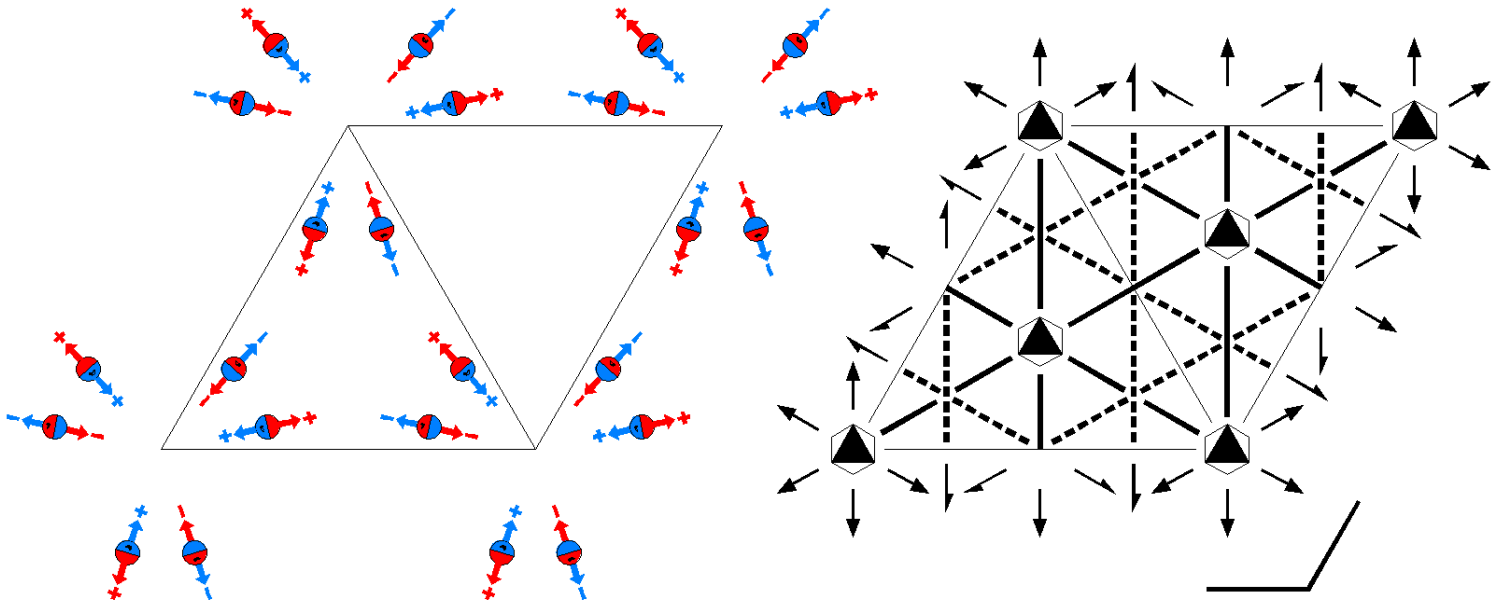
Along [2,1,0] p1m'1  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x/2,0



$P\bar{6}m2$   
187.1.1439

$\bar{6}m2$   
 $P\bar{6}m2$

Hexagonal



Origin on  $\bar{6}m2$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq 2y;$	$y \leq \min(1-x, 2x)$
Vertices	0,0,0 0,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/3,2/3,0 1/3,2/3,1/2		

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                          | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                         | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)               |
| (4) m x,y,0<br>( $m_z$  0,0,0)              | (5) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (6) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0) |
| (7) m $x, \bar{x}, z$<br>( $m_{xy}$  0,0,0) | (8) m x,2x,z<br>( $m_x$  0,0,0)                            | (9) m 2x,x,z<br>( $m_y$  0,0,0)                       |
| (10) 2 $x, \bar{x}, 0$<br>( $2_3$  0,0,0)   | (11) 2 x,2x,0<br>( $2_2$  0,0,0)                           | (12) 2 2x,x,0<br>( $2_1$  0,0,0)                      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

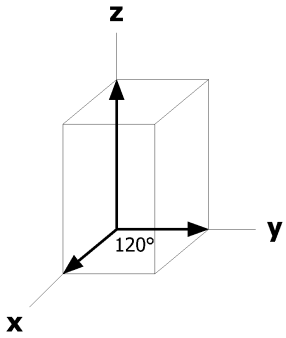
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	o	1	(1) $x,y,z$ [u,v,w] (4) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ] (7) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ] (10) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $\bar{y},x-y,\bar{z}$ [v, $\bar{u}+v,w$ ] (8) $\bar{x}+y,y,z$ [u-v, $\bar{v},\bar{w}$ ] (11) $\bar{x}+y,y,\bar{z}$ [ $\bar{u}+v,v,\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x}+y,\bar{x},\bar{z}$ [u-v,u,w] (9) $x,x-y,z$ [ $\bar{u},\bar{u}+v,\bar{w}$ ] (12) $x,x-y,\bar{z}$ [u,u-v, $\bar{w}$ ]
6	n	.m.	$x,\bar{x},z$ [u,u,0] $x,\bar{x},\bar{z}$ [ $\bar{u},\bar{u},0$ ]	$x,2x,z$ [ $\bar{u},0,0$ ] $x,2x,\bar{z}$ [u,0,0]	$2\bar{x},\bar{x},z$ [0, $\bar{u},0$ ] $2\bar{x},\bar{x},\bar{z}$ [0,u,0]
6	m	m..	$x,y,1/2$ [0,0,w] $\bar{y},\bar{x},1/2$ [0,0, $\bar{w}$ ]	$\bar{y},x-y,1/2$ [0,0,w] $\bar{x}+y,y,1/2$ [0,0, $\bar{w}$ ]	$\bar{x}+y,\bar{x},1/2$ [0,0,w] $x,x-y,1/2$ [0,0, $\bar{w}$ ]
6	l	m..	$\bar{y},y,0$ [0,0,w] $y,\bar{x},0$ [0,0, $\bar{w}$ ]	$\bar{y},x-y,0$ [0,0,w] $\bar{x}+y,y,0$ [0,0, $\bar{w}$ ]	$\bar{x}+y,\bar{x},0$ [0,0,w] $x,x-y,0$ [0,0, $\bar{w}$ ]
3	k	mm2	$x,\bar{x},1/2$ [0,0,0]	$x,2x,1/2$ [0,0,0]	$2\bar{x},\bar{x},1/2$ [0,0,0]
3	j	mm2	$x,\bar{x},0$ [0,0,0]	$x,2x,0$ [0,0,0]	$2\bar{x},\bar{x},0$ [0,0,0]
2	i	3m.	$2/3,1/3,z$ [0,0,0]	$2/3,1/3,\bar{z}$ [0,0,0]	
2	h	3m.	$1/3,2/3,z$ [0,0,0]	$1/3,2/3,\bar{z}$ [0,0,0]	
2	g	3m.	$0,0,z$ [0,0,0]	$0,0,\bar{z}$ [0,0,0]	
1	f	$\bar{6}$ m2	$2/3,1/3,1/2$ [0,0,0]		
1	e	$\bar{6}$ m2	$2/3,1/3,0$ [0,0,0]		
1	d	$\bar{6}$ m2	$1/3,2/3,1/2$ [0,0,0]		
1	c	$\bar{6}$ m2	$1/3,2/3,0$ [0,0,0]		
1	b	$\bar{6}$ m2	$0,0,1/2$ [0,0,0]		
1	a	$\bar{6}$ m2	$0,0,0$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p3m11'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0

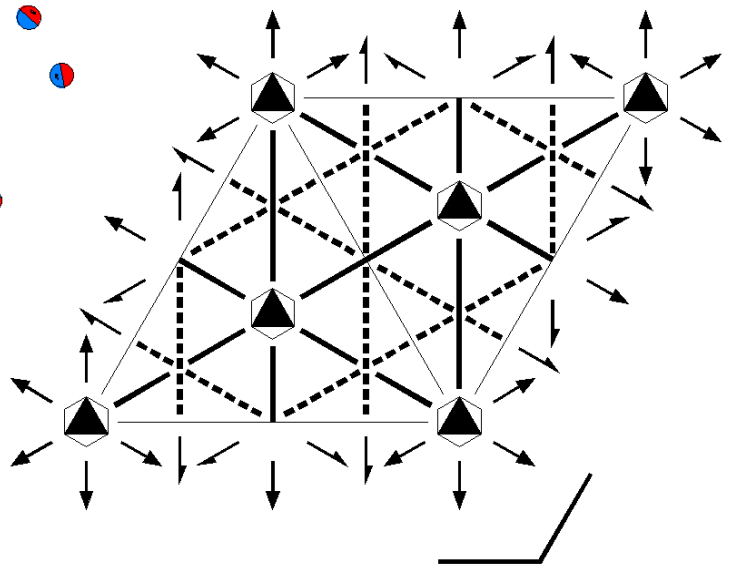
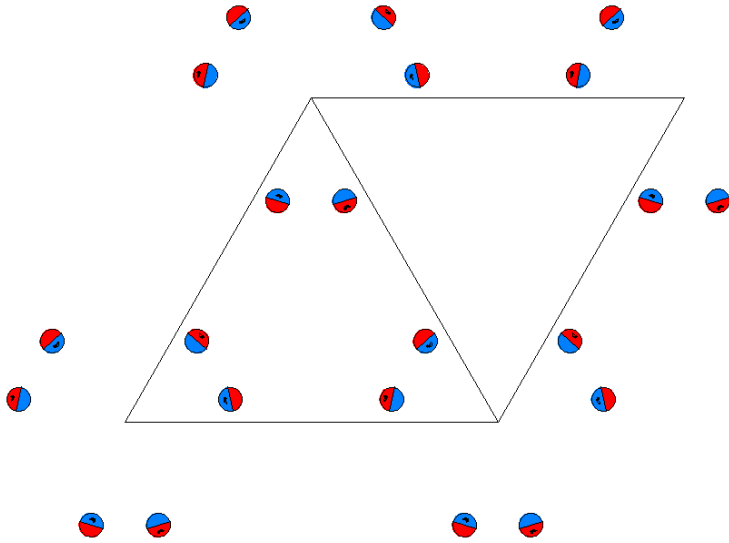


$P\bar{6}m21'$   
187.2.1440

$\bar{6}m21'$   
 $P\bar{6}m21'$

Hexagonal

1'



Origin on  $\bar{6}m21'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq 2y;$	$y \leq \min(1-x, 2x)$
Vertices	0,0,0 0,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/3,2/3,0 1/3,2/3,1/2		

**Symmetry Operations**

For 1 + set

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                          | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                         | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)               |
| (4) m x,y,0<br>( $m_z$  0,0,0)              | (5) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (6) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0) |
| (7) m x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0) | (8) m x,2x,z<br>( $m_x$  0,0,0)                            | (9) m 2x,x,z<br>( $m_y$  0,0,0)                       |
| (10) 2 x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)   | (11) 2 x,2x,0<br>( $2_2$  0,0,0)                           | (12) 2 2x,x,0<br>( $2_1$  0,0,0)                      |

For  $1'$  + set

(1) $1'$ ( $1 0,0,0$ )'	(2) $3^{+}$ $0,0,z$ ( $3_z 0,0,0$ )'	(3) $3^{-}$ $0,0,z$ ( $3_z^{-1} 0,0,0$ )'
(4) $m'$ $x,y,0$ ( $m_z 0,0,0$ )'	(5) $\bar{6}^{-}$ $0,0,z; 0,0,0$ ( $\bar{6}_z^{-1} 0,0,0$ )'	(6) $\bar{6}^{+}$ $0,0,z; 0,0,0$ ( $\bar{6}_z 0,0,0$ )'
(7) $m'$ $x,\bar{x},z$ ( $m_{xy} 0,0,0$ )'	(8) $m'$ $x,2x,z$ ( $m_x 0,0,0$ )'	(9) $m'$ $2x,x,z$ ( $m_y 0,0,0$ )'
(10) $2'$ $x,\bar{x},0$ ( $2_3 0,0,0$ )'	(11) $2'$ $x,2x,0$ ( $2_2 0,0,0$ )'	(12) $2'$ $2x,x,0$ ( $2_1 0,0,0$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			1 +	1' +	
12	o	11'	(1) $x,y,z$ [0,0,0]	(2) $\bar{y},x-y,z$ [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0]
			(4) $x,y,\bar{z}$ [0,0,0]	(5) $\bar{y},x-y,\bar{z}$ [0,0,0]	(6) $\bar{x}+y,\bar{x},\bar{z}$ [0,0,0]
			(7) $\bar{y},\bar{x},z$ [0,0,0]	(8) $\bar{x}+y,y,z$ [0,0,0]	(9) $x,x-y,z$ [0,0,0]
			(10) $\bar{y},\bar{x},\bar{z}$ [0,0,0]	(11) $\bar{x}+y,y,\bar{z}$ [0,0,0]	(12) $x,x-y,\bar{z}$ [0,0,0]
6	n	.m.1'	$x,\bar{x},z$ [0,0,0]	$x,2x,z$ [0,0,0]	$2\bar{x},\bar{x},z$ [0,0,0]
			$x,\bar{x},\bar{z}$ [0,0,0]	$x,2x,\bar{z}$ [0,0,0]	$2\bar{x},\bar{x},\bar{z}$ [0,0,0]
6	m	m..1'	$x,y,1/2$ [0,0,0]	$\bar{y},x-y,1/2$ [0,0,0]	$\bar{x}+y,\bar{x},1/2$ [0,0,0]
			$\bar{y},\bar{x},1/2$ [0,0,0]	$\bar{x}+y,y,1/2$ [0,0,0]	$x,x-y,1/2$ [0,0,0]
6	l	m..1'	$x,y,0$ [0,0,0]	$\bar{y},x-y,0$ [0,0,0]	$\bar{x}+y,\bar{x},0$ [0,0,0]
			$\bar{y},\bar{x},0$ [0,0,0]	$\bar{x}+y,y,0$ [0,0,0]	$x,x-y,0$ [0,0,0]
3	k	mm21'	$x,\bar{x},1/2$ [0,0,0]	$x,2x,1/2$ [0,0,0]	$2\bar{x},\bar{x},1/2$ [0,0,0]
3	j	mm21'	$x,\bar{x},0$ [0,0,0]	$x,2x,0$ [0,0,0]	$2\bar{x},\bar{x},0$ [0,0,0]
2	i	3m.1'	$2/3,1/3,z$ [0,0,0]	$2/3,1/3,\bar{z}$ [0,0,0]	
2	h	3m.1'	$1/3,2/3,z$ [0,0,0]	$1/3,2/3,\bar{z}$ [0,0,0]	
2	g	3m.1'	$0,0,z$ [0,0,0]	$0,0,\bar{z}$ [0,0,0]	
1	f	$\bar{6}m21'$	$2/3,1/3,1/2$ [0,0,0]		
1	e	$\bar{6}m21'$	$2/3,1/3,0$ [0,0,0]		

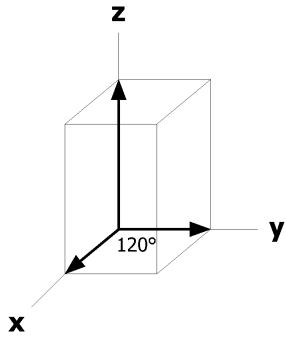
1	d	$\overline{6m21}'$ $1/3, 2/3, 1/2$ [0,0,0]
1	c	$\overline{6m21}'$ $1/3, 2/3, 0$ [0,0,0]
1	b	$\overline{6m21}'$ $0, 0, 1/2$ [0,0,0]
1	a	$\overline{6m21}'$ $0, 0, 0$ [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p3m11'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

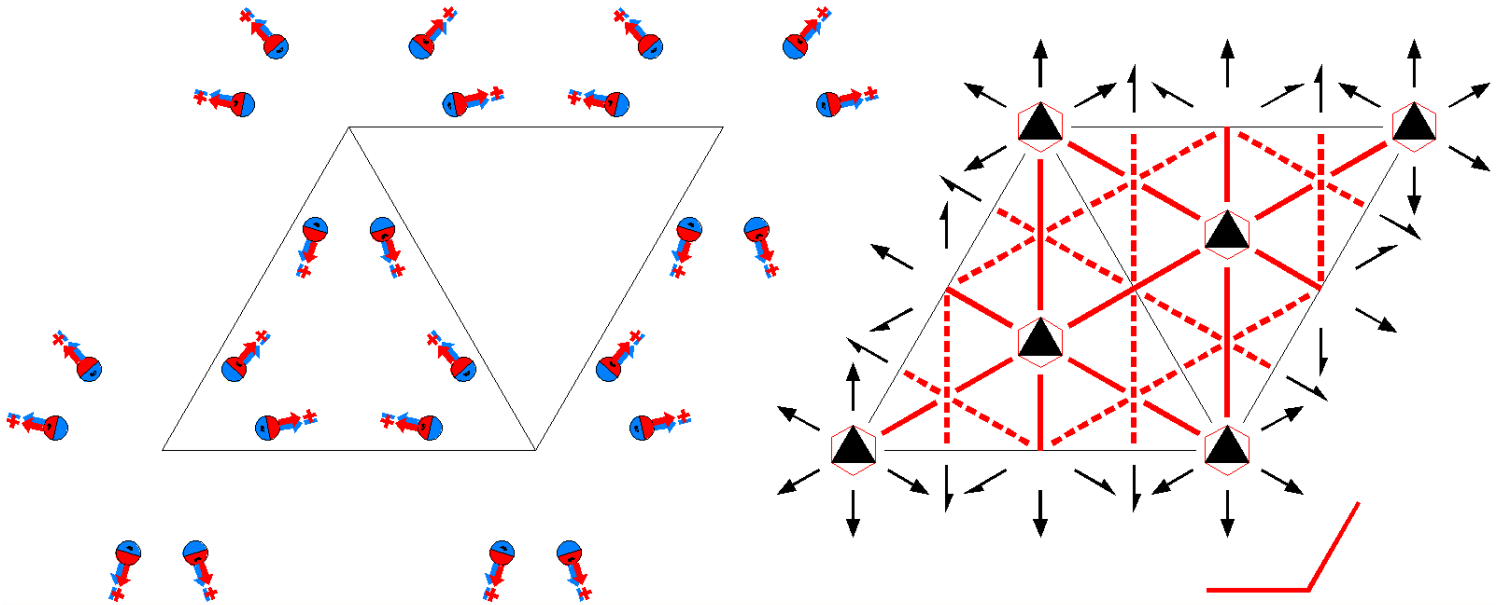
Along [2,1,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P\bar{6}'m'2$   
187.3.1441

$\bar{6}'m'2$   
 $P\bar{6}'m'2$

Hexagonal



Origin on  $\bar{6}'m'2$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq 2y;$	$y \leq \min(1-x, 2x)$
Vertices	0,0,0 0,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/3,2/3,0 1/3,2/3,1/2		

### Symmetry Operations

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                              | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                          | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                |
| (4) $m'$ x,y,0<br>( $m_z$  0,0,0)'              | (5) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0)' | (6) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0)' |
| (7) $m'$ x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0)' | (8) $m'$ x,2x,z<br>( $m_x$  0,0,0)'                         | (9) $m'$ 2x,x,z<br>( $m_y$  0,0,0)'                    |
| (10) 2 x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)       | (11) 2 x,2x,0<br>( $2_2$  0,0,0)                            | (12) 2 2x,x,0<br>( $2_1$  0,0,0)                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	o	1	(1) $x,y,z [u,v,w]$ (4) $x,y,\bar{z} [u,v,\bar{w}]$ (7) $\bar{y},\bar{x},z [\bar{v},\bar{u},w]$ (10) $\bar{y},\bar{x},\bar{z} [\bar{v},\bar{u},\bar{w}]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$ (5) $\bar{y},x-y,\bar{z} [\bar{v},u-v,\bar{w}]$ (8) $\bar{x}+y,y,z [\bar{u}+v,v,w]$ (11) $\bar{x}+y,y,\bar{z} [\bar{u}+v,v,\bar{w}]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$ (6) $\bar{x}+y,\bar{x},\bar{z} [\bar{u}+v,\bar{u},\bar{w}]$ (9) $x,x-y,z [u,u-v,w]$ (12) $x,x-y,\bar{z} [u,u-v,\bar{w}]$
6	n	.m'	$x,\bar{x},z [u,\bar{u},w]$ $x,\bar{x},\bar{z} [u,\bar{u},\bar{w}]$	$x,2x,z [u,2u,w]$ $x,2x,\bar{z} [u,2u,\bar{w}]$	$2\bar{x},\bar{x},z [2\bar{u},\bar{u},w]$ $2\bar{x},\bar{x},\bar{z} [2\bar{u},\bar{u},\bar{w}]$
6	m	m'..	$x,y,1/2 [u,v,0]$ $\bar{y},\bar{x},1/2 [\bar{v},\bar{u},0]$	$\bar{y},x-y,1/2 [\bar{v},u-v,0]$ $\bar{x}+y,y,1/2 [\bar{u}+v,v,0]$	$\bar{x}+y,\bar{x},1/2 [\bar{u}+v,\bar{u},0]$ $x,x-y,1/2 [u,u-v,0]$
6	l	m'..	$x,y,0 [u,v,0]$ $\bar{y},\bar{x},0 [\bar{v},\bar{u},0]$	$\bar{y},x-y,0 [\bar{v},u-v,0]$ $\bar{x}+y,y,0 [\bar{u}+v,v,0]$	$\bar{x}+y,\bar{x},0 [\bar{u}+v,\bar{u},0]$ $x,x-y,0 [u,u-v,0]$
3	k	m'm'2	$x,\bar{x},1/2 [u,\bar{u},0]$	$x,2x,1/2 [u,2u,0]$	$2\bar{x},\bar{x},1/2 [2\bar{u},\bar{u},0]$
3	j	m'm'2	$x,\bar{x},0 [u,\bar{u},0]$	$x,2x,0 [u,2u,0]$	$2\bar{x},\bar{x},0 [2\bar{u},\bar{u},0]$
2	i	3m'	$2/3,1/3,z [0,0,w]$	$2/3,1/3,\bar{z} [0,0,\bar{w}]$	
2	h	3m'	$1/3,2/3,z [0,0,w]$	$1/3,2/3,\bar{z} [0,0,\bar{w}]$	
2	g	3m'	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,\bar{w}]$	
1	f	$\bar{6}'m'2$	$2/3,1/3,1/2 [0,0,0]$		
1	e	$\bar{6}'m'2$	$2/3,1/3,0 [0,0,0]$		
1	d	$\bar{6}'m'2$	$1/3,2/3,1/2 [0,0,0]$		
1	c	$\bar{6}'m'2$	$1/3,2/3,0 [0,0,0]$		
1	b	$\bar{6}'m'2$	$0,0,1/2 [0,0,0]$		
1	a	$\bar{6}'m'2$	$0,0,0 [0,0,0]$		

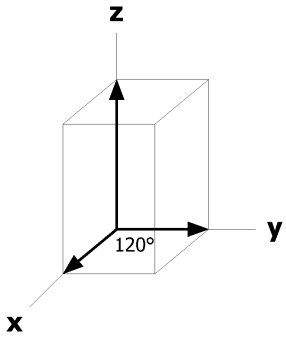
**Symmetry of Special Projections**

Along  $[0,0,1]$   $p3m'1$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p1m'1$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,0$

Along  $[2,1,0]$   $p2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,0$

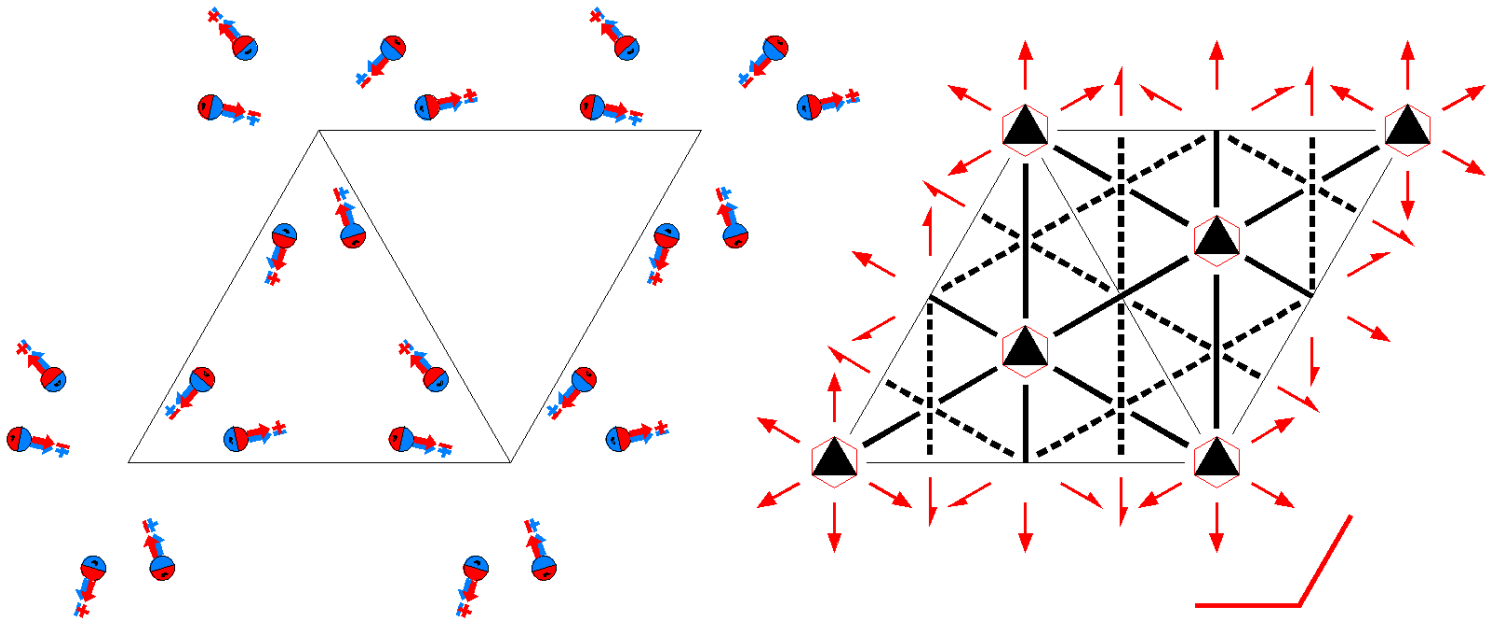




$P\bar{6}'m2'$   
187.4.1442

$\bar{6}'m2'$   
 $P\bar{6}'m2'$

Hexagonal



Origin on  $\bar{6}'m2'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq 2y;$	$y \leq \min(1-x, 2x)$
Vertices	0,0,0 0,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/3,2/3,0 1/3,2/3,1/2		

**Symmetry Operations**

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                            | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                            | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                  |
| (4) $m'$ x,y,0<br>( $m_z$  0,0,0)'            | (5) $\bar{6}^-$ ' 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0)' | (6) $\bar{6}^+$ ' 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0)' |
| (7) $m$ x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0) | (8) $m$ x,2x,z<br>( $m_x$  0,0,0)                             | (9) $m$ 2x,x,z<br>( $m_y$  0,0,0)                        |
| (10) $2'$ x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)' | (11) $2'$ x,2x,0<br>( $2_2$  0,0,0)'                          | (12) $2'$ 2x,x,0<br>( $2_1$  0,0,0)'                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

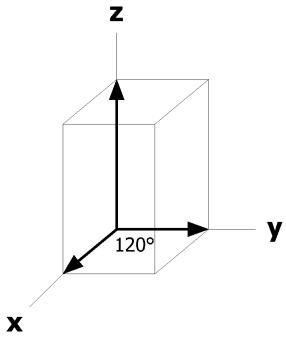
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	o	1	(1) $x,y,z$ [u,v,w] (4) $x,y,\bar{z}$ [u,v, $\bar{w}$ ] (7) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ] (10) $\bar{y},\bar{x},\bar{z}$ [v,u,w]	(2) $\bar{y},x-y,z$ [ $\bar{v}$ ,u-v,w] (5) $\bar{y},x-y,\bar{z}$ [ $\bar{v}$ ,u-v, $\bar{w}$ ] (8) $\bar{x}+y,y,z$ [u-v, $\bar{v}$ , $\bar{w}$ ] (11) $\bar{x}+y,y,\bar{z}$ [u-v, $\bar{v}$ ,w]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x}+y,\bar{x},\bar{z}$ [ $\bar{u}+v,\bar{u},\bar{w}$ ] (9) $x,x-y,z$ [ $\bar{u},\bar{u}+v,\bar{w}$ ] (12) $x,x-y,\bar{z}$ [ $\bar{u},\bar{u}+v,w$ ]
6	n	.m.	$x,\bar{x},z$ [u,u,0] $x,\bar{x},\bar{z}$ [u,u,0]	$x,2x,z$ [ $\bar{u},0,0$ ] $x,2x,\bar{z}$ [ $\bar{u},0,0$ ]	$2\bar{x},\bar{x},z$ [0, $\bar{u},0$ ] $2\bar{x},\bar{x},\bar{z}$ [0, $\bar{u},0$ ]
6	m	m'..	$x,y,1/2$ [u,v,0] $\bar{y},\bar{x},1/2$ [v,u,0]	$\bar{y},x-y,1/2$ [ $\bar{v}$ ,u-v,0] $\bar{x}+y,y,1/2$ [u-v, $\bar{v}$ ,0]	$\bar{x}+y,\bar{x},1/2$ [ $\bar{u}+v,\bar{u},0$ ] $x,x-y,1/2$ [ $\bar{u},\bar{u}+v,0$ ]
6	l	m'..	$x,y,0$ [u,v,0] $\bar{y},\bar{x},0$ [v,u,0]	$\bar{y},x-y,0$ [ $\bar{v}$ ,u-v,0] $\bar{x}+y,y,0$ [u-v, $\bar{v}$ ,0]	$\bar{x}+y,\bar{x},0$ [ $\bar{u}+v,\bar{u},0$ ] $x,x-y,0$ [ $\bar{u},\bar{u}+v,0$ ]
3	k	m'm2'	$x,\bar{x},1/2$ [u,u,0]	$x,2x,1/2$ [ $\bar{u},0,0$ ]	$2\bar{x},\bar{x},1/2$ [0, $\bar{u},0$ ]
3	j	m'm2'	$x,\bar{x},0$ [u,u,0]	$x,2x,0$ [ $\bar{u},0,0$ ]	$2\bar{x},\bar{x},0$ [0, $\bar{u},0$ ]
2	i	3m.	$2/3,1/3,z$ [0,0,0]	$2/3,1/3,\bar{z}$ [0,0,0]	
2	h	3m.	$1/3,2/3,z$ [0,0,0]	$1/3,2/3,\bar{z}$ [0,0,0]	
2	g	3m.	$0,0,z$ [0,0,0]	$0,0,\bar{z}$ [0,0,0]	
1	f	$\bar{6}'m2'$	$2/3,1/3,1/2$ [0,0,0]		
1	e	$\bar{6}'m2'$	$2/3,1/3,0$ [0,0,0]		
1	d	$\bar{6}'m2'$	$1/3,2/3,1/2$ [0,0,0]		
1	c	$\bar{6}'m2'$	$1/3,2/3,0$ [0,0,0]		
1	b	$\bar{6}'m2'$	$0,0,1/2$ [0,0,0]		
1	a	$\bar{6}'m2'$	$0,0,0$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p3m1$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0]  $p2'mm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x/2,0



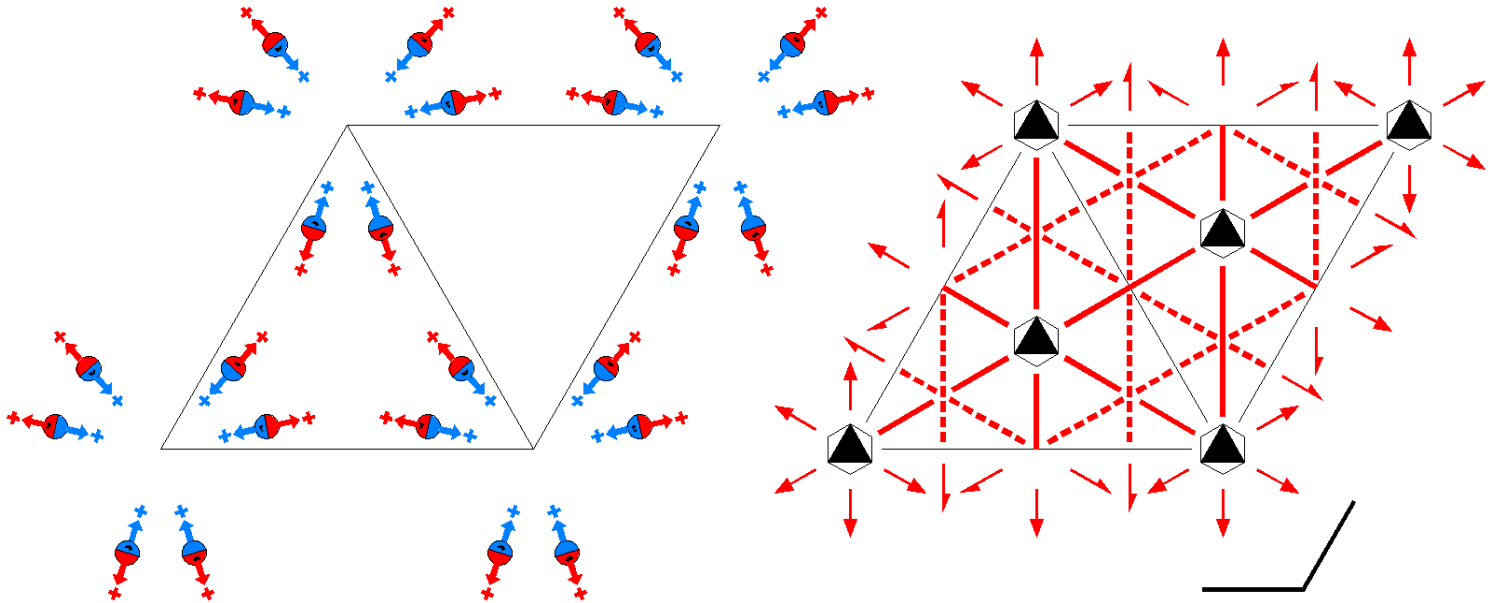
$P\bar{6}m'2'$

187.5.1443

$\bar{6}m'2'$

$P\bar{6}m'2'$

Hexagonal



Origin on  $\bar{6}m'2'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/2;$	$x \leq 2y;$	$y \leq \min(1-x, 2x)$
Vertices	0,0,0	2/3,1/3,0	1/3,2/3,0		
	0,0,1/2	2/3,1/3,1/2	1/3,2/3,1/2		

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                            | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                         | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)               |
| (4) m $x,y,0$<br>( $m_z$  0,0,0)              | (5) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (6) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0) |
| (7) $m'$ $x,\bar{x},z$<br>( $m_{xy}$  0,0,0)' | (8) $m'$ $x,2x,z$<br>( $m_x$  0,0,0)'                      | (9) $m'$ $2x,x,z$<br>( $m_y$  0,0,0)'                 |
| (10) $2'$ $x,\bar{x},0$<br>( $2_3$  0,0,0)'   | (11) $2'$ $x,2x,0$<br>( $2_2$  0,0,0)'                     | (12) $2'$ $2x,x,0$<br>( $2_1$  0,0,0)'                |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

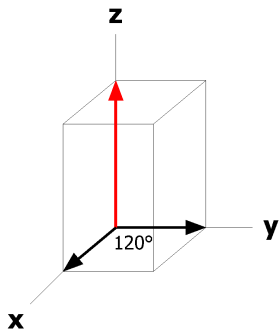
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
12	o	1	(1) $x,y,z$ [u,v,w] (4) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ] (7) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ] (10) $\bar{y},\bar{x},\bar{z}$ [v,u,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $\bar{y},x-y,\bar{z}$ [v, $\bar{u}+v,w$ ] (8) $\bar{x}+y,y,z$ [ $\bar{u}+v,v,w$ ] (11) $\bar{x}+y,y,\bar{z}$ [u-v, $\bar{v},w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x}+y,\bar{x},\bar{z}$ [u-v,u,w] (9) $x,x-y,z$ [u,u-v,w] (12) $x,x-y,\bar{z}$ [ $\bar{u},\bar{u}+v,w$ ]
6	n	.m'	$x,\bar{x},z$ [u, $\bar{u},w$ ] $x,\bar{x},\bar{z}$ [ $\bar{u},u,w$ ]	$x,2x,z$ [u,2u,w] $x,2x,\bar{z}$ [ $\bar{u},2\bar{u},w$ ]	$2\bar{x},\bar{x},z$ [2 $\bar{u},\bar{u},w$ ] $2\bar{x},\bar{x},\bar{z}$ [2 $\bar{u},\bar{u},w$ ]
6	m	m..	$x,y,1/2$ [0,0,w] $\bar{y},\bar{x},1/2$ [0,0,w]	$\bar{y},x-y,1/2$ [0,0,w] $\bar{x}+y,y,1/2$ [0,0,w]	$\bar{x}+y,\bar{x},1/2$ [0,0,w] $x,x-y,1/2$ [0,0,w]
6	l	m..	$x,y,0$ [0,0,w] $\bar{y},\bar{x},0$ [0,0,w]	$\bar{y},x-y,0$ [0,0,w] $\bar{x}+y,y,0$ [0,0,w]	$\bar{x}+y,\bar{x},0$ [0,0,w] $x,x-y,0$ [0,0,w]
3	k	mm'2'	$x,\bar{x},1/2$ [0,0,w]	$x,2x,1/2$ [0,0,w]	$2\bar{x},\bar{x},1/2$ [0,0,w]
3	j	mm'2'	$x,\bar{x},0$ [0,0,w]	$x,2x,0$ [0,0,w]	$2\bar{x},\bar{x},0$ [0,0,w]
2	i	3m'	$2/3,1/3,z$ [0,0,w]	$2/3,1/3,\bar{z}$ [0,0,w]	
2	h	3m'	$1/3,2/3,z$ [0,0,w]	$1/3,2/3,\bar{z}$ [0,0,w]	
2	g	3m'	$0,0,z$ [0,0,w]	$0,0,\bar{z}$ [0,0,w]	
1	f	$\bar{6}m'2'$	$2/3,1/3,1/2$ [0,0,w]		
1	e	$\bar{6}m'2'$	$2/3,1/3,0$ [0,0,w]		
1	d	$\bar{6}m'2'$	$1/3,2/3,1/2$ [0,0,w]		
1	c	$\bar{6}m'2'$	$1/3,2/3,0$ [0,0,w]		
1	b	$\bar{6}m'2'$	$0,0,1/2$ [0,0,w]		
1	a	$\bar{6}m'2'$	$0,0,0$ [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1]  $p3m11'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m1$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

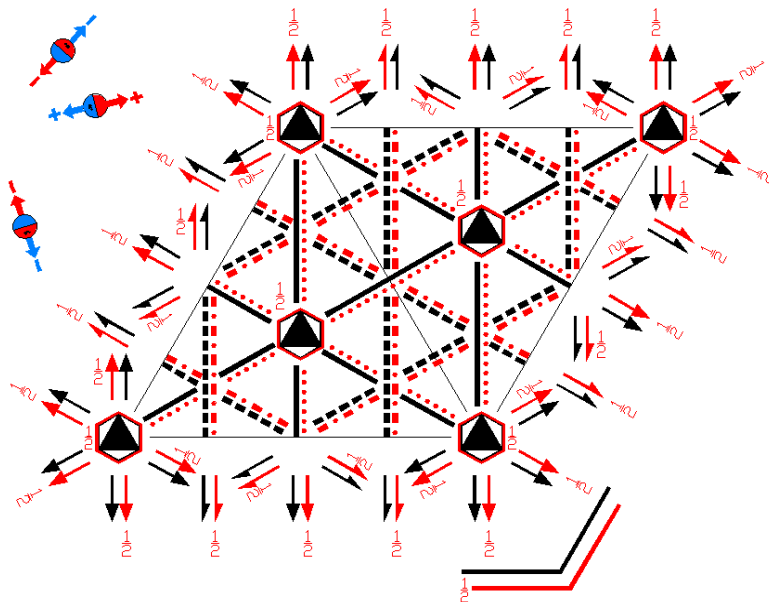
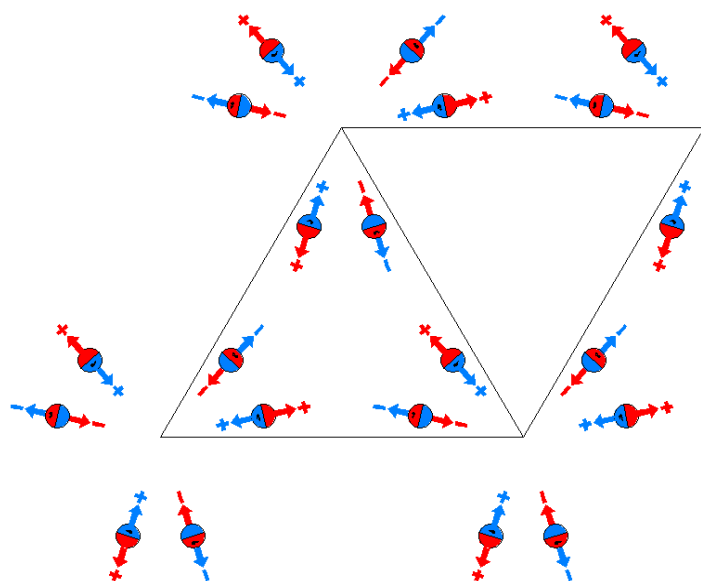
Along [2,1,0]  $p2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P_{2c}\bar{6}m2$   
187.6.1444

$\bar{6}m21'$   
 $P_{2c}\bar{6}m2$

Hexagonal



Origin on  $\bar{6}m2$

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $0 \leq z \leq 1/2$ ;  $x \leq 2y$ ;  $y \leq \min(1-x, 2x)$

Vertices  $0,0,0$   $2/3,1/3,0$   $1/3,2/3,0$   
 $0,0,1/2$   $2/3,1/3,1/2$   $1/3,2/3,1/2$

### Symmetry Operations

For  $(0,0,0)$  + set

- |   |  |   |
|---|--|---|
| (1) 1<br>( $1 0,0,0$ )                      | (2) $3^+$ $0,0,z$<br>( $3_z 0,0,0$ )                         | (3) $3^-$ $0,0,z$<br>( $3_z^{-1} 0,0,0$ )               |
| (4) $m$ $x,y,0$<br>( $m_z 0,0,0$ )          | (5) $\bar{6}^-$ $0,0,z; 0,0,0$<br>( $\bar{6}_z^{-1} 0,0,0$ ) | (6) $\bar{6}^+$ $0,0,z; 0,0,0$<br>( $\bar{6}_z 0,0,0$ ) |
| (7) $m$ $x,\bar{x},z$<br>( $m_{xy} 0,0,0$ ) | (8) $m$ $x,2x,z$<br>( $m_x 0,0,0$ )                          | (9) $m$ $2x,x,z$<br>( $m_y 0,0,0$ )                     |
| (10) 2 $x,\bar{x},0$<br>( $2_3 0,0,0$ )     | (11) 2 $x,2x,0$<br>( $2_2 0,0,0$ )                           | (12) 2 $2x,x,0$<br>( $2_1 0,0,0$ )                      |

For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 3 <sup>+</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub>  0,0,1)'	(3) 3 <sup>-</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,1)'
(4) m' x,y,1/2 (m <sub>z</sub>  0,0,1)'	(5) $\bar{6}^-$ ' 0,0,z; 0,0,1/2 ( $\bar{6}_z^{-1}$  0,0,1)'	(6) $\bar{6}^+$ ' 0,0,z; 0,0,1/2 ( $\bar{6}_z$  0,0,1)'
(7) c' (0,0,1) x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,1)'	(8) c' (0,0,1) x,2x,z (m <sub>x</sub>  0,0,1)'	(9) c' (0,0,1) 2x,x,z (m <sub>y</sub>  0,0,1)'
(10) 2' x, $\bar{x}$ ,1/2 (2 <sub>3</sub>  0,0,1)'	(11) 2' x,2x,1/2 (2 <sub>2</sub>  0,0,1)'	(12) 2' 2x,x,1/2 (2 <sub>1</sub>  0,0,1)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

**Positions**

			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(0,0,1)' +	
24	o	1	(1) x,y,z [u,v,w] (4) x,y, $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ ,w] (7) $\bar{y}$ , $\bar{x}$ ,z [v,u, $\bar{w}$ ] (10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w] (5) $\bar{y}$ ,x-y, $\bar{z}$ [v, $\bar{u}$ +v,w] (8) $\bar{x}$ +y,y,z [u-v, $\bar{v}$ , $\bar{w}$ ] (11) $\bar{x}$ +y,y, $\bar{z}$ [ $\bar{u}$ +v,v, $\bar{w}$ ]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w] (6) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ [u-v,u,w] (9) x,x-y,z [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ] (12) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ]
12	n	.m.	x, $\bar{x}$ ,z [u,u,0] x, $\bar{x}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ ,0]	x,2x,z [ $\bar{u}$ ,0,0] x,2x, $\bar{z}$ [u,0,0]	2 $\bar{x}$ , $\bar{x}$ ,z [0, $\bar{u}$ ,0] 2 $\bar{x}$ , $\bar{x}$ , $\bar{z}$ [0,u,0]
12	m	m'..	x,y,1/2 [u,v,0] $\bar{y}$ , $\bar{x}$ ,1/2 [v,u,0]	$\bar{y}$ ,x-y,1/2 [ $\bar{v}$ ,u-v,0] $\bar{x}$ +y,y,1/2 [u-v, $\bar{v}$ ,0]	$\bar{x}$ +y, $\bar{x}$ ,1/2 [ $\bar{u}$ +v, $\bar{u}$ ,0] x,x-y,1/2 [ $\bar{u}$ , $\bar{u}$ +v,0]
12	l	m..	x,y,0 [0,0,w] $\bar{y}$ , $\bar{x}$ ,0 [0,0,w]	$\bar{y}$ ,x-y,0 [0,0,w] $\bar{x}$ +y,y,0 [0,0,w]	$\bar{x}$ +y, $\bar{x}$ ,0 [0,0,w] x,x-y,0 [0,0,w]
6	k	m'm2'	x, $\bar{x}$ ,1/2 [u,u,0]	x,2x,1/2 [ $\bar{u}$ ,0,0]	2 $\bar{x}$ , $\bar{x}$ ,1/2 [0, $\bar{u}$ ,0]
6	j	mm2	x, $\bar{x}$ ,0 [0,0,0]	x,2x,0 [0,0,0]	2 $\bar{x}$ , $\bar{x}$ ,0 [0,0,0]
4	i	3m.	2/3,1/3,z [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	
4	h	3m.	1/3,2/3,z [0,0,0]	1/3,2/3, $\bar{z}$ [0,0,0]	
4	g	3m.	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]	
2	f	$\bar{6}^-m2'$	2/3,1/3,1/2 [0,0,0]		
2	e	$\bar{6}^-m2$	2/3,1/3,0 [0,0,0]		

2 d  $\bar{6}'m2'$   $1/3, 2/3, 1/2$  [0,0,0]

2 c  $\bar{6}m2$   $1/3, 2/3, 0$  [0,0,0]

2 b  $\bar{6}'m2'$   $0, 0, 1/2$  [0,0,0]

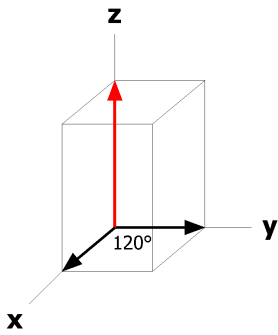
2 a  $\bar{6}m2$   $0, 0, 0$  [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p3m11'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

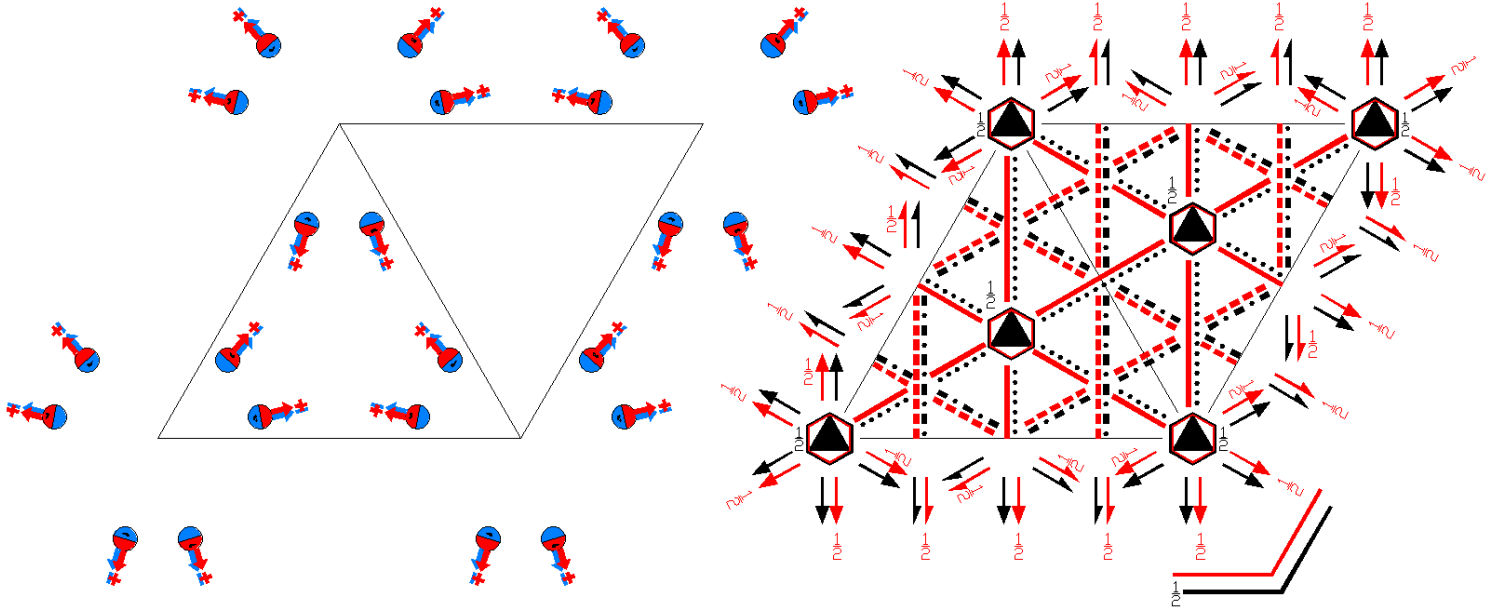
Along [2,1,0]  $p2mm$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P_{2c}\bar{6}m'2$   
187.7.1445

$\bar{6}m21'$   
 $P_{2c}\bar{6}m'2$

Hexagonal



Origin on  $\bar{6}'m'2$

**Asymmetric unit**  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $0 \leq z \leq 1/2$ ;  $x \leq 2y$ ;  $y \leq \min(1-x, 2x)$

**Vertices**  $0,0,0$   $2/3,1/3,0$   $1/3,2/3,0$   
 $0,0,1/2$   $2/3,1/3,1/2$   $1/3,2/3,1/2$

### Symmetry Operations

For  $(0,0,0)$  + set

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                              | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                          | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                |
| (4) $m'$ x,y,0<br>( $m_z$  0,0,0)'              | (5) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0)' | (6) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0)' |
| (7) $m'$ x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0)' | (8) $m'$ x,2x,z<br>( $m_x$  0,0,0)'                         | (9) $m'$ 2x,x,z<br>( $m_y$  0,0,0)'                    |
| (10) 2 x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)       | (11) 2 x,2x,0<br>( $2_2$  0,0,0)                            | (12) 2 2x,x,0<br>( $2_1$  0,0,0)                       |



## For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 3 <sup>+</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub>  0,0,1)'	(3) 3 <sup>-</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,1)'
(4) m <sub>x,y</sub> ,1/2 (m <sub>z</sub>  0,0,1)	(5) $\bar{6}^-$ 0,0,z; 0,0,1/2 ( $\bar{6}_z^{-1}$  0,0,1)	(6) $\bar{6}^+$ 0,0,z; 0,0,1/2 ( $\bar{6}_z$  0,0,1)
(7) c (0,0,1) x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,1)	(8) c (0,0,1) x,2x,z (m <sub>x</sub>  0,0,1)	(9) c (0,0,1) 2x,x,z (m <sub>y</sub>  0,0,1)
(10) 2' x, $\bar{x}$ ,1/2 (2 <sub>3</sub>  0,0,1)'	(11) 2' x,2x,1/2 (2 <sub>2</sub>  0,0,1)'	(12) 2' 2x,x,1/2 (2 <sub>1</sub>  0,0,1)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

**Positions**

			Coordinates		
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(0,0,1)' +	
24	o	1	(1) x,y,z [u,v,w] (4) x,y, $\bar{z}$ [u,v, $\bar{w}$ ] (7) $\bar{y}$ , $\bar{x}$ ,z [ $\bar{v}$ , $\bar{u}$ ,w] (10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w] (5) $\bar{y}$ ,x-y, $\bar{z}$ [ $\bar{v}$ ,u-v, $\bar{w}$ ] (8) $\bar{x}$ +y,y,z [ $\bar{u}$ +v,v,w] (11) $\bar{x}$ +y,y, $\bar{z}$ [ $\bar{u}$ +v,v, $\bar{w}$ ]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w] (6) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ [ $\bar{u}$ +v, $\bar{u}$ , $\bar{w}$ ] (9) x,x-y,z [u,u-v,w] (12) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ]
12	n	.m'	x, $\bar{x}$ ,z [u, $\bar{u}$ ,w] x, $\bar{x}$ , $\bar{z}$ [u, $\bar{u}$ , $\bar{w}$ ]	x,2x,z [u,2u,w] x,2x, $\bar{z}$ [u,2u, $\bar{w}$ ]	2 $\bar{x}$ , $\bar{x}$ ,z [2 $\bar{u}$ , $\bar{u}$ ,w] 2 $\bar{x}$ , $\bar{x}$ , $\bar{z}$ [2 $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]
12	m	m..	x,y,1/2 [0,0,w] $\bar{y}$ , $\bar{x}$ ,1/2 [0,0,w]	$\bar{y}$ ,x-y,1/2 [0,0,w] $\bar{x}$ +y,y,1/2 [0,0,w]	$\bar{x}$ +y, $\bar{x}$ ,1/2 [0,0,w] x,x-y,1/2 [0,0,w]
12	l	m'..	x,y,0 [u,v,0] $\bar{y}$ , $\bar{x}$ ,0 [ $\bar{v}$ , $\bar{u}$ ,0]	$\bar{y}$ ,x-y,0 [ $\bar{v}$ ,u-v,0] $\bar{x}$ +y,y,0 [ $\bar{u}$ +v,v,0]	$\bar{x}$ +y, $\bar{x}$ ,0 [ $\bar{u}$ +v, $\bar{u}$ ,0] x,x-y,0 [u,u-v,0]
6	k	mm'2'	x, $\bar{x}$ ,1/2 [0,0,w]	x,2x,1/2 [0,0,w]	2 $\bar{x}$ , $\bar{x}$ ,1/2 [0,0,w]
6	j	m'm'2	x, $\bar{x}$ ,0 [u, $\bar{u}$ ,0]	x,2x,0 [u,2u,0]	2 $\bar{x}$ , $\bar{x}$ ,0 [2 $\bar{u}$ , $\bar{u}$ ,0]
4	i	3m'	2/3,1/3,z [0,0,w]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	
4	h	3m'	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ [0,0, $\bar{w}$ ]	
4	g	3m'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	
2	f	$\bar{6}$ m'2'	2/3,1/3,1/2 [0,0,w]		
2	e	$\bar{6}$ 'm'2	2/3,1/3,0 [0,0,0]		

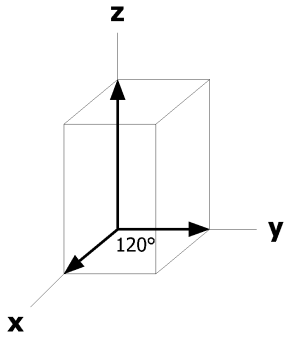
2	d	$\bar{6}'m'2'$	$1/3, 2/3, 1/2$	$[0, 0, w]$
2	c	$\bar{6}'m'2'$	$1/3, 2/3, 0$	$[0, 0, 0]$
2	b	$\bar{6}'m'2'$	$0, 0, 1/2$	$[0, 0, w]$
2	a	$\bar{6}'m'2'$	$0, 0, 0$	$[0, 0, 0]$

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p3m11'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$   $p_{2a'}1m'1$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x, 0, 1/2$

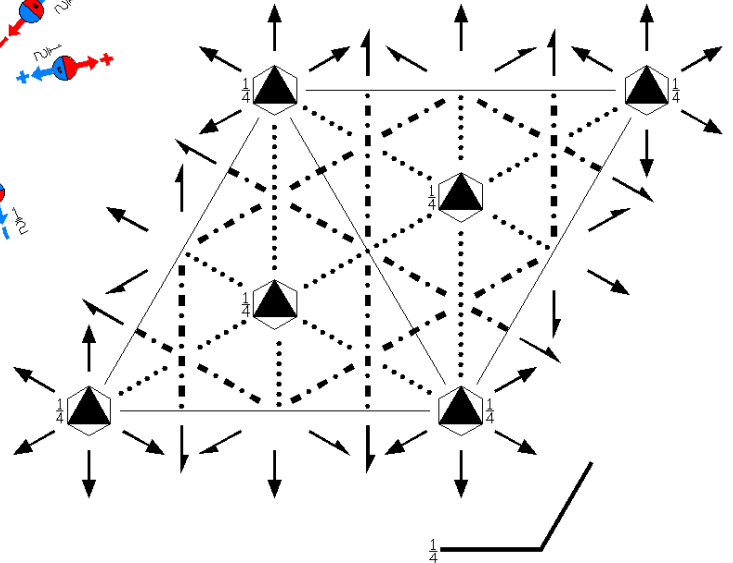
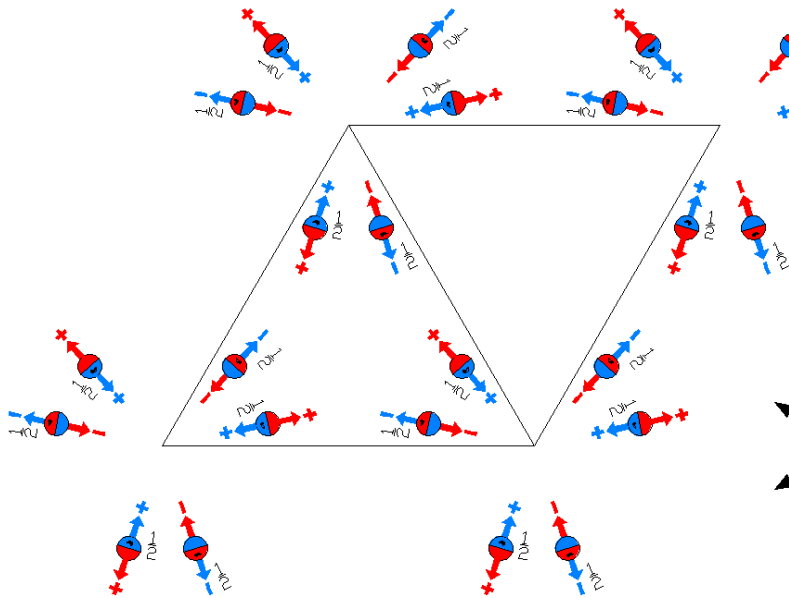
Along  $[2, 1, 0]$   $p_{2a'}2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x, x/2, 0$



$P\bar{6}c2$   
188.1.1446

$\bar{6}m2$   
 $P\bar{6}c2$

Hexagonal



**Origin on 3c2**

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,0,1/4

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                                      | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                             | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                   |
| (4) m x,y,1/4<br>( $m_z$  0,0,1/2)                      | (5) $\bar{6}^-$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2) | (6) $\bar{6}^+$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2) |
| (7) c (0,0,1/2) x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,1/2) | (8) c (0,0,1/2) x,2x,z<br>( $m_x$  0,0,1/2)                    | (9) c (0,0,1/2) 2x,x,z<br>( $m_y$  0,0,1/2)               |
| (10) 2 x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)               | (11) 2 x,2x,0<br>( $2_2$  0,0,0)                               | (12) 2 2x,x,0<br>( $2_1$  0,0,0)                          |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

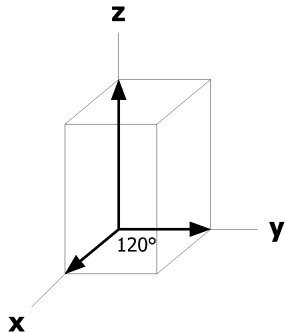
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates				
12	l	1	(1) x,y,z [u,v,w] (4) x,y, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ] (7) $\bar{y},\bar{x},z+1/2$ [v,u, $\bar{w}$ ] (10) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $\bar{y},x-y,\bar{z}+1/2$ [v, $\bar{u}+v,w$ ] (8) $\bar{x}+y,y,z+1/2$ [u-v, $\bar{v},\bar{w}$ ] (11) $\bar{x}+y,y,\bar{z}$ [ $\bar{u}+v,v,\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x}+y,\bar{x},\bar{z}+1/2$ [u-v,u,w] (9) x,x-y,z+1/2 [ $\bar{u},\bar{u}+v,\bar{w}$ ] (12) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ]		
6	k	m..	x,y,1/4 [0,0,w] $\bar{y},\bar{x},3/4$ [0,0, $\bar{w}$ ]	$\bar{y},x-y,1/4$ [0,0,w] $\bar{x}+y,y,3/4$ [0,0, $\bar{w}$ ]	$\bar{x}+y,\bar{x},1/4$ [0,0,w] x,x-y,3/4 [0,0, $\bar{w}$ ]		
6	j	..2	x, $\bar{x},0$ [u, $\bar{u},0$ ] x, $\bar{x},1/2$ [ $\bar{u},u,0$ ]	x,2x,0 [u,2u,0] x,2x,1/2 [ $\bar{u},2\bar{u},0$ ]	2 $\bar{x},\bar{x},0$ [2 $\bar{u},\bar{u},0$ ] 2 $\bar{x},\bar{x},1/2$ [2u,u,0]		
4	i	3..	2/3,1/3,z [0,0,w]	2/3,1/3, $\bar{z}+1/2$ [0,0,w]	2/3,1/3,z+1/2 [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	
4	h	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}+1/2$ [0,0,w]	1/3,2/3,z+1/2 [0,0, $\bar{w}$ ]	1/3,2/3, $\bar{z}$ [0,0, $\bar{w}$ ]	
4	g	3..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	
2	f	$\bar{6}$ ..	2/3,1/3,1/4 [0,0,w]	2/3,1/3,3/4 [0,0, $\bar{w}$ ]			
2	e	3.2	2/3,1/3,0 [0,0,0]	2/3,1/3,1/2 [0,0,0]			
2	d	$\bar{6}$ ..	1/3,2/3,1/4 [0,0,w]	1/3,2/3,3/4 [0,0, $\bar{w}$ ]			
2	c	3.2	1/3,2/3,0 [0,0,0]	1/3,2/3,1/2 [0,0,0]			
2	b	$\bar{6}$ ..	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]			
2	a	3.2	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p3m11'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>1m1  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/4

Along [2,1,0] p2mg  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



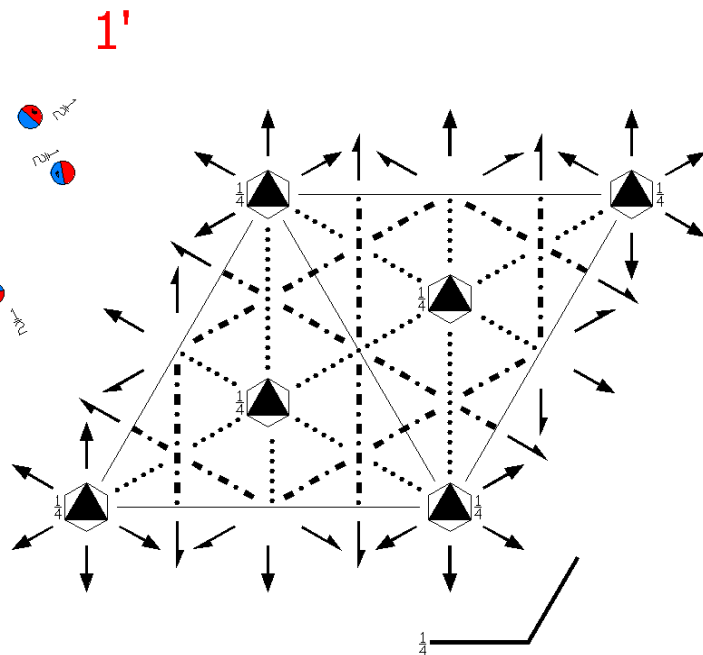
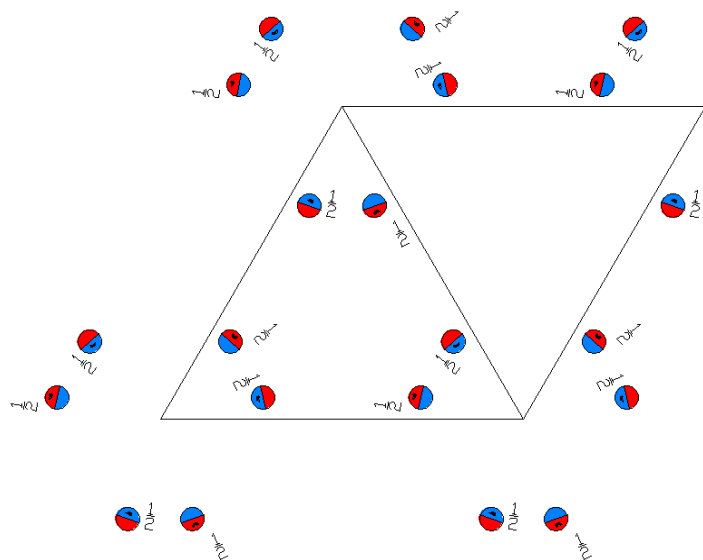
$P\bar{6}c21'$

188.2.1447

$\bar{6}m21'$

$P\bar{6}c21'$

Hexagonal



Origin on  $3c21'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,0 1/4

**Symmetry Operations**

For 1 + set

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                                    | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                             | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                   |
| (4) m $x,y,1/4$<br>( $m_z$  0,0,1/2)                  | (5) $\bar{6}^-$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2) | (6) $\bar{6}^+$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2) |
| (7) c (0,0,1/2) $x,\bar{x},z$<br>( $m_{xy}$  0,0,1/2) | (8) c (0,0,1/2) $x,2x,z$<br>( $m_x$  0,0,1/2)                  | (9) c (0,0,1/2) $2x,x,z$<br>( $m_y$  0,0,1/2)             |
| (10) 2 $x,\bar{x},0$<br>( $2_3$  0,0,0)               | (11) 2 $x,2x,0$<br>( $2_2$  0,0,0)                             | (12) 2 $2x,x,0$<br>( $2_1$  0,0,0)                        |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 3 <sup>+</sup> 0,0,z (3 <sub>z</sub>  0,0,0)'	(3) 3 <sup>-</sup> 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(4) m' x,y,1/4 (m <sub>z</sub>  0,0,1/2)'	(5) $\bar{6}^-$ 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1}$  0,0,1/2)'	(6) $\bar{6}^+$ 0,0,z; 0,0,1/4 ( $\bar{6}_z$  0,0,1/2)'
(7) c' (0,0,1/2) x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,1/2)'	(8) c' (0,0,1/2) x,2x,z (m <sub>x</sub>  0,0,1/2)'	(9) c' (0,0,1/2) 2x,x,z (m <sub>y</sub>  0,0,1/2)'
(10) 2' x, $\bar{x}$ ,0 (2 <sub>3</sub>  0,0,0)'	(11) 2' x,2x,0 (2 <sub>2</sub>  0,0,0)'	(12) 2' 2x,x,0 (2 <sub>1</sub>  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

**Positions**

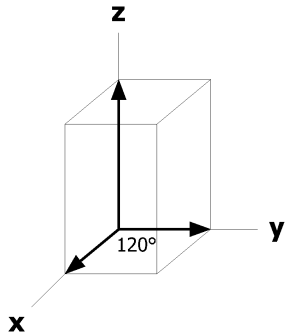
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			1 +	1' +		
12	l	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0]	
			(4) x,y, $\bar{z}+1/2$ [0,0,0]	(5) $\bar{y}$ ,x-y, $\bar{z}+1/2$ [0,0,0]	(6) $\bar{x}+y,\bar{x},\bar{z}+1/2$ [0,0,0]	
			(7) $\bar{y},\bar{x},z+1/2$ [0,0,0]	(8) $\bar{x}+y,y,z+1/2$ [0,0,0]	(9) x,x-y,z+1/2 [0,0,0]	
			(10) $\bar{y},\bar{x},\bar{z}$ [0,0,0]	(11) $\bar{x}+y,y,\bar{z}$ [0,0,0]	(12) x,x-y, $\bar{z}$ [0,0,0]	
6	k	m..1'	x,y,1/4 [0,0,0]	$\bar{y}$ ,x-y,1/4 [0,0,0]	$\bar{x}+y,\bar{x},1/4$ [0,0,0]	
			$\bar{y},\bar{x},3/4$ [0,0,0]	$\bar{x}+y,y,3/4$ [0,0,0]	x,x-y,3/4 [0,0,0]	
6	j	..21'	x, $\bar{x}$ ,0 [0,0,0]	x,2x,0 [0,0,0]	2 $\bar{x},\bar{x}$ ,0 [0,0,0]	
			x, $\bar{x}$ ,1/2 [0,0,0]	x,2x,1/2 [0,0,0]	2 $\bar{x},\bar{x},1/2$ [0,0,0]	
4	i	3..1'	2/3,1/3,z [0,0,0]	2/3,1/3, $\bar{z}+1/2$ [0,0,0]	2/3,1/3,z+1/2 [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]
4	h	3..1'	1/3,2/3,z [0,0,0]	1/3,2/3, $\bar{z}+1/2$ [0,0,0]	1/3,2/3,z+1/2 [0,0,0]	1/3,2/3, $\bar{z}$ [0,0,0]
4	g	3..1'	0,0,z [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]
2	f	$\bar{6}$ ..1'	2/3,1/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]		
2	e	3.21'	2/3,1/3,0 [0,0,0]	2/3,1/3,1/2 [0,0,0]		
2	d	$\bar{6}$ ..1'	1/3,2/3,1/4 [0,0,0]	1/3,2/3,3/4 [0,0,0]		
2	c	3.21'	1/3,2/3,0 [0,0,0]	1/3,2/3,1/2 [0,0,0]		
2	b	$\bar{6}$ ..1'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	a	3.21'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p3m11'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p1m11'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at  $x,0,0$

Along  $[2,1,0]$   $p2mg1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $x,x/2,0$



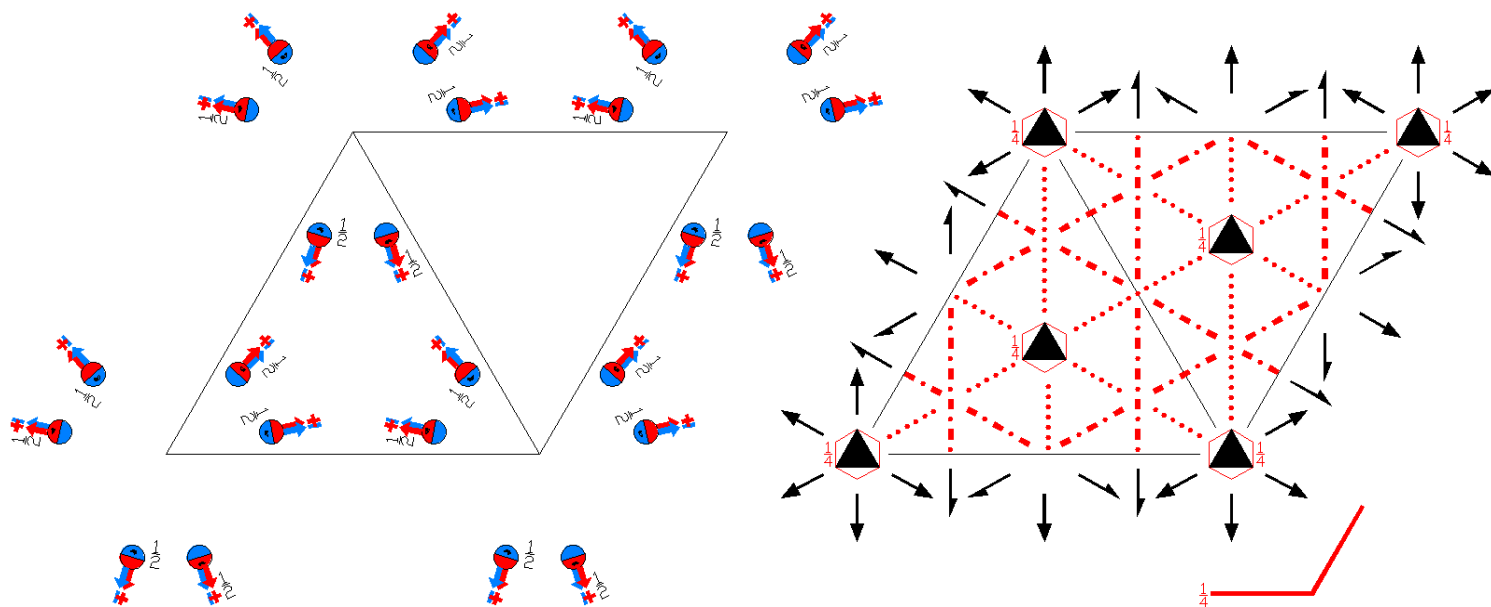
$P\bar{6}'c'2$

188.3.1448

$\bar{6}'m'2$

$P\bar{6}'c'2$

Hexagonal



Origin on  $3c'2$

Asymmetric unit	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,0 1/4

### Symmetry Operations

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)  | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                              | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) $m'$ x,y,1/4<br>( $m_z$  0,0,1/2)'                      | (5) $\bar{6}^-$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2)' | (6) $\bar{6}^+$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2)' |
| (7) $c'$ (0,0,1/2) x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,1/2)' | (8) $c'$ (0,0,1/2) x,2x,z<br>( $m_x$  0,0,1/2)'                 | (9) $c'$ (0,0,1/2) 2x,x,z<br>( $m_y$  0,0,1/2)'            |
| (10) 2 x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)                   | (11) 2 x,2x,0<br>( $2_2$  0,0,0)                                | (12) 2 2x,x,0<br>( $2_1$  0,0,0)                           |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

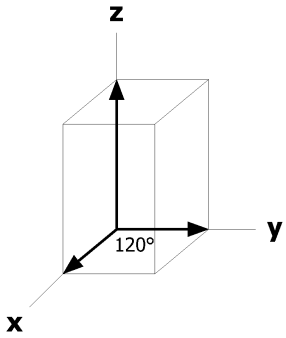
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates				
12	l	1	(1) x,y,z [u,v,w] (4) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ] (7) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ] (10) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $\bar{y},x-y,\bar{z}+1/2$ [ $\bar{v},u-v,\bar{w}$ ] (8) $\bar{x}+y,y,z+1/2$ [ $\bar{u}+v,v,w$ ] (11) $\bar{x}+y,y,\bar{z}$ [ $\bar{u}+v,v,\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x}+y,\bar{x},\bar{z}+1/2$ [ $\bar{u}+v,\bar{u},\bar{w}$ ] (9) x,x-y,z+1/2 [u,u-v,w] (12) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ]		
6	k	m'..	x,y,1/4 [u,v,0] $\bar{y},\bar{x},3/4$ [ $\bar{v},\bar{u},0$ ]	$\bar{y},x-y,1/4$ [ $\bar{v},u-v,0$ ] $\bar{x}+y,y,3/4$ [ $\bar{u}+v,v,0$ ]	$\bar{x}+y,\bar{x},1/4$ [ $\bar{u}+v,\bar{u},0$ ] x,x-y,3/4 [u,u-v,0]		
6	j	..2	x, $\bar{x},0$ [u, $\bar{u},0$ ] x, $\bar{x},1/2$ [u, $\bar{u},0$ ]	x,2x,0 [u,2u,0] x,2x,1/2 [u,2u,0]	2 $\bar{x},\bar{x},0$ [2 $\bar{u},\bar{u},0$ ] 2 $\bar{x},\bar{x},1/2$ [2 $\bar{u},\bar{u},0$ ]		
4	i	3..	2/3,1/3,z [0,0,w]	2/3,1/3, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	2/3,1/3,z+1/2 [0,0,w]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	
4	h	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/3,2/3,z+1/2 [0,0,w]	1/3,2/3, $\bar{z}$ [0,0, $\bar{w}$ ]	
4	g	3..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	
2	f	$\bar{6}'$ ..	2/3,1/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]			
2	e	3.2	2/3,1/3,0 [0,0,0]	2/3,1/3,1/2 [0,0,0]			
2	d	$\bar{6}'$ ..	1/3,2/3,1/4 [0,0,0]	1/3,2/3,3/4 [0,0,0]			
2	c	3.2	1/3,2/3,0 [0,0,0]	1/3,2/3,1/2 [0,0,0]			
2	b	$\bar{6}'$ ..	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]			
2	a	3.2	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p3m'1  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



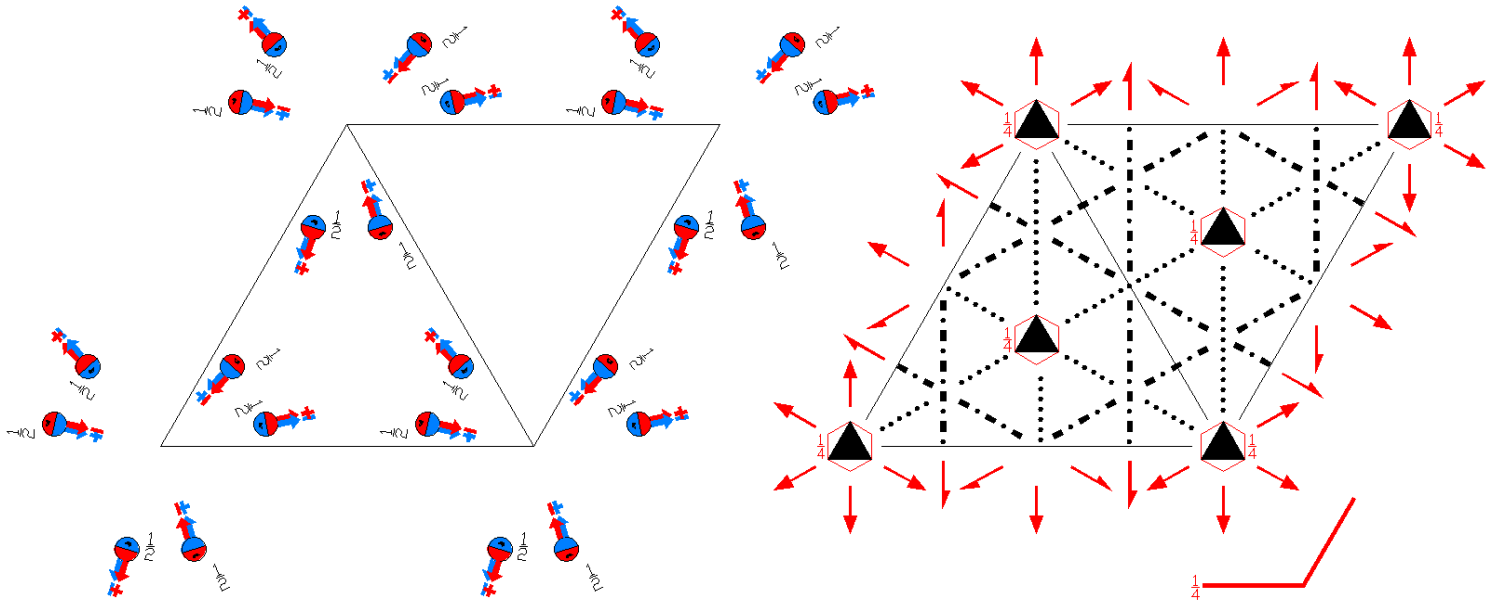
$P\bar{6}c2'$

188.4.1449

$\bar{6}m2'$

$P\bar{6}c2'$

Hexagonal



Origin on  $3c2'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,0 1/4

**Symmetry Operations**

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                                      | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                              | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) $m'$ x,y,1/4<br>( $m_z$  0,0,1/2)'                  | (5) $\bar{6}^-$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2)' | (6) $\bar{6}^+$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2)' |
| (7) c (0,0,1/2) x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,1/2) | (8) c (0,0,1/2) x,2x,z<br>( $m_x$  0,0,1/2)                     | (9) c (0,0,1/2) 2x,x,z<br>( $m_y$  0,0,1/2)                |
| (10) $2'$ x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)'           | (11) $2'$ x,2x,0<br>( $2_2$  0,0,0)'                            | (12) $2'$ 2x,x,0<br>( $2_1$  0,0,0)'                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

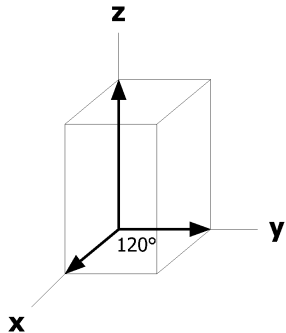
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates				
12	l	1	(1) x,y,z [u,v,w] (4) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ] (7) $\bar{y},\bar{x},z+1/2$ [v,u, $\bar{w}$ ] (10) $\bar{y},\bar{x},\bar{z}$ [v,u,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $\bar{y},x-y,\bar{z}+1/2$ [ $\bar{v},u-v,\bar{w}$ ] (8) $\bar{x}+y,y,z+1/2$ [u-v, $\bar{v},\bar{w}$ ] (11) $\bar{x}+y,y,\bar{z}$ [u-v, $\bar{v},w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x}+y,\bar{x},\bar{z}+1/2$ [ $\bar{u}+v,\bar{u},\bar{w}$ ] (9) x,x-y,z+1/2 [ $\bar{u},\bar{u}+v,\bar{w}$ ] (12) x,x-y, $\bar{z}$ [ $\bar{u},\bar{u}+v,w$ ]		
6	k	m'..	x,y,1/4 [u,v,0] $\bar{y},\bar{x},3/4$ [v,u,0]	$\bar{y},x-y,1/4$ [ $\bar{v},u-v,0$ ] $\bar{x}+y,y,3/4$ [u-v, $\bar{v},0$ ]	$\bar{x}+y,\bar{x},1/4$ [ $\bar{u}+v,\bar{u},0$ ] x,x-y,3/4 [ $\bar{u},\bar{u}+v,0$ ]		
6	j	..2'	x, $\bar{x},0$ [u,u,w] x, $\bar{x},1/2$ [u,u, $\bar{w}$ ]	x,2x,0 [ $\bar{u},0,w$ ] x,2x,1/2 [ $\bar{u},0,\bar{w}$ ]	2 $\bar{x},\bar{x},0$ [0, $\bar{u},w$ ] 2 $\bar{x},\bar{x},1/2$ [0, $\bar{u},\bar{w}$ ]		
4	i	3..	2/3,1/3,z [0,0,w]	2/3,1/3, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	2/3,1/3,z+1/2 [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0,w]	
4	h	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	1/3,2/3,z+1/2 [0,0, $\bar{w}$ ]	1/3,2/3, $\bar{z}$ [0,0,w]	
4	g	3..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	
2	f	$\bar{6}'..$	2/3,1/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]			
2	e	3.2'	2/3,1/3,0 [0,0,w]	2/3,1/3,1/2 [0,0, $\bar{w}$ ]			
2	d	$\bar{6}'..$	1/3,2/3,1/4 [0,0,0]	1/3,2/3,3/4 [0,0,0]			
2	c	3.2'	1/3,2/3,0 [0,0,w]	1/3,2/3,1/2 [0,0, $\bar{w}$ ]			
2	b	$\bar{6}'..$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]			
2	a	3.2'	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]			

**Symmetry of Special Projections**

Along [0,0,1] p3m1  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'1m1  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



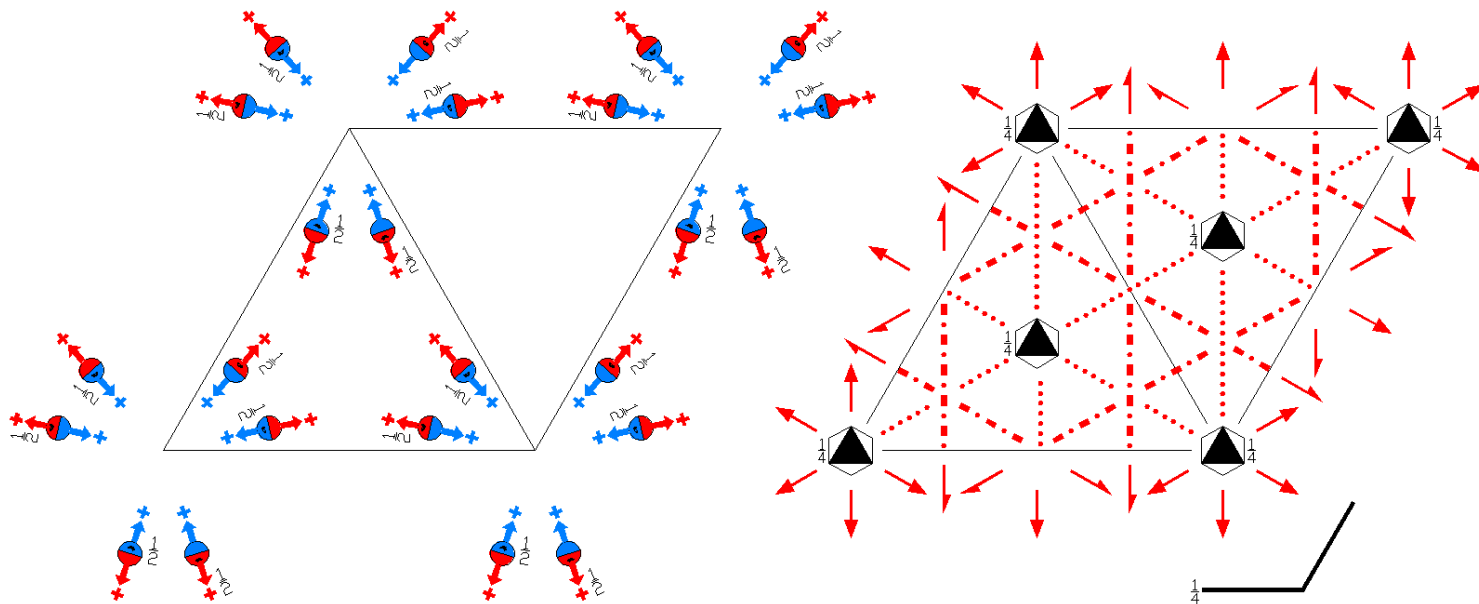
$P\bar{6}c'2'$

188.5.1450

$\bar{6}m'2'$

$P\bar{6}c'2'$

Hexagonal



Origin on  $3c'2'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,0,1/4

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                             | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                   |
| (4) m x,y,1/4<br>( $m_z$  0,0,1/2)                          | (5) $\bar{6}^-$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2) | (6) $\bar{6}^+$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2) |
| (7) $c'$ (0,0,1/2) x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,1/2)' | (8) $c'$ (0,0,1/2) x,2x,z<br>( $m_x$  0,0,1/2)'                | (9) $c'$ (0,0,1/2) 2x,x,z<br>( $m_y$  0,0,1/2)'           |
| (10) $2'$ x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)'               | (11) $2'$ x,2x,0<br>( $2_2$  0,0,0)'                           | (12) $2'$ 2x,x,0<br>( $2_1$  0,0,0)'                      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

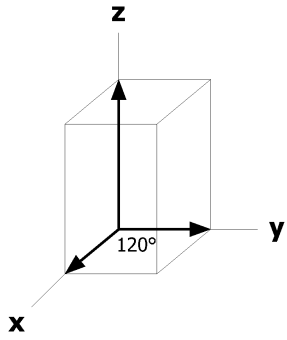
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates				
12	l	1	(1) x,y,z [u,v,w] (4) x,y, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ] (7) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ] (10) $\bar{y},\bar{x},\bar{z}$ [v,u,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $\bar{y},x-y,\bar{z}+1/2$ [v, $\bar{u}+v,w$ ] (8) $\bar{x}+y,y,z+1/2$ [ $\bar{u}+v,v,w$ ] (11) $\bar{x}+y,y,\bar{z}$ [u-v, $\bar{v},w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x}+y,\bar{x},\bar{z}+1/2$ [u-v,u,w] (9) x,x-y,z+1/2 [u,u-v,w] (12) x,x-y, $\bar{z}$ [ $\bar{u},\bar{u}+v,w$ ]		
6	k	m..	x,y,1/4 [0,0,w] $\bar{y},\bar{x},3/4$ [0,0,w]	$\bar{y},x-y,1/4$ [0,0,w] $\bar{x}+y,y,3/4$ [0,0,w]	$\bar{x}+y,\bar{x},1/4$ [0,0,w] x,x-y,3/4 [0,0,w]		
6	j	..2'	x, $\bar{x},0$ [u,u,w] x, $\bar{x},1/2$ [ $\bar{u},\bar{u},w$ ]	x,2x,0 [ $\bar{u},0,w$ ] x,2x,1/2 [u,0,w]	2 $\bar{x},\bar{x},0$ [0, $\bar{u},w$ ] 2 $\bar{x},\bar{x},1/2$ [0,u,w]		
4	i	3..	2/3,1/3,z [0,0,w]	2/3,1/3, $\bar{z}+1/2$ [0,0,w]	2/3,1/3,z+1/2 [0,0,w]	2/3,1/3, $\bar{z}$ [0,0,w]	
4	h	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}+1/2$ [0,0,w]	1/3,2/3,z+1/2 [0,0,w]	1/3,2/3, $\bar{z}$ [0,0,w]	
4	g	3..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}$ [0,0,w]	
2	f	$\bar{6}$ ..	2/3,1/3,1/4 [0,0,w]	2/3,1/3,3/4 [0,0,w]			
2	e	3.2'	2/3,1/3,0 [0,0,w]	2/3,1/3,1/2 [0,0,w]			
2	d	$\bar{6}$ ..	1/3,2/3,1/4 [0,0,w]	1/3,2/3,3/4 [0,0,w]			
2	c	3.2'	1/3,2/3,0 [0,0,w]	1/3,2/3,1/2 [0,0,w]			
2	b	$\bar{6}$ ..	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]			
2	a	3.2'	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]			

**Symmetry of Special Projections**

Along [0,0,1] p3m11'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p1m1  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

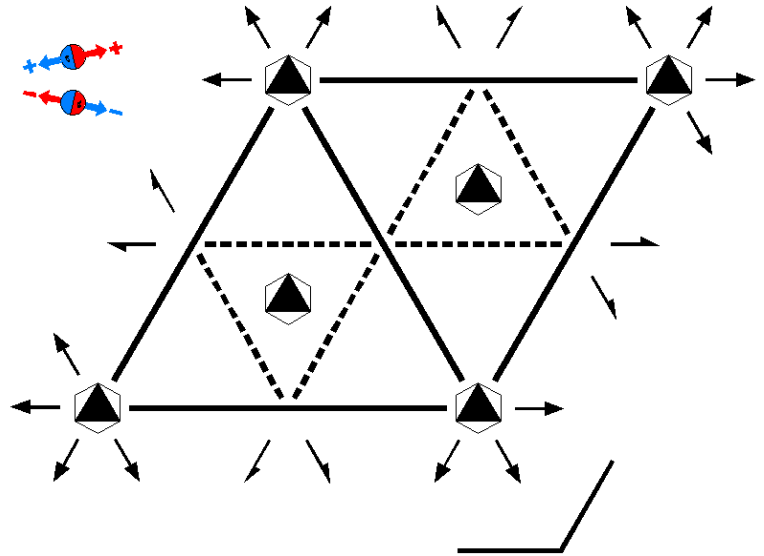
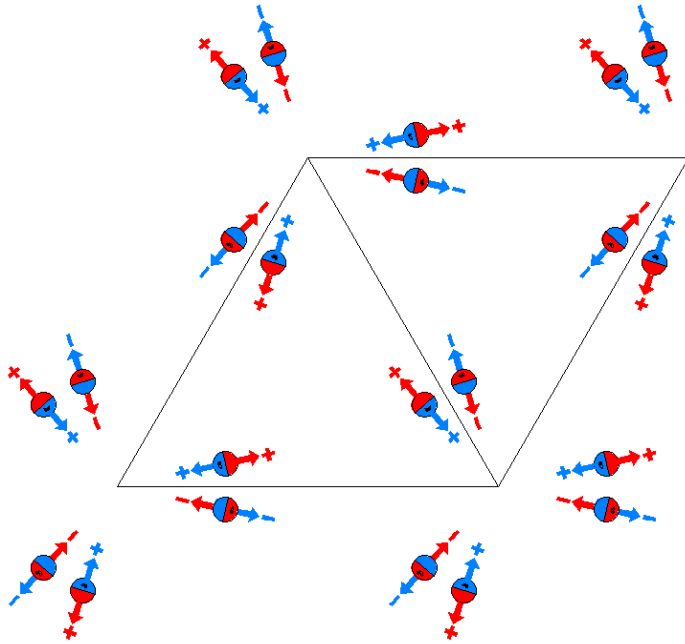
Along [2,1,0] p2'mg'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P\bar{6}2m$   
189.1.1451

$\bar{6}2m$   
 $P\bar{6}2m$

Hexagonal



Origin on  $\bar{6}2m$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

**Symmetry Operations**

- |                                   |  |   |
|-----------------------------------|--|---|
| (1) 1<br>(1 0,0,0)                | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                         | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)               |
| (4) m x,y,0<br>( $m_z$  0,0,0)    | (5) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (6) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0) |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0) | (8) 2 x,0,0<br>( $2_x$  0,0,0)                             | (9) 2 0,y,0<br>( $2_y$  0,0,0)                        |
| (10) m x,x,z<br>( $m_3$  0,0,0)   | (11) m x,0,z<br>( $m_2$  0,0,0)                            | (12) m 0,y,z<br>( $m_1$  0,0,0)                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

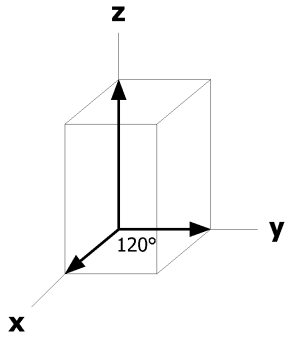
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	l	1	(1) x,y,z [u,v,w] (4) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ] (7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ] (10) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $\bar{y},x-y,\bar{z}$ [v, $\bar{u}+v,w$ ] (8) x-y, $\bar{y},\bar{z}$ [u-v, $\bar{v},\bar{w}$ ] (11) x-y, $\bar{y},z$ [ $\bar{u}+v,v,\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x}+y,\bar{x},\bar{z}$ [u-v,u,w] (9) $\bar{x},\bar{x}+y,\bar{z}$ [ $\bar{u},\bar{u}+v,\bar{w}$ ] (12) $\bar{x},\bar{x}+y,z$ [u,u-v, $\bar{w}$ ]	
6	k	m..	x,y,1/2 [0,0,w] y,x,1/2 [0,0, $\bar{w}$ ]	$\bar{y},x-y,1/2$ [0,0,w] x-y, $\bar{y},1/2$ [0,0, $\bar{w}$ ]	$\bar{x}+y,\bar{x},1/2$ [0,0,w] $\bar{x},\bar{x}+y,1/2$ [0,0, $\bar{w}$ ]	
6	j	m..	x,y,0 [0,0,w] y,x,0 [0,0, $\bar{w}$ ]	$\bar{y},x-y,0$ [0,0,w] x-y, $\bar{y},0$ [0,0, $\bar{w}$ ]	$\bar{x}+y,\bar{x},0$ [0,0,w] $\bar{x},\bar{x}+y,0$ [0,0, $\bar{w}$ ]	
6	i	..m	x,0,z [u,2u,0] x,0, $\bar{z}$ [ $\bar{u},2\bar{u},0$ ]	0,x,z [2 $\bar{u},\bar{u},0$ ] 0,x, $\bar{z}$ [2u,u,0]	$\bar{x},\bar{x},z$ [u, $\bar{u},0$ ] $\bar{x},\bar{x},\bar{z}$ [ $\bar{u},u,0$ ]	
4	h	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ [0,0,w]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	2/3,1/3,z [0,0, $\bar{w}$ ]
3	g	m2m	x,0,1/2 [0,0,0]	0,x,1/2 [0,0,0]	$\bar{x},\bar{x},1/2$ [0,0,0]	
3	f	m2m	x,0,0 [0,0,0]	0,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	
2	e	3.m	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	d	$\bar{6}..$	1/3,2/3,1/2 [0,0,w]	2/3,1/3,1/2 [0,0, $\bar{w}$ ]		
2	c	$\bar{6}..$	1/3,2/3,0 [0,0,w]	2/3,1/3,0 [0,0, $\bar{w}$ ]		
1	b	$\bar{6}2m$	0,0,1/2 [0,0,0]			
1	a	$\bar{6}2m$	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p31m1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

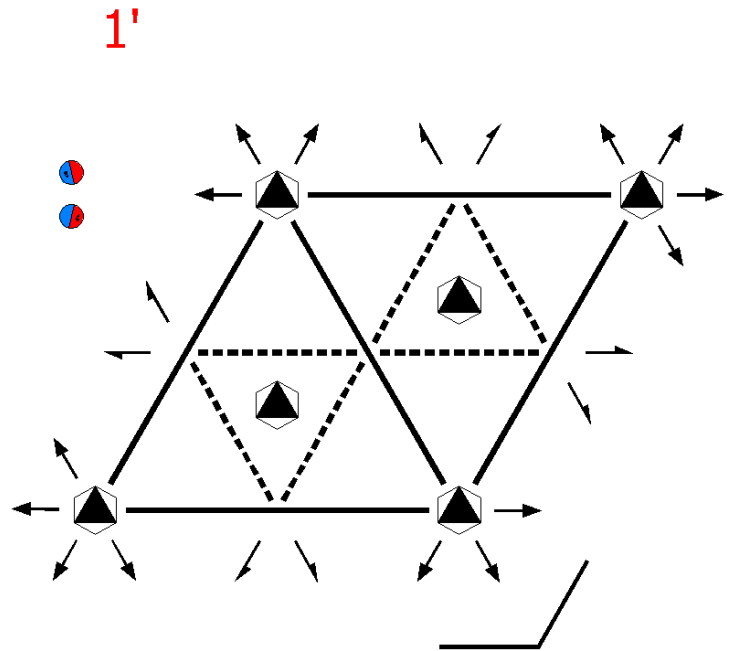
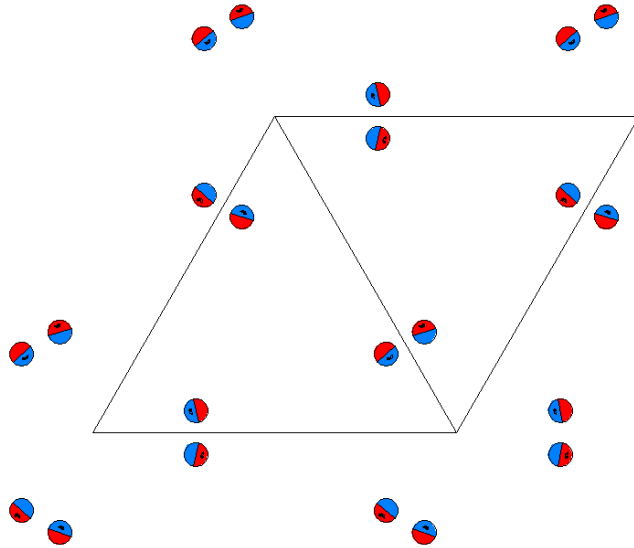
Along [2,1,0] p1m11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P\bar{6}2m1'$   
189.2.1452

$\bar{6}2m1'$   
 $P\bar{6}2m1'$

Hexagonal



Origin on  $\bar{6}2m1'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

**Symmetry Operations**

For 1 + set

- |                                   |  |   |
|-----------------------------------|--|---|
| (1) 1<br>(1 0,0,0)                | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                         | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)               |
| (4) m x,y,0<br>( $m_z$  0,0,0)    | (5) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (6) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0) |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0) | (8) 2 x,0,0<br>( $2_x$  0,0,0)                             | (9) 2 0,y,0<br>( $2_y$  0,0,0)                        |
| (10) m x,x,z<br>( $m_3$  0,0,0)   | (11) m x,0,z<br>( $m_2$  0,0,0)                            | (12) m 0,y,z<br>( $m_1$  0,0,0)                       |



For  $1'$  + set

(1) $1'$ ( $1 0,0,0$ )'	(2) $3^+'$ 0,0,z ( $3_z 0,0,0$ )'	(3) $3^-'$ 0,0,z ( $3_z^{-1} 0,0,0$ )'
(4) $m'$ x,y,0 ( $m_z 0,0,0$ )'	(5) $\bar{6}^-'$ 0,0,z; 0,0,0 ( $\bar{6}_z^{-1} 0,0,0$ )'	(6) $\bar{6}^+'$ 0,0,z; 0,0,0 ( $\bar{6}_z 0,0,0$ )'
(7) $2'$ x,x,0 ( $2_{xy} 0,0,0$ )'	(8) $2'$ x,0,0 ( $2_x 0,0,0$ )'	(9) $2'$ 0,y,0 ( $2_y 0,0,0$ )'
(10) $m'$ x,x,z ( $m_3 0,0,0$ )'	(11) $m'$ x,0,z ( $m_2 0,0,0$ )'	(12) $m'$ 0,y,z ( $m_1 0,0,0$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7);  $1'$ .

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			1 +		1' +	
12	l	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0]	
			(4) x,y, $\bar{z}$ [0,0,0]	(5) $\bar{y}$ ,x-y, $\bar{z}$ [0,0,0]	(6) $\bar{x}+y,\bar{x},\bar{z}$ [0,0,0]	
			(7) y,x, $\bar{z}$ [0,0,0]	(8) x-y, $\bar{y},\bar{z}$ [0,0,0]	(9) $\bar{x},\bar{x}+y,\bar{z}$ [0,0,0]	
			(10) y,x,z [0,0,0]	(11) x-y, $\bar{y},z$ [0,0,0]	(12) $\bar{x},\bar{x}+y,z$ [0,0,0]	
6	k	m..1'	x,y,1/2 [0,0,0]	$\bar{y}$ ,x-y,1/2 [0,0,0]	$\bar{x}+y,\bar{x},1/2$ [0,0,0]	
			y,x,1/2 [0,0,0]	x-y, $\bar{y},1/2$ [0,0,0]	$\bar{x},\bar{x}+y,1/2$ [0,0,0]	
6	j	m..1'	x,y,0 [0,0,0]	$\bar{y}$ ,x-y,0 [0,0,0]	$\bar{x}+y,\bar{x},0$ [0,0,0]	
			y,x,0 [0,0,0]	x-y, $\bar{y},0$ [0,0,0]	$\bar{x},\bar{x}+y,0$ [0,0,0]	
6	i	..m1'	x,0,z [0,0,0]	0,x,z [0,0,0]	$\bar{x},\bar{x},z$ [0,0,0]	
			x,0, $\bar{z}$ [0,0,0]	0,x, $\bar{z}$ [0,0,0]	$\bar{x},\bar{x},\bar{z}$ [0,0,0]	
4	h	3..1'	1/3,2/3,z [0,0,0]	1/3,2/3, $\bar{z}$ [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	2/3,1/3,z [0,0,0]
3	g	$\bar{m}2m1'$	x,0,1/2 [0,0,0]	0,x,1/2 [0,0,0]	$\bar{x},\bar{x},1/2$ [0,0,0]	
3	f	$m2m1'$	x,0,0 [0,0,0]	0,x,0 [0,0,0]	$\bar{x},\bar{x},0$ [0,0,0]	
2	e	3.m1'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	d	$\bar{6}^-..1'$	1/3,2/3,1/2 [0,0,0]	2/3,1/3,1/2 [0,0,0]		
2	c	$\bar{6}^-..1'$	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]		
1	b	$\bar{6}2m1'$	0,0,1/2 [0,0,0]			

1 a  $\overline{6}2m1'$  0,0,0 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p31m1'$

$\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$

Origin at 0,0,z

Along [1,0,0]  $p2mm1'$

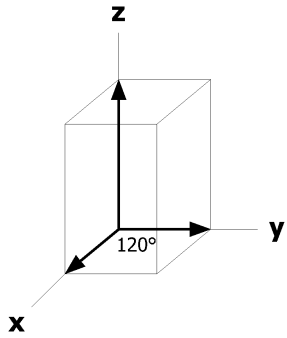
$\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$

Origin at x,0,0

Along [2,1,0]  $p1m11'$

$\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$

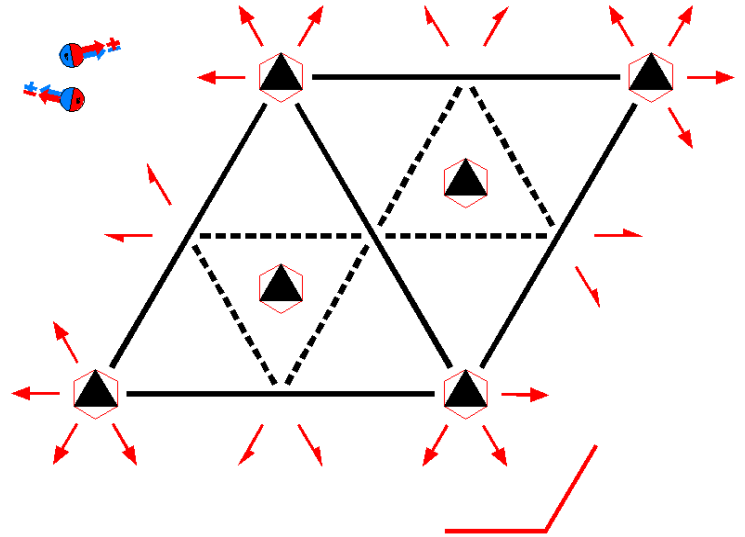
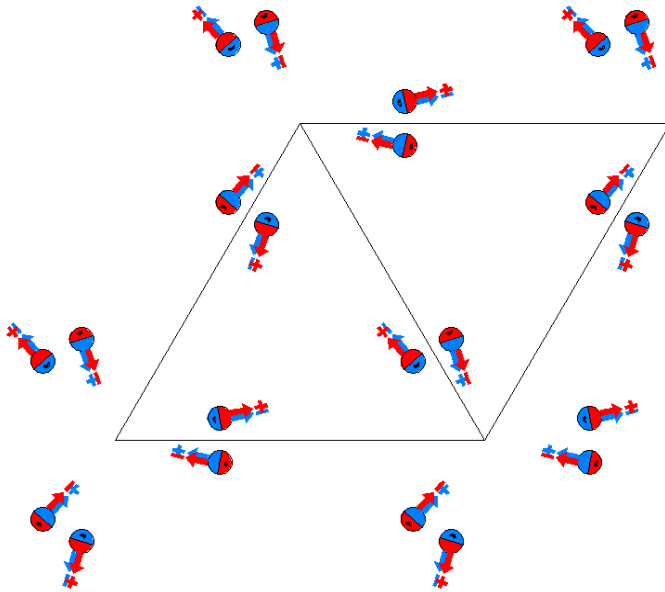
Origin at x,x/2,0



$P\bar{6}'2'm$   
189.3.1453

$\bar{6}'2'm$   
 $P\bar{6}'2'm$

Hexagonal



Origin on  $\bar{6}'2'm$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

### Symmetry Operations

- |                                       |  |   |
|---------------------------------------|--|---|
| (1) 1<br>(1 0,0,0)                    | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                           | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                 |
| (4) $m'$ x,y,0<br>( $m_z$  0,0,0)'    | (5) $\bar{6}^-'$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0)' | (6) $\bar{6}^+'$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0)' |
| (7) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)' | (8) $2'$ x,0,0<br>( $2_x$  0,0,0)'                           | (9) $2'$ 0,y,0<br>( $2_y$  0,0,0)'                      |
| (10) $m$ x,x,z<br>( $m_3$  0,0,0)     | (11) $m$ x,0,z<br>( $m_2$  0,0,0)                            | (12) $m$ 0,y,z<br>( $m_1$  0,0,0)                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

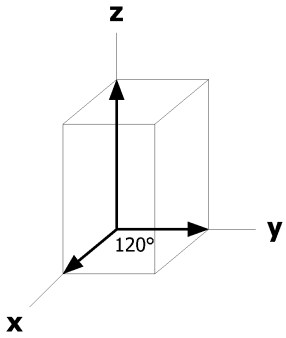
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	l	1	(1) x,y,z [u,v,w] (4) x,y, $\bar{z}$ [u,v, $\bar{w}$ ] (7) y,x, $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ ,w] (10) y,x,z [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w] (5) $\bar{y}$ ,x-y, $\bar{z}$ [ $\bar{v}$ ,u-v, $\bar{w}$ ] (8) x-y, $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ +v,v,w] (11) x-y, $\bar{y}$ ,z [ $\bar{u}$ +v,v, $\bar{w}$ ]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w] (6) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ [ $\bar{u}$ +v, $\bar{u}$ , $\bar{w}$ ] (9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ [u,u-v,w] (12) $\bar{x}$ , $\bar{x}$ +y,z [u,u-v, $\bar{w}$ ]	
6	k	m'..	x,y,1/2 [u,v,0] y,x,1/2 [ $\bar{v}$ , $\bar{u}$ ,0]	$\bar{y}$ ,x-y,1/2 [ $\bar{v}$ ,u-v,0] x-y, $\bar{y}$ ,1/2 [ $\bar{u}$ +v,v,0]	$\bar{x}$ +y, $\bar{x}$ ,1/2 [ $\bar{u}$ +v, $\bar{u}$ ,0] $\bar{x}$ , $\bar{x}$ +y,1/2 [u,u-v,0]	
6	j	m'..	x,y,0 [u,v,0] y,x,0 [ $\bar{v}$ , $\bar{u}$ ,0]	$\bar{y}$ ,x-y,0 [ $\bar{v}$ ,u-v,0] x-y, $\bar{y}$ ,0 [ $\bar{u}$ +v,v,0]	$\bar{x}$ +y, $\bar{x}$ ,0 [ $\bar{u}$ +v, $\bar{u}$ ,0] $\bar{x}$ , $\bar{x}$ +y,0 [u,u-v,0]	
6	i	..m	x,0,z [u,2u,0] x,0, $\bar{z}$ [u,2u,0]	0,x,z [2 $\bar{u}$ , $\bar{u}$ ,0] 0,x, $\bar{z}$ [2 $\bar{u}$ , $\bar{u}$ ,0]	$\bar{x}$ , $\bar{x}$ ,z [u, $\bar{u}$ ,0] $\bar{x}$ , $\bar{x}$ , $\bar{z}$ [u, $\bar{u}$ ,0]	
4	h	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0,w]      2/3,1/3,z [0,0, $\bar{w}$ ]	
3	g	m'2'm	x,0,1/2 [u,2u,0]	0,x,1/2 [2 $\bar{u}$ , $\bar{u}$ ,0]	$\bar{x}$ , $\bar{x}$ ,1/2 [u, $\bar{u}$ ,0]	
3	f	m'2'm	x,0,0 [u,2u,0]	0,x,0 [2 $\bar{u}$ , $\bar{u}$ ,0]	$\bar{x}$ , $\bar{x}$ ,0 [u, $\bar{u}$ ,0]	
2	e	3.m	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	d	$\bar{6}$ '..	1/3,2/3,1/2 [0,0,0]	2/3,1/3,1/2 [0,0,0]		
2	c	$\bar{6}$ '..	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]		
1	b	$\bar{6}$ '2'm	0,0,1/2 [0,0,0]			
1	a	$\bar{6}$ '2'm	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p31m  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,0,0

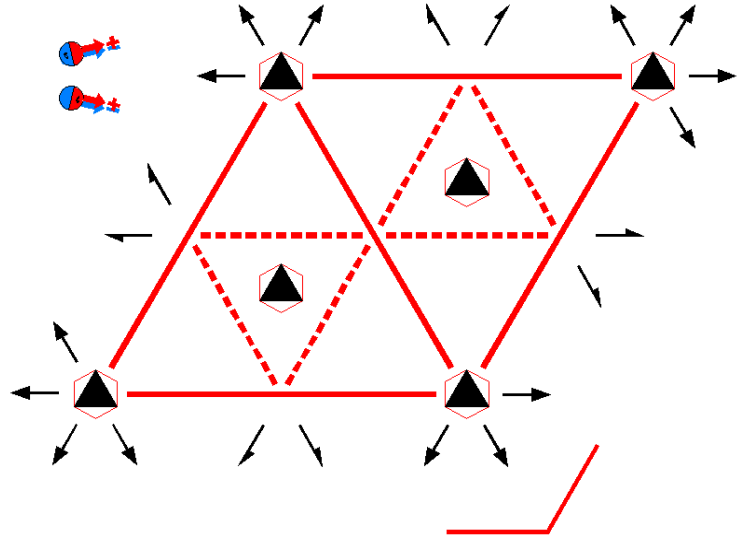
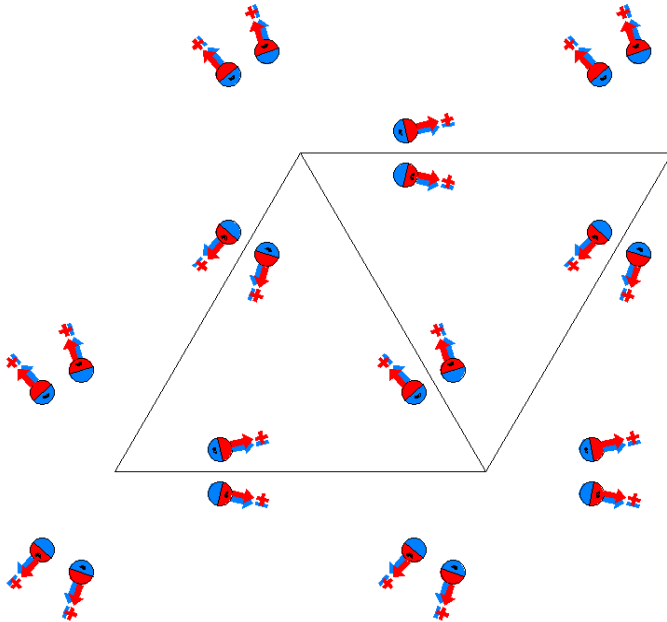
Along [2,1,0] p1m11'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P\bar{6}'2m'$   
189.4.1454

$\bar{6}'2m'$   
 $P\bar{6}'2m'$

Hexagonal



Origin on  $\bar{6}'2m'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

**Symmetry Operations**

- |                                     |   |  |
|-------------------------------------|---|--|
| (1) 1<br>(1 0,0,0)                  | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                          | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                |
| (4) $m'$ x,y,0<br>( $m_z$  0,0,0)'  | (5) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0)' | (6) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0)' |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0)   | (8) 2 x,0,0<br>( $2_x$  0,0,0)                              | (9) 2 0,y,0<br>( $2_y$  0,0,0)                         |
| (10) $m'$ x,x,z<br>( $m_3$  0,0,0)' | (11) $m'$ x,0,z<br>( $m_2$  0,0,0)'                         | (12) $m'$ 0,y,z<br>( $m_1$  0,0,0)'                    |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

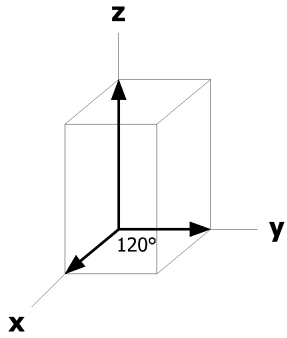
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	l	1	(1) x,y,z [u,v,w] (4) x,y, $\bar{z}$ [u,v, $\bar{w}$ ] (7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ] (10) y,x,z [v,u,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w] (5) $\bar{y}$ ,x-y, $\bar{z}$ [ $\bar{v}$ ,u-v, $\bar{w}$ ] (8) x-y, $\bar{y}$ , $\bar{z}$ [u-v, $\bar{v}$ , $\bar{w}$ ] (11) x-y, $\bar{y}$ ,z [u-v, $\bar{v}$ ,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w] (6) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ [ $\bar{u}$ +v, $\bar{u}$ , $\bar{w}$ ] (9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ] (12) $\bar{x}$ , $\bar{x}$ +y,z [ $\bar{u}$ , $\bar{u}$ +v,w]	
6	k	m'..	x,y,1/2 [u,v,0] y,x,1/2 [v,u,0]	$\bar{y}$ ,x-y,1/2 [ $\bar{v}$ ,u-v,0] x-y, $\bar{y}$ ,1/2 [u-v, $\bar{v}$ ,0]	$\bar{x}$ +y, $\bar{x}$ ,1/2 [ $\bar{u}$ +v, $\bar{u}$ ,0] $\bar{x}$ , $\bar{x}$ +y,1/2 [ $\bar{u}$ , $\bar{u}$ +v,0]	
6	j	m'..	x,y,0 [u,v,0] y,x,0 [v,u,0]	$\bar{y}$ ,x-y,0 [ $\bar{v}$ ,u-v,0] x-y, $\bar{y}$ ,0 [u-v, $\bar{v}$ ,0]	$\bar{x}$ +y, $\bar{x}$ ,0 [ $\bar{u}$ +v, $\bar{u}$ ,0] $\bar{x}$ , $\bar{x}$ +y,0 [ $\bar{u}$ , $\bar{u}$ +v,0]	
6	i	..m'	x,0,z [u,0,w] x,0, $\bar{z}$ [u,0, $\bar{w}$ ]	0,x,z [0,u,w] 0,x, $\bar{z}$ [0,u, $\bar{w}$ ]	$\bar{x}$ , $\bar{x}$ ,z [ $\bar{u}$ , $\bar{u}$ ,w] $\bar{x}$ , $\bar{x}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]	
4	h	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	2/3,1/3,z [0,0,w]
3	g	m'2m'	x,0,1/2 [u,0,0]	0,x,1/2 [0,u,0]	$\bar{x}$ , $\bar{x}$ ,1/2 [ $\bar{u}$ , $\bar{u}$ ,0]	
3	f	m'2m'	x,0,0 [u,0,0]	0,x,0 [0,u,0]	$\bar{x}$ , $\bar{x}$ ,0 [ $\bar{u}$ , $\bar{u}$ ,0]	
2	e	3.m'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
2	d	$\bar{6}$ '..	1/3,2/3,1/2 [0,0,0]	2/3,1/3,1/2 [0,0,0]		
2	c	$\bar{6}$ '..	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]		
1	b	$\bar{6}$ '2m'	0,0,1/2 [0,0,0]			
1	a	$\bar{6}$ '2m'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p31m'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p1m'1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



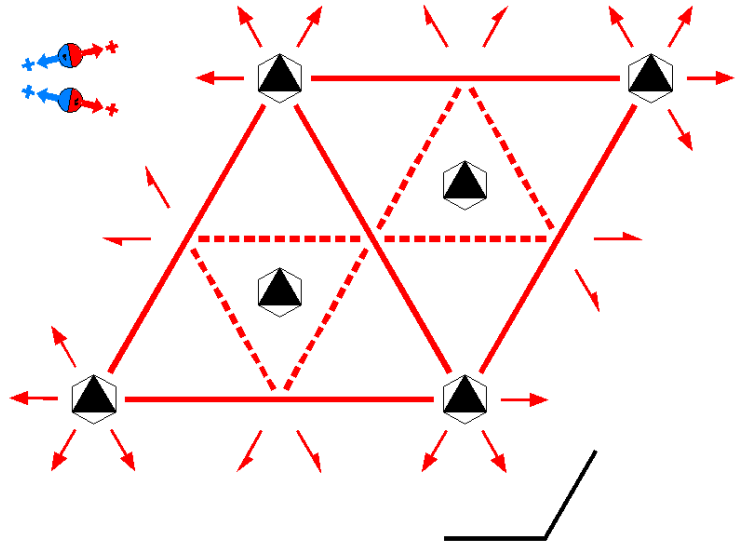
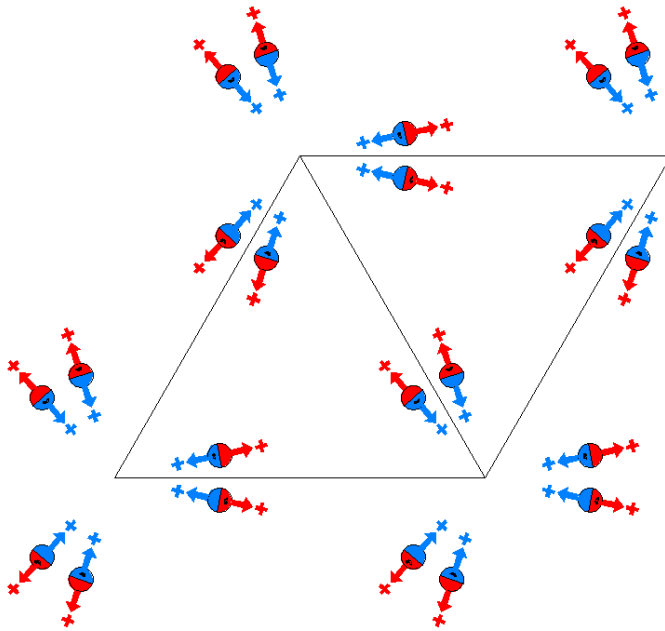
$P\bar{6}2'm'$

189.5.1455

$\bar{6}2'm'$

$P\bar{6}2'm'$

Hexagonal



Origin on  $\bar{6}2'm'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

**Symmetry Operations**

- |                                       |  |   |
|---------------------------------------|--|---|
| (1) 1<br>(1 0,0,0)                    | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                         | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)               |
| (4) m x,y,0<br>( $m_z$  0,0,0)        | (5) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (6) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0) |
| (7) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)' | (8) $2'$ x,0,0<br>( $2_x$  0,0,0)'                         | (9) $2'$ 0,y,0<br>( $2_y$  0,0,0)'                    |
| (10) $m'$ x,x,z<br>( $m_3$  0,0,0)'   | (11) $m'$ x,0,z<br>( $m_2$  0,0,0)'                        | (12) $m'$ 0,y,z<br>( $m_1$  0,0,0)'                   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	l	1	(1) x,y,z [u,v,w] (4) x,y, $\bar{z}$ [ $\bar{u},\bar{v},w$ ] (7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ] (10) y,x,z [v,u,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $\bar{y},x-y,\bar{z}$ [ $v,\bar{u}+v,w$ ] (8) x-y, $\bar{y},\bar{z}$ [ $\bar{u}+v,v,w$ ] (11) x-y, $\bar{y},z$ [u-v, $\bar{v},w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x}+y,\bar{x},\bar{z}$ [u-v,u,w] (9) $\bar{x},\bar{x}+y,\bar{z}$ [u,u-v,w] (12) $\bar{x},\bar{x}+y,z$ [ $\bar{u},\bar{u}+v,w$ ]	
6	k	m..	x,y,1/2 [0,0,w] y,x,1/2 [0,0,w]	$\bar{y},x-y,1/2$ [0,0,w] x-y, $\bar{y},1/2$ [0,0,w]	$\bar{x}+y,\bar{x},1/2$ [0,0,w] $\bar{x},\bar{x}+y,1/2$ [0,0,w]	
6	j	m..	x,y,0 [0,0,w] y,x,0 [0,0,w]	$\bar{y},x-y,0$ [0,0,w] x-y, $\bar{y},0$ [0,0,w]	$\bar{x}+y,\bar{x},0$ [0,0,w] $\bar{x},\bar{x}+y,0$ [0,0,w]	
6	i	..m'	x,0,z [u,0,w] x,0, $\bar{z}$ [ $\bar{u},0,w$ ]	0,x,z [0,u,w] 0,x, $\bar{z}$ [0, $\bar{u},w$ ]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},w$ ] $\bar{x},\bar{x},\bar{z}$ [u,u,w]	
4	h	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ [0,0,w]	2/3,1/3, $\bar{z}$ [0,0,w]	2/3,1/3,z [0,0,w]
3	g	m2'm'	x,0,1/2 [0,0,w]	0,x,1/2 [0,0,w]	$\bar{x},\bar{x},1/2$ [0,0,w]	
3	f	m2'm'	x,0,0 [0,0,w]	0,x,0 [0,0,w]	$\bar{x},\bar{x},0$ [0,0,w]	
2	e	3.m'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0,w]		
2	d	$\bar{6}..$	1/3,2/3,1/2 [0,0,w]	2/3,1/3,1/2 [0,0,w]		
2	c	$\bar{6}..$	1/3,2/3,0 [0,0,w]	2/3,1/3,0 [0,0,w]		
1	b	$\bar{6}2'm'$	0,0,1/2 [0,0,w]			
1	a	$\bar{6}2'm'$	0,0,0 [0,0,w]			

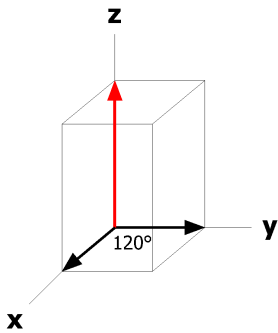
**Symmetry of Special Projections**

Along [0,0,1] p31m1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p1m1  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0

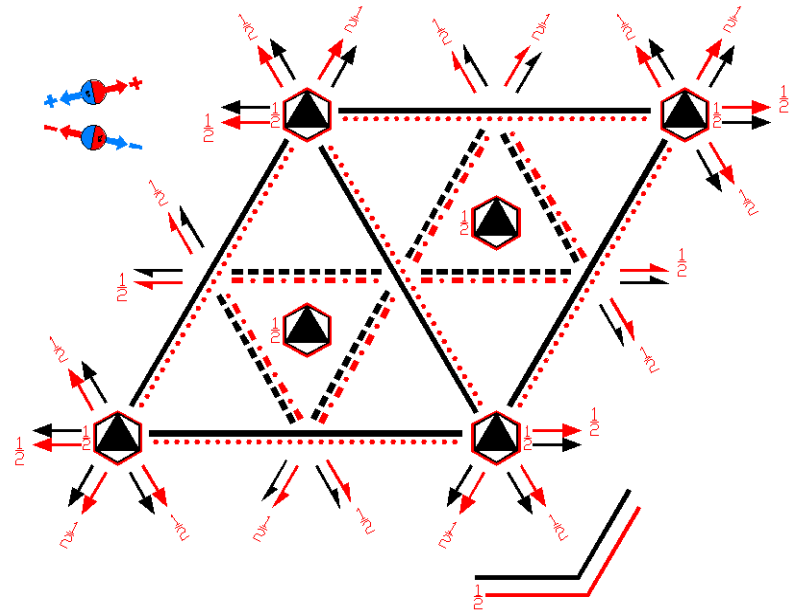
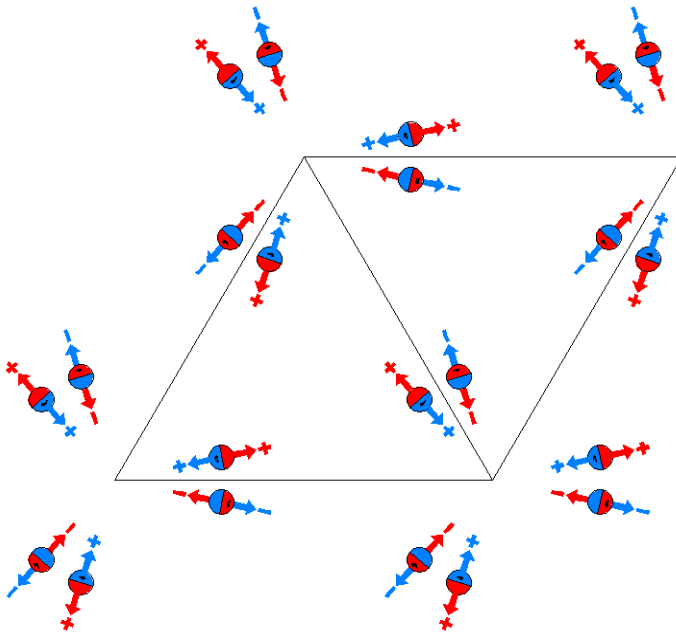




$P_{2c}\bar{6}2m$   
189.6.1456

$\bar{6}2m1'$   
 $P_{2c}\bar{6}2m$

Hexagonal



Origin on  $\bar{6}2m$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

**Symmetry Operations**

For (0,0,0) + set

- |                                   |  |   |
|-----------------------------------|--|---|
| (1) 1<br>(1 0,0,0)                | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                         | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)               |
| (4) m x,y,0<br>( $m_z$  0,0,0)    | (5) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (6) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0) |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0) | (8) 2 x,0,0<br>( $2_x$  0,0,0)                             | (9) 2 0,y,0<br>( $2_y$  0,0,0)                        |
| (10) m x,x,z<br>( $m_3$  0,0,0)   | (11) m x,0,z<br>( $m_2$  0,0,0)                            | (12) m 0,y,z<br>( $m_1$  0,0,0)                       |

## For (0,0,1)' + set

(1) $t' (0,0,1)$ $(1 0,0,1)'$	(2) $3^{+'} (0,0,1) 0,0,z$ $(3_z 0,0,1)'$	(3) $3^{-'} (0,0,1) 0,0,z$ $(3_z^{-1} 0,0,1)'$
(4) $m' x,y,1/2$ $(m_z 0,0,1)'$	(5) $\bar{6}^{-'} 0,0,z; 0,0,1/2$ $(\bar{6}_z^{-1} 0,0,1)'$	(6) $\bar{6}^{+'} 0,0,z; 0,0,1/2$ $(\bar{6}_z 0,0,1)'$
(7) $2' x,x,1/2$ $(2_{xy} 0,0,1)'$	(8) $2' x,0,1/2$ $(2_x 0,0,1)'$	(9) $2' 0,y,1/2$ $(2_y 0,0,1)'$
(10) $c' (0,0,1) x,x,z$ $(m_3 0,0,1)'$	(11) $c' (0,0,1) x,0,z$ $(m_2 0,0,1)'$	(12) $c' (0,0,1) 0,y,z$ $(m_1 0,0,1)'$

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t'(0,0,1)$ ; (2); (4); (7).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(0,0,1)' +		
24	l	1	(1) $x,y,z [u,v,w]$	(2) $\bar{y},x-y,z [\bar{v},u-v,w]$	(3) $\bar{x}+y,\bar{x},z [\bar{u}+v,\bar{u},w]$	
			(4) $x,y,\bar{z} [\bar{u},\bar{v},w]$	(5) $\bar{y},x-y,\bar{z} [v,\bar{u}+v,w]$	(6) $\bar{x}+y,\bar{x},\bar{z} [u-v,u,w]$	
			(7) $y,x,\bar{z} [v,u,\bar{w}]$	(8) $x-y,\bar{y},\bar{z} [u-v,\bar{v},\bar{w}]$	(9) $\bar{x},\bar{x}+y,\bar{z} [\bar{u},\bar{u}+v,\bar{w}]$	
			(10) $y,x,z [\bar{v},\bar{u},\bar{w}]$	(11) $x-y,\bar{y},z [\bar{u}+v,v,\bar{w}]$	(12) $\bar{x},\bar{x}+y,z [u,u-v,\bar{w}]$	
12	k	$m'..$	$x,y,1/2 [u,v,0]$	$\bar{y},x-y,1/2 [\bar{v},u-v,0]$	$\bar{x}+y,\bar{x},1/2 [\bar{u}+v,\bar{u},0]$	
			$y,x,1/2 [\bar{v},\bar{u},0]$	$x-y,\bar{y},1/2 [\bar{u}+v,v,0]$	$\bar{x},\bar{x}+y,1/2 [u,u-v,0]$	
12	j	$m..$	$x,y,0 [0,0,w]$	$\bar{y},x-y,0 [0,0,w]$	$\bar{x}+y,\bar{x},0 [0,0,w]$	
			$y,x,0 [0,0,\bar{w}]$	$x-y,\bar{y},0 [0,0,\bar{w}]$	$\bar{x},\bar{x}+y,0 [0,0,\bar{w}]$	
12	i	$..m$	$x,0,z [u,2u,0]$	$0,x,z [2\bar{u},\bar{u},0]$	$\bar{x},\bar{x},z [u,\bar{u},0]$	
			$x,0,\bar{z} [\bar{u},2\bar{u},0]$	$0,x,\bar{z} [2u,u,0]$	$\bar{x},\bar{x},\bar{z} [\bar{u},u,0]$	
8	h	$3..$	$1/3,2/3,z [0,0,w]$	$1/3,2/3,\bar{z} [0,0,w]$	$2/3,1/3,\bar{z} [0,0,\bar{w}]$	$2/3,1/3,z [0,0,\bar{w}]$
6	g	$m'2'm$	$x,0,1/2 [u,2u,0]$	$0,x,1/2 [2\bar{u},\bar{u},0]$	$\bar{x},\bar{x},1/2 [u,\bar{u},0]$	
6	f	$m2m$	$x,0,0 [0,0,0]$	$0,x,0 [0,0,0]$	$\bar{x},\bar{x},0 [0,0,0]$	
4	e	$3.m$	$0,0,z [0,0,0]$	$0,0,\bar{z} [0,0,0]$		
4	d	$\bar{6}'..$	$1/3,2/3,1/2 [0,0,0]$	$2/3,1/3,1/2 [0,0,0]$		
4	c	$\bar{6}..$	$1/3,2/3,0 [0,0,w]$	$2/3,1/3,0 [0,0,\bar{w}]$		
2	b	$\bar{6}'2'm$	$0,0,1/2 [0,0,0]$			

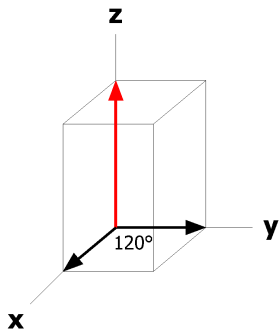
2 a  $\bar{6}2m$  0,0,0 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p31m1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a^*}2mm$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

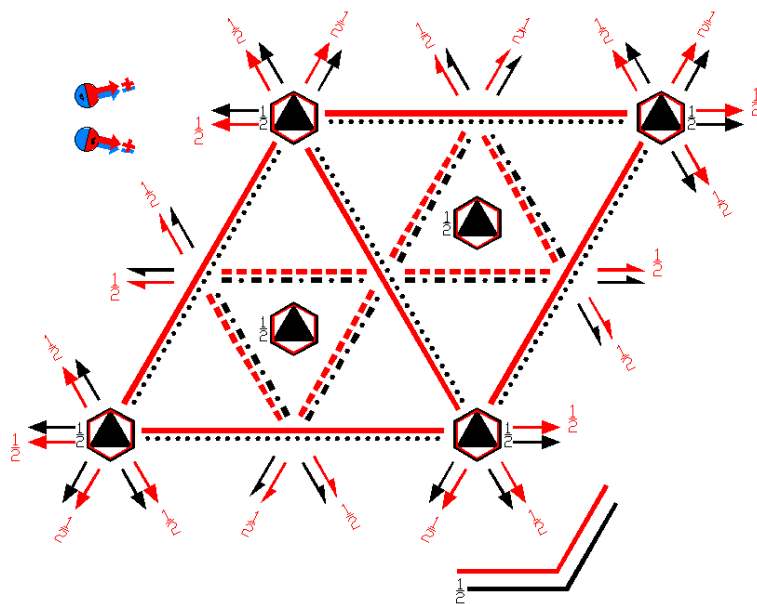
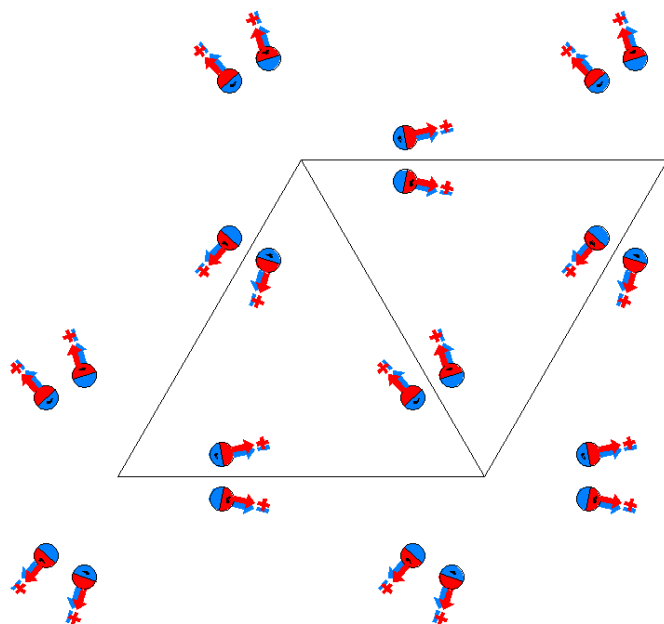
Along [2,1,0]  $p1m11'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P_{2c}\bar{6}'2m'$   
189.7.1457

$\bar{6}2m1'$   
 $P_{2c}\bar{6}'2m'$

Hexagonal



Origin on  $\bar{6}'2m'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq \min(1-x,x)$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2	1/2,1/2,0 1/2,1/2,1/2	

**Symmetry Operations**

For (0,0,0) + set

- |                                     |   |  |
|-------------------------------------|---|--|
| (1) 1<br>(1 0,0,0)                  | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                          | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                |
| (4) $m'$ x,y,0<br>( $m_z$  0,0,0)'  | (5) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0)' | (6) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0)' |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0)   | (8) 2 x,0,0<br>( $2_x$  0,0,0)                              | (9) 2 0,y,0<br>( $2_y$  0,0,0)                         |
| (10) $m'$ x,x,z<br>( $m_3$  0,0,0)' | (11) $m'$ x,0,z<br>( $m_2$  0,0,0)'                         | (12) $m'$ 0,y,z<br>( $m_1$  0,0,0)'                    |

## For (0,0,1)' + set

(1) t' (0,0,1) (1 0,0,1)'	(2) 3 <sup>+</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub>  0,0,1)'	(3) 3 <sup>-</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,1)'
(4) m <sub>x,y</sub> 1/2 (m <sub>z</sub>  0,0,1)	(5) $\bar{6}^-$ 0,0,z; 0,0,1/2 ( $\bar{6}_z^{-1}$  0,0,1)	(6) $\bar{6}^+$ 0,0,z; 0,0,1/2 ( $\bar{6}_z$  0,0,1)
(7) 2' <sub>x</sub> x,x,1/2 (2 <sub>xy</sub>  0,0,1)'	(8) 2' <sub>x</sub> x,0,1/2 (2 <sub>x</sub>  0,0,1)'	(9) 2' <sub>y</sub> 0,y,1/2 (2 <sub>y</sub>  0,0,1)'
(10) c (0,0,1) x,x,z (m <sub>3</sub>  0,0,1)	(11) c (0,0,1) x,0,z (m <sub>2</sub>  0,0,1)	(12) c (0,0,1) 0,y,z (m <sub>1</sub>  0,0,1)

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(0,0,1)' +		
24	l	1	(1) x,y,z [u,v,w] (4) x,y, $\bar{z}$ [u,v, $\bar{w}$ ] (7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ] (10) y,x,z [v,u,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w] (5) $\bar{y}$ ,x-y, $\bar{z}$ [ $\bar{v}$ ,u-v, $\bar{w}$ ] (8) x-y, $\bar{y}$ , $\bar{z}$ [u-v, $\bar{v}$ , $\bar{w}$ ] (11) x-y, $\bar{y}$ ,z [u-v, $\bar{v}$ ,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w] (6) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ [ $\bar{u}$ +v, $\bar{u}$ , $\bar{w}$ ] (9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ] (12) $\bar{x}$ , $\bar{x}$ +y,z [ $\bar{u}$ , $\bar{u}$ +v,w]	
12	k	m..	x,y,1/2 [0,0,w] y,x,1/2 [0,0,w]	$\bar{y}$ ,x-y,1/2 [0,0,w] x-y, $\bar{y}$ ,1/2 [0,0,w]	$\bar{x}$ +y, $\bar{x}$ ,1/2 [0,0,w] $\bar{x}$ , $\bar{x}$ +y,1/2 [0,0,w]	
12	j	m'..	x,y,0 [u,v,0] y,x,0 [v,u,0]	$\bar{y}$ ,x-y,0 [ $\bar{v}$ ,u-v,0] x-y, $\bar{y}$ ,0 [u-v, $\bar{v}$ ,0]	$\bar{x}$ +y, $\bar{x}$ ,0 [ $\bar{u}$ +v, $\bar{u}$ ,0] $\bar{x}$ , $\bar{x}$ +y,0 [ $\bar{u}$ , $\bar{u}$ +v,0]	
12	i	..m'	x,0,z [u,0,w] x,0, $\bar{z}$ [u,0, $\bar{w}$ ]	0,x,z [0,u,w] 0,x, $\bar{z}$ [0,u, $\bar{w}$ ]	$\bar{x}$ , $\bar{x}$ ,z [ $\bar{u}$ , $\bar{u}$ ,w] $\bar{x}$ , $\bar{x}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]	
8	h	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	2/3,1/3,z [0,0,w]
6	g	m <sup>2</sup> 'm'	x,0,1/2 [0,0,w]	0,x,1/2 [0,0,w]	$\bar{x}$ , $\bar{x}$ ,1/2 [0,0,w]	
6	f	m' <sup>2</sup> m'	x,0,0 [u,0,0]	0,x,0 [0,u,0]	$\bar{x}$ , $\bar{x}$ ,0 [ $\bar{u}$ , $\bar{u}$ ,0]	
4	e	3.m'	0,0,z [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]		
4	d	$\bar{6}$ ..	1/3,2/3,1/2 [0,0,w]	2/3,1/3,1/2 [0,0,w]		
4	c	$\bar{6}$ '..	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]		
2	b	$\bar{6}$ <sup>2</sup> 'm'	0,0,1/2 [0,0,w]			

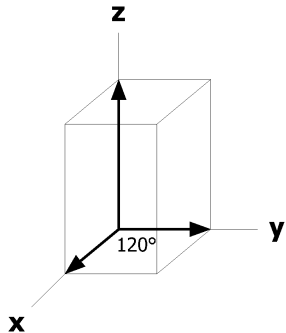
2 a  $\bar{6}'2m'$  0,0,0 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  $p31m1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a^*}2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

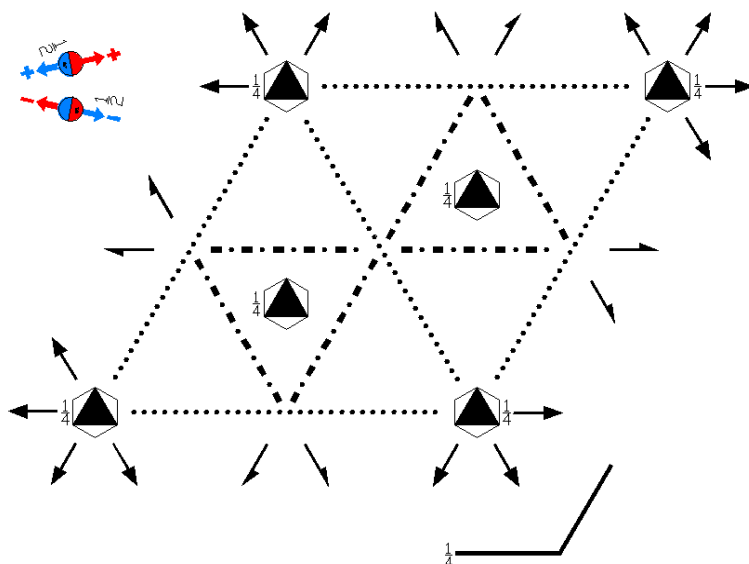
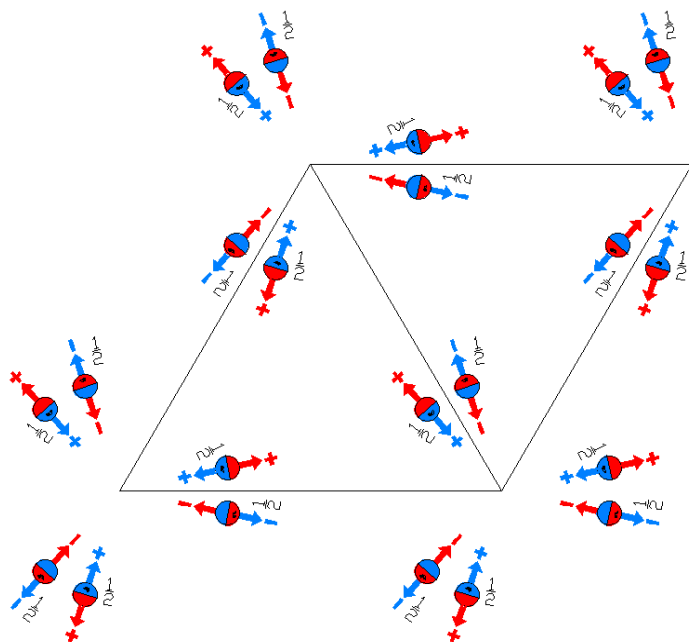
Along [2,1,0]  $p_{2a^*}1m1$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/2



$P\bar{6}2c$   
190.1.1458

$\bar{6}2m$   
 $P\bar{6}2c$

Hexagonal



Origin on 32c

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                          | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                             | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                   |
| (4) m x,y,1/4<br>( $m_z$  0,0,1/2)          | (5) $\bar{6}^-$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2) | (6) $\bar{6}^+$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2) |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0)           | (8) 2 x,0,0<br>( $2_x$  0,0,0)                                 | (9) 2 0,y,0<br>( $2_y$  0,0,0)                            |
| (10) c (0,0,1/2) x,x,z<br>( $m_3$  0,0,1/2) | (11) c (0,0,1/2) x,0,z<br>( $m_2$  0,0,1/2)                    | (12) c (0,0,1/2) 0,y,z<br>( $m_1$  0,0,1/2)               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
12	i	1	(1) x,y,z [u,v,w] (4) x,y, $\bar{z}+1/2$ [ $\bar{u},\bar{v},w$ ] (7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ] (10) y,x,z+1/2 [ $\bar{v},\bar{u},\bar{w}$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ] (5) $\bar{y},x-y,\bar{z}+1/2$ [v, $\bar{u}+v,w$ ] (8) x-y, $\bar{y},\bar{z}$ [u-v, $\bar{v},\bar{w}$ ] (11) x-y, $\bar{y},z+1/2$ [ $\bar{u}+v,v,\bar{w}$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ] (6) $\bar{x}+y,\bar{x},\bar{z}+1/2$ [u-v,u,w] (9) $\bar{x},\bar{x}+y,\bar{z}$ [ $\bar{u},\bar{u}+v,\bar{w}$ ] (12) $\bar{x},\bar{x}+y,z+1/2$ [u,u-v, $\bar{w}$ ]	
6	h	m..	x,y,1/4 [0,0,w] y,x,3/4 [0,0, $\bar{w}$ ]	$\bar{y},x-y,1/4$ [0,0,w] x-y, $\bar{y},3/4$ [0,0, $\bar{w}$ ]	$\bar{x}+y,\bar{x},1/4$ [0,0,w] $\bar{x},\bar{x}+y,3/4$ [0,0, $\bar{w}$ ]	
6	g	.2.	x,0,0 [u,0,0] x,0,1/2 [ $\bar{u},0,0$ ]	0,x,0 [0,u,0] 0,x,1/2 [0, $\bar{u},0$ ]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ] $\bar{x},\bar{x},1/2$ [u,u,0]	
4	f	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}+1/2$ [0,0,w]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	2/3,1/3,z+1/2 [0,0, $\bar{w}$ ]
4	e	3..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]
2	d	$\bar{6}$ ..	2/3,1/3,1/4 [0,0,w]	1/3,2/3,3/4 [0,0, $\bar{w}$ ]		
2	c	$\bar{6}$ ..	1/3,2/3,1/4 [0,0,w]	2/3,1/3,3/4 [0,0, $\bar{w}$ ]		
2	b	$\bar{6}$ ..	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		
2	a	32.	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

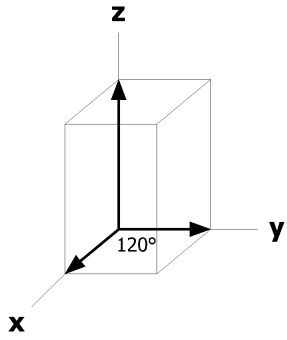
**Symmetry of Special Projections**

Along [0,0,1] p31m1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p<sub>2a</sub>1m1  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/4





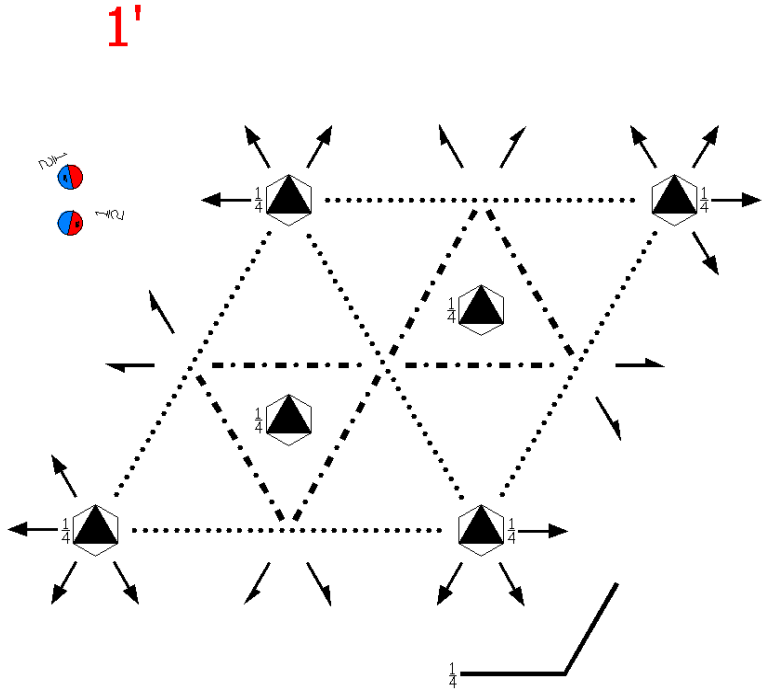
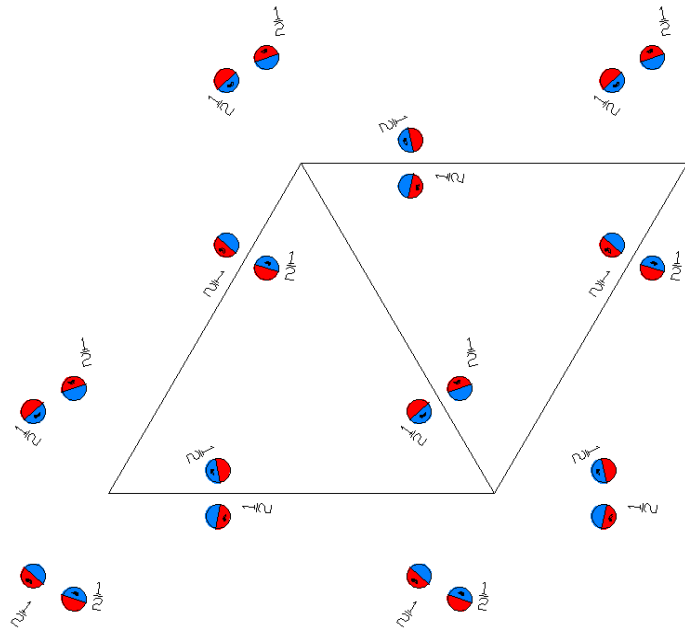
$P\bar{6}2c1'$

190.2.1459

$\bar{6}2m1'$

$P\bar{6}2c1'$

Hexagonal



Origin on  $32c1'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

### Symmetry Operations

For 1 + set

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                          | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                             | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                   |
| (4) m x,y,1/4<br>( $m_z$  0,0,1/2)          | (5) $\bar{6}^-$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2) | (6) $\bar{6}^+$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2) |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0)           | (8) 2 x,0,0<br>( $2_x$  0,0,0)                                 | (9) 2 0,y,0<br>( $2_y$  0,0,0)                            |
| (10) c (0,0,1/2) x,x,z<br>( $m_3$  0,0,1/2) | (11) c (0,0,1/2) x,0,z<br>( $m_2$  0,0,1/2)                    | (12) c (0,0,1/2) 0,y,z<br>( $m_1$  0,0,1/2)               |

For  $1'$  + set

(1) $1'$ ( $1 0,0,0$ )'	(2) $3^+ 1'$ 0,0,z ( $3_z 0,0,0$ )'	(3) $3^- 1'$ 0,0,z ( $3_z^{-1} 0,0,0$ )'
(4) $m'$ x,y,1/4 ( $m_z 0,0,1/2$ )'	(5) $\bar{6}^- 1'$ 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1} 0,0,1/2$ )'	(6) $\bar{6}^+ 1'$ 0,0,z; 0,0,1/4 ( $\bar{6}_z 0,0,1/2$ )'
(7) $2'$ x,x,0 ( $2_{xy} 0,0,0$ )'	(8) $2'$ x,0,0 ( $2_x 0,0,0$ )'	(9) $2'$ 0,y,0 ( $2_y 0,0,0$ )'
(10) $c'$ (0,0,1/2) x,x,z ( $m_3 0,0,1/2$ )'	(11) $c'$ (0,0,1/2) x,0,z ( $m_2 0,0,1/2$ )'	(12) $c'$ (0,0,1/2) 0,y,z ( $m_1 0,0,1/2$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7);  $1'$ .

**Positions**

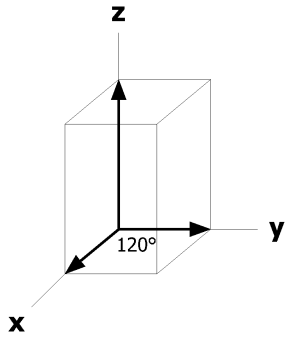
			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			1 +		1' +	
12	i	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0]	
			(4) x,y, $\bar{z}+1/2$ [0,0,0]	(5) $\bar{y}$ ,x-y, $\bar{z}+1/2$ [0,0,0]	(6) $\bar{x}+y,\bar{x},\bar{z}+1/2$ [0,0,0]	
			(7) y,x, $\bar{z}$ [0,0,0]	(8) x-y, $\bar{y},\bar{z}$ [0,0,0]	(9) $\bar{x},\bar{x}+y,\bar{z}$ [0,0,0]	
			(10) y,x,z+1/2 [0,0,0]	(11) x-y, $\bar{y},z+1/2$ [0,0,0]	(12) $\bar{x},\bar{x}+y,z+1/2$ [0,0,0]	
6	h	m..1'	x,y,1/4 [0,0,0]	$\bar{y}$ ,x-y,1/4 [0,0,0]	$\bar{x}+y,\bar{x},1/4$ [0,0,0]	
			y,x,3/4 [0,0,0]	x-y, $\bar{y},3/4$ [0,0,0]	$\bar{x},\bar{x}+y,3/4$ [0,0,0]	
6	g	.2.1'	x, $\bar{x},0$ [0,0,0]	x,2x,0 [0,0,0]	2 $\bar{x},\bar{x},0$ [0,0,0]	
			x, $\bar{x},1/2$ [0,0,0]	x,2x,1/2 [0,0,0]	2 $\bar{x},\bar{x},1/2$ [0,0,0]	
4	f	3..1'	1/3,2/3,z [0,0,0]	1/3,2/3, $\bar{z}+1/2$ [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	2/3,1/3,z+1/2 [0,0,0]
4	e	3..1'	0,0,z [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0,z+1/2 [0,0,0]
2	d	$\bar{6}..1'$	2/3,1/3,1/4 [0,0,0]	1/3,2/3,3/4 [0,0,0]		
2	c	$\bar{6}..1'$	1/3,2/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]		
2	b	$\bar{6}..1'$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	a	32.1'	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p31m1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mg1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at  $x,0,0$

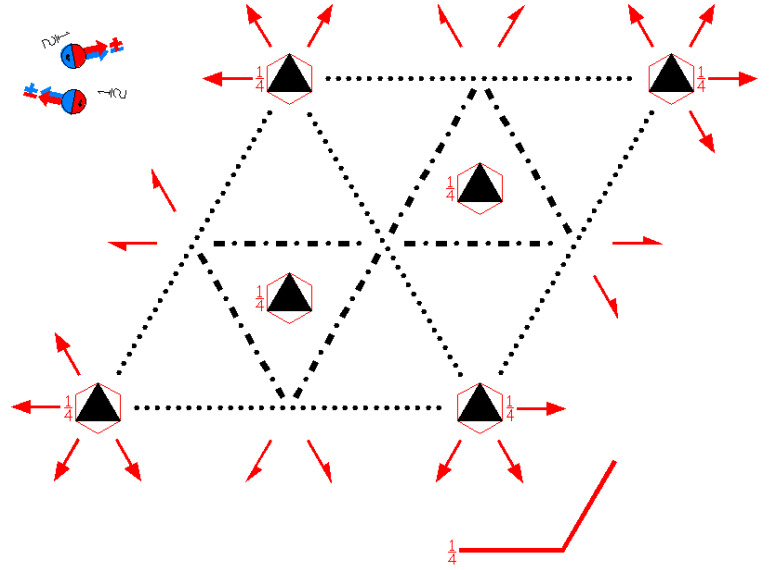
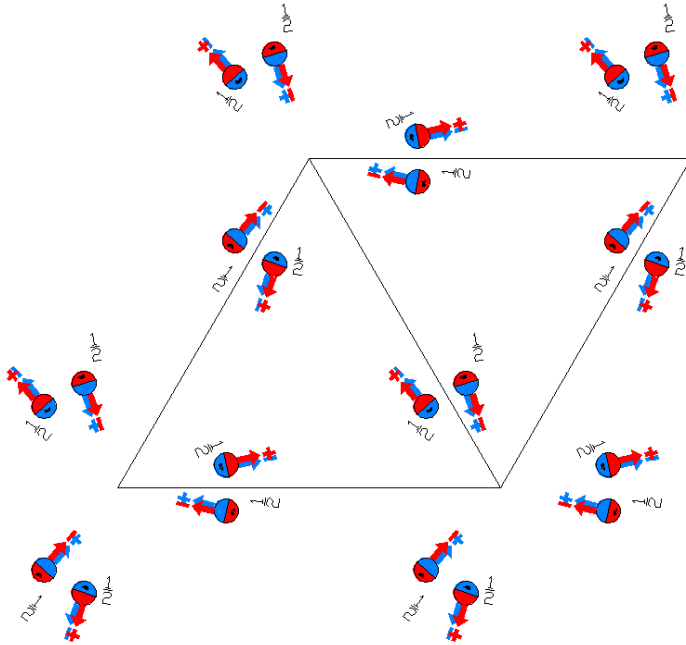
Along  $[2,1,0]$   $p1m11'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $x,x/2,0$



$P\bar{6}'2'c$   
190.3.1460

$\bar{6}'2'm$   
 $P\bar{6}'2'c$

Hexagonal



Origin on  $3'2'c$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

**Symmetry Operations**

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                          | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                                | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                      |
| (4) $m'$ x,y,1/4<br>( $m_z$  0,0,1/2)'      | (5) $\bar{6}^-$ ' 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2)' | (6) $\bar{6}^+$ ' 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2)' |
| (7) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)'       | (8) $2'$ x,0,0<br>( $2_x$  0,0,0)'                                | (9) $2'$ 0,y,0<br>( $2_y$  0,0,0)'                           |
| (10) c (0,0,1/2) x,x,z<br>( $m_3$  0,0,1/2) | (11) c (0,0,1/2) x,0,z<br>( $m_2$  0,0,1/2)                       | (12) c (0,0,1/2) 0,y,z<br>( $m_1$  0,0,1/2)                  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

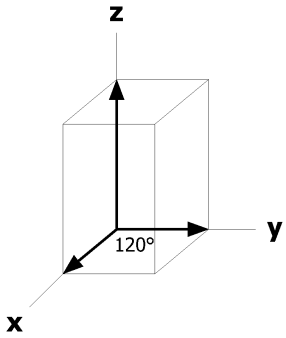
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
12	i	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w]	
			(4) x,y, $\bar{z}$ +1/2 [u,v, $\bar{w}$ ]	(5) $\bar{y}$ ,x-y, $\bar{z}$ +1/2 [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ +1/2 [ $\bar{u}$ +v, $\bar{u}$ , $\bar{w}$ ]	
			(7) y,x, $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ ,w]	(8) x-y, $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ +v,v,w]	(9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ [u,u-v,w]	
			(10) y,x,z+1/2 [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(11) x-y, $\bar{y}$ ,z+1/2 [ $\bar{u}$ +v,v, $\bar{w}$ ]	(12) $\bar{x}$ , $\bar{x}$ +y,z+1/2 [u,u-v, $\bar{w}$ ]	
6	h	m'..	x,y,1/4 [u,v,0]	$\bar{y}$ ,x-y,1/4 [ $\bar{v}$ ,u-v,0]	$\bar{x}$ +y, $\bar{x}$ ,1/4 [ $\bar{u}$ +v, $\bar{u}$ ,0]	
			y,x,3/4 [ $\bar{v}$ , $\bar{u}$ ,0]	x-y, $\bar{y}$ ,3/4 [ $\bar{u}$ +v,v,0]	$\bar{x}$ , $\bar{x}$ +y,3/4 [u,u-v,0]	
6	g	.2'	x, $\bar{x}$ ,0 [u,2u,w]	x,2x,0 [2 $\bar{u}$ , $\bar{u}$ ,w]	2 $\bar{x}$ , $\bar{x}$ ,0 [u, $\bar{u}$ ,w]	
			x, $\bar{x}$ ,1/2 [u,2u, $\bar{w}$ ]	x,2x,1/2 [2 $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]	2 $\bar{x}$ , $\bar{x}$ ,1/2 [u, $\bar{u}$ , $\bar{w}$ ]	
4	f	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ +1/2 [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0,w]	2/3,1/3,z+1/2 [0,0, $\bar{w}$ ]
4	e	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ +1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]
2	d	$\bar{6}$ '..	2/3,1/3,1/4 [0,0,0]	1/3,2/3,3/4 [0,0,0]		
2	c	$\bar{6}$ '..	1/3,2/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]		
2	b	$\bar{6}$ '..	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	a	32'	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		

**Symmetry of Special Projections**

Along [0,0,1] p31m  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p<sub>2a</sub>'1m1  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



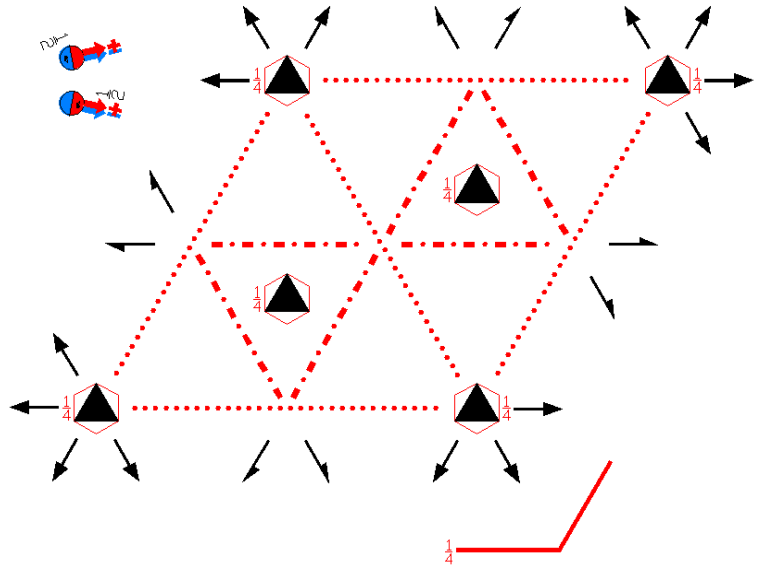
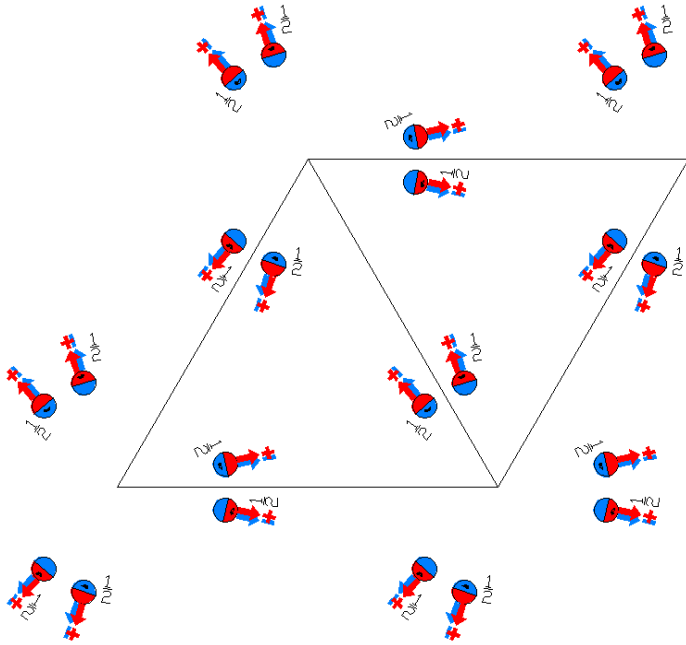
$P\bar{6}'2c'$

190.4.1461

$\bar{6}'2m'$

$P\bar{6}'2c'$

Hexagonal



Origin on  $32c'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

**Symmetry Operations**

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                              | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                              | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                    |
| (4) $m'$ x,y,1/4<br>( $m_z$  0,0,1/2)'          | (5) $\bar{6}^-$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2)' | (6) $\bar{6}^+$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2)' |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0)               | (8) 2 x,0,0<br>( $2_x$  0,0,0)                                  | (9) 2 0,y,0<br>( $2_y$  0,0,0)                             |
| (10) $c'$ (0,0,1/2) x,x,z<br>( $m_3$  0,0,1/2)' | (11) $c'$ (0,0,1/2) x,0,z<br>( $m_2$  0,0,1/2)'                 | (12) $c'$ (0,0,1/2) 0,y,z<br>( $m_1$  0,0,1/2)'            |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

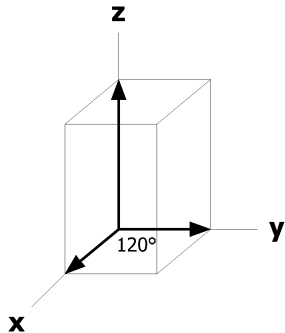
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
12	i	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w]	
			(4) x,y, $\bar{z}$ +1/2 [u,v, $\bar{w}$ ]	(5) $\bar{y}$ ,x-y, $\bar{z}$ +1/2 [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ +1/2 [ $\bar{u}$ +v, $\bar{u}$ , $\bar{w}$ ]	
			(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y}$ , $\bar{z}$ [u-v, $\bar{v}$ , $\bar{w}$ ]	(9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ]	
			(10) y,x,z+1/2 [v,u,w]	(11) x-y, $\bar{y}$ ,z+1/2 [u-v, $\bar{v}$ ,w]	(12) $\bar{x}$ , $\bar{x}$ +y,z+1/2 [ $\bar{u}$ , $\bar{u}$ +v,w]	
6	h	m'..	x,y,1/4 [u,v,0]	$\bar{y}$ ,x-y,1/4 [ $\bar{v}$ ,u-v,0]	$\bar{x}$ +y, $\bar{x}$ ,1/4 [ $\bar{u}$ +v, $\bar{u}$ ,0]	
			y,x,3/4 [v,u,0]	x-y, $\bar{y}$ ,3/4 [u-v, $\bar{v}$ ,0]	$\bar{x}$ , $\bar{x}$ +y,3/4 [ $\bar{u}$ , $\bar{u}$ +v,0]	
6	g	.2.	x, $\bar{x}$ ,0 [u,0,0]	x,2x,0 [0,u,0]	2 $\bar{x}$ , $\bar{x}$ ,0 [ $\bar{u}$ , $\bar{u}$ ,0]	
			x, $\bar{x}$ ,1/2 [u,0,0]	x,2x,1/2 [0,u,0]	2 $\bar{x}$ , $\bar{x}$ ,1/2 [ $\bar{u}$ , $\bar{u}$ ,0]	
4	f	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ +1/2 [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	2/3,1/3,z+1/2 [0,0,w]
4	e	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ +1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0,w]
2	d	$\bar{6}$ '..	2/3,1/3,1/4 [0,0,0]	1/3,2/3,3/4 [0,0,0]		
2	c	$\bar{6}$ '..	1/3,2/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]		
2	b	$\bar{6}$ '..	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	a	32.	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p31m'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p1m'1  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



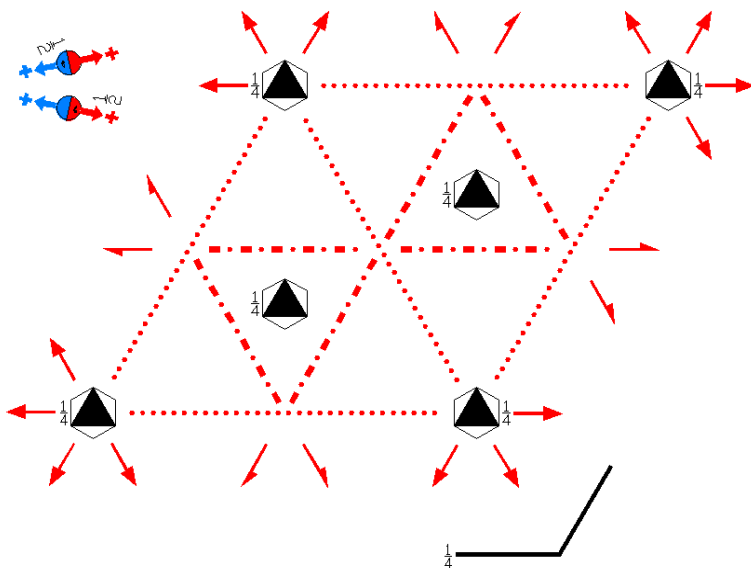
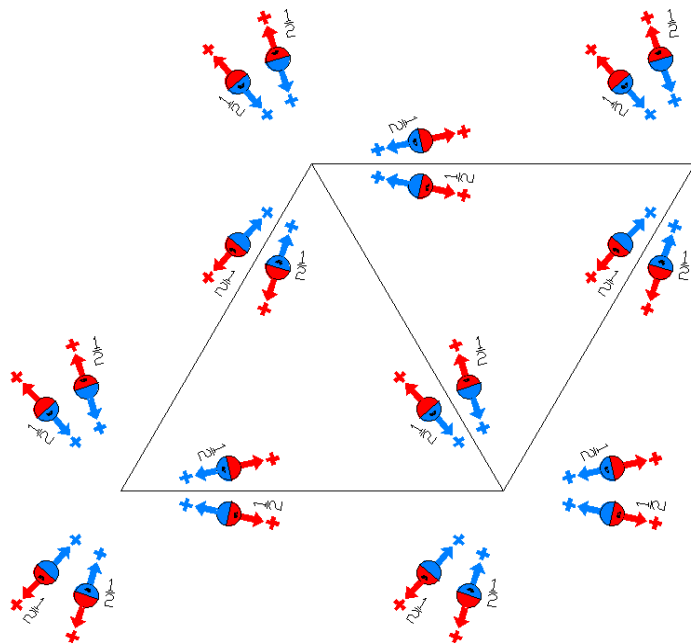
$P\bar{6}2'c'$

190.5.1462

$\bar{6}2'm'$

$P\bar{6}2'c'$

Hexagonal



Origin on  $32'c'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, (1+x)/2)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/3,2/3,0	0,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4	0,1/2,1/4

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                              | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                             | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)                   |
| (4) m x,y,1/4<br>( $m_z$  0,0,1/2)              | (5) $\bar{6}^-$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2) | (6) $\bar{6}^+$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2) |
| (7) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)'           | (8) $2'$ x,0,0<br>( $2_x$  0,0,0)'                             | (9) $2'$ 0,y,0<br>( $2_y$  0,0,0)'                        |
| (10) $c'$ (0,0,1/2) x,x,z<br>( $m_3$  0,0,1/2)' | (11) $c'$ (0,0,1/2) x,0,z<br>( $m_2$  0,0,1/2)'                | (12) $c'$ (0,0,1/2) 0,y,z<br>( $m_1$  0,0,1/2)'           |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

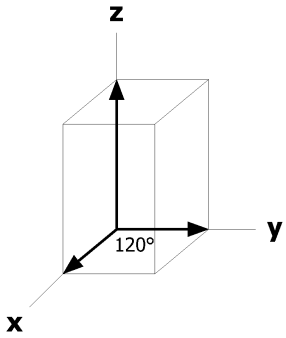
			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
12	i	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w]	
			(4) x,y, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(5) $\bar{y}$ ,x-y, $\bar{z}$ +1/2 [v, $\bar{u}$ +v,w]	(6) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ +1/2 [u-v,u,w]	
			(7) y,x, $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ ,w]	(8) x-y, $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ +v,v,w]	(9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ [u,u-v,w]	
			(10) y,x,z+1/2 [v,u,w]	(11) x-y, $\bar{y}$ ,z+1/2 [u-v, $\bar{v}$ ,w]	(12) $\bar{x}$ , $\bar{x}$ +y,z+1/2 [ $\bar{u}$ , $\bar{u}$ +v,w]	
6	h	m..	x,y,1/4 [0,0,w]	$\bar{y}$ ,x-y,1/4 [0,0,w]	$\bar{x}$ +y, $\bar{x}$ ,1/4 [0,0,w]	
			y,x,3/4 [0,0,w]	x-y, $\bar{y}$ ,3/4 [0,0,w]	$\bar{x}$ , $\bar{x}$ +y,3/4 [0,0,w]	
6	g	.2'	x, $\bar{x}$ ,0 [u,2u,w]	x,2x,0 [2 $\bar{u}$ , $\bar{u}$ ,w]	2 $\bar{x}$ , $\bar{x}$ ,0 [u, $\bar{u}$ ,w]	
			x, $\bar{x}$ ,1/2 [ $\bar{u}$ ,2 $\bar{u}$ ,w]	x,2x,1/2 [2u,u,w]	2 $\bar{x}$ , $\bar{x}$ ,1/2 [ $\bar{u}$ ,u,w]	
4	f	3..	1/3,2/3,z [0,0,w]	1/3,2/3, $\bar{z}$ +1/2 [0,0,w]	2/3,1/3, $\bar{z}$ [0,0,w]	2/3,1/3,z+1/2 [0,0,w]
4	e	3..	0,0,z [0,0,w]	0,0, $\bar{z}$ +1/2 [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0,z+1/2 [0,0,w]
2	d	$\bar{6}$ ..	2/3,1/3,1/4 [0,0,w]	1/3,2/3,3/4 [0,0,w]		
2	c	$\bar{6}$ ..	1/3,2/3,1/4 [0,0,w]	2/3,1/3,3/4 [0,0,w]		
2	b	$\bar{6}$ ..	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		
2	a	32'	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]		

**Symmetry of Special Projections**

Along [0,0,1] p31m1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

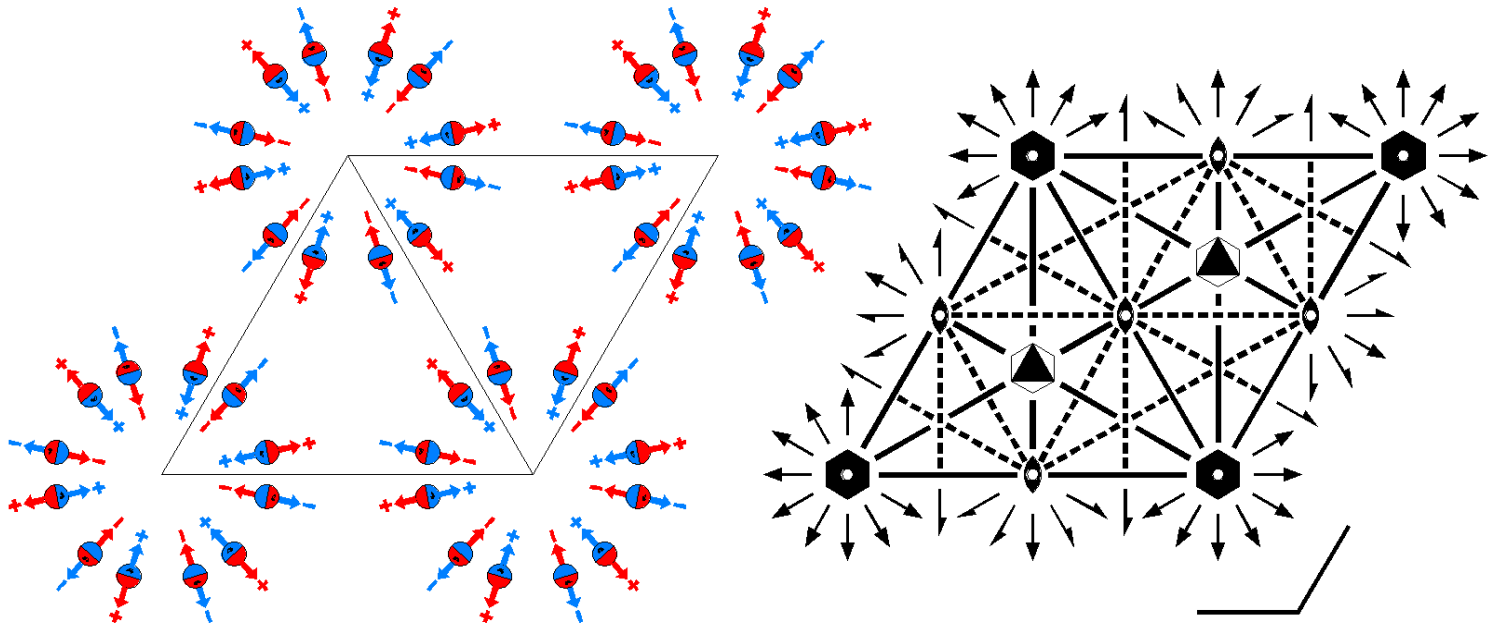
Along [2,1,0] p1m1  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P6/mmm  
191.1.1463

6/mmm  
P6/m2/m2/m

Hexagonal



Origin at center (6/mmm)

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2		

**Symmetry Operations**

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                       | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)  | (8) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                            | (9) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                            |
| (10) 2 x,x̄,0<br>(2 <sub>3</sub>  0,0,0) | (11) 2 x,2x,0<br>(2 <sub>2</sub>  0,0,0)                          | (12) 2 2x,x,0<br>(2 <sub>1</sub>  0,0,0)                          |

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)
(16) m $\bar{x}$ ,y,0 ( $m_z$  0,0,0)	(17) $\bar{6}^-$ 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,0)	(18) $\bar{6}^+$ 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,0)
(19) m $\bar{x}$ , $\bar{x}$ ,z ( $m_{xy}$  0,0,0)	(20) m $\bar{x}$ ,2x,z ( $m_x$  0,0,0)	(21) m 2x,x,z ( $m_y$  0,0,0)
(22) m $\bar{x}$ ,x,z ( $m_3$  0,0,0)	(23) m $\bar{x}$ ,0,z ( $m_2$  0,0,0)	(24) m 0,y,z ( $m_1$  0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	r	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w]	(5) y, $\bar{x}$ +y,z [v, $\bar{u}$ +v,w]	(6) x-y,x,z [u-v,u,w]
			(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y}$ , $\bar{z}$ [u-v, $\bar{v}$ , $\bar{w}$ ]	(9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(11) $\bar{x}$ +y,y, $\bar{z}$ [ $\bar{u}$ +v, $\bar{v}$ , $\bar{w}$ ]	(12) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(14) y, $\bar{x}$ +y, $\bar{z}$ [ $\bar{v}$ ,u-v,w]	(15) x-y,x, $\bar{z}$ [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(16) x,y, $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ ,w]	(17) $\bar{y}$ ,x-y, $\bar{z}$ [v, $\bar{u}$ +v,w]	(18) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ [u-v,u,w]
			(19) $\bar{y}$ , $\bar{x}$ ,z [v,u, $\bar{w}$ ]	(20) $\bar{x}$ +y,y,z [u-v, $\bar{v}$ , $\bar{w}$ ]	(21) x,x-y,z [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ]
			(22) y,x,z [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(23) x-y, $\bar{y}$ ,z [ $\bar{u}$ +v,v, $\bar{w}$ ]	(24) $\bar{x}$ , $\bar{x}$ +y,z [u,u-v, $\bar{w}$ ]
12	q	m..	x,y,1/2 [0,0,w]	$\bar{y}$ ,x-y,1/2 [0,0,w]	$\bar{x}$ +y, $\bar{x}$ ,1/2 [0,0,w]
			$\bar{x}$ , $\bar{y}$ ,1/2 [0,0,w]	y, $\bar{x}$ +y,1/2 [0,0,w]	x-y,x,1/2 [0,0,w]
			y,x,1/2 [0,0, $\bar{w}$ ]	x-y, $\bar{y}$ ,1/2 [0,0, $\bar{w}$ ]	$\bar{x}$ , $\bar{x}$ +y,1/2 [0,0, $\bar{w}$ ]
			$\bar{y}$ , $\bar{x}$ ,1/2 [0,0, $\bar{w}$ ]	$\bar{x}$ +y,y,1/2 [0,0, $\bar{w}$ ]	x,x-y,1/2 [0,0, $\bar{w}$ ]
12	p	m..	x,y,0 [0,0,w]	$\bar{y}$ ,x-y,0 [0,0,w]	$\bar{x}$ +y, $\bar{x}$ ,0 [0,0,w]
			$\bar{x}$ , $\bar{y}$ ,0 [0,0,w]	y, $\bar{x}$ +y,0 [0,0,w]	x-y,x,0 [0,0,w]
			y,x,0 [0,0, $\bar{w}$ ]	x-y, $\bar{y}$ ,0 [0,0, $\bar{w}$ ]	$\bar{x}$ , $\bar{x}$ +y,0 [0,0, $\bar{w}$ ]
			$\bar{y}$ , $\bar{x}$ ,0 [0,0, $\bar{w}$ ]	$\bar{x}$ +y,y,0 [0,0, $\bar{w}$ ]	x,x-y,0 [0,0, $\bar{w}$ ]

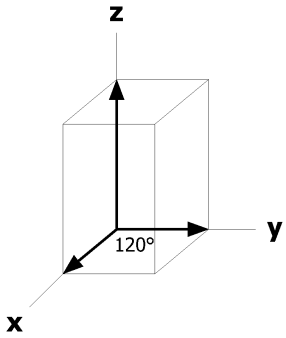
12	o	.m.	$x, 2x, z [u, 0, 0]$ $\bar{x}, 2\bar{x}, z [\bar{u}, 0, 0]$ $2x, x, \bar{z} [0, \bar{u}, 0]$ $2\bar{x}, \bar{x}, \bar{z} [u, 0, 0]$	$2\bar{x}, \bar{x}, z [0, u, 0]$ $2x, x, z [0, \bar{u}, 0]$ $\bar{x}, 2\bar{x}, \bar{z} [\bar{u}, 0, 0]$ $x, 2x, \bar{z} [0, u, 0]$	$x, \bar{x}, z [\bar{u}, \bar{u}, 0]$ $\bar{x}, x, z [u, u, 0]$ $\bar{x}, x, \bar{z} [u, u, 0]$ $x, \bar{x}, \bar{z} [\bar{u}, \bar{u}, 0]$	
12	n	..m	$x, 0, z [u, 2u, 0]$ $\bar{x}, 0, z [\bar{u}, 2\bar{u}, 0]$ $0, x, \bar{z} [2u, u, 0]$ $0, \bar{x}, \bar{z} [2\bar{u}, \bar{u}, 0]$	$0, x, z [2\bar{u}, \bar{u}, 0]$ $0, \bar{x}, z [2u, u, 0]$ $x, 0, \bar{z} [\bar{u}, 2\bar{u}, 0]$ $\bar{x}, 0, \bar{z} [u, 2u, 0]$	$\bar{x}, \bar{x}, z [u, \bar{u}, 0]$ $x, x, z [\bar{u}, u, 0]$ $\bar{x}, x, \bar{z} [\bar{u}, u, 0]$ $x, x, \bar{z} [u, \bar{u}, 0]$	
6	m	mm2	$x, 2x, 1/2 [0, 0, 0]$ $\bar{x}, 2\bar{x}, 1/2 [0, 0, 0]$	$2\bar{x}, \bar{x}, 1/2 [0, 0, 0]$ $2x, x, 1/2 [0, 0, 0]$	$x, \bar{x}, 1/2 [0, 0, 0]$ $\bar{x}, x, 1/2 [0, 0, 0]$	
6	l	mm2	$x, 2x, 0 [0, 0, 0]$ $\bar{x}, 2\bar{x}, 0 [0, 0, 0]$	$2\bar{x}, \bar{x}, 0 [0, 0, 0]$ $2x, x, 0 [0, 0, 0]$	$x, \bar{x}, 0 [0, 0, 0]$ $\bar{x}, x, 0 [0, 0, 0]$	
6	k	m2m	$x, 0, 1/2 [0, 0, 0]$ $\bar{x}, 0, 1/2 [0, 0, 0]$	$0, x, 1/2 [0, 0, 0]$ $0, \bar{x}, 1/2 [0, 0, 0]$	$\bar{x}, \bar{x}, 1/2 [0, 0, 0]$ $x, x, 1/2 [0, 0, 0]$	
6	j	m2m	$x, 0, 0 [0, 0, 0]$ $\bar{x}, 0, 0 [0, 0, 0]$	$0, x, 0 [0, 0, 0]$ $0, \bar{x}, 0 [0, 0, 0]$	$\bar{x}, \bar{x}, 0 [0, 0, 0]$ $x, x, 0 [0, 0, 0]$	
6	i	2mm	$1/2, 0, z [0, 0, 0]$ $0, 1/2, \bar{z} [0, 0, 0]$	$0, 1/2, z [0, 0, 0]$ $1/2, 0, \bar{z} [0, 0, 0]$	$1/2, 1/2, z [0, 0, 0]$ $1/2, 1/2, \bar{z} [0, 0, 0]$	
4	h	3m.	$1/3, 2/3, z [0, 0, 0]$	$2/3, 1/3, z [0, 0, 0]$	$2/3, 1/3, \bar{z} [0, 0, 0]$	$1/3, 2/3, \bar{z} [0, 0, 0]$
3	g	mmm	$1/2, 0, 1/2 [0, 0, 0]$	$0, 1/2, 1/2 [0, 0, 0]$		$1/2, 1/2, 1/2 [0, 0, 0]$
3	f	mmm	$1/2, 0, 0 [0, 0, 0]$	$0, 1/2, 0 [0, 0, 0]$		$1/2, 1/2, 0 [0, 0, 0]$
2	e	6mm	$0, 0, z [0, 0, 0]$	$0, 0, \bar{z} [0, 0, 0]$		
2	d	$\bar{6}m2$	$1/3, 2/3, 1/2 [0, 0, 0]$	$2/3, 1/3, 1/2 [0, 0, 0]$		
2	c	$\bar{6}m2$	$1/3, 2/3, 0 [0, 0, 0]$	$2/3, 1/3, 0 [0, 0, 0]$		
1	b	6/mmm	$0, 0, 1/2 [0, 0, 0]$			
1	a	6/mmm	$0, 0, 0 [0, 0, 0]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at  $x,0,0$

Along  $[2,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $x,x/2,0$



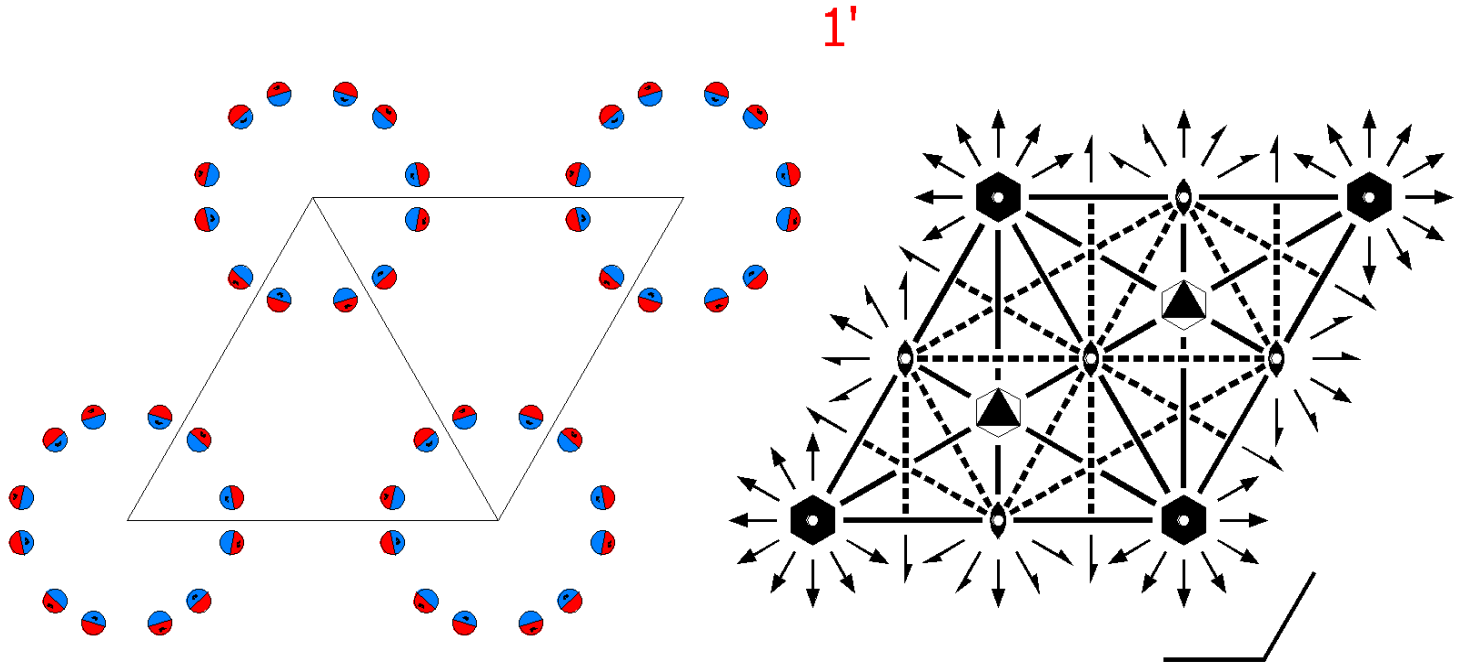
P6/mmm1'

191.2.1464

6/mmm1'

P6/m2/m2/m1'

Hexagonal



Origin at center (6/mmm1')

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/3$ ;  $0 \leq z \leq 1/2$ ;  $x \leq (1+y)/2$ ;  $y \leq x/2$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2

**Symmetry Operations**

For 1 + set

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                       | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)  | (8) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                            | (9) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                            |
| (10) 2 x,x̄,0<br>(2 <sub>3</sub>  0,0,0) | (11) 2 x,2x,0<br>(2 <sub>2</sub>  0,0,0)                          | (12) 2 2x,x,0<br>(2 <sub>1</sub>  0,0,0)                          |

- |  |   |   |
|--|---|---|
| (13) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)  | (14) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)      | (15) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (16) m x,y,0<br>( $m_z$  0,0,0)              | (17) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (18) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0)      |
| (19) m x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0) | (20) m x,2x,z<br>( $m_x$  0,0,0)                            | (21) m 2x,x,z<br>( $m_y$  0,0,0)                            |
| (22) m x,x,z<br>( $m_3$  0,0,0)              | (23) m x,0,z<br>( $m_2$  0,0,0)                             | (24) m 0,y,z<br>( $m_1$  0,0,0)                             |

For 1' + set

- |   |  |  |
|---|--|--|
| (1) 1'<br>(1 0,0,0)'                                | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)'               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (4) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'            | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)'               |
| (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'           | (8) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                           | (9) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                           |
| (10) 2' x, $\bar{x}$ ,0<br>(2 <sub>3</sub>  0,0,0)' | (11) 2' x,2x,0<br>(2 <sub>2</sub>  0,0,0)'                         | (12) 2' 2x,x,0<br>(2 <sub>1</sub>  0,0,0)'                         |
| (13) $\bar{1}$ '<br>( $\bar{1}$  0,0,0)'            | (14) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)'            | (15) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)'       |
| (16) m' x,y,0<br>( $m_z$  0,0,0)'                   | (17) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0)'       | (18) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0)'            |
| (19) m' x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0)'      | (20) m' x,2x,z<br>( $m_x$  0,0,0)'                                 | (21) m' 2x,x,z<br>( $m_y$  0,0,0)'                                 |
| (22) m' x,x,z<br>( $m_3$  0,0,0)'                   | (23) m' x,0,z<br>( $m_2$  0,0,0)'                                  | (24) m' 0,y,z<br>( $m_1$  0,0,0)'                                  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

			1 +	1' +	
24	r	11'	(1) x,y,z [0,0,0]	(2) $\bar{y}$ ,x-y,z [0,0,0]	(3) $\bar{x}+y,\bar{x},z$ [0,0,0]
			(4) $\bar{x},\bar{y},z$ [0,0,0]	(5) y, $\bar{x}+y,z$ [0,0,0]	(6) x-y,x,z [0,0,0]
			(7) y,x, $\bar{z}$ [0,0,0]	(8) x-y, $\bar{y},\bar{z}$ [0,0,0]	(9) $\bar{x},\bar{x}+y,\bar{z}$ [0,0,0]
			(10) $\bar{y},\bar{x},\bar{z}$ [0,0,0]	(11) $\bar{x}+y,y,\bar{z}$ [0,0,0]	(12) x,x-y, $\bar{z}$ [0,0,0]

			(13) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]	(14) $y, \bar{x} + y, \bar{z}$ [0,0,0]	(15) $x - y, x, \bar{z}$ [0,0,0]
			(16) $x, y, \bar{z}$ [0,0,0]	(17) $\bar{y}, x - y, \bar{z}$ [0,0,0]	(18) $\bar{x} + y, \bar{x}, \bar{z}$ [0,0,0]
			(19) $\bar{y}, \bar{x}, z$ [0,0,0]	(20) $\bar{x} + y, y, z$ [0,0,0]	(21) $x, x - y, z$ [0,0,0]
			(22) $y, x, z$ [0,0,0]	(23) $x - y, \bar{y}, z$ [0,0,0]	(24) $\bar{x}, \bar{x} + y, z$ [0,0,0]
12	q	m..1'	$x, y, 1/2$ [0,0,0]	$\bar{y}, x - y, 1/2$ [0,0,0]	$\bar{x} + y, \bar{x}, 1/2$ [0,0,0]
			$\bar{x}, \bar{y}, 1/2$ [0,0,0]	$y, \bar{x} + y, 1/2$ [0,0,0]	$x - y, x, 1/2$ [0,0,0]
			$y, x, 1/2$ [0,0,0]	$x - y, \bar{y}, 1/2$ [0,0,0]	$\bar{x}, \bar{x} + y, 1/2$ [0,0,0]
			$\bar{y}, \bar{x}, 1/2$ [0,0,0]	$\bar{x} + y, y, 1/2$ [0,0,0]	$x, x - y, 1/2$ [0,0,0]
12	p	m..1'	$x, y, 0$ [0,0,0]	$\bar{y}, x - y, 0$ [0,0,0]	$\bar{x} + y, \bar{x}, 0$ [0,0,0]
			$\bar{x}, \bar{y}, 0$ [0,0,0]	$y, \bar{x} + y, 0$ [0,0,0]	$x - y, x, 0$ [0,0,0]
			$y, x, 0$ [0,0,0]	$x - y, \bar{y}, 0$ [0,0,0]	$\bar{x}, \bar{x} + y, 0$ [0,0,0]
			$\bar{y}, \bar{x}, 0$ [0,0,0]	$\bar{x} + y, y, 0$ [0,0,0]	$x, x - y, 0$ [0,0,0]
12	o	.m.1'	$x, 2x, z$ [0,0,0]	$2\bar{x}, \bar{x}, z$ [0,0,0]	$x, \bar{x}, z$ [0,0,0]
			$\bar{x}, 2\bar{x}, z$ [0,0,0]	$2x, x, z$ [0,0,0]	$\bar{x}, x, z$ [0,0,0]
			$2x, x, \bar{z}$ [0,0,0]	$\bar{x}, 2\bar{x}, \bar{z}$ [0,0,0]	$\bar{x}, x, \bar{z}$ [0,0,0]
			$2\bar{x}, \bar{x}, \bar{z}$ [0,0,0]	$x, 2x, \bar{z}$ [0,0,0]	$x, \bar{x}, \bar{z}$ [0,0,0]
12	n	..m1'	$x, 0, z$ [0,0,0]	$0, x, z$ [0,0,0]	$\bar{x}, \bar{x}, z$ [0,0,0]
			$\bar{x}, 0, z$ [0,0,0]	$0, \bar{x}, z$ [0,0,0]	$x, x, z$ [0,0,0]
			$0, x, \bar{z}$ [0,0,0]	$x, 0, \bar{z}$ [0,0,0]	$\bar{x}, \bar{x}, \bar{z}$ [0,0,0]
			$0, \bar{x}, \bar{z}$ [0,0,0]	$\bar{x}, 0, \bar{z}$ [0,0,0]	$x, x, \bar{z}$ [0,0,0]
6	m	mm21'	$x, 2x, 1/2$ [0,0,0]	$2\bar{x}, \bar{x}, 1/2$ [0,0,0]	$x, \bar{x}, 1/2$ [0,0,0]
			$\bar{x}, 2\bar{x}, 1/2$ [0,0,0]	$2x, x, 1/2$ [0,0,0]	$\bar{x}, x, 1/2$ [0,0,0]
6	l	mm21'	$x, 2x, 0$ [0,0,0]	$2\bar{x}, \bar{x}, 0$ [0,0,0]	$x, \bar{x}, 0$ [0,0,0]
			$\bar{x}, 2\bar{x}, 0$ [0,0,0]	$2x, x, 0$ [0,0,0]	$\bar{x}, x, 0$ [0,0,0]
6	k	m2m1'	$x, 0, 1/2$ [0,0,0]	$0, x, 1/2$ [0,0,0]	$\bar{x}, \bar{x}, 1/2$ [0,0,0]
			$\bar{x}, 0, 1/2$ [0,0,0]	$0, \bar{x}, 1/2$ [0,0,0]	$x, x, 1/2$ [0,0,0]
6	j	m2m1'	$x, 0, 0$ [0,0,0]	$0, x, 0$ [0,0,0]	$\bar{x}, \bar{x}, 0$ [0,0,0]
			$\bar{x}, 0, 0$ [0,0,0]	$0, \bar{x}, 0$ [0,0,0]	$x, x, 0$ [0,0,0]



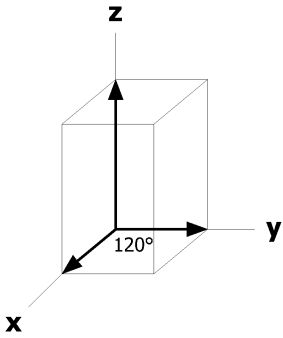
6	i	2mm1' 1/2,0,z [0,0,0]	0,1/2,z [0,0,0]	1/2,1/2,z [0,0,0]	
		0,1/2, $\bar{z}$ [0,0,0]	1/2,0, $\bar{z}$ [0,0,0]	1/2,1/2, $\bar{z}$ [0,0,0]	
4	h	3m.1' 1/3,2/3,z [0,0,0]	2/3,1/3,z [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	1/3,2/3, $\bar{z}$ [0,0,0]
3	g	mmm1' 1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
3	f	mmm1' 1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
2	e	6mm1' 0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
2	d	$\bar{6}m21'$ 1/3,2/3,1/2 [0,0,0]	2/3,1/3,1/2 [0,0,0]		
2	c	$\bar{6}m21'$ 1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]		
1	b	6/mmm1' 0,0,1/2 [0,0,0]			
1	a	6/mmm1' 0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

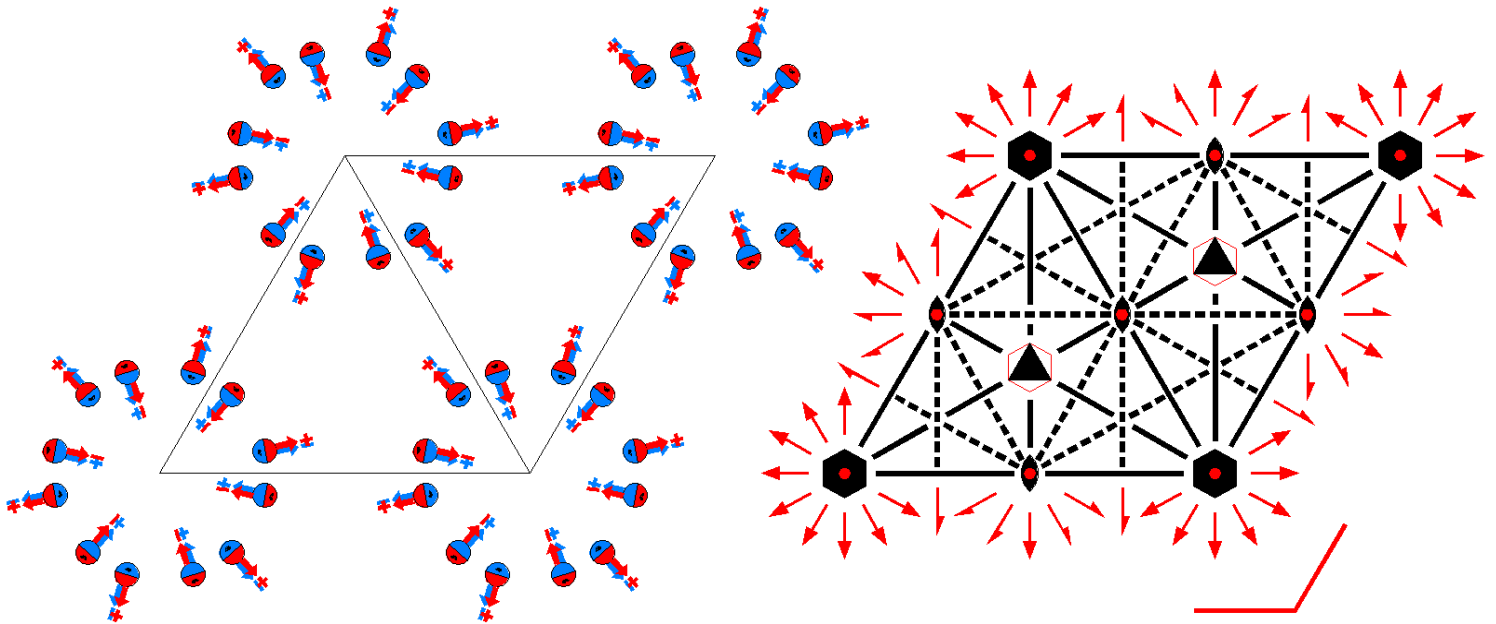
Along [2,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P6/m'mm  
191.3.1465

6/m'mm  
P6/m'2'/m2'/m

Hexagonal



Origin at center (6/m'mm)

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2		

**Symmetry Operations**

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                         | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)     | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'  | (8) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                          | (9) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                          |
| (10) 2' x,x̄,0<br>(2 <sub>3</sub>  0,0,0)' | (11) 2' x,2x,0<br>(2 <sub>2</sub>  0,0,0)'                        | (12) 2' 2x,x,0<br>(2 <sub>1</sub>  0,0,0)'                        |

(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(16) $m'$ x,y,0 ( $m_z$  0,0,0)'	(17) $\bar{6}^-$ 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,0)'	(18) $\bar{6}^+$ 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,0)'
(19) $m$ $\bar{x}, \bar{x}, z$ ( $m_{xy}$  0,0,0)	(20) $m$ x,2x,z ( $m_x$  0,0,0)	(21) $m$ 2x,x,z ( $m_y$  0,0,0)
(22) $m$ x,x,z ( $m_3$  0,0,0)	(23) $m$ x,0,z ( $m_2$  0,0,0)	(24) $m$ 0,y,z ( $m_1$  0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	r	1	(1) x,y,z [u,v,w]	(2) $\bar{y}, x-y, z$ [ $\bar{v}, u-v, w$ ]	(3) $\bar{x}+y, \bar{x}, z$ [ $\bar{u}+v, \bar{u}, w$ ]
			(4) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(5) $y, \bar{x}+y, z$ [ $v, \bar{u}+v, w$ ]	(6) x-y,x,z [u-v,u,w]
			(7) y,x, $\bar{z}$ [ $\bar{v}, \bar{u}, w$ ]	(8) x-y, $\bar{y}, \bar{z}$ [ $\bar{u}+v, v, w$ ]	(9) $\bar{x}, \bar{x}+y, \bar{z}$ [u,u-v,w]
			(10) $\bar{y}, \bar{x}, \bar{z}$ [v,u,w]	(11) $\bar{x}+y, \bar{y}, \bar{z}$ [u-v, $\bar{v}, w$ ]	(12) x,x-y, $\bar{z}$ [ $\bar{u}, \bar{u}+v, w$ ]
			(13) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(14) $y, \bar{x}+y, \bar{z}$ [v, $\bar{u}+v, \bar{w}$ ]	(15) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ]
			(16) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(17) $\bar{y}, x-y, \bar{z}$ [ $\bar{v}, u-v, \bar{w}$ ]	(18) $\bar{x}+y, \bar{x}, \bar{z}$ [ $\bar{u}+v, \bar{u}, \bar{w}$ ]
			(19) $\bar{y}, \bar{x}, z$ [v,u, $\bar{w}$ ]	(20) $\bar{x}+y, y, z$ [u-v, $\bar{v}, \bar{w}$ ]	(21) x,x-y,z [ $\bar{u}, \bar{u}+v, \bar{w}$ ]
			(22) y,x,z [ $\bar{v}, \bar{u}, \bar{w}$ ]	(23) x-y, $\bar{y}, z$ [ $\bar{u}+v, v, \bar{w}$ ]	(24) $\bar{x}, \bar{x}+y, z$ [u,u-v, $\bar{w}$ ]
12	q	m'..	x,y,1/2 [u,v,0]	$\bar{y}, x-y, 1/2$ [ $\bar{v}, u-v, 0$ ]	$\bar{x}+y, \bar{x}, 1/2$ [ $\bar{u}+v, \bar{u}, 0$ ]
			$\bar{x}, \bar{y}, 1/2$ [ $\bar{u}, \bar{v}, 0$ ]	$y, \bar{x}+y, 1/2$ [v, $\bar{u}+v, 0$ ]	x-y,x,1/2 [u-v,u,0]
			y,x,1/2 [ $\bar{v}, \bar{u}, 0$ ]	x-y, $\bar{y}, 1/2$ [ $\bar{u}+v, v, 0$ ]	$\bar{x}, \bar{x}+y, 1/2$ [u,u-v,0]
			$\bar{y}, \bar{x}, 1/2$ [v,u,0]	$\bar{x}+y, y, 1/2$ [u-v, $\bar{v}, 0$ ]	x,x-y,1/2 [ $\bar{u}, \bar{u}+v, 0$ ]
12	p	m'..	x,y,0 [u,v,0]	$\bar{y}, x-y, 0$ [ $\bar{v}, u-v, 0$ ]	$\bar{x}+y, \bar{x}, 0$ [ $\bar{u}+v, \bar{u}, 0$ ]
			$\bar{x}, \bar{y}, 0$ [ $\bar{u}, \bar{v}, 0$ ]	$y, \bar{x}+y, 0$ [v, $\bar{u}+v, 0$ ]	x-y,x,0 [u-v,u,0]
			y,x,0 [ $\bar{v}, \bar{u}, 0$ ]	x-y, $\bar{y}, 0$ [ $\bar{u}+v, v, 0$ ]	$\bar{x}, \bar{x}+y, 0$ [u,u-v,0]
			$\bar{y}, \bar{x}, 0$ [v,u,0]	$\bar{x}+y, y, 0$ [u-v, $\bar{v}, 0$ ]	x,x-y,0 [ $\bar{u}, \bar{u}+v, 0$ ]

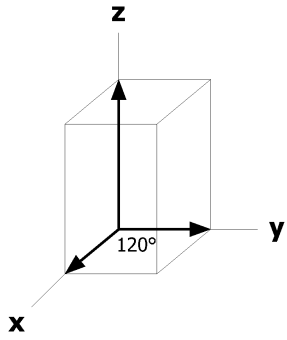
12	o	.m.	$x, 2x, z [u, 0, 0]$ $\bar{x}, 2\bar{x}, z [\bar{u}, 0, 0]$ $2x, x, \bar{z} [0, \bar{u}, 0]$ $2\bar{x}, \bar{x}, \bar{z} [0, u, 0]$	$2\bar{x}, \bar{x}, z [0, u, 0]$ $2x, x, z [0, \bar{u}, 0]$ $\bar{x}, 2\bar{x}, \bar{z} [\bar{u}, 0, 0]$ $x, 2x, \bar{z} [u, 0, 0]$	$x, \bar{x}, z [\bar{u}, \bar{u}, 0]$ $\bar{x}, x, z [u, u, 0]$ $\bar{x}, x, \bar{z} [u, u, 0]$ $x, \bar{x}, \bar{z} [\bar{u}, \bar{u}, 0]$	
12	n	..m	$x, 0, z [u, 2u, 0]$ $\bar{x}, 0, z [\bar{u}, 2\bar{u}, 0]$ $0, x, \bar{z} [2\bar{u}, \bar{u}, 0]$ $0, \bar{x}, \bar{z} [2u, u, 0]$	$0, x, z [2\bar{u}, \bar{u}, 0]$ $0, \bar{x}, z [2u, u, 0]$ $x, 0, \bar{z} [u, 2u, 0]$ $\bar{x}, 0, \bar{z} [\bar{u}, 2\bar{u}, 0]$	$\bar{x}, \bar{x}, z [u, \bar{u}, 0]$ $x, x, z [\bar{u}, u, 0]$ $\bar{x}, x, \bar{z} [u, \bar{u}, 0]$ $x, x, \bar{z} [\bar{u}, u, 0]$	
6	m	m'm2'	$x, 2x, 1/2 [u, 0, 0]$ $\bar{x}, 2\bar{x}, 1/2 [\bar{u}, 0, 0]$	$2\bar{x}, \bar{x}, 1/2 [0, u, 0]$ $2x, x, 1/2 [0, \bar{u}, 0]$	$x, \bar{x}, 1/2 [\bar{u}, \bar{u}, 0]$ $\bar{x}, x, 1/2 [u, u, 0]$	
6	l	m'm2'	$x, 2x, 0 [u, 0, 0]$ $\bar{x}, 2\bar{x}, 0 [\bar{u}, 0, 0]$	$2\bar{x}, \bar{x}, 0 [0, u, 0]$ $2x, x, 0 [0, \bar{u}, 0]$	$x, \bar{x}, 0 [\bar{u}, \bar{u}, 0]$ $\bar{x}, x, 0 [u, u, 0]$	
6	k	m'2'm	$x, 0, 1/2 [u, 2u, 0]$ $\bar{x}, 0, 1/2 [\bar{u}, 2\bar{u}, 0]$	$0, x, 1/2 [2\bar{u}, \bar{u}, 0]$ $0, \bar{x}, 1/2 [2u, u, 0]$	$\bar{x}, \bar{x}, 1/2 [u, \bar{u}, 0]$ $x, x, 1/2 [\bar{u}, u, 0]$	
6	j	m'2'm	$x, 0, 0 [u, 2u, 0]$ $\bar{x}, 0, 0 [\bar{u}, 2\bar{u}, 0]$	$0, x, 0 [2\bar{u}, \bar{u}, 0]$ $0, \bar{x}, 0 [2u, u, 0]$	$\bar{x}, \bar{x}, 0 [u, \bar{u}, 0]$ $x, x, 0 [\bar{u}, u, 0]$	
6	i	2mm	$1/2, 0, z [0, 0, 0]$ $0, 1/2, \bar{z} [0, 0, 0]$	$0, 1/2, z [0, 0, 0]$ $1/2, 0, \bar{z} [0, 0, 0]$	$1/2, 1/2, z [0, 0, 0]$ $1/2, 1/2, \bar{z} [0, 0, 0]$	
4	h	3m.	$1/3, 2/3, z [0, 0, 0]$	$2/3, 1/3, z [0, 0, 0]$	$2/3, 1/3, \bar{z} [0, 0, 0]$	$1/3, 2/3, \bar{z} [0, 0, 0]$
3	g	m'mm	$1/2, 0, 1/2 [0, 0, 0]$	$0, 1/2, 1/2 [0, 0, 0]$		$1/2, 1/2, 1/2 [0, 0, 0]$
3	f	m'mm	$1/2, 0, 0 [0, 0, 0]$	$0, 1/2, 0 [0, 0, 0]$		$1/2, 1/2, 0 [0, 0, 0]$
2	e	6mm	$0, 0, z [0, 0, 0]$	$0, 0, \bar{z} [0, 0, 0]$		
2	d	$\bar{6}'m2'$	$1/3, 2/3, 1/2 [0, 0, 0]$	$2/3, 1/3, 1/2 [0, 0, 0]$		
2	c	$\bar{6}'m2'$	$1/3, 2/3, 0 [0, 0, 0]$	$2/3, 1/3, 0 [0, 0, 0]$		
1	b	6/m'mm	$0, 0, 1/2 [0, 0, 0]$			
1	a	6/m'mm	$0, 0, 0 [0, 0, 0]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6mm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at  $x,0,0$

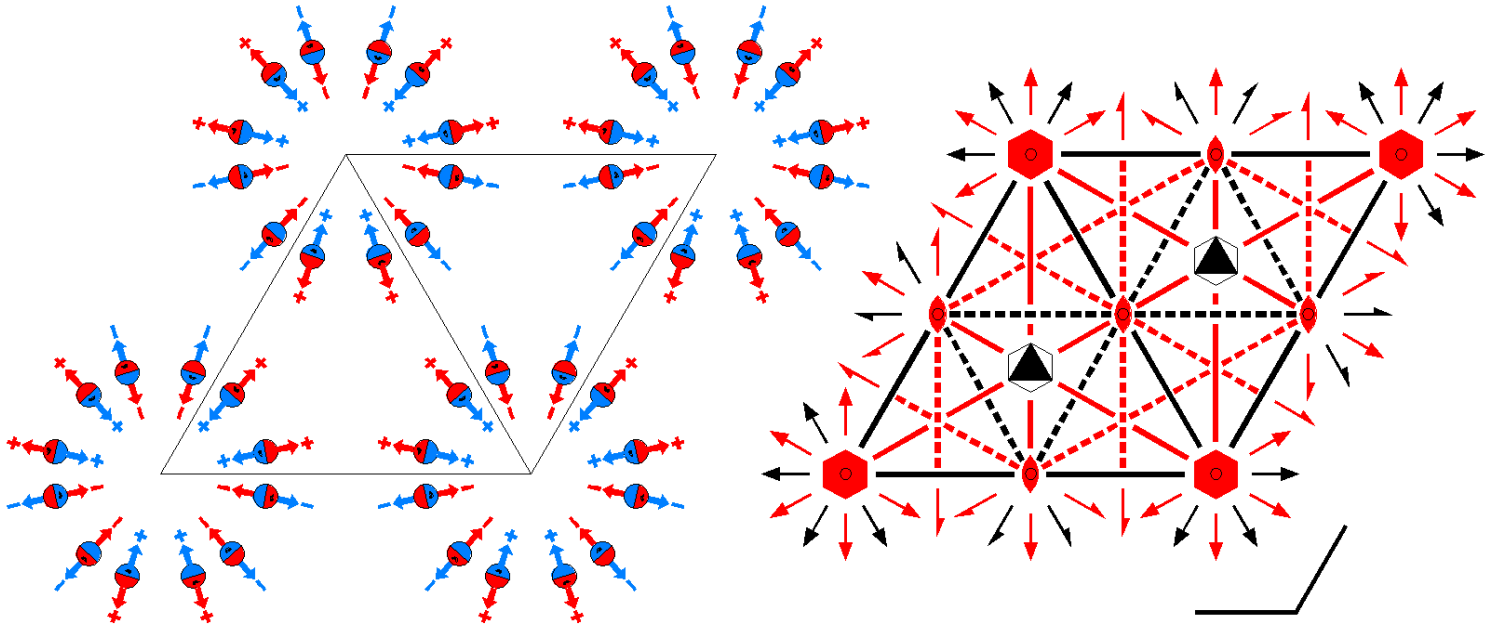
Along  $[2,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $x,x/2,0$



P6'/mm'm  
191.4.1466

6'/mm'm  
P6'/m2/m'2'/m

Hexagonal



Origin at center (6'/mm'm)

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2		

**Symmetry Operations**

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                         | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)                | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'   | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)'              |
| (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)    | (8) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                             | (9) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                            |
| (10) 2' x,x̄,0<br>(2 <sub>3</sub>  0,0,0)' | (11) 2' x,2x,0<br>(2 <sub>2</sub>  0,0,0)'                         | (12) 2' 2x,x,0<br>(2 <sub>1</sub>  0,0,0)'                        |

(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ ' 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(15) $\bar{3}^-$ ' 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(16) m $\bar{x}$ ,y,0 ( $m_z$  0,0,0)	(17) $\bar{6}^-$ 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,0)	(18) $\bar{6}^+$ 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,0)
(19) m' $\bar{x}$ , $\bar{x}$ ,z ( $m_{xy}$  0,0,0)'	(20) m' $\bar{x}$ ,2x,z ( $m_x$  0,0,0)'	(21) m' 2x,x,z ( $m_y$  0,0,0)'
(22) m $\bar{x}$ ,x,z ( $m_3$  0,0,0)	(23) m $\bar{x}$ ,0,z ( $m_2$  0,0,0)	(24) m 0,y,z ( $m_1$  0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	r	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z [u,v, $\bar{w}$ ]	(5) y, $\bar{x}$ +y,z [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) x-y,x,z [ $\bar{u}$ +v, $\bar{u}$ , $\bar{w}$ ]
			(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y}$ , $\bar{z}$ [u-v, $\bar{v}$ , $\bar{w}$ ]	(9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [v,u,w]	(11) $\bar{x}$ +y,y, $\bar{z}$ [u-v, $\bar{v}$ ,w]	(12) x,x-y, $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ +v,w]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(14) y, $\bar{x}$ +y, $\bar{z}$ [v, $\bar{u}$ +v, $\bar{w}$ ]	(15) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ]
			(16) x,y, $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ ,w]	(17) $\bar{y}$ ,x-y, $\bar{z}$ [v, $\bar{u}$ +v,w]	(18) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ [u-v,u,w]
			(19) $\bar{y}$ , $\bar{x}$ ,z [ $\bar{v}$ , $\bar{u}$ ,w]	(20) $\bar{x}$ +y,y,z [ $\bar{u}$ +v,v,w]	(21) x,x-y,z [u,u-v,w]
			(22) y,x,z [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(23) x-y, $\bar{y}$ ,z [ $\bar{u}$ +v,v, $\bar{w}$ ]	(24) $\bar{x}$ , $\bar{x}$ +y,z [u,u-v, $\bar{w}$ ]
12	q	m..	x,y,1/2 [0,0,w]	$\bar{y}$ ,x-y,1/2 [0,0,w]	$\bar{x}$ +y, $\bar{x}$ ,1/2 [0,0,w]
			$\bar{x}$ , $\bar{y}$ ,1/2 [0,0, $\bar{w}$ ]	y, $\bar{x}$ +y,1/2 [0,0, $\bar{w}$ ]	x-y,x,1/2 [0,0, $\bar{w}$ ]
			y,x,1/2 [0,0, $\bar{w}$ ]	x-y, $\bar{y}$ ,1/2 [0,0, $\bar{w}$ ]	$\bar{x}$ , $\bar{x}$ +y,1/2 [0,0, $\bar{w}$ ]
			$\bar{y}$ , $\bar{x}$ ,1/2 [0,0,w]	$\bar{x}$ +y,y,1/2 [0,0,w]	x,x-y,1/2 [0,0,w]
12	p	m..	x,y,0 [0,0,w]	$\bar{y}$ ,x-y,0 [0,0,w]	$\bar{x}$ +y, $\bar{x}$ ,0 [0,0,w]
			$\bar{x}$ , $\bar{y}$ ,0 [0,0, $\bar{w}$ ]	y, $\bar{x}$ +y,0 [0,0, $\bar{w}$ ]	x-y,x,0 [0,0, $\bar{w}$ ]
			y,x,0 [0,0, $\bar{w}$ ]	x-y, $\bar{y}$ ,0 [0,0, $\bar{w}$ ]	$\bar{x}$ , $\bar{x}$ +y,0 [0,0, $\bar{w}$ ]
			$\bar{y}$ , $\bar{x}$ ,0 [0,0,w]	$\bar{x}$ +y,y,0 [0,0,w]	x,x-y,0 [0,0,w]

12	o	.m'	$x, 2x, z [u, 2u, w]$ $\bar{x}, 2\bar{x}, z [u, 2u, \bar{w}]$ $2x, x, \bar{z} [2u, u, \bar{w}]$ $2\bar{x}, \bar{x}, \bar{z} [2u, u, w]$	$2\bar{x}, \bar{x}, z [2\bar{u}, \bar{u}, w]$ $2x, x, z [2\bar{u}, \bar{u}, \bar{w}]$ $\bar{x}, 2\bar{x}, \bar{z} [\bar{u}, 2\bar{u}, \bar{w}]$ $x, 2x, \bar{z} [\bar{u}, 2\bar{u}, w]$	$x, \bar{x}, z [u, \bar{u}, w]$ $\bar{x}, x, z [u, \bar{u}, \bar{w}]$ $\bar{x}, x, \bar{z} [\bar{u}, u, \bar{w}]$ $x, \bar{x}, \bar{z} [\bar{u}, u, w]$
12	n	..m	$x, 0, z [u, 2u, 0]$ $\bar{x}, 0, z [u, 2u, 0]$ $0, x, \bar{z} [2u, u, 0]$ $0, \bar{x}, \bar{z} [2u, u, 0]$	$0, x, z [2\bar{u}, \bar{u}, 0]$ $0, \bar{x}, z [2\bar{u}, \bar{u}, 0]$ $x, 0, \bar{z} [\bar{u}, 2\bar{u}, 0]$ $\bar{x}, 0, \bar{z} [\bar{u}, 2\bar{u}, 0]$	$\bar{x}, \bar{x}, z [u, \bar{u}, 0]$ $x, x, z [u, \bar{u}, 0]$ $\bar{x}, x, \bar{z} [\bar{u}, u, 0]$ $x, x, \bar{z} [\bar{u}, u, 0]$
6	m	mm'2'	$x, 2x, 1/2 [0, 0, w]$ $\bar{x}, 2\bar{x}, 1/2 [0, 0, \bar{w}]$	$2\bar{x}, \bar{x}, 1/2 [0, 0, w]$ $2x, x, 1/2 [0, 0, \bar{w}]$	$x, \bar{x}, 1/2 [0, 0, w]$ $\bar{x}, x, 1/2 [0, 0, \bar{w}]$
6	l	mm'2'	$x, 2x, 0 [0, 0, w]$ $\bar{x}, 2\bar{x}, 0 [0, 0, \bar{w}]$	$2\bar{x}, \bar{x}, 0 [0, 0, w]$ $2x, x, 0 [0, 0, \bar{w}]$	$x, \bar{x}, 0 [0, 0, w]$ $\bar{x}, x, 0 [0, 0, \bar{w}]$
6	k	m2m	$x, 0, 1/2 [0, 0, 0]$ $\bar{x}, 0, 1/2 [0, 0, 0]$	$0, x, 1/2 [0, 0, 0]$ $0, \bar{x}, 1/2 [0, 0, 0]$	$\bar{x}, \bar{x}, 1/2 [0, 0, 0]$ $x, x, 1/2 [0, 0, 0]$
6	j	m2m	$x, 0, 0 [0, 0, 0]$ $\bar{x}, 0, 0 [0, 0, 0]$	$0, x, 0 [0, 0, 0]$ $0, \bar{x}, 0 [0, 0, 0]$	$\bar{x}, \bar{x}, 0 [0, 0, 0]$ $x, x, 0 [0, 0, 0]$
6	i	2'm'm	$1/2, 0, z [u, 2u, 0]$ $0, 1/2, \bar{z} [u, 2u, 0]$	$0, 1/2, z [2\bar{u}, \bar{u}, 0]$ $1/2, 0, \bar{z} [2\bar{u}, \bar{u}, 0]$	$1/2, 1/2, z [u, \bar{u}, 0]$ $1/2, 1/2, \bar{z} [u, \bar{u}, 0]$
4	h	3m'	$1/3, 2/3, z [0, 0, w]$	$2/3, 1/3, z [0, 0, \bar{w}]$ $2/3, 1/3, \bar{z} [0, 0, \bar{w}]$	$1/3, 2/3, \bar{z} [0, 0, w]$
3	g	mm'm	$1/2, 0, 1/2 [0, 0, 0]$	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 1/2, 1/2 [0, 0, 0]$
3	f	mm'm	$1/2, 0, 0 [0, 0, 0]$	$0, 1/2, 0 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$
2	e	6'm'm	$0, 0, z [0, 0, 0]$	$0, 0, \bar{z} [0, 0, 0]$	
2	d	$\bar{6}m'2'$	$1/3, 2/3, 1/2 [0, 0, w]$	$2/3, 1/3, 1/2 [0, 0, \bar{w}]$	
2	c	$\bar{6}m'2'$	$1/3, 2/3, 0 [0, 0, w]$	$2/3, 1/3, 0 [0, 0, \bar{w}]$	
1	b	6'/mm'm	$0, 0, 1/2 [0, 0, 0]$		
1	a	6'/mm'm	$0, 0, 0 [0, 0, 0]$		

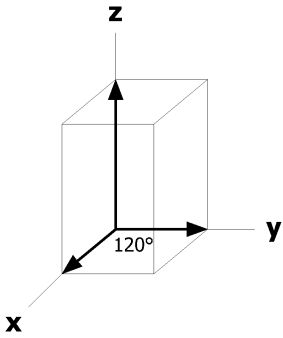


**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mm$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at  $x,0,0$

Along  $[2,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $x,x/2,0$



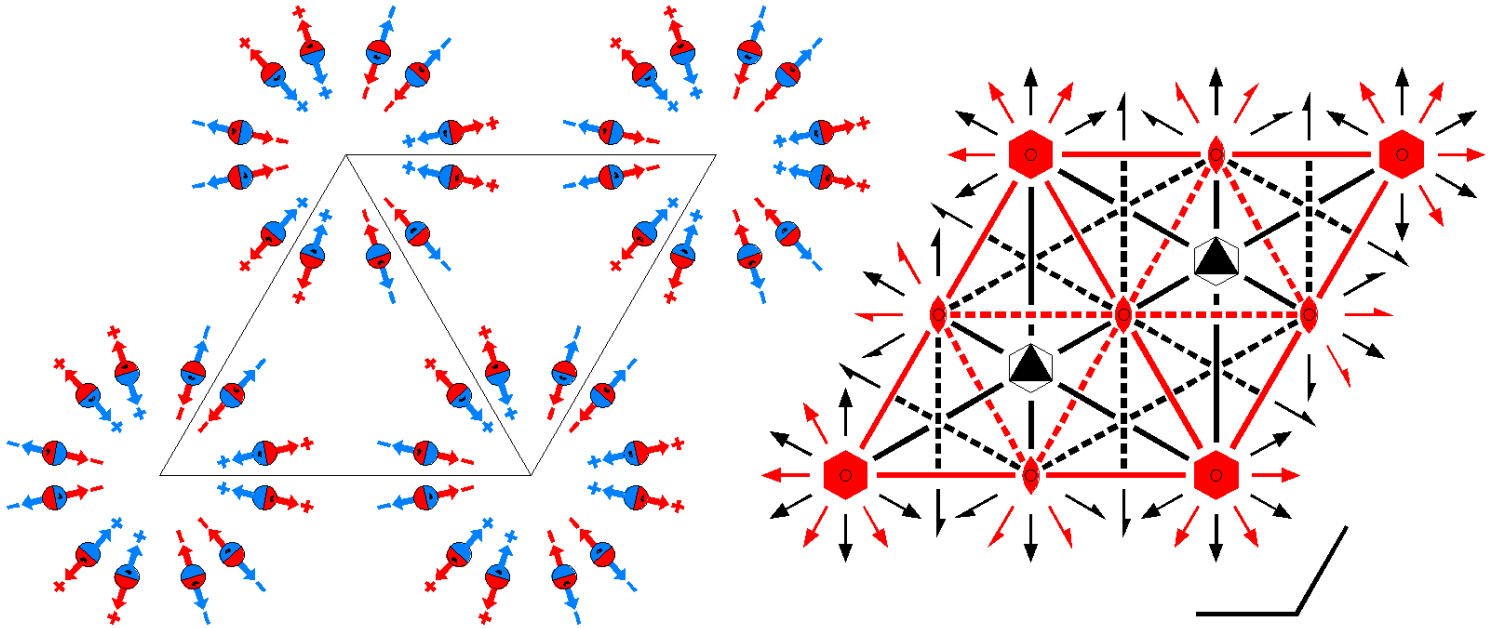
P6'/mmm'

191.5.1467

6'/mmm'

P6'/m2'/m2/m'

Hexagonal



Origin at center (6'/mmm')

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0		
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2		

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                        | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)                | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'  | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)'              |
| (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)' | (8) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                           | (9) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                          |
| (10) 2 x,x̄,0<br>(2 <sub>3</sub>  0,0,0)  | (11) 2 x,2x,0<br>(2 <sub>2</sub>  0,0,0)                           | (12) 2 2x,x,0<br>(2 <sub>1</sub>  0,0,0)                          |

(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(16) m $\bar{x},y,0$ ( $m_z$  0,0,0)	(17) $\bar{6}^-$ 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,0)	(18) $\bar{6}^+$ 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,0)
(19) m $\bar{x},\bar{x},z$ ( $m_{xy}$  0,0,0)	(20) m $\bar{x},2x,z$ ( $m_x$  0,0,0)	(21) m $2x,x,z$ ( $m_y$  0,0,0)
(22) m' $\bar{x},x,z$ ( $m_3$  0,0,0)'	(23) m' $\bar{x},0,z$ ( $m_2$  0,0,0)'	(24) m' $0,y,z$ ( $m_1$  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	r	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x,y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(5) $y,\bar{x}+y,z$ [ $\bar{v},u-v,\bar{w}$ ]	(6) $x-y,x,z$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]
			(7) $y,x,\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) $x-y,\bar{y},\bar{z}$ [ $\bar{u}+v,v,w$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}$ [u,u-v,w]
			(10) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(11) $\bar{x}+y,y,\bar{z}$ [ $\bar{u}+v,v,\bar{w}$ ]	(12) $x,x-y,\bar{z}$ [u,u-v, $\bar{w}$ ]
			(13) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $y,\bar{x}+y,\bar{z}$ [v, $\bar{u}+v,\bar{w}$ ]	(15) $x-y,x,\bar{z}$ [u-v,u, $\bar{w}$ ]
			(16) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(17) $\bar{y},x-y,\bar{z}$ [v, $\bar{u}+v,w$ ]	(18) $\bar{x}+y,\bar{x},\bar{z}$ [u-v,u,w]
			(19) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ]	(20) $\bar{x}+y,y,z$ [u-v, $\bar{v},\bar{w}$ ]	(21) $x,x-y,z$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
			(22) $y,x,z$ [v,u,w]	(23) $x-y,\bar{y},z$ [u-v, $\bar{v},w$ ]	(24) $\bar{x},\bar{x}+y,z$ [ $\bar{u},\bar{u}+v,w$ ]
12	q	m..	$x,y,1/2$ [0,0,w]	$\bar{y},x-y,1/2$ [0,0,w]	$\bar{x}+y,\bar{x},1/2$ [0,0,w]
			$\bar{x},\bar{y},1/2$ [0,0, $\bar{w}$ ]	$y,\bar{x}+y,1/2$ [0,0, $\bar{w}$ ]	$x-y,x,1/2$ [0,0, $\bar{w}$ ]
			$y,x,1/2$ [0,0,w]	$x-y,\bar{y},1/2$ [0,0,w]	$\bar{x},\bar{x}+y,1/2$ [0,0,w]
			$\bar{y},\bar{x},1/2$ [0,0, $\bar{w}$ ]	$\bar{x}+y,y,1/2$ [0,0, $\bar{w}$ ]	$x,x-y,1/2$ [0,0, $\bar{w}$ ]
12	p	m..	$x,y,0$ [0,0,w]	$\bar{y},x-y,0$ [0,0,w]	$\bar{x}+y,\bar{x},0$ [0,0,w]
			$\bar{x},\bar{y},0$ [0,0, $\bar{w}$ ]	$y,\bar{x}+y,0$ [0,0, $\bar{w}$ ]	$x-y,x,0$ [0,0, $\bar{w}$ ]
			$y,x,0$ [0,0,w]	$x-y,\bar{y},0$ [0,0,w]	$\bar{x},\bar{x}+y,0$ [0,0,w]
			$\bar{y},\bar{x},0$ [0,0, $\bar{w}$ ]	$\bar{x}+y,y,0$ [0,0, $\bar{w}$ ]	$x,x-y,0$ [0,0, $\bar{w}$ ]

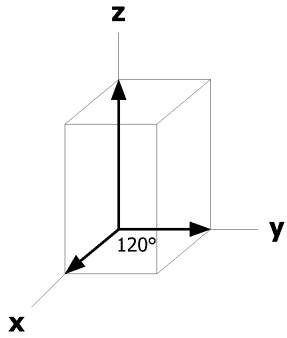
12	o	.m.	$x, 2x, z [u, 0, 0]$	$2\bar{x}, \bar{x}, z [0, u, 0]$	$x, \bar{x}, z [\bar{u}, \bar{u}, 0]$
			$\bar{x}, 2\bar{x}, z [u, 0, 0]$	$2x, x, z [0, u, 0]$	$\bar{x}, x, z [\bar{u}, \bar{u}, 0]$
			$2x, x, \bar{z} [0, \bar{u}, 0]$	$\bar{x}, 2\bar{x}, \bar{z} [\bar{u}, 0, 0]$	$\bar{x}, x, \bar{z} [u, u, 0]$
			$2\bar{x}, \bar{x}, \bar{z} [0, \bar{u}, 0]$	$x, 2x, \bar{z} [\bar{u}, 0, 0]$	$x, \bar{x}, \bar{z} [u, u, 0]$
12	n	..m'	$x, 0, z [u, 0, w]$	$0, x, z [0, u, w]$	$\bar{x}, \bar{x}, z [\bar{u}, \bar{u}, w]$
			$\bar{x}, 0, z [u, 0, \bar{w}]$	$0, \bar{x}, z [0, u, \bar{w}]$	$x, x, z [\bar{u}, \bar{u}, \bar{w}]$
			$0, x, \bar{z} [0, \bar{u}, w]$	$x, 0, \bar{z} [\bar{u}, 0, w]$	$\bar{x}, \bar{x}, \bar{z} [u, u, w]$
			$0, \bar{x}, \bar{z} [0, \bar{u}, \bar{w}]$	$\bar{x}, 0, \bar{z} [\bar{u}, 0, \bar{w}]$	$x, x, \bar{z} [u, u, \bar{w}]$
6	m	mm2	$x, 2x, 1/2 [0, 0, 0]$	$2\bar{x}, \bar{x}, 1/2 [0, 0, 0]$	$x, \bar{x}, 1/2 [0, 0, 0]$
			$\bar{x}, 2\bar{x}, 1/2 [0, 0, 0]$	$2x, x, 1/2 [0, 0, 0]$	$\bar{x}, x, 1/2 [0, 0, 0]$
6	l	mm2	$x, 2x, 0 [0, 0, 0]$	$2\bar{x}, \bar{x}, 0 [0, 0, 0]$	$x, \bar{x}, 0 [0, 0, 0]$
			$\bar{x}, 2\bar{x}, 0 [0, 0, 0]$	$2x, x, 0 [0, 0, 0]$	$\bar{x}, x, 0 [0, 0, 0]$
6	k	m2'm'	$x, 0, 1/2 [0, 0, w]$	$0, x, 1/2 [0, 0, w]$	$\bar{x}, \bar{x}, 1/2 [0, 0, w]$
			$\bar{x}, 0, 1/2 [0, 0, \bar{w}]$	$0, \bar{x}, 1/2 [0, 0, \bar{w}]$	$x, x, 1/2 [0, 0, \bar{w}]$
6	j	m2'm'	$x, 0, 0 [0, 0, w]$	$0, x, 0 [0, 0, w]$	$\bar{x}, \bar{x}, 0 [0, 0, w]$
			$\bar{x}, 0, 0 [0, 0, \bar{w}]$	$0, \bar{x}, 0 [0, 0, \bar{w}]$	$x, x, 0 [0, 0, \bar{w}]$
6	i	2'mm'	$1/2, 0, z [u, 0, 0]$	$0, 1/2, z [0, u, 0]$	$1/2, 1/2, z [\bar{u}, \bar{u}, 0]$
			$0, 1/2, \bar{z} [0, \bar{u}, 0]$	$1/2, 0, \bar{z} [\bar{u}, 0, 0]$	$1/2, 1/2, \bar{z} [u, u, 0]$
4	h	3m.	$1/3, 2/3, z [0, 0, 0]$	$2/3, 1/3, z [0, 0, 0]$	$2/3, 1/3, \bar{z} [0, 0, 0]$
					$1/3, 2/3, \bar{z} [0, 0, 0]$
3	g	mmm'	$1/2, 0, 1/2 [0, 0, 0]$	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 1/2, 1/2 [0, 0, 0]$
3	f	mmm'	$1/2, 0, 0 [0, 0, 0]$	$0, 1/2, 0 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$
2	e	6'mm'	$0, 0, z [0, 0, 0]$	$0, 0, \bar{z} [0, 0, 0]$	
2	d	$\bar{6}m2$	$1/3, 2/3, 1/2 [0, 0, 0]$	$2/3, 1/3, 1/2 [0, 0, 0]$	
2	c	$\bar{6}m2$	$1/3, 2/3, 0 [0, 0, 0]$	$2/3, 1/3, 0 [0, 0, 0]$	
1	b	6'mmm'	$0, 0, 1/2 [0, 0, 0]$		
1	a	6'mmm'	$0, 0, 0 [0, 0, 0]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at  $x,0,0$

Along  $[2,1,0]$   $p2mm$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $x,x/2,0$



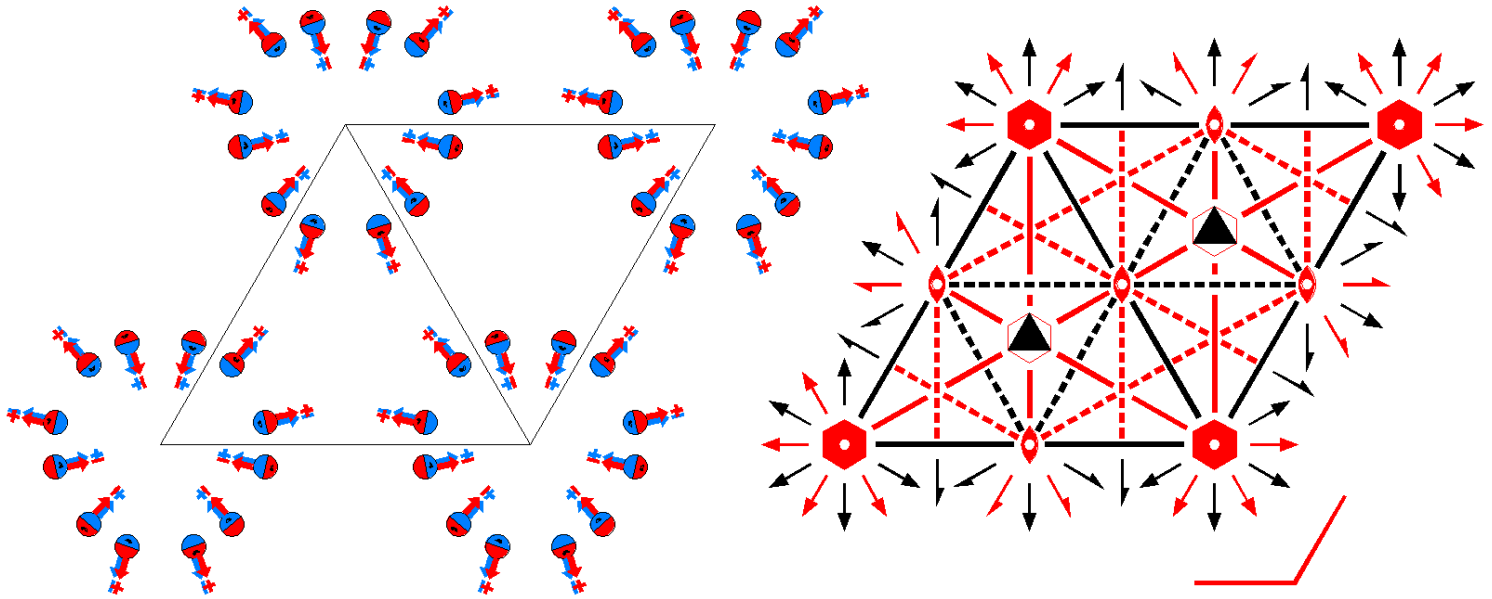
P6'/m'm'm

191.6.1468

6'/m'm'm

P6'/m'2'/m'2'/m

Hexagonal



**Origin at center (6'/m'm'm)**

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0		
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2		

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                        | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)                | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'  | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)'              |
| (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)' | (8) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                           | (9) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                          |
| (10) 2 x,x̄,0<br>(2 <sub>3</sub>  0,0,0)  | (11) 2 x,2x,0<br>(2 <sub>2</sub>  0,0,0)                           | (12) 2 2x,x,0<br>(2 <sub>1</sub>  0,0,0)                          |

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)
(16) $m'$ x,y,0 ( $m_z$  0,0,0)'	(17) $\bar{6}^-$ 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,0)'	(18) $\bar{6}^+$ 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,0)'
(19) $m'$ x, $\bar{x}$ ,z ( $m_{xy}$  0,0,0)'	(20) $m'$ x,2x,z ( $m_x$  0,0,0)'	(21) $m'$ 2x,x,z ( $m_y$  0,0,0)'
(22) $m$ x,x,z ( $m_3$  0,0,0)	(23) $m$ x,0,z ( $m_2$  0,0,0)	(24) $m$ 0,y,z ( $m_1$  0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	r	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y$ , $\bar{x}$ ,z [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z [u,v, $\bar{w}$ ]	(5) y, $\bar{x}+y$ ,z [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) x-y,x,z [ $\bar{u}+v$ , $\bar{u}$ , $\bar{w}$ ]
			(7) y,x, $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ ,w]	(8) x-y, $\bar{y}$ , $\bar{z}$ [ $\bar{u}+v$ ,v,w]	(9) $\bar{x}$ , $\bar{x}+y$ , $\bar{z}$ [u,u-v,w]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(11) $\bar{x}+y$ ,y, $\bar{z}$ [ $\bar{u}+v$ ,v, $\bar{w}$ ]	(12) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(14) y, $\bar{x}+y$ , $\bar{z}$ [ $\bar{v}$ ,u-v,w]	(15) x-y,x, $\bar{z}$ [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(16) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(17) $\bar{y}$ ,x-y, $\bar{z}$ [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(18) $\bar{x}+y$ , $\bar{x}$ , $\bar{z}$ [ $\bar{u}+v$ , $\bar{u}$ , $\bar{w}$ ]
			(19) $\bar{y}$ , $\bar{x}$ ,z [ $\bar{v}$ , $\bar{u}$ ,w]	(20) $\bar{x}+y$ ,y,z [ $\bar{u}+v$ ,v,w]	(21) x,x-y,z [u,u-v,w]
			(22) y,x,z [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(23) x-y, $\bar{y}$ ,z [ $\bar{u}+v$ ,v, $\bar{w}$ ]	(24) $\bar{x}$ , $\bar{x}+y$ ,z [u,u-v, $\bar{w}$ ]
12	q	m'..	x,y,1/2 [u,v,0]	$\bar{y}$ ,x-y,1/2 [ $\bar{v}$ ,u-v,0]	$\bar{x}+y$ , $\bar{x}$ ,1/2 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			$\bar{x}$ , $\bar{y}$ ,1/2 [u,v,0]	y, $\bar{x}+y$ ,1/2 [ $\bar{v}$ ,u-v,0]	x-y,x,1/2 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			y,x,1/2 [ $\bar{v}$ , $\bar{u}$ ,0]	x-y, $\bar{y}$ ,1/2 [ $\bar{u}+v$ ,v,0]	$\bar{x}$ , $\bar{x}+y$ ,1/2 [u,u-v,0]
			$\bar{y}$ , $\bar{x}$ ,1/2 [ $\bar{v}$ , $\bar{u}$ ,0]	$\bar{x}+y$ ,y,1/2 [ $\bar{u}+v$ ,v,0]	x,x-y,1/2 [u,u-v,0]
12	p	m'..	x,y,0 [u,v,0]	$\bar{y}$ ,x-y,0 [ $\bar{v}$ ,u-v,0]	$\bar{x}+y$ , $\bar{x}$ ,0 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			$\bar{x}$ , $\bar{y}$ ,0 [u,v,0]	y, $\bar{x}+y$ ,0 [ $\bar{v}$ ,u-v,0]	x-y,x,0 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			y,x,0 [ $\bar{v}$ , $\bar{u}$ ,0]	x-y, $\bar{y}$ ,0 [ $\bar{u}+v$ ,v,0]	$\bar{x}$ , $\bar{x}+y$ ,0 [u,u-v,0]
			$\bar{y}$ , $\bar{x}$ ,0 [ $\bar{v}$ , $\bar{u}$ ,0]	$\bar{x}+y$ ,y,0 [ $\bar{u}+v$ ,v,0]	x,x-y,0 [u,u-v,0]

12	o	.m'	$x, 2x, z [u, 2u, w]$ $\bar{x}, 2\bar{x}, z [u, 2u, \bar{w}]$ $2x, x, \bar{z} [2\bar{u}, \bar{u}, w]$ $2\bar{x}, \bar{x}, \bar{z} [2\bar{u}, \bar{u}, \bar{w}]$	$2\bar{x}, \bar{x}, z [2\bar{u}, \bar{u}, w]$ $2x, x, z [2\bar{u}, \bar{u}, \bar{w}]$ $\bar{x}, 2\bar{x}, \bar{z} [u, 2u, w]$ $x, 2x, \bar{z} [u, 2u, \bar{w}]$	$x, \bar{x}, z [u, \bar{u}, w]$ $\bar{x}, x, z [u, \bar{u}, \bar{w}]$ $\bar{x}, x, \bar{z} [u, \bar{u}, w]$ $x, \bar{x}, \bar{z} [u, \bar{u}, \bar{w}]$
12	n	..m	$x, 0, z [u, 2u, 0]$ $\bar{x}, 0, z [u, 2u, 0]$ $0, x, \bar{z} [2\bar{u}, \bar{u}, 0]$ $0, \bar{x}, \bar{z} [2\bar{u}, \bar{u}, 0]$	$0, x, z [2\bar{u}, \bar{u}, 0]$ $0, \bar{x}, z [2\bar{u}, \bar{u}, 0]$ $x, 0, \bar{z} [u, 2u, 0]$ $\bar{x}, 0, \bar{z} [u, 2u, 0]$	$\bar{x}, \bar{x}, z [u, \bar{u}, 0]$ $x, x, z [u, \bar{u}, 0]$ $\bar{x}, \bar{x}, \bar{z} [u, \bar{u}, 0]$ $x, x, \bar{z} [u, \bar{u}, 0]$
6	m	m'm'2	$x, 2x, 1/2 [u, 2u, 0]$ $\bar{x}, 2\bar{x}, 1/2 [u, 2u, 0]$	$2\bar{x}, \bar{x}, 1/2 [2\bar{u}, \bar{u}, 0]$ $2x, x, 1/2 [2\bar{u}, \bar{u}, 0]$	$x, \bar{x}, 1/2 [u, \bar{u}, 0]$ $\bar{x}, x, 1/2 [u, \bar{u}, 0]$
6	l	m'm'2	$x, 2x, 0 [u, 2u, 0]$ $\bar{x}, 2\bar{x}, 0 [u, 2u, 0]$	$2\bar{x}, \bar{x}, 0 [2\bar{u}, \bar{u}, 0]$ $2x, x, 0 [2\bar{u}, \bar{u}, 0]$	$x, \bar{x}, 0 [u, \bar{u}, 0]$ $\bar{x}, x, 0 [u, \bar{u}, 0]$
6	k	m'2'm	$x, 0, 1/2 [u, 2u, 0]$ $\bar{x}, 0, 1/2 [u, 2u, 0]$	$0, x, 1/2 [2\bar{u}, \bar{u}, 0]$ $0, \bar{x}, 1/2 [2\bar{u}, \bar{u}, 0]$	$\bar{x}, \bar{x}, 1/2 [u, \bar{u}, 0]$ $x, x, 1/2 [u, \bar{u}, 0]$
6	j	m'2'm	$x, 0, 0 [u, 2u, 0]$ $\bar{x}, 0, 0 [u, 2u, 0]$	$0, x, 0 [2\bar{u}, \bar{u}, 0]$ $0, \bar{x}, 0 [2\bar{u}, \bar{u}, 0]$	$\bar{x}, \bar{x}, 0 [u, \bar{u}, 0]$ $x, x, 0 [u, \bar{u}, 0]$
6	i	2'm'm	$1/2, 0, z [u, 2u, 0]$ $0, 1/2, \bar{z} [2\bar{u}, \bar{u}, 0]$	$0, 1/2, z [2\bar{u}, \bar{u}, 0]$ $1/2, 0, \bar{z} [u, 2u, 0]$	$1/2, 1/2, z [u, \bar{u}, 0]$ $1/2, 1/2, \bar{z} [u, \bar{u}, 0]$
4	h	3m'	$1/3, 2/3, z [0, 0, w]$	$2/3, 1/3, z [0, 0, \bar{w}]$ $2/3, 1/3, \bar{z} [0, 0, w]$	$1/3, 2/3, \bar{z} [0, 0, \bar{w}]$
3	g	m'm'm	$1/2, 0, 1/2 [u, 2u, 0]$	$0, 1/2, 1/2 [2\bar{u}, \bar{u}, 0]$	$1/2, 1/2, 1/2 [u, \bar{u}, 0]$
3	f	m'm'm	$1/2, 0, 0 [u, 2u, 0]$	$0, 1/2, 0 [2\bar{u}, \bar{u}, 0]$	$1/2, 1/2, 0 [u, \bar{u}, 0]$
2	e	6'm'm	$0, 0, z [0, 0, 0]$	$0, 0, \bar{z} [0, 0, 0]$	
2	d	$\bar{6}'m'2$	$1/3, 2/3, 1/2 [0, 0, 0]$	$2/3, 1/3, 1/2 [0, 0, 0]$	
2	c	$\bar{6}'m'2$	$1/3, 2/3, 0 [0, 0, 0]$	$2/3, 1/3, 0 [0, 0, 0]$	
1	b	6'/m'm'm	$0, 0, 1/2 [0, 0, 0]$		
1	a	6'/m'm'm	$0, 0, 0 [0, 0, 0]$		

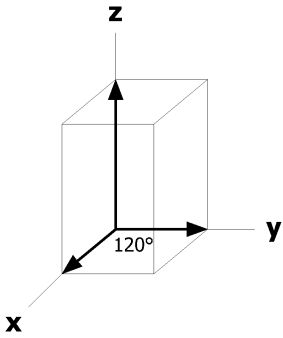


**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6'm'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2'mm'$   
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,0,0$

Along  $[2,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $x,x/2,0$



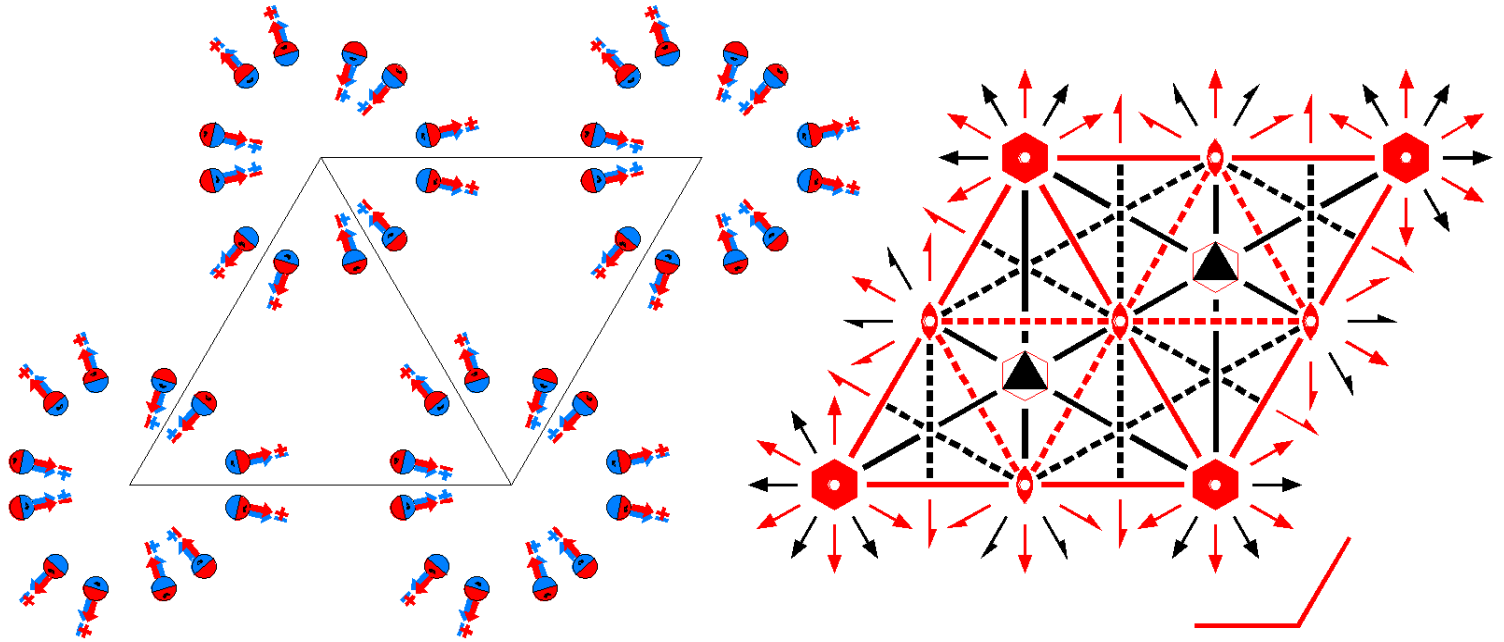
P6'/m'mm'

191.7.1469

6'/m'mm'

P6'/m'2/m2'/m'

Hexagonal



Origin at center (6'/m'mm')

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2		

**Symmetry Operations**

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                         | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)                | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'   | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)'              |
| (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)    | (8) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                             | (9) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                            |
| (10) 2' x,x̄,0<br>(2 <sub>3</sub>  0,0,0)' | (11) 2' x,2x,0<br>(2 <sub>2</sub>  0,0,0)'                         | (12) 2' 2x,x,0<br>(2 <sub>1</sub>  0,0,0)'                        |

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)
(16) $m'$ x,y,0 ( $m_z$  0,0,0)'	(17) $\bar{6}^-$ 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,0)'	(18) $\bar{6}^+$ 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,0)'
(19) $m$ x, $\bar{x}$ ,z ( $m_{xy}$  0,0,0)	(20) $m$ x,2x,z ( $m_x$  0,0,0)	(21) $m$ 2x,x,z ( $m_y$  0,0,0)
(22) $m'$ x,x,z ( $m_3$  0,0,0)'	(23) $m'$ x,0,z ( $m_2$  0,0,0)'	(24) $m'$ 0,y,z ( $m_1$  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	r	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y$ , $\bar{x}$ ,z [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z [u,v, $\bar{w}$ ]	(5) y, $\bar{x}+y$ ,z [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) x-y,x,z [ $\bar{u}+v$ , $\bar{u}$ , $\bar{w}$ ]
			(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y}$ , $\bar{z}$ [u-v, $\bar{v}$ , $\bar{w}$ ]	(9) $\bar{x}$ , $\bar{x}+y$ , $\bar{z}$ [ $\bar{u}$ , $\bar{u}+v$ , $\bar{w}$ ]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [v,u,w]	(11) $\bar{x}+y$ , $\bar{y}$ , $\bar{z}$ [u-v, $\bar{v}$ ,w]	(12) x,x-y, $\bar{z}$ [ $\bar{u}$ , $\bar{u}+v$ ,w]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(14) y, $\bar{x}+y$ , $\bar{z}$ [ $\bar{v}$ ,u-v,w]	(15) x-y,x, $\bar{z}$ [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(16) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(17) $\bar{y}$ ,x-y, $\bar{z}$ [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(18) $\bar{x}+y$ , $\bar{x}$ , $\bar{z}$ [ $\bar{u}+v$ , $\bar{u}$ , $\bar{w}$ ]
			(19) $\bar{y}$ , $\bar{x}$ ,z [v,u, $\bar{w}$ ]	(20) $\bar{x}+y$ ,y,z [u-v, $\bar{v}$ , $\bar{w}$ ]	(21) x,x-y,z [ $\bar{u}$ , $\bar{u}+v$ , $\bar{w}$ ]
			(22) y,x,z [v,u,w]	(23) x-y, $\bar{y}$ ,z [u-v, $\bar{v}$ ,w]	(24) $\bar{x}$ , $\bar{x}+y$ ,z [ $\bar{u}$ , $\bar{u}+v$ ,w]
12	q	m'..	x,y,1/2 [u,v,0]	$\bar{y}$ ,x-y,1/2 [ $\bar{v}$ ,u-v,0]	$\bar{x}+y$ , $\bar{x}$ ,1/2 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			$\bar{x}$ , $\bar{y}$ ,1/2 [u,v,0]	y, $\bar{x}+y$ ,1/2 [ $\bar{v}$ ,u-v,0]	x-y,x,1/2 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			y,x,1/2 [v,u,0]	x-y, $\bar{y}$ ,1/2 [u-v, $\bar{v}$ ,0]	$\bar{x}$ , $\bar{x}+y$ ,1/2 [ $\bar{u}$ , $\bar{u}+v$ ,0]
			$\bar{y}$ , $\bar{x}$ ,1/2 [v,u,0]	$\bar{x}+y$ ,y,1/2 [u-v, $\bar{v}$ ,0]	x,x-y,1/2 [ $\bar{u}$ , $\bar{u}+v$ ,0]
12	p	m'..	x,y,0 [u,v,0]	$\bar{y}$ ,x-y,0 [ $\bar{v}$ ,u-v,0]	$\bar{x}+y$ , $\bar{x}$ ,0 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			$\bar{x}$ , $\bar{y}$ ,0 [u,v,0]	y, $\bar{x}+y$ ,0 [ $\bar{v}$ ,u-v,0]	x-y,x,0 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			y,x,0 [v,u,0]	x-y, $\bar{y}$ ,0 [u-v, $\bar{v}$ ,0]	$\bar{x}$ , $\bar{x}+y$ ,0 [ $\bar{u}$ , $\bar{u}+v$ ,0]
			$\bar{y}$ , $\bar{x}$ ,0 [v,u,0]	$\bar{x}+y$ ,y,0 [u-v, $\bar{v}$ ,0]	x,x-y,0 [ $\bar{u}$ , $\bar{u}+v$ ,0]

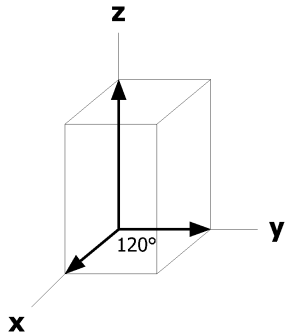
12	o	.m.	$x, 2x, z [u, 0, 0]$	$2\bar{x}, \bar{x}, z [0, u, 0]$	$x, \bar{x}, z [\bar{u}, \bar{u}, 0]$
			$\bar{x}, 2\bar{x}, z [u, 0, 0]$	$2x, x, z [0, u, 0]$	$\bar{x}, x, z [\bar{u}, \bar{u}, 0]$
			$2x, x, \bar{z} [0, u, 0]$	$\bar{x}, 2\bar{x}, \bar{z} [u, 0, 0]$	$\bar{x}, x, \bar{z} [\bar{u}, \bar{u}, 0]$
			$2\bar{x}, \bar{x}, \bar{z} [0, u, 0]$	$x, 2x, \bar{z} [u, 0, 0]$	$x, \bar{x}, \bar{z} [\bar{u}, \bar{u}, 0]$
12	n	..m'	$x, 0, z [u, 0, w]$	$0, x, z [0, u, w]$	$\bar{x}, \bar{x}, z [\bar{u}, \bar{u}, w]$
			$\bar{x}, 0, z [u, 0, \bar{w}]$	$0, \bar{x}, z [0, u, \bar{w}]$	$x, x, z [\bar{u}, \bar{u}, \bar{w}]$
			$0, x, \bar{z} [0, u, \bar{w}]$	$x, 0, \bar{z} [u, 0, \bar{w}]$	$\bar{x}, \bar{x}, \bar{z} [\bar{u}, \bar{u}, \bar{w}]$
			$0, \bar{x}, \bar{z} [0, u, w]$	$\bar{x}, 0, \bar{z} [u, 0, w]$	$x, x, \bar{z} [\bar{u}, \bar{u}, w]$
6	m	m'm2'	$x, 2x, 1/2 [u, 0, 0]$	$2\bar{x}, \bar{x}, 1/2 [0, u, 0]$	$x, \bar{x}, 1/2 [\bar{u}, \bar{u}, 0]$
			$\bar{x}, 2\bar{x}, 1/2 [u, 0, 0]$	$2x, x, 1/2 [0, u, 0]$	$\bar{x}, x, 1/2 [\bar{u}, \bar{u}, 0]$
6	l	m'm2'	$x, 2x, 0 [u, 0, 0]$	$2\bar{x}, \bar{x}, 0 [0, u, 0]$	$x, \bar{x}, 0 [\bar{u}, \bar{u}, 0]$
			$\bar{x}, 2\bar{x}, 0 [u, 0, 0]$	$2x, x, 0 [0, u, 0]$	$\bar{x}, x, 0 [\bar{u}, \bar{u}, 0]$
6	k	m'2m'	$x, 0, 1/2 [u, 0, 0]$	$0, x, 1/2 [0, u, 0]$	$\bar{x}, \bar{x}, 1/2 [\bar{u}, \bar{u}, 0]$
			$\bar{x}, 0, 1/2 [u, 0, 0]$	$0, \bar{x}, 1/2 [0, u, 0]$	$x, x, 1/2 [\bar{u}, \bar{u}, 0]$
6	j	m'2m'	$x, 0, 0 [u, 0, 0]$	$0, x, 0 [0, u, 0]$	$\bar{x}, \bar{x}, 0 [\bar{u}, \bar{u}, 0]$
			$\bar{x}, 0, 0 [u, 0, 0]$	$0, \bar{x}, 0 [0, u, 0]$	$x, x, 0 [\bar{u}, \bar{u}, 0]$
6	i	2'mm'	$1/2, 0, z [u, 0, 0]$	$0, 1/2, z [0, u, 0]$	$1/2, 1/2, z [\bar{u}, \bar{u}, 0]$
			$0, 1/2, \bar{z} [0, u, 0]$	$1/2, 0, \bar{z} [u, 0, 0]$	$1/2, 1/2, \bar{z} [\bar{u}, \bar{u}, 0]$
4	h	3m.	$1/3, 2/3, z [0, 0, 0]$	$2/3, 1/3, z [0, 0, 0]$	$2/3, 1/3, \bar{z} [0, 0, 0]$
					$1/3, 2/3, \bar{z} [0, 0, 0]$
3	g	m'mm'	$1/2, 0, 1/2 [u, 0, 0]$	$0, 1/2, 1/2 [0, u, 0]$	$1/2, 1/2, 1/2 [\bar{u}, \bar{u}, 0]$
3	f	m'mm'	$1/2, 0, 0 [u, 0, 0]$	$0, 1/2, 0 [0, u, 0]$	$1/2, 1/2, 0 [\bar{u}, \bar{u}, 0]$
2	e	6'mm'	$0, 0, z [0, 0, 0]$	$0, 0, \bar{z} [0, 0, 0]$	
2	d	$\bar{6}'m2'$	$1/3, 2/3, 1/2 [0, 0, 0]$	$2/3, 1/3, 1/2 [0, 0, 0]$	
2	c	$\bar{6}'m2'$	$1/3, 2/3, 0 [0, 0, 0]$	$2/3, 1/3, 0 [0, 0, 0]$	
1	b	6'/m'mm'	$0, 0, 1/2 [0, 0, 0]$		
1	a	6'/m'mm'	$0, 0, 0 [0, 0, 0]$		

**Symmetry of Special Projections**

Along [0,0,1]  $p6'mm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,0

Along [2,1,0]  $p2'mm'$   
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,x/2,0



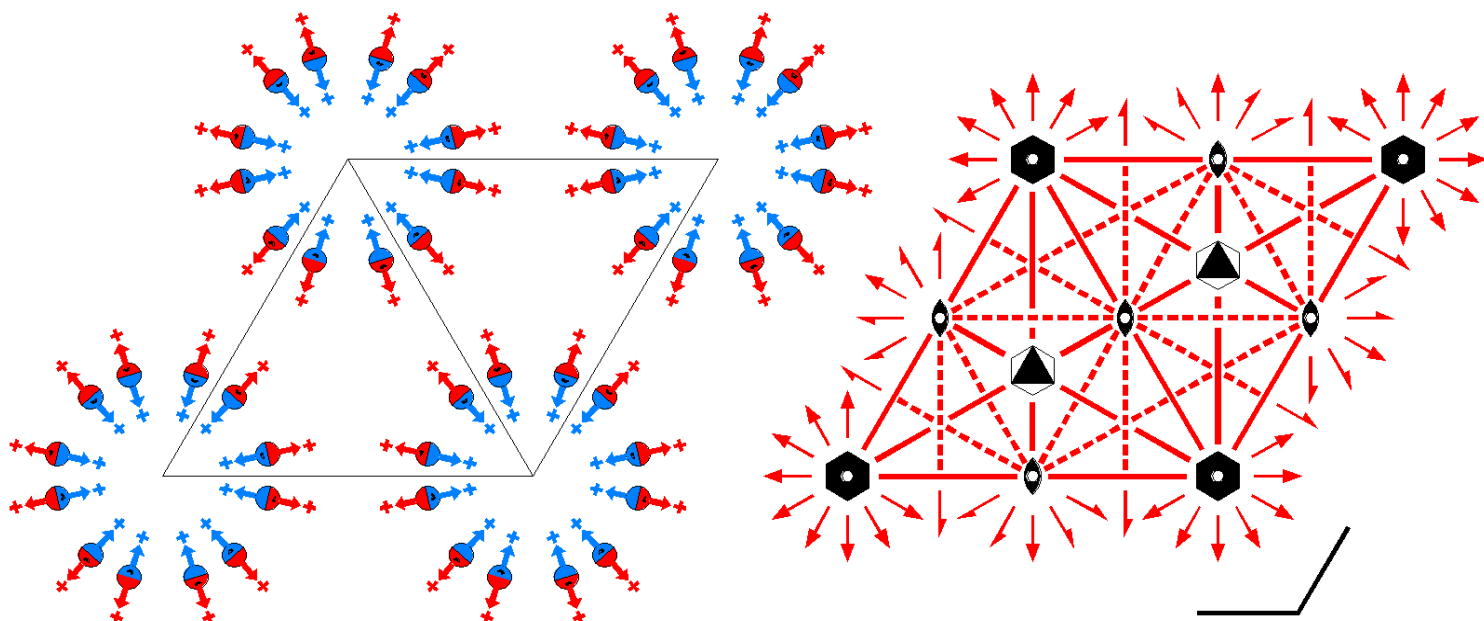
P6/mm'm'

191.8.1470

6/mm'm'

P6/m2'/m'2'/m'

Hexagonal



Origin at center (6/mm'm')

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/3$ ;  $0 \leq z \leq 1/2$ ;  $x \leq (1+y)/2$ ;  $y \leq x/2$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2

### Symmetry Operations

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                         | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)     | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) 2' x,x,0<br>(2 <sub>xy</sub>  0,0,0)'  | (8) 2' x,0,0<br>(2 <sub>x</sub>  0,0,0)'                          | (9) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                          |
| (10) 2' x,x̄,0<br>(2 <sub>3</sub>  0,0,0)' | (11) 2' x,2x,0<br>(2 <sub>2</sub>  0,0,0)'                        | (12) 2' 2x,x,0<br>(2 <sub>1</sub>  0,0,0)'                        |

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)
(16) m $\bar{x}$ ,y,0 ( $m_z$  0,0,0)	(17) $\bar{6}^-$ 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,0)	(18) $\bar{6}^+$ 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,0)
(19) m' $\bar{x}$ , $\bar{x}$ ,z ( $m_{xy}$  0,0,0)'	(20) m' $\bar{x}$ ,2x,z ( $m_x$  0,0,0)'	(21) m' 2x,x,z ( $m_y$  0,0,0)'
(22) m' $\bar{x}$ ,x,z ( $m_3$  0,0,0)'	(23) m' $\bar{x}$ ,0,z ( $m_2$  0,0,0)'	(24) m' 0,y,z ( $m_1$  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	r	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w]	(5) y, $\bar{x}$ +y,z [v, $\bar{u}$ +v,w]	(6) x-y,x,z [u-v,u,w]
			(7) y,x, $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ ,w]	(8) x-y, $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ +v,v,w]	(9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ [u,u-v,w]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [v,u,w]	(11) $\bar{x}$ +y,y, $\bar{z}$ [u-v, $\bar{v}$ ,w]	(12) x,x-y, $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ +v,w]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(14) y, $\bar{x}$ +y, $\bar{z}$ [ $\bar{v}$ ,u-v,w]	(15) x-y,x, $\bar{z}$ [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(16) x,y, $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ ,w]	(17) $\bar{y}$ ,x-y, $\bar{z}$ [v, $\bar{u}$ +v,w]	(18) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ [u-v,u,w]
			(19) $\bar{y}$ , $\bar{x}$ ,z [ $\bar{v}$ , $\bar{u}$ ,w]	(20) $\bar{x}$ +y,y,z [ $\bar{u}$ +v,v,w]	(21) x,x-y,z [u,u-v,w]
			(22) y,x,z [v,u,w]	(23) x-y, $\bar{y}$ ,z [u-v, $\bar{v}$ ,w]	(24) $\bar{x}$ , $\bar{x}$ +y,z [ $\bar{u}$ , $\bar{u}$ +v,w]
12	q	m..	x,y,1/2 [0,0,w]	$\bar{y}$ ,x-y,1/2 [0,0,w]	$\bar{x}$ +y, $\bar{x}$ ,1/2 [0,0,w]
			$\bar{x}$ , $\bar{y}$ ,1/2 [0,0,w]	y, $\bar{x}$ +y,1/2 [0,0,w]	x-y,x,1/2 [0,0,w]
			y,x,1/2 [0,0,w]	x-y, $\bar{y}$ ,1/2 [0,0,w]	$\bar{x}$ , $\bar{x}$ +y,1/2 [0,0,w]
			$\bar{y}$ , $\bar{x}$ ,1/2 [0,0,w]	$\bar{x}$ +y,y,1/2 [0,0,w]	x,x-y,1/2 [0,0,w]
12	p	m..	x,y,0 [0,0,w]	$\bar{y}$ ,x-y,0 [0,0,w]	$\bar{x}$ +y, $\bar{x}$ ,0 [0,0,w]
			$\bar{x}$ , $\bar{y}$ ,0 [0,0,w]	y, $\bar{x}$ +y,0 [0,0,w]	x-y,x,0 [0,0,w]
			y,x,0 [0,0,w]	x-y, $\bar{y}$ ,0 [0,0,w]	$\bar{x}$ , $\bar{x}$ +y,0 [0,0,w]
			$\bar{y}$ , $\bar{x}$ ,0 [0,0,w]	$\bar{x}$ +y,y,0 [0,0,w]	x,x-y,0 [0,0,w]

12	o	.m'	$x, 2x, z [u, 2u, w]$ $\bar{x}, 2\bar{x}, z [\bar{u}, 2\bar{u}, w]$ $2x, x, \bar{z} [2\bar{u}, \bar{u}, w]$ $2\bar{x}, \bar{x}, \bar{z} [2u, u, w]$	$2\bar{x}, \bar{x}, z [2\bar{u}, \bar{u}, w]$ $2x, x, z [2u, u, w]$ $\bar{x}, 2\bar{x}, \bar{z} [u, 2u, w]$ $x, 2x, \bar{z} [\bar{u}, 2\bar{u}, w]$	$x, \bar{x}, z [u, \bar{u}, w]$ $\bar{x}, x, z [\bar{u}, u, w]$ $\bar{x}, x, \bar{z} [u, \bar{u}, w]$ $x, \bar{x}, \bar{z} [\bar{u}, u, w]$	
12	n	..m'	$x, 0, z [u, 0, w]$ $\bar{x}, 0, z [\bar{u}, 0, w]$ $0, x, \bar{z} [0, \bar{u}, w]$ $0, \bar{x}, \bar{z} [0, u, w]$	$0, x, z [0, u, w]$ $0, \bar{x}, z [0, \bar{u}, w]$ $x, 0, \bar{z} [\bar{u}, 0, w]$ $\bar{x}, 0, \bar{z} [u, 0, w]$	$\bar{x}, \bar{x}, z [\bar{u}, \bar{u}, w]$ $x, x, z [u, u, w]$ $\bar{x}, x, \bar{z} [u, u, w]$ $x, x, \bar{z} [\bar{u}, \bar{u}, w]$	
6	m	mm'2'	$x, 2x, 1/2 [0, 0, w]$ $\bar{x}, 2\bar{x}, 1/2 [0, 0, w]$	$2\bar{x}, \bar{x}, 1/2 [0, 0, w]$ $2x, x, 1/2 [0, 0, w]$	$x, \bar{x}, 1/2 [0, 0, w]$ $\bar{x}, x, 1/2 [0, 0, w]$	
6	l	mm'2'	$x, 2x, 0 [0, 0, w]$ $\bar{x}, 2\bar{x}, 0 [0, 0, w]$	$2\bar{x}, \bar{x}, 0 [0, 0, w]$ $2x, x, 0 [0, 0, w]$	$x, \bar{x}, 0 [0, 0, w]$ $\bar{x}, x, 0 [0, 0, w]$	
6	k	m2'm'	$x, 0, 1/2 [0, 0, w]$ $\bar{x}, 0, 1/2 [0, 0, w]$	$0, x, 1/2 [0, 0, w]$ $0, \bar{x}, 1/2 [0, 0, w]$	$\bar{x}, \bar{x}, 1/2 [0, 0, w]$ $x, x, 1/2 [0, 0, w]$	
6	j	m2'm'	$x, 0, 0 [0, 0, w]$ $\bar{x}, 0, 0 [0, 0, w]$	$0, x, 0 [0, 0, w]$ $0, \bar{x}, 0 [0, 0, w]$	$\bar{x}, \bar{x}, 0 [0, 0, w]$ $x, x, 0 [0, 0, w]$	
6	i	2m'm'	$1/2, 0, z [0, 0, w]$ $0, 1/2, \bar{z} [0, 0, w]$	$0, 1/2, z [0, 0, w]$ $1/2, 0, \bar{z} [0, 0, w]$	$1/2, 1/2, z [0, 0, w]$ $1/2, 1/2, \bar{z} [0, 0, w]$	
4	h	3m'	$1/3, 2/3, z [0, 0, w]$	$2/3, 1/3, z [0, 0, w]$	$2/3, 1/3, \bar{z} [0, 0, w]$	$1/3, 2/3, \bar{z} [0, 0, w]$
3	g	mm'm'	$1/2, 0, 1/2 [0, 0, w]$	$0, 1/2, 1/2 [0, 0, w]$	$1/2, 1/2, 1/2 [0, 0, w]$	
3	f	mm'm'	$1/2, 0, 0 [0, 0, w]$	$0, 1/2, 0 [0, 0, w]$	$1/2, 1/2, 0 [0, 0, w]$	
2	e	6m'm'	$0, 0, z [0, 0, w]$	$0, 0, \bar{z} [0, 0, w]$		
2	d	$\bar{6}m'2'$	$1/3, 2/3, 1/2 [0, 0, w]$	$2/3, 1/3, 1/2 [0, 0, w]$		
2	c	$\bar{6}m'2'$	$1/3, 2/3, 0 [0, 0, w]$	$2/3, 1/3, 0 [0, 0, w]$		
1	b	6/mm'm'	$0, 0, 1/2 [0, 0, w]$			
1	a	6/mm'm'	$0, 0, 0 [0, 0, w]$			

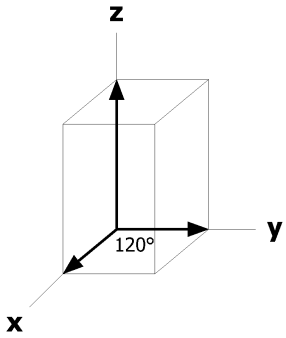


**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,0,0]$   $p2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at  $x,0,0$

Along  $[2,1,0]$   $p2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $x,x/2,0$



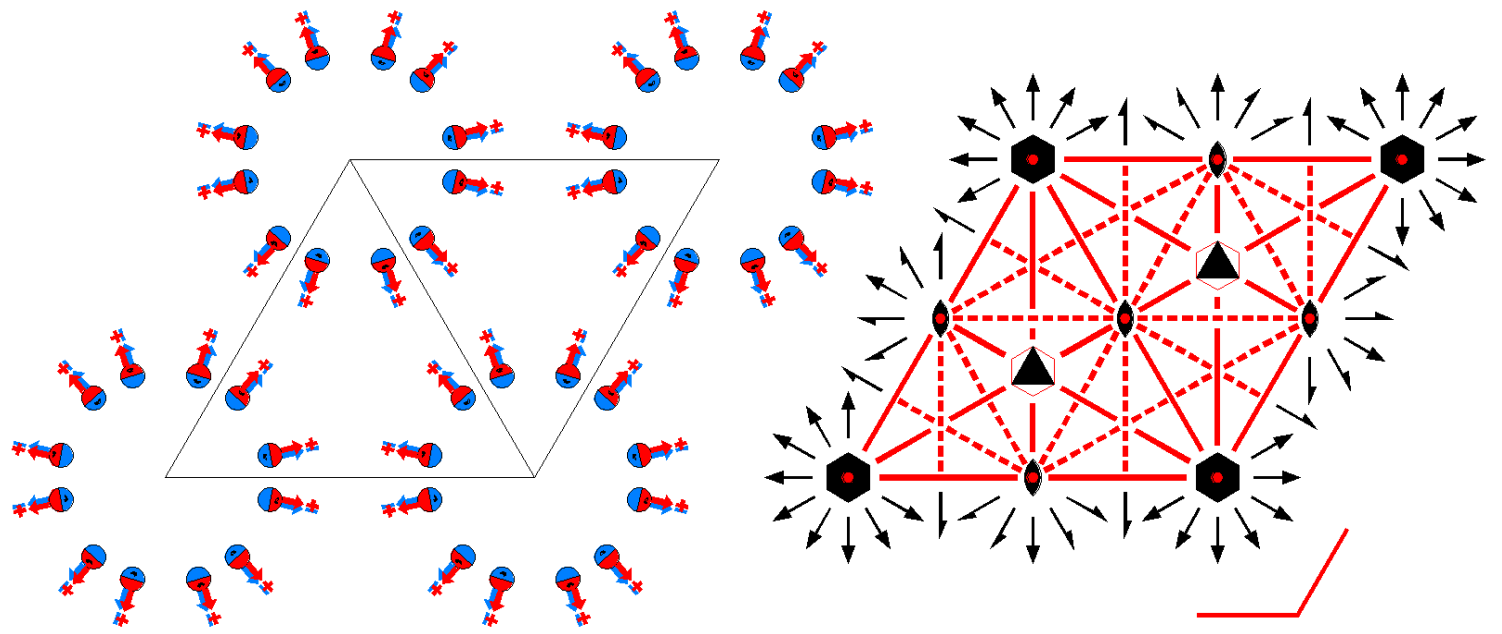
P6/m'm'm'

191.9.1471

6/m'm'm'

P6/m'2/m'2/m'

Hexagonal



Origin at center (6/m'm'm')

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/3;$	$0 \leq z \leq 1/2;$	$x \leq (1+y)/2;$	$y \leq x/2$
Vertices	0,0,0 0,0,1/2	1/2,0,0 1/2,0,1/2	2/3,1/3,0 2/3,1/3,1/2		

**Symmetry Operations**

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                                | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)            | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)           | (8) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)                            | (9) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)                            |
| (10) 2 x, $\bar{x}$ ,0<br>(2 <sub>3</sub>  0,0,0) | (11) 2 x,2x,0<br>(2 <sub>2</sub>  0,0,0)                          | (12) 2 2x,x,0<br>(2 <sub>1</sub>  0,0,0)                          |

(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ ' 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(15) $\bar{3}^-$ ' 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(16) $m'$ x,y,0 ( $m_z$  0,0,0)'	(17) $\bar{6}^-$ ' 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,0)'	(18) $\bar{6}^+$ ' 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,0)'
(19) $m'$ x, $\bar{x}$ ,z ( $m_{xy}$  0,0,0)'	(20) $m'$ x,2x,z ( $m_x$  0,0,0)'	(21) $m'$ 2x,x,z ( $m_y$  0,0,0)'
(22) $m'$ x,x,z ( $m_3$  0,0,0)'	(23) $m'$ x,0,z ( $m_2$  0,0,0)'	(24) $m'$ 0,y,z ( $m_1$  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	r	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y$ , $\bar{x}$ ,z [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w]	(5) y, $\bar{x}+y$ ,z [v, $\bar{u}+v$ ,w]	(6) x-y,x,z [u-v,u,w]
			(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y}$ , $\bar{z}$ [u-v, $\bar{v}$ , $\bar{w}$ ]	(9) $\bar{x}$ , $\bar{x}+y$ , $\bar{z}$ [ $\bar{u}$ , $\bar{u}+v$ , $\bar{w}$ ]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(11) $\bar{x}+y$ ,y, $\bar{z}$ [ $\bar{u}+v$ ,v, $\bar{w}$ ]	(12) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(14) y, $\bar{x}+y$ , $\bar{z}$ [v, $\bar{u}+v$ , $\bar{w}$ ]	(15) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ]
			(16) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(17) $\bar{y}$ ,x-y, $\bar{z}$ [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(18) $\bar{x}+y$ , $\bar{x}$ , $\bar{z}$ [ $\bar{u}+v$ , $\bar{u}$ , $\bar{w}$ ]
			(19) $\bar{y}$ , $\bar{x}$ ,z [ $\bar{v}$ , $\bar{u}$ ,w]	(20) $\bar{x}+y$ ,y,z [ $\bar{u}+v$ ,v,w]	(21) x,x-y,z [u,u-v,w]
			(22) y,x,z [v,u,w]	(23) x-y, $\bar{y}$ ,z [u-v, $\bar{v}$ ,w]	(24) $\bar{x}$ , $\bar{x}+y$ ,z [ $\bar{u}$ , $\bar{u}+v$ ,w]
12	q	m'..	x,y,1/2 [u,v,0]	$\bar{y}$ ,x-y,1/2 [ $\bar{v}$ ,u-v,0]	$\bar{x}+y$ , $\bar{x}$ ,1/2 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			$\bar{x}$ , $\bar{y}$ ,1/2 [ $\bar{u}$ , $\bar{v}$ ,0]	y, $\bar{x}+y$ ,1/2 [v, $\bar{u}+v$ ,0]	x-y,x,1/2 [u-v,u,0]
			y,x,1/2 [v,u,0]	x-y, $\bar{y}$ ,1/2 [u-v, $\bar{v}$ ,0]	$\bar{x}$ , $\bar{x}+y$ ,1/2 [ $\bar{u}$ , $\bar{u}+v$ ,0]
			$\bar{y}$ , $\bar{x}$ ,1/2 [ $\bar{v}$ , $\bar{u}$ ,0]	$\bar{x}+y$ ,y,1/2 [ $\bar{u}+v$ ,v,0]	x,x-y,1/2 [u,u-v,0]
12	p	m'..	x,y,0 [u,v,0]	$\bar{y}$ ,x-y,0 [ $\bar{v}$ ,u-v,0]	$\bar{x}+y$ , $\bar{x}$ ,0 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			$\bar{x}$ , $\bar{y}$ ,0 [ $\bar{u}$ , $\bar{v}$ ,0]	y, $\bar{x}+y$ ,0 [v, $\bar{u}+v$ ,0]	x-y,x,0 [u-v,u,0]
			y,x,0 [v,u,0]	x-y, $\bar{y}$ ,0 [u-v, $\bar{v}$ ,0]	$\bar{x}$ , $\bar{x}+y$ ,0 [ $\bar{u}$ , $\bar{u}+v$ ,0]
			$\bar{y}$ , $\bar{x}$ ,0 [ $\bar{v}$ , $\bar{u}$ ,0]	$\bar{x}+y$ ,y,0 [ $\bar{u}+v$ ,v,0]	x,x-y,0 [u,u-v,0]

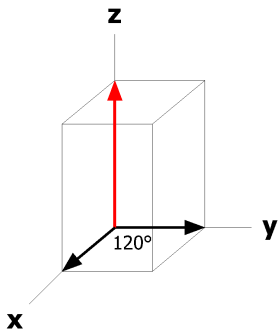
12	o	.m'	$x, 2x, z [u, 2u, w]$ $\bar{x}, 2\bar{x}, z [\bar{u}, 2\bar{u}, w]$ $2x, x, \bar{z} [2u, u, \bar{w}]$ $2\bar{x}, \bar{x}, \bar{z} [2\bar{u}, \bar{u}, \bar{w}]$	$2\bar{x}, \bar{x}, z [2\bar{u}, \bar{u}, w]$ $2x, x, z [2u, u, w]$ $\bar{x}, 2\bar{x}, \bar{z} [\bar{u}, 2\bar{u}, \bar{w}]$ $x, 2x, \bar{z} [u, 2u, \bar{w}]$	$x, \bar{x}, z [u, \bar{u}, w]$ $\bar{x}, x, z [\bar{u}, u, w]$ $\bar{x}, x, \bar{z} [\bar{u}, u, \bar{w}]$ $x, \bar{x}, \bar{z} [u, \bar{u}, \bar{w}]$
12	n	..m'	$x, 0, z [u, 0, w]$ $\bar{x}, 0, z [\bar{u}, 0, w]$ $0, x, \bar{z} [0, u, \bar{w}]$ $0, \bar{x}, \bar{z} [0, \bar{u}, \bar{w}]$	$0, x, z [0, u, w]$ $0, \bar{x}, z [0, \bar{u}, w]$ $x, 0, \bar{z} [u, 0, \bar{w}]$ $\bar{x}, 0, \bar{z} [\bar{u}, 0, \bar{w}]$	$\bar{x}, \bar{x}, z [\bar{u}, \bar{u}, w]$ $x, x, z [u, u, w]$ $\bar{x}, x, \bar{z} [\bar{u}, u, \bar{w}]$ $x, x, \bar{z} [u, u, \bar{w}]$
6	m	m'm'2	$x, 2x, 1/2 [u, 2u, 0]$ $\bar{x}, 2\bar{x}, 1/2 [\bar{u}, 2\bar{u}, 0]$	$2\bar{x}, \bar{x}, 1/2 [2\bar{u}, \bar{u}, 0]$ $2x, x, 1/2 [2u, u, 0]$	$x, \bar{x}, 1/2 [u, \bar{u}, 0]$ $\bar{x}, x, 1/2 [\bar{u}, u, 0]$
6	l	m'm'2	$x, 2x, 0 [u, 2u, 0]$ $\bar{x}, 2\bar{x}, 0 [\bar{u}, 2\bar{u}, 0]$	$2\bar{x}, \bar{x}, 0 [2\bar{u}, \bar{u}, 0]$ $2x, x, 0 [2u, u, 0]$	$x, \bar{x}, 0 [u, \bar{u}, 0]$ $\bar{x}, x, 0 [\bar{u}, u, 0]$
6	k	m'2m'	$x, 0, 1/2 [u, 0, 0]$ $\bar{x}, 0, 1/2 [\bar{u}, 0, 0]$	$0, x, 1/2 [0, u, 0]$ $0, \bar{x}, 1/2 [0, \bar{u}, 0]$	$\bar{x}, \bar{x}, 1/2 [\bar{u}, \bar{u}, 0]$ $x, x, 1/2 [u, u, 0]$
6	j	m'2m'	$x, 0, 0 [u, 0, 0]$ $\bar{x}, 0, 0 [\bar{u}, 0, 0]$	$0, x, 0 [0, u, 0]$ $0, \bar{x}, 0 [0, \bar{u}, 0]$	$\bar{x}, \bar{x}, 0 [\bar{u}, \bar{u}, 0]$ $x, x, 0 [u, u, 0]$
6	i	2m'm'	$1/2, 0, z [0, 0, w]$ $0, 1/2, \bar{z} [0, 0, \bar{w}]$	$0, 1/2, z [0, 0, w]$ $1/2, 0, \bar{z} [0, 0, \bar{w}]$	$1/2, 1/2, z [0, 0, w]$ $1/2, 1/2, \bar{z} [0, 0, \bar{w}]$
4	h	3m'	$1/3, 2/3, z [0, 0, w]$	$2/3, 1/3, z [0, 0, w]$ $2/3, 1/3, \bar{z} [0, 0, \bar{w}]$	$1/3, 2/3, \bar{z} [0, 0, \bar{w}]$
3	g	m'm'm'	$1/2, 0, 1/2 [0, 0, 0]$	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 1/2, 1/2 [0, 0, 0]$
3	f	m'm'm'	$1/2, 0, 0 [0, 0, 0]$	$0, 1/2, 0 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$
2	e	6m'm'	$0, 0, z [0, 0, w]$	$0, 0, \bar{z} [0, 0, \bar{w}]$	
2	d	$\bar{6}'m'2$	$1/3, 2/3, 1/2 [0, 0, 0]$	$2/3, 1/3, 1/2 [0, 0, 0]$	
2	c	$\bar{6}'m'2$	$1/3, 2/3, 0 [0, 0, 0]$	$2/3, 1/3, 0 [0, 0, 0]$	
1	b	6/m'm'm'	$0, 0, 1/2 [0, 0, 0]$		
1	a	6/m'm'm'	$0, 0, 0 [0, 0, 0]$		

**Symmetry of Special Projections**

Along [0,0,1]  $p6m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,0

Along [2,1,0]  $p2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,x/2,0



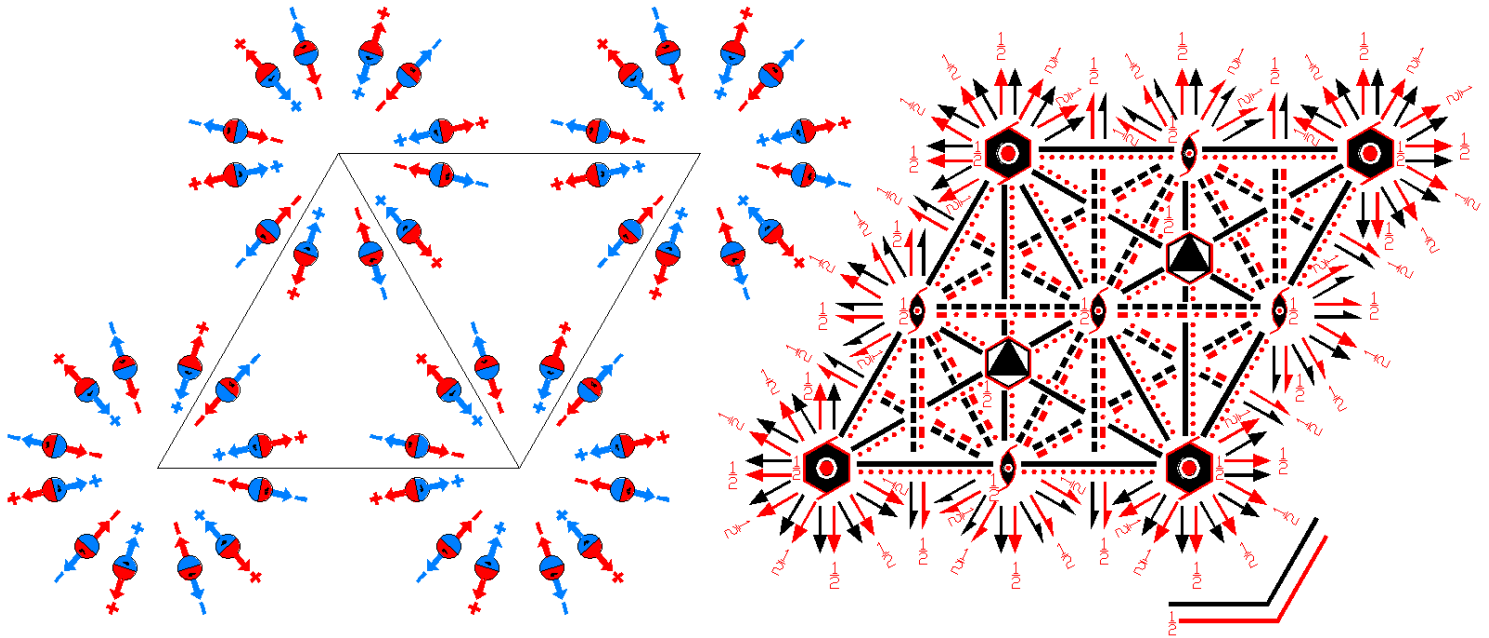
$P_{2c} 6/mmm$

191.10.1472

$6/mmm1'$

$P_{2c} 6/m2/m2/m$

Hexagonal



Origin at center ( $6/mmm$ )

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/3$ ;  $0 \leq z \leq 1/2$ ;  $x \leq (1+y)/2$ ;  $y \leq x/2$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2

### Symmetry Operations

For (0,0,0) + set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                        | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)      | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) 2 0,0,z<br>( $2_z$  0,0,0)            | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0) | (6) $6^+$ 0,0,z<br>( $6_z$  0,0,0)      |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0)         | (8) 2 x,0,0<br>( $2_x$  0,0,0)          | (9) 2 0,y,0<br>( $2_y$  0,0,0)          |
| (10) 2 $x, \bar{x}, 0$<br>( $2_3$  0,0,0) | (11) 2 x,2x,0<br>( $2_2$  0,0,0)        | (12) 2 2x,x,0<br>( $2_1$  0,0,0)        |

- |  |   |   |
|--|---|---|
| (13) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)      | (14) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)      | (15) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (16) m x,y,0<br>( $m_z$  0,0,0)                  | (17) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (18) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0)      |
| (19) m $\bar{x},\bar{x},z$<br>( $m_{xy}$  0,0,0) | (20) m x,2x,z<br>( $m_x$  0,0,0)                            | (21) m 2x,x,z<br>( $m_y$  0,0,0)                            |
| (22) m x,x,z<br>( $m_3$  0,0,0)                  | (23) m x,0,z<br>( $m_2$  0,0,0)                             | (24) m 0,y,z<br>( $m_1$  0,0,0)                             |

For (0,0,1)' + set

- |  |  |  |
|--|--|--|
| (1) t' (0,0,1)<br>( $\bar{1}$  0,0,1)'                 | (2) $3^+$ ' (0,0,1) 0,0,z<br>( $3_z$  0,0,1)'                    | (3) $3^-$ ' (0,0,1) 0,0,z<br>( $3_z^{-1}$  0,0,1)'               |
| (4) $2'$ (0,0,1) 0,0,z<br>( $2_z$  0,0,1)'             | (5) $6^-$ ' (0,0,1) 0,0,z<br>( $6_z^{-1}$  0,0,1)'               | (6) $6^+$ ' (0,0,1) 0,0,z<br>( $6_z$  0,0,1)'                    |
| (7) $2'$ x,x,1/2<br>( $2_{xy}$  0,0,1)'                | (8) $2'$ x,0,1/2<br>( $2_x$  0,0,1)'                             | (9) $2'$ 0,y,1/2<br>( $2_y$  0,0,1)'                             |
| (10) $2'$ x, $\bar{x}$ ,1/2<br>( $2_3$  0,0,1)'        | (11) $2'$ x,2x,1/2<br>( $2_2$  0,0,1)'                           | (12) $2'$ 2x,x,1/2<br>( $2_1$  0,0,1)'                           |
| (13) $\bar{1}'$ 0,0,1/2<br>( $\bar{1}$  0,0,1)'        | (14) $\bar{3}^+$ ' 0,0,z; 0,0,1/2<br>( $\bar{3}_z$  0,0,1)'      | (15) $\bar{3}^-$ ' 0,0,z; 0,0,1/2<br>( $\bar{3}_z^{-1}$  0,0,1)' |
| (16) m' x,y,1/2<br>( $m_z$  0,0,1)'                    | (17) $\bar{6}^-$ ' 0,0,z; 0,0,1/2<br>( $\bar{6}_z^{-1}$  0,0,1)' | (18) $\bar{6}^+$ ' 0,0,z; 0,0,1/2<br>( $\bar{6}_z$  0,0,1)'      |
| (19) c' (0,0,1) x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,1)' | (20) c' (0,0,1) x,2x,z<br>( $m_x$  0,0,1)'                       | (21) c' (0,0,1) 2x,x,z<br>( $m_y$  0,0,1)'                       |
| (22) c' (0,0,1) x,x,z<br>( $m_3$  0,0,1)'              | (23) c' (0,0,1) x,0,z<br>( $m_2$  0,0,1)'                        | (24) c' (0,0,1) 0,y,z<br>( $m_1$  0,0,1)'                        |

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7); (13).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

			(0,0,0) +	(0,0,1)' +	
48	r	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(5) $y,\bar{x}+y,z$ [ $v,\bar{u}+v,w$ ]	(6) x-y,x,z [u-v,u,w]
			(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y},\bar{z}$ [u-v, $\bar{v},\bar{w}$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
			(10) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(11) $\bar{x}+y,y,\bar{z}$ [ $\bar{u}+v,v,\bar{w}$ ]	(12) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ]

			(13) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(14) $y, \bar{x} + y, \bar{z}$ [ $\bar{v}, u - v, w$ ]	(15) $x - y, x, \bar{z}$ [ $\bar{u} + v, \bar{u}, w$ ]
			(16) $x, y, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(17) $\bar{y}, x - y, \bar{z}$ [ $v, \bar{u} + v, w$ ]	(18) $\bar{x} + y, \bar{x}, \bar{z}$ [u-v,u,w]
			(19) $\bar{y}, \bar{x}, z$ [v,u, $\bar{w}$ ]	(20) $\bar{x} + y, y, z$ [u-v, $\bar{v}, \bar{w}$ ]	(21) $x, x - y, z$ [ $\bar{u}, \bar{u} + v, \bar{w}$ ]
			(22) $y, x, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(23) $x - y, \bar{y}, z$ [ $\bar{u} + v, v, \bar{w}$ ]	(24) $\bar{x}, \bar{x} + y, z$ [u,u-v, $\bar{w}$ ]
24	q	m'..	$x, y, 1/2$ [u,v,0]	$\bar{y}, x - y, 1/2$ [ $\bar{v}, u - v, 0$ ]	$\bar{x} + y, \bar{x}, 1/2$ [ $\bar{u} + v, \bar{u}, 0$ ]
			$\bar{x}, \bar{y}, 1/2$ [ $\bar{u}, \bar{v}, 0$ ]	$y, \bar{x} + y, 1/2$ [ $v, \bar{u} + v, 0$ ]	$x - y, x, 1/2$ [u-v,u,0]
			$y, x, 1/2$ [ $\bar{v}, \bar{u}, 0$ ]	$x - y, \bar{y}, 1/2$ [ $\bar{u} + v, v, 0$ ]	$\bar{x}, \bar{x} + y, 1/2$ [u,u-v,0]
			$\bar{y}, \bar{x}, 1/2$ [v,u,0]	$\bar{x} + y, y, 1/2$ [u-v, $\bar{v}, 0$ ]	$x, x - y, 1/2$ [ $\bar{u}, \bar{u} + v, 0$ ]
24	p	m..	$x, y, 0$ [0,0,w]	$\bar{y}, x - y, 0$ [0,0,w]	$\bar{x} + y, \bar{x}, 0$ [0,0,w]
			$\bar{x}, \bar{y}, 0$ [0,0,w]	$y, \bar{x} + y, 0$ [0,0,w]	$x - y, x, 0$ [0,0,w]
			$y, x, 0$ [0,0, $\bar{w}$ ]	$x - y, \bar{y}, 0$ [0,0, $\bar{w}$ ]	$\bar{x}, \bar{x} + y, 0$ [0,0, $\bar{w}$ ]
			$\bar{y}, \bar{x}, 0$ [0,0, $\bar{w}$ ]	$\bar{x} + y, y, 0$ [0,0, $\bar{w}$ ]	$x, x - y, 0$ [0,0, $\bar{w}$ ]
24	o	.m.	$x, 2x, z$ [u,0,0]	$2\bar{x}, \bar{x}, z$ [0,u,0]	$x, \bar{x}, z$ [ $\bar{u}, \bar{u}, 0$ ]
			$\bar{x}, 2\bar{x}, z$ [ $\bar{u}, 0, 0$ ]	$2x, x, z$ [0, $\bar{u}, 0$ ]	$\bar{x}, x, z$ [u,u,0]
			$2x, x, \bar{z}$ [0, $\bar{u}, 0$ ]	$\bar{x}, 2\bar{x}, \bar{z}$ [ $\bar{u}, 0, 0$ ]	$\bar{x}, x, \bar{z}$ [u,u,0]
			$2\bar{x}, \bar{x}, \bar{z}$ [u,0,0]	$x, 2x, \bar{z}$ [0,u,0]	$x, \bar{x}, \bar{z}$ [ $\bar{u}, \bar{u}, 0$ ]
24	n	..m	$x, 0, z$ [u,2u,0]	$0, x, z$ [2 $\bar{u}, \bar{u}, 0$ ]	$\bar{x}, \bar{x}, z$ [u, $\bar{u}, 0$ ]
			$\bar{x}, 0, z$ [ $\bar{u}, 2\bar{u}, 0$ ]	$0, \bar{x}, z$ [2u,u,0]	$x, x, z$ [ $\bar{u}, u, 0$ ]
			$0, x, \bar{z}$ [2u,u,0]	$x, 0, \bar{z}$ [ $\bar{u}, 2\bar{u}, 0$ ]	$\bar{x}, \bar{x}, \bar{z}$ [ $\bar{u}, u, 0$ ]
			$0, \bar{x}, \bar{z}$ [2 $\bar{u}, \bar{u}, 0$ ]	$\bar{x}, 0, \bar{z}$ [u,2u,0]	$x, x, \bar{z}$ [u, $\bar{u}, 0$ ]
12	m	m'm2'	$x, 2x, 1/2$ [u,0,0]	$2\bar{x}, \bar{x}, 1/2$ [0,u,0]	$x, \bar{x}, 1/2$ [ $\bar{u}, \bar{u}, 0$ ]
			$\bar{x}, 2\bar{x}, 1/2$ [ $\bar{u}, 0, 0$ ]	$2x, x, 1/2$ [0, $\bar{u}, 0$ ]	$\bar{x}, x, 1/2$ [u,u,0]
12	l	mm2	$x, 2x, 0$ [0,0,0]	$2\bar{x}, \bar{x}, 0$ [0,0,0]	$x, \bar{x}, 0$ [0,0,0]
			$\bar{x}, 2\bar{x}, 0$ [0,0,0]	$2x, x, 0$ [0,0,0]	$\bar{x}, x, 0$ [0,0,0]
12	k	m'2'm	$x, 0, 1/2$ [u,2u,0]	$0, x, 1/2$ [2 $\bar{u}, \bar{u}, 0$ ]	$\bar{x}, \bar{x}, 1/2$ [u, $\bar{u}, 0$ ]
			$\bar{x}, 0, 1/2$ [ $\bar{u}, 2\bar{u}, 0$ ]	$0, \bar{x}, 1/2$ [2u,u,0]	$x, x, 1/2$ [ $\bar{u}, u, 0$ ]
12	j	m2m	$x, 0, 0$ [0,0,0]	$0, x, 0$ [0,0,0]	$\bar{x}, \bar{x}, 0$ [0,0,0]
			$\bar{x}, 0, 0$ [0,0,0]	$0, \bar{x}, 0$ [0,0,0]	$x, x, 0$ [0,0,0]



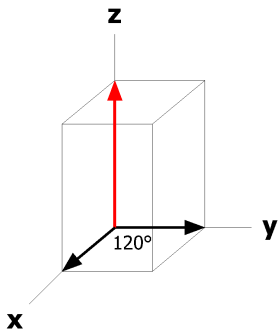
12	i	2mm	1/2,0,z [0,0,0] 0,1/2, $\bar{z}$ [0,0,0]	0,1/2,z [0,0,0] 1/2,0, $\bar{z}$ [0,0,0]	1/2,1/2,z [0,0,0] 1/2,1/2, $\bar{z}$ [0,0,0]	
8	h	3m.	1/3,2/3,z [0,0,0]	2/3,1/3,z [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	1/3,2/3, $\bar{z}$ [0,0,0]
6	g	m'mm	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
6	f	mmm	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
4	e	6mm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4	d	$\bar{6}$ 'm2'	1/3,2/3,1/2 [0,0,0]	2/3,1/3,1/2 [0,0,0]		
4	c	$\bar{6}$ m2	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]		
2	b	6/m'mm	0,0,1/2 [0,0,0]			
2	a	6/mmm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



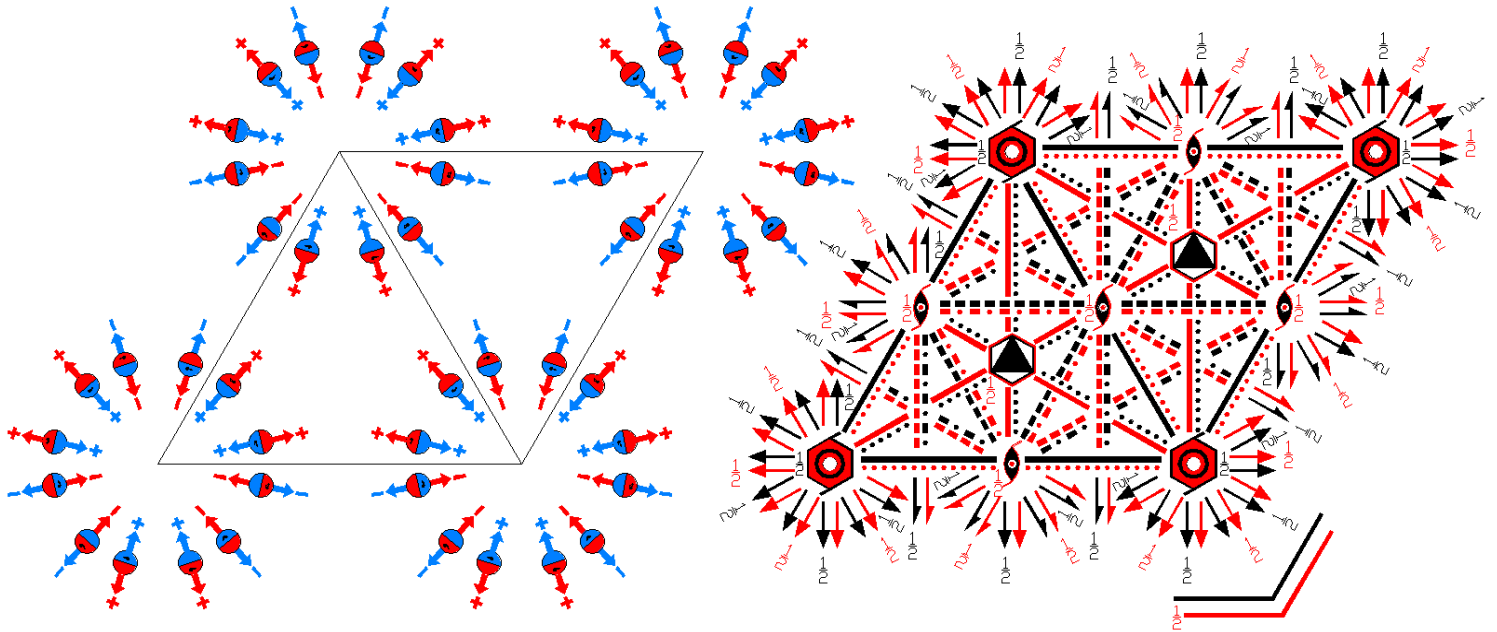
$P_{2c} 6'/mm'm$

191.11.1473

$6/mmm1'$

$P_{2c} 6'/m2/m'2'/m$

Hexagonal



Origin at center ( $6'/mm'm$ )

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/3$ ;  $0 \leq z \leq 1/2$ ;  $x \leq (1+y)/2$ ;  $y \leq x/2$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2

### Symmetry Operations

For (0,0,0) + set

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                            | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)       | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) $2'$ 0,0,z<br>( $2_z$  0,0,0)'            | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0)' | (6) $6^{+}$ 0,0,z<br>( $6_z$  0,0,0)'   |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0)             | (8) 2 x,0,0<br>( $2_x$  0,0,0)           | (9) 2 0,y,0<br>( $2_y$  0,0,0)          |
| (10) $2'$ x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)' | (11) $2'$ x,2x,0<br>( $2_2$  0,0,0)'     | (12) $2'$ 2x,x,0<br>( $2_1$  0,0,0)'    |

- |  |   |  |
|--|---|--|
| (13) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)'         | (14) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)'     | (15) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)' |
| (16) m x,y,0<br>(m <sub>z</sub>  0,0,0)              | (17) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,0) | (18) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,0)       |
| (19) m' x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)' | (20) m' x,2x,z<br>(m <sub>x</sub>  0,0,0)'                  | (21) m' 2x,x,z<br>(m <sub>y</sub>  0,0,0)'                   |
| (22) m x,x,z<br>(m <sub>3</sub>  0,0,0)              | (23) m x,0,z<br>(m <sub>2</sub>  0,0,0)                     | (24) m 0,y,z<br>(m <sub>1</sub>  0,0,0)                      |

For (0,0,1)' + set

- |  |  |   |
|--|--|---|
| (1) t' (0,0,1)<br>( $\bar{1}$  0,0,1)'                     | (2) $3^+$ (0,0,1) 0,0,z<br>( $3_z$  0,0,1)'                    | (3) $3^-$ (0,0,1) 0,0,z<br>( $3_z^{-1}$  0,0,1)'              |
| (4) 2 (0,0,1) 0,0,z<br>(2 <sub>z</sub>  0,0,1)             | (5) $6^-$ (0,0,1) 0,0,z<br>( $6_z^{-1}$  0,0,1)                | (6) $6^+$ (0,0,1) 0,0,z<br>( $6_z$  0,0,1)                    |
| (7) 2' x,x,1/2<br>(2 <sub>xy</sub>  0,0,1)'                | (8) 2' x,0,1/2<br>(2 <sub>x</sub>  0,0,1)'                     | (9) 2' 0,y,1/2<br>(2 <sub>y</sub>  0,0,1)'                    |
| (10) 2 x, $\bar{x}$ ,1/2<br>(2 <sub>3</sub>  0,0,1)        | (11) 2 x,2x,1/2<br>(2 <sub>2</sub>  0,0,1)                     | (12) 2 2x,x,1/2<br>(2 <sub>1</sub>  0,0,1)                    |
| (13) $\bar{1}$ 0,0,1/2<br>( $\bar{1}$  0,0,1)              | (14) $\bar{3}^+$ 0,0,z; 0,0,1/2<br>( $\bar{3}_z$  0,0,1)       | (15) $\bar{3}^-$ 0,0,z; 0,0,1/2<br>( $\bar{3}_z^{-1}$  0,0,1) |
| (16) m' x,y,1/2<br>(m <sub>z</sub>  0,0,1)'                | (17) $\bar{6}^-$ 0,0,z; 0,0,1/2<br>( $\bar{6}_z^{-1}$  0,0,1)' | (18) $\bar{6}^+$ 0,0,z; 0,0,1/2<br>( $\bar{6}_z$  0,0,1)'     |
| (19) c (0,0,1) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,1) | (20) c (0,0,1) x,2x,z<br>(m <sub>x</sub>  0,0,1)               | (21) c (0,0,1) 2x,x,z<br>(m <sub>y</sub>  0,0,1)              |
| (22) c' (0,0,1) x,x,z<br>(m <sub>3</sub>  0,0,1)'          | (23) c' (0,0,1) x,0,z<br>(m <sub>2</sub>  0,0,1)'              | (24) c' (0,0,1) 0,y,z<br>(m <sub>1</sub>  0,0,1)'             |

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7); (13).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

			(0,0,0) +	(0,0,1)' +	
48	r	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(5) y, $\bar{x}+y,z$ [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) x-y,x,z [ $\bar{u}+v,\bar{u},\bar{w}$ ]
			(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y},\bar{z}$ [u-v, $\bar{v},\bar{w}$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
			(10) $\bar{y},\bar{x},\bar{z}$ [v,u,w]	(11) $\bar{x}+y,y,\bar{z}$ [u-v, $\bar{v},w$ ]	(12) x,x-y, $\bar{z}$ [ $\bar{u},\bar{u}+v,w$ ]

			(13) $\bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$	(14) $y, \bar{x} + y, \bar{z} [v, \bar{u} + v, \bar{w}]$	(15) $x - y, x, \bar{z} [u - v, u, \bar{w}]$
			(16) $x, y, \bar{z} [\bar{u}, \bar{v}, w]$	(17) $\bar{y}, x - y, \bar{z} [v, \bar{u} + v, w]$	(18) $\bar{x} + y, \bar{x}, \bar{z} [u - v, u, w]$
			(19) $\bar{y}, \bar{x}, z [\bar{v}, \bar{u}, w]$	(20) $\bar{x} + y, y, z [\bar{u} + v, v, w]$	(21) $x, x - y, z [u, u - v, w]$
			(22) $y, x, z [\bar{v}, \bar{u}, \bar{w}]$	(23) $x - y, \bar{y}, z [\bar{u} + v, v, \bar{w}]$	(24) $\bar{x}, \bar{x} + y, z [u, u - v, \bar{w}]$
24	q	m'..	$x, y, 1/2 [u, v, 0]$	$\bar{y}, x - y, 1/2 [\bar{v}, u - v, 0]$	$\bar{x} + y, \bar{x}, 1/2 [\bar{u} + v, \bar{u}, 0]$
			$\bar{x}, \bar{y}, 1/2 [u, v, 0]$	$y, \bar{x} + y, 1/2 [\bar{v}, u - v, 0]$	$x - y, x, 1/2 [\bar{u} + v, \bar{u}, 0]$
			$y, x, 1/2 [\bar{v}, \bar{u}, 0]$	$x - y, \bar{y}, 1/2 [\bar{u} + v, v, 0]$	$\bar{x}, \bar{x} + y, 1/2 [u, u - v, 0]$
			$\bar{y}, \bar{x}, 1/2 [\bar{v}, \bar{u}, 0]$	$\bar{x} + y, y, 1/2 [\bar{u} + v, v, 0]$	$x, x - y, 1/2 [u, u - v, 0]$
24	p	m..	$x, y, 0 [0, 0, w]$	$\bar{y}, x - y, 0 [0, 0, w]$	$\bar{x} + y, \bar{x}, 0 [u, u - v, 0]$
			$\bar{x}, \bar{y}, 0 [0, 0, \bar{w}]$	$y, \bar{x} + y, 0 [0, 0, \bar{w}]$	$x - y, x, 0 [0, 0, \bar{w}]$
			$y, x, 0 [0, 0, \bar{w}]$	$x - y, \bar{y}, 0 [0, 0, \bar{w}]$	$\bar{x}, \bar{x} + y, 0 [0, 0, \bar{w}]$
			$\bar{y}, \bar{x}, 0 [0, 0, w]$	$\bar{x} + y, y, 0 [0, 0, w]$	$x, x - y, 0 [0, 0, w]$
24	o	.m'.	$x, 2x, z [u, 2u, w]$	$2\bar{x}, \bar{x}, z [2\bar{u}, \bar{u}, w]$	$x, \bar{x}, z [u, \bar{u}, w]$
			$\bar{x}, 2\bar{x}, z [u, 2u, \bar{w}]$	$2x, x, z [2\bar{u}, \bar{u}, \bar{w}]$	$\bar{x}, x, z [u, \bar{u}, \bar{w}]$
			$2x, x, \bar{z} [2u, u, \bar{w}]$	$\bar{x}, 2\bar{x}, \bar{z} [\bar{u}, 2\bar{u}, \bar{w}]$	$\bar{x}, x, \bar{z} [\bar{u}, u, \bar{w}]$
			$2\bar{x}, \bar{x}, \bar{z} [2u, u, w]$	$x, 2x, \bar{z} [\bar{u}, 2\bar{u}, w]$	$x, \bar{x}, \bar{z} [\bar{u}, u, w]$
24	n	..m	$x, 0, z [u, 2u, 0]$	$0, x, z [2\bar{u}, \bar{u}, 0]$	$\bar{x}, \bar{x}, z [u, \bar{u}, 0]$
			$\bar{x}, 0, z [u, 2u, 0]$	$0, \bar{x}, z [2\bar{u}, \bar{u}, 0]$	$x, x, z [u, \bar{u}, 0]$
			$0, x, \bar{z} [2u, u, 0]$	$x, 0, \bar{z} [\bar{u}, 2\bar{u}, 0]$	$\bar{x}, \bar{x}, \bar{z} [\bar{u}, u, 0]$
			$0, \bar{x}, \bar{z} [2u, u, 0]$	$\bar{x}, 0, \bar{z} [\bar{u}, 2\bar{u}, 0]$	$x, x, \bar{z} [\bar{u}, u, 0]$
12	m	m'm'2	$x, 2x, 1/2 [u, 2u, 0]$	$2\bar{x}, \bar{x}, 1/2 [2\bar{u}, \bar{u}, 0]$	$x, \bar{x}, 1/2 [u, \bar{u}, 0]$
			$\bar{x}, 2\bar{x}, 1/2 [u, 2u, 0]$	$2x, x, 1/2 [2\bar{u}, \bar{u}, 0]$	$\bar{x}, x, 1/2 [u, \bar{u}, 0]$
12	l	mm'2'	$x, 2x, 0 [0, 0, w]$	$2\bar{x}, \bar{x}, 0 [0, 0, w]$	$x, \bar{x}, 0 [0, 0, w]$
			$\bar{x}, 2\bar{x}, 0 [0, 0, \bar{w}]$	$2x, x, 0 [0, 0, \bar{w}]$	$\bar{x}, x, 0 [0, 0, \bar{w}]$
12	k	m'2'm	$x, 0, 1/2 [u, 2u, 0]$	$0, x, 1/2 [2\bar{u}, \bar{u}, 0]$	$\bar{x}, \bar{x}, 1/2 [u, \bar{u}, 0]$
			$\bar{x}, 0, 1/2 [u, 2u, 0]$	$0, \bar{x}, 1/2 [2\bar{u}, \bar{u}, 0]$	$x, x, 1/2 [u, \bar{u}, 0]$
12	j	m2m	$x, 0, 0 [0, 0, 0]$	$0, x, 0 [0, 0, 0]$	$\bar{x}, \bar{x}, 0 [0, 0, 0]$
			$\bar{x}, 0, 0 [0, 0, 0]$	$0, \bar{x}, 0 [0, 0, 0]$	$x, x, 0 [0, 0, 0]$

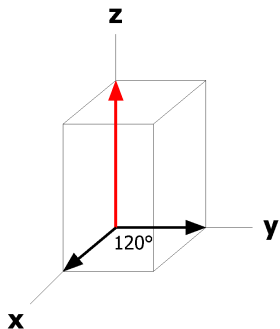
12	i	2'm'm	1/2,0,z [u,2u,0]	0,1/2,z [2 $\bar{u}$ , $\bar{u}$ ,0]	1/2,1/2,z [u, $\bar{u}$ ,0]	
			0,1/2, $\bar{z}$ [u,2u,0]	1/2,0, $\bar{z}$ [2 $\bar{u}$ , $\bar{u}$ ,0]	1/2,1/2, $\bar{z}$ [u, $\bar{u}$ ,0]	
8	h	3m'	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	1/3,2/3, $\bar{z}$ [0,0,w]
6	g	m'm'm	1/2,0,1/2 [u,2u,0]	0,1/2,1/2 [2 $\bar{u}$ , $\bar{u}$ ,0]	1/2,1/2,1/2 [u, $\bar{u}$ ,0]	
6	f	mm'm	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
4	e	6'm'm	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4	d	$\bar{6}$ 'm'2	1/3,2/3,1/2 [0,0,0]	2/3,1/3,1/2 [0,0,0]		
4	c	$\bar{6}$ 'm'2'	1/3,2/3,0 [0,0,w]	2/3,1/3,0 [0,0, $\bar{w}$ ]		
2	b	6'/m'm'm	0,0,1/2 [0,0,0]			
2	a	6'/mm'm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



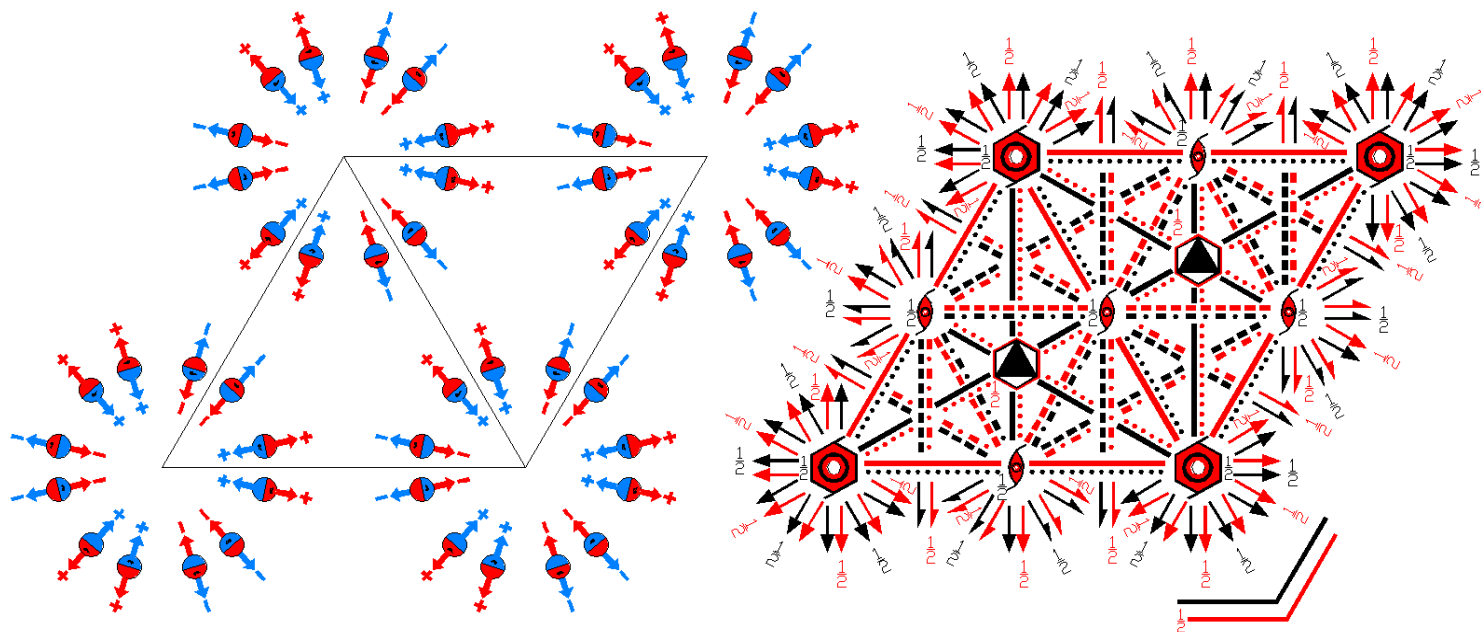
$P_{2c} 6'/mmm'$

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$6/mmm1'$

$P_{2c} 6'/m2'/m2/m'$

Hexagonal



Origin at center ( $6'/mmm'$ )

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/3$ ;  $0 \leq z \leq 1/2$ ;  $x \leq (1+y)/2$ ;  $y \leq x/2$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0
	0,0,1/2	1/2,0,1/2	2/3,1/3,1/2

### Symmetry Operations

For (0,0,0) + set

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                        | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)       | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) $2'$ 0,0,z<br>( $2_z$  0,0,0)'        | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0)' | (6) $6^+$ 0,0,z<br>( $6_z$  0,0,0)'     |
| (7) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)'     | (8) $2'$ x,0,0<br>( $2_x$  0,0,0)'       | (9) $2'$ 0,y,0<br>( $2_y$  0,0,0)'      |
| (10) 2 $x, \bar{x}, 0$<br>( $2_3$  0,0,0) | (11) 2 x,2x,0<br>( $2_2$  0,0,0)         | (12) 2 2x,x,0<br>( $2_1$  0,0,0)        |

(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ ' 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(15) $\bar{3}^-$ ' 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(16) m x,y,0 (m <sub>z</sub>  0,0,0)	(17) $\bar{6}^-$ 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,0)	(18) $\bar{6}^+$ 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,0)
(19) m x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)	(20) m x,2x,z (m <sub>x</sub>  0,0,0)	(21) m 2x,x,z (m <sub>y</sub>  0,0,0)
(22) m' x,x,z (m <sub>3</sub>  0,0,0)'	(23) m' x,0,z (m <sub>2</sub>  0,0,0)'	(24) m' 0,y,z (m <sub>1</sub>  0,0,0)'
(1) t' (0,0,1) (1 0,0,1)'	(2) 3 <sup>+</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub>  0,0,1)'	(3) 3 <sup>-</sup> ' (0,0,1) 0,0,z (3 <sub>z</sub> <sup>-1</sup>  0,0,1)'
(4) 2 (0,0,1) 0,0,z (2 <sub>z</sub>  0,0,1)	(5) 6 <sup>-</sup> (0,0,1) 0,0,z (6 <sub>z</sub> <sup>-1</sup>  0,0,1)	(6) 6 <sup>+</sup> (0,0,1) 0,0,z (6 <sub>z</sub>  0,0,1)
(7) 2 x,x,1/2 (2 <sub>xy</sub>  0,0,1)	(8) 2 x,0,1/2 (2 <sub>x</sub>  0,0,1)	(9) 2 0,y,1/2 (2 <sub>y</sub>  0,0,1)
(10) 2' x, $\bar{x}$ ,1/2 (2 <sub>3</sub>  0,0,1)'	(11) 2' x,2x,1/2 (2 <sub>2</sub>  0,0,1)'	(12) 2' 2x,x,1/2 (2 <sub>1</sub>  0,0,1)'
(13) $\bar{1}$ 0,0,1/2 ( $\bar{1}$  0,0,1)	(14) $\bar{3}^+$ 0,0,z; 0,0,1/2 ( $\bar{3}_z$  0,0,1)	(15) $\bar{3}^-$ 0,0,z; 0,0,1/2 ( $\bar{3}_z^{-1}$  0,0,1)
(16) m' x,y,1/2 (m <sub>z</sub>  0,0,1)'	(17) $\bar{6}^-$ ' 0,0,z; 0,0,1/2 ( $\bar{6}_z^{-1}$  0,0,1)'	(18) $\bar{6}^+$ ' 0,0,z; 0,0,1/2 ( $\bar{6}_z$  0,0,1)'
(19) c' (0,0,1) x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,1)'	(20) c' (0,0,1) x,2x,z (m <sub>x</sub>  0,0,1)'	(21) c' (0,0,1) 2x,x,z (m <sub>y</sub>  0,0,1)'
(22) c (0,0,1) x,x,z (m <sub>3</sub>  0,0,1)	(23) c (0,0,1) x,0,z (m <sub>2</sub>  0,0,1)	(24) c (0,0,1) 0,y,z (m <sub>1</sub>  0,0,1)

**Generators selected** (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7); (13).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (0,0,1)' +

48	r	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z$ [u,v, $\bar{w}$ ]	(5) y, $\bar{x}+y,z$ [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) x-y,x,z [ $\bar{u}+v,\bar{u},\bar{w}$ ]
			(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) x-y, $\bar{y},\bar{z}$ [ $\bar{u}+v,v,w$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}$ [u,u-v,w]
			(10) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(11) $\bar{x}+y,y,\bar{z}$ [ $\bar{u}+v,v,\bar{w}$ ]	(12) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ]

			(13) $\bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$	(14) $y, \bar{x} + y, \bar{z} [v, \bar{u} + v, \bar{w}]$	(15) $x - y, x, \bar{z} [u - v, u, \bar{w}]$
			(16) $x, y, \bar{z} [\bar{u}, \bar{v}, w]$	(17) $\bar{y}, x - y, \bar{z} [v, \bar{u} + v, w]$	(18) $\bar{x} + y, \bar{x}, \bar{z} [u - v, u, w]$
			(19) $\bar{y}, \bar{x}, z [v, u, \bar{w}]$	(20) $\bar{x} + y, y, z [u - v, \bar{v}, \bar{w}]$	(21) $x, x - y, z [\bar{u}, \bar{u} + v, \bar{w}]$
			(22) $y, x, z [v, u, w]$	(23) $x - y, \bar{y}, z [u - v, \bar{v}, w]$	(24) $\bar{x}, \bar{x} + y, z [\bar{u}, \bar{u} + v, w]$
24	q	m'..	$x, y, 1/2 [u, v, 0]$	$\bar{y}, x - y, 1/2 [\bar{v}, u - v, 0]$	$\bar{x} + y, \bar{x}, 1/2 [\bar{u} + v, \bar{u}, 0]$
			$\bar{x}, \bar{y}, 1/2 [u, v, 0]$	$y, \bar{x} + y, 1/2 [\bar{v}, u - v, 0]$	$x - y, x, 1/2 [\bar{u} + v, \bar{u}, 0]$
			$y, x, 1/2 [v, u, 0]$	$x - y, \bar{y}, 1/2 [u - v, \bar{v}, 0]$	$\bar{x}, \bar{x} + y, 1/2 [\bar{u}, \bar{u} + v, 0]$
			$\bar{y}, \bar{x}, 1/2 [v, u, 0]$	$\bar{x} + y, y, 1/2 [u - v, \bar{v}, 0]$	$x, x - y, 1/2 [\bar{u}, \bar{u} + v, 0]$
24	p	m..	$x, y, 0 [0, 0, w]$	$\bar{y}, x - y, 0 [0, 0, w]$	$\bar{x} + y, \bar{x}, 0 [0, 0, w]$
			$\bar{x}, \bar{y}, 0 [0, 0, \bar{w}]$	$y, \bar{x} + y, 0 [0, 0, \bar{w}]$	$x - y, x, 0 [0, 0, \bar{w}]$
			$y, x, 0 [0, 0, w]$	$x - y, \bar{y}, 0 [0, 0, w]$	$\bar{x}, \bar{x} + y, 0 [0, 0, w]$
			$\bar{y}, \bar{x}, 0 [0, 0, \bar{w}]$	$\bar{x} + y, y, 0 [0, 0, \bar{w}]$	$x, x - y, 0 [0, 0, \bar{w}]$
24	o	.m.	$x, 2x, z [u, 0, 0]$	$2\bar{x}, \bar{x}, z [0, u, 0]$	$x, \bar{x}, z [\bar{u}, \bar{u}, 0]$
			$\bar{x}, 2\bar{x}, z [u, 0, 0]$	$2x, x, z [0, u, 0]$	$\bar{x}, x, z [\bar{u}, \bar{u}, 0]$
			$2x, x, \bar{z} [0, \bar{u}, 0]$	$\bar{x}, 2\bar{x}, \bar{z} [\bar{u}, 0, 0]$	$\bar{x}, x, \bar{z} [u, u, 0]$
			$2\bar{x}, \bar{x}, \bar{z} [0, \bar{u}, 0]$	$x, 2x, \bar{z} [\bar{u}, 0, 0]$	$x, \bar{x}, \bar{z} [u, u, 0]$
24	n	..m'	$x, 0, z [u, 0, w]$	$0, x, z [0, u, w]$	$\bar{x}, \bar{x}, z [\bar{u}, \bar{u}, w]$
			$\bar{x}, 0, z [u, 0, \bar{w}]$	$0, \bar{x}, z [0, u, \bar{w}]$	$x, x, z [\bar{u}, \bar{u}, \bar{w}]$
			$0, x, \bar{z} [0, \bar{u}, w]$	$x, 0, \bar{z} [\bar{u}, 0, w]$	$\bar{x}, \bar{x}, \bar{z} [u, u, w]$
			$0, \bar{x}, \bar{z} [0, \bar{u}, \bar{w}]$	$\bar{x}, 0, \bar{z} [\bar{u}, 0, \bar{w}]$	$x, x, \bar{z} [u, u, \bar{w}]$
12	m	mm2	$x, 2x, 1/2 [u, 0, 0]$	$2\bar{x}, \bar{x}, 1/2 [0, u, 0]$	$x, \bar{x}, 1/2 [\bar{u}, \bar{u}, 0]$
			$\bar{x}, 2\bar{x}, 1/2 [u, 0, 0]$	$2x, x, 1/2 [0, u, 0]$	$\bar{x}, x, 1/2 [\bar{u}, \bar{u}, 0]$
12	l	mm2	$x, 2x, 0 [0, 0, 0]$	$2\bar{x}, \bar{x}, 0 [0, 0, 0]$	$x, \bar{x}, 0 [0, 0, 0]$
			$\bar{x}, 2\bar{x}, 0 [0, 0, 0]$	$2x, x, 0 [0, 0, 0]$	$\bar{x}, x, 0 [0, 0, 0]$
12	k	m'2m'	$x, 0, 1/2 [u, 0, 0]$	$0, x, 1/2 [0, u, 0]$	$\bar{x}, \bar{x}, 1/2 [\bar{u}, \bar{u}, 0]$
			$\bar{x}, 0, 1/2 [u, 0, 0]$	$0, \bar{x}, 1/2 [0, u, 0]$	$x, x, 1/2 [\bar{u}, \bar{u}, 0]$
12	j	m2'm'	$x, 0, 0 [0, 0, w]$	$0, x, 0 [0, 0, w]$	$\bar{x}, \bar{x}, 0 [0, 0, w]$
			$\bar{x}, 0, 0 [0, 0, \bar{w}]$	$0, \bar{x}, 0 [0, 0, \bar{w}]$	$x, x, 0 [0, 0, \bar{w}]$



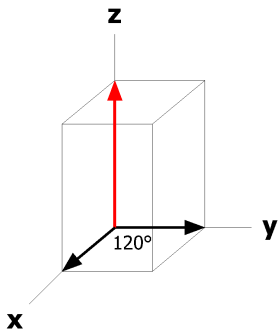
12	i	2'mm'	1/2,0,z [u,0,0]	0,1/2,z [0,u,0]	1/2,1/2,z [ $\bar{u},\bar{u},0$ ]	
			0,1/2, $\bar{z}$ [0, $\bar{u},0$ ]	1/2,0, $\bar{z}$ [ $\bar{u},0,0$ ]	1/2,1/2, $\bar{z}$ [u,u,0]	
8	h	3m.	1/3,2/3,z [0,0,0]	2/3,1/3,z [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	1/3,2/3, $\bar{z}$ [0,0,0]
6	g	m'mm'	1/2,0,1/2 [u,0,0]	0,1/2,1/2 [0,u,0]	1/2,1/2,1/2 [ $\bar{u},\bar{u},0$ ]	
6	f	mmm'	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
4	e	6'mm'	0,0,z [0,0,0]	0,0, $\bar{z}$ [0,0,0]		
4	d	$\bar{6}$ 'm2'	1/3,2/3,1/2 [0,0,0]	2/3,1/3,1/2 [0,0,0]		
4	c	$\bar{6}$ m2	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]		
2	b	6'/m'mm'	0,0,1/2 [0,0,0]			
2	a	6'/mmm'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p<sub>2a</sub>-2mm  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



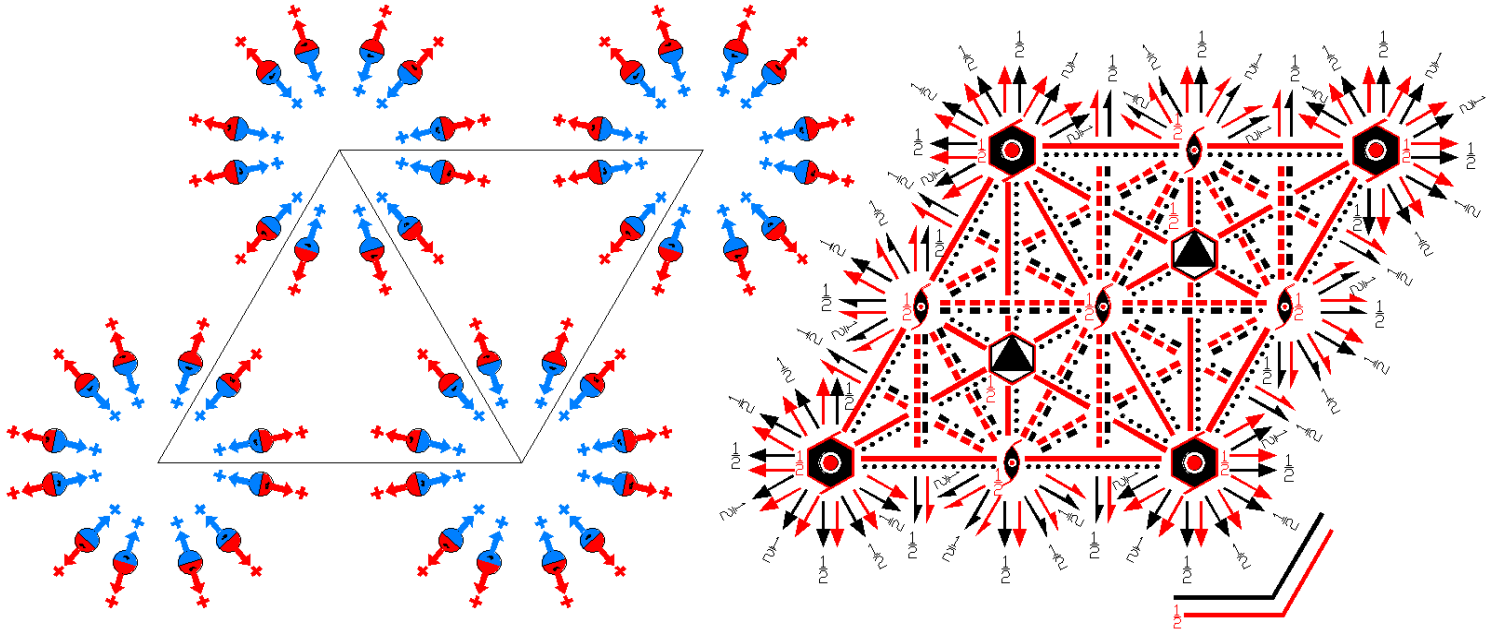
$P_{2c} 6/m\bar{m}'m'$

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$6/m\bar{m}m1'$

$P_{2c} 6/m2'/m'2'/m'$

Hexagonal



Origin at center ( $6/m\bar{m}'m'$ )

Asymmetric unit  $0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/3; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq x/2$

Vertices  $0,0,0 \quad 1/2,0,0 \quad 2/3,1/3,0$   
 $0,0,1/2 \quad 1/2,0,1/2 \quad 2/3,1/3,1/2$

### Symmetry Operations

For  $(0,0,0) +$  set

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)      | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) 2 0,0,z<br>( $2_z$  0,0,0)                | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0) | (6) $6^+$ 0,0,z<br>( $6_z$  0,0,0)      |
| (7) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)'         | (8) $2'$ x,0,0<br>( $2_x$  0,0,0)'      | (9) $2'$ 0,y,0<br>( $2_y$  0,0,0)'      |
| (10) $2'$ x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)' | (11) $2'$ x,2x,0<br>( $2_2$  0,0,0)'    | (12) $2'$ 2x,x,0<br>( $2_1$  0,0,0)'    |

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)
(16) m x,y,0 (m <sub>z</sub>  0,0,0)	(17) $\bar{6}^-$ 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,0)	(18) $\bar{6}^+$ 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,0)
(19) m' x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)'	(20) m' x,2x,z (m <sub>x</sub>  0,0,0)'	(21) m' 2x,x,z (m <sub>y</sub>  0,0,0)'
(22) m' x,x,z (m <sub>3</sub>  0,0,0)'	(23) m' x,0,z (m <sub>2</sub>  0,0,0)'	(24) m' 0,y,z (m <sub>1</sub>  0,0,0)'

For (0,0,1)' + set

(1) t' (0,0,1) ( $\bar{1}$  0,0,1)'	(2) $3^+$ ' (0,0,1) 0,0,z ( $3_z$  0,0,1)'	(3) $3^-$ ' (0,0,1) 0,0,z ( $3_z^{-1}$  0,0,1)'
(4) 2' (0,0,1) 0,0,z ( $2_z$  0,0,1)'	(5) $6^-$ ' (0,0,1) 0,0,z ( $6_z^{-1}$  0,0,1)'	(6) $6^+$ ' (0,0,1) 0,0,z ( $6_z$  0,0,1)'
(7) 2 x,x,1/2 ( $2_{xy}$  0,0,1)	(8) 2 x,0,1/2 ( $2_x$  0,0,1)	(9) 2 0,y,1/2 ( $2_y$  0,0,1)
(10) 2 x, $\bar{x}$ ,1/2 ( $2_3$  0,0,1)	(11) 2 x,2x,1/2 ( $2_2$  0,0,1)	(12) 2 2x,x,1/2 ( $2_1$  0,0,1)
(13) $\bar{1}$ ' 0,0,1/2 ( $\bar{1}$  0,0,1)'	(14) $\bar{3}^+$ ' 0,0,z; 0,0,1/2 ( $\bar{3}_z$  0,0,1)'	(15) $\bar{3}^-$ ' 0,0,z; 0,0,1/2 ( $\bar{3}_z^{-1}$  0,0,1)'
(16) m' x,y,1/2 (m <sub>z</sub>  0,0,1)'	(17) $\bar{6}^-$ ' 0,0,z; 0,0,1/2 ( $\bar{6}_z^{-1}$  0,0,1)'	(18) $\bar{6}^+$ ' 0,0,z; 0,0,1/2 ( $\bar{6}_z$  0,0,1)'
(19) c (0,0,1) x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,1)	(20) c (0,0,1) x,2x,z (m <sub>x</sub>  0,0,1)	(21) c (0,0,1) 2x,x,z (m <sub>y</sub>  0,0,1)
(22) c (0,0,1) x,x,z (m <sub>3</sub>  0,0,1)	(23) c (0,0,1) x,0,z (m <sub>2</sub>  0,0,1)	(24) c (0,0,1) 0,y,z (m <sub>1</sub>  0,0,1)

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7); (13).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

			(0,0,0) +	(0,0,1)' +	
48	r	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(5) y, $\bar{x}+y,z$ [ $v,\bar{u}+v,w$ ]	(6) x-y,x,z [u-v,u,w]
			(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) x-y, $\bar{y},\bar{z}$ [ $\bar{u}+v,v,w$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}$ [u,u-v,w]
			(10) $\bar{y},\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(11) $\bar{x}+y,y,\bar{z}$ [u-v, $\bar{v},w$ ]	(12) x,x-y, $\bar{z}$ [ $\bar{u},\bar{u}+v,w$ ]

			(13) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(14) $y, \bar{x} + y, \bar{z}$ [ $\bar{v}, u - v, w$ ]	(15) $x - y, x, \bar{z}$ [ $\bar{u} + v, \bar{u}, w$ ]
			(16) $x, y, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(17) $\bar{y}, x - y, \bar{z}$ [ $v, \bar{u} + v, w$ ]	(18) $\bar{x} + y, \bar{x}, \bar{z}$ [ $u - v, u, w$ ]
			(19) $\bar{y}, \bar{x}, z$ [ $\bar{v}, \bar{u}, w$ ]	(20) $\bar{x} + y, y, z$ [ $\bar{u} + v, v, w$ ]	(21) $x, x - y, z$ [ $\bar{u}, \bar{u} + v, \bar{w}$ ]
			(22) $y, x, z$ [v,u,w]	(23) $x - y, \bar{y}, z$ [ $u - v, \bar{v}, w$ ]	(24) $\bar{x}, \bar{x} + y, z$ [ $u, u - v, w$ ]
24	q	m'..	$x, y, 1/2$ [u,v,0]	$\bar{y}, x - y, 1/2$ [ $\bar{v}, u - v, 0$ ]	$\bar{x} + y, \bar{x}, 1/2$ [ $\bar{u} + v, \bar{u}, 0$ ]
			$\bar{x}, \bar{y}, 1/2$ [ $\bar{u}, \bar{v}, 0$ ]	$y, \bar{x} + y, 1/2$ [ $v, \bar{u} + v, 0$ ]	$x - y, x, 1/2$ [ $u - v, u, 0$ ]
			$y, x, 1/2$ [v,u,0]	$x - y, \bar{y}, 1/2$ [ $u - v, \bar{v}, 0$ ]	$\bar{x}, \bar{x} + y, 1/2$ [ $\bar{u}, \bar{u} + v, 0$ ]
			$\bar{y}, \bar{x}, 1/2$ [ $\bar{v}, \bar{u}, 0$ ]	$\bar{x} + y, y, 1/2$ [ $\bar{u} + v, v, 0$ ]	$x, x - y, 1/2$ [ $u, u - v, 0$ ]
24	p	m..	$x, y, 0$ [0,0,w]	$\bar{y}, x - y, 0$ [0,0,w]	$\bar{x} + y, \bar{x}, 0$ [0,0,w]
			$\bar{x}, \bar{y}, 0$ [0,0,w]	$y, \bar{x} + y, 0$ [0,0,w]	$x - y, x, 0$ [0,0,w]
			$y, x, 0$ [0,0,w]	$x - y, \bar{y}, 0$ [0,0,w]	$\bar{x}, \bar{x} + y, 0$ [0,0,w]
			$\bar{y}, \bar{x}, 0$ [0,0,w]	$\bar{x} + y, y, 0$ [0,0,w]	$x, x - y, 0$ [0,0,w]
24	o	.m'.	$x, 2x, z$ [u,2u,w]	$2\bar{x}, \bar{x}, z$ [ $2\bar{u}, \bar{u}, w$ ]	$x, \bar{x}, z$ [ $u, \bar{u}, w$ ]
			$\bar{x}, 2\bar{x}, z$ [ $\bar{u}, 2\bar{u}, w$ ]	$2x, x, z$ [2u,u,w]	$\bar{x}, x, z$ [ $\bar{u}, u, w$ ]
			$2x, x, \bar{z}$ [ $2\bar{u}, \bar{u}, w$ ]	$\bar{x}, 2\bar{x}, \bar{z}$ [ $u, 2u, w$ ]	$\bar{x}, x, \bar{z}$ [ $u, \bar{u}, w$ ]
			$2\bar{x}, \bar{x}, \bar{z}$ [ $2u, u, w$ ]	$x, 2x, \bar{z}$ [ $\bar{u}, 2\bar{u}, w$ ]	$x, \bar{x}, \bar{z}$ [ $\bar{u}, u, w$ ]
24	n	..m'	$x, 0, z$ [u,0,w]	$0, x, z$ [0,u,w]	$\bar{x}, \bar{x}, z$ [ $\bar{u}, \bar{u}, w$ ]
			$\bar{x}, 0, z$ [ $\bar{u}, 0, w$ ]	$0, \bar{x}, z$ [0, $\bar{u}$ ,w]	$x, x, z$ [u,u,w]
			$0, x, \bar{z}$ [0, $\bar{u}$ ,w]	$x, 0, \bar{z}$ [ $\bar{u}, 0, w$ ]	$\bar{x}, \bar{x}, \bar{z}$ [u,u,w]
			$0, \bar{x}, \bar{z}$ [0,u,w]	$\bar{x}, 0, \bar{z}$ [u,0,w]	$x, x, \bar{z}$ [ $\bar{u}, \bar{u}, w$ ]
12	m	m'm'2	$x, 2x, 1/2$ [u,2u,0]	$2\bar{x}, \bar{x}, 1/2$ [ $2\bar{u}, \bar{u}, 0$ ]	$x, \bar{x}, 1/2$ [u, $\bar{u}$ ,0]
			$\bar{x}, 2\bar{x}, 1/2$ [ $\bar{u}, 2\bar{u}, 0$ ]	$2x, x, 1/2$ [2u,u,0]	$\bar{x}, x, 1/2$ [ $\bar{u}, u, 0$ ]
12	l	mm'2'	$x, 2x, 0$ [0,0,w]	$2\bar{x}, \bar{x}, 0$ [0,0,w]	$x, \bar{x}, 0$ [0,0,w]
			$\bar{x}, 2\bar{x}, 0$ [0,0,w]	$2x, x, 0$ [0,0,w]	$\bar{x}, x, 0$ [0,0,w]
12	k	m'2m'	$x, 0, 1/2$ [u,0,0]	$0, x, 1/2$ [0,u,0]	$\bar{x}, \bar{x}, 1/2$ [ $\bar{u}, \bar{u}, 0$ ]
			$\bar{x}, 0, 1/2$ [ $\bar{u}, 0, 0$ ]	$0, \bar{x}, 1/2$ [0, $\bar{u}$ ,0]	$x, x, 1/2$ [u,u,0]
12	j	m2'm'	$x, 0, 0$ [0,0,w]	$0, x, 0$ [0,0,w]	$\bar{x}, \bar{x}, 0$ [0,0,w]
			$\bar{x}, 0, 0$ [0,0,w]	$0, \bar{x}, 0$ [0,0,w]	$x, x, 0$ [0,0,w]

Continued

191.13.1475

 $P_{2c} 6/mm'm'$ 

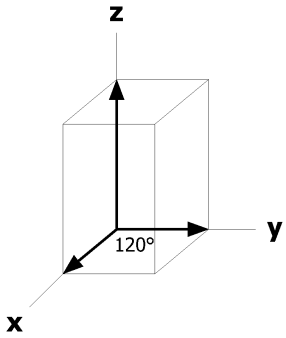
12	i	$2m'm'$	$1/2,0,z [0,0,w]$	$0,1/2,z [0,0,w]$	$1/2,1/2,z [0,0,w]$
			$0,1/2,\bar{z} [0,0,w]$	$1/2,0,\bar{z} [0,0,w]$	$1/2,1/2,\bar{z} [0,0,w]$
8	h	$3m'$	$1/3,2/3,z [0,0,w]$	$2/3,1/3,z [0,0,w]$	$2/3,1/3,\bar{z} [0,0,w]$
					$1/3,2/3,\bar{z} [0,0,w]$
6	g	$m'm'm'$	$1/2,0,1/2 [0,0,0]$	$0,1/2,1/2 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$
6	f	$mm'm'$	$1/2,0,0 [0,0,w]$	$0,1/2,0 [0,0,w]$	$1/2,1/2,0 [0,0,w]$
4	e	$6m'm'$	$0,0,z [0,0,w]$	$0,0,\bar{z} [0,0,w]$	
4	d	$\bar{6}m'2$	$1/3,2/3,1/2 [0,0,0]$	$2/3,1/3,1/2 [0,0,0]$	
4	c	$\bar{6}m'2'$	$1/3,2/3,0 [0,0,w]$	$2/3,1/3,0 [0,0,w]$	
2	b	$6/m'm'm'$	$0,0,1/2 [0,0,0]$		
2	a	$6/mm'm'$	$0,0,0 [0,0,w]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p6mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,0,0]$   $p_{2a} 2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x,0,1/2$

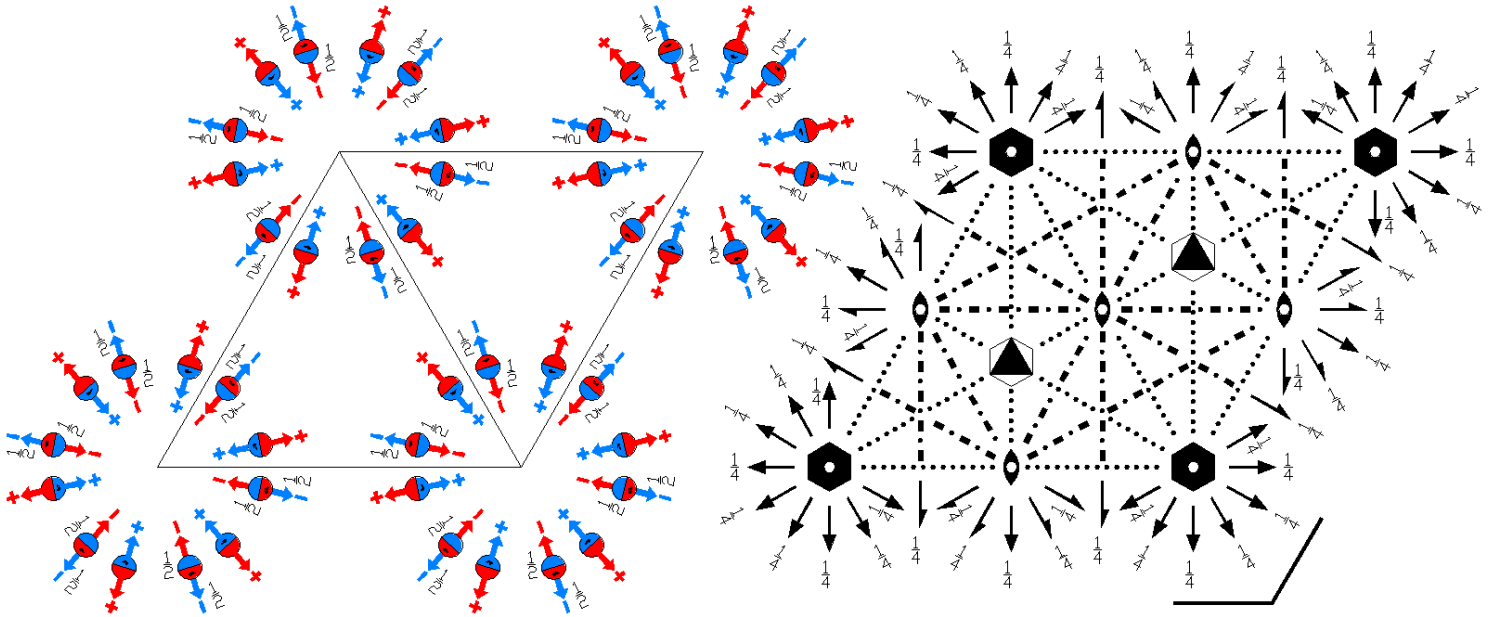
Along  $[2,1,0]$   $p_{2a} 2m'm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x,x/2,1/2$



P6/mcc  
192.1.1476

6/mmm  
P6/m2/c2/c

Hexagonal



Origin at center (6/m) at 6/mcc

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, x)$
Vertices	0,0,0 0,0,1/4	1/2,0,0 1/2,0,1/4	2/3,1/3,0 2/3,1/3,1/4	1/2,1/2,0 1/2,1/2,1/4	

**Symmetry Operations**

- |   |   |   |
|---|---|---|
| (1) 1<br>(1 0,0,0)                                    | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)           | (8) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)                        | (9) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)                        |
| (10) 2 x, $\bar{x}$ ,1/4<br>(2 <sub>3</sub>  0,0,1/2) | (11) 2 x,2x,1/4<br>(2 <sub>2</sub>  0,0,1/2)                      | (12) 2 2x,x,1/4<br>(2 <sub>1</sub>  0,0,1/2)                      |

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)
(16) m $x,y,0$ ( $m_z$  0,0,1/2)	(17) $\bar{6}^-$ 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,1/2)	(18) $\bar{6}^+$ 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,1/2)
(19) c (0,0,1/2) $x,\bar{x},z$ ( $m_{xy}$  0,0,1/2)	(20) c (0,0,1/2) $x,2x,z$ ( $m_x$  0,0,1/2)	(21) c (0,0,1/2) $2x,x,z$ ( $m_y$  0,0,1/2)
(22) c (0,0,1/2) $x,x,z$ ( $m_3$  0,0,1/2)	(23) c (0,0,1/2) $x,0,z$ ( $m_2$  0,0,1/2)	(24) c (0,0,1/2) $0,y,z$ ( $m_1$  0,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	m	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(5) $y,\bar{x}+y,z$ [ $v,\bar{u}+v,w$ ]	(6) $x-y,x,z$ [u-v,u,w]
			(7) $y,x,\bar{z}+1/2$ [v,u, $\bar{w}$ ]	(8) $x-y,\bar{y},\bar{z}+1/2$ [u-v, $\bar{v},\bar{w}$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}+1/2$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
			(10) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(11) $\bar{x}+y,y,\bar{z}+1/2$ [ $\bar{u}+v,v,\bar{w}$ ]	(12) $x,x-y,\bar{z}+1/2$ [u,u-v, $\bar{w}$ ]
			(13) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(14) $y,\bar{x}+y,\bar{z}$ [ $\bar{v},u-v,w$ ]	(15) $x-y,x,\bar{z}$ [ $\bar{u}+v,\bar{u},w$ ]
			(16) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(17) $\bar{y},x-y,\bar{z}$ [ $v,\bar{u}+v,w$ ]	(18) $\bar{x}+y,\bar{x},\bar{z}$ [u-v,u,w]
			(19) $\bar{y},\bar{x},z+1/2$ [v,u, $\bar{w}$ ]	(20) $\bar{x}+y,y,z+1/2$ [u-v, $\bar{v},\bar{w}$ ]	(21) $x,x-y,z+1/2$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
			(22) $y,x,z+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(23) $x-y,\bar{y},z+1/2$ [ $\bar{u}+v,v,\bar{w}$ ]	(24) $\bar{x},\bar{x}+y,z+1/2$ [u,u-v, $\bar{w}$ ]
12	l	m..	$x,y,0$ [0,0,w]	$\bar{y},x-y,0$ [0,0,w]	$\bar{x}+y,\bar{x},0$ [0,0,w]
			$\bar{x},\bar{y},0$ [0,0,w]	$y,\bar{x}+y,0$ [0,0,w]	$x-y,x,0$ [0,0,w]
			$y,x,1/2$ [0,0, $\bar{w}$ ]	$x-y,\bar{y},1/2$ [0,0, $\bar{w}$ ]	$\bar{x},\bar{x}+y,1/2$ [0,0, $\bar{w}$ ]
			$\bar{y},\bar{x},1/2$ [0,0, $\bar{w}$ ]	$\bar{x}+y,y,1/2$ [0,0, $\bar{w}$ ]	$x,x-y,1/2$ [0,0, $\bar{w}$ ]
12	k	..2	$x,2x,1/4$ [u,2u,0]	$2\bar{x},\bar{x},1/4$ [ $2\bar{u},\bar{u},0$ ]	$x,\bar{x},1/4$ [u, $\bar{u},0$ ]
			$\bar{x},2\bar{x},1/4$ [ $\bar{u},2\bar{u},0$ ]	$2x,x,1/4$ [2u,u,0]	$\bar{x},x,1/4$ [ $\bar{u},u,0$ ]
			$\bar{x},2\bar{x},3/4$ [u,2u,0]	$2x,x,3/4$ [ $2\bar{u},\bar{u},0$ ]	$\bar{x},x,3/4$ [u, $\bar{u},0$ ]
			$x,2x,3/4$ [ $\bar{u},2\bar{u},0$ ]	$2\bar{x},\bar{x},3/4$ [2u,u,0]	$x,\bar{x},3/4$ [ $\bar{u},u,0$ ]

12	j	.2.	x,0,1/4 [u,0,0]	0,x,1/4 [0,u,0]	$\bar{x},\bar{x},1/4 [\bar{u},\bar{u},0]$
			$\bar{x},0,1/4 [\bar{u},0,0]$	0, $\bar{x},1/4 [0,\bar{u},0]$	x,x,1/4 [u,u,0]
			$\bar{x},0,3/4 [u,0,0]$	0, $\bar{x},3/4 [0,u,0]$	x,x,3/4 [ $\bar{u},\bar{u},0$ ]
			x,0,3/4 [ $\bar{u},0,0$ ]	0,x,3/4 [0, $\bar{u},0$ ]	$\bar{x},\bar{x},3/4 [u,u,0]$
12	i	2..	1/2,0,z [0,0,w]	0,1/2,z [0,0,w]	1/2,1/2,z [0,0,w]
			0,1/2, $\bar{z}+1/2 [0,0,\bar{w}]$	1/2,0, $\bar{z}+1/2 [0,0,\bar{w}]$	1/2,1/2, $\bar{z}+1/2 [0,0,\bar{w}]$
			1/2,0, $\bar{z} [0,0,w]$	0,1/2, $\bar{z} [0,0,w]$	1/2,1/2, $\bar{z} [0,0,w]$
			0,1/2,z+1/2 [0,0, $\bar{w}$ ]	1/2,0,z+1/2 [0,0, $\bar{w}$ ]	1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]
8	h	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0,w]	2/3,1/3, $\bar{z}+1/2 [0,0,\bar{w}]$
			2/3,1/3, $\bar{z} [0,0,w]$	1/3,2/3, $\bar{z} [0,0,w]$	1/3,2/3,z+1/2 [0,0, $\bar{w}$ ]
6	g	2/m..	1/2,0,0 [0,0,w]	0,1/2,0 [0,0,w]	1/2,1/2,0 [0,0,w]
			0,1/2,1/2 [0,0, $\bar{w}$ ]	1/2,0,1/2 [0,0, $\bar{w}$ ]	1/2,1/2,1/2 [0,0, $\bar{w}$ ]
6	f	222	1/2,0,1/4 [0,0,0]	0,1/2,1/4 [0,0,0]	1/2,1/2,1/4 [0,0,0]
			1/2,0,3/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]
4	e	6..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2 [0,0,\bar{w}]$	0,0, $\bar{z} [0,0,w]$
					0,0,z+1/2 [0,0, $\bar{w}$ ]
4	d	$\bar{6}$ ..	1/3,2/3,0 [0,0,w]	2/3,1/3,0 [0,0,w]	2/3,1/3,1/2 [0,0, $\bar{w}$ ]
					1/3,2/3,1/2 [0,0, $\bar{w}$ ]
4	c	3.2	1/3,2/3,1/4 [0,0,0]	2/3,1/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]
					1/3,2/3,3/4 [0,0,0]
2	b	6/m..	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]	
2	a	622	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]	

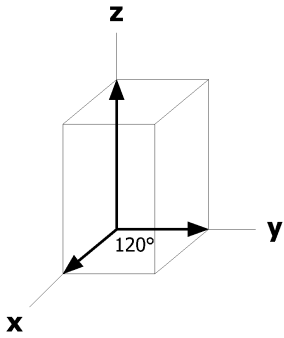
### Symmetry of Special Projections

Along [0,0,1]  $p6mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a'}2m'm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/2

Along [2,1,0]  $p_{2a'}2m'm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/2





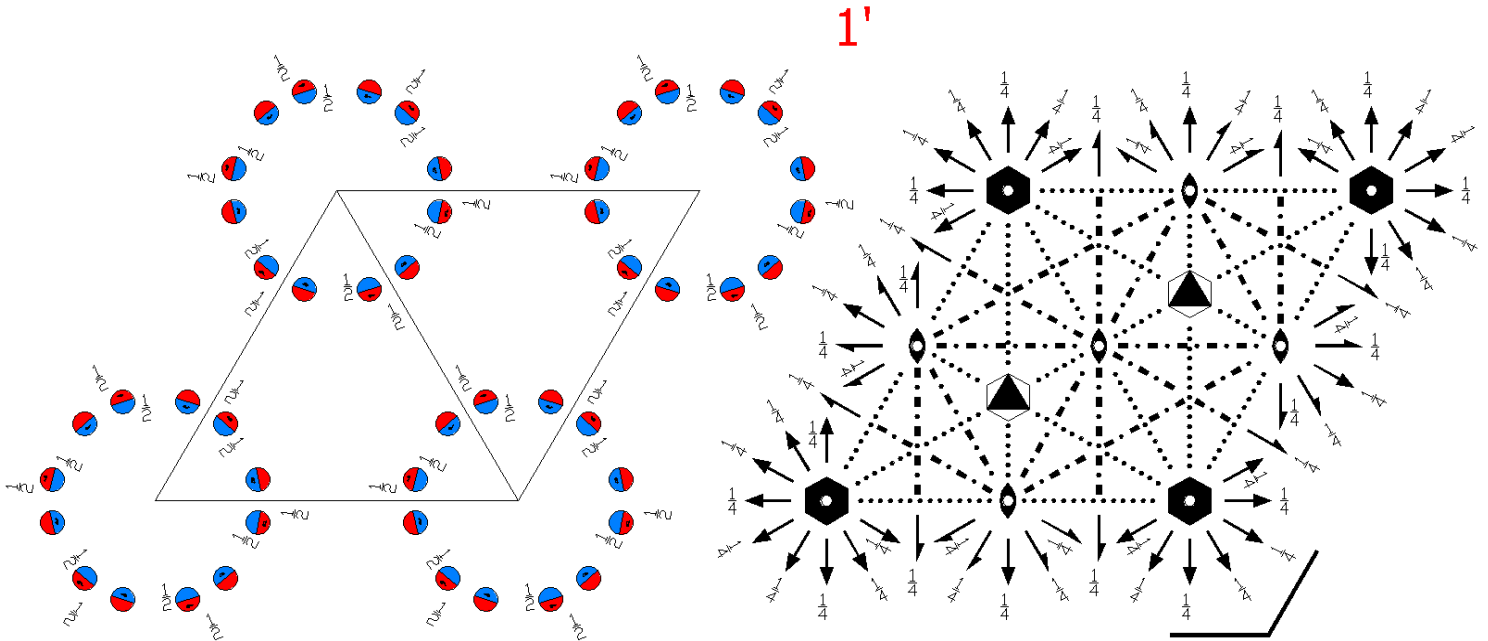
P6/mcc1'

192.2.1477

6/mmm1'

P6/m2/c2/c1'

Hexagonal



Origin at center (6/m1') at 6/mcc1'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/2,1/2,1/4	

**Symmetry Operations**

- |  |   |   |
|--|---|---|
|  | For 1 + set   |   |
| (1) 1<br>(1 0,0,0)                           | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)       | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)  | (8) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)                        | (9) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)                        |
| (10) 2 x,x̄,1/4<br>(2 <sub>3</sub>  0,0,1/2) | (11) 2 x,2x,1/4<br>(2 <sub>2</sub>  0,0,1/2)                      | (12) 2 2x,x,1/4<br>(2 <sub>1</sub>  0,0,1/2)                      |

- |  |   |   |
|--|---|---|
| (13) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)              | (14) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)        | (15) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (16) m x,y,0<br>( $m_z$  0,0,1/2)                        | (17) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$  0,0,1/2) | (18) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$  0,0,1/2)    |
| (19) c (0,0,1/2) x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,1/2) | (20) c (0,0,1/2) x,2x,z<br>( $m_x$  0,0,1/2)                  | (21) c (0,0,1/2) 2x,x,z<br>( $m_y$  0,0,1/2)                |
| (22) c (0,0,1/2) x,x,z<br>( $m_3$  0,0,1/2)              | (23) c (0,0,1/2) x,0,z<br>( $m_2$  0,0,1/2)                   | (24) c (0,0,1/2) 0,y,z<br>( $m_1$  0,0,1/2)                 |

For 1' + set

- |   |  |  |
|---|--|--|
| (1) 1'<br>(1 0,0,0)'  | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)'               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (4) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                    | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)'               |
| (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'               | (8) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'                       | (9) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'                       |
| (10) 2' x, $\bar{x}$ ,1/4<br>(2 <sub>3</sub>  0,0,1/2)'     | (11) 2' x,2x,1/4<br>(2 <sub>2</sub>  0,0,1/2)'                     | (12) 2' 2x,x,1/4<br>(2 <sub>1</sub>  0,0,1/2)'                     |
| (13) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$ ' 0,0,0)'             | (14) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$ ' 0,0,0)'           | (15) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$ ' 0,0,0)'      |
| (16) m' x,y,0<br>( $m_z$ ' 0,0,1/2)'                        | (17) $\bar{6}^-$ 0,0,z; 0,0,0<br>( $\bar{6}_z^{-1}$ ' 0,0,1/2)'    | (18) $\bar{6}^+$ 0,0,z; 0,0,0<br>( $\bar{6}_z$ ' 0,0,1/2)'         |
| (19) c' (0,0,1/2) x, $\bar{x}$ ,z<br>( $m_{xy}$ ' 0,0,1/2)' | (20) c' (0,0,1/2) x,2x,z<br>( $m_x$ ' 0,0,1/2)'                    | (21) c' (0,0,1/2) 2x,x,z<br>( $m_y$ ' 0,0,1/2)'                    |
| (22) c' (0,0,1/2) x,x,z<br>( $m_3$ ' 0,0,1/2)'              | (23) c' (0,0,1/2) x,0,z<br>( $m_2$ ' 0,0,1/2)'                     | (24) c' (0,0,1/2) 0,y,z<br>( $m_1$ ' 0,0,1/2)'                     |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

- |    |   |     |  |  |   |
|----|---|-----|--|--|---|
| 24 | m | 11' | (1) x,y,z [0,0,0]                          | (2) $\bar{y}$ ,x-y,z [0,0,0]           | (3) $\bar{x}+y,\bar{x},z$ [0,0,0]           |
|    |   |     | (4) $\bar{x},\bar{y},z$ [0,0,0]            | (5) y, $\bar{x}+y,z$ [0,0,0]           | (6) x-y,x,z [0,0,0]                         |
|    |   |     | (7) y,x, $\bar{z}+1/2$ [0,0,0]             | (8) x-y, $\bar{y},\bar{z}+1/2$ [0,0,0] | (9) $\bar{x},\bar{x}+y,\bar{z}+1/2$ [0,0,0] |
|    |   |     | (10) $\bar{y},\bar{x},\bar{z}+1/2$ [0,0,0] | (11) $\bar{x}+y,y,\bar{z}+1/2$ [0,0,0] | (12) x,x-y, $\bar{z}+1/2$ [0,0,0]           |

			(13) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]	(14) $y, \bar{x} + y, \bar{z}$ [0,0,0]	(15) $x - y, x, \bar{z}$ [0,0,0]
			(16) $x, y, \bar{z}$ [0,0,0]	(17) $\bar{y}, x - y, \bar{z}$ [0,0,0]	(18) $\bar{x} + y, \bar{x}, \bar{z}$ [0,0,0]
			(19) $\bar{y}, \bar{x}, z + 1/2$ [0,0,0]	(20) $\bar{x} + y, y, z + 1/2$ [0,0,0]	(21) $x, x - y, z + 1/2$ [0,0,0]
			(22) $y, x, z + 1/2$ [0,0,0]	(23) $x - y, \bar{y}, z + 1/2$ [0,0,0]	(24) $\bar{x}, \bar{x} + y, z + 1/2$ [0,0,0]
12	l	m..1'	$x, y, 0$ [0,0,0]	$\bar{y}, x - y, 0$ [0,0,0]	$\bar{x} + y, \bar{x}, 0$ [0,0,0]
			$\bar{x}, \bar{y}, 0$ [0,0,0]	$y, \bar{x} + y, 0$ [0,0,0]	$x - y, x, 0$ [0,0,0]
			$y, x, 1/2$ [0,0,0]	$x - y, \bar{y}, 1/2$ [0,0,0]	$\bar{x}, \bar{x} + y, 1/2$ [0,0,0]
			$\bar{y}, \bar{x}, 1/2$ [0,0,0]	$\bar{x} + y, y, 1/2$ [0,0,0]	$x, x - y, 1/2$ [0,0,0]
12	k	..21'	$x, 2x, 1/4$ [0,0,0]	$2\bar{x}, \bar{x}, 1/4$ [0,0,0]	$x, \bar{x}, 1/4$ [0,0,0]
			$\bar{x}, 2\bar{x}, 1/4$ [0,0,0]	$2x, x, 1/4$ [0,0,0]	$\bar{x}, x, 1/4$ [0,0,0]
			$\bar{x}, 2\bar{x}, 3/4$ [0,0,0]	$2x, x, 3/4$ [0,0,0]	$\bar{x}, x, 3/4$ [0,0,0]
			$x, 2x, 3/4$ [0,0,0]	$2\bar{x}, \bar{x}, 3/4$ [0,0,0]	$x, \bar{x}, 3/4$ [0,0,0]
12	j	.2.1'	$x, 0, 1/4$ [0,0,0]	$0, x, 1/4$ [0,0,0]	$\bar{x}, \bar{x}, 1/4$ [0,0,0]
			$\bar{x}, 0, 1/4$ [0,0,0]	$0, \bar{x}, 1/4$ [0,0,0]	$x, x, 1/4$ [0,0,0]
			$\bar{x}, 0, 3/4$ [0,0,0]	$0, \bar{x}, 3/4$ [0,0,0]	$x, x, 3/4$ [0,0,0]
			$x, 0, 3/4$ [0,0,0]	$0, x, 3/4$ [0,0,0]	$\bar{x}, \bar{x}, 3/4$ [0,0,0]
12	i	2..1'	$1/2, 0, z$ [0,0,0]	$0, 1/2, z$ [0,0,0]	$1/2, 1/2, z$ [0,0,0]
			$0, 1/2, \bar{z} + 1/2$ [0,0,0]	$1/2, 0, \bar{z} + 1/2$ [0,0,0]	$1/2, 1/2, \bar{z} + 1/2$ [0,0,0]
			$1/2, 0, \bar{z}$ [0,0,0]	$0, 1/2, \bar{z}$ [0,0,0]	$1/2, 1/2, \bar{z}$ [0,0,0]
			$0, 1/2, z + 1/2$ [0,0,0]	$1/2, 0, z + 1/2$ [0,0,0]	$1/2, 1/2, z + 1/2$ [0,0,0]
8	h	3..1'	$1/3, 2/3, z$ [0,0,0]	$2/3, 1/3, z$ [0,0,0]	$2/3, 1/3, \bar{z} + 1/2$ [0,0,0]
			$2/3, 1/3, \bar{z}$ [0,0,0]	$1/3, 2/3, \bar{z}$ [0,0,0]	$1/3, 2/3, z + 1/2$ [0,0,0]
6	g	2/m..1'	$1/2, 0, 0$ [0,0,0]	$0, 1/2, 0$ [0,0,0]	$1/2, 1/2, 0$ [0,0,0]
			$0, 1/2, 1/2$ [0,0,0]	$1/2, 0, 1/2$ [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]
6	f	2221'	$1/2, 0, 1/4$ [0,0,0]	$0, 1/2, 1/4$ [0,0,0]	$1/2, 1/2, 1/4$ [0,0,0]
			$1/2, 0, 3/4$ [0,0,0]	$0, 1/2, 3/4$ [0,0,0]	$1/2, 1/2, 3/4$ [0,0,0]
4	e	6..1'	$0, 0, z$ [0,0,0]	$0, 0, \bar{z} + 1/2$ [0,0,0]	$0, 0, \bar{z}$ [0,0,0]
			$0, 0, z + 1/2$ [0,0,0]		
4	d	$\bar{6}$ ..1'	$1/3, 2/3, 0$ [0,0,0]	$2/3, 1/3, 0$ [0,0,0]	$2/3, 1/3, 1/2$ [0,0,0]
			$1/3, 2/3, 1/2$ [0,0,0]		
4	c	3.21'	$1/3, 2/3, 1/4$ [0,0,0]	$2/3, 1/3, 1/4$ [0,0,0]	$2/3, 1/3, 3/4$ [0,0,0]
			$1/3, 2/3, 3/4$ [0,0,0]		

Continued

192.2.1477

P6/mcc1'

2      b      6/m..1' 0,0,0 [0,0,0]

0,0,1/2 [0,0,0]

2      a      6221' 0,0,1/4 [0,0,0]

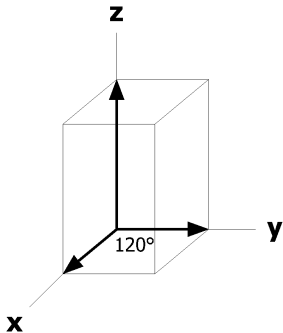
0,0,3/4 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]    p6mm1'  
**a\* = a    b\* = b**  
Origin at 0,0,z

Along [1,0,0]    p2mm1'  
**a\* = c/2    b\* = (a + 2b)/2**  
Origin at x,0,0

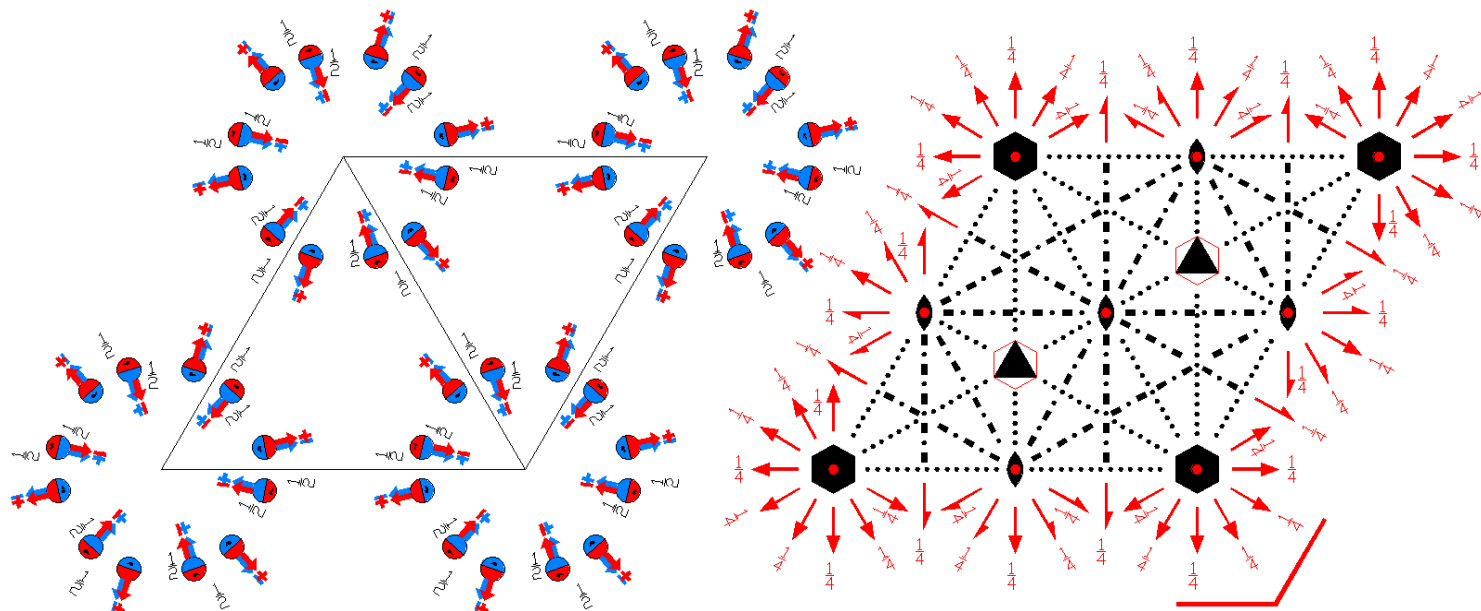
Along [2,1,0]    p2mm1'  
**a\* = c/2    b\* = b/2**  
Origin at x,x/2,0



P6/m'cc  
192.3.1478

6/m'mm  
P6/m'2'/c2'/c

Hexagonal



Origin at center (6/m') at 6/m'cc

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/2,1/2,1/4	

### Symmetry Operations

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                             | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)         | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'  | (8) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'                      | (9) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'                      |
| (10) 2' x,x̄,1/4<br>(2 <sub>3</sub>  0,0,1/2)' | (11) 2' x,2x,1/4<br>(2 <sub>2</sub>  0,0,1/2)'                    | (12) 2' 2x,x,1/4<br>(2 <sub>1</sub>  0,0,1/2)'                    |

(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ ' 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(15) $\bar{3}^-$ ' 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(16) $m'$ x,y,0 ( $m_z$  0,0,1/2)'	(17) $\bar{6}^-$ ' 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,1/2)'	(18) $\bar{6}^+$ ' 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,1/2)'
(19) c (0,0,1/2) x, $\bar{x}$ ,z ( $m_{xy}$  0,0,1/2)	(20) c (0,0,1/2) x,2x,z ( $m_x$  0,0,1/2)	(21) c (0,0,1/2) 2x,x,z ( $m_y$  0,0,1/2)
(22) c (0,0,1/2) x,x,z ( $m_3$  0,0,1/2)	(23) c (0,0,1/2) x,0,z ( $m_2$  0,0,1/2)	(24) c (0,0,1/2) 0,y,z ( $m_1$  0,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	m	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w]	(5) y, $\bar{x}$ +y,z [v, $\bar{u}$ +v,w]	(6) x-y,x,z [u-v,u,w]
			(7) y,x, $\bar{z}$ +1/2 [ $\bar{v}$ , $\bar{u}$ ,w]	(8) x-y, $\bar{y}$ , $\bar{z}$ +1/2 [ $\bar{u}$ +v,v,w]	(9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ +1/2 [u,u-v,w]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ +1/2 [v,u,w]	(11) $\bar{x}$ +y,y, $\bar{z}$ +1/2 [u-v, $\bar{v}$ ,w]	(12) x,x-y, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{u}$ +v,w]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(14) y, $\bar{x}$ +y, $\bar{z}$ [v, $\bar{u}$ +v, $\bar{w}$ ]	(15) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ]
			(16) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(17) $\bar{y}$ ,x-y, $\bar{z}$ [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(18) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ [ $\bar{u}$ +v, $\bar{u}$ , $\bar{w}$ ]
			(19) $\bar{y}$ , $\bar{x}$ ,z+1/2 [v,u, $\bar{w}$ ]	(20) $\bar{x}$ +y,y,z+1/2 [u-v, $\bar{v}$ , $\bar{w}$ ]	(21) x,x-y,z+1/2 [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ]
			(22) y,x,z+1/2 [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(23) x-y, $\bar{y}$ ,z+1/2 [ $\bar{u}$ +v,v, $\bar{w}$ ]	(24) $\bar{x}$ , $\bar{x}$ +y,z+1/2 [u,u-v, $\bar{w}$ ]
12	l	m'..	x,y,0 [u,v,0]	$\bar{y}$ ,x-y,0 [ $\bar{v}$ ,u-v,0]	$\bar{x}$ +y, $\bar{x}$ ,0 [ $\bar{u}$ +v, $\bar{u}$ ,0]
			$\bar{x}$ , $\bar{y}$ ,0 [ $\bar{u}$ , $\bar{v}$ ,0]	y, $\bar{x}$ +y,0 [v, $\bar{u}$ +v,0]	x-y,x,0 [u-v,u,0]
			y,x,1/2 [ $\bar{v}$ , $\bar{u}$ ,0]	x-y, $\bar{y}$ ,1/2 [ $\bar{u}$ +v,v,0]	$\bar{x}$ , $\bar{x}$ +y,1/2 [u,u-v,0]
			$\bar{y}$ , $\bar{x}$ ,1/2 [v,u,0]	$\bar{x}$ +y,y,1/2 [u-v, $\bar{v}$ ,0]	x,x-y,1/2 [ $\bar{u}$ , $\bar{u}$ +v,0]
12	k	..2'	x,2x,1/4 [u,0,w]	$2\bar{x}$ , $\bar{x}$ ,1/4 [0,u,w]	x, $\bar{x}$ ,1/4 [ $\bar{u}$ , $\bar{u}$ ,w]
			$\bar{x}$ , $2\bar{x}$ ,1/4 [ $\bar{u}$ ,0,w]	2x,x,1/4 [0, $\bar{u}$ ,w]	$\bar{x}$ ,x,1/4 [u,u,w]
			$\bar{x}$ , $2\bar{x}$ ,3/4 [ $\bar{u}$ ,0, $\bar{w}$ ]	2x,x,3/4 [0, $\bar{u}$ , $\bar{w}$ ]	$\bar{x}$ ,x,3/4 [u,u, $\bar{w}$ ]
			x,2x,3/4 [u,0, $\bar{w}$ ]	$2\bar{x}$ , $\bar{x}$ ,3/4 [0,u, $\bar{w}$ ]	x, $\bar{x}$ ,3/4 [ $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]

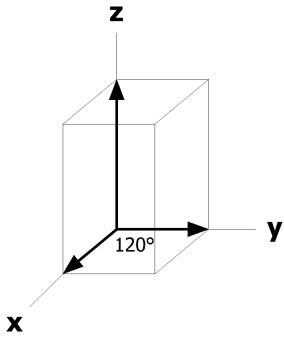
Continued			192.3.1478			P6/m'cc
12	j	.2'	x,0,1/4 [u,2u,w] $\bar{x}$ ,0,1/4 [ $\bar{u}$ ,2 $\bar{u}$ ,w] $\bar{x}$ ,0,3/4 [ $\bar{u}$ ,2 $\bar{u}$ , $\bar{w}$ ] x,0,3/4 [u,2u, $\bar{w}$ ]	0,x,1/4 [2 $\bar{u}$ , $\bar{u}$ ,w] 0, $\bar{x}$ ,1/4 [2u,u,w] 0, $\bar{x}$ ,3/4 [2u,u, $\bar{w}$ ] 0,x,3/4 [2 $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]		$\bar{x}$ , $\bar{x}$ ,1/4 [u, $\bar{u}$ ,w] x,x,1/4 [ $\bar{u}$ ,u,w] x,x,3/4 [ $\bar{u}$ ,u, $\bar{w}$ ] $\bar{x}$ , $\bar{x}$ ,3/4 [u, $\bar{u}$ , $\bar{w}$ ]
12	i	2..	1/2,0,z [0,0,w] 0,1/2, $\bar{z}$ +1/2 [0,0,w] 1/2,0, $\bar{z}$ [0,0, $\bar{w}$ ] 0,1/2,z+1/2 [0,0, $\bar{w}$ ]	0,1/2,z [0,0,w] 1/2,0, $\bar{z}$ +1/2 [0,0,w] 0,1/2, $\bar{z}$ [0,0, $\bar{w}$ ] 1/2,0,z+1/2 [0,0, $\bar{w}$ ]		1/2,1/2,z [0,0,w] 1/2,1/2, $\bar{z}$ +1/2 [0,0,w] 1/2,1/2, $\bar{z}$ [0,0, $\bar{w}$ ] 1/2,1/2,z+1/2 [0,0, $\bar{w}$ ]
8	h	3..	1/3,2/3,z [0,0,w] 2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	2/3,1/3,z [0,0,w] 1/3,2/3, $\bar{z}$ [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ +1/2 [0,0,w] 1/3,2/3,z+1/2 [0,0, $\bar{w}$ ]	1/3,2/3, $\bar{z}$ +1/2 [0,0,w] 2/3,1/3,z+1/2 [0,0, $\bar{w}$ ]
6	g	2/m'..	1/2,0,0 [0,0,0] 0,1/2,1/2 [0,0,0]	0,1/2,0 [0,0,0] 1/2,0,1/2 [0,0,0]		1/2,1/2,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]
6	f	22'2'	1/2,0,1/4 [0,0,w] 1/2,0,3/4 [0,0, $\bar{w}$ ]	0,1/2,1/4 [0,0,w] 0,1/2,3/4 [0,0, $\bar{w}$ ]		1/2,1/2,1/4 [0,0,w] 1/2,1/2,3/4 [0,0, $\bar{w}$ ]
4	e	6..	0,0,z [0,0,w]	0,0, $\bar{z}$ +1/2 [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0,z+1/2 [0,0, $\bar{w}$ ]
4	d	$\bar{6}$ '..	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]	2/3,1/3,1/2 [0,0,0]	1/3,2/3,1/2 [0,0,0]
4	c	3.2'	1/3,2/3,1/4 [0,0,w]	2/3,1/3,1/4 [0,0,w]	2/3,1/3,3/4 [0,0, $\bar{w}$ ]	1/3,2/3,3/4 [0,0, $\bar{w}$ ]
2	b	6/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
2	a	62'2'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		

### Symmetry of Special Projections

Along [0,0,1] p6mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0]  $p_{2a'}2m'm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

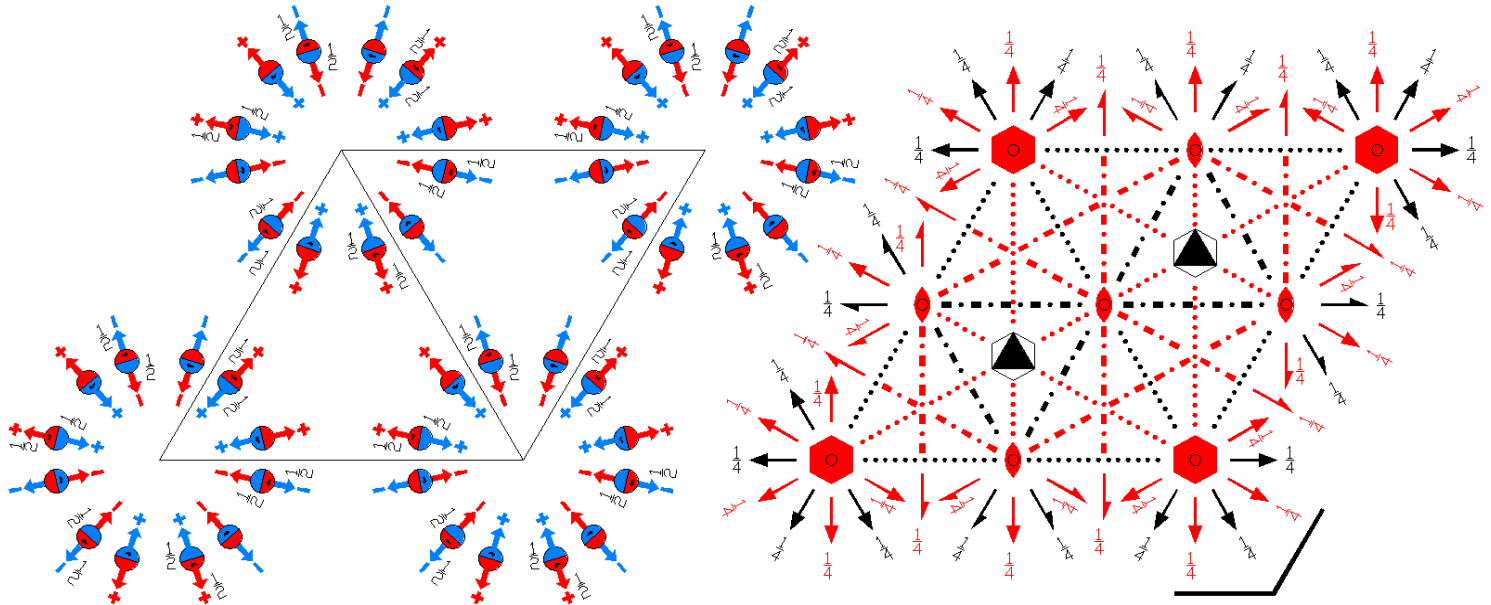
Along [2,1,0]  $p_{2a'}2m'm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P6'/mc'c  
192.4.1479

6'/mm'm  
P6'/m2/c'2'/c

Hexagonal



Origin at center (6'/m) at 6'/mc'c

**Asymmetric unit**     $0 \leq x \leq 2/3$ ;     $0 \leq y \leq 1/2$ ;     $0 \leq z \leq 1/4$ ;     $x \leq (1+y)/2$ ;     $y \leq \min(1-x, x)$

Vertices             $0,0,0$              $1/2,0,0$              $2/3,1/3,0$              $1/2,1/2,0$   
                           $0,0,1/4$              $1/2,0,1/4$              $2/3,1/3,1/4$              $1/2,1/2,1/4$

**Symmetry Operations**

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                             | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)                | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'       | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)'              |
| (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)    | (8) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)                         | (9) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)                        |
| (10) 2' x,x̄,1/4<br>(2 <sub>3</sub>  0,0,1/2)' | (11) 2' x,2x,1/4<br>(2 <sub>2</sub>  0,0,1/2)'                     | (12) 2' 2x,x,1/4<br>(2 <sub>1</sub>  0,0,1/2)'                    |



(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ ' 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(15) $\bar{3}^-$ ' 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(16) m x,y,0 ( $m_z$  0,0,1/2)	(17) $\bar{6}^-$ 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,1/2)	(18) $\bar{6}^+$ 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,1/2)
(19) c' (0,0,1/2) x, $\bar{x}$ ,z ( $m_{xy}$  0,0,1/2)'	(20) c' (0,0,1/2) x,2x,z ( $m_x$  0,0,1/2)'	(21) c' (0,0,1/2) 2x,x,z ( $m_y$  0,0,1/2)'
(22) c (0,0,1/2) x,x,z ( $m_3$  0,0,1/2)	(23) c (0,0,1/2) x,0,z ( $m_2$  0,0,1/2)	(24) c (0,0,1/2) 0,y,z ( $m_1$  0,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	m	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z [u,v, $\bar{w}$ ]	(5) y, $\bar{x}$ +y,z [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) x-y,x,z [ $\bar{u}$ +v, $\bar{u}$ , $\bar{w}$ ]
			(7) y,x, $\bar{z}$ +1/2 [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y}$ , $\bar{z}$ +1/2 [u-v, $\bar{v}$ , $\bar{w}$ ]	(9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ +1/2 [v,u,w]	(11) $\bar{x}$ +y,y, $\bar{z}$ +1/2 [u-v, $\bar{v}$ ,w]	(12) x,x-y, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{u}$ +v,w]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(14) y, $\bar{x}$ +y, $\bar{z}$ [v, $\bar{u}$ +v, $\bar{w}$ ]	(15) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ]
			(16) x,y, $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ ,w]	(17) $\bar{y}$ ,x-y, $\bar{z}$ [v, $\bar{u}$ +v,w]	(18) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ [u-v,u,w]
			(19) $\bar{y}$ , $\bar{x}$ ,z+1/2 [ $\bar{v}$ , $\bar{u}$ ,w]	(20) $\bar{x}$ +y,y,z+1/2 [ $\bar{u}$ +v,v,w]	(21) x,x-y,z+1/2 [u,u-v,w]
			(22) y,x,z+1/2 [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(23) x-y, $\bar{y}$ ,z+1/2 [ $\bar{u}$ +v,v, $\bar{w}$ ]	(24) $\bar{x}$ , $\bar{x}$ +y,z+1/2 [u,u-v, $\bar{w}$ ]
12	l	m..	x,y,0 [0,0,w]	$\bar{y}$ ,x-y,0 [0,0,w]	$\bar{x}$ +y, $\bar{x}$ ,0 [0,0,w]
			$\bar{x}$ , $\bar{y}$ ,0 [0,0, $\bar{w}$ ]	y, $\bar{x}$ +y,0 [0,0, $\bar{w}$ ]	x-y,x,0 [0,0, $\bar{w}$ ]
			y,x,1/2 [0,0, $\bar{w}$ ]	x-y, $\bar{y}$ ,1/2 [0,0, $\bar{w}$ ]	$\bar{x}$ , $\bar{x}$ +y,1/2 [0,0, $\bar{w}$ ]
			$\bar{y}$ , $\bar{x}$ ,1/2 [0,0,w]	$\bar{x}$ +y,y,1/2 [0,0,w]	x,x-y,1/2 [0,0,w]
12	k	..2'	x,2x,1/4 [u,0,w]	2 $\bar{x}$ , $\bar{x}$ ,1/4 [0,u,w]	x, $\bar{x}$ ,1/4 [ $\bar{u}$ , $\bar{u}$ ,w]
			$\bar{x}$ ,2 $\bar{x}$ ,1/4 [u,0, $\bar{w}$ ]	2x,x,1/4 [0,u, $\bar{w}$ ]	$\bar{x}$ ,x,1/4 [ $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]
			$\bar{x}$ ,2 $\bar{x}$ ,3/4 [ $\bar{u}$ ,0, $\bar{w}$ ]	2x,x,3/4 [0, $\bar{u}$ , $\bar{w}$ ]	$\bar{x}$ ,x,3/4 [u,u, $\bar{w}$ ]
			x,2x,3/4 [ $\bar{u}$ ,0,w]	2 $\bar{x}$ , $\bar{x}$ ,3/4 [0, $\bar{u}$ ,w]	x, $\bar{x}$ ,3/4 [u,u,w]

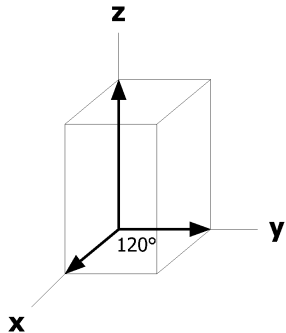
Continued			192.4.1479			P6'/mc'c		
12	j	.2.	x,0,1/4 [u,0,0]	0,x,1/4 [0,u,0]	$\bar{x},\bar{x},1/4 [\bar{u},\bar{u},0]$			
			$\bar{x},0,1/4 [u,0,0]$	0, $\bar{x},1/4 [0,u,0]$	x,x,1/4 [ $\bar{u},\bar{u},0$ ]			
			$\bar{x},0,3/4 [\bar{u},0,0]$	0, $\bar{x},3/4 [0,\bar{u},0]$	x,x,3/4 [u,u,0]			
			x,0,3/4 [ $\bar{u},0,0$ ]	0,x,3/4 [0, $\bar{u},0$ ]	$\bar{x},\bar{x},3/4 [u,u,0]$			
12	i	2'..	1/2,0,z [u,v,0]	0,1/2,z [ $\bar{v},u-v,0$ ]	1/2,1/2,z [ $\bar{u}+v,\bar{u},0$ ]			
			0,1/2, $\bar{z}+1/2 [v,u,0]$	1/2,0, $\bar{z}+1/2 [u-v,\bar{v},0]$	1/2,1/2, $\bar{z}+1/2 [\bar{u},\bar{u}+v,0]$			
			1/2,0, $\bar{z} [\bar{u},\bar{v},0]$	0,1/2, $\bar{z} [v,\bar{u}+v,0]$	1/2,1/2, $\bar{z} [u-v,u,0]$			
			0,1/2,z+1/2 [ $\bar{v},\bar{u},0$ ]	1/2,0,z+1/2 [ $\bar{u}+v,v,0$ ]	1/2,1/2,z+1/2 [u,u-v,0]			
8	h	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}+1/2 [0,0,\bar{w}]$	1/3,2/3, $\bar{z}+1/2 [0,0,w]$		
			2/3,1/3, $\bar{z} [0,0,\bar{w}]$	1/3,2/3, $\bar{z} [0,0,w]$	1/3,2/3,z+1/2 [0,0,w]	2/3,1/3,z+1/2 [0,0, $\bar{w}$ ]		
6	g	2'/m..	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]			
			0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]			
6	f	2'22'	1/2,0,1/4 [u,0,0]	0,1/2,1/4 [0,u,0]	1/2,1/2,1/4 [ $\bar{u},\bar{u},0$ ]			
			1/2,0,3/4 [ $\bar{u},0,0$ ]	0,1/2,3/4 [0, $\bar{u},0$ ]	1/2,1/2,3/4 [u,u,0]			
4	e	6'..	0,0,z [0,0,0]	0,0, $\bar{z}+1/2 [0,0,0]$	0,0, $\bar{z} [0,0,0]$	0,0,z+1/2 [0,0,0]		
4	d	$\bar{6}$ ..	1/3,2/3,0 [0,0,w]	2/3,1/3,0 [0,0, $\bar{w}$ ]	2/3,1/3,1/2 [0,0, $\bar{w}$ ]	1/3,2/3,1/2 [0,0,w]		
4	c	3.2'	1/3,2/3,1/4 [0,0,w]	2/3,1/3,1/4 [0,0, $\bar{w}$ ]	2/3,1/3,3/4 [0,0, $\bar{w}$ ]	1/3,2/3,3/4 [0,0,w]		
2	b	6'/m..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]				
2	a	6'22'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]				

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p<sub>2a</sub>'2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



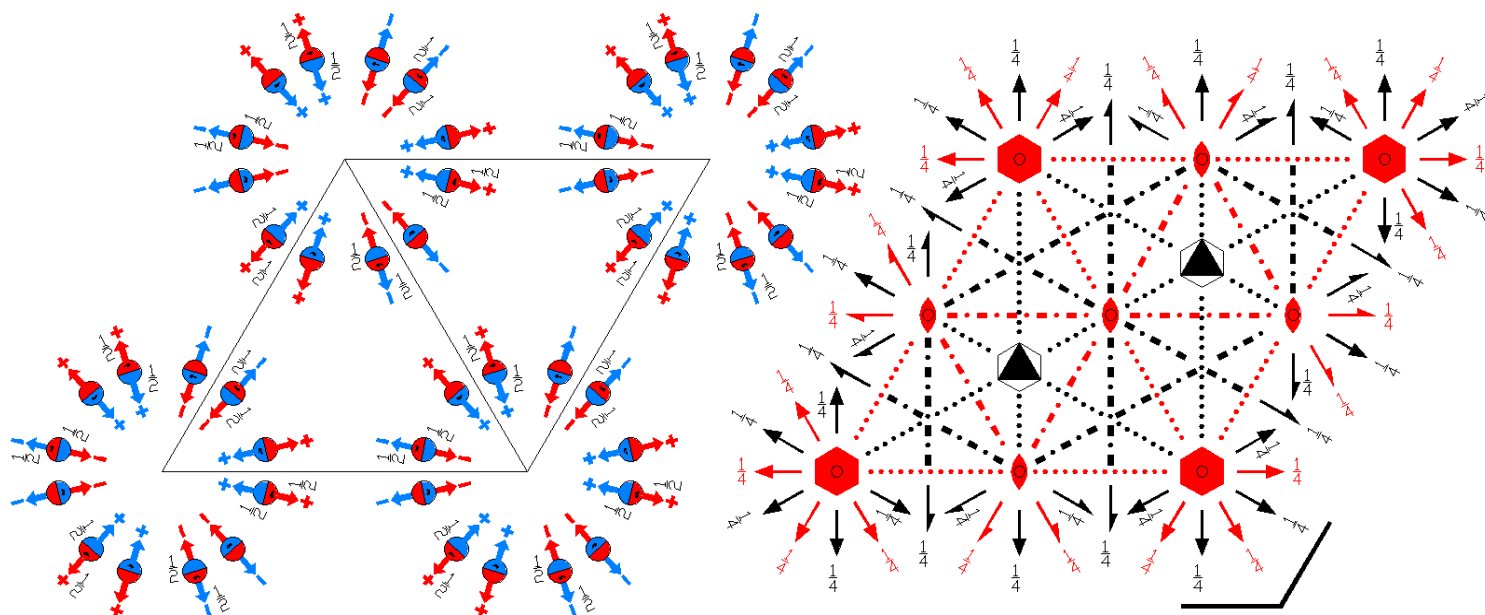
P6'/mcc'

192.5.1480

6'/mmm'

P6'/m2'/c2/c'

Hexagonal



Origin at center (6'/m) at 6'/mcc'

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $x \leq (1+y)/2$ ;  $y \leq \min(1-x, x)$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/2,1/2,1/4

### Symmetry Operations

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                            | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)                | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2' 0,0,z<br>(2 <sub>z</sub>  0,0,0)'      | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0)' | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)'              |
| (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)' | (8) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'                       | (9) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'                      |
| (10) 2 x,x̄,1/4<br>(2 <sub>3</sub>  0,0,1/2)  | (11) 2 x,2x,1/4<br>(2 <sub>2</sub>  0,0,1/2)                       | (12) 2 2x,x,1/4<br>(2 <sub>1</sub>  0,0,1/2)                      |

(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ ' 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(15) $\bar{3}^-$ ' 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(16) m $x,y,0$ ( $m_z$  0,0,1/2)	(17) $\bar{6}^-$ 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,1/2)	(18) $\bar{6}^+$ 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,1/2)
(19) c (0,0,1/2) $x,\bar{x},z$ ( $m_{xy}$  0,0,1/2)	(20) c (0,0,1/2) $x,2x,z$ ( $m_x$  0,0,1/2)	(21) c (0,0,1/2) $2x,x,z$ ( $m_y$  0,0,1/2)
(22) c' (0,0,1/2) $x,x,z$ ( $m_3$  0,0,1/2)'	(23) c' (0,0,1/2) $x,0,z$ ( $m_2$  0,0,1/2)'	(24) c' (0,0,1/2) $0,y,z$ ( $m_1$  0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	m	1	(1) $x,y,z$ [ $u,v,w$ ]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z$ [ $u,v,\bar{w}$ ]	(5) $y,\bar{x}+y,z$ [ $\bar{v},u-v,\bar{w}$ ]	(6) $x-y,x,z$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]
			(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $x-y,\bar{y},\bar{z}+1/2$ [ $\bar{u}+v,v,w$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}+1/2$ [ $u,u-v,w$ ]
			(10) $\bar{y},\bar{x},\bar{z}+1/2$ [ $\bar{v},\bar{u},\bar{w}$ ]	(11) $\bar{x}+y,y,\bar{z}+1/2$ [ $\bar{u}+v,v,\bar{w}$ ]	(12) $x,x-y,\bar{z}+1/2$ [ $u,u-v,\bar{w}$ ]
			(13) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) $y,\bar{x}+y,\bar{z}$ [ $v,\bar{u}+v,\bar{w}$ ]	(15) $x-y,x,\bar{z}$ [ $u-v,u,\bar{w}$ ]
			(16) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(17) $\bar{y},x-y,\bar{z}$ [ $v,\bar{u}+v,w$ ]	(18) $\bar{x}+y,\bar{x},\bar{z}$ [ $u-v,u,w$ ]
			(19) $\bar{y},\bar{x},z+1/2$ [ $v,u,\bar{w}$ ]	(20) $\bar{x}+y,y,z+1/2$ [ $u-v,\bar{v},\bar{w}$ ]	(21) $x,x-y,z+1/2$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
			(22) $y,x,z+1/2$ [ $v,u,w$ ]	(23) $x-y,\bar{y},z+1/2$ [ $u-v,\bar{v},w$ ]	(24) $\bar{x},\bar{x}+y,z+1/2$ [ $\bar{u},\bar{u}+v,w$ ]
12	l	m..	$x,y,0$ [0,0,w]	$\bar{y},x-y,0$ [0,0,w]	$\bar{x}+y,\bar{x},0$ [0,0,w]
			$\bar{x},\bar{y},0$ [0,0, $\bar{w}$ ]	$y,\bar{x}+y,0$ [0,0, $\bar{w}$ ]	$x-y,x,0$ [0,0, $\bar{w}$ ]
			$y,x,1/2$ [0,0,w]	$x-y,\bar{y},1/2$ [0,0,w]	$\bar{x},\bar{x}+y,1/2$ [0,0,w]
			$\bar{y},\bar{x},1/2$ [0,0, $\bar{w}$ ]	$\bar{x}+y,y,1/2$ [0,0, $\bar{w}$ ]	$x,x-y,1/2$ [0,0, $\bar{w}$ ]
12	k	..2	$x,2x,1/4$ [ $u,2u,0$ ]	$2\bar{x},\bar{x},1/4$ [ $2\bar{u},\bar{u},0$ ]	$x,\bar{x},1/4$ [ $u,\bar{u},0$ ]
			$\bar{x},2\bar{x},1/4$ [ $u,2u,0$ ]	$2x,x,1/4$ [ $2\bar{u},\bar{u},0$ ]	$\bar{x},x,1/4$ [ $u,\bar{u},0$ ]
			$\bar{x},2\bar{x},3/4$ [ $\bar{u},2\bar{u},0$ ]	$2x,x,3/4$ [ $2u,u,0$ ]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]
			$x,2x,3/4$ [ $\bar{u},2\bar{u},0$ ]	$2\bar{x},\bar{x},3/4$ [ $2u,u,0$ ]	$x,\bar{x},3/4$ [ $\bar{u},u,0$ ]

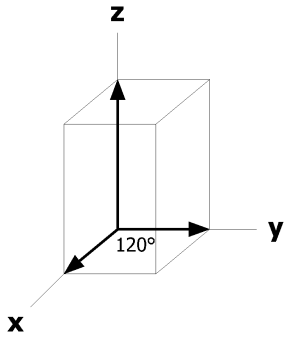
Continued			192.5.1480			P6'/mcc'		
12	j	.2'	x,0,1/4 [u,2u,w]	0,x,1/4 [2 $\bar{u}$ , $\bar{u}$ ,w]	$\bar{x}$ , $\bar{x}$ ,1/4 [u, $\bar{u}$ ,w]			
			$\bar{x}$ ,0,1/4 [u,2u, $\bar{w}$ ]	0, $\bar{x}$ ,1/4 [2 $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]	x,x,1/4 [u, $\bar{u}$ , $\bar{w}$ ]			
			$\bar{x}$ ,0,3/4 [ $\bar{u}$ ,2 $\bar{u}$ , $\bar{w}$ ]	0, $\bar{x}$ ,3/4 [2u,u, $\bar{w}$ ]	x,x,3/4 [ $\bar{u}$ ,u, $\bar{w}$ ]			
			x,0,3/4 [ $\bar{u}$ ,2 $\bar{u}$ ,w]	0,x,3/4 [2u,u,w]	$\bar{x}$ , $\bar{x}$ ,3/4 [ $\bar{u}$ ,u,w]			
12	i	2'..	1/2,0,z [u,v,0]	0,1/2,z [ $\bar{v}$ ,u-v,0]	1/2,1/2,z [ $\bar{u}$ +v, $\bar{u}$ ,0]			
			0,1/2, $\bar{z}$ +1/2 [ $\bar{v}$ , $\bar{u}$ ,0]	1/2,0, $\bar{z}$ +1/2 [ $\bar{u}$ +v,v,0]	1/2,1/2, $\bar{z}$ +1/2 [u,u-v,0]			
			1/2,0, $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ ,0]	0,1/2, $\bar{z}$ [v, $\bar{u}$ +v,0]	1/2,1/2, $\bar{z}$ [u-v,u,0]			
			0,1/2,z+1/2 [v,u,0]	1/2,0,z+1/2 [u-v, $\bar{v}$ ,0]	1/2,1/2,z+1/2 [ $\bar{u}$ , $\bar{u}$ +v,0]			
8	h	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ +1/2 [0,0,w]	1/3,2/3, $\bar{z}$ +1/2 [0,0, $\bar{w}$ ]		
			2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	1/3,2/3, $\bar{z}$ [0,0,w]	1/3,2/3,z+1/2 [0,0, $\bar{w}$ ]	2/3,1/3,z+1/2 [0,0,w]		
6	g	2'/m..	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]			
			0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]			
6	f	2'2'2	1/2,0,1/4 [u,2u,0]	0,1/2,1/4 [2 $\bar{u}$ , $\bar{u}$ ,0]	1/2,1/2,1/4 [u, $\bar{u}$ ,0]			
			1/2,0,3/4 [ $\bar{u}$ ,2 $\bar{u}$ ,0]	0,1/2,3/4 [2u,u,0]	1/2,1/2,3/4 [ $\bar{u}$ ,u,0]			
4	e	6'..	0,0,z [0,0,0]	0,0, $\bar{z}$ +1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0,z+1/2 [0,0,0]		
4	d	$\bar{6}$ ..	1/3,2/3,0 [0,0,w]	2/3,1/3,0 [0,0, $\bar{w}$ ]	2/3,1/3,1/2 [0,0,w]	1/3,2/3,1/2 [0,0, $\bar{w}$ ]		
4	c	3.2	1/3,2/3,1/4 [0,0,0]	2/3,1/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]	1/3,2/3,3/4 [0,0,0]		
2	b	6'/m..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]				
2	a	6'2'2	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]				

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

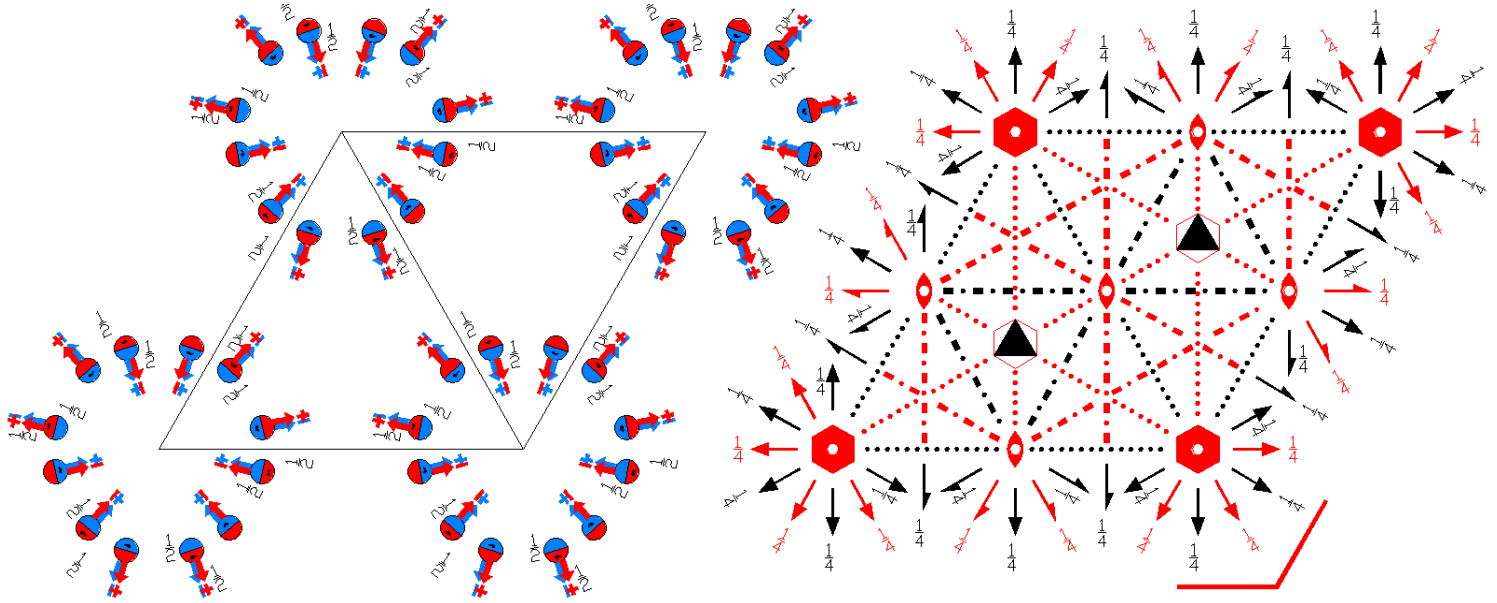
Along [2,1,0] p2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P6'/m'c'c$   
192.6.1481

$6'/m'm'm$   
 $P6'/m'2'/c'2/c$

Hexagonal



Origin at center ( $6'/m'$ ) at  $6'/m'c'c$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, x)$
Vertices	0,0,0 0,0,1/4	1/2,0,0 1/2,0,1/4	2/3,1/3,0 2/3,1/3,1/4	1/2,1/2,0 1/2,1/2,1/4	

**Symmetry Operations**

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                              | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)       | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0) |
| (4) $2'$ 0,0,z<br>( $2_z$  0,0,0)'              | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0)' | (6) $6^+$ 0,0,z<br>( $6_z$  0,0,0)'     |
| (7) $2'$ x,x,1/4<br>( $2_{xy}$  0,0,1/2)'       | (8) $2'$ x,0,1/4<br>( $2_x$  0,0,1/2)'   | (9) $2'$ 0,y,1/4<br>( $2_y$  0,0,1/2)'  |
| (10) $2$ x, $\bar{x}$ ,1/4<br>( $2_3$  0,0,1/2) | (11) $2$ x,2x,1/4<br>( $2_2$  0,0,1/2)   | (12) $2$ 2x,x,1/4<br>( $2_1$  0,0,1/2)  |

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)
(16) $m'$ x,y,0 ( $m_z$  0,0,1/2)'	(17) $\bar{6}^-$ 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,1/2)'	(18) $\bar{6}^+$ 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,1/2)'
(19) $c'$ (0,0,1/2) x, $\bar{x}$ ,z ( $m_{xy}$  0,0,1/2)'	(20) $c'$ (0,0,1/2) x,2x,z ( $m_x$  0,0,1/2)'	(21) $c'$ (0,0,1/2) 2x,x,z ( $m_y$  0,0,1/2)'
(22) $c$ (0,0,1/2) x,x,z ( $m_3$  0,0,1/2)	(23) $c$ (0,0,1/2) x,0,z ( $m_2$  0,0,1/2)	(24) $c$ (0,0,1/2) 0,y,z ( $m_1$  0,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	m	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y$ , $\bar{x}$ ,z [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z [u,v, $\bar{w}$ ]	(5) y, $\bar{x}+y$ ,z [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) x-y,x,z [ $\bar{u}+v$ , $\bar{u}$ , $\bar{w}$ ]
			(7) y,x, $\bar{z}+1/2$ [ $\bar{v}$ , $\bar{u}$ ,w]	(8) x-y, $\bar{y}$ , $\bar{z}+1/2$ [ $\bar{u}+v$ ,v,w]	(9) $\bar{x}$ , $\bar{x}+y$ , $\bar{z}+1/2$ [u,u-v,w]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}+1/2$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(11) $\bar{x}+y$ ,y, $\bar{z}+1/2$ [ $\bar{u}+v$ ,v, $\bar{w}$ ]	(12) x,x-y, $\bar{z}+1/2$ [u,u-v, $\bar{w}$ ]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(14) y, $\bar{x}+y$ , $\bar{z}$ [ $\bar{v}$ ,u-v,w]	(15) x-y,x, $\bar{z}$ [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(16) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(17) $\bar{y}$ ,x-y, $\bar{z}$ [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(18) $\bar{x}+y$ , $\bar{x}$ , $\bar{z}$ [ $\bar{u}+v$ , $\bar{u}$ , $\bar{w}$ ]
			(19) $\bar{y}$ , $\bar{x}$ ,z+1/2 [ $\bar{v}$ , $\bar{u}$ ,w]	(20) $\bar{x}+y$ ,y,z+1/2 [ $\bar{u}+v$ ,v,w]	(21) x,x-y,z+1/2 [u,u-v,w]
			(22) y,x,z+1/2 [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(23) x-y, $\bar{y}$ ,z+1/2 [ $\bar{u}+v$ ,v, $\bar{w}$ ]	(24) $\bar{x}$ , $\bar{x}+y$ ,z+1/2 [u,u-v, $\bar{w}$ ]
12	l	m'..	x,y,0 [u,v,0]	$\bar{y}$ ,x-y,0 [ $\bar{v}$ ,u-v,0]	$\bar{x}+y$ , $\bar{x}$ ,0 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			$\bar{x}$ , $\bar{y}$ ,0 [u,v,0]	y, $\bar{x}+y$ ,0 [ $\bar{v}$ ,u-v,0]	x-y,x,0 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			y,x,1/2 [ $\bar{v}$ , $\bar{u}$ ,0]	x-y, $\bar{y}$ ,1/2 [ $\bar{u}+v$ ,v,0]	$\bar{x}$ , $\bar{x}+y$ ,1/2 [u,u-v,0]
			$\bar{y}$ , $\bar{x}$ ,1/2 [ $\bar{v}$ , $\bar{u}$ ,0]	$\bar{x}+y$ ,y,1/2 [ $\bar{u}+v$ ,v,0]	x,x-y,1/2 [u,u-v,0]
12	k	..2	x,2x,1/4 [u,2u,0]	2 $\bar{x}$ , $\bar{x}$ ,1/4 [2 $\bar{u}$ , $\bar{u}$ ,0]	x, $\bar{x}$ ,1/4 [u, $\bar{u}$ ,0]
			$\bar{x}$ ,2 $\bar{x}$ ,1/4 [u,2u,0]	2x,x,1/4 [2 $\bar{u}$ , $\bar{u}$ ,0]	$\bar{x}$ ,x,1/4 [u, $\bar{u}$ ,0]
			$\bar{x}$ ,2 $\bar{x}$ ,3/4 [u,2u,0]	2x,x,3/4 [2 $\bar{u}$ , $\bar{u}$ ,0]	$\bar{x}$ ,x,3/4 [u, $\bar{u}$ ,0]
			x,2x,3/4 [u,2u,0]	2 $\bar{x}$ , $\bar{x}$ ,3/4 [2 $\bar{u}$ , $\bar{u}$ ,0]	x, $\bar{x}$ ,3/4 [u, $\bar{u}$ ,0]

12	j	.2'	x,0,1/4 [u,2u,w]	0,x,1/4 [2 $\bar{u}$ , $\bar{u}$ ,w]	$\bar{x},\bar{x},1/4 [u,\bar{u},w]$	
			$\bar{x},0,1/4 [u,2u,\bar{w}]$	0, $\bar{x},1/4 [2\bar{u},\bar{u},\bar{w}]$	x,x,1/4 [u, $\bar{u},\bar{w}]$	
			$\bar{x},0,3/4 [u,2u,w]$	0, $\bar{x},3/4 [2\bar{u},\bar{u},w]$	x,x,3/4 [u, $\bar{u},w]$	
			x,0,3/4 [u,2u, $\bar{w}]$	0,x,3/4 [2 $\bar{u}$ , $\bar{u},\bar{w}]$	$\bar{x},\bar{x},3/4 [u,\bar{u},\bar{w}]$	
12	i	2'..	1/2,0,z [u,v,0]	0,1/2,z [ $\bar{v}$ ,u-v,0]	1/2,1/2,z [ $\bar{u}+v,\bar{u},0]$	
			0,1/2, $\bar{z}+1/2 [\bar{v},\bar{u},0]$	1/2,0, $\bar{z}+1/2 [\bar{u}+v,v,0]$	1/2,1/2, $\bar{z}+1/2 [u,u-v,0]$	
			1/2,0, $\bar{z} [u,v,0]$	0,1/2, $\bar{z} [\bar{v},u-v,0]$	1/2,1/2, $\bar{z} [\bar{u}+v,\bar{u},0]$	
			0,1/2,z+1/2 [ $\bar{v},\bar{u},0]$	1/2,0,z+1/2 [ $\bar{u}+v,v,0]$	1/2,1/2,z+1/2 [u,u-v,0]	
8	h	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0, $\bar{w}]$	2/3,1/3, $\bar{z}+1/2 [0,0,w]$	1/3,2/3, $\bar{z}+1/2 [0,0,\bar{w}]$
			2/3,1/3, $\bar{z} [0,0,w]$	1/3,2/3, $\bar{z} [0,0,\bar{w}]$	1/3,2/3,z+1/2 [0,0,w]	2/3,1/3,z+1/2 [0,0, $\bar{w}]$
6	g	2'/m'..	1/2,0,0 [u,v,0]	0,1/2,0 [ $\bar{v}$ ,u-v,0]	1/2,1/2,0 [ $\bar{u}+v,\bar{u},0]$	
			0,1/2,1/2 [ $\bar{v},\bar{u},0]$	1/2,0,1/2 [ $\bar{u}+v,v,0]$	1/2,1/2,1/2 [u,u-v,0]	
6	f	2'2'2	1/2,0,1/4 [u,2u,0]	0,1/2,1/4 [2 $\bar{u}$ , $\bar{u},0]$	1/2,1/2,1/4 [u, $\bar{u},0]$	
			1/2,0,3/4 [u,2u,0]	0,1/2,3/4 [2 $\bar{u}$ , $\bar{u},0]$	1/2,1/2,3/4 [u, $\bar{u},0]$	
4	e	6'..	0,0,z [0,0,0]	0,0, $\bar{z}+1/2 [0,0,0]$	0,0, $\bar{z} [0,0,0]$	0,0,z+1/2 [0,0,0]
4	d	$\bar{6}'..$	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]	2/3,1/3,1/2 [0,0,0]	1/3,2/3,1/2 [0,0,0]
4	c	3.2	1/3,2/3,1/4 [0,0,0]	2/3,1/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]	1/3,2/3,3/4 [0,0,0]
2	b	6'/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
2	a	6'2'2	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

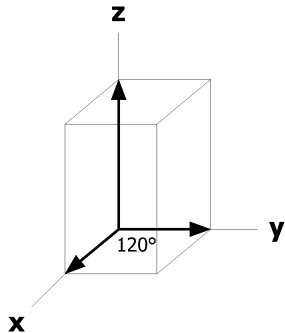
### Symmetry of Special Projections

Along [0,0,1] p6'm'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,0,0

Along [2,1,0] p<sub>2a</sub>'2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/4

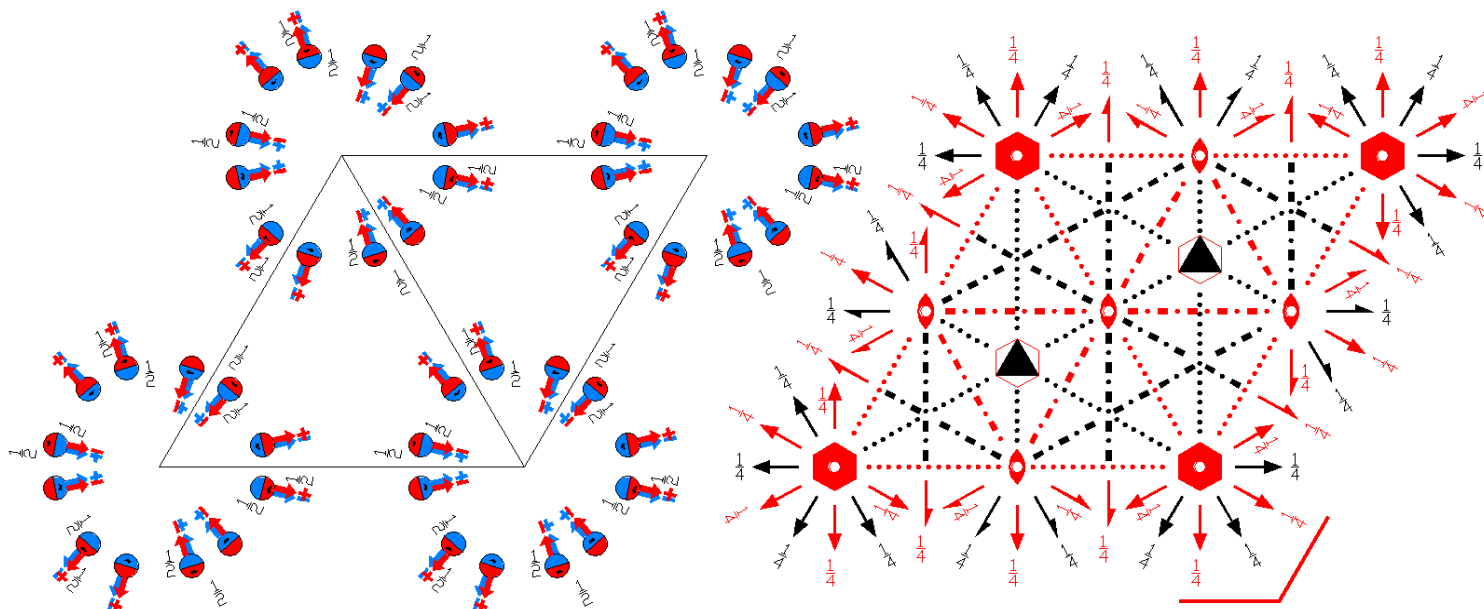




$P6'/m'cc'$   
192.7.1482

$6'/m'mm'$   
 $P6'/m'2/c2'/c'$

Hexagonal



Origin at center ( $6'/m'$ ) at  $6'/m'cc'$

**Asymmetric unit**  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $x \leq (1+y)/2$ ;  $y \leq \min(1-x, x)$

Vertices  $0,0,0$   $1/2,0,0$   $2/3,1/3,0$   $1/2,1/2,0$   
 $0,0,1/4$   $1/2,0,1/4$   $2/3,1/3,1/4$   $1/2,1/2,1/4$

### Symmetry Operations

- |   |  |  |
|---|--|--|
| (1) 1<br>(1 0,0,0)                                | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)       | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)  |
| (4) $2'$ 0,0,z<br>( $2_z$  0,0,0)'                | (5) $6^-$ 0,0,z<br>( $6_z^{-1}$  0,0,0)' | (6) $6^+$ 0,0,z<br>( $6_z$  0,0,0)'      |
| (7) 2 x,x,1/4<br>( $2_{xy}$  0,0,1/2)             | (8) 2 x,0,1/4<br>( $2_x$  0,0,1/2)       | (9) 2 0,y,1/4<br>( $2_y$  0,0,1/2)       |
| (10) $2'$ $x, \bar{x}, 1/4$<br>( $2_3$  0,0,1/2)' | (11) $2'$ x,2x,1/4<br>( $2_2$  0,0,1/2)' | (12) $2'$ 2x,x,1/4<br>( $2_1$  0,0,1/2)' |

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)
(16) $m'$ x,y,0 ( $m_z$  0,0,1/2)'	(17) $\bar{6}^-$ 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,1/2)'	(18) $\bar{6}^+$ 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,1/2)'
(19) c (0,0,1/2) x, $\bar{x}$ ,z ( $m_{xy}$  0,0,1/2)	(20) c (0,0,1/2) x,2x,z ( $m_x$  0,0,1/2)	(21) c (0,0,1/2) 2x,x,z ( $m_y$  0,0,1/2)
(22) c' (0,0,1/2) x,x,z ( $m_3$  0,0,1/2)'	(23) c' (0,0,1/2) x,0,z ( $m_2$  0,0,1/2)'	(24) c' (0,0,1/2) 0,y,z ( $m_1$  0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	m	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y$ , $\bar{x}$ ,z [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z [u,v, $\bar{w}$ ]	(5) y, $\bar{x}+y$ ,z [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) x-y,x,z [ $\bar{u}+v$ , $\bar{u}$ , $\bar{w}$ ]
			(7) y,x, $\bar{z}+1/2$ [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y}$ , $\bar{z}+1/2$ [u-v, $\bar{v}$ , $\bar{w}$ ]	(9) $\bar{x}$ , $\bar{x}+y$ , $\bar{z}+1/2$ [ $\bar{u}$ , $\bar{u}+v$ , $\bar{w}$ ]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}+1/2$ [v,u,w]	(11) $\bar{x}+y$ ,y, $\bar{z}+1/2$ [u-v, $\bar{v}$ ,w]	(12) x,x-y, $\bar{z}+1/2$ [ $\bar{u}$ , $\bar{u}+v$ ,w]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(14) y, $\bar{x}+y$ , $\bar{z}$ [ $\bar{v}$ ,u-v,w]	(15) x-y,x, $\bar{z}$ [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(16) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(17) $\bar{y}$ ,x-y, $\bar{z}$ [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(18) $\bar{x}+y$ , $\bar{x}$ , $\bar{z}$ [ $\bar{u}+v$ , $\bar{u}$ , $\bar{w}$ ]
			(19) $\bar{y}$ , $\bar{x}$ ,z+1/2 [v,u, $\bar{w}$ ]	(20) $\bar{x}+y$ ,y,z+1/2 [u-v, $\bar{v}$ , $\bar{w}$ ]	(21) x,x-y,z+1/2 [ $\bar{u}$ , $\bar{u}+v$ , $\bar{w}$ ]
			(22) y,x,z+1/2 [v,u,w]	(23) x-y, $\bar{y}$ ,z+1/2 [u-v, $\bar{v}$ ,w]	(24) $\bar{x}$ , $\bar{x}+y$ ,z+1/2 [ $\bar{u}$ , $\bar{u}+v$ ,w]
12	l	m'..	x,y,0 [u,v,0]	$\bar{y}$ ,x-y,0 [ $\bar{v}$ ,u-v,0]	$\bar{x}+y$ , $\bar{x}$ ,0 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			$\bar{x}$ , $\bar{y}$ ,0 [u,v,0]	y, $\bar{x}+y$ ,0 [ $\bar{v}$ ,u-v,0]	x-y,x,0 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			y,x,1/2 [v,u,0]	x-y, $\bar{y}$ ,1/2 [u-v, $\bar{v}$ ,0]	$\bar{x}$ , $\bar{x}+y$ ,1/2 [ $\bar{u}$ , $\bar{u}+v$ ,0]
			$\bar{y}$ , $\bar{x}$ ,1/2 [v,u,0]	$\bar{x}+y$ ,y,1/2 [u-v, $\bar{v}$ ,0]	x,x-y,1/2 [ $\bar{u}$ , $\bar{u}+v$ ,0]
12	k	..2'	x,2x,1/4 [u,0,w]	2 $\bar{x}$ , $\bar{x}$ ,1/4 [0,u,w]	x, $\bar{x}$ ,1/4 [ $\bar{u}$ , $\bar{u}$ ,w]
			$\bar{x}$ ,2 $\bar{x}$ ,1/4 [u,0, $\bar{w}$ ]	2x,x,1/4 [0,u, $\bar{w}$ ]	$\bar{x}$ ,x,1/4 [ $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]
			$\bar{x}$ ,2 $\bar{x}$ ,3/4 [u,0,w]	2x,x,3/4 [0,u,w]	$\bar{x}$ ,x,3/4 [ $\bar{u}$ , $\bar{u}$ ,w]
			x,2x,3/4 [u,0, $\bar{w}$ ]	2 $\bar{x}$ , $\bar{x}$ ,3/4 [0,u, $\bar{w}$ ]	x, $\bar{x}$ ,3/4 [ $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]

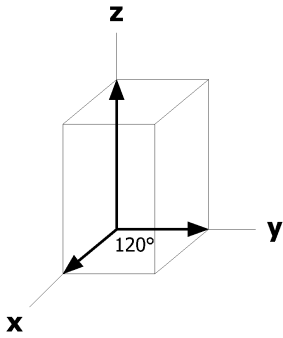
Continued			192.7.1482			P6'/m'cc'		
12	j	.2.	x,0,1/4 [u,0,0]	0,x,1/4 [0,u,0]	$\bar{x},\bar{x},1/4 [\bar{u},\bar{u},0]$			
			$\bar{x},0,1/4 [u,0,0]$	0, $\bar{x},1/4 [0,u,0]$	x,x,1/4 [ $\bar{u},\bar{u},0]$			
			$\bar{x},0,3/4 [u,0,0]$	0, $\bar{x},3/4 [0,u,0]$	x,x,3/4 [ $\bar{u},\bar{u},0]$			
			x,0,3/4 [u,0,0]	0,x,3/4 [0,u,0]	$\bar{x},\bar{x},3/4 [\bar{u},\bar{u},0]$			
12	i	2'..	1/2,0,z [u,v,0]	0,1/2,z [ $\bar{v},u-v,0]$	1/2,1/2,z [ $\bar{u}+v,\bar{u},0]$			
			0,1/2, $\bar{z}+1/2 [v,u,0]$	1/2,0, $\bar{z}+1/2 [u-v,\bar{v},0]$	1/2,1/2, $\bar{z}+1/2 [\bar{u},\bar{u}+v,0]$			
			1/2,0, $\bar{z} [u,v,0]$	0,1/2, $\bar{z} [\bar{v},u-v,0]$	1/2,1/2, $\bar{z} [\bar{u}+v,\bar{u},0]$			
			0,1/2,z+1/2 [v,u,0]	1/2,0,z+1/2 [u-v, $\bar{v},0]$	1/2,1/2,z+1/2 [ $\bar{u},\bar{u}+v,0]$			
8	h	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}+1/2 [0,0,\bar{w}]$	1/3,2/3, $\bar{z}+1/2 [0,0,w]$		
			2/3,1/3, $\bar{z} [0,0,w]$	1/3,2/3, $\bar{z} [0,0,\bar{w}]$	1/3,2/3,z+1/2 [0,0, $\bar{w}]$	2/3,1/3,z+1/2 [0,0,w]		
6	g	2'/m'..	1/2,0,0 [u,v,0]	0,1/2,0 [ $\bar{v},u-v,0]$	1/2,1/2,0 [ $\bar{u}+v,\bar{u},0]$			
			0,1/2,1/2 [v,u,0]	1/2,0,1/2 [u-v, $\bar{v},0]$	1/2,1/2,1/2 [ $\bar{u},\bar{u}+v,0]$			
6	f	2'22'	1/2,0,1/4 [u,0,0]	0,1/2,1/4 [0,u,0]	1/2,1/2,1/4 [ $\bar{u},\bar{u},0]$			
			1/2,0,3/4 [u,0,0]	0,1/2,3/4 [0,u,0]	1/2,1/2,3/4 [ $\bar{u},\bar{u},0]$			
4	e	6'..	0,0,z [0,0,0]	0,0, $\bar{z}+1/2 [0,0,0]$	0,0, $\bar{z} [0,0,0]$	0,0,z+1/2 [0,0,0]		
4	d	$\bar{6}'..$	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]	2/3,1/3,1/2 [0,0,0]	1/3,2/3,1/2 [0,0,0]		
4	c	3.2'	1/3,2/3,1/4 [0,0,w]	2/3,1/3,1/4 [0,0, $\bar{w}]$	2/3,1/3,3/4 [0,0,w]	1/3,2/3,3/4 [0,0, $\bar{w}]$		
2	b	6'/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]				
2	a	6'22'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]				

### Symmetry of Special Projections

Along [0,0,1] p6'mm'  
 $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>'2'm'm  
 $\mathbf{a}^* = \mathbf{c}/2 \quad \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/4

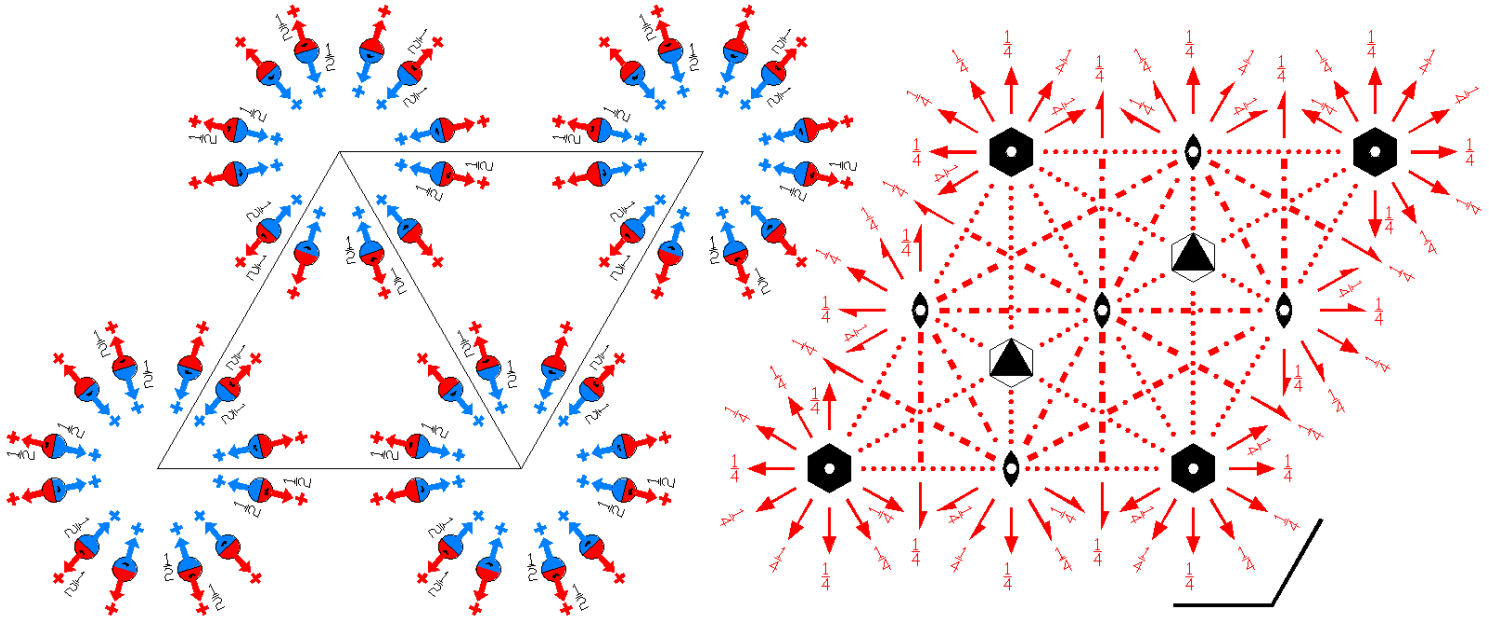
Along [2,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{b}/2 \quad \mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x/2,0



P6/mc'c'  
192.8.1483

6/mm'm'  
P6/m2'/c2'/c'

Hexagonal



Origin at center (6/m) at 6/mc'c'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/2,1/2,1/4	

### Symmetry Operations

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                             | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)         | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'  | (8) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'                      | (9) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'                      |
| (10) 2' x,x̄,1/4<br>(2 <sub>3</sub>  0,0,1/2)' | (11) 2' x,2x,1/4<br>(2 <sub>2</sub>  0,0,1/2)'                    | (12) 2' 2x,x,1/4<br>(2 <sub>1</sub>  0,0,1/2)'                    |

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)
(16) m $x,y,0$ ( $m_z$  0,0,1/2)	(17) $\bar{6}^-$ 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,1/2)	(18) $\bar{6}^+$ 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,1/2)
(19) c' (0,0,1/2) $x,\bar{x},z$ ( $m_{xy}$  0,0,1/2)'	(20) c' (0,0,1/2) $x,2x,z$ ( $m_x$  0,0,1/2)'	(21) c' (0,0,1/2) $2x,x,z$ ( $m_y$  0,0,1/2)'
(22) c' (0,0,1/2) $x,x,z$ ( $m_3$  0,0,1/2)'	(23) c' (0,0,1/2) $x,0,z$ ( $m_2$  0,0,1/2)'	(24) c' (0,0,1/2) $0,y,z$ ( $m_1$  0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	m	1	(1) $x,y,z$ [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(5) $y,\bar{x}+y,z$ [ $v,\bar{u}+v,w$ ]	(6) $x-y,x,z$ [u-v,u,w]
			(7) $y,x,\bar{z}+1/2$ [ $\bar{v},\bar{u},w$ ]	(8) $x-y,\bar{y},\bar{z}+1/2$ [ $\bar{u}+v,v,w$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}+1/2$ [u,u-v,w]
			(10) $\bar{y},\bar{x},\bar{z}+1/2$ [v,u,w]	(11) $\bar{x}+y,y,\bar{z}+1/2$ [u-v, $\bar{v},w$ ]	(12) $x,x-y,\bar{z}+1/2$ [ $\bar{u},\bar{u}+v,w$ ]
			(13) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(14) $y,\bar{x}+y,\bar{z}$ [ $\bar{v},u-v,w$ ]	(15) $x-y,x,\bar{z}$ [ $\bar{u}+v,\bar{u},w$ ]
			(16) $x,y,\bar{z}$ [ $\bar{u},\bar{v},w$ ]	(17) $\bar{y},x-y,\bar{z}$ [ $v,\bar{u}+v,w$ ]	(18) $\bar{x}+y,\bar{x},\bar{z}$ [u-v,u,w]
			(19) $\bar{y},\bar{x},z+1/2$ [ $\bar{v},\bar{u},w$ ]	(20) $\bar{x}+y,y,z+1/2$ [ $\bar{u}+v,v,w$ ]	(21) $x,x-y,z+1/2$ [u,u-v,w]
			(22) $y,x,z+1/2$ [v,u,w]	(23) $x-y,\bar{y},z+1/2$ [u-v, $\bar{v},w$ ]	(24) $\bar{x},\bar{x}+y,z+1/2$ [ $\bar{u},\bar{u}+v,w$ ]
12	l	m..	$x,y,0$ [0,0,w]	$\bar{y},x-y,0$ [0,0,w]	$\bar{x}+y,\bar{x},0$ [0,0,w]
			$\bar{x},\bar{y},0$ [0,0,w]	$y,\bar{x}+y,0$ [0,0,w]	$x-y,x,0$ [0,0,w]
			$y,x,1/2$ [0,0,w]	$x-y,\bar{y},1/2$ [0,0,w]	$\bar{x},\bar{x}+y,1/2$ [0,0,w]
			$\bar{y},\bar{x},1/2$ [0,0,w]	$\bar{x}+y,y,1/2$ [0,0,w]	$x,x-y,1/2$ [0,0,w]
12	k	..2'	$x,2x,1/4$ [u,0,w]	$2\bar{x},\bar{x},1/4$ [0,u,w]	$x,\bar{x},1/4$ [ $\bar{u},\bar{u},w$ ]
			$\bar{x},2\bar{x},1/4$ [ $\bar{u},0,w$ ]	$2x,x,1/4$ [0, $\bar{u},w$ ]	$\bar{x},x,1/4$ [u,u,w]
			$\bar{x},2\bar{x},3/4$ [u,0,w]	$2x,x,3/4$ [0,u,w]	$\bar{x},x,3/4$ [ $\bar{u},\bar{u},w$ ]
			$x,2x,3/4$ [ $\bar{u},0,w$ ]	$2\bar{x},\bar{x},3/4$ [0, $\bar{u},w$ ]	$x,\bar{x},3/4$ [u,u,w]

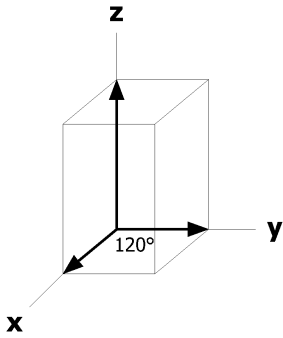
Continued			192.8.1483			P6/mc'c'		
12	j	.2'	x,0,1/4 [u,2u,w]	0,x,1/4 [2 $\bar{u}$ , $\bar{u}$ ,w]	$\bar{x},\bar{x},1/4 [u,\bar{u},w]$	$\bar{x},\bar{x},1/4 [u,\bar{u},w]$	$\bar{x},\bar{x},1/4 [u,\bar{u},w]$	$\bar{x},\bar{x},1/4 [u,\bar{u},w]$
			$\bar{x},0,1/4 [\bar{u},2\bar{u},w]$	0, $\bar{x},1/4 [2u,u,w]$	x,x,1/4 [ $\bar{u}$ ,u,w]	x,x,1/4 [ $\bar{u}$ ,u,w]	x,x,1/4 [ $\bar{u}$ ,u,w]	x,x,1/4 [ $\bar{u}$ ,u,w]
			$\bar{x},0,3/4 [u,2u,w]$	0, $\bar{x},3/4 [2\bar{u},\bar{u},w]$	x,x,3/4 [u, $\bar{u}$ ,w]	x,x,3/4 [u, $\bar{u}$ ,w]	x,x,3/4 [u, $\bar{u}$ ,w]	x,x,3/4 [u, $\bar{u}$ ,w]
			x,0,3/4 [ $\bar{u},2\bar{u},w]$	0,x,3/4 [2u,u,w]	$\bar{x},\bar{x},3/4 [\bar{u},u,w]$	$\bar{x},\bar{x},3/4 [\bar{u},u,w]$	$\bar{x},\bar{x},3/4 [\bar{u},u,w]$	$\bar{x},\bar{x},3/4 [\bar{u},u,w]$
12	i	2..	1/2,0,z [0,0,w]	0,1/2,z [0,0,w]	1/2,1/2,z [0,0,w]	1/2,1/2,z [0,0,w]	1/2,1/2,z [0,0,w]	1/2,1/2,z [0,0,w]
			0,1/2, $\bar{z}+1/2 [0,0,w]$	1/2,0, $\bar{z}+1/2 [0,0,w]$	1/2,1/2, $\bar{z}+1/2 [0,0,w]$	1/2,1/2, $\bar{z}+1/2 [0,0,w]$	1/2,1/2, $\bar{z}+1/2 [0,0,w]$	1/2,1/2, $\bar{z}+1/2 [0,0,w]$
			1/2,0, $\bar{z} [0,0,w]$	0,1/2, $\bar{z} [0,0,w]$	1/2,1/2, $\bar{z} [0,0,w]$	1/2,1/2, $\bar{z} [0,0,w]$	1/2,1/2, $\bar{z} [0,0,w]$	1/2,1/2, $\bar{z} [0,0,w]$
			0,1/2,z+1/2 [0,0,w]	1/2,0,z+1/2 [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2,z+1/2 [0,0,w]	1/2,1/2,z+1/2 [0,0,w]
8	h	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0,w]	2/3,1/3, $\bar{z}+1/2 [0,0,w]$	1/3,2/3, $\bar{z}+1/2 [0,0,w]$	1/3,2/3, $\bar{z}+1/2 [0,0,w]$	1/3,2/3, $\bar{z}+1/2 [0,0,w]$
			2/3,1/3, $\bar{z} [0,0,w]$	1/3,2/3, $\bar{z} [0,0,w]$	1/3,2/3,z+1/2 [0,0,w]	2/3,1/3,z+1/2 [0,0,w]	2/3,1/3,z+1/2 [0,0,w]	2/3,1/3,z+1/2 [0,0,w]
6	g	2/m..	1/2,0,0 [0,0,w]	0,1/2,0 [0,0,w]	1/2,1/2,0 [0,0,w]	1/2,1/2,0 [0,0,w]	1/2,1/2,0 [0,0,w]	1/2,1/2,0 [0,0,w]
			0,1/2,1/2 [0,0,w]	1/2,0,1/2 [0,0,w]	1/2,1/2,1/2 [0,0,w]	1/2,1/2,1/2 [0,0,w]	1/2,1/2,1/2 [0,0,w]	1/2,1/2,1/2 [0,0,w]
6	f	22'2'	1/2,0,1/4 [0,0,w]	0,1/2,1/4 [0,0,w]	1/2,1/2,1/4 [0,0,w]	1/2,1/2,1/4 [0,0,w]	1/2,1/2,1/4 [0,0,w]	1/2,1/2,1/4 [0,0,w]
			1/2,0,3/4 [0,0,w]	0,1/2,3/4 [0,0,w]	1/2,1/2,3/4 [0,0,w]	1/2,1/2,3/4 [0,0,w]	1/2,1/2,3/4 [0,0,w]	1/2,1/2,3/4 [0,0,w]
4	e	6..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2 [0,0,w]$	0,0, $\bar{z} [0,0,w]$	0,0,z+1/2 [0,0,w]	0,0,z+1/2 [0,0,w]	0,0,z+1/2 [0,0,w]
4	d	$\bar{6}$ ..	1/3,2/3,0 [0,0,w]	2/3,1/3,0 [0,0,w]	2/3,1/3,1/2 [0,0,w]	1/3,2/3,1/2 [0,0,w]	1/3,2/3,1/2 [0,0,w]	1/3,2/3,1/2 [0,0,w]
4	c	3.2'	1/3,2/3,1/4 [0,0,w]	2/3,1/3,1/4 [0,0,w]	2/3,1/3,3/4 [0,0,w]	1/3,2/3,3/4 [0,0,w]	1/3,2/3,3/4 [0,0,w]	1/3,2/3,3/4 [0,0,w]
2	b	6/m..	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]				
2	a	62'2'	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]				

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,0

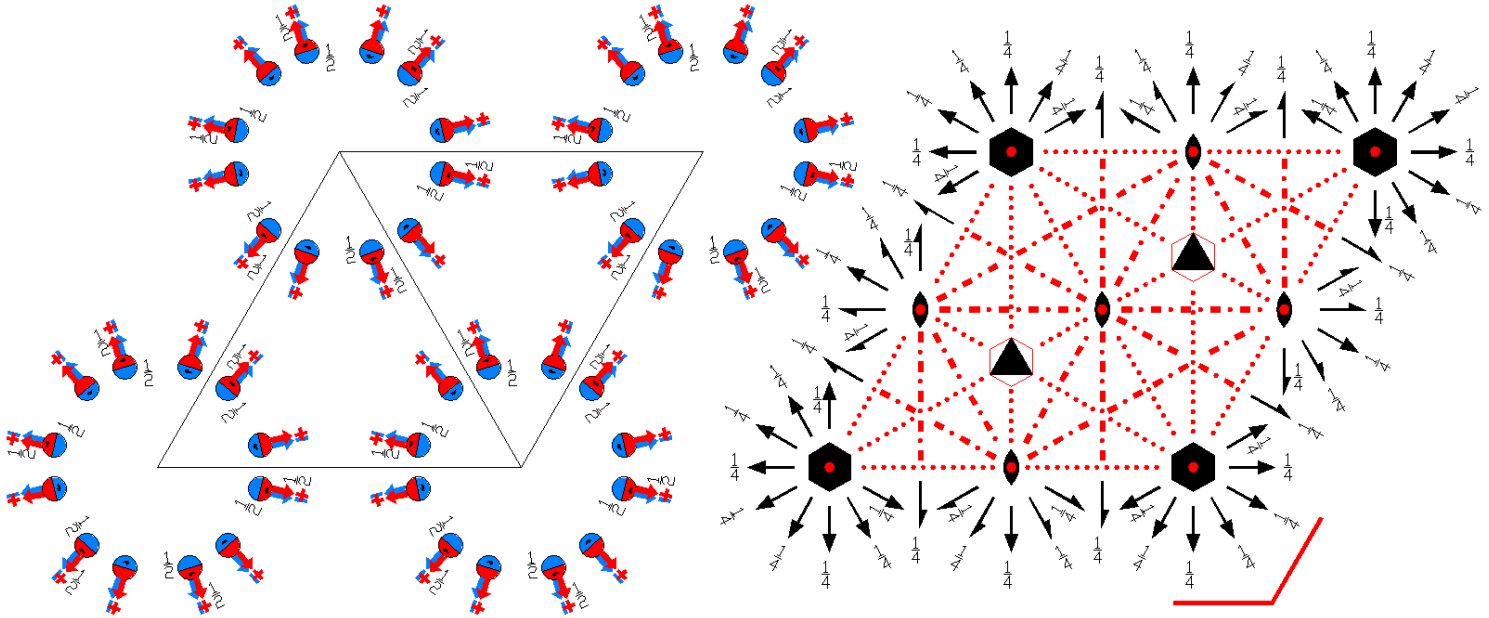
Along [2,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,x/2,0



P6/m'c'c'  
192.9.1484

6/m'm'm'  
P6/m'2/c'2/c'

Hexagonal



Origin at center (6/m') at 6/m'c'c'

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, x)$
Vertices	0,0,0 0,0,1/4	1/2,0,0 1/2,0,1/4	2/3,1/3,0 2/3,1/3,1/4	1/2,1/2,0 1/2,1/2,1/4	

**Symmetry Operations**

- |  |   |   |
|--|---|---|
| (1) 1<br>(1 0,0,0)                           | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)               | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0) |
| (4) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)       | (5) 6 <sup>-</sup> 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,0) | (6) 6 <sup>+</sup> 0,0,z<br>(6 <sub>z</sub>  0,0,0)               |
| (7) 2 x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)  | (8) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)                        | (9) 2 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)                        |
| (10) 2 x,x̄,1/4<br>(2 <sub>3</sub>  0,0,1/2) | (11) 2 x,2x,1/4<br>(2 <sub>2</sub>  0,0,1/2)                      | (12) 2 2x,x,1/4<br>(2 <sub>1</sub>  0,0,1/2)                      |

(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ ' 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(15) $\bar{3}^-$ ' 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(16) $m'$ x,y,0 ( $m_z$  0,0,1/2)'	(17) $\bar{6}^-$ ' 0,0,z; 0,0,0 ( $\bar{6}_z^{-1}$  0,0,1/2)'	(18) $\bar{6}^+$ ' 0,0,z; 0,0,0 ( $\bar{6}_z$  0,0,1/2)'
(19) $c'$ (0,0,1/2) x, $\bar{x}$ ,z ( $m_{xy}$  0,0,1/2)'	(20) $c'$ (0,0,1/2) x,2x,z ( $m_x$  0,0,1/2)'	(21) $c'$ (0,0,1/2) 2x,x,z ( $m_y$  0,0,1/2)'
(22) $c'$ (0,0,1/2) x,x,z ( $m_3$  0,0,1/2)'	(23) $c'$ (0,0,1/2) x,0,z ( $m_2$  0,0,1/2)'	(24) $c'$ (0,0,1/2) 0,y,z ( $m_1$  0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	m	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y$ , $\bar{x}$ ,z [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w]	(5) y, $\bar{x}+y$ ,z [v, $\bar{u}+v$ ,w]	(6) x-y,x,z [u-v,u,w]
			(7) y,x, $\bar{z}+1/2$ [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y}$ , $\bar{z}+1/2$ [u-v, $\bar{v}$ , $\bar{w}$ ]	(9) $\bar{x}$ , $\bar{x}+y$ , $\bar{z}+1/2$ [ $\bar{u}$ , $\bar{u}+v$ , $\bar{w}$ ]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}+1/2$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(11) $\bar{x}+y$ ,y, $\bar{z}+1/2$ [ $\bar{u}+v$ ,v, $\bar{w}$ ]	(12) x,x-y, $\bar{z}+1/2$ [u,u-v, $\bar{w}$ ]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(14) y, $\bar{x}+y$ , $\bar{z}$ [v, $\bar{u}+v$ , $\bar{w}$ ]	(15) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ]
			(16) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(17) $\bar{y}$ ,x-y, $\bar{z}$ [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(18) $\bar{x}+y$ , $\bar{x}$ , $\bar{z}$ [ $\bar{u}+v$ , $\bar{u}$ , $\bar{w}$ ]
			(19) $\bar{y}$ , $\bar{x}$ ,z+1/2 [ $\bar{v}$ , $\bar{u}$ ,w]	(20) $\bar{x}+y$ ,y,z+1/2 [ $\bar{u}+v$ ,v,w]	(21) x,x-y,z+1/2 [u,u-v,w]
			(22) y,x,z+1/2 [v,u,w]	(23) x-y, $\bar{y}$ ,z+1/2 [u-v, $\bar{v}$ ,w]	(24) $\bar{x}$ , $\bar{x}+y$ ,z+1/2 [ $\bar{u}$ , $\bar{u}+v$ ,w]
12	l	m'..	x,y,0 [u,v,0]	$\bar{y}$ ,x-y,0 [ $\bar{v}$ ,u-v,0]	$\bar{x}+y$ , $\bar{x}$ ,0 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			$\bar{x}$ , $\bar{y}$ ,0 [ $\bar{u}$ , $\bar{v}$ ,0]	y, $\bar{x}+y$ ,0 [v, $\bar{u}+v$ ,0]	x-y,x,0 [u-v,u,0]
			y,x,1/2 [ $\bar{u}$ , $\bar{v}$ ,0]	x-y, $\bar{y}$ ,1/2 [v, $\bar{u}+v$ ,0]	$\bar{x}$ , $\bar{x}+y$ ,1/2 [u-v,u,0]
			$\bar{y}$ , $\bar{x}$ ,1/2 [u,v,0]	$\bar{x}+y$ ,y,1/2 [ $\bar{v}$ ,u-v,0]	x,x-y,1/2 [ $\bar{u}+v$ , $\bar{u}$ ,0]
12	k	..2	x,2x,1/4 [u,2u,0]	2 $\bar{x}$ , $\bar{x}$ ,1/4 [2 $\bar{u}$ , $\bar{u}$ ,0]	x, $\bar{x}$ ,1/4 [u, $\bar{u}$ ,0]
			$\bar{x}$ ,2 $\bar{x}$ ,1/4 [ $\bar{u}$ ,2 $\bar{u}$ ,0]	2x,x,1/4 [2u,u,0]	$\bar{x}$ ,x,1/4 [ $\bar{u}$ ,u,0]
			$\bar{x}$ ,2 $\bar{x}$ ,3/4 [ $\bar{u}$ ,2 $\bar{u}$ ,0]	2x,x,3/4 [2u,u,0]	$\bar{x}$ ,x,3/4 [ $\bar{u}$ ,u,0]
			x,2x,3/4 [u,2u,0]	2 $\bar{x}$ , $\bar{x}$ ,3/4 [2 $\bar{u}$ , $\bar{u}$ ,0]	x, $\bar{x}$ ,3/4 [u, $\bar{u}$ ,0]



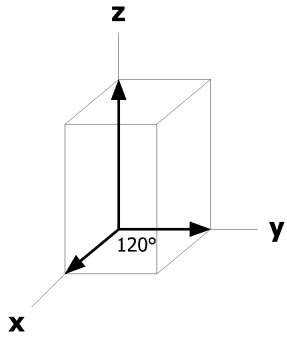
Continued			192.9.1484			P6/m'c'c'		
12	j	.2.	x,0,1/4 [u,0,0]	0,x,1/4 [0,u,0]	$\bar{x},\bar{x},1/4 [\bar{u},\bar{u},0]$			
			$\bar{x},0,1/4 [\bar{u},0,0]$	0, $\bar{x},1/4 [0,\bar{u},0]$	x,x,1/4 [u,u,0]			
			$\bar{x},0,3/4 [\bar{u},0,0]$	0, $\bar{x},3/4 [0,\bar{u},0]$	x,x,3/4 [u,u,0]			
			x,0,3/4 [u,0,0]	0,x,3/4 [0,u,0]	$\bar{x},\bar{x},3/4 [\bar{u},\bar{u},0]$			
12	i	2..	1/2,0,z [0,0,w]	0,1/2,z [0,0,w]	1/2,1/2,z [0,0,w]			
			0,1/2, $\bar{z}+1/2 [0,0,\bar{w}]$	1/2,0, $\bar{z}+1/2 [0,0,\bar{w}]$	1/2,1/2, $\bar{z}+1/2 [0,0,\bar{w}]$			
			1/2,0, $\bar{z} [0,0,\bar{w}]$	0,1/2, $\bar{z} [0,0,\bar{w}]$	1/2,1/2, $\bar{z} [0,0,\bar{w}]$			
			0,1/2,z+1/2 [0,0,w]	1/2,0,z+1/2 [0,0,w]	1/2,1/2,z+1/2 [0,0,w]			
8	h	3..	1/3,2/3,z [0,0,w]	2/3,1/3,z [0,0,w]	2/3,1/3, $\bar{z}+1/2 [0,0,\bar{w}]$	1/3,2/3, $\bar{z}+1/2 [0,0,\bar{w}]$		
			2/3,1/3, $\bar{z} [0,0,\bar{w}]$	1/3,2/3, $\bar{z} [0,0,\bar{w}]$	1/3,2/3,z+1/2 [0,0,w]	2/3,1/3,z+1/2 [0,0,w]		
6	g	2/m'..	1/2,0,0 [0,0,w]	0,1/2,0 [0,0,w]	1/2,1/2,0 [0,0,w]			
			0,1/2,1/2 [0,0, $\bar{w}]$	1/2,0,1/2 [0,0, $\bar{w}]$	1/2,1/2,1/2 [0,0, $\bar{w}]$			
6	f	222	1/2,0,1/4 [0,0,0]	0,1/2,1/4 [0,0,0]	1/2,1/2,1/4 [0,0,0]			
			1/2,0,3/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,1/2,3/4 [0,0,0]			
4	e	6..	0,0,z [0,0,w]	0,0, $\bar{z}+1/2 [0,0,\bar{w}]$	0,0, $\bar{z} [0,0,\bar{w}]$	0,0,z+1/2 [0,0,w]		
4	d	$\bar{6}'..$	1/3,2/3,0 [0,0,0]	2/3,1/3,0 [0,0,0]	2/3,1/3,1/2 [0,0,0]	1/3,2/3,1/2 [0,0,0]		
4	c	3.2	1/3,2/3,1/4 [0,0,0]	2/3,1/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]	1/3,2/3,3/4 [0,0,0]		
2	b	6/m'..	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]				
2	a	622	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]				

### Symmetry of Special Projections

Along [0,0,1] p6m'm'  
 $\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2 \quad \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

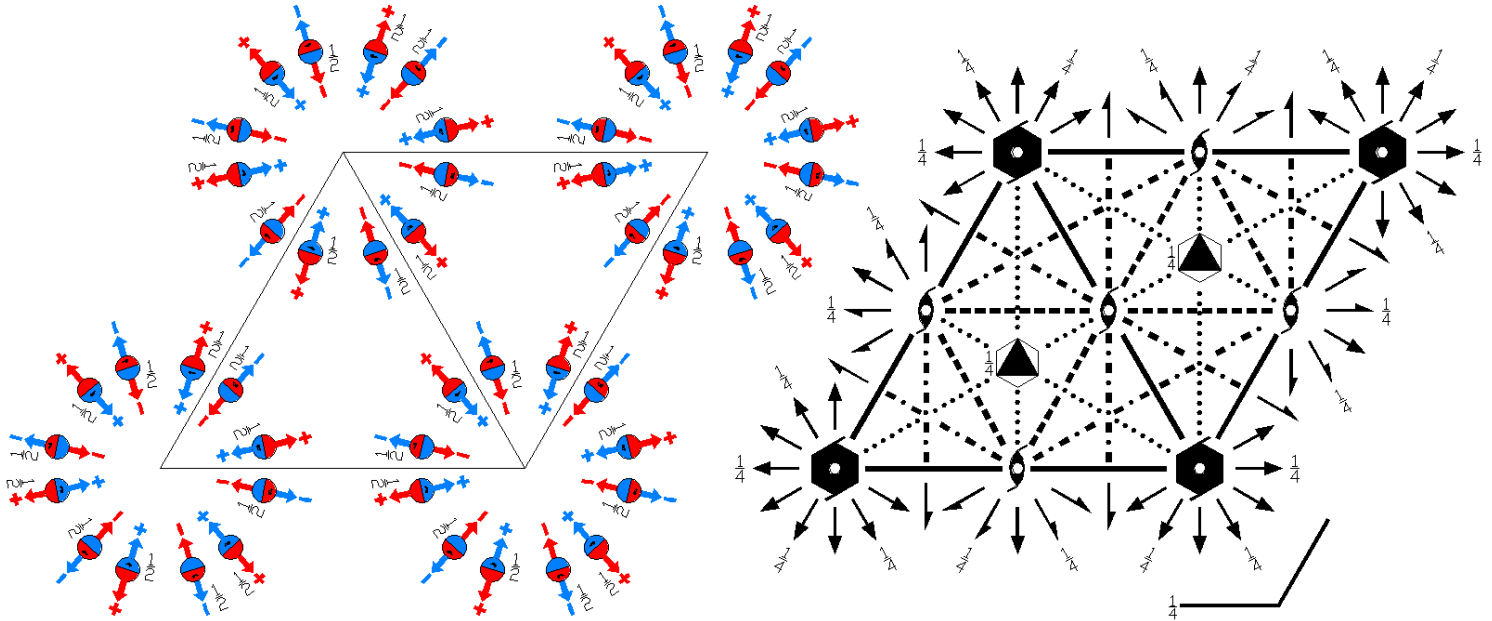
Along [2,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2 \quad \mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P6_3/mcm$   
193.1.1485

$6/mmm$   
 $P6_3/m2/c2/m$

Hexagonal



Origin at center ( $\bar{3}1m$ ) at  $\bar{3}c2/m$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/2,1/2,1/4	

### Symmetry Operations

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                         | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)        |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2) | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2) |
| (7) 2 x,x,1/4<br>( $2_{xy}$  0,0,1/2)      | (8) 2 x,0,1/4<br>( $2_x$  0,0,1/2)                  | (9) 2 0,y,1/4<br>( $2_y$  0,0,1/2)             |
| (10) 2 $x, \bar{x}, 0$<br>( $2_3$  0,0,0)  | (11) 2 x,2x,0<br>( $2_2$  0,0,0)                    | (12) 2 2x,x,0<br>( $2_1$  0,0,0)               |

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)
(16) m $\bar{x}$ ,y,1/4 ( $m_z$  0,0,1/2)	(17) $\bar{6}^-$ 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1}$  0,0,1/2)	(18) $\bar{6}^+$ 0,0,z; 0,0,1/4 ( $\bar{6}_z$  0,0,1/2)
(19) c (0,0,1/2) $\bar{x}$ , $\bar{x}$ ,z ( $m_{xy}$  0,0,1/2)	(20) c (0,0,1/2) $\bar{x}$ ,2 $\bar{x}$ ,z ( $m_x$  0,0,1/2)	(21) c (0,0,1/2) 2 $\bar{x}$ , $\bar{x}$ ,z ( $m_y$  0,0,1/2)
(22) m $\bar{x}$ ,x,z ( $m_3$  0,0,0)	(23) m $\bar{x}$ ,0,z ( $m_2$  0,0,0)	(24) m 0,y,z ( $m_1$  0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	l	1	(1) $\bar{x}$ ,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(5) y, $\bar{x}$ +y,z+1/2 [v, $\bar{u}$ +v,w]	(6) x-y,x,z+1/2 [u-v,u,w]
			(7) y,x, $\bar{z}$ +1/2 [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y}$ , $\bar{z}$ +1/2 [u-v, $\bar{v}$ , $\bar{w}$ ]	(9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(11) $\bar{x}$ +y,y, $\bar{z}$ [ $\bar{u}$ +v,v, $\bar{w}$ ]	(12) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(14) y, $\bar{x}$ +y, $\bar{z}$ [ $\bar{v}$ ,u-v,w]	(15) x-y,x, $\bar{z}$ [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(16) x,y, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(17) $\bar{y}$ ,x-y, $\bar{z}$ +1/2 [v, $\bar{u}$ +v,w]	(18) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ +1/2 [u-v,u,w]
			(19) $\bar{y}$ , $\bar{x}$ ,z+1/2 [v,u, $\bar{w}$ ]	(20) $\bar{x}$ +y,y,z+1/2 [u-v, $\bar{v}$ , $\bar{w}$ ]	(21) x,x-y,z+1/2 [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ]
			(22) y,x,z [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(23) x-y, $\bar{y}$ ,z [ $\bar{u}$ +v,v, $\bar{w}$ ]	(24) $\bar{x}$ , $\bar{x}$ +y,z [u,u-v, $\bar{w}$ ]
12	k	..m	x,0,z [u,2u,0]	0,x,z [2 $\bar{u}$ , $\bar{u}$ ,0]	$\bar{x}$ , $\bar{x}$ ,z [u, $\bar{u}$ ,0]
			$\bar{x}$ ,0,z+1/2 [ $\bar{u}$ ,2 $\bar{u}$ ,0]	0, $\bar{x}$ ,z+1/2 [2u,u,0]	x,x,z+1/2 [ $\bar{u}$ ,u,0]
			0,x, $\bar{z}$ +1/2 [2u,u,0]	x,0, $\bar{z}$ +1/2 [ $\bar{u}$ ,2 $\bar{u}$ ,0]	$\bar{x}$ , $\bar{x}$ , $\bar{z}$ +1/2 [ $\bar{u}$ ,u,0]
			0, $\bar{x}$ , $\bar{z}$ [2 $\bar{u}$ , $\bar{u}$ ,0]	$\bar{x}$ ,0, $\bar{z}$ [u,2u,0]	x,x, $\bar{z}$ [u, $\bar{u}$ ,0]
12	j	m..	x,y,1/4 [0,0,w]	$\bar{y}$ ,x-y,1/4 [0,0,w]	$\bar{x}$ +y, $\bar{x}$ ,1/4 [0,0,w]
			$\bar{x}$ , $\bar{y}$ ,3/4 [0,0,w]	y, $\bar{x}$ +y,3/4 [0,0,w]	x-y,x,3/4 [0,0,w]
			y,x,1/4 [0,0, $\bar{w}$ ]	x-y, $\bar{y}$ ,1/4 [0,0, $\bar{w}$ ]	$\bar{x}$ , $\bar{x}$ +y,1/4 [0,0, $\bar{w}$ ]
			$\bar{y}$ , $\bar{x}$ ,3/4 [0,0, $\bar{w}$ ]	$\bar{x}$ +y,y,3/4 [0,0, $\bar{w}$ ]	x,x-y,3/4 [0,0, $\bar{w}$ ]

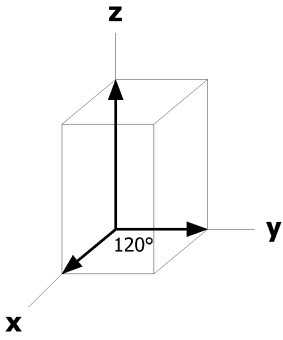
12	i	..2	x,2x,0 [u,2u,0] $\bar{x},2\bar{x},1/2 [\bar{u},2\bar{u},0]$ $\bar{x},2\bar{x},0 [u,2u,0]$ x,2x,1/2 [ $\bar{u},2\bar{u},0$ ]	$2\bar{x},\bar{x},0 [2\bar{u},\bar{u},0]$ 2x,x,1/2 [2u,u,0] 2x,x,0 [2 $\bar{u},\bar{u},0$ ] $2\bar{x},\bar{x},1/2 [2u,u,0]$	$x,\bar{x},0 [u,\bar{u},0]$ $\bar{x},x,1/2 [\bar{u},u,0]$ $\bar{x},x,0 [u,\bar{u},0]$ $x,\bar{x},1/2 [\bar{u},u,0]$	
8	h	3..	1/3,2/3,z [0,0,w] 2/3,1/3, $\bar{z}$ [0,0,w]	2/3,1/3,z+1/2 [0,0,w] 1/3,2/3, $\bar{z}+1/2$ [0,0,w]	2/3,1/3, $\bar{z}+1/2$ [0,0, $\bar{w}$ ] 1/3,2/3,z+1/2 [0,0, $\bar{w}$ ]	1/3,2/3, $\bar{z}$ [0,0, $\bar{w}$ ] 2/3,1/3,z [0,0, $\bar{w}$ ]
6	g	m2m	x,0,1/4 [0,0,0]	0,x,1/4 [0,0,0]	$\bar{x},\bar{x},1/4 [0,0,0]$	
6	f	..2/m	1/2,0,0 [u,2u,0] 1/2,0,1/2 [ $\bar{u},2\bar{u},0$ ]	0,1/2,0 [2 $\bar{u},\bar{u},0$ ] 0,1/2,1/2 [2u,u,0]	1/2,1/2,0 [u, $\bar{u},0$ ] 1/2,1/2,1/2 [ $\bar{u},u,0$ ]	
4	e	3.m	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	d	3.2	1/3,2/3,0 [0,0,0]	2/3,1/3,1/2 [0,0,0]	2/3,1/3,0 [0,0,0]	1/3,2/3,1/2 [0,0,0]
4	c	$\bar{6}..$	1/3,2/3,1/4 [0,0,w]	2/3,1/3,3/4 [0,0,w]	2/3,1/3,1/4 [0,0, $\bar{w}$ ]	1/3,2/3,3/4 [0,0, $\bar{w}$ ]
2	b	$\bar{3}.m$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
2	a	$\bar{6}2m$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/4

Along [2,1,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



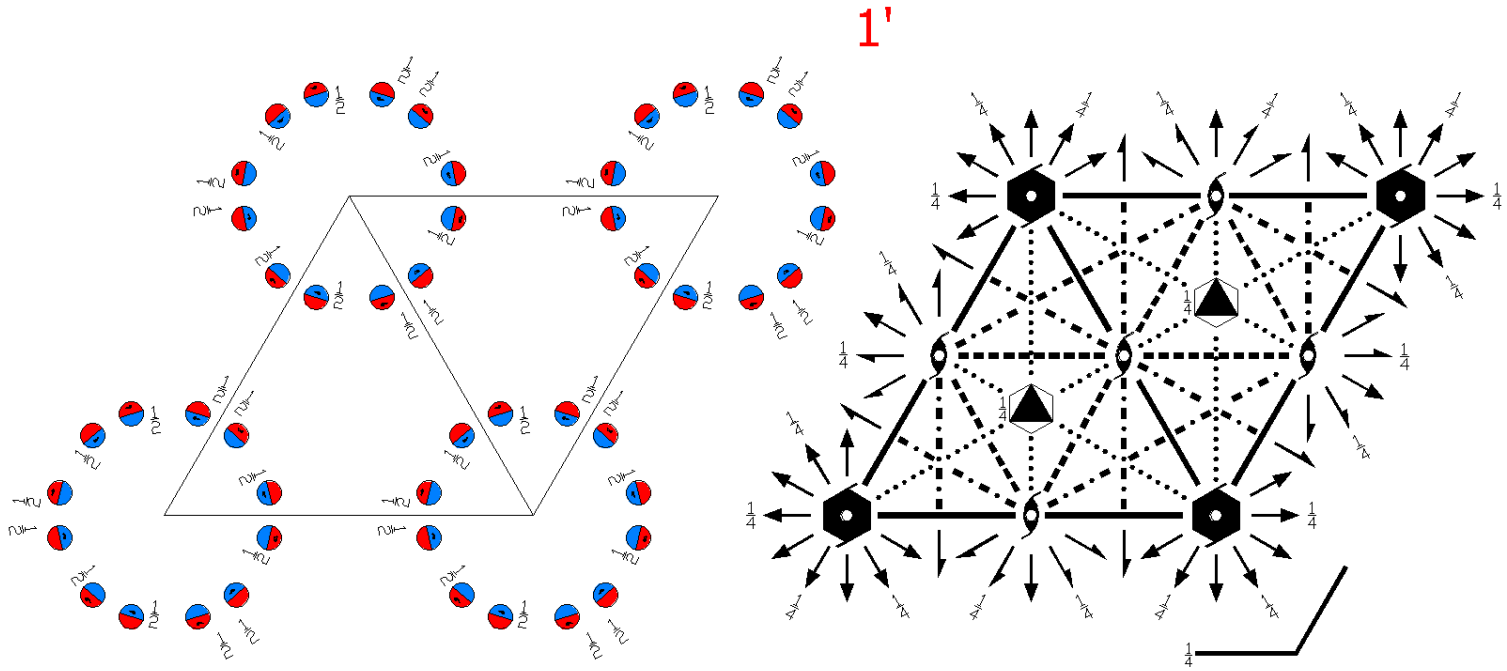
$P6_3/mcm1'$

193.2.1486

$6/mmm1'$

$P6_3/m2/c2/m1'$

Hexagonal



Origin at center ( $\bar{3}1m1'$ ) at  $\bar{3}c2/m1'$

Asymmetric unit  $0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad x \leq (1+y)/2; \quad y \leq \min(1-x, x)$

Vertices  $0,0,0 \quad 1/2,0,0 \quad 2/3,1/3,0 \quad 1/2,1/2,0$   
 $0,0,1/4 \quad 1/2,0,1/4 \quad 2/3,1/3,1/4 \quad 1/2,1/2,1/4$

**Symmetry Operations**

For 1 + set

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                         | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)        |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2) | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2) |
| (7) 2 x,x,1/4<br>( $2_{xy}$  0,0,1/2)      | (8) 2 x,0,1/4<br>( $2_x$  0,0,1/2)                  | (9) 2 0,y,1/4<br>( $2_y$  0,0,1/2)             |
| (10) 2 $x, \bar{x}, 0$<br>( $2_3$  0,0,0)  | (11) 2 x,2x,0<br>( $2_2$  0,0,0)                    | (12) 2 2x,x,0<br>( $2_1$  0,0,0)               |

- |  |   |   |
|--|---|---|
| (13) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)              | (14) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)          | (15) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (16) m x,y,1/4<br>( $m_z$  0,0,1/2)                      | (17) $\bar{6}^-$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2) | (18) $\bar{6}^+$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2)  |
| (19) c (0,0,1/2) x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,1/2) | (20) c (0,0,1/2) x,2x,z<br>( $m_x$  0,0,1/2)                    | (21) c (0,0,1/2) 2x,x,z<br>( $m_y$  0,0,1/2)                |
| (22) m x,x,z<br>( $m_3$  0,0,0)                          | (23) m x,0,z<br>( $m_2$  0,0,0)                                 | (24) m 0,y,z<br>( $m_1$  0,0,0)                             |

## For 1' + set

- |  |  |  |
|--|--|--|
| (1) 1'<br>(1 0,0,0)'                                       | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)'                           | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (4) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)'       | (5) 6 <sup>-</sup> (0,0,1/2) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' | (6) 6 <sup>+</sup> (0,0,1/2) 0,0,z<br>(6 <sub>z</sub>  0,0,1/2)'   |
| (7) 2' x,x,1/4<br>(2 <sub>xy</sub>  0,0,1/2)'              | (8) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'                                   | (9) 2' 0,y,1/4<br>(2 <sub>y</sub>  0,0,1/2)'                       |
| (10) 2' x, $\bar{x}$ ,0<br>(2 <sub>3</sub>  0,0,0)'        | (11) 2' x,2x,0<br>(2 <sub>2</sub>  0,0,0)'                                     | (12) 2' 2x,x,0<br>(2 <sub>1</sub>  0,0,0)'                         |
| (13) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)'             | (14) $\bar{3}^+$ ' 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)'                      | (15) $\bar{3}^-$ ' 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)'     |
| (16) m' x,y,1/4<br>( $m_z$  0,0,1/2)'                      | (17) $\bar{6}^-$ ' 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2)'             | (18) $\bar{6}^+$ ' 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2)'      |
| (19) c' (0,0,1/2) x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,1/2)' | (20) c' (0,0,1/2) x,2x,z<br>( $m_x$  0,0,1/2)'                                 | (21) c' (0,0,1/2) 2x,x,z<br>( $m_y$  0,0,1/2)'                     |
| (22) m' x,x,z<br>( $m_3$  0,0,0)'                          | (23) m' x,0,z<br>( $m_2$  0,0,0)'  | (24) m' 0,y,z<br>( $m_1$  0,0,0)'                                  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

- |    |   |     | 1 +                                    | 1' +                                   |   |
|----|---|-----|--|--|---|
| 24 | I | 11' | (1) x,y,z [0,0,0]                      | (2) $\bar{y}$ ,x-y,z [0,0,0]           | (3) $\bar{x}+y,\bar{x},z$ [0,0,0]           |
|    |   |     | (4) $\bar{x},\bar{y},z+1/2$ [0,0,0]    | (5) y, $\bar{x}+y,z+1/2$ [0,0,0]       | (6) x-y,x,z+1/2 [0,0,0]                     |
|    |   |     | (7) y,x, $\bar{z}+1/2$ [0,0,0]         | (8) x-y, $\bar{y},\bar{z}+1/2$ [0,0,0] | (9) $\bar{x},\bar{x}+y,\bar{z}+1/2$ [0,0,0] |
|    |   |     | (10) $\bar{y},\bar{x},\bar{z}$ [0,0,0] | (11) $\bar{x}+y,y,\bar{z}$ [0,0,0]     | (12) x,x-y, $\bar{z}$ [0,0,0]               |

			(13) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]	(14) $y, \bar{x} + y, \bar{z}$ [0,0,0]	(15) $x - y, x, \bar{z}$ [0,0,0]
			(16) $x, y, \bar{z} + 1/2$ [0,0,0]	(17) $\bar{y}, x - y, \bar{z} + 1/2$ [0,0,0]	(18) $\bar{x} + y, \bar{x}, \bar{z} + 1/2$ [0,0,0]
			(19) $\bar{y}, \bar{x}, z + 1/2$ [0,0,0]	(20) $\bar{x} + y, y, z + 1/2$ [0,0,0]	(21) $x, x - y, z + 1/2$ [0,0,0]
			(22) $y, x, z$ [0,0,0]	(23) $x - y, \bar{y}, z$ [0,0,0]	(24) $\bar{x}, \bar{x} + y, z$ [0,0,0]
12	k	..m1'	$x, 0, z$ [0,0,0]	$0, x, z$ [0,0,0]	$\bar{x}, \bar{x}, z$ [0,0,0]
			$\bar{x}, 0, z + 1/2$ [0,0,0]	$0, \bar{x}, z + 1/2$ [0,0,0]	$x, x, z + 1/2$ [0,0,0]
			$0, x, \bar{z} + 1/2$ [0,0,0]	$x, 0, \bar{z} + 1/2$ [0,0,0]	$\bar{x}, \bar{x}, \bar{z} + 1/2$ [0,0,0]
			$0, \bar{x}, \bar{z}$ [0,0,0]	$\bar{x}, 0, \bar{z}$ [0,0,0]	$x, x, \bar{z}$ [0,0,0]
12	j	m..1'	$x, y, 1/4$ [0,0,0]	$\bar{y}, x - y, 1/4$ [0,0,0]	$\bar{x} + y, \bar{x}, 1/4$ [0,0,0]
			$\bar{x}, \bar{y}, 3/4$ [0,0,0]	$y, \bar{x} + y, 3/4$ [0,0,0]	$x - y, x, 3/4$ [0,0,0]
			$y, x, 1/4$ [0,0,0]	$x - y, \bar{y}, 1/4$ [0,0,0]	$\bar{x}, \bar{x} + y, 1/4$ [0,0,0]
			$\bar{y}, \bar{x}, 3/4$ [0,0,0]	$\bar{x} + y, y, 3/4$ [0,0,0]	$x, x - y, 3/4$ [0,0,0]
12	i	..21'	$x, 2x, 0$ [0,0,0]	$2\bar{x}, \bar{x}, 0$ [0,0,0]	$x, \bar{x}, 0$ [0,0,0]
			$\bar{x}, 2\bar{x}, 1/2$ [0,0,0]	$2x, x, 1/2$ [0,0,0]	$\bar{x}, x, 1/2$ [0,0,0]
			$\bar{x}, 2\bar{x}, 0$ [0,0,0]	$2x, x, 0$ [0,0,0]	$\bar{x}, x, 0$ [0,0,0]
			$x, 2x, 1/2$ [0,0,0]	$2\bar{x}, \bar{x}, 1/2$ [0,0,0]	$x, \bar{x}, 1/2$ [0,0,0]
8	h	3..1'	$1/3, 2/3, z$ [0,0,0]	$2/3, 1/3, z + 1/2$ [0,0,0]	$2/3, 1/3, \bar{z} + 1/2$ [0,0,0]
			$2/3, 1/3, \bar{z}$ [0,0,0]	$1/3, 2/3, \bar{z} + 1/2$ [0,0,0]	$1/3, 2/3, z$ [0,0,0]
6	g	m2m1'	$x, 0, 1/4$ [0,0,0]	$0, x, 1/4$ [0,0,0]	$\bar{x}, \bar{x}, 1/4$ [0,0,0]
			$\bar{x}, 0, 3/4$ [0,0,0]	$0, \bar{x}, 3/4$ [0,0,0]	$x, x, 3/4$ [0,0,0]
6	f	..2/m1'	$1/2, 0, 0$ [0,0,0]	$0, 1/2, 0$ [0,0,0]	$1/2, 1/2, 0$ [0,0,0]
			$1/2, 0, 1/2$ [0,0,0]	$0, 1/2, 1/2$ [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]
4	e	3.m1'	$0, 0, z$ [0,0,0]	$0, 0, z + 1/2$ [0,0,0]	$0, 0, \bar{z} + 1/2$ [0,0,0]
					$0, 0, \bar{z}$ [0,0,0]
4	d	3.21'	$1/3, 2/3, 0$ [0,0,0]	$2/3, 1/3, 1/2$ [0,0,0]	$2/3, 1/3, 0$ [0,0,0]
					$1/3, 2/3, 1/2$ [0,0,0]
4	c	$\bar{6}$ ..1'	$1/3, 2/3, 1/4$ [0,0,0]	$2/3, 1/3, 3/4$ [0,0,0]	$2/3, 1/3, 1/4$ [0,0,0]
					$1/3, 2/3, 3/4$ [0,0,0]
2	b	$\bar{3}$ .m1'	$0, 0, 0$ [0,0,0]	$0, 0, 1/2$ [0,0,0]	
2	a	$\bar{6}2m1'$	$0, 0, 1/4$ [0,0,0]	$0, 0, 3/4$ [0,0,0]	

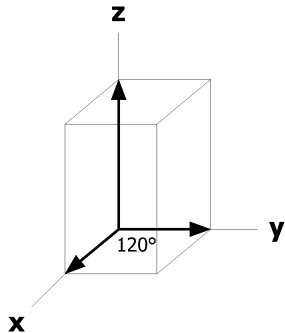
**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,0

Along [2,1,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,x/2,0





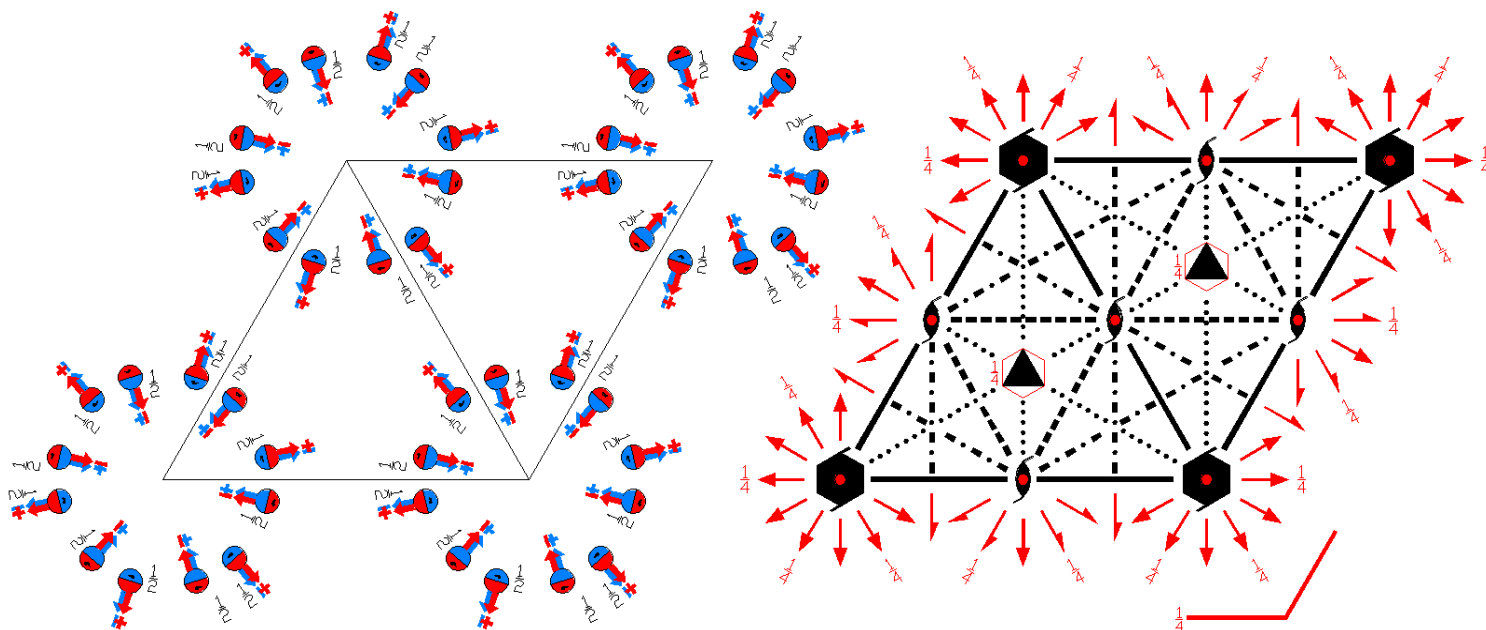
$P6_3/m'cm$

193.3.1487

$6/m'mm$

$P6_3/m'2'/c2'/m$

Hexagonal



Origin at center ( $\bar{3}'1m$ ) at  $\bar{3}'c2'/m$

**Asymmetric unit**  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $x \leq (1+y)/2$ ;  $y \leq \min(1-x, x)$

Vertices  $0,0,0$   $1/2,0,0$   $2/3,1/3,0$   $1/2,1/2,0$   
 $0,0,1/4$   $1/2,0,1/4$   $2/3,1/3,1/4$   $1/2,1/2,1/4$

### Symmetry Operations

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                            | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)        |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)    | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2) |
| (7) $2'$ x,x,1/4<br>( $2_{xy}$  0,0,1/2)'     | (8) $2'$ x,0,1/4<br>( $2_x$  0,0,1/2)'              | (9) $2'$ 0,y,1/4<br>( $2_y$  0,0,1/2)'         |
| (10) $2'$ x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)' | (11) $2'$ x,2x,0<br>( $2_2$  0,0,0)'                | (12) $2'$ 2x,x,0<br>( $2_1$  0,0,0)'           |

(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ ' 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(15) $\bar{3}^-$ ' 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(16) m' x,y,1/4 ( $m_z$  0,0,1/2)'	(17) $\bar{6}^-$ ' 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1}$  0,0,1/2)'	(18) $\bar{6}^+$ ' 0,0,z; 0,0,1/4 ( $\bar{6}_z$  0,0,1/2)'
(19) c (0,0,1/2) x, $\bar{x}$ ,z ( $m_{xy}$  0,0,1/2)	(20) c (0,0,1/2) x,2x,z ( $m_x$  0,0,1/2)	(21) c (0,0,1/2) 2x,x,z ( $m_y$  0,0,1/2)
(22) m x,x,z ( $m_3$  0,0,0)	(23) m x,0,z ( $m_2$  0,0,0)	(24) m 0,y,z ( $m_1$  0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
24	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(5) y, $\bar{x}$ +y,z+1/2 [v, $\bar{u}$ +v,w]	(6) x-y,x,z+1/2 [u-v,u,w]
			(7) y,x, $\bar{z}$ +1/2 [ $\bar{v}$ , $\bar{u}$ ,w]	(8) x-y, $\bar{y}$ , $\bar{z}$ +1/2 [ $\bar{u}$ +v,v,w]	(9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ +1/2 [u,u-v,w]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [v,u,w]	(11) $\bar{x}$ +y,y, $\bar{z}$ [u-v, $\bar{v}$ ,w]	(12) x,x-y, $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ +v,w]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(14) y, $\bar{x}$ +y, $\bar{z}$ [v, $\bar{u}$ +v, $\bar{w}$ ]	(15) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ]
			(16) x,y, $\bar{z}$ +1/2 [u,v, $\bar{w}$ ]	(17) $\bar{y}$ ,x-y, $\bar{z}$ +1/2 [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(18) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ +1/2 [ $\bar{u}$ +v, $\bar{u}$ , $\bar{w}$ ]
			(19) $\bar{y}$ , $\bar{x}$ ,z+1/2 [v,u, $\bar{w}$ ]	(20) $\bar{x}$ +y,y,z+1/2 [u-v, $\bar{v}$ , $\bar{w}$ ]	(21) x,x-y,z+1/2 [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ]
			(22) y,x,z [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(23) x-y, $\bar{y}$ ,z [ $\bar{u}$ +v,v, $\bar{w}$ ]	(24) $\bar{x}$ , $\bar{x}$ +y,z [u,u-v, $\bar{w}$ ]
12	k	..m	x,0,z [u,2u,0]	0,x,z [2 $\bar{u}$ , $\bar{u}$ ,0]	$\bar{x}$ , $\bar{x}$ ,z [u, $\bar{u}$ ,0]
			$\bar{x}$ ,0,z+1/2 [ $\bar{u}$ ,2 $\bar{u}$ ,0]	0, $\bar{x}$ ,z+1/2 [2u,u,0]	x,x,z+1/2 [ $\bar{u}$ ,u,0]
			0,x, $\bar{z}$ +1/2 [2 $\bar{u}$ , $\bar{u}$ ,0]	x,0, $\bar{z}$ +1/2 [u,2u,0]	$\bar{x}$ , $\bar{x}$ , $\bar{z}$ +1/2 [u, $\bar{u}$ ,0]
			0, $\bar{x}$ , $\bar{z}$ [2u,u,0]	$\bar{x}$ ,0, $\bar{z}$ [ $\bar{u}$ ,2 $\bar{u}$ ,0]	x,x, $\bar{z}$ [ $\bar{u}$ ,u,0]
12	j	m'..	x,y,1/4 [u,v,0]	$\bar{y}$ ,x-y,1/4 [ $\bar{v}$ ,u-v,0]	$\bar{x}$ +y, $\bar{x}$ ,1/4 [ $\bar{u}$ +v, $\bar{u}$ ,0]
			$\bar{x}$ , $\bar{y}$ ,3/4 [ $\bar{u}$ , $\bar{v}$ ,0]	y, $\bar{x}$ +y,3/4 [v, $\bar{u}$ +v,0]	x-y,x,3/4 [u-v,u,0]
			y,x,1/4 [ $\bar{v}$ , $\bar{u}$ ,0]	x-y, $\bar{y}$ ,1/4 [ $\bar{u}$ +v,v,0]	$\bar{x}$ , $\bar{x}$ +y,1/4 [u,u-v,0]
			$\bar{y}$ , $\bar{x}$ ,3/4 [v,u,0]	$\bar{x}$ +y,y,3/4 [u-v, $\bar{v}$ ,0]	x,x-y,3/4 [ $\bar{u}$ , $\bar{u}$ +v,0]

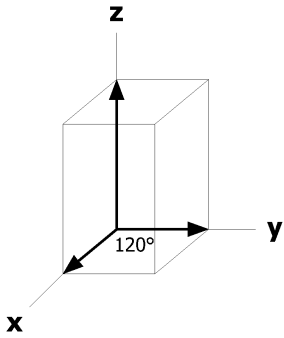
12	i	..2'	$x, 2x, 0 [u, 0, w]$	$2\bar{x}, \bar{x}, 0 [0, u, w]$	$x, \bar{x}, 0 [\bar{u}, \bar{u}, w]$	
			$\bar{x}, 2\bar{x}, 1/2 [\bar{u}, 0, w]$	$2x, x, 1/2 [0, \bar{u}, w]$	$\bar{x}, x, 1/2 [u, u, w]$	
			$\bar{x}, 2\bar{x}, 0 [\bar{u}, 0, \bar{w}]$	$2x, x, 0 [0, \bar{u}, \bar{w}]$	$\bar{x}, x, 0 [u, u, \bar{w}]$	
			$x, 2x, 1/2 [u, 0, \bar{w}]$	$2\bar{x}, \bar{x}, 1/2 [0, u, \bar{w}]$	$x, \bar{x}, 1/2 [\bar{u}, \bar{u}, \bar{w}]$	
8	h	3..	$1/3, 2/3, z [0, 0, w]$	$2/3, 1/3, z+1/2 [0, 0, w]$	$2/3, 1/3, \bar{z}+1/2 [0, 0, w]$	$1/3, 2/3, \bar{z} [0, 0, w]$
			$2/3, 1/3, \bar{z} [0, 0, \bar{w}]$	$1/3, 2/3, \bar{z}+1/2 [0, 0, \bar{w}]$	$1/3, 2/3, z+1/2 [0, 0, \bar{w}]$	$2/3, 1/3, z [0, 0, \bar{w}]$
6	g	m'2'm	$x, 0, 1/4 [u, 2u, 0]$	$0, x, 1/4 [2\bar{u}, \bar{u}, 0]$	$\bar{x}, \bar{x}, 1/4 [u, \bar{u}, 0]$	
			$\bar{x}, 0, 3/4 [\bar{u}, 2\bar{u}, 0]$	$0, \bar{x}, 3/4 [2u, u, 0]$	$x, x, 3/4 [\bar{u}, u, 0]$	
6	f	..2'/m	$1/2, 0, 0 [0, 0, 0]$	$0, 1/2, 0 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$	
			$1/2, 0, 1/2 [0, 0, 0]$	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 1/2, 1/2 [0, 0, 0]$	
4	e	3.m	$0, 0, z [0, 0, 0]$	$0, 0, z+1/2 [0, 0, 0]$	$0, 0, \bar{z}+1/2 [0, 0, 0]$	$0, 0, \bar{z} [0, 0, 0]$
4	d	3.2'	$1/3, 2/3, 0 [0, 0, w]$	$2/3, 1/3, 1/2 [0, 0, w]$	$2/3, 1/3, 0 [0, 0, \bar{w}]$	$1/3, 2/3, 1/2 [0, 0, \bar{w}]$
4	c	$\bar{6}'..$	$1/3, 2/3, 1/4 [0, 0, 0]$	$2/3, 1/3, 3/4 [0, 0, 0]$	$2/3, 1/3, 1/4 [0, 0, 0]$	$1/3, 2/3, 3/4 [0, 0, 0]$
2	b	$\bar{3}'..m$	$0, 0, 0 [0, 0, 0]$	$0, 0, 1/2 [0, 0, 0]$		
2	a	$\bar{6}'2'm$	$0, 0, 1/4 [0, 0, 0]$	$0, 0, 3/4 [0, 0, 0]$		

### Symmetry of Special Projections

Along  $[0, 0, 1]$  p6mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$  p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at  $x, 0, 0$

Along  $[2, 1, 0]$  p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x, x/2, 0$



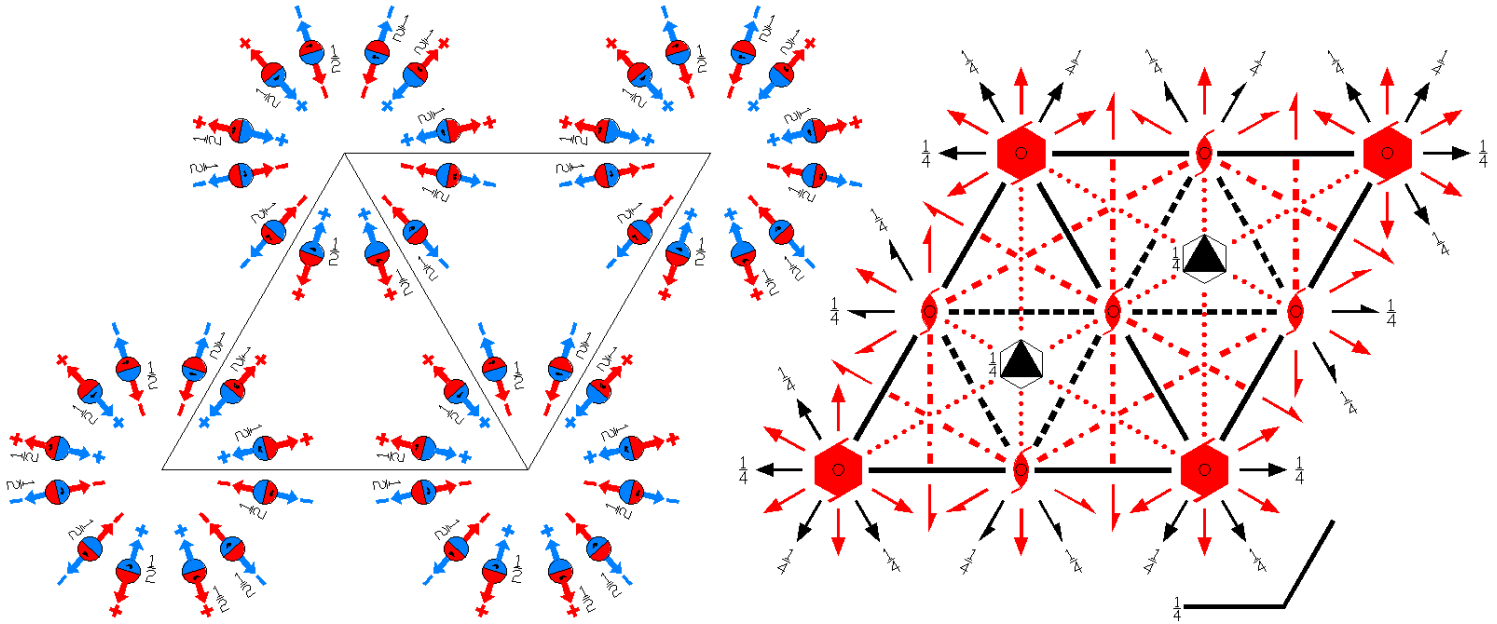
$P6_3'/mc'm$

193.4.1488

$6'/mm'm$

$P6_3'/m2/c'2'/m$

Hexagonal



Origin at center ( $\bar{3}'1m$ ) at  $\bar{3}'c'2'/m$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, x)$
Vertices	0,0,0 0,0,1/4	1/2,0,0 1/2,0,1/4	2/3,1/3,0 2/3,1/3,1/4	1/2,1/2,0 1/2,1/2,1/4	

### Symmetry Operations

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                             | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                   | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)         |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)' | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)' | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)' |
| (7) 2 x,x,1/4<br>( $2_{xy}$  0,0,1/2)          | (8) 2 x,0,1/4<br>( $2_x$  0,0,1/2)                   | (9) 2 0,y,1/4<br>( $2_y$  0,0,1/2)              |
| (10) $2'$ x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)'  | (11) $2'$ x,2x,0<br>( $2_2$  0,0,0)'                 | (12) $2'$ 2x,x,0<br>( $2_1$  0,0,0)'            |

(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ ' 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(15) $\bar{3}^-$ ' 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(16) m x,y,1/4 ( $m_z$  0,0,1/2)	(17) $\bar{6}^-$ 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1}$  0,0,1/2)	(18) $\bar{6}^+$ 0,0,z; 0,0,1/4 ( $\bar{6}_z$  0,0,1/2)
(19) c' (0,0,1/2) x, $\bar{x}$ ,z ( $m_{xy}$  0,0,1/2)'	(20) c' (0,0,1/2) x,2x,z ( $m_x$  0,0,1/2)'	(21) c' (0,0,1/2) 2x,x,z ( $m_y$  0,0,1/2)'
(22) m x,x,z ( $m_3$  0,0,0)	(23) m x,0,z ( $m_2$  0,0,0)	(24) m 0,y,z ( $m_1$  0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y$ , $\bar{x}$ ,z [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [u,v, $\bar{w}$ ]	(5) y, $\bar{x}+y$ ,z+1/2 [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) x-y,x,z+1/2 [ $\bar{u}+v$ , $\bar{u}$ , $\bar{w}$ ]
			(7) y,x, $\bar{z}+1/2$ [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y}$ , $\bar{z}+1/2$ [u-v, $\bar{v}$ , $\bar{w}$ ]	(9) $\bar{x}$ , $\bar{x}+y$ , $\bar{z}+1/2$ [ $\bar{u}$ , $\bar{u}+v$ , $\bar{w}$ ]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [v,u,w]	(11) $\bar{x}+y$ ,y, $\bar{z}$ [u-v, $\bar{v}$ ,w]	(12) x,x-y, $\bar{z}$ [ $\bar{u}$ , $\bar{u}+v$ ,w]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(14) y, $\bar{x}+y$ , $\bar{z}$ [v, $\bar{u}+v$ , $\bar{w}$ ]	(15) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ]
			(16) x,y, $\bar{z}+1/2$ [ $\bar{u}$ , $\bar{v}$ ,w]	(17) $\bar{y}$ ,x-y, $\bar{z}+1/2$ [v, $\bar{u}+v$ ,w]	(18) $\bar{x}+y$ , $\bar{x}$ , $\bar{z}+1/2$ [u-v,u,w]
			(19) $\bar{y}$ , $\bar{x}$ ,z+1/2 [ $\bar{v}$ , $\bar{u}$ ,w]	(20) $\bar{x}+y$ ,y,z+1/2 [ $\bar{u}+v$ ,v,w]	(21) x,x-y,z+1/2 [u,u-v,w]
			(22) y,x,z [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(23) x-y, $\bar{y}$ ,z [ $\bar{u}+v$ ,v, $\bar{w}$ ]	(24) $\bar{x}$ , $\bar{x}+y$ ,z [u,u-v, $\bar{w}$ ]
12	k	..m	x,0,z [u,2u,0]	0,x,z [2 $\bar{u}$ , $\bar{u}$ ,0]	$\bar{x}$ , $\bar{x}$ ,z [u, $\bar{u}$ ,0]
			$\bar{x}$ ,0,z+1/2 [u,2u,0]	0, $\bar{x}$ ,z+1/2 [2 $\bar{u}$ , $\bar{u}$ ,0]	x,x,z+1/2 [u, $\bar{u}$ ,0]
			0,x, $\bar{z}+1/2$ [2u,u,0]	x,0, $\bar{z}+1/2$ [ $\bar{u}$ ,2 $\bar{u}$ ,0]	$\bar{x}$ , $\bar{x}$ , $\bar{z}+1/2$ [ $\bar{u}$ ,u,0]
			0, $\bar{x}$ , $\bar{z}$ [2u,u,0]	$\bar{x}$ ,0, $\bar{z}$ [ $\bar{u}$ ,2 $\bar{u}$ ,0]	x,x, $\bar{z}$ [ $\bar{u}$ ,u,0]
12	j	m..	x,y,1/4 [0,0,w]	$\bar{y}$ ,x-y,1/4 [0,0,w]	$\bar{x}+y$ , $\bar{x}$ ,1/4 [0,0,w]
			$\bar{x}$ , $\bar{y}$ ,3/4 [0,0, $\bar{w}$ ]	y, $\bar{x}+y$ ,3/4 [0,0, $\bar{w}$ ]	x-y,x,3/4 [0,0, $\bar{w}$ ]
			y,x,1/4 [0,0, $\bar{w}$ ]	x-y, $\bar{y}$ ,1/4 [0,0, $\bar{w}$ ]	$\bar{x}$ , $\bar{x}+y$ ,1/4 [0,0, $\bar{w}$ ]
			$\bar{y}$ , $\bar{x}$ ,3/4 [0,0,w]	$\bar{x}+y$ ,y,3/4 [0,0,w]	x,x-y,3/4 [0,0,w]

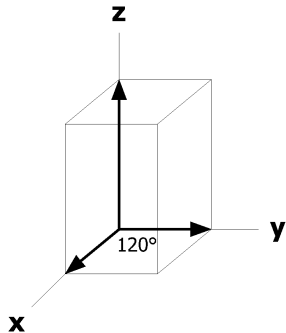
12	i	..2'	x,2x,0 [u,0,w] $\bar{x},2\bar{x},1/2$ [u,0,w] $\bar{x},2\bar{x},0$ [ $\bar{u},0,\bar{w}$ ] x,2x,1/2 [ $\bar{u},0,\bar{w}$ ]	$2\bar{x},\bar{x},0$ [0,u,w] 2x,x,1/2 [0,u,w] 2x,x,0 [0, $\bar{u},\bar{w}$ ] $2\bar{x},\bar{x},1/2$ [0, $\bar{u},\bar{w}$ ]	x, $\bar{x},0$ [ $\bar{u},\bar{u},w$ ] $\bar{x},x,1/2$ [ $\bar{u},\bar{u},w$ ] $\bar{x},x,0$ [u,u, $\bar{w}$ ] x, $\bar{x},1/2$ [u,u, $\bar{w}$ ]	
8	h	3..	1/3,2/3,z [0,0,w] 2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	2/3,1/3,z+1/2 [0,0, $\bar{w}$ ] 1/3,2/3, $\bar{z}+1/2$ [0,0,w]	2/3,1/3, $\bar{z}+1/2$ [0,0, $\bar{w}$ ] 1/3,2/3,z+1/2 [0,0,w]	1/3,2/3, $\bar{z}$ [0,0,w] 2/3,1/3,z [0,0, $\bar{w}$ ]
6	g	m2m	x,0,1/4 [0,0,0] $\bar{x},0,3/4$ [0,0,0]	0,x,1/4 [0,0,0] 0, $\bar{x},3/4$ [0,0,0]	$\bar{x},\bar{x},1/4$ [0,0,0] x,x,3/4 [0,0,0]	
6	f	..2'/m	1/2,0,0 [0,0,0] 1/2,0,1/2 [0,0,0]	0,1/2,0 [0,0,0] 0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]	
4	e	3.m	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]	0,0, $\bar{z}$ [0,0,0]
4	d	3.2'	1/3,2/3,0 [0,0,w]	2/3,1/3,1/2 [0,0, $\bar{w}$ ]	2/3,1/3,0 [0,0,w]	1/3,2/3,1/2 [0,0, $\bar{w}$ ]
4	c	$\bar{6}..$	1/3,2/3,1/4 [0,0,w]	2/3,1/3,3/4 [0,0, $\bar{w}$ ]	2/3,1/3,1/4 [0,0,w]	1/3,2/3,3/4 [0,0, $\bar{w}$ ]
2	b	$\bar{3}'$ .m	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		
2	a	$\bar{6}2m$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



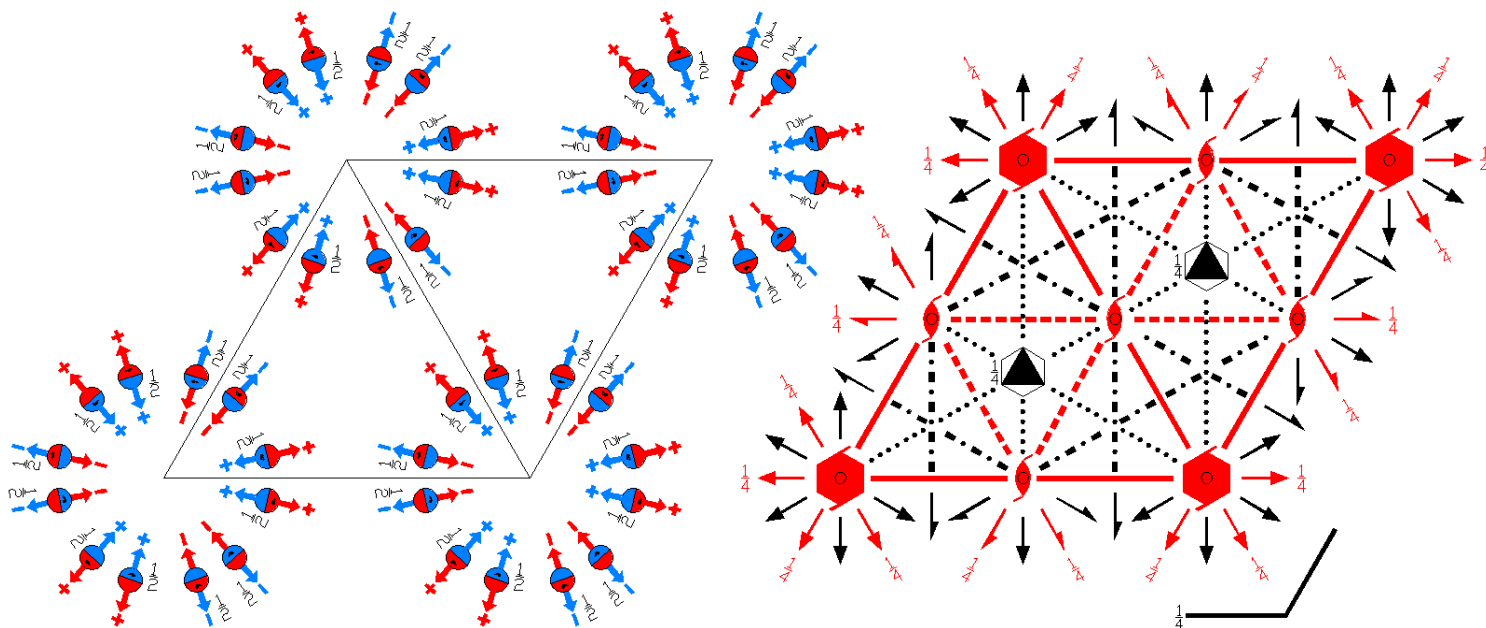
$P6_3'/mcm'$

193.5.1489

$6'/mmm'$

$P6_3'/m'2/c2/m'$

Hexagonal



Origin at center ( $\bar{3}'1m'$ ) at  $\bar{3}'c2/m'$

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $x \leq (1+y)/2$ ;  $y \leq \min(1-x, x)$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/2,1/2,1/4

### Symmetry Operations

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                             | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                   | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)         |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)' | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)' | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)' |
| (7) $2'$ x,x,1/4<br>( $2_{xy}$  0,0,1/2)'      | (8) $2'$ x,0,1/4<br>( $2_x$  0,0,1/2)'               | (9) $2'$ 0,y,1/4<br>( $2_y$  0,0,1/2)'          |
| (10) $2$ x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)    | (11) $2$ x,2x,0<br>( $2_2$  0,0,0)                   | (12) $2$ 2x,x,0<br>( $2_1$  0,0,0)              |

(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ ' 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(15) $\bar{3}^-$ ' 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(16) m x,y,1/4 ( $m_z$  0,0,1/2)	(17) $\bar{6}^-$ 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1}$  0,0,1/2)	(18) $\bar{6}^+$ 0,0,z; 0,0,1/4 ( $\bar{6}_z$  0,0,1/2)
(19) c (0,0,1/2) x, $\bar{x}$ ,z ( $m_{xy}$  0,0,1/2)	(20) c (0,0,1/2) x,2x,z ( $m_x$  0,0,1/2)	(21) c (0,0,1/2) 2x,x,z ( $m_y$  0,0,1/2)
(22) m' x,x,z ( $m_3$  0,0,0)'	(23) m' x,0,z ( $m_2$  0,0,0)'	(24) m' 0,y,z ( $m_1$  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y$ , $\bar{x}$ ,z [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [u,v, $\bar{w}$ ]	(5) y, $\bar{x}+y$ ,z+1/2 [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) x-y,x,z+1/2 [ $\bar{u}+v$ , $\bar{u}$ , $\bar{w}$ ]
			(7) y,x, $\bar{z}+1/2$ [ $\bar{v}$ , $\bar{u}$ ,w]	(8) x-y, $\bar{y}$ , $\bar{z}+1/2$ [ $\bar{u}+v$ ,v,w]	(9) $\bar{x}$ , $\bar{x}+y$ , $\bar{z}+1/2$ [u,u-v,w]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(11) $\bar{x}+y$ ,y, $\bar{z}$ [ $\bar{u}+v$ ,v, $\bar{w}$ ]	(12) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(14) y, $\bar{x}+y$ , $\bar{z}$ [v, $\bar{u}+v$ , $\bar{w}$ ]	(15) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ]
			(16) x,y, $\bar{z}+1/2$ [ $\bar{u}$ , $\bar{v}$ ,w]	(17) $\bar{y}$ ,x-y, $\bar{z}+1/2$ [v, $\bar{u}+v$ ,w]	(18) $\bar{x}+y$ , $\bar{x}$ , $\bar{z}+1/2$ [u-v,u,w]
			(19) $\bar{y}$ , $\bar{x}$ ,z+1/2 [v,u, $\bar{w}$ ]	(20) $\bar{x}+y$ ,y,z+1/2 [u-v, $\bar{v}$ , $\bar{w}$ ]	(21) x,x-y,z+1/2 [ $\bar{u}$ , $\bar{u}+v$ , $\bar{w}$ ]
			(22) y,x,z [v,u,w]	(23) x-y, $\bar{y}$ ,z [u-v, $\bar{v}$ ,w]	(24) $\bar{x}$ , $\bar{x}+y$ ,z [ $\bar{u}$ , $\bar{u}+v$ ,w]
12	k	..m'	x,0,z [u,0,w]	0,x,z [0,u,w]	$\bar{x}$ , $\bar{x}$ ,z [ $\bar{u}$ , $\bar{u}$ ,w]
			$\bar{x}$ ,0,z+1/2 [u,0, $\bar{w}$ ]	0, $\bar{x}$ ,z+1/2 [0,u, $\bar{w}$ ]	x,x,z+1/2 [ $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]
			0,x, $\bar{z}+1/2$ [0, $\bar{u}$ ,w]	x,0, $\bar{z}+1/2$ [ $\bar{u}$ ,0,w]	$\bar{x}$ , $\bar{x}$ , $\bar{z}+1/2$ [u,u,w]
			0, $\bar{x}$ , $\bar{z}$ [0, $\bar{u}$ , $\bar{w}$ ]	$\bar{x}$ ,0, $\bar{z}$ [ $\bar{u}$ ,0, $\bar{w}$ ]	x,x, $\bar{z}$ [u,u, $\bar{w}$ ]
12	j	m..	x,y,1/4 [0,0,w]	$\bar{y}$ ,x-y,1/4 [0,0,w]	$\bar{x}+y$ , $\bar{x}$ ,1/4 [0,0,w]
			$\bar{x}$ , $\bar{y}$ ,3/4 [0,0, $\bar{w}$ ]	y, $\bar{x}+y$ ,3/4 [0,0, $\bar{w}$ ]	x-y,x,3/4 [0,0, $\bar{w}$ ]
			y,x,1/4 [0,0,w]	x-y, $\bar{y}$ ,1/4 [0,0,w]	$\bar{x}$ , $\bar{x}+y$ ,1/4 [0,0,w]
			$\bar{y}$ , $\bar{x}$ ,3/4 [0,0, $\bar{w}$ ]	$\bar{x}+y$ ,y,3/4 [0,0, $\bar{w}$ ]	x,x-y,3/4 [0,0, $\bar{w}$ ]



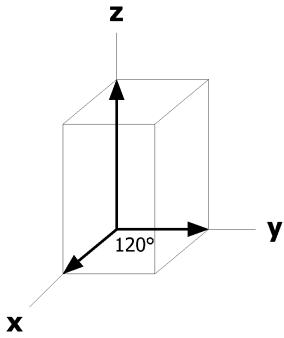
12	i	..2	x,2x,0 [u,2u,0]	$2\bar{x},\bar{x},0 [2\bar{u},\bar{u},0]$	$x,\bar{x},0 [u,\bar{u},0]$	
			$\bar{x},2\bar{x},1/2 [u,2u,0]$	$2x,x,1/2 [2\bar{u},\bar{u},0]$	$\bar{x},x,1/2 [u,\bar{u},0]$	
			$\bar{x},2\bar{x},0 [\bar{u},2\bar{u},0]$	$2x,x,0 [2u,u,0]$	$\bar{x},x,0 [\bar{u},u,0]$	
			$x,2x,1/2 [\bar{u},2\bar{u},0]$	$2\bar{x},\bar{x},1/2 [2u,u,0]$	$x,\bar{x},1/2 [\bar{u},u,0]$	
8	h	3..	$1/3,2/3,z [0,0,w]$	$2/3,1/3,z+1/2 [0,0,\bar{w}]$	$2/3,1/3,\bar{z}+1/2 [0,0,w]$	$1/3,2/3,\bar{z} [0,0,\bar{w}]$
			$2/3,1/3,\bar{z} [0,0,\bar{w}]$	$1/3,2/3,\bar{z}+1/2 [0,0,w]$	$1/3,2/3,z+1/2 [0,0,\bar{w}]$	$2/3,1/3,z [0,0,w]$
6	g	m2'm'	$x,0,1/4 [0,0,w]$	$0,x,1/4 [0,0,w]$	$\bar{x},\bar{x},1/4 [0,0,w]$	
			$\bar{x},0,3/4 [0,0,\bar{w}]$	$0,\bar{x},3/4 [0,0,\bar{w}]$	$x,x,3/4 [0,0,\bar{w}]$	
6	f	..2/m'	$1/2,0,0 [0,0,0]$	$0,1/2,0 [0,0,0]$	$1/2,1/2,0 [0,0,0]$	
			$1/2,0,1/2 [0,0,0]$	$0,1/2,1/2 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$	
4	e	3.m'	$0,0,z [0,0,w]$	$0,0,z+1/2 [0,0,\bar{w}]$	$0,0,\bar{z}+1/2 [0,0,w]$	$0,0,\bar{z} [0,0,\bar{w}]$
4	d	3.2	$1/3,2/3,0 [0,0,0]$	$2/3,1/3,1/2 [0,0,0]$	$2/3,1/3,0 [0,0,0]$	$1/3,2/3,1/2 [0,0,0]$
4	c	$\bar{6}..$	$1/3,2/3,1/4 [0,0,w]$	$2/3,1/3,3/4 [0,0,\bar{w}]$	$2/3,1/3,1/4 [0,0,\bar{w}]$	$1/3,2/3,3/4 [0,0,w]$
2	b	$\bar{3}'m'$	$0,0,0 [0,0,0]$	$0,0,1/2 [0,0,0]$		
2	a	$\bar{6}2'm'$	$0,0,1/4 [0,0,w]$	$0,0,3/4 [0,0,\bar{w}]$		

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2mg  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



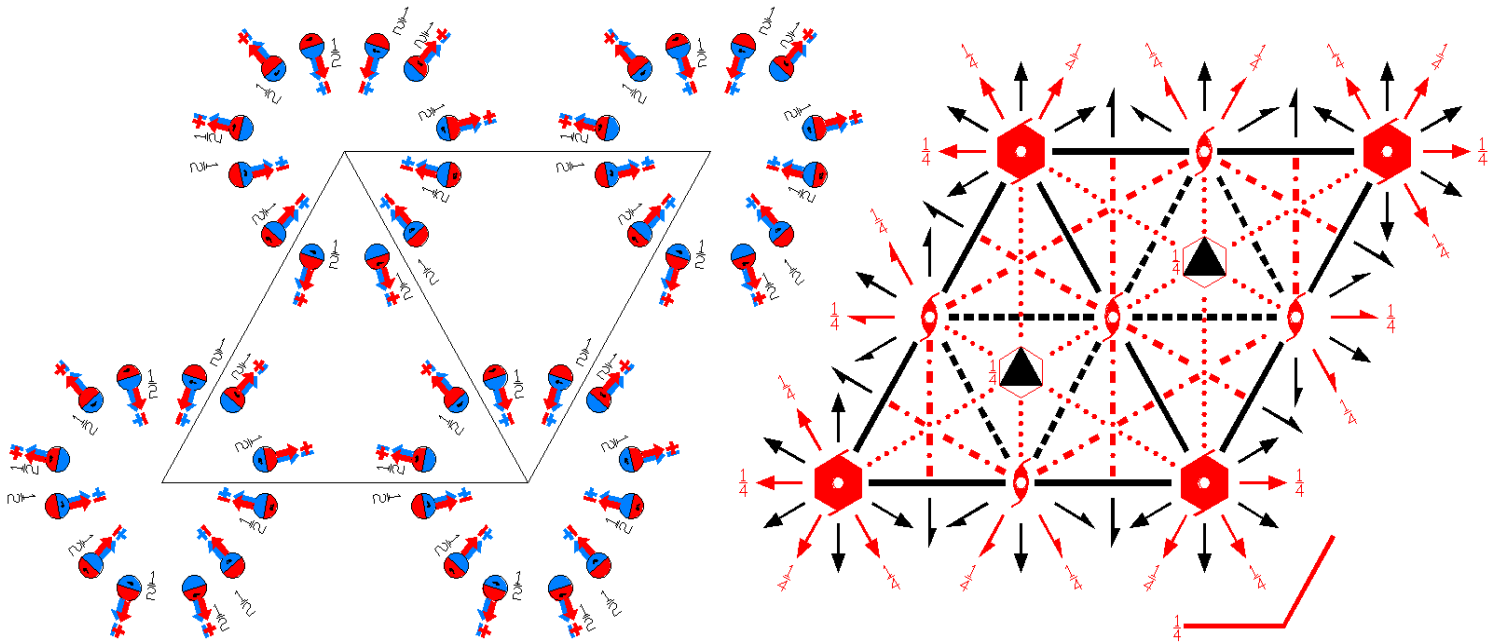
$P6_3'/m'c'm$

193.6.1490

$6'/m'm'm$

$P6_3'/m'2'/c'2'/m$

Hexagonal



Origin at center ( $\bar{3}1m$ ) at  $\bar{3}c'2/m$

Asymmetric unit	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, x)$
Vertices	0,0,0 0,0,1/4	1/2,0,0 1/2,0,1/4	2/3,1/3,0 2/3,1/3,1/4	1/2,1/2,0 1/2,1/2,1/4	

### Symmetry Operations

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                             | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                   | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)         |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)' | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)' | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)' |
| (7) $2'$ x,x,1/4<br>( $2_{xy}$  0,0,1/2)'      | (8) $2'$ x,0,1/4<br>( $2_x$  0,0,1/2)'               | (9) $2'$ 0,y,1/4<br>( $2_y$  0,0,1/2)'          |
| (10) $2$ x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)    | (11) $2$ x,2x,0<br>( $2_2$  0,0,0)                   | (12) $2$ 2x,x,0<br>( $2_1$  0,0,0)              |

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)
(16) m' x,y,1/4 ( $m_z$  0,0,1/2)'	(17) $\bar{6}^-$ 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1}$  0,0,1/2)'	(18) $\bar{6}^+$ 0,0,z; 0,0,1/4 ( $\bar{6}_z$  0,0,1/2)'
(19) c' (0,0,1/2) x, $\bar{x}$ ,z ( $m_{xy}$  0,0,1/2)'	(20) c' (0,0,1/2) x,2x,z ( $m_x$  0,0,1/2)'	(21) c' (0,0,1/2) 2x,x,z ( $m_y$  0,0,1/2)'
(22) m x,x,z ( $m_3$  0,0,0)	(23) m x,0,z ( $m_2$  0,0,0)	(24) m 0,y,z ( $m_1$  0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [u,v, $\bar{w}$ ]	(5) y, $\bar{x}$ +y,z+1/2 [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) x-y,x,z+1/2 [ $\bar{u}$ +v, $\bar{u}$ , $\bar{w}$ ]
			(7) y,x, $\bar{z}$ +1/2 [ $\bar{v}$ , $\bar{u}$ ,w]	(8) x-y, $\bar{y}$ , $\bar{z}$ +1/2 [ $\bar{u}$ +v,v,w]	(9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ +1/2 [u,u-v,w]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(11) $\bar{x}$ +y,y, $\bar{z}$ [ $\bar{u}$ +v,v, $\bar{w}$ ]	(12) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(14) y, $\bar{x}$ +y, $\bar{z}$ [ $\bar{v}$ ,u-v,w]	(15) x-y,x, $\bar{z}$ [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(16) x,y, $\bar{z}$ +1/2 [u,v, $\bar{w}$ ]	(17) $\bar{y}$ ,x-y, $\bar{z}$ +1/2 [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(18) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ +1/2 [ $\bar{u}$ +v, $\bar{u}$ , $\bar{w}$ ]
			(19) $\bar{y}$ , $\bar{x}$ ,z+1/2 [ $\bar{v}$ , $\bar{u}$ ,w]	(20) $\bar{x}$ +y,y,z+1/2 [ $\bar{u}$ +v,v,w]	(21) x,x-y,z+1/2 [u,u-v,w]
			(22) y,x,z [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(23) x-y, $\bar{y}$ ,z [ $\bar{u}$ +v,v, $\bar{w}$ ]	(24) $\bar{x}$ , $\bar{x}$ +y,z [u,u-v, $\bar{w}$ ]
12	k	..m	x,0,z [u,2u,0]	0,x,z [2 $\bar{u}$ , $\bar{u}$ ,0]	$\bar{x}$ , $\bar{x}$ ,z [u, $\bar{u}$ ,0]
			$\bar{x}$ ,0,z+1/2 [u,2u,0]	0, $\bar{x}$ ,z+1/2 [2 $\bar{u}$ , $\bar{u}$ ,0]	x,x,z+1/2 [u, $\bar{u}$ ,0]
			0,x, $\bar{z}$ +1/2 [2 $\bar{u}$ , $\bar{u}$ ,0]	x,0, $\bar{z}$ +1/2 [u,2u,0]	$\bar{x}$ , $\bar{x}$ , $\bar{z}$ +1/2 [u, $\bar{u}$ ,0]
			0, $\bar{x}$ , $\bar{z}$ [2 $\bar{u}$ , $\bar{u}$ ,0]	$\bar{x}$ ,0, $\bar{z}$ [u,2u,0]	x,x, $\bar{z}$ [u, $\bar{u}$ ,0]
12	j	m'..	x,y,1/4 [u,v,0]	$\bar{y}$ ,x-y,1/4 [ $\bar{v}$ ,u-v,0]	$\bar{x}$ +y, $\bar{x}$ ,1/4 [ $\bar{u}$ +v, $\bar{u}$ ,0]
			$\bar{x}$ , $\bar{y}$ ,3/4 [u,v,0]	y, $\bar{x}$ +y,3/4 [ $\bar{v}$ ,u-v,0]	x-y,x,3/4 [ $\bar{u}$ +v, $\bar{u}$ ,0]
			y,x,1/4 [ $\bar{v}$ , $\bar{u}$ ,0]	x-y, $\bar{y}$ ,1/4 [ $\bar{u}$ +v,v,0]	$\bar{x}$ , $\bar{x}$ +y,1/4 [u,u-v,0]
			$\bar{y}$ , $\bar{x}$ ,3/4 [ $\bar{v}$ , $\bar{u}$ ,0]	$\bar{x}$ +y,y,3/4 [ $\bar{u}$ +v,v,0]	x,x-y,3/4 [u,u-v,0]

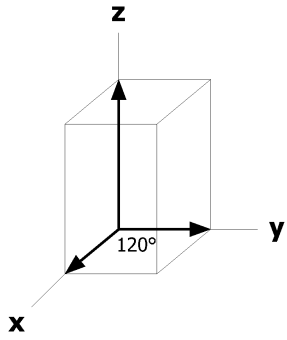
12	i	..2	$x, 2x, 0 [u, 2u, 0]$	$2\bar{x}, \bar{x}, 0 [2\bar{u}, \bar{u}, 0]$	$x, \bar{x}, 0 [u, \bar{u}, 0]$	
			$\bar{x}, 2\bar{x}, 1/2 [u, 2u, 0]$	$2x, x, 1/2 [2\bar{u}, \bar{u}, 0]$	$\bar{x}, x, 1/2 [u, \bar{u}, 0]$	
			$\bar{x}, 2\bar{x}, 0 [u, 2u, 0]$	$2x, x, 0 [2\bar{u}, \bar{u}, 0]$	$\bar{x}, x, 0 [u, \bar{u}, 0]$	
			$x, 2x, 1/2 [u, 2u, 0]$	$2\bar{x}, \bar{x}, 1/2 [2\bar{u}, \bar{u}, 0]$	$x, \bar{x}, 1/2 [u, \bar{u}, 0]$	
8	h	3..	$1/3, 2/3, z [0, 0, w]$	$2/3, 1/3, z+1/2 [0, 0, \bar{w}]$	$2/3, 1/3, \bar{z}+1/2 [0, 0, w]$	$1/3, 2/3, \bar{z} [0, 0, \bar{w}]$
			$2/3, 1/3, \bar{z} [0, 0, w]$	$1/3, 2/3, \bar{z}+1/2 [0, 0, \bar{w}]$	$1/3, 2/3, z+1/2 [0, 0, w]$	$2/3, 1/3, z [0, 0, \bar{w}]$
6	g	m'2'm	$x, 0, 1/4 [u, 2u, 0]$	$0, x, 1/4 [2\bar{u}, \bar{u}, 0]$	$\bar{x}, \bar{x}, 1/4 [u, \bar{u}, 0]$	
			$\bar{x}, 0, 3/4 [u, 2u, 0]$	$0, \bar{x}, 3/4 [2\bar{u}, \bar{u}, 0]$	$x, x, 3/4 [u, \bar{u}, 0]$	
6	f	..2/m	$1/2, 0, 0 [u, 2u, 0]$	$0, 1/2, 0 [2\bar{u}, \bar{u}, 0]$	$1/2, 1/2, 0 [u, \bar{u}, 0]$	
			$1/2, 0, 1/2 [u, 2u, 0]$	$0, 1/2, 1/2 [2\bar{u}, \bar{u}, 0]$	$1/2, 1/2, 1/2 [u, \bar{u}, 0]$	
4	e	3.m	$0, 0, z [0, 0, 0]$	$0, 0, z+1/2 [0, 0, 0]$	$0, 0, \bar{z}+1/2 [0, 0, 0]$	$0, 0, \bar{z} [0, 0, 0]$
4	d	3.2	$1/3, 2/3, 0 [0, 0, 0]$	$2/3, 1/3, 1/2 [0, 0, 0]$	$2/3, 1/3, 0 [0, 0, 0]$	$1/3, 2/3, 1/2 [0, 0, 0]$
4	c	$\bar{6}'..$	$1/3, 2/3, 1/4 [0, 0, 0]$	$2/3, 1/3, 3/4 [0, 0, 0]$	$2/3, 1/3, 1/4 [0, 0, 0]$	$1/3, 2/3, 3/4 [0, 0, 0]$
2	b	$\bar{3}.m$	$0, 0, 0 [0, 0, 0]$	$0, 0, 1/2 [0, 0, 0]$		
2	a	$\bar{6}'2'm$	$0, 0, 1/4 [0, 0, 0]$	$0, 0, 3/4 [0, 0, 0]$		

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p6'm'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 0, 0]$   $p2'mm'$   
 $\mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, 0, 0$

Along  $[2, 1, 0]$   $p2mg1'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $x, x/2, 0$



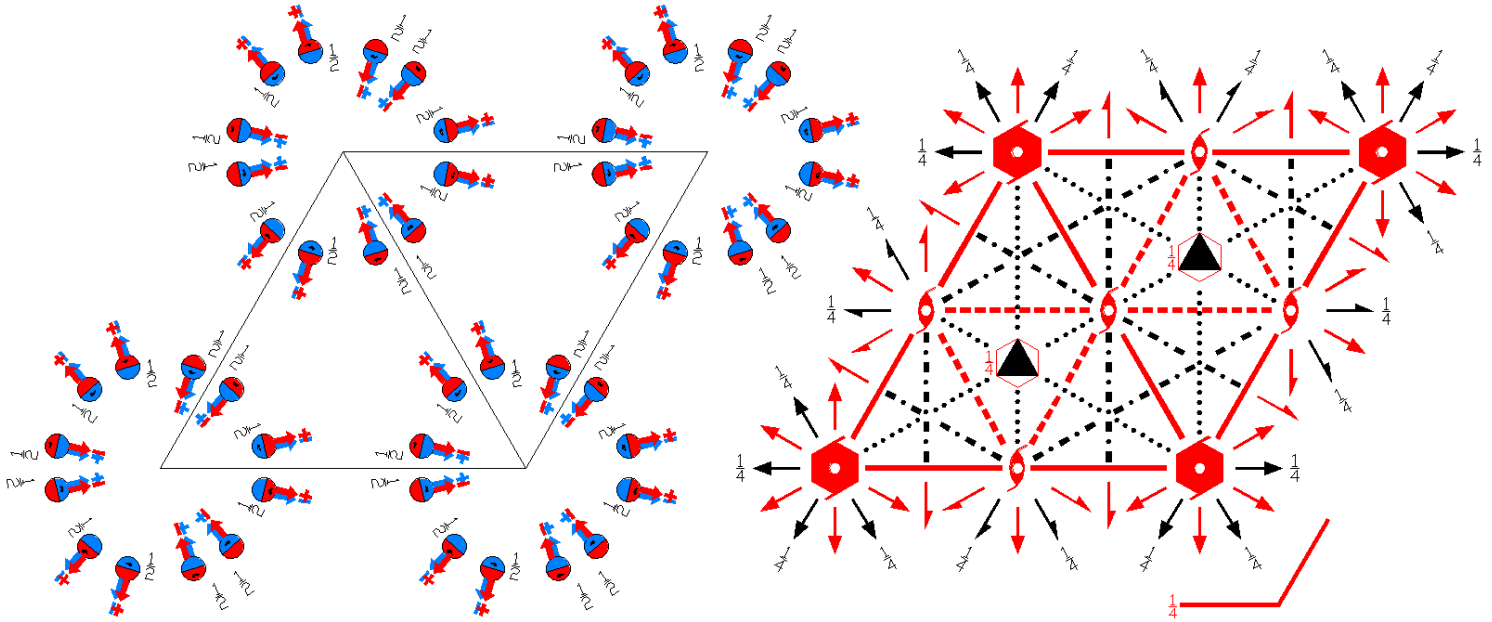
$P6_3'/m'cm'$

193.7.1491

$6'/m'mm'$

$P6_3'/m'2/c2'/m'$

Hexagonal



Origin at center ( $\bar{3}1m'$ ) at  $\bar{3}c2'/m'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/4;$	$x \leq (1+y)/2;$	$y \leq \min(1-x, x)$
Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0	
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/2,1/2,1/4	

### Symmetry Operations

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                             | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                   | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)         |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)' | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)' | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)' |
| (7) 2 x,x,1/4<br>( $2_{xy}$  0,0,1/2)          | (8) 2 x,0,1/4<br>( $2_x$  0,0,1/2)                   | (9) 2 0,y,1/4<br>( $2_y$  0,0,1/2)              |
| (10) $2'$ x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)'  | (11) $2'$ x,2x,0<br>( $2_2$  0,0,0)'                 | (12) $2'$ 2x,x,0<br>( $2_1$  0,0,0)'            |

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)
(16) m' x,y,1/4 ( $m_z$  0,0,1/2)'	(17) $\bar{6}^-$ 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1}$  0,0,1/2)'	(18) $\bar{6}^+$ 0,0,z; 0,0,1/4 ( $\bar{6}_z$  0,0,1/2)'
(19) c (0,0,1/2) x, $\bar{x}$ ,z ( $m_{xy}$  0,0,1/2)	(20) c (0,0,1/2) x,2x,z ( $m_x$  0,0,1/2)	(21) c (0,0,1/2) 2x,x,z ( $m_y$  0,0,1/2)
(22) m' x,x,z ( $m_3$  0,0,0)'	(23) m' x,0,z ( $m_2$  0,0,0)'	(24) m' 0,y,z ( $m_1$  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [u,v, $\bar{w}$ ]	(5) y, $\bar{x}$ +y,z+1/2 [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) x-y,x,z+1/2 [ $\bar{u}$ +v, $\bar{u}$ , $\bar{w}$ ]
			(7) y,x, $\bar{z}$ +1/2 [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y}$ , $\bar{z}$ +1/2 [u-v, $\bar{v}$ , $\bar{w}$ ]	(9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [v,u,w]	(11) $\bar{x}$ +y,y, $\bar{z}$ [u-v, $\bar{v}$ ,w]	(12) x,x-y, $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ +v,w]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(14) y, $\bar{x}$ +y, $\bar{z}$ [ $\bar{v}$ ,u-v,w]	(15) x-y,x, $\bar{z}$ [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(16) x,y, $\bar{z}$ +1/2 [u,v, $\bar{w}$ ]	(17) $\bar{y}$ ,x-y, $\bar{z}$ +1/2 [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(18) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ +1/2 [ $\bar{u}$ +v, $\bar{u}$ , $\bar{w}$ ]
			(19) $\bar{y}$ , $\bar{x}$ ,z+1/2 [v,u, $\bar{w}$ ]	(20) $\bar{x}$ +y,y,z+1/2 [u-v, $\bar{v}$ , $\bar{w}$ ]	(21) x,x-y,z+1/2 [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ]
			(22) y,x,z [v,u,w]	(23) x-y, $\bar{y}$ ,z [u-v, $\bar{v}$ ,w]	(24) $\bar{x}$ , $\bar{x}$ +y,z [ $\bar{u}$ , $\bar{u}$ +v,w]
12	k	..m'	x,0,z [u,0,w]	0,x,z [0,u,w]	$\bar{x}$ , $\bar{x}$ ,z [ $\bar{u}$ , $\bar{u}$ ,w]
			$\bar{x}$ ,0,z+1/2 [u,0, $\bar{w}$ ]	0, $\bar{x}$ ,z+1/2 [0,u, $\bar{w}$ ]	x,x,z+1/2 [ $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]
			0,x, $\bar{z}$ +1/2 [0,u, $\bar{w}$ ]	x,0, $\bar{z}$ +1/2 [u,0, $\bar{w}$ ]	$\bar{x}$ , $\bar{x}$ , $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]
			0, $\bar{x}$ , $\bar{z}$ [0,u,w]	$\bar{x}$ ,0, $\bar{z}$ [u,0,w]	x,x, $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ ,w]
12	j	m'..	x,y,1/4 [u,v,0]	$\bar{y}$ ,x-y,1/4 [ $\bar{v}$ ,u-v,0]	$\bar{x}$ +y, $\bar{x}$ ,1/4 [ $\bar{u}$ +v, $\bar{u}$ ,0]
			$\bar{x}$ , $\bar{y}$ ,3/4 [u,v,0]	y, $\bar{x}$ +y,3/4 [ $\bar{v}$ ,u-v,0]	x-y,x,3/4 [ $\bar{u}$ +v, $\bar{u}$ ,0]
			y,x,1/4 [v,u,0]	x-y, $\bar{y}$ ,1/4 [u-v, $\bar{v}$ ,0]	$\bar{x}$ , $\bar{x}$ +y,1/4 [ $\bar{u}$ , $\bar{u}$ +v,0]
			$\bar{y}$ , $\bar{x}$ ,3/4 [v,u,0]	$\bar{x}$ +y,y,3/4 [u-v, $\bar{v}$ ,0]	x,x-y,3/4 [ $\bar{u}$ , $\bar{u}$ +v,0]

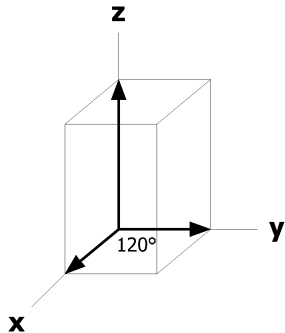
12	i	..2'	x,2x,0 [u,0,w] $\bar{x},2\bar{x},1/2 [u,0,\bar{w}]$ $\bar{x},2\bar{x},0 [u,0,w]$ x,2x,1/2 [u,0, $\bar{w}]$	$2\bar{x},\bar{x},0 [0,u,w]$ 2x,x,1/2 [0,u, $\bar{w}]$ 2x,x,0 [0,u,w] $2\bar{x},\bar{x},1/2 [0,u,\bar{w}]$	$x,\bar{x},0 [\bar{u},\bar{u},w]$ $\bar{x},x,1/2 [\bar{u},\bar{u},\bar{w}]$ $\bar{x},x,0 [\bar{u},\bar{u},w]$ $x,\bar{x},1/2 [\bar{u},\bar{u},\bar{w}]$	
8	h	3..	1/3,2/3,z [0,0,w] 2/3,1/3, $\bar{z}$ [0,0,w]	2/3,1/3,z+1/2 [0,0, $\bar{w}]$ 1/3,2/3, $\bar{z}$ +1/2 [0,0, $\bar{w}]$	2/3,1/3, $\bar{z}$ +1/2 [0,0, $\bar{w}]$ 1/3,2/3,z+1/2 [0,0, $\bar{w}]$	1/3,2/3, $\bar{z}$ [0,0,w] 2/3,1/3,z [0,0,w]
6	g	m'2m'	x,0,1/4 [u,0,0] $\bar{x},0,3/4 [u,0,0]$	0,x,1/4 [0,u,0] 0, $\bar{x}$ ,3/4 [0,u,0]	$\bar{x},\bar{x},1/4 [\bar{u},\bar{u},0]$ x,x,3/4 [ $\bar{u},\bar{u},0]$	
6	f	..2'/m'	1/2,0,0 [u,2u,0] 1/2,0,1/2 [u,2u,0]	0,1/2,0 [2 $\bar{u},\bar{u},0]$ 0,1/2,1/2 [2 $\bar{u},\bar{u},0]$	1/2,1/2,0 [u, $\bar{u},0]$ 1/2,1/2,1/2 [u, $\bar{u},0]$	
4	e	3.m'	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}]$	0,0, $\bar{z}$ +1/2 [0,0, $\bar{w}]$	0,0, $\bar{z}$ [0,0,w]
4	d	3.2'	1/3,2/3,0 [0,0,w]	2/3,1/3,1/2 [0,0, $\bar{w}]$	2/3,1/3,0 [0,0, $\bar{w}]$	1/3,2/3,1/2 [0,0,w]
4	c	$\bar{6}$ '..	1/3,2/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]	2/3,1/3,1/4 [0,0,0]	1/3,2/3,3/4 [0,0,0]
2	b	$\bar{3}$ .m'	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}]$		
2	a	$\bar{6}$ '2m'	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p6'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p<sub>2a</sub>2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,1/4

Along [2,1,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



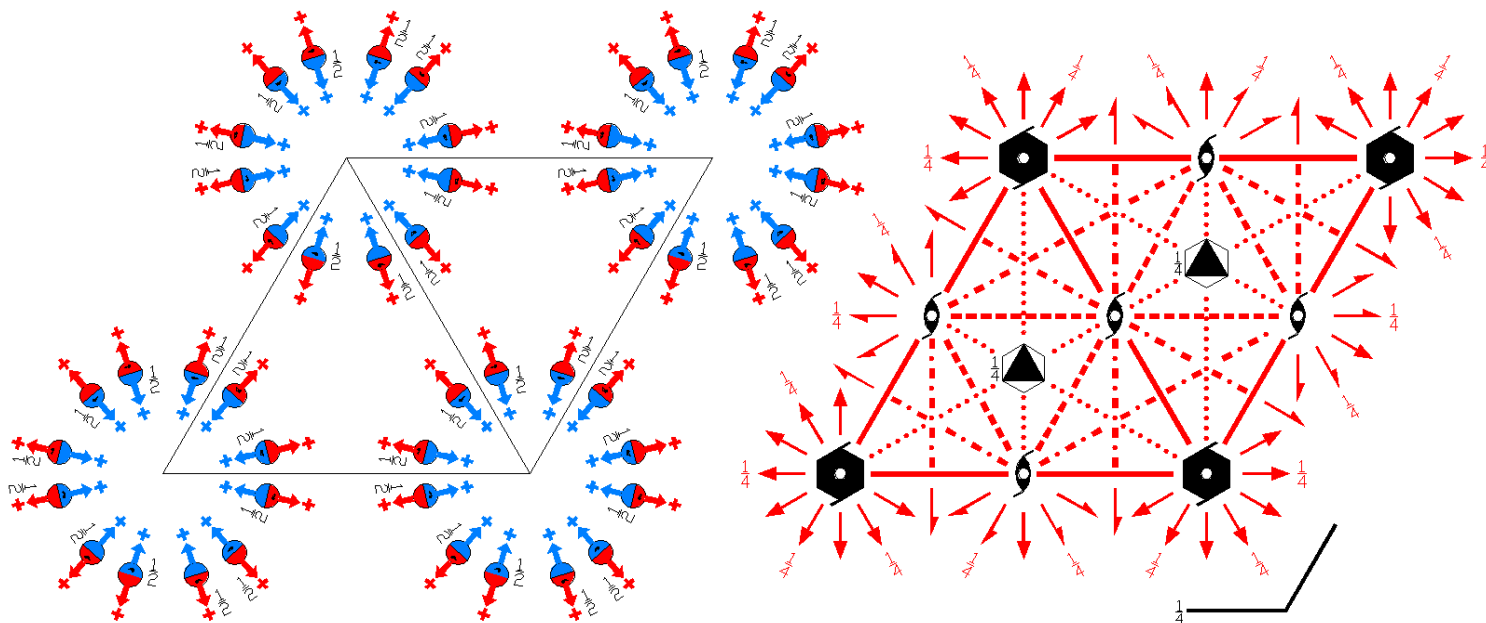
$P6_3/mc'm'$

193.8.1492

$6/mm'm'$

$P6_3/m2'/c'2'/m'$

Hexagonal



Origin at center ( $\bar{3}1m'$ ) at  $\bar{3}c'2'/m'$

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $x \leq (1+y)/2$ ;  $y \leq \min(1-x, x)$

Vertices	0,0,0	1/2,0,0	2/3,1/3,0	1/2,1/2,0
	0,0,1/4	1/2,0,1/4	2/3,1/3,1/4	1/2,1/2,1/4

### Symmetry Operations

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                            | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)        |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)    | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2) |
| (7) $2'$ x,x,1/4<br>( $2_{xy}$  0,0,1/2)'     | (8) $2'$ x,0,1/4<br>( $2_x$  0,0,1/2)'              | (9) $2'$ 0,y,1/4<br>( $2_y$  0,0,1/2)'         |
| (10) $2'$ x, $\bar{x}$ ,0<br>( $2_3$  0,0,0)' | (11) $2'$ x,2x,0<br>( $2_2$  0,0,0)'                | (12) $2'$ 2x,x,0<br>( $2_1$  0,0,0)'           |



(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)
(16) m x,y,1/4 ( $m_z$  0,0,1/2)	(17) $\bar{6}^-$ 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1}$  0,0,1/2)	(18) $\bar{6}^+$ 0,0,z; 0,0,1/4 ( $\bar{6}_z$  0,0,1/2)
(19) c' (0,0,1/2) x, $\bar{x}$ ,z ( $m_{xy}$  0,0,1/2)'	(20) c' (0,0,1/2) x,2x,z ( $m_x$  0,0,1/2)'	(21) c' (0,0,1/2) 2x,x,z ( $m_y$  0,0,1/2)'
(22) m' x,x,z ( $m_3$  0,0,0)'	(23) m' x,0,z ( $m_2$  0,0,0)'	(24) m' 0,y,z ( $m_1$  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
24	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(5) y, $\bar{x}$ +y,z+1/2 [v, $\bar{u}$ +v,w]	(6) x-y,x,z+1/2 [u-v,u,w]
			(7) y,x, $\bar{z}$ +1/2 [ $\bar{v}$ , $\bar{u}$ ,w]	(8) x-y, $\bar{y}$ , $\bar{z}$ +1/2 [ $\bar{u}$ +v,v,w]	(9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ +1/2 [u,u-v,w]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [v,u,w]	(11) $\bar{x}$ +y,y, $\bar{z}$ [u-v, $\bar{v}$ ,w]	(12) x,x-y, $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ +v,w]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(14) y, $\bar{x}$ +y, $\bar{z}$ [ $\bar{v}$ ,u-v,w]	(15) x-y,x, $\bar{z}$ [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(16) x,y, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(17) $\bar{y}$ ,x-y, $\bar{z}$ +1/2 [v, $\bar{u}$ +v,w]	(18) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ +1/2 [u-v,u,w]
			(19) $\bar{y}$ , $\bar{x}$ ,z+1/2 [ $\bar{v}$ , $\bar{u}$ ,w]	(20) $\bar{x}$ +y,y,z+1/2 [ $\bar{u}$ +v,v,w]	(21) x,x-y,z+1/2 [u,u-v,w]
			(22) y,x,z [v,u,w]	(23) x-y, $\bar{y}$ ,z [u-v, $\bar{v}$ ,w]	(24) $\bar{x}$ , $\bar{x}$ +y,z [ $\bar{u}$ , $\bar{u}$ +v,w]
12	k	..m'	x,0,z [u,0,w]	0,x,z [0,u,w]	$\bar{x}$ , $\bar{x}$ ,z [ $\bar{u}$ , $\bar{u}$ ,w]
			$\bar{x}$ ,0,z+1/2 [ $\bar{u}$ ,0,w]	0, $\bar{x}$ ,z+1/2 [0, $\bar{u}$ ,w]	x,x,z+1/2 [u,u,w]
			0,x, $\bar{z}$ +1/2 [0, $\bar{u}$ ,w]	x,0, $\bar{z}$ +1/2 [ $\bar{u}$ ,0,w]	$\bar{x}$ , $\bar{x}$ , $\bar{z}$ +1/2 [u,u,w]
			0, $\bar{x}$ , $\bar{z}$ [0,u,w]	$\bar{x}$ ,0, $\bar{z}$ [u,0,w]	x,x, $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ ,w]
12	j	m..	x,y,1/4 [0,0,w]	$\bar{y}$ ,x-y,1/4 [0,0,w]	$\bar{x}$ +y, $\bar{x}$ ,1/4 [0,0,w]
			$\bar{x}$ , $\bar{y}$ ,3/4 [0,0,w]	y, $\bar{x}$ +y,3/4 [0,0,w]	x-y,x,3/4 [0,0,w]
			y,x,1/4 [0,0,w]	x-y, $\bar{y}$ ,1/4 [0,0,w]	$\bar{x}$ , $\bar{x}$ +y,1/4 [0,0,w]
			$\bar{y}$ , $\bar{x}$ ,3/4 [0,0,w]	$\bar{x}$ +y,y,3/4 [0,0,w]	x,x-y,3/4 [0,0,w]

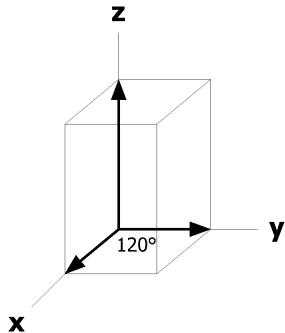
12	i	..2'	x,2x,0 [u,0,w] $\bar{x},2\bar{x},1/2 [\bar{u},0,w]$ $\bar{x},2\bar{x},0 [u,0,w]$ x,2x,1/2 [ $\bar{u},0,w]$	$2\bar{x},\bar{x},0 [0,u,w]$ 2x,x,1/2 [0, $\bar{u},w]$ 2x,x,0 [0,u,w] $2\bar{x},\bar{x},1/2 [0,\bar{u},w]$	$x,\bar{x},0 [\bar{u},\bar{u},w]$ $\bar{x},x,1/2 [u,u,w]$ $\bar{x},x,0 [\bar{u},\bar{u},w]$ x, $\bar{x},1/2 [u,u,w]$	
8	h	3..	1/3,2/3,z [0,0,w] 2/3,1/3, $\bar{z}$ [0,0,w]	2/3,1/3,z+1/2 [0,0,w] 1/3,2/3, $\bar{z}+1/2 [0,0,w]$	2/3,1/3, $\bar{z}+1/2 [0,0,w]$ 1/3,2/3,z+1/2 [0,0,w]	1/3,2/3, $\bar{z}$ [0,0,w] 2/3,1/3,z [0,0,w]
6	g	m2'm'	x,0,1/4 [0,0,w] $\bar{x},0,3/4 [0,0,w]$	0,x,1/4 [0,0,w] 0, $\bar{x},3/4 [0,0,w]$	$\bar{x},\bar{x},1/4 [0,0,w]$ x,x,3/4 [0,0,w]	
6	f	..2'/m'	1/2,0,0 [u,0,w] 1/2,0,1/2 [ $\bar{u},0,w]$	0,1/2,0 [0,u,w] 0,1/2,1/2 [0, $\bar{u},w]$	1/2,1/2,0 [ $\bar{u},\bar{u},w]$ 1/2,1/2,1/2 [u,u,w]	
4	e	3.m'	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}+1/2 [0,0,w]$	0,0, $\bar{z}$ [0,0,w]
4	d	3.2'	1/3,2/3,0 [0,0,w]	2/3,1/3,1/2 [0,0,w]	2/3,1/3,0 [0,0,w]	1/3,2/3,1/2 [0,0,w]
4	c	$\bar{6}..$	1/3,2/3,1/4 [0,0,w]	2/3,1/3,3/4 [0,0,w]	2/3,1/3,1/4 [0,0,w]	1/3,2/3,3/4 [0,0,w]
2	b	$\bar{3}.m'$	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]		
2	a	$\bar{6}2'm'$	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2'mg'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



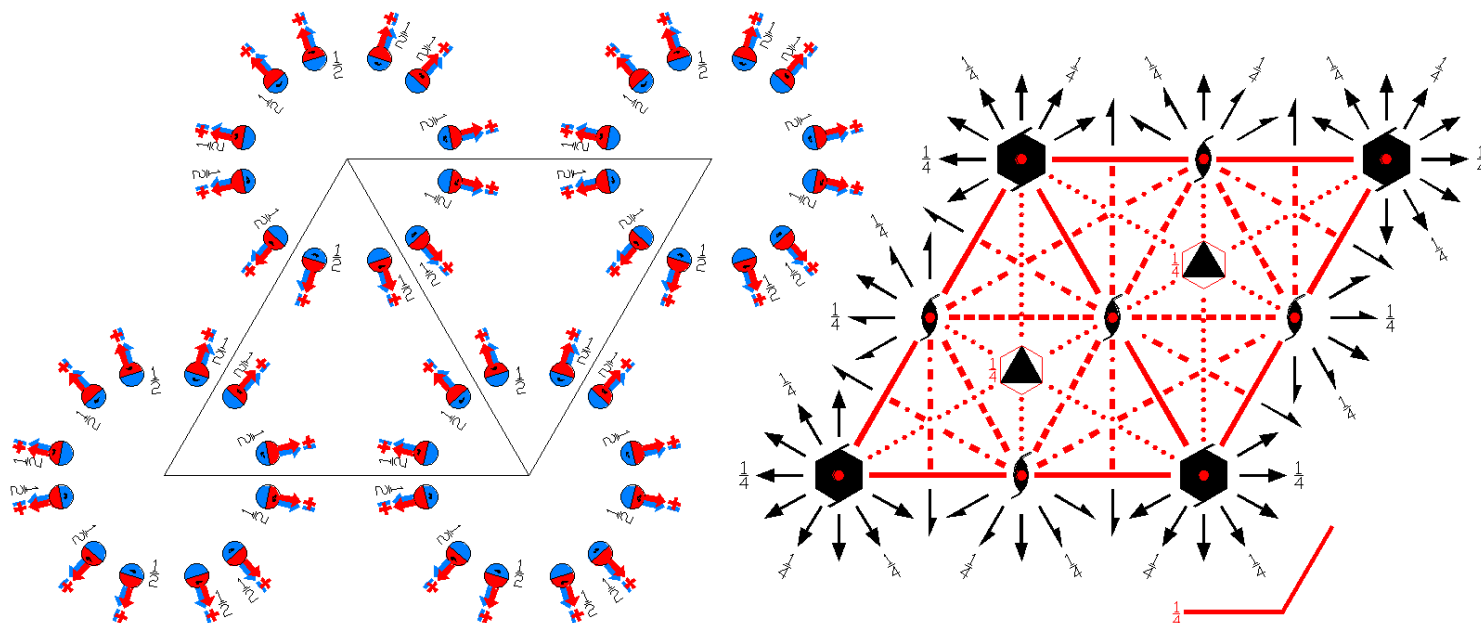
$P6_3/m'c'm'$

193.9.1493

$6/m'm'm'$

$P6_3/m'2/c'2/m'$

Hexagonal



Origin at center ( $\bar{3}'1m'$ ) at  $\bar{3}'c'2/m'$

**Asymmetric unit**  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $x \leq (1+y)/2$ ;  $y \leq \min(1-x, x)$

Vertices  $0,0,0$   $1/2,0,0$   $2/3,1/3,0$   $1/2,1/2,0$   
 $0,0,1/4$   $1/2,0,1/4$   $2/3,1/3,1/4$   $1/2,1/2,1/4$

### Symmetry Operations

- |  |   |  |
|--|---|--|
| (1) 1<br>(1 0,0,0)                         | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)        |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2) | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2) |
| (7) 2 x,x,1/4<br>( $2_{xy}$  0,0,1/2)      | (8) 2 x,0,1/4<br>( $2_x$  0,0,1/2)                  | (9) 2 0,y,1/4<br>( $2_y$  0,0,1/2)             |
| (10) 2 $x,\bar{x},0$<br>( $2_3$  0,0,0)    | (11) 2 x,2x,0<br>( $2_2$  0,0,0)                    | (12) 2 2x,x,0<br>( $2_1$  0,0,0)               |

(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ ' 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(15) $\bar{3}^-$ ' 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(16) m' x,y,1/4 ( $m_z$  0,0,1/2)'	(17) $\bar{6}^-$ ' 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1}$  0,0,1/2)'	(18) $\bar{6}^+$ ' 0,0,z; 0,0,1/4 ( $\bar{6}_z$  0,0,1/2)'
(19) c' (0,0,1/2) x, $\bar{x}$ ,z ( $m_{xy}$  0,0,1/2)'	(20) c' (0,0,1/2) x,2x,z ( $m_x$  0,0,1/2)'	(21) c' (0,0,1/2) 2x,x,z ( $m_y$  0,0,1/2)'
(22) m' x,x,z ( $m_3$  0,0,0)'	(23) m' x,0,z ( $m_2$  0,0,0)'	(24) m' 0,y,z ( $m_1$  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y$ , $\bar{x}$ ,z [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(5) y, $\bar{x}+y$ ,z+1/2 [v, $\bar{u}+v$ ,w]	(6) x-y,x,z+1/2 [u-v,u,w]
			(7) y,x, $\bar{z}+1/2$ [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y}$ , $\bar{z}+1/2$ [u-v, $\bar{v}$ , $\bar{w}$ ]	(9) $\bar{x}$ , $\bar{x}+y$ , $\bar{z}+1/2$ [ $\bar{u}$ , $\bar{u}+v$ , $\bar{w}$ ]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(11) $\bar{x}+y$ ,y, $\bar{z}$ [ $\bar{u}+v$ ,v, $\bar{w}$ ]	(12) x,x-y, $\bar{z}$ [u,u-v, $\bar{w}$ ]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(14) y, $\bar{x}+y$ , $\bar{z}$ [v, $\bar{u}+v$ , $\bar{w}$ ]	(15) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ]
			(16) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(17) $\bar{y}$ ,x-y, $\bar{z}+1/2$ [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(18) $\bar{x}+y$ , $\bar{x}$ , $\bar{z}+1/2$ [ $\bar{u}+v$ , $\bar{u}$ , $\bar{w}$ ]
			(19) $\bar{y}$ , $\bar{x}$ ,z+1/2 [ $\bar{v}$ , $\bar{u}$ ,w]	(20) $\bar{x}+y$ ,y,z+1/2 [ $\bar{u}+v$ ,v,w]	(21) x,x-y,z+1/2 [u,u-v,w]
			(22) y,x,z [v,u,w]	(23) x-y, $\bar{y}$ ,z [u-v, $\bar{v}$ ,w]	(24) $\bar{x}$ , $\bar{x}+y$ ,z [ $\bar{u}$ , $\bar{u}+v$ ,w]
12	k	..m'	x,0,z [u,0,w]	0,x,z [0,u,w]	$\bar{x}$ , $\bar{x}$ ,z [ $\bar{u}$ , $\bar{u}$ ,w]
			$\bar{x}$ ,0,z+1/2 [ $\bar{u}$ ,0,w]	0, $\bar{x}$ ,z+1/2 [0, $\bar{u}$ ,w]	x,x,z+1/2 [u,u,w]
			0,x, $\bar{z}+1/2$ [0,u, $\bar{w}$ ]	x,0, $\bar{z}+1/2$ [u,0, $\bar{w}$ ]	$\bar{x}$ , $\bar{x}$ , $\bar{z}+1/2$ [ $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]
			0, $\bar{x}$ , $\bar{z}$ [0, $\bar{u}$ , $\bar{w}$ ]	$\bar{x}$ ,0, $\bar{z}$ [ $\bar{u}$ ,0, $\bar{w}$ ]	x,x, $\bar{z}$ [u,u, $\bar{w}$ ]
12	j	m'..	x,y,1/4 [u,v,0]	$\bar{y}$ ,x-y,1/4 [ $\bar{v}$ ,u-v,0]	$\bar{x}+y$ , $\bar{x}$ ,1/4 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			$\bar{x}$ , $\bar{y}$ ,3/4 [ $\bar{u}$ , $\bar{v}$ ,0]	y, $\bar{x}+y$ ,3/4 [v, $\bar{u}+v$ ,0]	x-y,x,3/4 [u-v,u,0]
			y,x,1/4 [v,u,0]	x-y, $\bar{y}$ ,1/4 [u-v, $\bar{v}$ ,0]	$\bar{x}$ , $\bar{x}+y$ ,1/4 [ $\bar{u}$ , $\bar{u}+v$ ,0]
			$\bar{y}$ , $\bar{x}$ ,3/4 [ $\bar{v}$ , $\bar{u}$ ,0]	$\bar{x}+y$ ,y,3/4 [ $\bar{u}+v$ ,v,0]	x,x-y,3/4 [u,u-v,0]

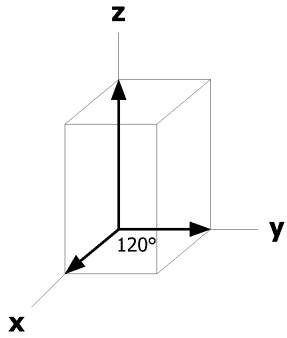
12	i	..2	x,2x,0 [u,2u,0]	$2\bar{x},\bar{x},0 [2\bar{u},\bar{u},0]$	$x,\bar{x},0 [u,\bar{u},0]$	
			$\bar{x},2\bar{x},1/2 [\bar{u},2\bar{u},0]$	$2x,x,1/2 [2u,u,0]$	$\bar{x},x,1/2 [\bar{u},u,0]$	
			$\bar{x},2\bar{x},0 [2u,u,0]$	$2x,x,0 [\bar{u},2\bar{u},0]$	$\bar{x},x,0 [\bar{u},u,0]$	
			$x,2x,1/2 [2\bar{u},\bar{u},0]$	$2\bar{x},\bar{x},1/2 [u,2u,0]$	$x,\bar{x},1/2 [u,\bar{u},0]$	
8	h	3..	$1/3,2/3,z [0,0,w]$	$2/3,1/3,z+1/2 [0,0,w]$	$2/3,1/3,\bar{z}+1/2 [0,0,\bar{w}]$	$1/3,2/3,\bar{z} [0,0,\bar{w}]$
			$2/3,1/3,\bar{z} [0,0,\bar{w}]$	$1/3,2/3,\bar{z}+1/2 [0,0,\bar{w}]$	$1/3,2/3,z+1/2 [0,0,w]$	$2/3,1/3,z [0,0,w]$
6	g	m'2m'	$x,0,1/4 [u,0,0]$	$0,x,1/4 [0,u,0]$	$\bar{x},\bar{x},1/4 [\bar{u},\bar{u},0]$	
			$\bar{x},0,3/4 [\bar{u},0,0]$	$0,\bar{x},3/4 [0,\bar{u},0]$	$x,x,3/4 [u,u,0]$	
6	f	..2/m'	$1/2,0,0 [0,0,0]$	$0,1/2,0 [0,0,0]$	$1/2,1/2,0 [0,0,0]$	
			$1/2,0,1/2 [0,0,0]$	$0,1/2,1/2 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$	
4	e	3.m'	$0,0,z [0,0,w]$	$0,0,z+1/2 [0,0,w]$	$0,0,\bar{z}+1/2 [0,0,\bar{w}]$	$0,0,\bar{z} [0,0,\bar{w}]$
4	d	3.2	$1/3,2/3,0 [0,0,0]$	$2/3,1/3,1/2 [0,0,0]$	$2/3,1/3,0 [0,0,0]$	$1/3,2/3,1/2 [0,0,0]$
4	c	$\bar{6}'..$	$1/3,2/3,1/4 [0,0,0]$	$2/3,1/3,3/4 [0,0,0]$	$2/3,1/3,1/4 [0,0,0]$	$1/3,2/3,3/4 [0,0,0]$
2	b	$\bar{3}'m'$	$0,0,0 [0,0,0]$	$0,0,1/2 [0,0,0]$		
2	a	$\bar{6}'2m'$	$0,0,1/4 [0,0,0]$	$0,0,3/4 [0,0,0]$		

### Symmetry of Special Projections

Along [0,0,1] p6m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

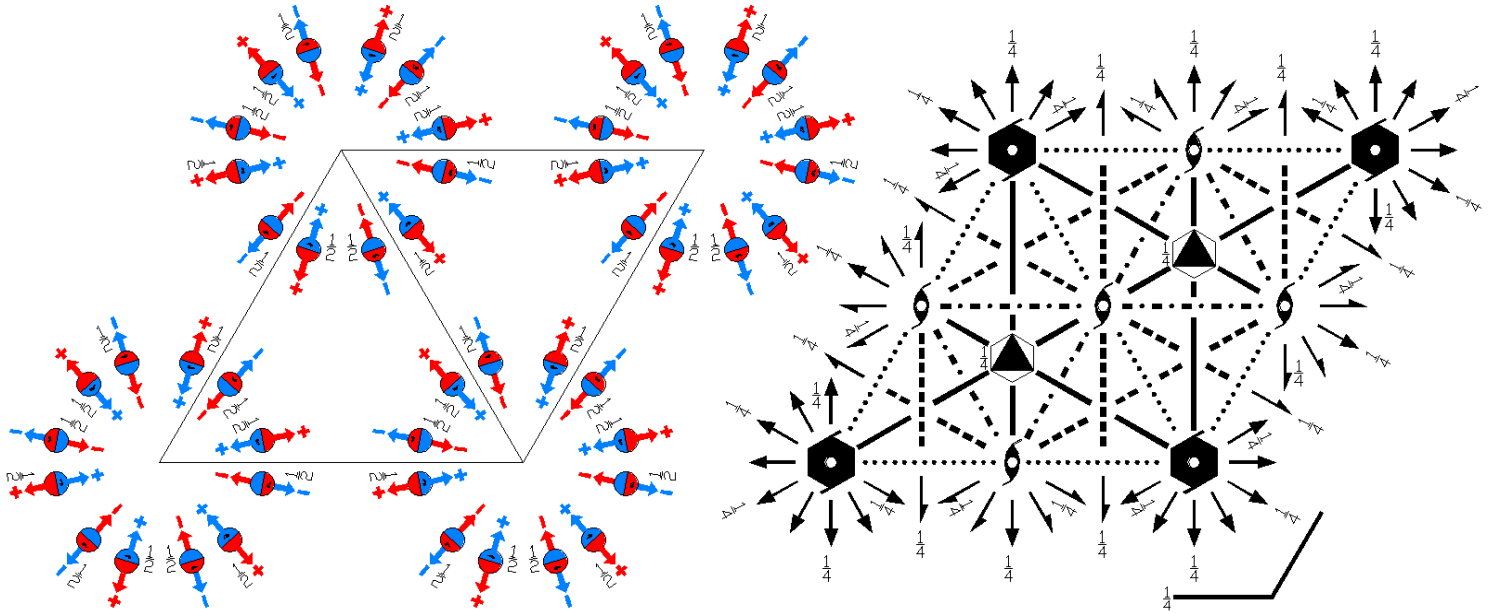
Along [2,1,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



$P6_3/mmc$   
194.1.1494

$6/mmm$   
 $P6_3/m2/m2/c$

Hexagonal



Origin at center ( $\bar{3}m1$ ) at  $\bar{3}2/mc$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq 2y;$	$y \leq \min(1-x, 2x)$
Vertices	0,0,0	$2/3, 1/3, 0$	$1/3, 2/3, 0$		
	0,0,1/4	$2/3, 1/3, 1/4$	$1/3, 2/3, 1/4$		

**Symmetry Operations**

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                            | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)        |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)    | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2) |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0)             | (8) 2 x,0,0<br>( $2_x$  0,0,0)                      | (9) 2 0,y,0<br>( $2_y$  0,0,0)                 |
| (10) 2 $x, \bar{x}, 1/4$<br>( $2_3$  0,0,1/2) | (11) 2 x,2x,1/4<br>( $2_2$  0,0,1/2)                | (12) 2 2x,x,1/4<br>( $2_1$  0,0,1/2)           |

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)
(16) m $\bar{x}$ ,y,1/4 ( $m_z$  0,0,1/2)	(17) $\bar{6}^-$ 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1}$  0,0,1/2)	(18) $\bar{6}^+$ 0,0,z; 0,0,1/4 ( $\bar{6}_z$  0,0,1/2)
(19) m $\bar{x}$ , $\bar{x}$ ,z ( $m_{xy}$  0,0,0)	(20) m $\bar{x}$ ,2x,z ( $m_x$  0,0,0)	(21) m 2x,x,z ( $m_y$  0,0,0)
(22) c (0,0,1/2) $\bar{x}$ ,x,z ( $m_3$  0,0,1/2)	(23) c (0,0,1/2) $\bar{x}$ ,0,z ( $m_2$  0,0,1/2)	(24) c (0,0,1/2) 0,y,z ( $m_1$  0,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	l	1	(1) $\bar{x}$ ,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y$ , $\bar{x}$ ,z [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(5) y, $\bar{x}+y$ ,z+1/2 [v, $\bar{u}+v$ ,w]	(6) x-y,x,z+1/2 [u-v,u,w]
			(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y}$ , $\bar{z}$ [u-v, $\bar{v}$ , $\bar{w}$ ]	(9) $\bar{x}$ , $\bar{x}+y$ , $\bar{z}$ [ $\bar{u}$ , $\bar{u}+v$ , $\bar{w}$ ]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}+1/2$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(11) $\bar{x}+y$ ,y, $\bar{z}+1/2$ [ $\bar{u}+v$ ,v, $\bar{w}$ ]	(12) x,x-y, $\bar{z}+1/2$ [u,u-v, $\bar{w}$ ]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(14) y, $\bar{x}+y$ , $\bar{z}$ [ $\bar{v}$ ,u-v,w]	(15) x-y,x, $\bar{z}$ [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(16) x,y, $\bar{z}+1/2$ [ $\bar{u}$ , $\bar{v}$ ,w]	(17) $\bar{y}$ ,x-y, $\bar{z}+1/2$ [v, $\bar{u}+v$ ,w]	(18) $\bar{x}+y$ , $\bar{x}$ , $\bar{z}+1/2$ [u-v,u,w]
			(19) $\bar{y}$ , $\bar{x}$ ,z [v,u, $\bar{w}$ ]	(20) $\bar{x}+y$ ,y,z [u-v, $\bar{v}$ , $\bar{w}$ ]	(21) x,x-y,z [ $\bar{u}$ , $\bar{u}+v$ , $\bar{w}$ ]
			(22) y,x,z+1/2 [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(23) x-y, $\bar{y}$ ,z+1/2 [ $\bar{u}+v$ ,v, $\bar{w}$ ]	(24) $\bar{x}$ , $\bar{x}+y$ ,z+1/2 [u,u-v, $\bar{w}$ ]
12	k	.m.	x,2x,z [u,0,0]	2 $\bar{x}$ , $\bar{x}$ ,z [0,u,0]	x, $\bar{x}$ ,z [ $\bar{u}$ , $\bar{u}$ ,0]
			$\bar{x}$ ,2 $\bar{x}$ ,z+1/2 [ $\bar{u}$ ,0,0]	2x,x,z+1/2 [0, $\bar{u}$ ,0]	$\bar{x}$ ,x,z+1/2 [u,u,0]
			2x,x, $\bar{z}$ [0,u,0]	$\bar{x}$ ,2 $\bar{x}$ , $\bar{z}$ [u,0,0]	$\bar{x}$ ,x, $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ ,0]
			2 $\bar{x}$ , $\bar{x}$ , $\bar{z}+1/2$ [0, $\bar{u}$ ,0]	x,2x, $\bar{z}+1/2$ [ $\bar{u}$ ,0,0]	x, $\bar{x}$ , $\bar{z}+1/2$ [u,u,0]
12	j	m..	x,y,1/4 [0,0,w]	$\bar{y}$ ,x-y,1/4 [0,0,w]	$\bar{x}+y$ , $\bar{x}$ ,1/4 [0,0,w]
			$\bar{x}$ , $\bar{y}$ ,3/4 [0,0,w]	y, $\bar{x}+y$ ,3/4 [0,0,w]	x-y,x,3/4 [0,0,w]
			y,x,3/4 [0,0, $\bar{w}$ ]	x-y, $\bar{y}$ ,3/4 [0,0, $\bar{w}$ ]	$\bar{x}$ , $\bar{x}+y$ ,3/4 [0,0, $\bar{w}$ ]
			$\bar{y}$ , $\bar{x}$ ,1/4 [0,0, $\bar{w}$ ]	$\bar{x}+y$ ,y,1/4 [0,0, $\bar{w}$ ]	x,x-y,1/4 [0,0, $\bar{w}$ ]

12	i	.2.	x,0,0 [u,0,0]	0,x,0 [0,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	
			$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	$0,\bar{x},1/2$ [0, $\bar{u},0$ ]	x,x,1/2 [u,u,0]	
			$\bar{x},0,0$ [u,0,0]	$0,\bar{x},0$ [0,u,0]	x,x,0 [ $\bar{u},\bar{u},0$ ]	
			x,0,1/2 [ $\bar{u},0,0$ ]	$0,x,1/2$ [0, $\bar{u},0$ ]	$\bar{x},\bar{x},1/2$ [u,u,0]	
6	h	mm2	x,2x,1/4 [0,0,0]	$2\bar{x},\bar{x},1/4$ [0,0,0]	x, $\bar{x},1/4$ [0,0,0]	
			$\bar{x},2\bar{x},3/4$ [0,0,0]	2x,x,3/4 [0,0,0]	$\bar{x},x,3/4$ [0,0,0]	
6	g	.2/m.	1/2,0,0 [u,0,0]	0,1/2,0 [0,u,0]	1/2,1/2,0 [ $\bar{u},\bar{u},0$ ]	
			1/2,0,1/2 [ $\bar{u},0,0$ ]	0,1/2,1/2 [0, $\bar{u},0$ ]	1/2,1/2,1/2 [u,u,0]	
4	f	3m.	1/3,2/3,z [0,0,0]	2/3,1/3,z+1/2 [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	1/3,2/3, $\bar{z}+1/2$ [0,0,0]
4	e	3m.	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]
2	d	$\bar{6}m2$	1/3,2/3,3/4 [0,0,0]	2/3,1/3,1/4 [0,0,0]		
2	c	$\bar{6}m2$	1/3,2/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]		
2	b	$\bar{6}m2$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	a	$\bar{3}m.$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

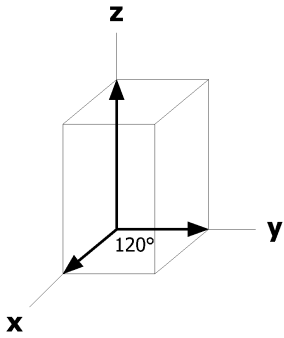
### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/4





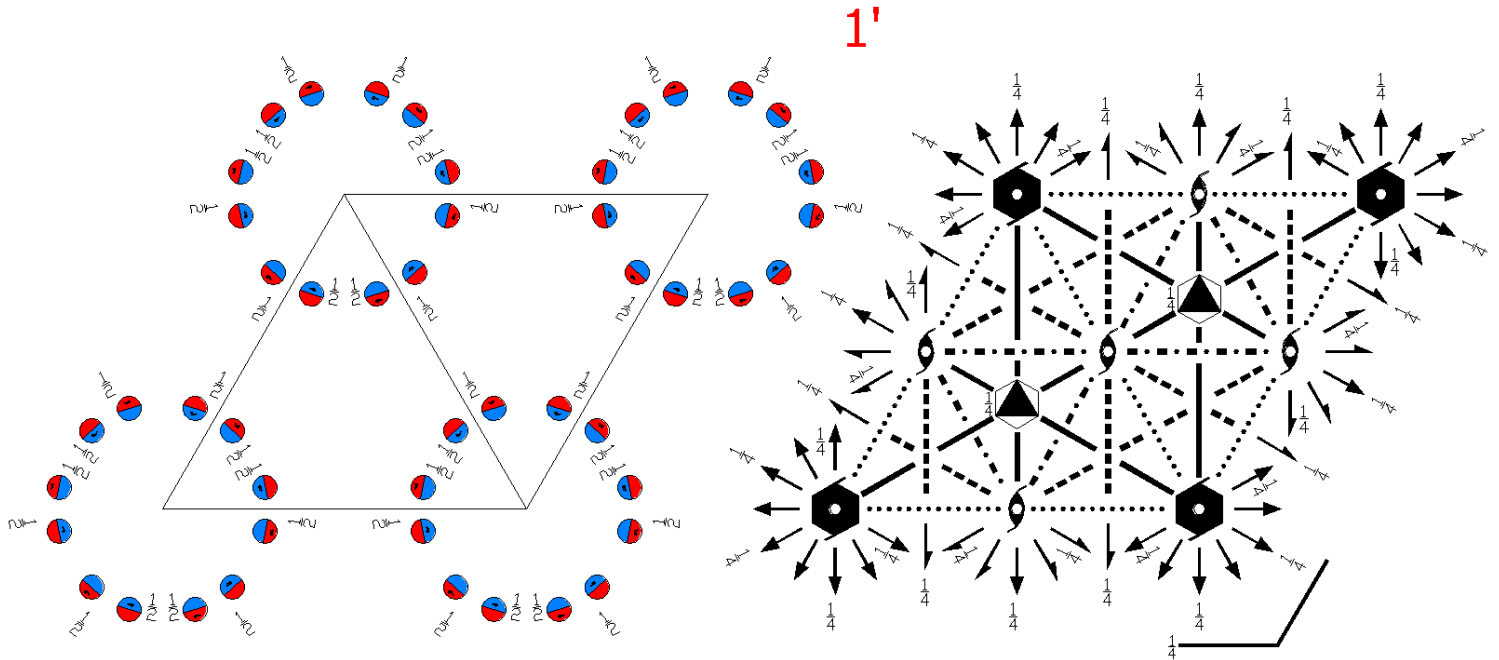
$P6_3/mmc1'$

194.2.1495

$6/mmm1'$

$P6_3/m2/m2/c1'$

Hexagonal



Origin at center ( $\bar{3}m11'$ ) at  $\bar{3}2/mc1'$

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $0 \leq z \leq 1/4$ ;  $x \leq 2y$ ;  $y \leq \min(1-x, 2x)$

Vertices  $0,0,0$   $2/3,1/3,0$   $1/3,2/3,0$   
 $0,0,1/4$   $2/3,1/3,1/4$   $1/3,2/3,1/4$

### Symmetry Operations

For 1 + set

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                            | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)        |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)    | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2) |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0)             | (8) 2 x,0,0<br>( $2_x$  0,0,0)                      | (9) 2 0,y,0<br>( $2_y$  0,0,0)                 |
| (10) 2 $x, \bar{x}, 1/4$<br>( $2_3$  0,0,1/2) | (11) 2 x,2x,1/4<br>( $2_2$  0,0,1/2)                | (12) 2 2x,x,1/4<br>( $2_1$  0,0,1/2)           |

- |   |   |   |
|---|---|---|
| (13) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)           | (14) $\bar{3}^+$ 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)          | (15) $\bar{3}^-$ 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0) |
| (16) m $\bar{x}$ ,y,1/4<br>( $m_z$  0,0,1/2)          | (17) $\bar{6}^-$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2) | (18) $\bar{6}^+$ 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2)  |
| (19) m $\bar{x}$ , $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0) | (20) m $\bar{x}$ ,2x,z<br>( $m_x$  0,0,0)                       | (21) m 2x,x,z<br>( $m_y$  0,0,0)                            |
| (22) c (0,0,1/2) $\bar{x}$ ,x,z<br>( $m_3$  0,0,1/2)  | (23) c (0,0,1/2) $\bar{x}$ ,0,z<br>( $m_2$  0,0,1/2)            | (24) c (0,0,1/2) 0,y,z<br>( $m_1$  0,0,1/2)                 |

## For 1' + set

- |  |  |  |
|--|--|--|
| (1) 1'<br>(1 0,0,0)'   | (2) 3 <sup>+</sup> 0,0,z<br>(3 <sub>z</sub>  0,0,0)'                           | (3) 3 <sup>-</sup> 0,0,z<br>(3 <sub>z</sub> <sup>-1</sup>  0,0,0)' |
| (4) 2' (0,0,1/2) 0,0,z<br>(2 <sub>z</sub>  0,0,1/2)'             | (5) 6 <sup>-</sup> (0,0,1/2) 0,0,z<br>(6 <sub>z</sub> <sup>-1</sup>  0,0,1/2)' | (6) 6 <sup>+</sup> (0,0,1/2) 0,0,z<br>(6 <sub>z</sub>  0,0,1/2)'   |
| (7) 2' $\bar{x}$ ,x,0<br>(2 <sub>xy</sub>  0,0,0)'               | (8) 2' $\bar{x}$ ,0,0<br>(2 <sub>x</sub>  0,0,0)'                              | (9) 2' 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                           |
| (10) 2' $\bar{x}$ , $\bar{x}$ ,1/4<br>(2 <sub>3</sub>  0,0,1/2)' | (11) 2' $\bar{x}$ ,2x,1/4<br>(2 <sub>2</sub>  0,0,1/2)'                        | (12) 2' 2x,x,1/4<br>(2 <sub>1</sub>  0,0,1/2)'                     |
| (13) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)'                   | (14) $\bar{3}^+$ ' 0,0,z; 0,0,0<br>( $\bar{3}_z$  0,0,0)'                      | (15) $\bar{3}^-$ ' 0,0,z; 0,0,0<br>( $\bar{3}_z^{-1}$  0,0,0)'     |
| (16) m' $\bar{x}$ ,y,1/4<br>( $m_z$  0,0,1/2)'                   | (17) $\bar{6}^-$ ' 0,0,z; 0,0,1/4<br>( $\bar{6}_z^{-1}$  0,0,1/2)'             | (18) $\bar{6}^+$ ' 0,0,z; 0,0,1/4<br>( $\bar{6}_z$  0,0,1/2)'      |
| (19) m' $\bar{x}$ , $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0)'          | (20) m' $\bar{x}$ ,2x,z<br>( $m_x$  0,0,0)'                                    | (21) m' 2x,x,z<br>( $m_y$  0,0,0)'                                 |
| (22) c' (0,0,1/2) $\bar{x}$ ,x,z<br>( $m_3$  0,0,1/2)'           | (23) c' (0,0,1/2) $\bar{x}$ ,0,z<br>( $m_2$  0,0,1/2)'                         | (24) c' (0,0,1/2) 0,y,z<br>( $m_1$  0,0,1/2)'                      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

- |    |   |     |  |  |   |
|----|---|-----|--|--|---|
|    |   |     | 1 +  |  | 1' +                                    |
| 24 | I | 11' | (1) x,y,z [0,0,0]                          | (2) $\bar{y}$ ,x-y,z [0,0,0]           | (3) $\bar{x}+y,\bar{x}$ ,z [0,0,0]      |
|    |   |     | (4) $\bar{x},\bar{y}$ ,z+1/2 [0,0,0]       | (5) y, $\bar{x}+y$ ,z+1/2 [0,0,0]      | (6) x-y,x,z+1/2 [0,0,0]                 |
|    |   |     | (7) y,x, $\bar{z}$ [0,0,0]                 | (8) x-y, $\bar{y},\bar{z}$ [0,0,0]     | (9) $\bar{x},\bar{x}+y,\bar{z}$ [0,0,0] |
|    |   |     | (10) $\bar{y},\bar{x},\bar{z}+1/2$ [0,0,0] | (11) $\bar{x}+y,y,\bar{z}+1/2$ [0,0,0] | (12) x,x-y, $\bar{z}+1/2$ [0,0,0]       |

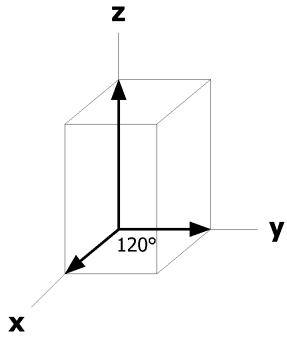
			(13) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]	(14) $y, \bar{x} + y, \bar{z}$ [0,0,0]	(15) $x - y, x, \bar{z}$ [0,0,0]
			(16) $x, y, \bar{z} + 1/2$ [0,0,0]	(17) $\bar{y}, x - y, \bar{z} + 1/2$ [0,0,0]	(18) $\bar{x} + y, \bar{x}, \bar{z} + 1/2$ [0,0,0]
			(19) $\bar{y}, \bar{x}, z$ [0,0,0]	(20) $\bar{x} + y, y, z$ [0,0,0]	(21) $x, x - y, z$ [0,0,0]
			(22) $y, x, z + 1/2$ [0,0,0]	(23) $x - y, \bar{y}, z + 1/2$ [0,0,0]	(24) $\bar{x}, \bar{x} + y, z + 1/2$ [0,0,0]
12	k	.m.1'	$x, 2x, z$ [0,0,0]	$2\bar{x}, \bar{x}, z$ [0,0,0]	$x, \bar{x}, z$ [0,0,0]
			$\bar{x}, 2\bar{x}, z + 1/2$ [0,0,0]	$2x, x, z + 1/2$ [0,0,0]	$\bar{x}, x, z + 1/2$ [0,0,0]
			$2x, x, \bar{z}$ [0,0,0]	$\bar{x}, 2\bar{x}, \bar{z}$ [0,0,0]	$\bar{x}, x, \bar{z}$ [0,0,0]
			$2\bar{x}, \bar{x}, \bar{z} + 1/2$ [0,0,0]	$x, 2x, \bar{z} + 1/2$ [0,0,0]	$x, \bar{x}, \bar{z} + 1/2$ [0,0,0]
12	j	m..1'	$x, y, 1/4$ [0,0,0]	$\bar{y}, x - y, 1/4$ [0,0,0]	$\bar{x} + y, \bar{x}, 1/4$ [0,0,0]
			$\bar{x}, \bar{y}, 3/4$ [0,0,0]	$y, \bar{x} + y, 3/4$ [0,0,0]	$x - y, x, 3/4$ [0,0,0]
			$y, x, 3/4$ [0,0,0]	$x - y, \bar{y}, 3/4$ [0,0,0]	$\bar{x}, \bar{x} + y, 3/4$ [0,0,0]
			$\bar{y}, \bar{x}, 1/4$ [0,0,0]	$\bar{x} + y, y, 1/4$ [0,0,0]	$x, x - y, 1/4$ [0,0,0]
12	i	.2.1'	$x, 0, 0$ [0,0,0]	$0, x, 0$ [0,0,0]	$\bar{x}, \bar{x}, 0$ [0,0,0]
			$\bar{x}, 0, 1/2$ [0,0,0]	$0, \bar{x}, 1/2$ [0,0,0]	$x, x, 1/2$ [0,0,0]
			$\bar{x}, 0, 0$ [0,0,0]	$0, \bar{x}, 0$ [0,0,0]	$x, x, 0$ [0,0,0]
			$x, 0, 1/2$ [0,0,0]	$0, x, 1/2$ [0,0,0]	$\bar{x}, \bar{x}, 1/2$ [0,0,0]
6	h	mm21'	$x, 2x, 1/4$ [0,0,0]	$2\bar{x}, \bar{x}, 1/4$ [0,0,0]	$x, \bar{x}, 1/4$ [0,0,0]
			$\bar{x}, 2\bar{x}, 3/4$ [0,0,0]	$2x, x, 3/4$ [0,0,0]	$\bar{x}, x, 3/4$ [0,0,0]
6	g	.2/m.1'	$1/2, 0, 0$ [0,0,0]	$0, 1/2, 0$ [0,0,0]	$1/2, 1/2, 0$ [0,0,0]
			$1/2, 0, 1/2$ [0,0,0]	$0, 1/2, 1/2$ [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]
4	f	3m.1'	$1/3, 2/3, z$ [0,0,0]	$2/3, 1/3, z + 1/2$ [0,0,0]	$2/3, 1/3, \bar{z}$ [0,0,0]
					$1/3, 2/3, \bar{z} + 1/2$ [0,0,0]
4	e	3m.1'	$0, 0, z$ [0,0,0]	$0, 0, z + 1/2$ [0,0,0]	$0, 0, \bar{z}$ [0,0,0]
					$0, 0, \bar{z} + 1/2$ [0,0,0]
2	d	$\bar{6}m21'$	$1/3, 2/3, 3/4$ [0,0,0]	$2/3, 1/3, 1/4$ [0,0,0]	
2	c	$\bar{6}m21'$	$1/3, 2/3, 1/4$ [0,0,0]	$2/3, 1/3, 3/4$ [0,0,0]	
2	b	$\bar{6}m21'$	$0, 0, 1/4$ [0,0,0]	$0, 0, 3/4$ [0,0,0]	
2	a	$\bar{3}m.1'$	$0, 0, 0$ [0,0,0]	$0, 0, 1/2$ [0,0,0]	

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
Origin at x,0,0

Along [2,1,0] p2mm1'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at x,x/2,0



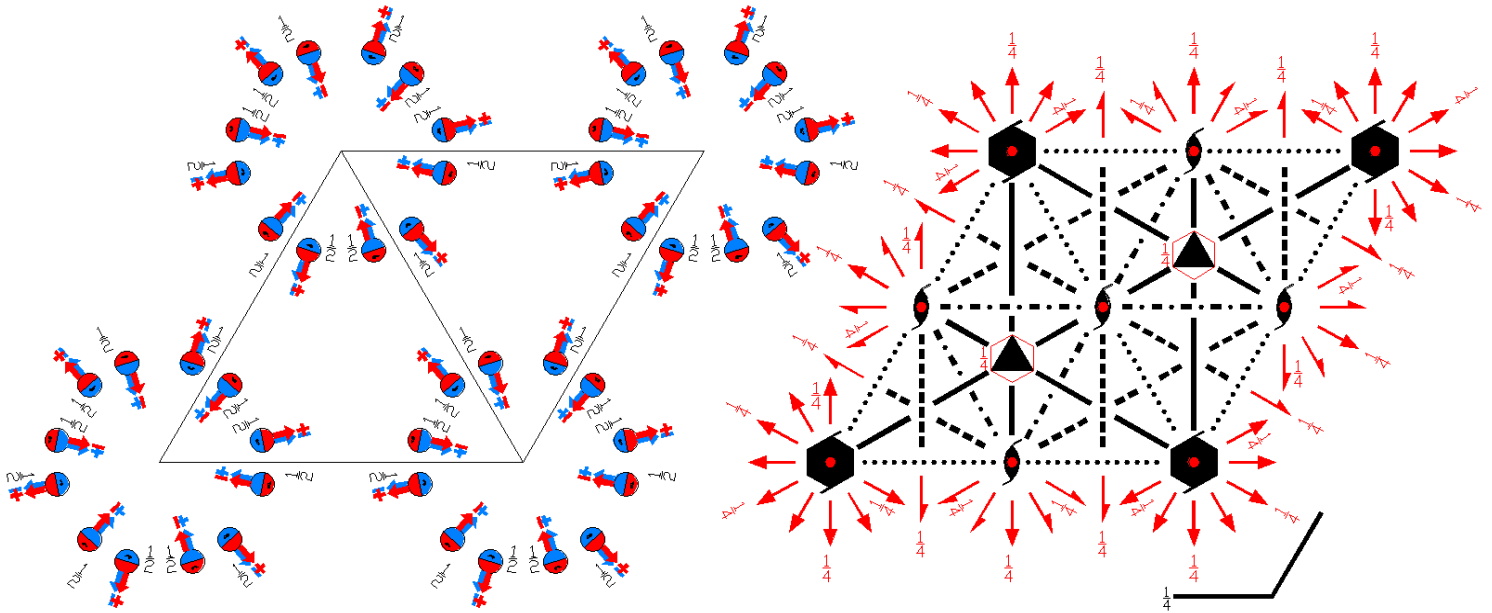
$P6_3/m'mc$

194.3.1496

$6/m'mm$

$P6_3/m'2'/m2'/c$

Hexagonal



Origin at center ( $\bar{3}'m1$ ) at  $\bar{3}'2'/mc$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq 2y;$	$y \leq \min(1-x, 2x)$
Vertices	0,0,0	$2/3, 1/3, 0$	$1/3, 2/3, 0$		
	0,0,1/4	$2/3, 1/3, 1/4$	$1/3, 2/3, 1/4$		

**Symmetry Operations**

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                                | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)        |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)        | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2) |
| (7) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)'             | (8) $2'$ x,0,0<br>( $2_x$  0,0,0)'                  | (9) $2'$ 0,y,0<br>( $2_y$  0,0,0)'             |
| (10) $2'$ x, $\bar{x}$ ,1/4<br>( $2_3$  0,0,1/2)' | (11) $2'$ x,2x,1/4<br>( $2_2$  0,0,1/2)'            | (12) $2'$ 2x,x,1/4<br>( $2_1$  0,0,1/2)'       |

(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ ' 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(15) $\bar{3}^-$ ' 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(16) m' x,y,1/4 ( $m_z$  0,0,1/2)'	(17) $\bar{6}^-$ ' 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1}$  0,0,1/2)'	(18) $\bar{6}^+$ ' 0,0,z; 0,0,1/4 ( $\bar{6}_z$  0,0,1/2)'
(19) m $\bar{x},\bar{x},z$ ( $m_{xy}$  0,0,0)	(20) m x,2x,z ( $m_x$  0,0,0)	(21) m 2x,x,z ( $m_y$  0,0,0)
(22) c (0,0,1/2) x,x,z ( $m_3$  0,0,1/2)	(23) c (0,0,1/2) x,0,z ( $m_2$  0,0,1/2)	(24) c (0,0,1/2) 0,y,z ( $m_1$  0,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z+1/2$ [ $\bar{u},\bar{v},w$ ]	(5) $y,\bar{x}+y,z+1/2$ [ $v,\bar{u}+v,w$ ]	(6) x-y,x,z+1/2 [u-v,u,w]
			(7) y,x, $\bar{z}$ [ $\bar{v},\bar{u},w$ ]	(8) x-y, $\bar{y},\bar{z}$ [ $\bar{u}+v,v,w$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}$ [u,u-v,w]
			(10) $\bar{y},\bar{x},\bar{z}+1/2$ [v,u,w]	(11) $\bar{x}+y,\bar{y},\bar{z}+1/2$ [u-v, $\bar{v},w$ ]	(12) x,x-y, $\bar{z}+1/2$ [ $\bar{u},\bar{u}+v,w$ ]
			(13) $\bar{x},\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]	(14) y, $\bar{x}+y,\bar{z}$ [v, $\bar{u}+v,\bar{w}$ ]	(15) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ]
			(16) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(17) $\bar{y},x-y,\bar{z}+1/2$ [ $\bar{v},u-v,\bar{w}$ ]	(18) $\bar{x}+y,\bar{x},\bar{z}+1/2$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]
			(19) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ]	(20) $\bar{x}+y,y,z$ [u-v, $\bar{v},\bar{w}$ ]	(21) x,x-y,z [ $\bar{u},\bar{u}+v,\bar{w}$ ]
			(22) y,x,z+1/2 [ $\bar{v},\bar{u},\bar{w}$ ]	(23) x-y, $\bar{y},z+1/2$ [ $\bar{u}+v,v,\bar{w}$ ]	(24) $\bar{x},\bar{x}+y,z+1/2$ [u,u-v, $\bar{w}$ ]
12	k	.m.	x,2x,z [u,0,0]	$2\bar{x},\bar{x},z$ [0,u,0]	x, $\bar{x},z$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},2\bar{x},z+1/2$ [ $\bar{u},0,0$ ]	2x,x,z+1/2 [0, $\bar{u},0$ ]	$\bar{x},x,z+1/2$ [u,u,0]
			2x,x, $\bar{z}$ [0, $\bar{u},0$ ]	$\bar{x},2\bar{x},\bar{z}$ [ $\bar{u},0,0$ ]	$\bar{x},x,\bar{z}$ [u,u,0]
			$2\bar{x},\bar{x},\bar{z}+1/2$ [0,u,0]	x,2x, $\bar{z}+1/2$ [u,0,0]	x, $\bar{x},\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]
12	j	m'..	x,y,1/4 [u,v,0]	$\bar{y},x-y,1/4$ [ $\bar{v},u-v,0$ ]	$\bar{x}+y,\bar{x},1/4$ [ $\bar{u}+v,\bar{u},0$ ]
			$\bar{x},\bar{y},3/4$ [ $\bar{u},\bar{v},0$ ]	y, $\bar{x}+y,3/4$ [v, $\bar{u}+v,0$ ]	x-y,x,3/4 [u-v,u,0]
			y,x,3/4 [ $\bar{v},\bar{u},0$ ]	x-y, $\bar{y},3/4$ [ $\bar{u}+v,v,0$ ]	$\bar{x},\bar{x}+y,3/4$ [u,u-v,0]
			$\bar{y},\bar{x},1/4$ [v,u,0]	$\bar{x}+y,y,1/4$ [u-v, $\bar{v},0$ ]	x,x-y,1/4 [ $\bar{u},\bar{u}+v,0$ ]

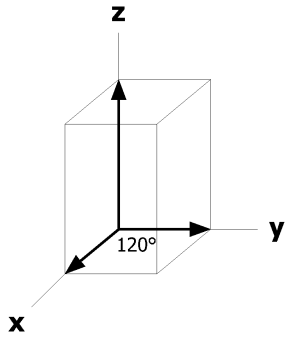
12	i	.2'	x,0,0 [u,2u,w]	0,x,0 [2 $\bar{u}$ , $\bar{u}$ ,w]	$\bar{x},\bar{x},0$ [u, $\bar{u}$ ,w]	
			$\bar{x},0,1/2$ [ $\bar{u}$ ,2 $\bar{u}$ ,w]	0, $\bar{x},1/2$ [2u,u,w]	x,x,1/2 [ $\bar{u}$ ,u,w]	
			$\bar{x},0,0$ [ $\bar{u}$ ,2 $\bar{u}$ , $\bar{w}$ ]	0, $\bar{x},0$ [2u,u, $\bar{w}$ ]	x,x,0 [ $\bar{u}$ ,u, $\bar{w}$ ]	
			x,0,1/2 [u,2u, $\bar{w}$ ]	0,x,1/2 [2 $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]	$\bar{x},\bar{x},1/2$ [u, $\bar{u}$ , $\bar{w}$ ]	
6	h	m'm2'	x,2x,1/4 [u,0,0]	2 $\bar{x},\bar{x},1/4$ [0,u,0]	x, $\bar{x},1/4$ [ $\bar{u}$ , $\bar{u}$ ,0]	
			$\bar{x},2\bar{x},3/4$ [ $\bar{u}$ ,0,0]	2x,x,3/4 [0, $\bar{u}$ ,0]	$\bar{x},x,3/4$ [u,u,0]	
6	g	.2'/m.	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
			1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
4	f	3m.	1/3,2/3,z [0,0,0]	2/3,1/3,z+1/2 [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	1/3,2/3, $\bar{z}+1/2$ [0,0,0]
4	e	3m.	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]
2	d	$\bar{6}'m2'$	1/3,2/3,3/4 [0,0,0]	2/3,1/3,1/4 [0,0,0]		
2	c	$\bar{6}'m2'$	1/3,2/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]		
2	b	$\bar{6}'m2'$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	a	$\bar{3}'m.$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p6mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p<sub>2a</sub>2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



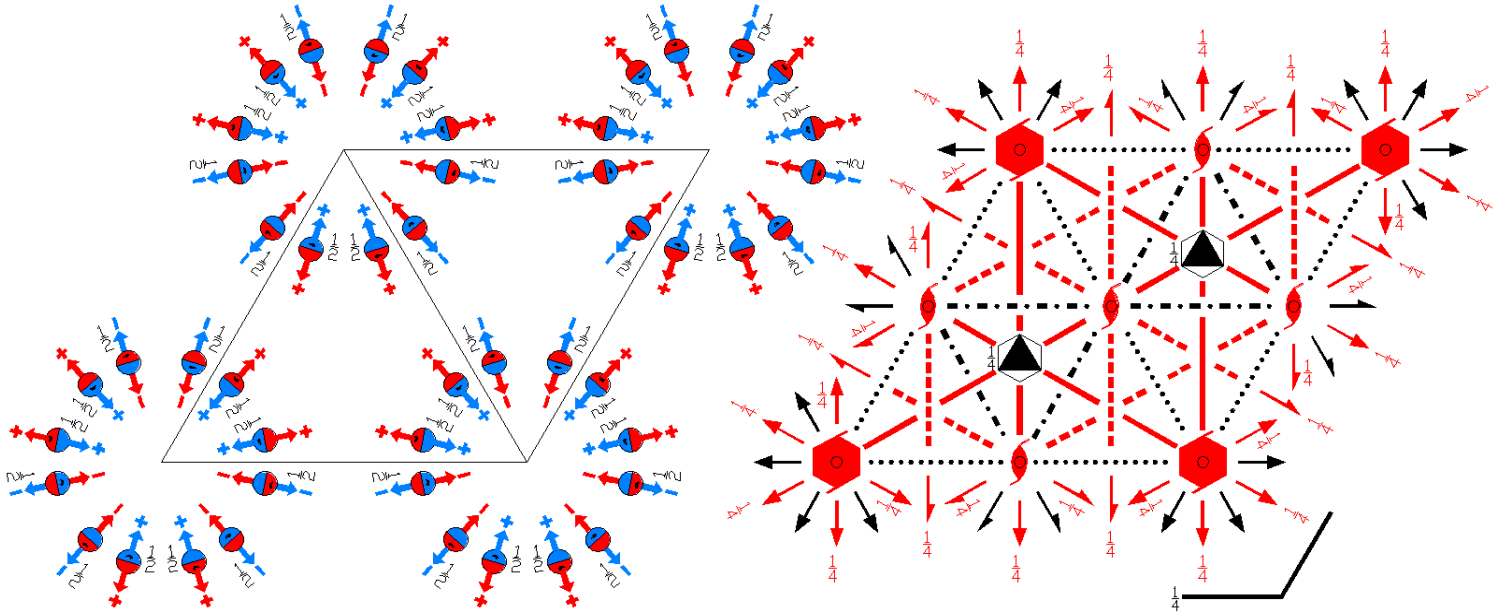
$P6_3'/mm'c$

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$6'/mm'm$

$P6_3'/m2/m'2'/c$

Hexagonal



Origin at center ( $\bar{3}'m'1$ ) at  $\bar{3}'2/m'c$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq 2y;$	$y \leq \min(1-x, 2x)$
Vertices	0,0,0	$2/3, 1/3, 0$	$1/3, 2/3, 0$		
	0,0,1/4	$2/3, 1/3, 1/4$	$1/3, 2/3, 1/4$		

### Symmetry Operations

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                                | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                   | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)         |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)'    | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)' | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)' |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0)                 | (8) 2 x,0,0<br>( $2_x$  0,0,0)                       | (9) 2 0,y,0<br>( $2_y$  0,0,0)                  |
| (10) $2'$ x, $\bar{x}$ ,1/4<br>( $2_3$  0,0,1/2)' | (11) $2'$ x,2x,1/4<br>( $2_2$  0,0,1/2)'             | (12) $2'$ 2x,x,1/4<br>( $2_1$  0,0,1/2)'        |



(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ ' 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(15) $\bar{3}^-$ ' 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(16) m $\bar{x}$ ,y,1/4 ( $m_z$  0,0,1/2)	(17) $\bar{6}^-$ 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1}$  0,0,1/2)	(18) $\bar{6}^+$ 0,0,z; 0,0,1/4 ( $\bar{6}_z$  0,0,1/2)
(19) m' $\bar{x}$ , $\bar{x}$ ,z ( $m_{xy}$  0,0,0)'	(20) m' $\bar{x}$ ,2x,z ( $m_x$  0,0,0)'	(21) m' 2x,x,z ( $m_y$  0,0,0)'
(22) c (0,0,1/2) $\bar{x}$ ,x,z ( $m_3$  0,0,1/2)	(23) c (0,0,1/2) $\bar{x}$ ,0,z ( $m_2$  0,0,1/2)	(24) c (0,0,1/2) 0,y,z ( $m_1$  0,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [u,v, $\bar{w}$ ]	(5) y, $\bar{x}$ +y,z+1/2 [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) x-y,x,z+1/2 [ $\bar{u}$ +v, $\bar{u}$ , $\bar{w}$ ]
			(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y}$ , $\bar{z}$ [u-v, $\bar{v}$ , $\bar{w}$ ]	(9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ [ $\bar{u}$ , $\bar{u}$ +v, $\bar{w}$ ]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ +1/2 [v,u,w]	(11) $\bar{x}$ +y, $\bar{y}$ , $\bar{z}$ +1/2 [u-v, $\bar{v}$ ,w]	(12) x,x-y, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{u}$ +v,w]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(14) y, $\bar{x}$ +y, $\bar{z}$ [v, $\bar{u}$ +v, $\bar{w}$ ]	(15) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ]
			(16) x,y, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(17) $\bar{y}$ ,x-y, $\bar{z}$ +1/2 [v, $\bar{u}$ +v,w]	(18) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ +1/2 [u-v,u,w]
			(19) $\bar{y}$ , $\bar{x}$ ,z [ $\bar{v}$ , $\bar{u}$ ,w]	(20) $\bar{x}$ +y,y,z [ $\bar{u}$ +v,v,w]	(21) x,x-y,z [u,u-v,w]
			(22) y,x,z+1/2 [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(23) x-y, $\bar{y}$ ,z+1/2 [ $\bar{u}$ +v,v, $\bar{w}$ ]	(24) $\bar{x}$ , $\bar{x}$ +y,z+1/2 [u,u-v, $\bar{w}$ ]
12	k	.m'	x,2x,z [u,2u,w]	2 $\bar{x}$ , $\bar{x}$ ,z [2 $\bar{u}$ , $\bar{u}$ ,w]	x, $\bar{x}$ ,z [u, $\bar{u}$ ,w]
			$\bar{x}$ ,2 $\bar{x}$ ,z+1/2 [u,2u, $\bar{w}$ ]	2x,x,z+1/2 [2 $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]	$\bar{x}$ ,x,z+1/2 [u, $\bar{u}$ , $\bar{w}$ ]
			2x,x, $\bar{z}$ [2u,u, $\bar{w}$ ]	$\bar{x}$ ,2 $\bar{x}$ , $\bar{z}$ [ $\bar{u}$ ,2 $\bar{u}$ , $\bar{w}$ ]	$\bar{x}$ ,x, $\bar{z}$ [ $\bar{u}$ ,u, $\bar{w}$ ]
			2 $\bar{x}$ , $\bar{x}$ , $\bar{z}$ +1/2 [2u,u,w]	x,2x, $\bar{z}$ +1/2 [ $\bar{u}$ ,2 $\bar{u}$ ,w]	x, $\bar{x}$ , $\bar{z}$ +1/2 [ $\bar{u}$ ,u,w]
12	j	m..	x,y,1/4 [0,0,w]	$\bar{y}$ ,x-y,1/4 [0,0,w]	$\bar{x}$ +y, $\bar{x}$ ,1/4 [0,0,w]
			$\bar{x}$ , $\bar{y}$ ,3/4 [0,0, $\bar{w}$ ]	y, $\bar{x}$ +y,3/4 [0,0, $\bar{w}$ ]	x-y,x,3/4 [0,0, $\bar{w}$ ]
			y,x,3/4 [0,0, $\bar{w}$ ]	x-y, $\bar{y}$ ,3/4 [0,0, $\bar{w}$ ]	$\bar{x}$ , $\bar{x}$ +y,3/4 [0,0, $\bar{w}$ ]
			$\bar{y}$ , $\bar{x}$ ,1/4 [0,0,w]	$\bar{x}$ +y,y,1/4 [0,0,w]	x,x-y,1/4 [0,0,w]

Continued

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P6<sub>3</sub>'/mm'c

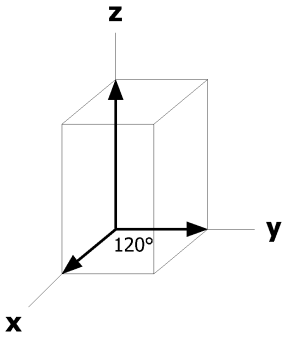
12	i	.2.	x,0,0 [u,0,0]	0,x,0 [0,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	
			$\bar{x},0,1/2$ [u,0,0]	0, $\bar{x},1/2$ [0,u,0]	x,x,1/2 [ $\bar{u},\bar{u},0$ ]	
			$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0, $\bar{x},0$ [0, $\bar{u},0$ ]	x,x,0 [u,u,0]	
			x,0,1/2 [ $\bar{u},0,0$ ]	0,x,1/2 [0, $\bar{u},0$ ]	$\bar{x},\bar{x},1/2$ [u,u,0]	
6	h	mm'2'	x,2x,1/4 [0,0,w]	2 $\bar{x},\bar{x},1/4$ [0,0,w]	x, $\bar{x},1/4$ [0,0,w]	
			$\bar{x},2\bar{x},3/4$ [0,0, $\bar{w}$ ]	2x,x,3/4 [0,0, $\bar{w}$ ]	$\bar{x},x,3/4$ [0,0, $\bar{w}$ ]	
6	g	.2/m'.	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
			1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
4	f	3m'.	1/3,2/3,z [0,0,w]	2/3,1/3,z+1/2 [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	1/3,2/3, $\bar{z}+1/2$ [0,0,w]
4	e	3m'.	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0,w]
2	d	$\bar{6}m'2'$	1/3,2/3,3/4 [0,0,w]	2/3,1/3,1/4 [0,0, $\bar{w}$ ]		
2	c	$\bar{6}m'2'$	1/3,2/3,1/4 [0,0,w]	2/3,1/3,3/4 [0,0, $\bar{w}$ ]		
2	b	$\bar{6}m'2'$	0,0,1/4 [0,0,w]	0,0,3/4 [0,0, $\bar{w}$ ]		
2	a	$\bar{3}m'$ .	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p<sub>2a</sub>'2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



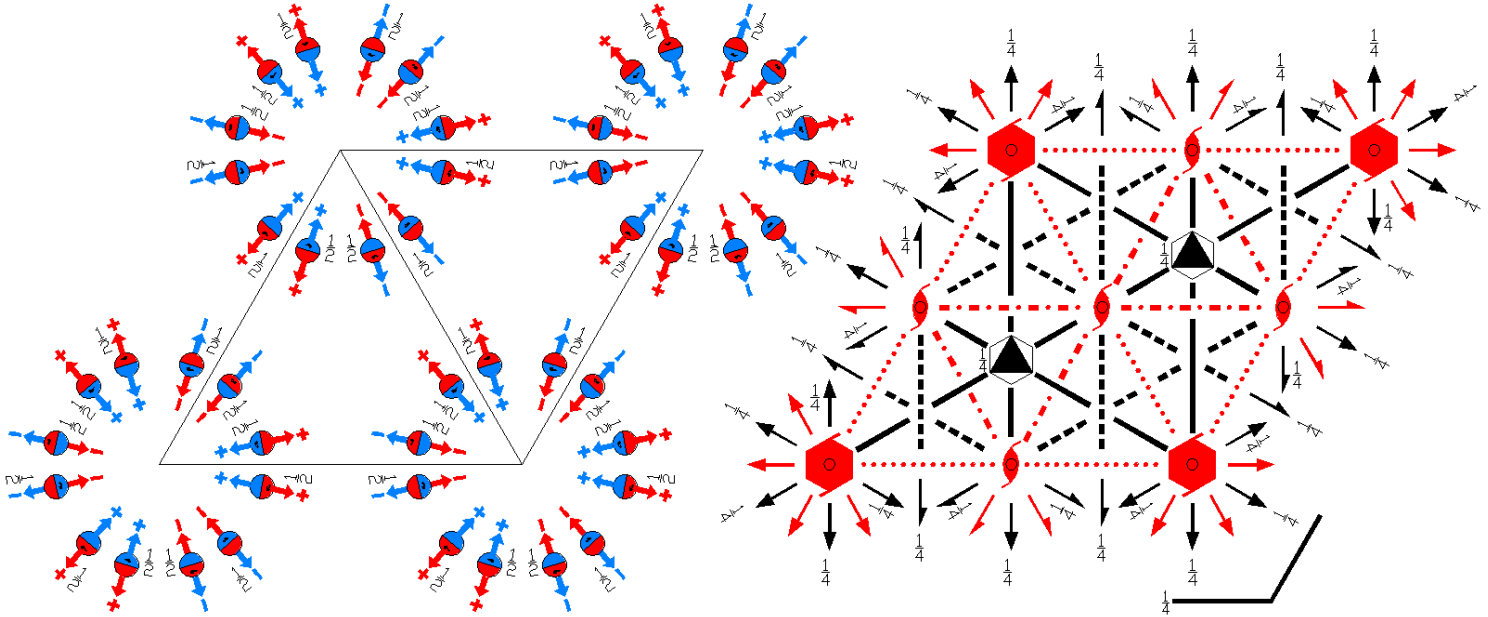
$P6_3'/mmc'$

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$6'/mmm'$

$P6_3'/m2'/m2'/c'$

Hexagonal



Origin at center ( $\bar{3}'m1$ ) at  $\bar{3}'2'/mc'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq 2y;$	$y \leq \min(1-x, 2x)$
Vertices	0,0,0	2/3,1/3,0	1/3,2/3,0		
	0,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4		

**Symmetry Operations**

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                             | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                   | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)         |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)' | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)' | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)' |
| (7) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)'          | (8) $2'$ x,0,0<br>( $2_x$  0,0,0)'                   | (9) $2'$ 0,y,0<br>( $2_y$  0,0,0)'              |
| (10) 2 x, $\bar{x}$ ,1/4<br>( $2_3$  0,0,1/2)  | (11) 2 x,2x,1/4<br>( $2_2$  0,0,1/2)                 | (12) 2 2x,x,1/4<br>( $2_1$  0,0,1/2)            |

(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(16) m $\bar{x}$ ,y,1/4 ( $m_z$  0,0,1/2)	(17) $\bar{6}^-$ 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1}$  0,0,1/2)	(18) $\bar{6}^+$ 0,0,z; 0,0,1/4 ( $\bar{6}_z$  0,0,1/2)
(19) m $\bar{x}$ , $\bar{x}$ ,z ( $m_{xy}$  0,0,0)	(20) m $\bar{x}$ ,2x,z ( $m_x$  0,0,0)	(21) m 2x,x,z ( $m_y$  0,0,0)
(22) c' (0,0,1/2) $\bar{x}$ ,x,z ( $m_3$  0,0,1/2)'	(23) c' (0,0,1/2) $\bar{x}$ ,0,z ( $m_2$  0,0,1/2)'	(24) c' (0,0,1/2) 0,y,z ( $m_1$  0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	l	1	(1) $\bar{x}$ ,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y$ , $\bar{x}$ ,z [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [u,v, $\bar{w}$ ]	(5) y, $\bar{x}+y$ ,z+1/2 [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) x-y,x,z+1/2 [ $\bar{u}+v$ , $\bar{u}$ , $\bar{w}$ ]
			(7) y,x, $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ ,w]	(8) x-y, $\bar{y}$ , $\bar{z}$ [ $\bar{u}+v$ ,v,w]	(9) $\bar{x}$ , $\bar{x}+y$ , $\bar{z}$ [u,u-v,w]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}+1/2$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(11) $\bar{x}+y$ ,y, $\bar{z}+1/2$ [ $\bar{u}+v$ ,v, $\bar{w}$ ]	(12) x,x-y, $\bar{z}+1/2$ [u,u-v, $\bar{w}$ ]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(14) y, $\bar{x}+y$ , $\bar{z}$ [v, $\bar{u}+v$ , $\bar{w}$ ]	(15) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ]
			(16) x,y, $\bar{z}+1/2$ [ $\bar{u}$ , $\bar{v}$ ,w]	(17) $\bar{y}$ ,x-y, $\bar{z}+1/2$ [v, $\bar{u}+v$ ,w]	(18) $\bar{x}+y$ , $\bar{x}$ , $\bar{z}+1/2$ [u-v,u,w]
			(19) $\bar{y}$ , $\bar{x}$ ,z [v,u, $\bar{w}$ ]	(20) $\bar{x}+y$ ,y,z [u-v, $\bar{v}$ , $\bar{w}$ ]	(21) x,x-y,z [ $\bar{u}$ , $\bar{u}+v$ , $\bar{w}$ ]
			(22) y,x,z+1/2 [v,u,w]	(23) x-y, $\bar{y}$ ,z+1/2 [u-v, $\bar{v}$ ,w]	(24) $\bar{x}$ , $\bar{x}+y$ ,z+1/2 [ $\bar{u}$ , $\bar{u}+v$ ,w]
12	k	.m.	x,2x,z [u,0,0]	2 $\bar{x}$ , $\bar{x}$ ,z [0,u,0]	x, $\bar{x}$ ,z [ $\bar{u}$ , $\bar{u}$ ,0]
			$\bar{x}$ ,2 $\bar{x}$ ,z+1/2 [u,0,0]	2x,x,z+1/2 [0,u,0]	$\bar{x}$ ,x,z+1/2 [ $\bar{u}$ , $\bar{u}$ ,0]
			2x,x, $\bar{z}$ [0, $\bar{u}$ ,0]	$\bar{x}$ ,2 $\bar{x}$ , $\bar{z}$ [ $\bar{u}$ ,0,0]	$\bar{x}$ ,x, $\bar{z}$ [u,u,0]
			2 $\bar{x}$ , $\bar{x}$ , $\bar{z}+1/2$ [0, $\bar{u}$ ,0]	x,2x, $\bar{z}+1/2$ [ $\bar{u}$ ,0,0]	x, $\bar{x}$ , $\bar{z}+1/2$ [u,u,0]
12	j	m..	x,y,1/4 [0,0,w]	$\bar{y}$ ,x-y,1/4 [0,0,w]	$\bar{x}+y$ , $\bar{x}$ ,1/4 [0,0,w]
			$\bar{x}$ , $\bar{y}$ ,3/4 [0,0, $\bar{w}$ ]	y, $\bar{x}+y$ ,3/4 [0,0, $\bar{w}$ ]	x-y,x,3/4 [0,0, $\bar{w}$ ]
			y,x,3/4 [0,0,w]	x-y, $\bar{y}$ ,3/4 [0,0,w]	$\bar{x}$ , $\bar{x}+y$ ,3/4 [0,0,w]
			$\bar{y}$ , $\bar{x}$ ,1/4 [0,0, $\bar{w}$ ]	$\bar{x}+y$ ,y,1/4 [0,0, $\bar{w}$ ]	x,x-y,1/4 [0,0, $\bar{w}$ ]

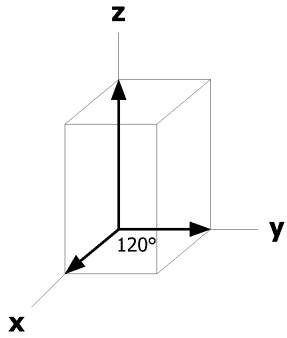
12	i	.2'	x,0,0 [u,2u,w]	0,x,0 [2 $\bar{u}$ , $\bar{u}$ ,w]	$\bar{x},\bar{x},0$ [u, $\bar{u}$ ,w]	
			$\bar{x},0,1/2$ [u,2u, $\bar{w}$ ]	0, $\bar{x},1/2$ [2 $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]	x,x,1/2 [u, $\bar{u}$ , $\bar{w}$ ]	
			$\bar{x},0,0$ [ $\bar{u}$ ,2 $\bar{u}$ , $\bar{w}$ ]	0, $\bar{x},0$ [2u,u, $\bar{w}$ ]	x,x,0 [ $\bar{u}$ ,u, $\bar{w}$ ]	
			x,0,1/2 [ $\bar{u}$ ,2 $\bar{u}$ ,w]	0,x,1/2 [2u,u,w]	$\bar{x},\bar{x},1/2$ [ $\bar{u}$ ,u,w]	
6	h	mm2	x,2x,1/4 [0,0,0]	2 $\bar{x},\bar{x},1/4$ [0,0,0]	x, $\bar{x},1/4$ [0,0,0]	
			$\bar{x},2\bar{x},3/4$ [0,0,0]	2x,x,3/4 [0,0,0]	$\bar{x},x,3/4$ [0,0,0]	
6	g	.2'/m.	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
			1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
4	f	3m.	1/3,2/3,z [0,0,0]	2/3,1/3,z+1/2 [0,0,0]	2/3,1/3, $\bar{z}$ [0,0,0]	1/3,2/3, $\bar{z}+1/2$ [0,0,0]
4	e	3m.	0,0,z [0,0,0]	0,0,z+1/2 [0,0,0]	0,0, $\bar{z}$ [0,0,0]	0,0, $\bar{z}+1/2$ [0,0,0]
2	d	$\bar{6}m2$	1/3,2/3,3/4 [0,0,0]	2/3,1/3,1/4 [0,0,0]		
2	c	$\bar{6}m2$	1/3,2/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]		
2	b	$\bar{6}m2$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	a	$\bar{3}'m.$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2mm  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



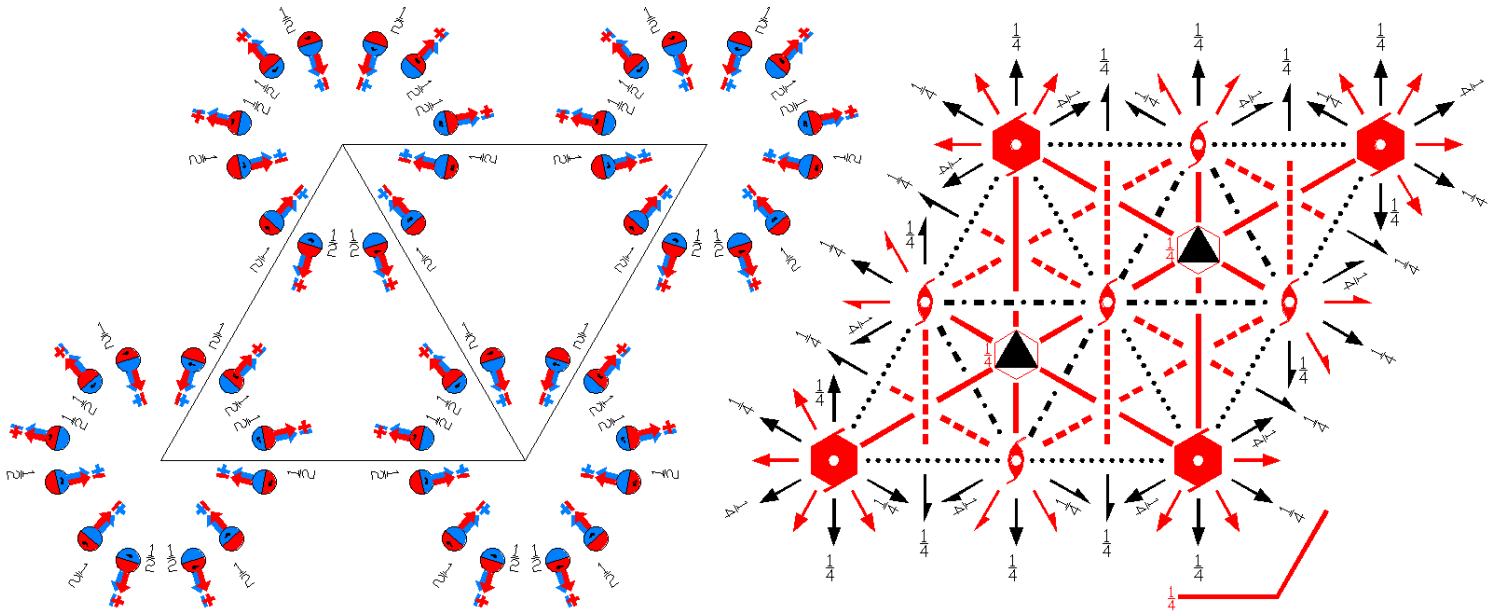
$P6_3'/m'm'c$

194.6.1499

$6'/m'm'm$

$P6_3'/m'2'/m'2'/c$

Hexagonal



Origin at center ( $\bar{3}m'1$ ) at  $\bar{3}2'/m'c$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq 2y;$	$y \leq \min(1-x, 2x)$
Vertices	0,0,0	2/3,1/3,0	1/3,2/3,0		
	0,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4		

**Symmetry Operations**

- |  |  |   |
|--|--|---|
| (1) 1<br>(1 0,0,0)                             | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                   | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)         |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)' | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)' | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)' |
| (7) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)'          | (8) $2'$ x,0,0<br>( $2_x$  0,0,0)'                   | (9) $2'$ 0,y,0<br>( $2_y$  0,0,0)'              |
| (10) 2 x, $\bar{x}$ ,1/4<br>( $2_3$  0,0,1/2)  | (11) 2 x,2x,1/4<br>( $2_2$  0,0,1/2)                 | (12) 2 2x,x,1/4<br>( $2_1$  0,0,1/2)            |

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)
(16) m' x,y,1/4 ( $m_z$  0,0,1/2)'	(17) $\bar{6}^-$ 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1}$  0,0,1/2)'	(18) $\bar{6}^+$ 0,0,z; 0,0,1/4 ( $\bar{6}_z$  0,0,1/2)'
(19) m' x, $\bar{x}$ ,z ( $m_{xy}$  0,0,0)'	(20) m' x,2x,z ( $m_x$  0,0,0)'	(21) m' 2x,x,z ( $m_y$  0,0,0)'
(22) c (0,0,1/2) x,x,z ( $m_3$  0,0,1/2)	(23) c (0,0,1/2) x,0,z ( $m_2$  0,0,1/2)	(24) c (0,0,1/2) 0,y,z ( $m_1$  0,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y$ , $\bar{x}$ ,z [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [u,v, $\bar{w}$ ]	(5) y, $\bar{x}+y$ ,z+1/2 [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(6) x-y,x,z+1/2 [ $\bar{u}+v$ , $\bar{u}$ , $\bar{w}$ ]
			(7) y,x, $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ ,w]	(8) x-y, $\bar{y}$ , $\bar{z}$ [ $\bar{u}+v$ ,v,w]	(9) $\bar{x}$ , $\bar{x}+y$ , $\bar{z}$ [u,u-v,w]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}+1/2$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(11) $\bar{x}+y$ ,y, $\bar{z}+1/2$ [ $\bar{u}+v$ ,v, $\bar{w}$ ]	(12) x,x-y, $\bar{z}+1/2$ [u,u-v, $\bar{w}$ ]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(14) y, $\bar{x}+y$ , $\bar{z}$ [ $\bar{v}$ ,u-v,w]	(15) x-y,x, $\bar{z}$ [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(16) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(17) $\bar{y}$ ,x-y, $\bar{z}+1/2$ [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(18) $\bar{x}+y$ , $\bar{x}$ , $\bar{z}+1/2$ [ $\bar{u}+v$ , $\bar{u}$ , $\bar{w}$ ]
			(19) $\bar{y}$ , $\bar{x}$ ,z [ $\bar{v}$ , $\bar{u}$ ,w]	(20) $\bar{x}+y$ ,y,z [ $\bar{u}+v$ ,v,w]	(21) x,x-y,z [u,u-v,w]
			(22) y,x,z+1/2 [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(23) x-y, $\bar{y}$ ,z+1/2 [ $\bar{u}+v$ ,v, $\bar{w}$ ]	(24) $\bar{x}$ , $\bar{x}+y$ ,z+1/2 [u,u-v, $\bar{w}$ ]
12	k	.m'	x,2x,z [u,2u,w]	$2\bar{x}$ , $\bar{x}$ ,z [2 $\bar{u}$ , $\bar{u}$ ,w]	x, $\bar{x}$ ,z [u, $\bar{u}$ ,w]
			$\bar{x}$ , $2\bar{x}$ ,z+1/2 [u,2u, $\bar{w}$ ]	2x,x,z+1/2 [2 $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]	$\bar{x}$ ,x,z+1/2 [u, $\bar{u}$ , $\bar{w}$ ]
			2x,x, $\bar{z}$ [2 $\bar{u}$ , $\bar{u}$ ,w]	$\bar{x}$ , $2\bar{x}$ , $\bar{z}$ [u,2u,w]	$\bar{x}$ ,x, $\bar{z}$ [u, $\bar{u}$ ,w]
			$2\bar{x}$ , $\bar{x}$ , $\bar{z}+1/2$ [2 $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]	x,2x, $\bar{z}+1/2$ [u,2u, $\bar{w}$ ]	x, $\bar{x}$ , $\bar{z}+1/2$ [u, $\bar{u}$ , $\bar{w}$ ]
12	j	m'..	x,y,1/4 [u,v,0]	$\bar{y}$ ,x-y,1/4 [ $\bar{v}$ ,u-v,0]	$\bar{x}+y$ , $\bar{x}$ ,1/4 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			$\bar{x}$ , $\bar{y}$ ,3/4 [u,v,0]	y, $\bar{x}+y$ ,3/4 [ $\bar{v}$ ,u-v,0]	x-y,x,3/4 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			y,x,3/4 [ $\bar{v}$ , $\bar{u}$ ,0]	x-y, $\bar{y}$ ,3/4 [ $\bar{u}+v$ ,v,0]	$\bar{x}$ , $\bar{x}+y$ ,3/4 [u,u-v,0]
			$\bar{y}$ , $\bar{x}$ ,1/4 [ $\bar{v}$ , $\bar{u}$ ,0]	$\bar{x}+y$ ,y,1/4 [ $\bar{u}+v$ ,v,0]	x,x-y,1/4 [u,u-v,0]

12	i	.2'	x,0,0 [u,2u,w]	0,x,0 [2 $\bar{u}$ , $\bar{u}$ ,w]	$\bar{x},\bar{x},0$ [u, $\bar{u}$ ,w]	
			$\bar{x},0,1/2$ [u,2u, $\bar{w}$ ]	0, $\bar{x},1/2$ [2 $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]	x,x,1/2 [u, $\bar{u}$ , $\bar{w}$ ]	
			$\bar{x},0,0$ [u,2u,w]	0, $\bar{x},0$ [2 $\bar{u}$ , $\bar{u}$ ,w]	x,x,0 [u, $\bar{u}$ ,w]	
			x,0,1/2 [u,2u, $\bar{w}$ ]	0,x,1/2 [2 $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]	$\bar{x},\bar{x},1/2$ [u, $\bar{u}$ , $\bar{w}$ ]	
6	h	m'm'2	x,2x,1/4 [u,2u,0]	2 $\bar{x},\bar{x},1/4$ [2 $\bar{u}$ , $\bar{u}$ ,0]	x, $\bar{x},1/4$ [u, $\bar{u}$ ,0]	
			$\bar{x},2\bar{x},3/4$ [u,2u,0]	2x,x,3/4 [2 $\bar{u}$ , $\bar{u}$ ,0]	$\bar{x},x,3/4$ [u, $\bar{u}$ ,0]	
6	g	.2'/m'	1/2,0,0 [u,2u,w]	0,1/2,0 [2 $\bar{u}$ , $\bar{u}$ ,w]	1/2,1/2,0 [u, $\bar{u}$ ,w]	
			1/2,0,1/2 [u,2u, $\bar{w}$ ]	0,1/2,1/2 [2 $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]	1/2,1/2,1/2 [u, $\bar{u}$ , $\bar{w}$ ]	
4	f	3m'	1/3,2/3,z [0,0,w]	2/3,1/3,z+1/2 [0,0, $\bar{w}$ ]	2/3,1/3, $\bar{z}$ [0,0,w]	1/3,2/3, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	e	3m'	0,0,z [0,0,w]	0,0,z+1/2 [0,0, $\bar{w}$ ]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
2	d	$\bar{6}$ 'm'2	1/3,2/3,3/4 [0,0,0]	2/3,1/3,1/4 [0,0,0]		
2	c	$\bar{6}$ 'm'2	1/3,2/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]		
2	b	$\bar{6}$ 'm'2	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	a	$\bar{3}$ m'	0,0,0 [0,0,w]	0,0,1/2 [0,0, $\bar{w}$ ]		

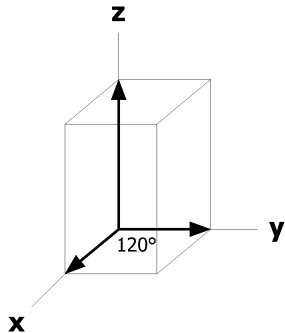
### Symmetry of Special Projections

Along [0,0,1] p6m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'm'g  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p<sub>2a</sub>'2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,1/4





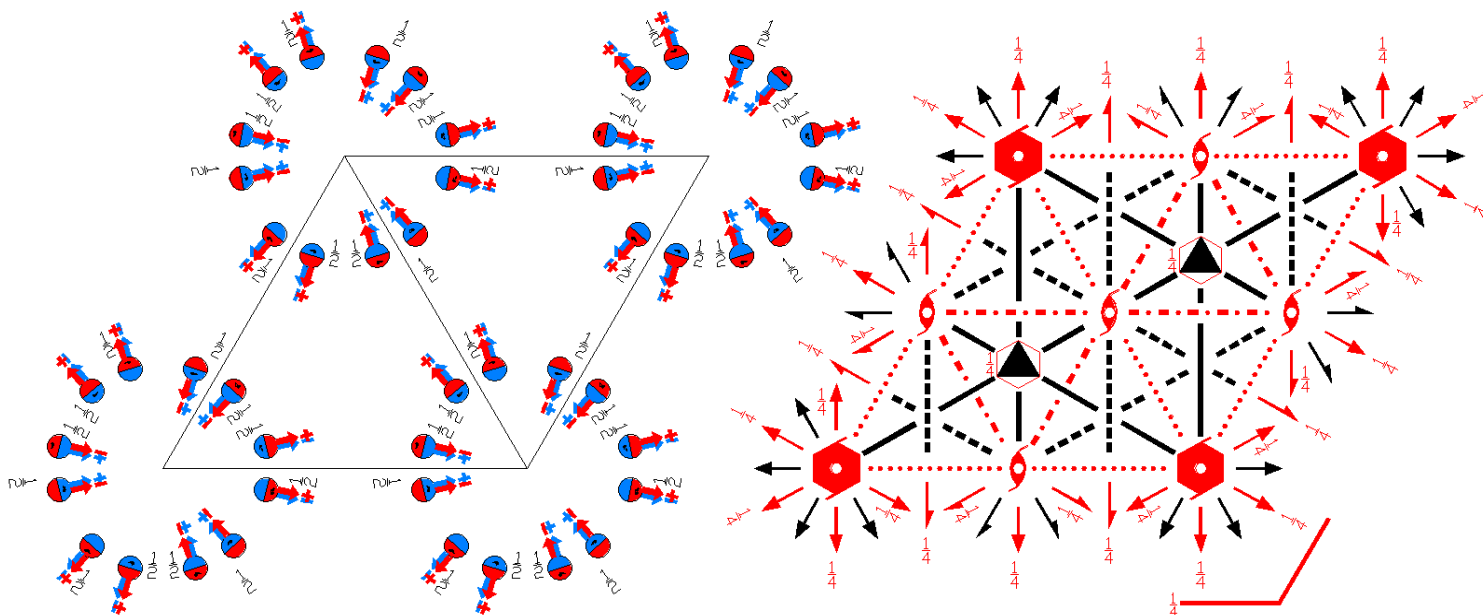
$P6_3'/m'mc'$

194.7.1500

$6'/m'mm'$

$P6_3'/m'2/m2'/c'$

Hexagonal



Origin at center ( $\bar{3}m1$ ) at  $\bar{3}2/mc'$

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $0 \leq z \leq 1/4$ ;  $x \leq 2y$ ;  $y \leq \min(1-x, 2x)$

Vertices  $0,0,0$   $2/3,1/3,0$   $1/3,2/3,0$   
 $0,0,1/4$   $2/3,1/3,1/4$   $1/3,2/3,1/4$

### Symmetry Operations

- |   |  |   |
|---|--|---|
| (1) 1<br>(1 0,0,0)                                | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                   | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)         |
| (4) $2'$ (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)'    | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2)' | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2)' |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0)                 | (8) 2 x,0,0<br>( $2_x$  0,0,0)                       | (9) 2 0,y,0<br>( $2_y$  0,0,0)                  |
| (10) $2'$ x, $\bar{x}$ ,1/4<br>( $2_3$  0,0,1/2)' | (11) $2'$ x,2x,1/4<br>( $2_2$  0,0,1/2)'             | (12) $2'$ 2x,x,1/4<br>( $2_1$  0,0,1/2)'        |

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)
(16) m' x,y,1/4 ( $m_z$  0,0,1/2)'	(17) $\bar{6}^-$ 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1}$  0,0,1/2)'	(18) $\bar{6}^+$ 0,0,z; 0,0,1/4 ( $\bar{6}_z$  0,0,1/2)'
(19) m $\bar{x},\bar{x},z$ ( $m_{xy}$  0,0,0)	(20) m x,2x,z ( $m_x$  0,0,0)	(21) m 2x,x,z ( $m_y$  0,0,0)
(22) c' (0,0,1/2) x,x,z ( $m_3$  0,0,1/2)'	(23) c' (0,0,1/2) x,0,z ( $m_2$  0,0,1/2)'	(24) c' (0,0,1/2) 0,y,z ( $m_1$  0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y},x-y,z$ [ $\bar{v},u-v,w$ ]	(3) $\bar{x}+y,\bar{x},z$ [ $\bar{u}+v,\bar{u},w$ ]
			(4) $\bar{x},\bar{y},z+1/2$ [u,v, $\bar{w}$ ]	(5) y, $\bar{x}+y,z+1/2$ [ $\bar{v},u-v,\bar{w}$ ]	(6) x-y,x,z+1/2 [ $\bar{u}+v,\bar{u},\bar{w}$ ]
			(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y},\bar{z}$ [u-v, $\bar{v},\bar{w}$ ]	(9) $\bar{x},\bar{x}+y,\bar{z}$ [ $\bar{u},\bar{u}+v,\bar{w}$ ]
			(10) $\bar{y},\bar{x},\bar{z}+1/2$ [v,u,w]	(11) $\bar{x}+y,\bar{y},\bar{z}+1/2$ [u-v, $\bar{v},w$ ]	(12) x,x-y, $\bar{z}+1/2$ [ $\bar{u},\bar{u}+v,w$ ]
			(13) $\bar{x},\bar{y},\bar{z}$ [u,v,w]	(14) y, $\bar{x}+y,\bar{z}$ [ $\bar{v},u-v,w$ ]	(15) x-y,x, $\bar{z}$ [ $\bar{u}+v,\bar{u},w$ ]
			(16) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(17) $\bar{y},x-y,\bar{z}+1/2$ [ $\bar{v},u-v,\bar{w}$ ]	(18) $\bar{x}+y,\bar{x},\bar{z}+1/2$ [ $\bar{u}+v,\bar{u},\bar{w}$ ]
			(19) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ]	(20) $\bar{x}+y,y,z$ [u-v, $\bar{v},\bar{w}$ ]	(21) x,x-y,z [ $\bar{u},\bar{u}+v,\bar{w}$ ]
			(22) y,x,z+1/2 [v,u,w]	(23) x-y, $\bar{y},z+1/2$ [u-v, $\bar{v},w$ ]	(24) $\bar{x},\bar{x}+y,z+1/2$ [ $\bar{u},\bar{u}+v,w$ ]
12	k	.m.	x,2x,z [u,0,0]	$2\bar{x},\bar{x},z$ [0,u,0]	x, $\bar{x},z$ [ $\bar{u},\bar{u},0$ ]
			$\bar{x},2\bar{x},z+1/2$ [u,0,0]	2x,x,z+1/2 [0,u,0]	$\bar{x},x,z+1/2$ [ $\bar{u},\bar{u},0$ ]
			2x,x, $\bar{z}$ [0,u,0]	$\bar{x},2\bar{x},\bar{z}$ [u,0,0]	$\bar{x},x,\bar{z}$ [ $\bar{u},\bar{u},0$ ]
			$2\bar{x},\bar{x},\bar{z}+1/2$ [0,u,0]	x,2x, $\bar{z}+1/2$ [u,0,0]	x, $\bar{x},\bar{z}+1/2$ [ $\bar{u},\bar{u},0$ ]
12	j	m'..	x,y,1/4 [u,v,0]	$\bar{y},x-y,1/4$ [ $\bar{v},u-v,0$ ]	$\bar{x}+y,\bar{x},1/4$ [ $\bar{u}+v,\bar{u},0$ ]
			$\bar{x},\bar{y},3/4$ [u,v,0]	y, $\bar{x}+y,3/4$ [ $\bar{v},u-v,0$ ]	x-y,x,3/4 [ $\bar{u}+v,\bar{u},0$ ]
			y,x,3/4 [v,u,0]	x-y, $\bar{y},3/4$ [u-v, $\bar{v},0$ ]	$\bar{x},\bar{x}+y,3/4$ [ $\bar{u},\bar{u}+v,0$ ]
			$\bar{y},\bar{x},1/4$ [v,u,0]	$\bar{x}+y,y,1/4$ [u-v, $\bar{v},0$ ]	x,x-y,1/4 [ $\bar{u},\bar{u}+v,0$ ]

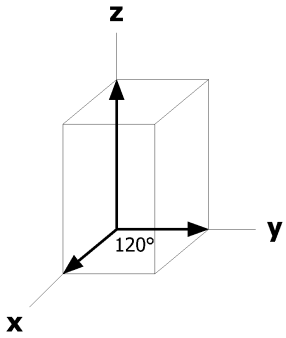
Continued		194.7.1500		P6 <sub>3</sub> '/m'mc'		
12	i	.2.	x,0,0 [u,0,0]	0,x,0 [0,u,0]	$\bar{x},\bar{x},0 [\bar{u},\bar{u},0]$	
			$\bar{x},0,1/2 [u,0,0]$	$0,\bar{x},1/2 [0,u,0]$	$x,x,1/2 [\bar{u},\bar{u},0]$	
			$\bar{x},0,0 [u,0,0]$	$0,\bar{x},0 [0,u,0]$	$x,x,0 [\bar{u},\bar{u},0]$	
			x,0,1/2 [u,0,0]	0,x,1/2 [0,u,0]	$\bar{x},\bar{x},1/2 [\bar{u},\bar{u},0]$	
6	h	m'm2'	x,2x,1/4 [u,0,0]	$2\bar{x},\bar{x},1/4 [0,u,0]$	$x,\bar{x},1/4 [\bar{u},\bar{u},0]$	
			$\bar{x},2\bar{x},3/4 [u,0,0]$	$2x,x,3/4 [0,u,0]$	$\bar{x},x,3/4 [\bar{u},\bar{u},0]$	
6	g	.2/m.	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
			1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
4	f	3m.	1/3,2/3,z [0,0,0]	$2/3,1/3,z+1/2 [0,0,0]$	$2/3,1/3,\bar{z} [0,0,0]$	$1/3,2/3,\bar{z}+1/2 [0,0,0]$
4	e	3m.	0,0,z [0,0,0]	$0,0,z+1/2 [0,0,0]$	$0,0,\bar{z} [0,0,0]$	$0,0,\bar{z}+1/2 [0,0,0]$
2	d	$\bar{6}'m2'$	$1/3,2/3,3/4 [0,0,0]$	$2/3,1/3,1/4 [0,0,0]$		
2	c	$\bar{6}'m2'$	$1/3,2/3,1/4 [0,0,0]$	$2/3,1/3,3/4 [0,0,0]$		
2	b	$\bar{6}'m2'$	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	a	$\bar{3}m.$	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p6'mm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x/2,0



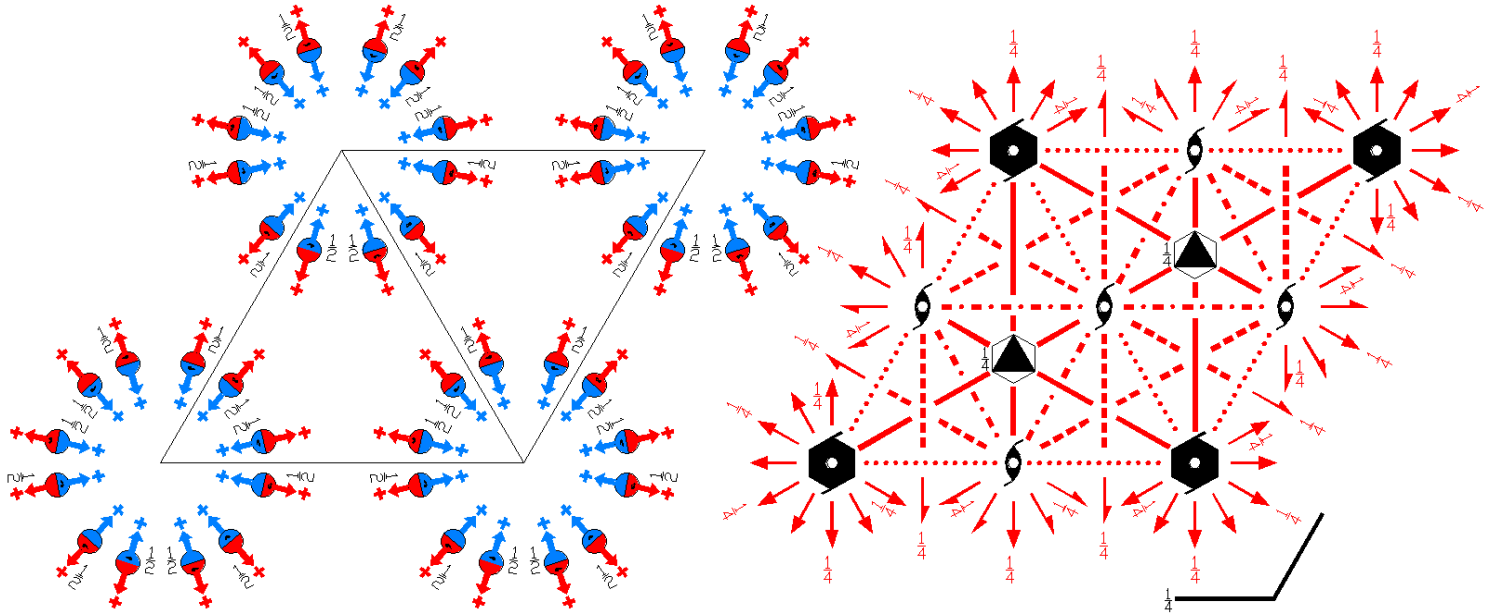
$P6_3/mm'c'$

194.8.1501

$6/mm'm'$

$P6_3/m2'/m'2'/c'$

Hexagonal



Origin at center ( $\bar{3}m'1$ ) at  $\bar{3}2'/m'c'$

<b>Asymmetric unit</b>	$0 \leq x \leq 2/3;$	$0 \leq y \leq 2/3;$	$0 \leq z \leq 1/4;$	$x \leq 2y;$	$y \leq \min(1-x, 2x)$
Vertices	0,0,0	2/3,1/3,0	1/3,2/3,0		
	0,0,1/4	2/3,1/3,1/4	1/3,2/3,1/4		

**Symmetry Operations**

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                                | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)        |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)        | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2) |
| (7) $2'$ x,x,0<br>( $2_{xy}$  0,0,0)'             | (8) $2'$ x,0,0<br>( $2_x$  0,0,0)'                  | (9) $2'$ 0,y,0<br>( $2_y$  0,0,0)'             |
| (10) $2'$ x, $\bar{x}$ ,1/4<br>( $2_3$  0,0,1/2)' | (11) $2'$ x,2x,1/4<br>( $2_2$  0,0,1/2)'            | (12) $2'$ 2x,x,1/4<br>( $2_1$  0,0,1/2)'       |

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(14) $\bar{3}^+$ 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)	(15) $\bar{3}^-$ 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)
(16) m $\bar{x}$ ,y,1/4 ( $m_z$  0,0,1/2)	(17) $\bar{6}^-$ 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1}$  0,0,1/2)	(18) $\bar{6}^+$ 0,0,z; 0,0,1/4 ( $\bar{6}_z$  0,0,1/2)
(19) m' $\bar{x}$ , $\bar{x}$ ,z ( $m_{xy}$  0,0,0)'	(20) m' $\bar{x}$ ,2x,z ( $m_x$  0,0,0)'	(21) m' 2x,x,z ( $m_y$  0,0,0)'
(22) c' (0,0,1/2) $\bar{x}$ ,x,z ( $m_3$  0,0,1/2)'	(23) c' (0,0,1/2) $\bar{x}$ ,0,z ( $m_2$  0,0,1/2)'	(24) c' (0,0,1/2) 0,y,z ( $m_1$  0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}$ +y, $\bar{x}$ ,z [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(5) y, $\bar{x}$ +y,z+1/2 [v, $\bar{u}$ +v,w]	(6) x-y,x,z+1/2 [u-v,u,w]
			(7) y,x, $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ ,w]	(8) x-y, $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ +v,v,w]	(9) $\bar{x}$ , $\bar{x}$ +y, $\bar{z}$ [u,u-v,w]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ +1/2 [v,u,w]	(11) $\bar{x}$ +y,y, $\bar{z}$ +1/2 [u-v, $\bar{v}$ ,w]	(12) x,x-y, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{u}$ +v,w]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(14) y, $\bar{x}$ +y, $\bar{z}$ [ $\bar{v}$ ,u-v,w]	(15) x-y,x, $\bar{z}$ [ $\bar{u}$ +v, $\bar{u}$ ,w]
			(16) x,y, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(17) $\bar{y}$ ,x-y, $\bar{z}$ +1/2 [v, $\bar{u}$ +v,w]	(18) $\bar{x}$ +y, $\bar{x}$ , $\bar{z}$ +1/2 [u-v,u,w]
			(19) $\bar{y}$ , $\bar{x}$ ,z [ $\bar{v}$ , $\bar{u}$ ,w]	(20) $\bar{x}$ +y,y,z [ $\bar{u}$ +v,v,w]	(21) x,x-y,z [u,u-v,w]
			(22) y,x,z+1/2 [v,u,w]	(23) x-y, $\bar{y}$ ,z+1/2 [u-v, $\bar{v}$ ,w]	(24) $\bar{x}$ , $\bar{x}$ +y,z+1/2 [ $\bar{u}$ , $\bar{u}$ +v,w]
12	k	.m'	x,2x,z [u,2u,w]	2 $\bar{x}$ , $\bar{x}$ ,z [2 $\bar{u}$ , $\bar{u}$ ,w]	x, $\bar{x}$ ,z [u, $\bar{u}$ ,w]
			$\bar{x}$ ,2 $\bar{x}$ ,z+1/2 [ $\bar{u}$ ,2 $\bar{u}$ ,w]	2x,x,z+1/2 [2u,u,w]	$\bar{x}$ ,x,z+1/2 [ $\bar{u}$ ,u,w]
			2x,x, $\bar{z}$ [2 $\bar{u}$ , $\bar{u}$ ,w]	$\bar{x}$ ,2 $\bar{x}$ , $\bar{z}$ [u,2u,w]	$\bar{x}$ ,x, $\bar{z}$ [u, $\bar{u}$ ,w]
			2 $\bar{x}$ , $\bar{x}$ , $\bar{z}$ +1/2 [2u,u,w]	x,2x, $\bar{z}$ +1/2 [ $\bar{u}$ ,2 $\bar{u}$ ,w]	x, $\bar{x}$ , $\bar{z}$ +1/2 [ $\bar{u}$ ,u,w]
12	j	m..	x,y,1/4 [0,0,w]	$\bar{y}$ ,x-y,1/4 [0,0,w]	$\bar{x}$ +y, $\bar{x}$ ,1/4 [0,0,w]
			$\bar{x}$ , $\bar{y}$ ,3/4 [0,0,w]	y, $\bar{x}$ +y,3/4 [0,0,w]	x-y,x,3/4 [0,0,w]
			y,x,3/4 [0,0,w]	x-y, $\bar{y}$ ,3/4 [0,0,w]	$\bar{x}$ , $\bar{x}$ +y,3/4 [0,0,w]
			$\bar{y}$ , $\bar{x}$ ,1/4 [0,0,w]	$\bar{x}$ +y,y,1/4 [0,0,w]	x,x-y,1/4 [0,0,w]

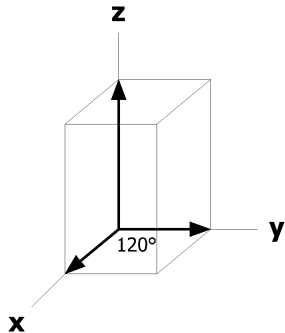
12	i	.2'	x,0,0 [u,2u,w]	0,x,0 [2 $\bar{u}$ , $\bar{u}$ ,w]	$\bar{x},\bar{x},0$ [u, $\bar{u}$ ,w]	
			$\bar{x},0,1/2$ [ $\bar{u}$ ,2 $\bar{u}$ ,w]	0, $\bar{x},1/2$ [2u,u,w]	x,x,1/2 [ $\bar{u}$ ,u,w]	
			$\bar{x},0,0$ [u,2u,w]	0, $\bar{x},0$ [2 $\bar{u}$ , $\bar{u}$ ,w]	x,x,0 [u, $\bar{u}$ ,w]	
			x,0,1/2 [ $\bar{u}$ ,2 $\bar{u}$ ,w]	0,x,1/2 [2u,u,w]	$\bar{x},\bar{x},1/2$ [ $\bar{u}$ ,u,w]	
6	h	mm'2'	x,2x,1/4 [0,0,w]	2 $\bar{x},\bar{x},1/4$ [0,0,w]	x, $\bar{x},1/4$ [0,0,w]	
			$\bar{x},2\bar{x},3/4$ [0,0,w]	2x,x,3/4 [0,0,w]	$\bar{x},x,3/4$ [0,0,w]	
6	g	.2'/m'	1/2,0,0 [u,2u,w]	0,1/2,0 [2 $\bar{u}$ , $\bar{u}$ ,w]	1/2,1/2,0 [u, $\bar{u}$ ,w]	
			1/2,0,1/2 [ $\bar{u}$ ,2 $\bar{u}$ ,w]	0,1/2,1/2 [2u,u,w]	1/2,1/2,1/2 [ $\bar{u}$ ,u,w]	
4	f	3m'	1/3,2/3,z [0,0,w]	2/3,1/3,z+1/2 [0,0,w]	2/3,1/3, $\bar{z}$ [0,0,w]	1/3,2/3, $\bar{z}+1/2$ [0,0,w]
4	e	3m'	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}$ [0,0,w]	0,0, $\bar{z}+1/2$ [0,0,w]
2	d	$\bar{6}m'2'$	1/3,2/3,3/4 [0,0,w]	2/3,1/3,1/4 [0,0,w]		
2	c	$\bar{6}m'2'$	1/3,2/3,1/4 [0,0,w]	2/3,1/3,3/4 [0,0,w]		
2	b	$\bar{6}m'2'$	0,0,1/4 [0,0,w]	0,0,3/4 [0,0,w]		
2	a	$\bar{3}m'$	0,0,0 [0,0,w]	0,0,1/2 [0,0,w]		

### Symmetry of Special Projections

Along [0,0,1] p6mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2'mg'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

Along [2,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



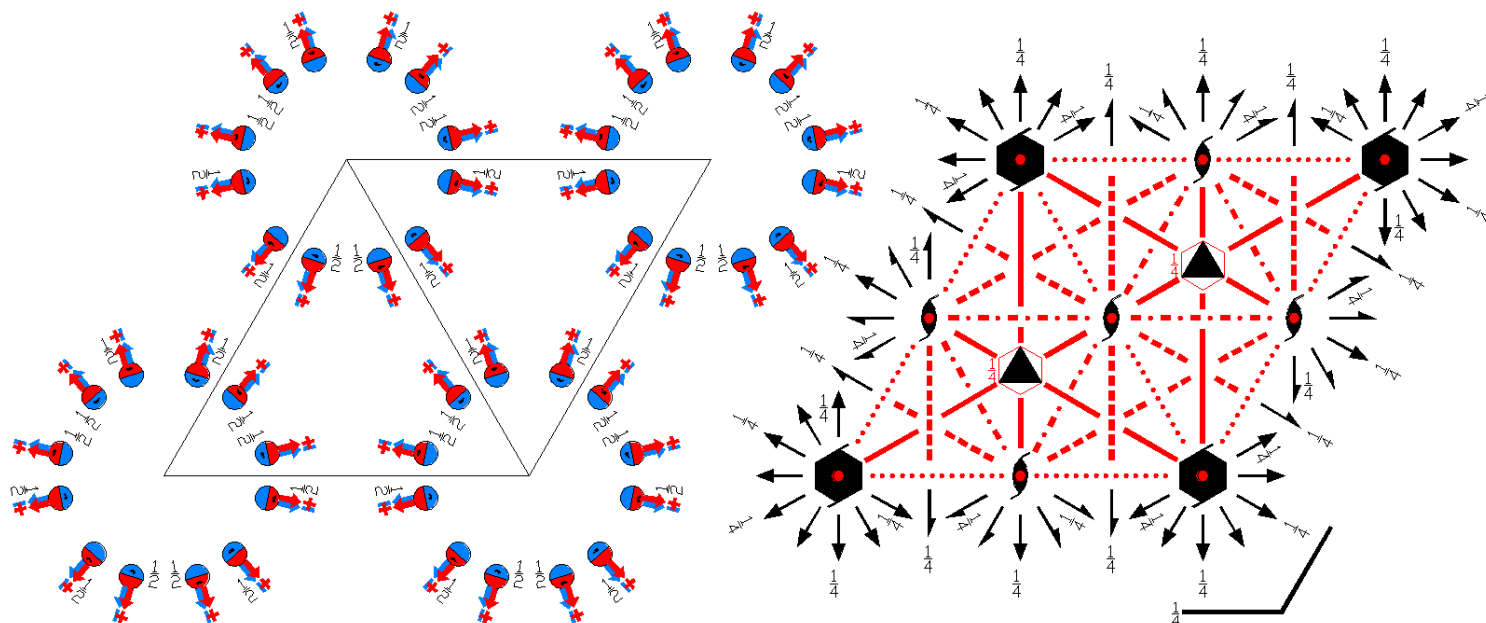
$P6_3/m'm'c'$

194.9.1502

$6/m'm'm'$

$P6_3/m'2/m'2/c'$

Hexagonal



Origin at center ( $\bar{3}'m'1$ ) at  $\bar{3}'2/m'c'$

Asymmetric unit  $0 \leq x \leq 2/3$ ;  $0 \leq y \leq 2/3$ ;  $0 \leq z \leq 1/4$ ;  $x \leq 2y$ ;  $y \leq \min(1-x, 2x)$

Vertices  $0,0,0$   $2/3,1/3,0$   $1/3,2/3,0$   
 $0,0,1/4$   $2/3,1/3,1/4$   $1/3,2/3,1/4$

### Symmetry Operations

- |   |   |  |
|---|---|--|
| (1) 1<br>(1 0,0,0)                            | (2) $3^+$ 0,0,z<br>( $3_z$  0,0,0)                  | (3) $3^-$ 0,0,z<br>( $3_z^{-1}$  0,0,0)        |
| (4) 2 (0,0,1/2) 0,0,z<br>( $2_z$  0,0,1/2)    | (5) $6^-$ (0,0,1/2) 0,0,z<br>( $6_z^{-1}$  0,0,1/2) | (6) $6^+$ (0,0,1/2) 0,0,z<br>( $6_z$  0,0,1/2) |
| (7) 2 x,x,0<br>( $2_{xy}$  0,0,0)             | (8) 2 x,0,0<br>( $2_x$  0,0,0)                      | (9) 2 0,y,0<br>( $2_y$  0,0,0)                 |
| (10) 2 $x, \bar{x}, 1/4$<br>( $2_3$  0,0,1/2) | (11) 2 x,2x,1/4<br>( $2_2$  0,0,1/2)                | (12) 2 2x,x,1/4<br>( $2_1$  0,0,1/2)           |

(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) $\bar{3}^+$ ' 0,0,z; 0,0,0 ( $\bar{3}_z$  0,0,0)'	(15) $\bar{3}^-$ ' 0,0,z; 0,0,0 ( $\bar{3}_z^{-1}$  0,0,0)'
(16) m' x,y,1/4 ( $m_z$  0,0,1/2)'	(17) $\bar{6}^-$ ' 0,0,z; 0,0,1/4 ( $\bar{6}_z^{-1}$  0,0,1/2)'	(18) $\bar{6}^+$ ' 0,0,z; 0,0,1/4 ( $\bar{6}_z$  0,0,1/2)'
(19) m' x, $\bar{x}$ ,z ( $m_{xy}$  0,0,0)'	(20) m' x,2x,z ( $m_x$  0,0,0)'	(21) m' 2x,x,z ( $m_y$  0,0,0)'
(22) c' (0,0,1/2) x,x,z ( $m_3$  0,0,1/2)'	(23) c' (0,0,1/2) x,0,z ( $m_2$  0,0,1/2)'	(24) c' (0,0,1/2) 0,y,z ( $m_1$  0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

			Coordinates		
Multiplicity,	Wyckoff letter,	Site Symmetry.			
24	l	1	(1) x,y,z [u,v,w]	(2) $\bar{y}$ ,x-y,z [ $\bar{v}$ ,u-v,w]	(3) $\bar{x}+y$ , $\bar{x}$ ,z [ $\bar{u}+v$ , $\bar{u}$ ,w]
			(4) $\bar{x}$ , $\bar{y}$ ,z+1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(5) y, $\bar{x}+y$ ,z+1/2 [v, $\bar{u}+v$ ,w]	(6) x-y,x,z+1/2 [u-v,u,w]
			(7) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(8) x-y, $\bar{y}$ , $\bar{z}$ [u-v, $\bar{v}$ , $\bar{w}$ ]	(9) $\bar{x}$ , $\bar{x}+y$ , $\bar{z}$ [ $\bar{u}$ , $\bar{u}+v$ , $\bar{w}$ ]
			(10) $\bar{y}$ , $\bar{x}$ , $\bar{z}+1/2$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(11) $\bar{x}+y$ ,y, $\bar{z}+1/2$ [ $\bar{u}+v$ ,v, $\bar{w}$ ]	(12) x,x-y, $\bar{z}+1/2$ [u,u-v, $\bar{w}$ ]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(14) y, $\bar{x}+y$ , $\bar{z}$ [v, $\bar{u}+v$ , $\bar{w}$ ]	(15) x-y,x, $\bar{z}$ [u-v,u, $\bar{w}$ ]
			(16) x,y, $\bar{z}+1/2$ [u,v, $\bar{w}$ ]	(17) $\bar{y}$ ,x-y, $\bar{z}+1/2$ [ $\bar{v}$ ,u-v, $\bar{w}$ ]	(18) $\bar{x}+y$ , $\bar{x}$ , $\bar{z}+1/2$ [ $\bar{u}+v$ , $\bar{u}$ , $\bar{w}$ ]
			(19) $\bar{y}$ , $\bar{x}$ ,z [ $\bar{v}$ , $\bar{u}$ ,w]	(20) $\bar{x}+y$ ,y,z [ $\bar{u}+v$ ,v,w]	(21) x,x-y,z [u,u-v,w]
			(22) y,x,z+1/2 [v,u,w]	(23) x-y, $\bar{y}$ ,z+1/2 [u-v, $\bar{v}$ ,w]	(24) $\bar{x}$ , $\bar{x}+y$ ,z+1/2 [ $\bar{u}$ , $\bar{u}+v$ ,w]
12	k	.m'	x,2x,z [u,2u,w]	$2\bar{x}$ , $\bar{x}$ ,z [2 $\bar{u}$ , $\bar{u}$ ,w]	x, $\bar{x}$ ,z [u, $\bar{u}$ ,w]
			$\bar{x}$ , $2\bar{x}$ ,z+1/2 [ $\bar{u}$ ,2 $\bar{u}$ ,w]	2x,x,z+1/2 [2u,u,w]	$\bar{x}$ ,x,z+1/2 [ $\bar{u}$ ,u,w]
			2x,x, $\bar{z}$ [2u,u, $\bar{w}$ ]	$\bar{x}$ , $2\bar{x}$ , $\bar{z}$ [ $\bar{u}$ ,2 $\bar{u}$ , $\bar{w}$ ]	$\bar{x}$ ,x, $\bar{z}$ [ $\bar{u}$ ,u, $\bar{w}$ ]
			$2\bar{x}$ , $\bar{x}$ , $\bar{z}+1/2$ [2 $\bar{u}$ , $\bar{u}$ , $\bar{w}$ ]	x,2x, $\bar{z}+1/2$ [u,2u, $\bar{w}$ ]	x, $\bar{x}$ , $\bar{z}+1/2$ [u, $\bar{u}$ , $\bar{w}$ ]
12	j	m'..	x,y,1/4 [u,v,0]	$\bar{y}$ ,x-y,1/4 [ $\bar{v}$ ,u-v,0]	$\bar{x}+y$ , $\bar{x}$ ,1/4 [ $\bar{u}+v$ , $\bar{u}$ ,0]
			$\bar{x}$ , $\bar{y}$ ,3/4 [ $\bar{u}$ , $\bar{v}$ ,0]	y, $\bar{x}+y$ ,3/4 [v, $\bar{u}+v$ ,0]	x-y,x,3/4 [u-v,u,0]
			y,x,3/4 [v,u,0]	x-y, $\bar{y}$ ,3/4 [u-v, $\bar{v}$ ,0]	$\bar{x}$ , $\bar{x}+y$ ,3/4 [ $\bar{u}$ , $\bar{u}+v$ ,0]
			$\bar{y}$ , $\bar{x}$ ,1/4 [ $\bar{v}$ , $\bar{u}$ ,0]	$\bar{x}+y$ ,y,1/4 [ $\bar{u}+v$ ,v,0]	x,x-y,1/4 [u,u-v,0]



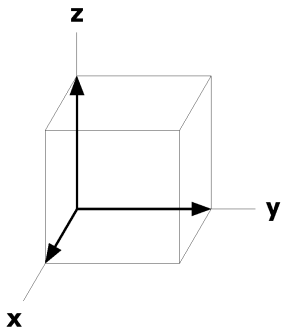
12	i	.2.	x,0,0 [u,0,0]	0,x,0 [0,u,0]	$\bar{x},\bar{x},0$ [ $\bar{u},\bar{u},0$ ]	
			$\bar{x},0,1/2$ [ $\bar{u},0,0$ ]	$0,\bar{x},1/2$ [0, $\bar{u},0$ ]	x,x,1/2 [u,u,0]	
			$\bar{x},0,0$ [ $\bar{u},0,0$ ]	$0,\bar{x},0$ [0, $\bar{u},0$ ]	x,x,0 [u,u,0]	
			x,0,1/2 [u,0,0]	0,x,1/2 [0,u,0]	$\bar{x},\bar{x},1/2$ [ $\bar{u},\bar{u},0$ ]	
6	h	m'm'2	x,2x,1/4 [u,2u,0]	$2\bar{x},\bar{x},1/4$ [2 $\bar{u},\bar{u},0$ ]	x, $\bar{x},1/4$ [u, $\bar{u},0$ ]	
			$\bar{x},2\bar{x},3/4$ [ $\bar{u},2\bar{u},0$ ]	2x,x,3/4 [2u,u,0]	$\bar{x},x,3/4$ [ $\bar{u},u,0$ ]	
6	g	.2/m'.	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]	
			1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,1/2 [0,0,0]	
4	f	3m'.	1/3,2/3,z [0,0,w]	2/3,1/3,z+1/2 [0,0,w]	2/3,1/3, $\bar{z}$ [0,0, $\bar{w}$ ]	1/3,2/3, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
4	e	3m'.	0,0,z [0,0,w]	0,0,z+1/2 [0,0,w]	0,0, $\bar{z}$ [0,0, $\bar{w}$ ]	0,0, $\bar{z}+1/2$ [0,0, $\bar{w}$ ]
2	d	$\bar{6}$ 'm'2	1/3,2/3,3/4 [0,0,0]	2/3,1/3,1/4 [0,0,0]		
2	c	$\bar{6}$ 'm'2	1/3,2/3,1/4 [0,0,0]	2/3,1/3,3/4 [0,0,0]		
2	b	$\bar{6}$ 'm'2	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]		
2	a	$\bar{3}$ 'm'.	0,0,0 [0,0,0]	0,0,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p6m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,0,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2$   
 Origin at x,0,0

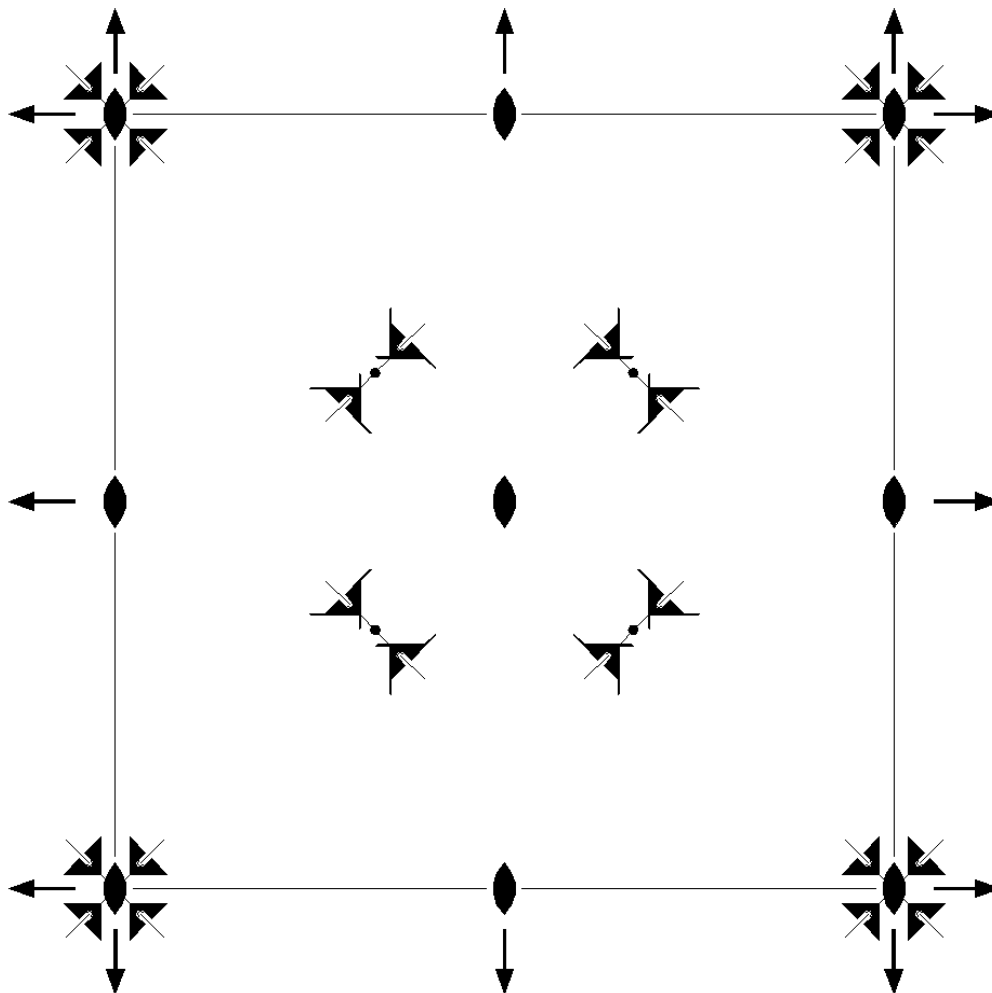
Along [2,1,0] p2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at x,x/2,0



P23  
195.1.1503

23  
P23

Cubic



Origin at 23

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$ ;  $y \leq 1-x$ ;  $z \leq \min(x,y)$

Vertices  $0,0,0$   $1,0,0$   $0,1,0$   $1/2,1/2,1/2$

**Symmetry Operations**

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>+</sup>  0,0,0)  | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>+</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>+</sup> <sup>-1</sup>  0,0,0)            | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>+</sup> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-</sup>  0,0,0)                  | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-</sup>  0,0,0) | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-</sup>  0,0,0)                    |

Continued

195.1.1503

P23

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

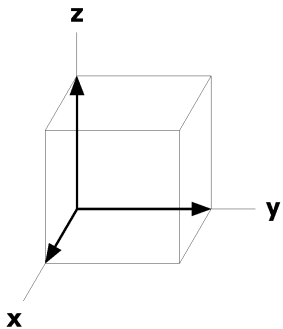
			Coordinates								
			Multiplicity, Wyckoff letter, Site Symmetry.								
12	j	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}, \bar{y}, z$	$[\bar{u}, \bar{v}, w]$	(3)	$\bar{x}, y, \bar{z}$	$[\bar{u}, v, \bar{w}]$	(4)	$x, \bar{y}, \bar{z}$	$[u, \bar{v}, \bar{w}]$
(5)	z,x,y	[w,u,v]	(6)	$z, \bar{x}, \bar{y}$	$[w, \bar{u}, \bar{v}]$	(7)	$\bar{z}, \bar{x}, y$	$[\bar{w}, \bar{u}, v]$	(8)	$\bar{z}, x, \bar{y}$	$[\bar{w}, u, \bar{v}]$
(9)	y,z,x	[v,w,u]	(10)	$\bar{y}, z, \bar{x}$	$[\bar{v}, w, \bar{u}]$	(11)	$y, \bar{z}, \bar{x}$	$[v, \bar{w}, \bar{u}]$	(12)	$\bar{y}, \bar{z}, x$	$[\bar{v}, \bar{w}, u]$
6	i	2..	x,1/2,1/2	[u,0,0]	$\bar{x}, 1/2, 1/2$	$[\bar{u}, 0, 0]$	1/2,x,1/2	[0,u,0]	1/2,1/2, $\bar{x}$	[0,0, $\bar{u}$ ]	
			1/2, $\bar{x}$ ,1/2	[0, $\bar{u}$ ,0]	1/2,1/2,x	[0,0,u]					
6	h	2..	x,1/2,0	[u,0,0]	$\bar{x}, 1/2, 0$	$[\bar{u}, 0, 0]$	0,x,1/2	[0,u,0]	1/2,0, $\bar{x}$	[0,0, $\bar{u}$ ]	
			0, $\bar{x}$ ,1/2	[0, $\bar{u}$ ,0]	1/2,0,x	[0,0,u]					
6	g	2..	x,0,1/2	[u,0,0]	$\bar{x}, 0, 1/2$	$[\bar{u}, 0, 0]$	1/2,x,0	[0,u,0]	0,1/2, $\bar{x}$	[0,0, $\bar{u}$ ]	
			1/2, $\bar{x}$ ,0	[0, $\bar{u}$ ,0]	0,1/2,x	[0,0,u]					
6	f	2..	x,0,0	[u,0,0]	$\bar{x}, 0, 0$	$[\bar{u}, 0, 0]$	0,x,0	[0,u,0]	0,0, $\bar{x}$	[0,0, $\bar{u}$ ]	
			0, $\bar{x}$ ,0	[0, $\bar{u}$ ,0]	0,0,x	[0,0,u]					
4	e	.3.	x,x,x	[u,u,u]	$\bar{x}, \bar{x}, x$	$[\bar{u}, \bar{u}, u]$	$\bar{x}, x, \bar{x}$	$[\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x}$	$[u, \bar{u}, \bar{u}]$	
3	d	222..	1/2,0,0	[0,0,0]	0,1/2,0	[0,0,0]	0,0,1/2	[0,0,0]			
3	c	222..	0,1/2,1/2	[0,0,0]	1/2,0,1/2	[0,0,0]	1/2,1/2,0	[0,0,0]			
1	b	23.	1/2,1/2,1/2	[0,0,0]							
1	a	23.	0,0,0	[0,0,0]							

**Symmetry of Special Projections**

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,1,1] p3  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

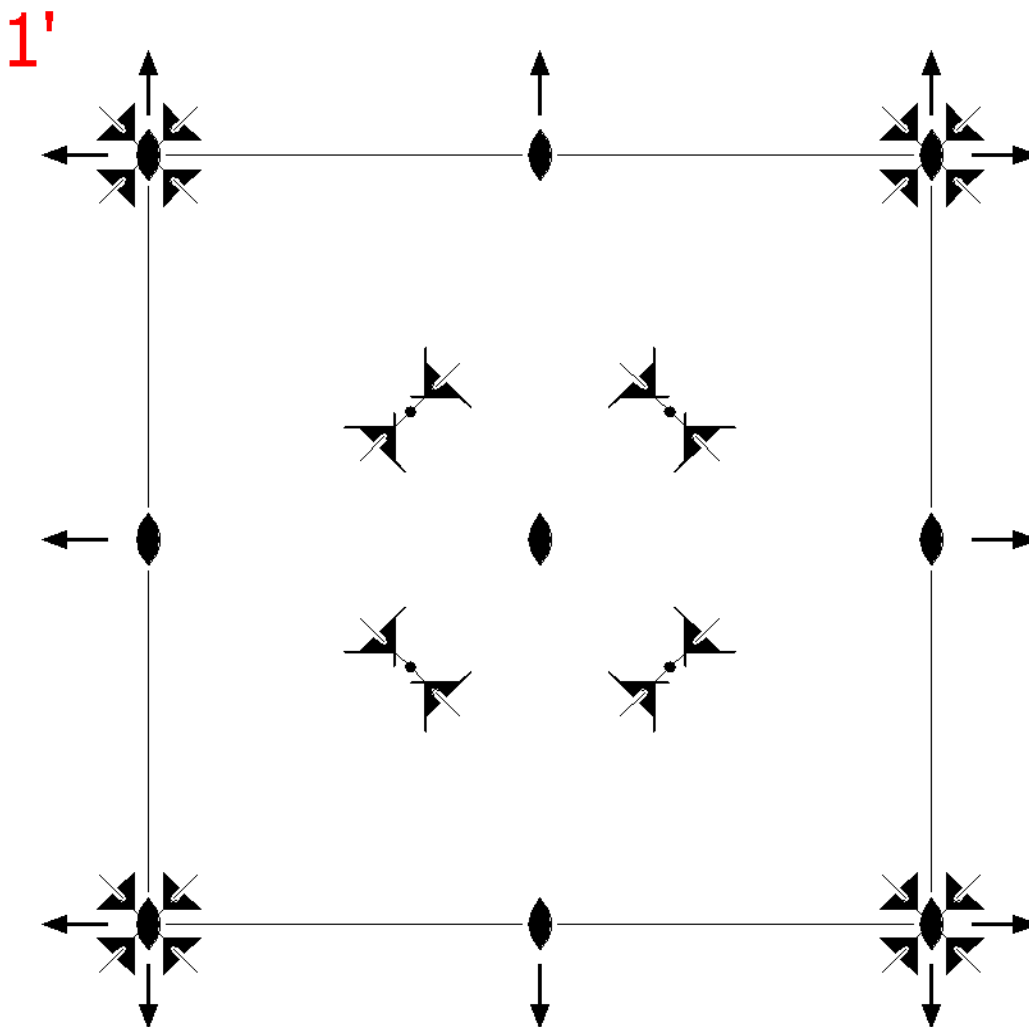
Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P231'  
195.2.1504

231'  
P231'

Cubic



Origin at 231'

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1;$   $0 \leq z \leq 1/2;$   $y \leq 1-x;$   $z \leq \min(x,y)$   
**Vertices** 0,0,0 1,0,0 0,1,0 1/2,1/2,1/2

**Symmetry Operations**

For 1 + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)              |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(4) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'
(5) 3 <sup>+</sup> x,x,x (3 <sub>xyz</sub>  0,0,0)'	(6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$ (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0)'	(7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)'	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x (3 <sub><math>\bar{yz}</math></sub> <sup>-1</sup>  0,0,0)'
(9) 3 <sup>-</sup> x,x,x (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)'	(10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub>  0,0,0)'	(11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x (3 <sub><math>\bar{yz}</math></sub>  0,0,0)'	(12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$ (3 <sub><math>\bar{yz}</math></sub>  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5): 1'.

**Positions**

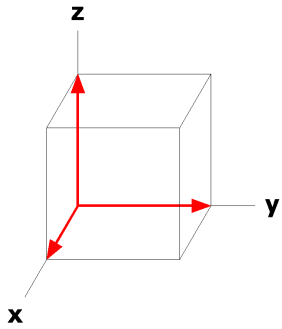
			Coordinates				
Multiplicity, Wyckoff letter, Site Symmetry.			1 +		1' +		
12	j	11'					
(1)	x,y,z	[0,0,0]	(2)	$\bar{x}$ , $\bar{y}$ ,z	[0,0,0]	(3)	$\bar{x}$ ,y, $\bar{z}$ [0,0,0]
(5)	z,x,y	[0,0,0]	(6)	z, $\bar{x}$ , $\bar{y}$	[0,0,0]	(7)	$\bar{z}$ , $\bar{x}$ ,y [0,0,0]
(9)	y,z,x	[0,0,0]	(10)	$\bar{y}$ ,z, $\bar{x}$	[0,0,0]	(11)	y, $\bar{z}$ , $\bar{x}$ [0,0,0]
6	i	2..1'	x,1/2,1/2	[0,0,0]	$\bar{x}$ ,1/2,1/2	[0,0,0]	1/2,x,1/2
			1/2, $\bar{x}$ ,1/2	[0,0,0]	1/2,1/2,x	[0,0,0]	1/2,1/2, $\bar{x}$
6	h	2..1'	x,1/2,0	[0,0,0]	$\bar{x}$ ,1/2,0	[0,0,0]	0,x,1/2
			0, $\bar{x}$ ,1/2	[0,0,0]	1/2,0,x	[0,0,0]	1/2,0, $\bar{x}$
6	g	2..1'	x,0,1/2	[0,0,0]	$\bar{x}$ ,0,1/2	[0,0,0]	1/2,x,0
			1/2, $\bar{x}$ ,0	[0,0,0]	0,1/2,x	[0,0,0]	0,1/2, $\bar{x}$
6	f	2..1'	x,0,0	[0,0,0]	$\bar{x}$ ,0,0	[0,0,0]	0,x,0
			0, $\bar{x}$ ,0	[0,0,0]	0,0,x	[0,0,0]	0,0, $\bar{x}$
4	e	.3.1'	x,x,x	[0,0,0]	$\bar{x}$ , $\bar{x}$ ,x	[0,0,0]	$\bar{x}$ ,x, $\bar{x}$
							x, $\bar{x}$ , $\bar{x}$
3	d	222..1'	1/2,0,0	[0,0,0]	0,1/2,0	[0,0,0]	0,0,1/2
3	c	222..1'	0,1/2,1/2	[0,0,0]	1/2,0,1/2	[0,0,0]	1/2,1/2,0
1	b	23.1'	1/2,1/2,1/2	[0,0,0]			
1	a	23.1'	0,0,0	[0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,1,1]  $p31'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
Origin at x,x,x

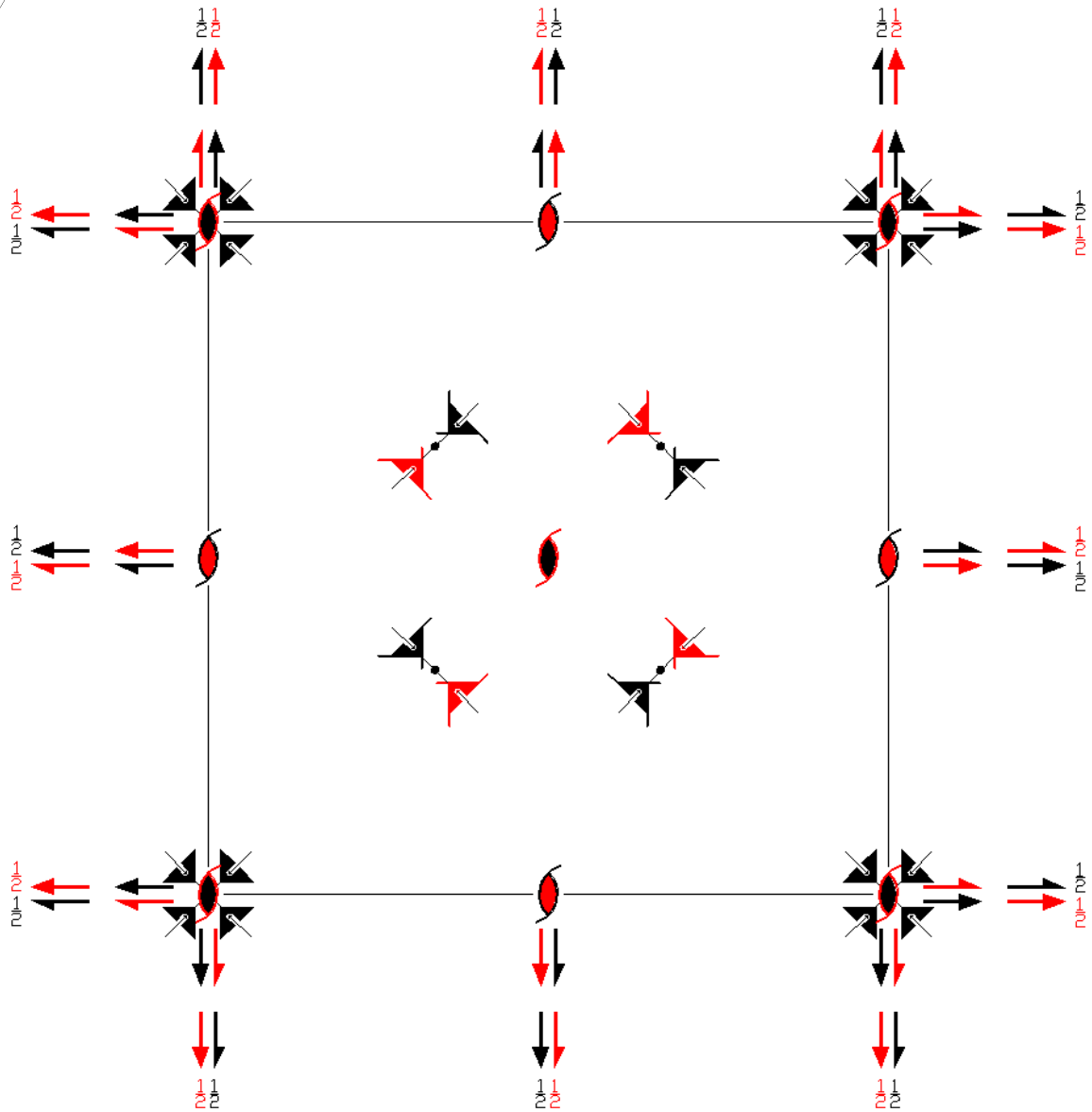
Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,x,0



P<sub>F</sub>23  
195.3.1505

231'  
P<sub>F</sub>23

Cubic



Origin at 23

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$ ;  $0 \leq z \leq 1/2$ ;  $y \leq 1-x$ ;  $z \leq \min(x,y)$

Vertices 0,0,0    1,0,0    0,1,0    1/2,1/2,1/2

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)              |

For (1,0,0)<sup>l</sup> + set

(1) t <sup>l</sup> (1,0,0) (1 1,0,0) <sup>l</sup>	(2) 2 <sup>l</sup> 1/2,0,z (2 <sub>z</sub>  1,0,0) <sup>l</sup>	(3) 2 <sup>l</sup> 1/2,y,0 (2 <sub>y</sub>  1,0,0) <sup>l</sup>	(4) 2 <sup>l</sup> (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0) <sup>l</sup>
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x+2/3,x+1/3,x (3 <sub>xyz</sub>  1,0,0) <sup>l</sup>	(6) 3 <sup>+</sup> (1/3,-1/3,1/3) x+2/3,x-1/3,x (3 <sub>xyz</sub> <sup>-1</sup>  1,0,0) <sup>l</sup>	(7) 3 <sup>+</sup> (1/3,-1/3,-1/3) x+2/3,x-1/3,x (3 <sub>xyz</sub> <sup>-1</sup>  1,0,0) <sup>l</sup>	(8) 3 <sup>+</sup> (1/3,1/3,-1/3) x+2/3,x-1/3,x (3 <sub>xyz</sub> <sup>-1</sup>  1,0,0) <sup>l</sup>
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x+1/3,x-1/3,x (3 <sub>xyz</sub> <sup>-1</sup>  1,0,0) <sup>l</sup>	(10) 3 <sup>-</sup> (1/3,-1/3,-1/3) x+1/3,x+1/3,x (3 <sub>xyz</sub>  1,0,0) <sup>l</sup>	(11) 3 <sup>-</sup> (1/3,1/3,-1/3) x+1/3,x-1/3,x (3 <sub>xyz</sub>  1,0,0) <sup>l</sup>	(12) 3 <sup>-</sup> (1/3,-1/3,1/3) x+1/3,x+1/3,x (3 <sub>xyz</sub>  1,0,0) <sup>l</sup>

**Generators selected** (1); t<sup>l</sup>(1,0,0); t<sup>l</sup>(0,1,0); t<sup>l</sup>(0,0,1); (2); (3); (5).**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates		
	(0,0,0) +	(1,0,0) <sup>l</sup> +	
24 j 1			
(1) x,y,z [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
(5) z,x,y [w,u,v]	(6) z, $\bar{x}, \bar{y}$ [ $\bar{w}, \bar{u}, \bar{v}$ ]	(7) $\bar{z}, \bar{x}, y$ [ $\bar{w}, \bar{u}, v$ ]	(8) $\bar{z}, x, \bar{y}$ [ $\bar{w}, u, \bar{v}$ ]
(9) y,z,x [v,w,u]	(10) $\bar{y}, z, \bar{x}$ [ $\bar{v}, w, \bar{u}$ ]	(11) y, $\bar{z}, \bar{x}$ [v, $\bar{w}, \bar{u}$ ]	(12) $\bar{y}, \bar{z}, x$ [ $\bar{v}, \bar{w}, u$ ]
12 i 2..	x, 1/2, 1/2 [u,0,0] 1/2, $\bar{x}$ , 1/2 [0,u,0]	$\bar{x}$ , 1/2, 1/2 [u,0,0] 1/2, 1/2, x [0,0,u]	1/2, x, 1/2 [0,u,0] 1/2, 1/2, $\bar{x}$ [0,0,u]
12 h 2'..	x, 1/2, 0 [0,v,w] 0, $\bar{x}$ , 1/2 [ $\bar{w}$ ,0,v]	$\bar{x}$ , 1/2, 0 [0,v, $\bar{w}$ ] 1/2, 0, x [v,w,0]	0, x, 1/2 [w,0,v] 1/2, 0, $\bar{x}$ [v, $\bar{w}$ ,0]
12 g 2'..	x, 0, 1/2 [0,v,w] 1/2, $\bar{x}$ , 0 [w,0, $\bar{v}$ ]	$\bar{x}$ , 0, 1/2 [0, $\bar{v}$ ,w] 0, 1/2, x [v,w,0]	1/2, x, 0 [w,0,v] 0, 1/2, $\bar{x}$ [ $\bar{v}$ , w,0]
12 f 2..	x, 0, 0 [u,0,0] 0, $\bar{x}$ , 0 [0, $\bar{u}$ ,0]	$\bar{x}$ , 0, 0 [ $\bar{u}$ ,0,0] 0, 0, x [0,0,u]	0, x, 0 [0,u,0] 0, 0, $\bar{x}$ [0,0, $\bar{u}$ ]
8 e .3.	x, x, x [u,u,u]	$\bar{x}, \bar{x}, x$ [ $\bar{u}, \bar{u}, u$ ]	$\bar{x}, x, \bar{x}$ [ $\bar{u}, u, \bar{u}$ ]
6 d 22'2'..	1/2, 0, 0 [u,0,0]	0, 1/2, 0 [0,u,0]	0, 0, 1/2 [0,0,u]
6 c 22'2'..	0, 1/2, 1/2 [u,0,0]	1/2, 0, 1/2 [0,u,0]	1/2, 1/2, 0 [0,0,u]
2 b 23.	1/2, 1/2, 1/2 [0,0,0]		
2 a 23.	0, 0, 0 [0,0,0]		

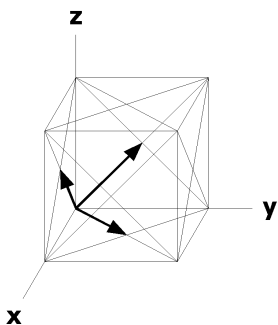


**Symmetry of Special Projections**

Along [0,0,1]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,1,1]  $p31'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
Origin at x,x,x

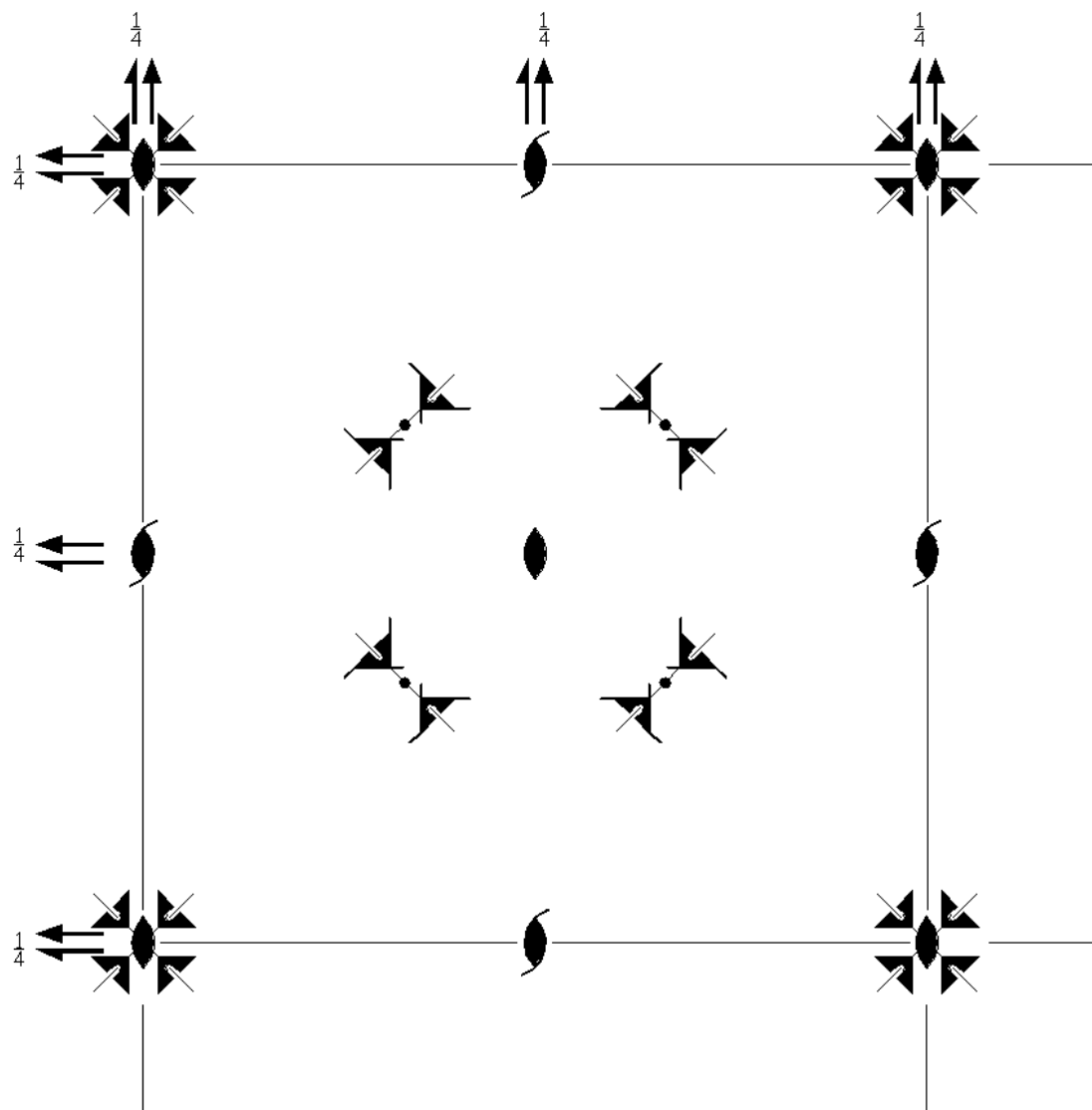
Along [1,1,0]  $p_c-1m1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x-1/4, x+1/4, 0$



F23  
196.1.1506

23  
F23

Cubic



Origin at 23

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $-1/4 \leq z \leq 1/4$ ;  $y \leq x$ ;  $\max(x-1/2, -y) \leq z \leq \min(1/2 - x, y)$

Vertices 0,0,0    1/2,0,0    1/2,1/2,0    1/4,1/4,1/4    1/4,1/4,-1/4

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                         | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xyz}^{-1}</math></sub>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}^{-1}</math></sub>  0,0,0)  | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{yz}^{-1}</math></sub>  0,0,0)    |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{xyz}^{-1}</math></sub>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)    | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0) | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0) |

## For (0,1/2,1/2) + set

- |   |  |   |   |
|---|--|---|---|
| (1) $t(0,1/2,1/2)$<br>(1 0,1/2,1/2)   | (2) $2(0,0,1/2) \ 0,1/4,z$<br>(2 <sub>z</sub>  0,1/2,1/2)  | (3) $2(0,1/2,0) \ 0,y,1/4$<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) $2 \ x,1/4,1/4$<br>(2 <sub>x</sub>  0,1/2,1/2)  |
| (5) $3^+(1/3,1/3,1/3)$<br>$x-1/3,x-1/6,x$<br>(3 <sub>xyz</sub>  0,1/2,1/2)  | (6) $3^+ \ \bar{x},x+1/2,\bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  0,1/2,1/2)  | (7) $3^+ (-1/3,1/3,1/3)$<br>$x+1/3,\bar{x}-1/6,\bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  0,1/2,1/2) | (8) $3^+ \ \bar{x},\bar{x}+1/2,x$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  0,1/2,1/2) |
| (9) $3^-(1/3,1/3,1/3)$<br>$x-1/6,x+1/6,x$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  0,1/2,1/2) | (10) $3^-(1/3,1/3,1/3)$<br>$x+1/6,x+1/6,\bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub>  0,1/2,1/2) | (11) $3^- \ \bar{x}+1/2,\bar{x}+1/2,x$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub>  0,1/2,1/2)                                | (12) $3^- \ \bar{x}-1/2,x+1/2,\bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub>  0,1/2,1/2)          |

## For (1/2,0,1/2) + set

- |   |  |   |   |
|---|--|---|---|
| (1) $t(1/2,0,1/2)$<br>(1 1/2,0,1/2)   | (2) $2(0,0,1/2) \ 1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,1/2)  | (3) $2 \ 1/4,y,1/4$<br>(2 <sub>y</sub>  1/2,0,1/2)  | (4) $2(1/2,0,0) \ x,0,1/2$<br>(2 <sub>x</sub>  1/2,0,1/2)   |
| (5) $3^+(1/3,1/3,1/3)$<br>$x+1/6,x-1/6,x$<br>(3 <sub>xyz</sub>  1/2,0,1/2)  | (6) $3^+(1/3,-1/3,1/3)$<br>$x+1/6,x+1/6,\bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1/2,0,1/2) | (7) $3^+ \ x+1/2,\bar{x}-1/2,\bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1/2,0,1/2) | (8) $3^+ \ \bar{x}+1/2,\bar{x}+1/2,x$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1/2,0,1/2)     |
| (9) $3^-(1/3,1/3,1/3)$<br>$x-1/6,x-1/3,x$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1/2,0,1/2) | (10) $3^- \ x+1/2,\bar{x},\bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub>  1/2,0,1/2)                             | (11) $3^- \ \bar{x}+1/2,\bar{x},x$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub>  1/2,0,1/2)                  | (12) $3^-(1/3,-1/3,1/3)$<br>$\bar{x}-1/6,x+1/3,\bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub>  1/2,0,1/2) |

## For (1/2,1/2,0) + set

- |   |   |   |  |
|---|---|---|--|
| (1) $t(1/2,1/2,0)$<br>(1 1/2,1/2,0)   | (2) $2 \ 1/4,1/4,z$<br>(2 <sub>z</sub>  1/2,1/2,0)  | (3) $2(0,1/2,0) \ 1/4,y,0$<br>(2 <sub>y</sub>  1/2,1/2,0)   | (4) $2(1/2,0,0) \ x,1/4,0$<br>(2 <sub>x</sub>  1/2,1/2,0)  |
| (5) $3^+(1/3,1/3,1/3)$<br>$x+1/6,x+1/3,x$<br>(3 <sub>xyz</sub>  1/2,1/2,0)  | (6) $3^+ \ \bar{x}+1/2,x,\bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1/2,1/2,0) | (7) $3^+ \ x+1/2,\bar{x},\bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1/2,1/2,0)         | (8) $3^+(1/3,1/3,-1/3)$<br>$\bar{x}+1/6,\bar{x}+1/3,x$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1/2,1/2,0) |
| (9) $3^-(1/3,1/3,1/3)$<br>$x+1/3,x+1/6,x$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1/2,1/2,0) | (10) $3^- \ x,\bar{x}+1/2,\bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub>  1/2,1/2,0)              | (11) $3^-(1/3,1/3,-1/3)$<br>$\bar{x}+1/3,\bar{x}+1/6,x$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub>  1/2,1/2,0) | (12) $3^- \ \bar{x},x+1/2,\bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub>  1/2,1/2,0)                                   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
48	h	1		
(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]	
(5) z,x,y [w,u,v]	(6) $z,\bar{x},\bar{y}$ [ $w,\bar{u},\bar{v}$ ]	(7) $\bar{z},\bar{x},y$ [ $\bar{w},\bar{u},v$ ]	(8) $\bar{z},x,\bar{y}$ [ $\bar{w},u,\bar{v}$ ]	
(9) y,z,x [v,w,u]	(10) $\bar{y},z,\bar{x}$ [ $\bar{v},w,\bar{u}$ ]	(11) $y,\bar{z},\bar{x}$ [ $v,\bar{w},\bar{u}$ ]	(12) $\bar{y},\bar{z},x$ [ $\bar{v},\bar{w},u$ ]	

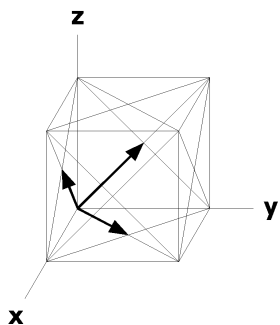
24	g	2..	$x, 1/4, 1/4 [u, 0, 0]$	$\bar{x}, 3/4, 1/4 [\bar{u}, 0, 0]$	$1/4, x, 1/4 [0, u, 0]$
			$1/4, \bar{x}, 3/4 [0, \bar{u}, 0]$	$1/4, 1/4, x [0, 0, u]$	$3/4, 1/4, \bar{x} [0, 0, \bar{u}]$
24	f	2..	$x, 0, 0 [u, 0, 0]$	$\bar{x}, 0, 0 [\bar{u}, 0, 0]$	$0, x, 0 [0, u, 0]$
			$0, \bar{x}, 0 [0, \bar{u}, 0]$	$0, 0, x [0, 0, u]$	$0, 0, \bar{x} [0, 0, \bar{u}]$
16	e	.3.	$x, x, x [u, u, u]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$	$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$
					$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
4	d	23.	$3/4, 3/4, 3/4 [0, 0, 0]$		
4	c	23.	$1/4, 1/4, 1/4 [0, 0, 0]$		
4	b	23.	$1/2, 1/2, 1/2 [0, 0, 0]$		
4	a	23.	$0, 0, 0 [0, 0, 0]$		

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p2m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $0, 0, z$

Along  $[1, 1, 1]$   $p3$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at  $x, x, x$

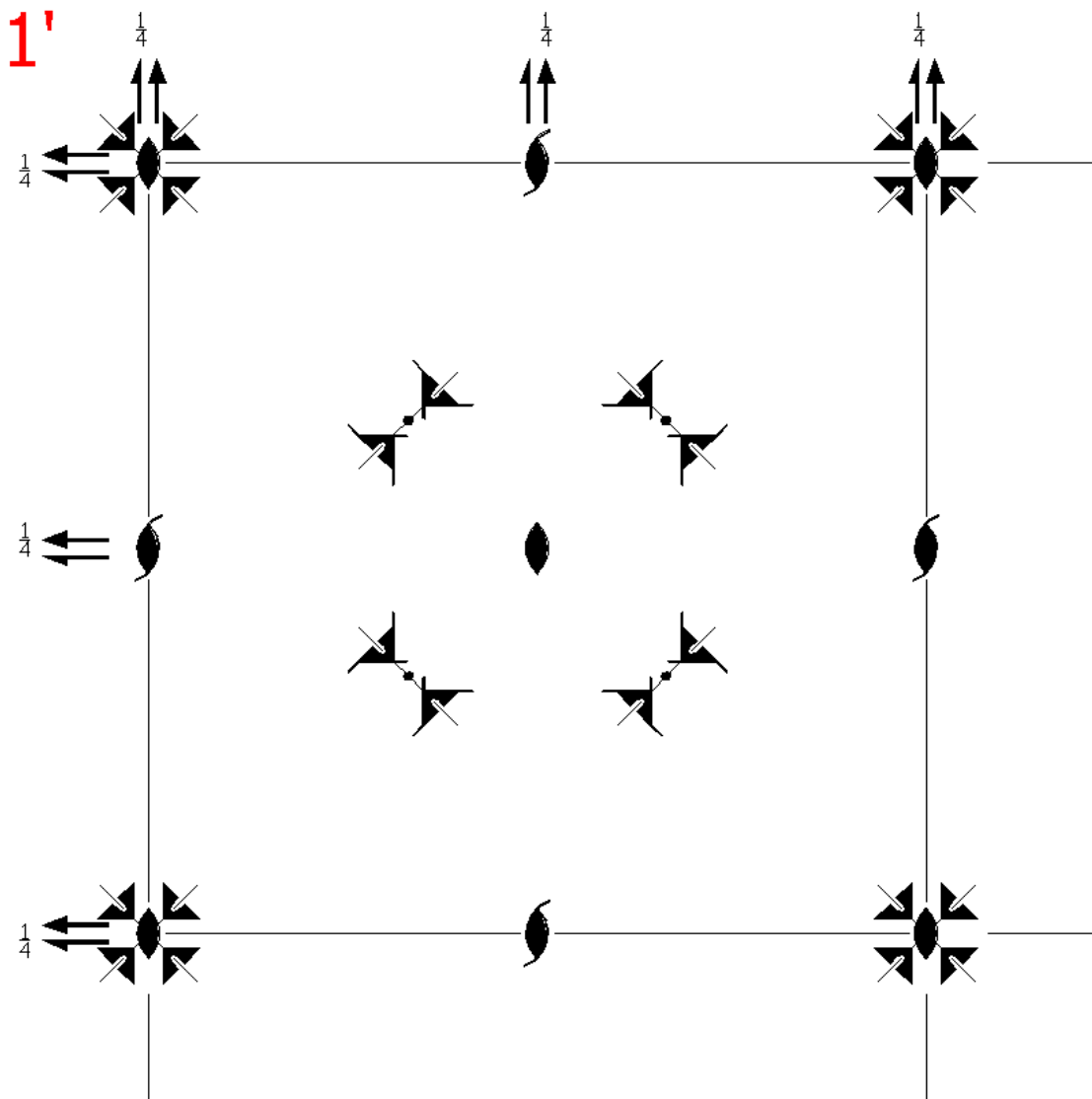
Along  $[1, 1, 0]$   $c1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 0$



F231'  
196.2.1507

231'  
F231'

Cubic



Origin at 231'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $-1/4 \leq z \leq 1/4$ ;  $y \leq x$ ;  $\max(x-1/2, -y) \leq z \leq \min(1/2 - x, y)$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/4,1/4,1/4$   $1/4,1/4,-1/4$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)              |

## For (0,1/2,1/2) + set

- |  |  |   |  |
|--|--|---|--|
| (1) $t(0,1/2,1/2)$<br>(1 0,1/2,1/2)  | (2) $2(0,0,1/2) 0,1/4,z$<br>(2 <sub>z</sub>  0,1/2,1/2)                                  | (3) $2(0,1/2,0) 0,y,1/4$<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) $2x,1/4,1/4$<br>(2 <sub>x</sub>  0,1/2,1/2)                                |
| (5) $3^+(1/3,1/3,1/3)$<br>$x-1/3,x-1/6,x$<br>(3 <sub>xyz</sub>  0,1/2,1/2)               | (6) $3^+ \bar{x},x+1/2,\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)           | (7) $3^+(-1/3,1/3,1/3)$<br>$x+1/3,\bar{x}-1/6,\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2) | (8) $3^+ \bar{x},\bar{x}+1/2,x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2) |
| (9) $3^-(1/3,1/3,1/3)$<br>$x-1/6,x+1/6,x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2) | (10) $3^-(-1/3,1/3,1/3)$<br>$x+1/6,\bar{x}+1/6,\bar{x}$<br>(3 <sub>xyz</sub>  0,1/2,1/2) | (11) $3^- \bar{x}+1/2,\bar{x}+1/2,x$<br>(3 <sub>xyz</sub>  0,1/2,1/2)                                 | (12) $3^- \bar{x}-1/2,x+1/2,\bar{x}$<br>(3 <sub>xyz</sub>  0,1/2,1/2)          |

## For (1/2,0,1/2) + set

- |  |   |  |  |
|--|---|--|--|
| (1) $t(1/2,0,1/2)$<br>(1 1/2,0,1/2)  | (2) $2(0,0,1/2) 1/4,0,z$<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) $2(1/4,y,1/4)$<br>(2 <sub>y</sub>  1/2,0,1/2)                                  | (4) $2(1/2,0,0) x,0,1/2$<br>(2 <sub>x</sub>  1/2,0,1/2)                                  |
| (5) $3^+(1/3,1/3,1/3)$<br>$x+1/6,x-1/6,x$<br>(3 <sub>xyz</sub>  1/2,0,1/2)               | (6) $3^+(1/3,-1/3,1/3)$<br>$x+1/6,x+1/6,\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) | (7) $3^+ x+1/2,\bar{x}-1/2,\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) | (8) $3^+ \bar{x}+1/2,\bar{x}+1/2,x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2)       |
| (9) $3^-(1/3,1/3,1/3)$<br>$x-1/6,x-1/3,x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) | (10) $3^- x+1/2,\bar{x},\bar{x}$<br>(3 <sub>xyz</sub>  1/2,0,1/2)                               | (11) $3^- \bar{x}+1/2,\bar{x},x$<br>(3 <sub>xyz</sub>  1/2,0,1/2)                  | (12) $3^-(1/3,-1/3,1/3)$<br>$\bar{x}-1/6,x+1/3,\bar{x}$<br>(3 <sub>xyz</sub>  1/2,0,1/2) |

## For (1/2,1/2,0) + set

- |  |  |  |   |
|--|--|--|---|
| (1) $t(1/2,1/2,0)$<br>(1 1/2,1/2,0)  | (2) $2(1/4,1/4,z)$<br>(2 <sub>z</sub>  1/2,1/2,0)                              | (3) $2(0,1/2,0) 1/4,y,0$<br>(2 <sub>y</sub>  1/2,1/2,0)                                  | (4) $2(1/2,0,0) x,1/4,0$<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) $3^+(1/3,1/3,1/3)$<br>$x+1/6,x+1/3,x$<br>(3 <sub>xyz</sub>  1/2,1/2,0)               | (6) $3^+ \bar{x}+1/2,x,\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0) | (7) $3^+ x+1/2,\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0)           | (8) $3^+(1/3,1/3,-1/3)$<br>$\bar{x}+1/6,\bar{x}+1/3,x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0) |
| (9) $3^-(1/3,1/3,1/3)$<br>$x+1/3,x+1/6,x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0) | (10) $3^- x,\bar{x}+1/2,\bar{x}$<br>(3 <sub>xyz</sub>  1/2,1/2,0)              | (11) $3^-(1/3,1/3,-1/3)$<br>$\bar{x}+1/3,\bar{x}+1/6,x$<br>(3 <sub>xyz</sub>  1/2,1/2,0) | (12) $3^- \bar{x},x+1/2,\bar{x}$<br>(3 <sub>xyz</sub>  1/2,1/2,0)                                     |

## For (0,0,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $1'$<br>(1 0,0,0)'   | (2) $2' 0,0,z$<br>(2 <sub>z</sub>  0,0,0)'                                 | (3) $2' 0,y,0$<br>(2 <sub>y</sub>  0,0,0)'                                 | (4) $2' x,0,0$<br>(2 <sub>x</sub>  0,0,0)'                                 |
| (5) $3^{+'} x,x,x$<br>(3 <sub>xyz</sub>  0,0,0)'               | (6) $3^{+'} \bar{x},x,\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)' | (7) $3^{+'} x,\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)' | (8) $3^{+'} \bar{x},\bar{x},x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)' |
| (9) $3^{-'} x,x,x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)' | (10) $3^{-'} x,\bar{x},\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)'              | (11) $3^{-'} \bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)'              | (12) $3^{-'} \bar{x},x,\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)'              |

## For (0,1/2,1/2)' + set

(1) $t' (0,1/2,1/2)$ (1   0,1/2,1/2)'	(2) $2' (0,0,1/2) \quad 0,1/4,z$ (2 <sub>z</sub>   0,1/2,1/2)'	(3) $2' (0,1/2,0) \quad 0,y,1/4$ (2 <sub>y</sub>   0,1/2,1/2)'	(4) $2' \quad x,1/4,1/4$ (2 <sub>x</sub>   0,1/2,1/2)'
(5) $3^{+'} (1/3,1/3,1/3)$ $x-1/3,x-1/6,x$ (3 <sub>xyz</sub>   0,1/2,1/2)'	(6) $3^{+'} \quad \bar{x},x+1/2,\bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   0,1/2,1/2)'	(7) $3^{+'} (-1/3,1/3,1/3)$ $x+1/3,\bar{x}-1/6,\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   0,1/2,1/2)'	(8) $3^{+'} \quad \bar{x},\bar{x}+1/2,x$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   0,1/2,1/2)'
(9) $3^{-'} (1/3,1/3,1/3)$ $x-1/6,x+1/6,x$ (3 <sub>xyz</sub> <sup>-1</sup>   0,1/2,1/2)'	(10) $3^{-'} (-1/3,1/3,1/3)$ $x+1/6,\bar{x}+1/6,\bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   0,1/2,1/2)'	(11) $3^{-'} \quad \bar{x}+1/2,\bar{x}+1/2,x$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   0,1/2,1/2)'	(12) $3^{-'} \quad \bar{x}-1/2,x+1/2,\bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   0,1/2,1/2)'

## For (1/2,0,1/2)' + set

(1) $t' (1/2,0,1/2)$ (1   1/2,0,1/2)'	(2) $2' (0,0,1/2) \quad 1/4,0,z$ (2 <sub>z</sub>   1/2,0,1/2)'	(3) $2' \quad 1/4,y,1/4$ (2 <sub>y</sub>   1/2,0,1/2)'	(4) $2' (1/2,0,0) \quad x,0,1/2$ (2 <sub>x</sub>   1/2,0,1/2)'
(5) $3^{+'} (1/3,1/3,1/3)$ $x+1/6,x-1/6,x$ (3 <sub>xyz</sub>   1/2,0,1/2)'	(6) $3^{+'} (1/3,-1/3,1/3)$ $x+1/6,x+1/6,\bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2,0,1/2)'	(7) $3^{+'} \quad x+1/2,\bar{x}-1/2,\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,0,1/2)'	(8) $3^{+'} \quad \bar{x}+1/2,\bar{x}+1/2,x$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2,0,1/2)'
(9) $3^{-'} (1/3,1/3,1/3)$ $x-1/6,x-1/3,x$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,0,1/2)'	(10) $3^{-'} \quad x+1/2,\bar{x},\bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,0,1/2)'	(11) $3^{-'} \quad \bar{x}+1/2,\bar{x},x$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,0,1/2)'	(12) $3^{-'} (1/3,-1/3,1/3)$ $x-1/6,x+1/3,\bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,0,1/2)'

## For (1/2,1/2,0)' + set

(1) $t' (1/2,1/2,0)$ (1   1/2,1/2,0)'	(2) $2' \quad 1/4,1/4,z$ (2 <sub>z</sub>   1/2,1/2,0)'	(3) $2' (0,1/2,0) \quad 1/4,y,0$ (2 <sub>y</sub>   1/2,1/2,0)'	(4) $2' (1/2,0,0) \quad x,1/4,0$ (2 <sub>x</sub>   1/2,1/2,0)'
(5) $3^{+'} (1/3,1/3,1/3)$ $x+1/6,x+1/3,x$ (3 <sub>xyz</sub>   1/2,1/2,0)'	(6) $3^{+'} \quad \bar{x}+1/2,x,\bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2,1/2,0)'	(7) $3^{+'} \quad x+1/2,\bar{x},\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)'	(8) $3^{+'} (1/3,1/3,-1/3)$ $x+1/6,\bar{x}+1/3,x$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2,1/2,0)'
(9) $3^{-'} (1/3,1/3,1/3)$ $x+1/3,x+1/6,x$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)'	(10) $3^{-'} \quad x,\bar{x}+1/2,\bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,1/2,0)'	(11) $3^{-'} (1/3,1/3,-1/3)$ $x+1/3,\bar{x}+1/6,x$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,1/2,0)'	(12) $3^{-'} \quad \bar{x},x+1/2,\bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +  
(0,0,0)' + (0,1/2,1/2)' + (1/2,0,1/2)' + (1/2,1/2,0)'

48 h 11'

(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{x},y,\bar{z}$ [0,0,0]	(4) $x,\bar{y},\bar{z}$ [0,0,0]
(5) z,x,y [0,0,0]	(6) $z,\bar{x},\bar{y}$ [0,0,0]	(7) $\bar{z},\bar{x},y$ [0,0,0]	(8) $\bar{z},x,\bar{y}$ [0,0,0]
(9) y,z,x [0,0,0]	(10) $\bar{y},z,\bar{x}$ [0,0,0]	(11) $y,\bar{z},\bar{x}$ [0,0,0]	(12) $\bar{y},\bar{z},x$ [0,0,0]

24	g	2..1'	$x, 1/4, 1/4 [0,0,0]$	$\bar{x}, 3/4, 1/4 [0,0,0]$	$1/4, x, 1/4 [0,0,0]$
			$1/4, \bar{x}, 3/4 [0,0,0]$	$1/4, 1/4, x [0,0,0]$	$3/4, 1/4, \bar{x} [0,0,0]$
24	f	2..1'	$x, 0, 0 [0,0,0]$	$\bar{x}, 0, 0 [0,0,0]$	$0, x, 0 [0,0,0]$
			$0, \bar{x}, 0 [0,0,0]$	$0, 0, x [0,0,0]$	$0, 0, \bar{x} [0,0,0]$
16	e	.3.1'	$x, x, x [0,0,0]$	$\bar{x}, \bar{x}, x [0,0,0]$	$\bar{x}, x, \bar{x} [0,0,0]$
4	d	23.1'	$3/4, 3/4, 3/4 [0,0,0]$		
4	c	23.1'	$1/4, 1/4, 1/4 [0,0,0]$		
4	b	23.1'	$1/2, 1/2, 1/2 [0,0,0]$		
4	a	23.1'	$0, 0, 0 [0,0,0]$		

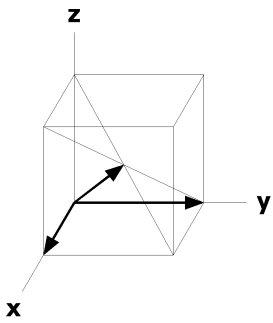
### Symmetry of Special Projections

Along  $[0,0,1]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p31'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at  $x,x,x$

Along  $[1,1,0]$   $c1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$

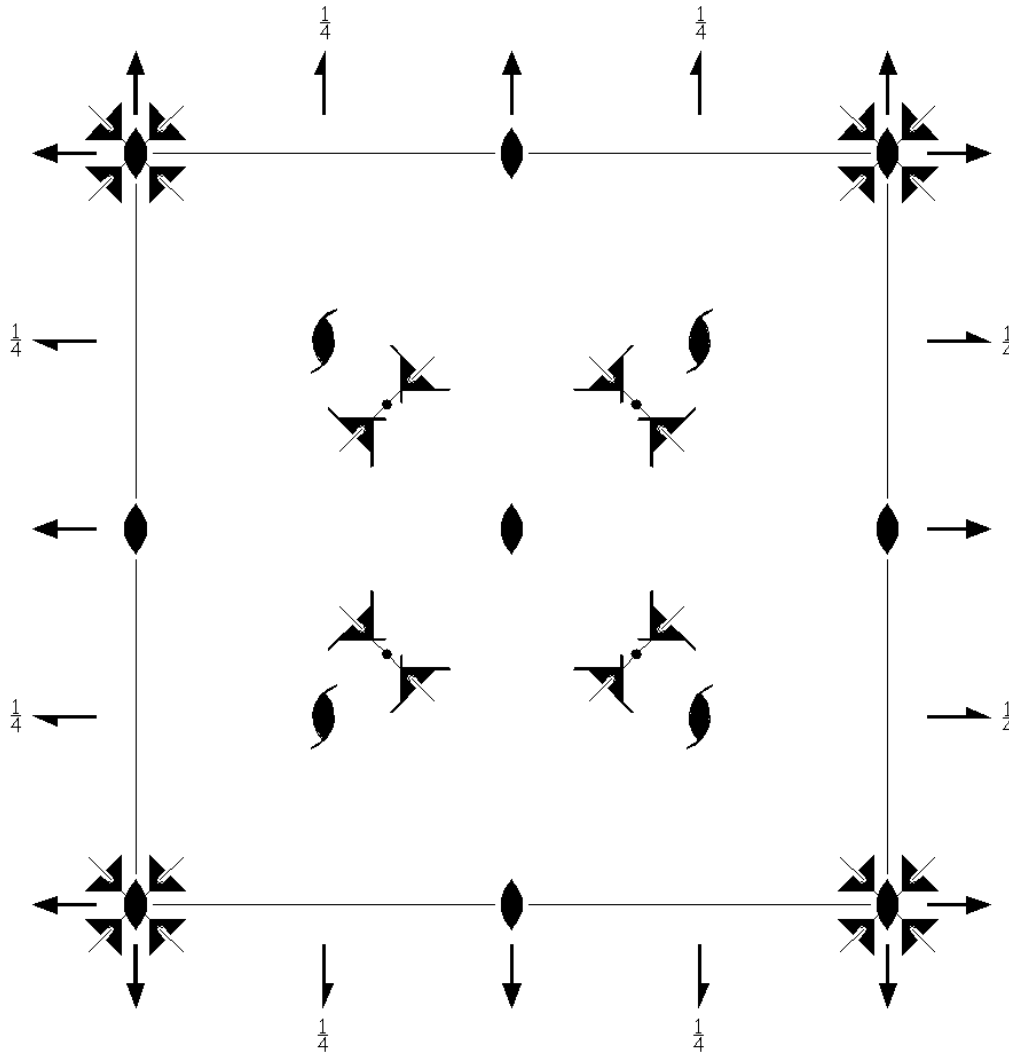




I23  
197.1.1508

23  
I23

Cubic



Origin at 23

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq \min(x, 1-x);$   $z \leq y$   
**Vertices** 0,0,0 1,0,0 1/2,1/2,0 1/2,1/2,1/2

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)              |

## For (1/2,1/2,1/2) + set

(1) $t(1/2,1/2,1/2)$ (1   1/2,1/2,1/2)	(2) $2(0,0,1/2)$ 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,1/2)	(3) $2(0,1/2,0)$ 1/4,y,1/4 (2 <sub>y</sub>   1/2,1/2,1/2)	(4) $2(1/2,0,0)$ x,1/4,1/4 (2 <sub>x</sub>   1/2,1/2,1/2)
(5) $3^+(1/2,1/2,1/2)$ x,x,x (3 <sub>xyz</sub>   1/2,1/2,1/2)	(6) $3^+(1/6,-1/6,1/6)$ $\bar{x}+1/3, \bar{x}+1/3, \bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2,1/2,1/2)	(7) $3^+(-1/6,1/6,1/6)$ $\bar{x}+2/3, \bar{x}-1/3, \bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2,1/2,1/2)	(8) $3^+(1/6,1/6,-1/6)$ $\bar{x}+1/3, \bar{x}+2/3, \bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2,1/2,1/2)
(9) $3^-(1/2,1/2,1/2)$ x,x,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,1/2)	(10) $3^-(-1/6,1/6,1/6)$ $\bar{x}+1/3, \bar{x}+1/3, \bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,1/2,1/2)	(11) $3^-(1/6,1/6,-1/6)$ $\bar{x}+2/3, \bar{x}+1/3, \bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,1/2,1/2)	(12) $3^-(1/6,-1/6,1/6)$ $\bar{x}-1/3, \bar{x}+2/3, \bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

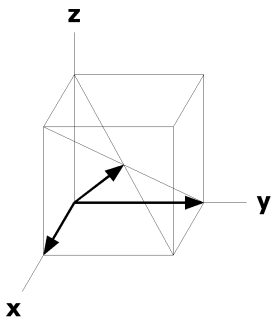
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates								
			(0,0,0) +	(1/2,1/2,1/2) +							
24	f	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}, \bar{y}, z$	$[\bar{u}, \bar{v}, w]$	(3)	$\bar{x}, y, \bar{z}$	$[\bar{u}, v, \bar{w}]$	(4)	$x, \bar{y}, \bar{z}$	$[u, \bar{v}, \bar{w}]$
(5)	z,x,y	[w,u,v]	(6)	$z, \bar{x}, \bar{y}$	$[w, \bar{u}, \bar{v}]$	(7)	$\bar{z}, \bar{x}, y$	$[\bar{w}, \bar{u}, v]$	(8)	$\bar{z}, x, \bar{y}$	$[\bar{w}, u, \bar{v}]$
(9)	y,z,x	[v,w,u]	(10)	$\bar{y}, z, \bar{x}$	$[\bar{v}, w, \bar{u}]$	(11)	$y, \bar{z}, \bar{x}$	$[v, \bar{w}, \bar{u}]$	(12)	$\bar{y}, \bar{z}, x$	$[\bar{v}, \bar{w}, u]$
12	e	2..	x,1/2,0 [u,0,0]	$\bar{x}, 1/2, 0$	$[\bar{u}, 0, 0]$	0,x,1/2 [0,u,0]					
			0, $\bar{x}$ ,1/2 [0, $\bar{u}$ ,0]	1/2,0,x [0,0,u]		1/2,0, $\bar{x}$ [0,0, $\bar{u}$ ]					
12	d	2..	x,0,0 [u,0,0]	$\bar{x}, 0, 0$	$[\bar{u}, 0, 0]$	0,x,0 [0,u,0]					
			0, $\bar{x}$ ,0 [0, $\bar{u}$ ,0]	0,0,x [0,0,u]		0,0, $\bar{x}$ [0,0, $\bar{u}$ ]					
8	c	.3.	x,x,x [u,u,u]	$\bar{x}, \bar{x}, x$	$[\bar{u}, \bar{u}, u]$	$\bar{x}, x, \bar{x}$	$[\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x}$	$[u, \bar{u}, \bar{u}]$		
6	b	222..	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		1/2,1/2,0 [0,0,0]					
2	a	23.	0,0,0 [0,0,0]								

**Symmetry of Special Projections**

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,1,1] p3  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

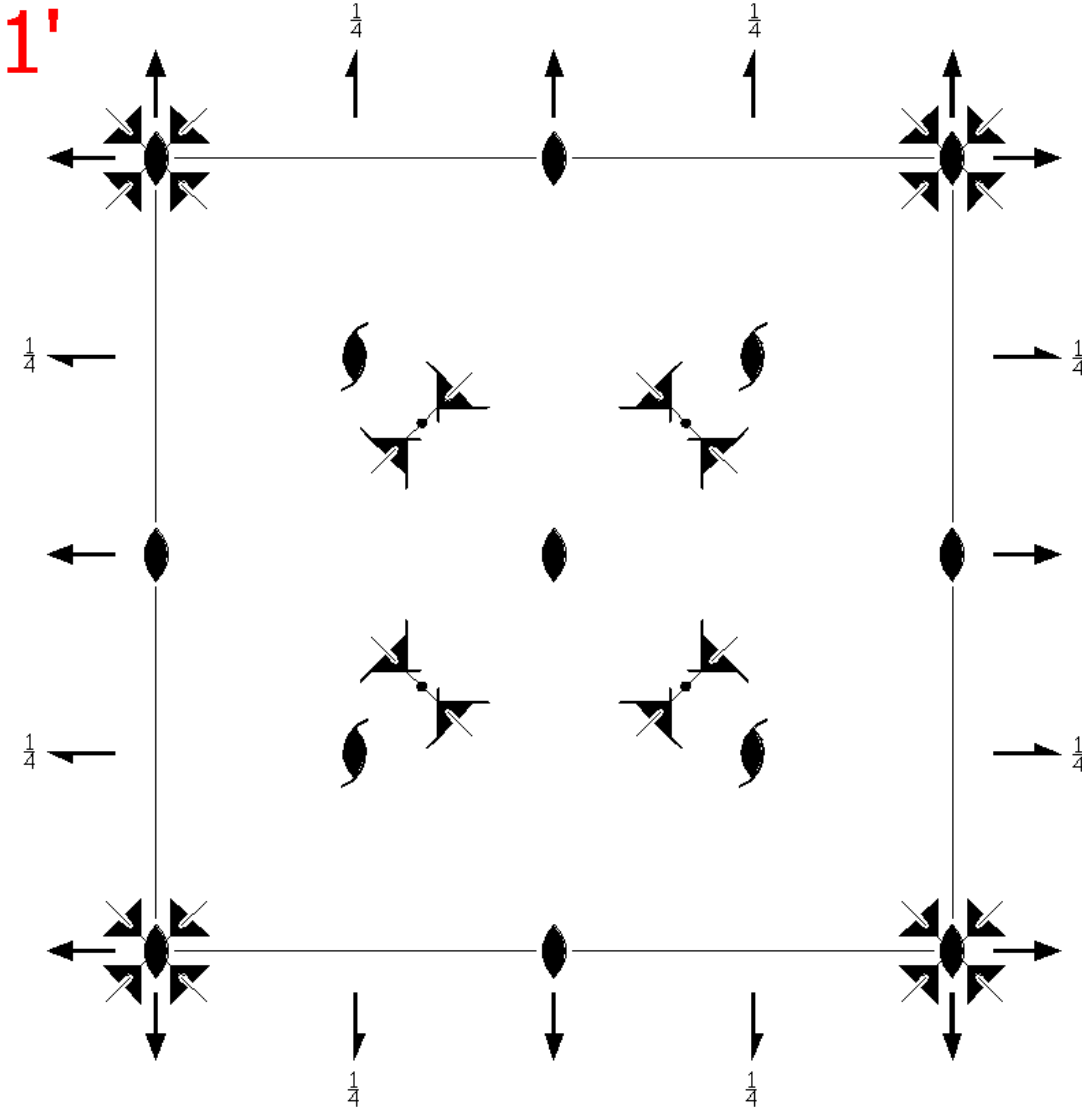
Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



I231'  
197.2.1509

231'  
I231'

Cubic



Origin at 231'

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$ ;  $y \leq \min(x, 1-x)$ ;  $z \leq y$

Vertices 0,0,0 1,0,0 1/2,1/2,0 1/2,1/2,1/2

**Symmetry Operations**

For (0,0,0) + set

- (1) 1  
(1|0,0,0)
- (2) 2 0,0,z  
(2<sub>z</sub>|0,0,0)
- (3) 2 0,y,0  
(2<sub>y</sub>|0,0,0)
- (4) 2 x,0,0  
(2<sub>x</sub>|0,0,0)
- (5) 3<sup>+</sup> x,x,x  
(3<sub>xyz</sub>|0,0,0)
- (6) 3<sup>+</sup>  $\bar{x},x,\bar{x}$   
(3 <sub>$\bar{x}yz^{-1}$</sub> |0,0,0)
- (7) 3<sup>+</sup> x, $\bar{x},\bar{x}$   
(3 <sub>$\bar{x}yz^{-1}$</sub> |0,0,0)
- (8) 3<sup>+</sup>  $\bar{x},\bar{x},x$   
(3 <sub>$\bar{x}yz^{-1}$</sub> |0,0,0)
- (9) 3<sup>-</sup> x,x,x  
(3 <sub>$\bar{x}yz^{-1}$</sub> |0,0,0)
- (10) 3<sup>-</sup> x, $\bar{x},\bar{x}$   
(3 <sub>$\bar{x}yz$</sub> |0,0,0)
- (11) 3<sup>-</sup>  $\bar{x},\bar{x},x$   
(3 <sub>$\bar{x}yz$</sub> |0,0,0)
- (12) 3<sup>-</sup>  $\bar{x},x,\bar{x}$   
(3 <sub>$\bar{x}yz$</sub> |0,0,0)

## For (1/2,1/2,1/2) + set

- |   |  |   |  |
|---|--|---|--|
| (1) $t$ (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)                                      | (2) $2$ (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2)  | (3) $2$ (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,1/2,1/2)   | (4) $2$ (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>   1/2,1/2,1/2)  |
| (5) $3^+$ (1/2,1/2,1/2) x,x,x<br>(3 <sub>xyz</sub>   1/2,1/2,1/2)               | (6) $3^+$ (1/6,-1/6,1/6)<br>$\bar{x}+1/3, \bar{x}+1/3, \bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2,1/2,1/2) | (7) $3^+$ (-1/6,1/6,1/6)<br>$\bar{x}+2/3, \bar{x}-1/3, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,1/2)             | (8) $3^+$ (1/6,1/6,-1/6)<br>$\bar{x}+1/3, \bar{x}+2/3, \bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2,1/2,1/2) |
| (9) $3^-$ (1/2,1/2,1/2) x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,1/2) | (10) $3^-$ (-1/6,1/6,1/6)<br>$\bar{x}+1/3, \bar{x}+1/3, \bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,1/2,1/2)              | (11) $3^-$ (1/6,1/6,-1/6)<br>$\bar{x}+2/3, \bar{x}+1/3, \bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,1/2,1/2) | (12) $3^-$ (1/6,-1/6,1/6)<br>$\bar{x}-1/3, \bar{x}+2/3, \bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,1/2,1/2)              |

## For (0,0,0)' + set

- |  |   |  |   |
|--|---|--|---|
| (1) $1'$<br>(1   0,0,0)'                                       | (2) $2'$ 0,0,z<br>(2 <sub>z</sub>   0,0,0)'   | (3) $2'$ 0,y,0<br>(2 <sub>y</sub>   0,0,0)'  | (4) $2'$ x,0,0<br>(2 <sub>x</sub>   0,0,0)'   |
| (5) $3^+$ ' x,x,x<br>(3 <sub>xyz</sub>   0,0,0)'               | (6) $3^+$ ' $\bar{x}, \bar{x}, \bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   0,0,0)' | (7) $3^+$ ' $\bar{x}, \bar{x}, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   0,0,0)'             | (8) $3^+$ ' $\bar{x}, \bar{x}, \bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   0,0,0)' |
| (9) $3^-$ ' x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   0,0,0)' | (10) $3^-$ ' $\bar{x}, \bar{x}, \bar{x}$<br>(3 <sub>xyz</sub>   0,0,0)'                                       | (11) $3^-$ ' $\bar{x}, \bar{x}, \bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub>   0,0,0)' | (12) $3^-$ ' $\bar{x}, \bar{x}, \bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub>   0,0,0)'              |

## For (1/2,1/2,1/2)' + set

- |  |   |  |   |
|--|---|--|---|
| (1) $t'$ (1/2,1/2,1/2)<br>(1   1/2,1/2,1/2)'                                       | (2) $2'$ (0,0,1/2) 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,1/2)'   | (3) $2'$ (0,1/2,0) 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,1/2,1/2)'  | (4) $2'$ (1/2,0,0) x,1/4,1/4<br>(2 <sub>x</sub>   1/2,1/2,1/2)'   |
| (5) $3^+$ ' (1/2,1/2,1/2) x,x,x<br>(3 <sub>xyz</sub>   1/2,1/2,1/2)'               | (6) $3^+$ ' (1/6,-1/6,1/6)<br>$\bar{x}+1/3, \bar{x}+1/3, \bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2,1/2,1/2)' | (7) $3^+$ ' (-1/6,1/6,1/6)<br>$\bar{x}+2/3, \bar{x}-1/3, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,1/2)'             | (8) $3^+$ ' (1/6,1/6,-1/6)<br>$\bar{x}+1/3, \bar{x}+2/3, \bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2,1/2,1/2)' |
| (9) $3^-$ ' (1/2,1/2,1/2) x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,1/2)' | (10) $3^-$ ' (-1/6,1/6,1/6)<br>$\bar{x}+1/3, \bar{x}+1/3, \bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,1/2,1/2)'              | (11) $3^-$ ' (1/6,1/6,-1/6)<br>$\bar{x}+2/3, \bar{x}+1/3, \bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,1/2,1/2)' | (12) $3^-$ ' (1/6,-1/6,1/6)<br>$\bar{x}-1/3, \bar{x}+2/3, \bar{x}$<br>(3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,1/2,1/2)'              |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

- |                   |                                    |                                    |                                    |                                   |
|-------------------|------------------------------------|------------------------------------|------------------------------------|-----------------------------------|
| 24                | f                                  | 11'                                | (0,0,0) +<br>(0,0,0)'              | (1/2,1/2,1/2) +<br>(1/2,1/2,1/2)' |
| (1) x,y,z [0,0,0] | (2) $\bar{x}, \bar{y}, z$ [0,0,0]  | (3) $\bar{x}, y, \bar{z}$ [0,0,0]  | (4) $x, \bar{y}, \bar{z}$ [0,0,0]  |                                   |
| (5) z,x,y [0,0,0] | (6) $z, \bar{x}, \bar{y}$ [0,0,0]  | (7) $\bar{z}, \bar{x}, y$ [0,0,0]  | (8) $\bar{z}, x, \bar{y}$ [0,0,0]  |                                   |
| (9) y,z,x [0,0,0] | (10) $\bar{y}, z, \bar{x}$ [0,0,0] | (11) $y, \bar{z}, \bar{x}$ [0,0,0] | (12) $\bar{y}, \bar{z}, x$ [0,0,0] |                                   |

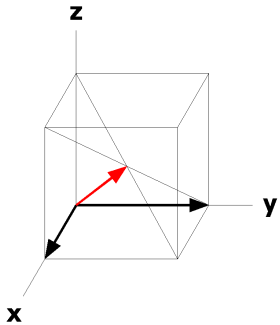
12	e	2..1'	$x, 1/2, 0 [0,0,0]$	$\bar{x}, 1/2, 0 [0,0,0]$	$0, x, 1/2 [0,0,0]$
			$0, \bar{x}, 1/2 [0,0,0]$	$1/2, 0, x [0,0,0]$	$1/2, 0, \bar{x} [0,0,0]$
12	d	2..1'	$x, 0, 0 [0,0,0]$	$\bar{x}, 0, 0 [0,0,0]$	$0, x, 0 [0,0,0]$
			$0, \bar{x}, 0 [0,0,0]$	$0, 0, x [0,0,0]$	$0, 0, \bar{x} [0,0,0]$
8	c	.3.1'	$x, x, x [0,0,0]$	$\bar{x}, \bar{x}, x [0,0,0]$	$\bar{x}, x, \bar{x} [0,0,0]$
					$x, \bar{x}, \bar{x} [0,0,0]$
6	b	222..1'	$0, 1/2, 1/2 [0,0,0]$	$1/2, 0, 1/2 [0,0,0]$	$1/2, 1/2, 0 [0,0,0]$
2	a	23.1'	$0, 0, 0 [0,0,0]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $c2mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p31'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x,x,x$

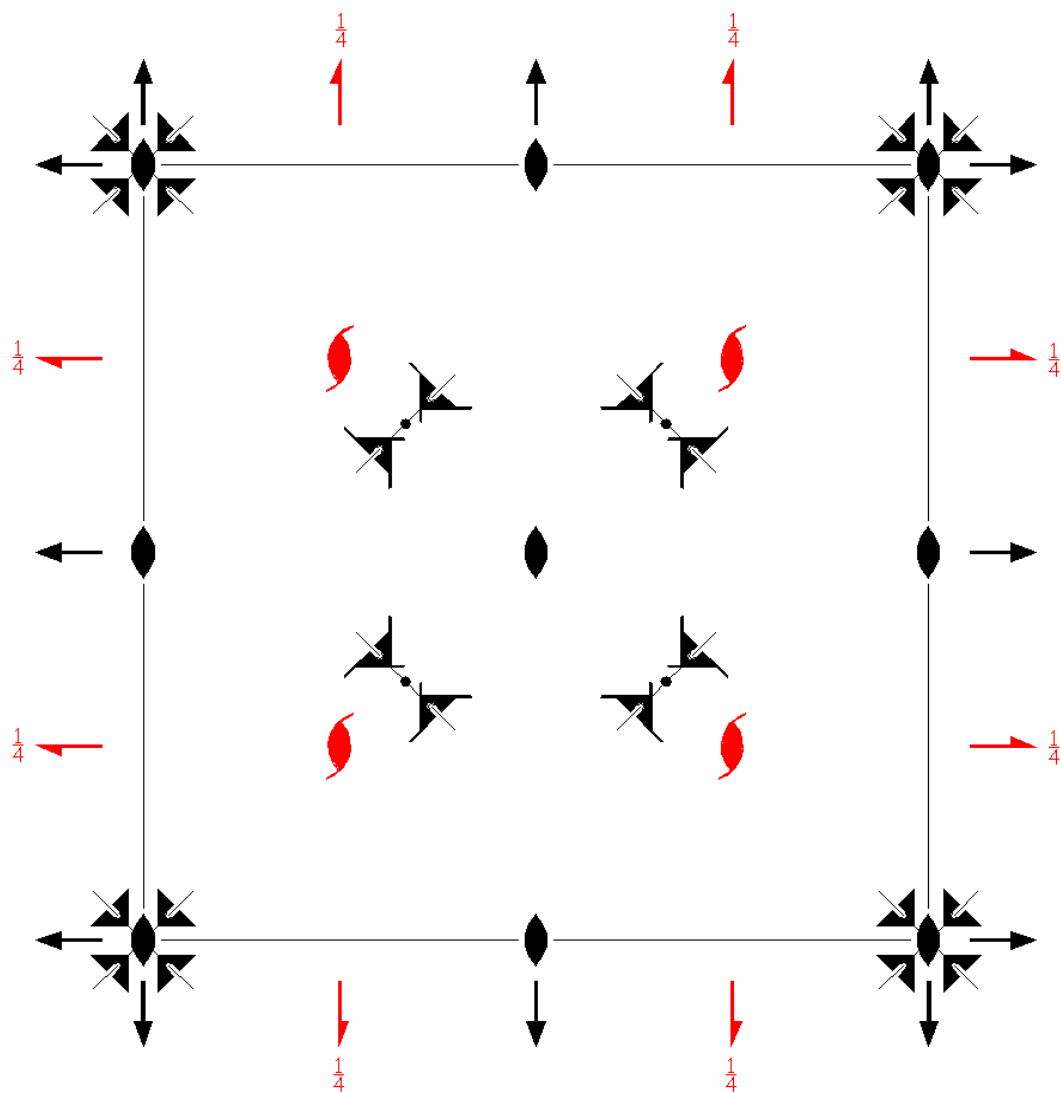
Along  $[1,1,0]$   $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



$I_{P23}$   
197.3.1510

$231'$   
 $I_{P23}$

Cubic



Origin at 23

<b>Asymmetric unit</b>	$0 \leq x \leq 1;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$y \leq \min(x, 1-x);$	$z \leq y$
Vertices	0,0,0	1,0,0	1/2,1/2,0	1/2,1/2,1/2	

**Symmetry Operations**

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                         | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xyz}^{-1}</math></sub>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}^{-1}</math></sub>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xyz}^{-1}</math></sub>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{xyz}^{-1}</math></sub>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)    | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)      | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)     |

## For (1/2,1/2,1/2)' + set

(1) $t' (1/2, 1/2, 1/2)$ (1   1/2, 1/2, 1/2)'	(2) $2' (0, 0, 1/2)$ 1/4, 1/4, z (2 <sub>z</sub>   1/2, 1/2, 1/2)'	(3) $2' (0, 1/2, 0)$ 1/4, y, 1/4 (2 <sub>y</sub>   1/2, 1/2, 1/2)'	(4) $2' (1/2, 0, 0)$ x, 1/4, 1/4 (2 <sub>x</sub>   1/2, 1/2, 1/2)'
(5) $3^{+'} (1/2, 1/2, 1/2)$ x, x, x (3 <sub>xyz</sub>   1/2, 1/2, 1/2)'	(6) $3^{+'} (1/6, -1/6, 1/6)$ $\bar{x} + 1/3, \bar{x} + 1/3, \bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2, 1/2, 1/2)'	(7) $3^{+'} (-1/6, 1/6, 1/6)$ $\bar{x} + 2/3, \bar{x} - 1/3, \bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2, 1/2, 1/2)'	(8) $3^{+'} (1/6, 1/6, -1/6)$ $\bar{x} + 1/3, \bar{x} + 2/3, \bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2, 1/2, 1/2)'
(9) $3^{-'} (1/2, 1/2, 1/2)$ x, x, x (3 <sub>xyz</sub> <sup>-1</sup>   1/2, 1/2, 1/2)'	(10) $3^{-'} (-1/6, 1/6, 1/6)$ $\bar{x} + 1/3, \bar{x} + 1/3, \bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2, 1/2, 1/2)'	(11) $3^{-'} (1/6, 1/6, -1/6)$ $\bar{x} + 2/3, \bar{x} + 1/3, \bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2, 1/2, 1/2)'	(12) $3^{-'} (1/6, -1/6, 1/6)$ $\bar{x} - 1/3, \bar{x} + 2/3, \bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2, 1/2, 1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

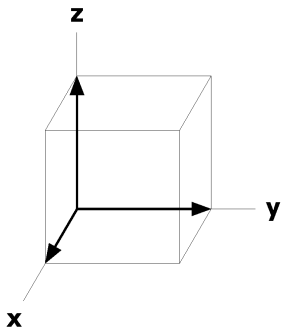
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates								
			(0,0,0) +	(1/2,1/2,1/2)' +							
24	f	1									
(1)	x, y, z	[u, v, w]	(2)	$\bar{x}, \bar{y}, z$	$[\bar{u}, \bar{v}, w]$	(3)	$\bar{x}, y, \bar{z}$	$[\bar{u}, v, \bar{w}]$	(4)	$x, \bar{y}, \bar{z}$	$[u, \bar{v}, \bar{w}]$
(5)	z, x, y	[w, u, v]	(6)	$z, \bar{x}, \bar{y}$	$[w, \bar{u}, \bar{v}]$	(7)	$\bar{z}, \bar{x}, y$	$[\bar{w}, \bar{u}, v]$	(8)	$\bar{z}, x, \bar{y}$	$[\bar{w}, u, \bar{v}]$
(9)	y, z, x	[v, w, u]	(10)	$\bar{y}, z, \bar{x}$	$[\bar{v}, w, \bar{u}]$	(11)	$y, \bar{z}, \bar{x}$	$[v, \bar{w}, \bar{u}]$	(12)	$\bar{y}, \bar{z}, x$	$[\bar{v}, \bar{w}, u]$
12	e	2..	x, 1/2, 0	[u, 0, 0]	$\bar{x}, 1/2, 0$	$[\bar{u}, 0, 0]$	0, x, 1/2	[0, u, 0]	1/2, 0, $\bar{x}$	[0, 0, $\bar{u}$ ]	
			0, $\bar{x}$ , 1/2	[0, $\bar{u}$ , 0]	1/2, 0, x	[0, 0, u]					
12	d	2..	x, 0, 0	[u, 0, 0]	$\bar{x}, 0, 0$	$[\bar{u}, 0, 0]$	0, x, 0	[0, u, 0]	0, 0, $\bar{x}$	[0, 0, $\bar{u}$ ]	
			0, $\bar{x}$ , 0	[0, $\bar{u}$ , 0]	0, 0, x	[0, 0, u]					
8	c	.3.	x, x, x	[u, u, u]	$\bar{x}, \bar{x}, x$	$[\bar{u}, \bar{u}, u]$	$\bar{x}, x, \bar{x}$	$[\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x}$	$[u, \bar{u}, \bar{u}]$	
6	b	222..	0, 1/2, 1/2	[0, 0, 0]	1/2, 0, 1/2	[0, 0, 0]	1/2, 1/2, 0	[0, 0, 0]			
2	a	23.	0, 0, 0	[0, 0, 0]							

**Symmetry of Special Projections**

Along [0,0,1]  $c_p$ -2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,1,1]  $p31'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

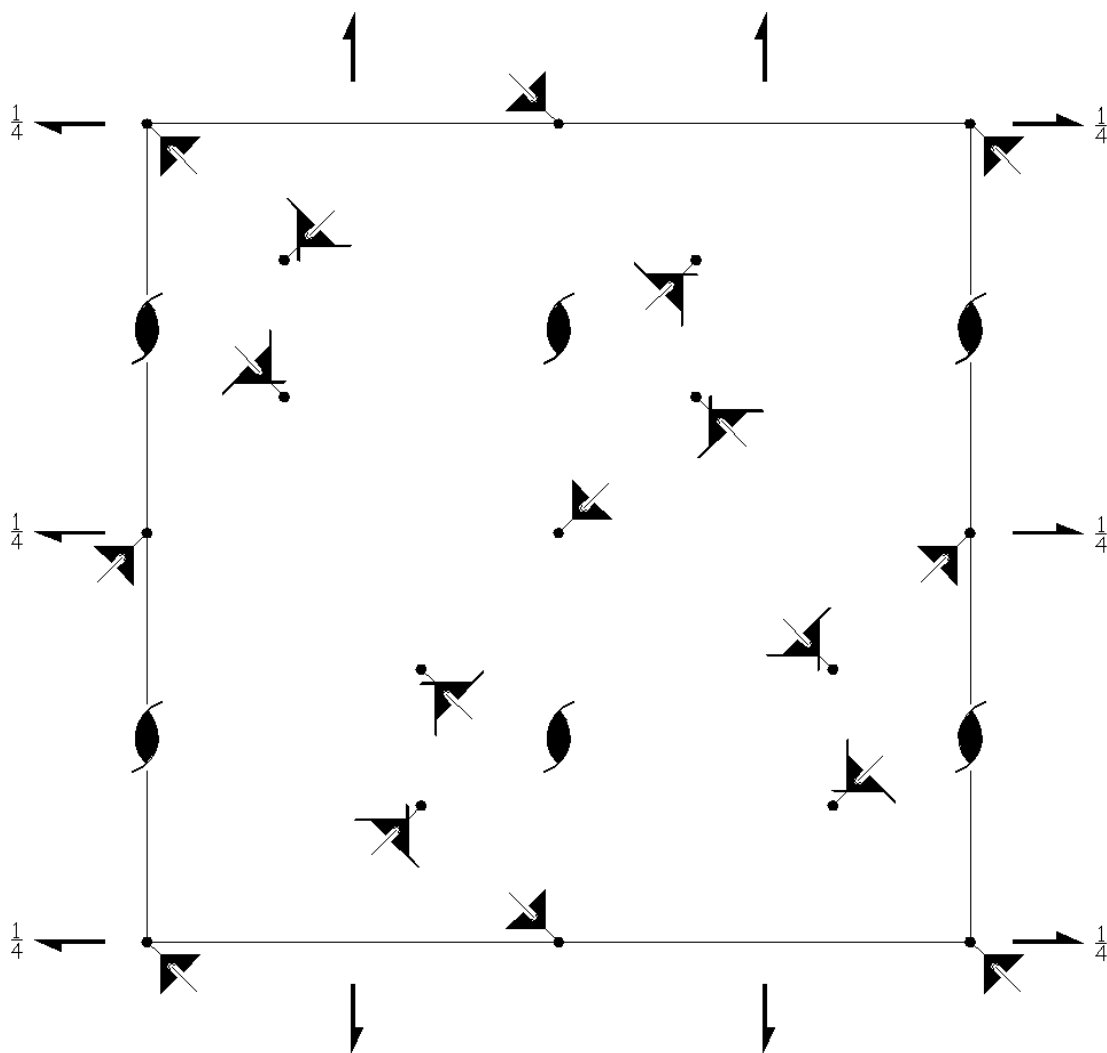
Along [1,1,0]  $p_{2b}$ -1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



P2<sub>1</sub>3  
198.1.1511

23  
P2<sub>1</sub>3

Cubic



**Origin** on 3 [1,1,1] at midpoint of three non-intersecting pairs of parallel 2<sub>1</sub> axes

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $-1/2 \leq z \leq 1/2$ ;  $\max(x-1/2, -y) \leq z \leq \min(x, y)$

Vertices 0,0,0      1/2,0,0      1/2,1/2,0      0,1/2,0      1/2,1/2,1/2      0,1/2,-1/2

### Symmetry Operations

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)  | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)  | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}+1/2, \bar{x}, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,1/2,0)      | (7) 3 <sup>+</sup> $x+1/2, \bar{x}-1/2, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,0,1/2)        | (8) 3 <sup>+</sup> $\bar{x}, \bar{x}+1/2, x$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,1/2,1/2)            |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> (-1/3, 1/3, 1/3)<br>$x+1/6, \bar{x}+1/6, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,1/2,1/2) | (11) 3 <sup>-</sup> (1/3, 1/3, -1/3)<br>$\bar{x}+1/3, \bar{x}+1/6, x$<br>(3 <sub><math>\bar{xyz}</math></sub>  1/2,1/2,0) | (12) 3 <sup>-</sup> (1/3, -1/3, 1/3)<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  1/2,0,1/2) |



**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

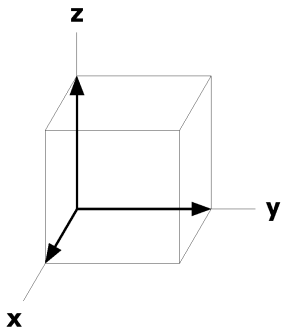
		Coordinates					
Multiplicity, Wyckoff letter, Site Symmetry.							
12	b 1						
(1)	x,y,z [u,v,w]	(2)	$\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3)	$\bar{x}, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4)	$x+1/2, \bar{y}+1/2, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]
(5)	z,x,y [w,u,v]	(6)	$z+1/2, \bar{x}+1/2, \bar{y}$ [ $w, \bar{u}, \bar{v}$ ]	(7)	$\bar{z}+1/2, \bar{x}, y+1/2$ [ $\bar{w}, \bar{u}, v$ ]	(8)	$\bar{z}, x+1/2, \bar{y}+1/2$ [ $\bar{w}, u, \bar{v}$ ]
(9)	y,z,x [v,w,u]	(10)	$\bar{y}, z+1/2, \bar{x}+1/2$ [ $\bar{v}, w, \bar{u}$ ]	(11)	$y+1/2, \bar{z}+1/2, \bar{x}$ [ $v, \bar{w}, \bar{u}$ ]	(12)	$\bar{y}+1/2, \bar{z}, x+1/2$ [ $\bar{v}, \bar{w}, u$ ]
4	a .3. x,x,x [u,u,u]	$\bar{x}+1/2, \bar{x}, x+1/2$ [ $\bar{u}, \bar{u}, u$ ]	$\bar{x}, x+1/2, \bar{x}+1/2$ [ $\bar{u}, u, \bar{u}$ ]	$x+1/2, \bar{x}+1/2, \bar{x}$ [ $u, \bar{u}, \bar{u}$ ]			

**Symmetry of Special Projections**

Along [0,0,1] p2g'g'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,1,1] p3  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

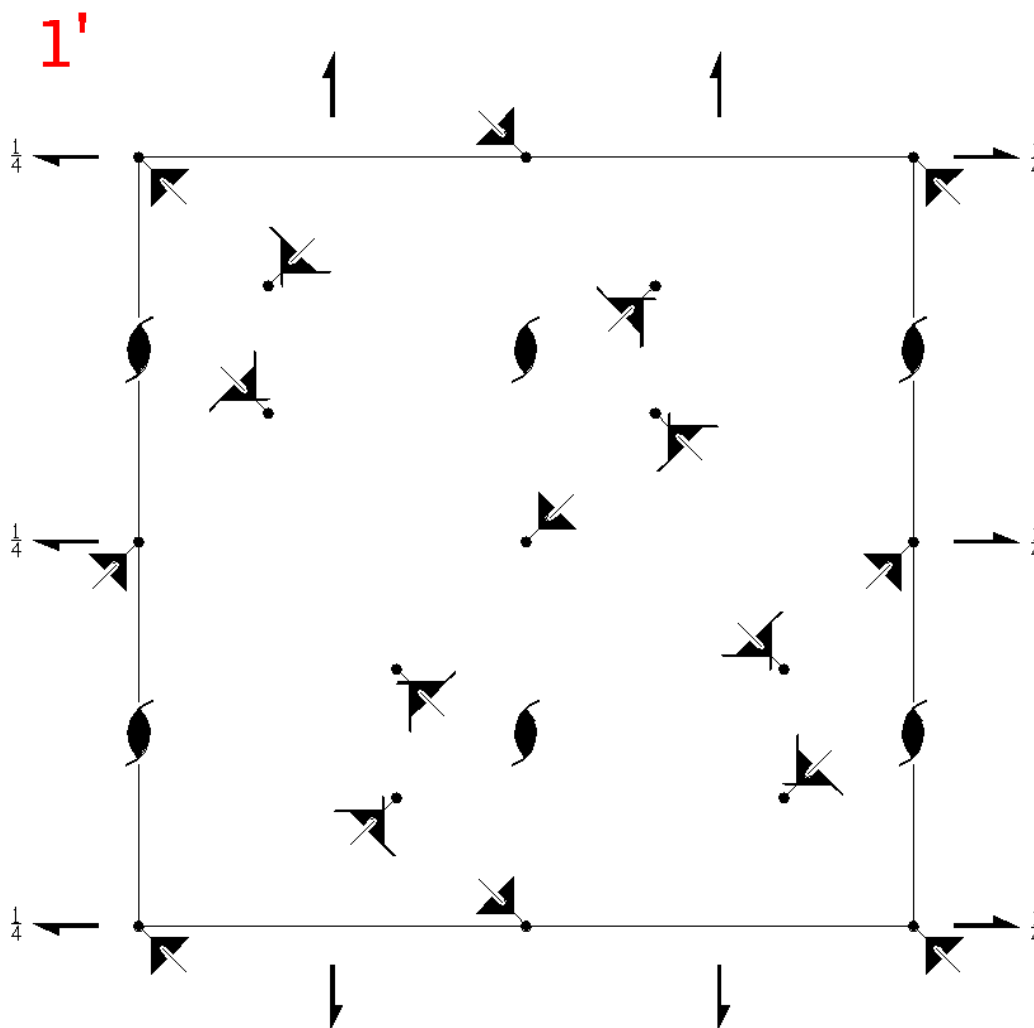
Along [1,1,0] p1g'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x+1/4,x,0



P2<sub>1</sub>31'  
198.2.1512

231'  
P2<sub>1</sub>31'

Cubic



**Origin** on 31' [1,1,1] at midpoint of three non-intersecting pairs of parallel 2<sub>1</sub> axes

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $-1/2 \leq z \leq 1/2$ ;  $\max(x-1/2, -y) \leq z \leq \min(x, y)$

**Vertices** 0,0,0      1/2,0,0      1/2,1/2,0      1/2,1/2,1/2      0,1/2,-1/2

**Symmetry Operations**

For 1 + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)  | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)  | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}+1/2, x, \bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  1/2,1/2,0)      | (7) 3 <sup>+</sup> $x+1/2, \bar{x}-1/2, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,0,1/2)        | (8) 3 <sup>+</sup> $\bar{x}, \bar{x}+1/2, x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,1/2,1/2)            |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> (-1/3, 1/3, 1/3)<br>$x+1/6, \bar{x}+1/6, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,1/2,1/2) | (11) 3 <sup>-</sup> (1/3, 1/3, -1/3)<br>$\bar{x}+1/3, \bar{x}+1/6, x$<br>(3 <sub><math>\bar{xyz}</math></sub>  1/2,1/2,0) | (12) 3 <sup>-</sup> (1/3, -1/3, 1/3)<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  1/2,0,1/2) |

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' (0,0,1/2) 1/4,0,z (2 <sub>z</sub>  1/2,0,1/2)'	(3) 2' (0,1/2,0) 0,y,1/4 (2 <sub>y</sub>  0,1/2,1/2)'	(4) 2' (1/2,0,0) x,1/4,0 (2 <sub>x</sub>  1/2,1/2,0)'
(5) 3 <sup>+</sup> ' x,x,x (3 <sub>xyz</sub>  0,0,0)'	(6) 3 <sup>+</sup> ' $\bar{x}+1/2, \bar{x}, \bar{x}$ (3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  1/2,1/2,0)'	(7) 3 <sup>+</sup> ' $x+1/2, \bar{x}-1/2, \bar{x}$ (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,0,1/2)'	(8) 3 <sup>+</sup> ' $\bar{x}, \bar{x}+1/2, \bar{x}$ (3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,1/2,1/2)'
(9) 3 <sup>-</sup> ' x,x,x (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)'	(10) 3 <sup>-</sup> ' (-1/3,1/3,1/3) x+1/6, $\bar{x}+1/6, \bar{x}$ (3 <sub>xyz</sub>  0,1/2,1/2)'	(11) 3 <sup>-</sup> ' (1/3,1/3,-1/3) x+1/3, $\bar{x}+1/6, \bar{x}$ (3 <sub><math>\bar{xy}\bar{z}</math></sub>  1/2,1/2,0)'	(12) 3 <sup>-</sup> ' (1/3,-1/3,1/3) x-1/6, $\bar{x}+1/3, \bar{x}$ (3 <sub><math>\bar{xy}\bar{z}</math></sub>  1/2,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

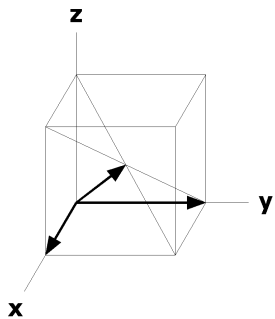
			Coordinates	
Multiplicity,	Wyckoff letter,	Site Symmetry.	1 +	1' +
12	b	11'		
(1) x,y,z [0,0,0]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [0,0,0]	(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [0,0,0]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [0,0,0]	
(5) z,x,y [0,0,0]	(6) $z+1/2, \bar{x}+1/2, \bar{y}$ [0,0,0]	(7) $\bar{z}+1/2, \bar{x}, y+1/2$ [0,0,0]	(8) $\bar{z}, x+1/2, \bar{y}+1/2$ [0,0,0]	
(9) y,z,x [0,0,0]	(10) $\bar{y}, z+1/2, \bar{x}+1/2$ [0,0,0]	(11) $y+1/2, \bar{z}+1/2, \bar{x}$ [0,0,0]	(12) $\bar{y}+1/2, \bar{z}, x+1/2$ [0,0,0]	
4	a	.3.1'	x,x,x [0,0,0]	$\bar{x}+1/2, \bar{x}, x+1/2$ [0,0,0] $\bar{x}, x+1/2, \bar{x}+1/2$ [0,0,0] $x+1/2, \bar{x}+1/2, \bar{x}$ [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p2gg1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,1,1] p31'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

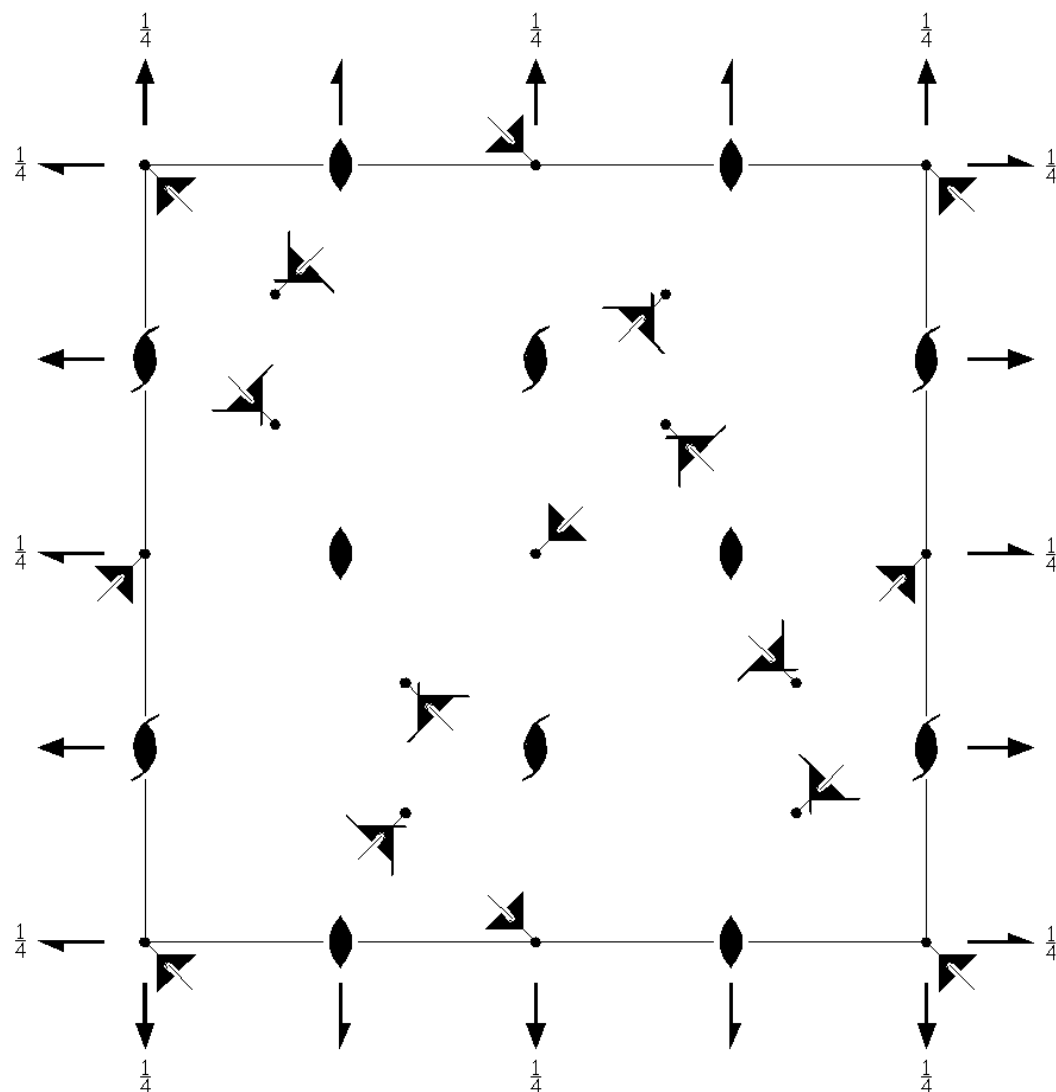
Along [1,1,0] p1g11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x+1/4,x,0



$I_{2,3}$   
199.1.1513

$23$   
 $I_{2,3}$

Cubic



**Origin** on  $3 [1,1,1]$  at midpoint of three non-intersecting pairs of parallel  $2_1$  axes and of three non-intersecting pairs of parallel  $2_1$  axes

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$ ;  $z \leq \min(x,y)$

Vertices 0,0,0       $1/2, 0, 0$        $1/2, 1/2, 0$        $0, 1/2, 0$        $1/2, 1/2, 1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>$(1   0,0,0)$                          | (2) 2 (0,0,1/2) $1/4, 0, z$<br>$(2_z   1/2, 0, 1/2)$  | (3) 2 (0,1/2,0) $0, y, 1/4$<br>$(2_y   0, 1/2, 1/2)$  | (4) 2 (1/2,0,0) $x, 1/4, 0$<br>$(2_x   1/2, 1/2, 0)$  |
| (5) $3^+$ $x, x, x$<br>$(3_{xyz}   0,0,0)$      | (6) $3^+$ $\bar{x} + 1/2, x, \bar{x}$<br>$(3_{x\bar{y}z}^{-1}   1/2, 1/2, 0)$                         | (7) $3^+$ $x + 1/2, \bar{x} - 1/2, \bar{x}$<br>$(3_{x\bar{y}z}^{-1}   1/2, 0, 1/2)$                   | (8) $3^+$ $\bar{x}, \bar{x} + 1/2, x$<br>$(3_{x\bar{y}z}^{-1}   0, 1/2, 1/2)$                         |
| (9) $3^-$ $x, x, x$<br>$(3_{xyz}^{-1}   0,0,0)$ | (10) $3^-$ $(-1/3, 1/3, 1/3)$<br>$x + 1/6, \bar{x} + 1/6, \bar{x}$<br>$(3_{x\bar{y}z}   0, 1/2, 1/2)$ | (11) $3^-$ $(1/3, 1/3, -1/3)$<br>$\bar{x} + 1/3, \bar{x} + 1/6, x$<br>$(3_{x\bar{y}z}   1/2, 1/2, 0)$ | (12) $3^-$ $(1/3, -1/3, 1/3)$<br>$\bar{x} - 1/6, x + 1/3, \bar{x}$<br>$(3_{x\bar{y}z}   1/2, 0, 1/2)$ |

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) 2 0,1/4,z (2 <sub>z</sub>   0,1/2,0)	(3) 2 1/4,y,0 (2 <sub>y</sub>   1/2,0,0)	(4) 2 x,0,1/4 (2 <sub>x</sub>   0,0,1/2)
(5) 3 <sup>+</sup> (1/2,1/2,1/2) x,x,x (3 <sub>xyz</sub>   1/2,1/2,1/2)	(6) 3 <sup>+</sup> (1/6,-1/6,1/6) $\bar{x}-1/6, \bar{x}+1/3, \bar{x}$ (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>   0,0,1/2)	(7) 3 <sup>+</sup> (-1/6,1/6,1/6) $\bar{x}+1/6, \bar{x}+1/6, \bar{x}$ (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>   0,1/2,0)	(8) 3 <sup>+</sup> (1/6,1/6,-1/6) $\bar{x}+1/3, \bar{x}+1/6, \bar{x}$ (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2,0,0)
(9) 3 <sup>-</sup> (1/2,1/2,1/2) x,x,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,1/2)	(10) 3 <sup>-</sup> (1/6,-1/6,-1/6) $\bar{x}+1/6, \bar{x}+1/6, \bar{x}$ (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2,0,0)	(11) 3 <sup>-</sup> (-1/6,-1/6,1/6) $\bar{x}+1/3, \bar{x}+1/6, \bar{x}$ (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>   0,0,1/2)	(12) 3 <sup>-</sup> (-1/6,1/6,-1/6) $\bar{x}-1/6, \bar{x}+1/3, \bar{x}$ (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>   0,1/2,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

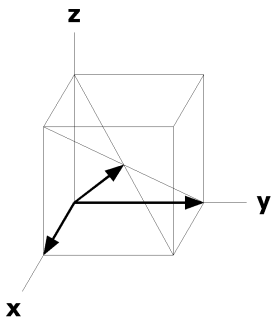
			Coordinates					
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) +	(1/2,1/2,1/2) +				
24	c	1						
(1)	x,y,z	[u,v,w]	(2) $\bar{x}+1/2, \bar{y}, \bar{z}+1/2$	$[\bar{u}, \bar{v}, \bar{w}]$	(3) $\bar{x}, \bar{y}+1/2, \bar{z}+1/2$	$[\bar{u}, \bar{v}, \bar{w}]$		
(4)	x+1/2, $\bar{y}+1/2, \bar{z}$	$[\bar{u}, \bar{v}, \bar{w}]$	(5)	z,x,y	[w,u,v]	(6) $\bar{z}+1/2, \bar{x}+1/2, \bar{y}$	$[\bar{w}, \bar{u}, \bar{v}]$	
(7)	$\bar{z}+1/2, \bar{x}, \bar{y}+1/2$	$[\bar{w}, \bar{u}, \bar{v}]$	(8)	$\bar{z}, \bar{x}+1/2, \bar{y}+1/2$	$[\bar{w}, \bar{u}, \bar{v}]$	(9)	y,z,x	[v,w,u]
(10)	$\bar{y}, \bar{z}+1/2, \bar{x}+1/2$	$[\bar{v}, \bar{w}, \bar{u}]$	(11)	$\bar{y}+1/2, \bar{z}+1/2, \bar{x}$	$[\bar{v}, \bar{w}, \bar{u}]$	(12)	$\bar{y}+1/2, \bar{z}, \bar{x}+1/2$	$[\bar{v}, \bar{w}, \bar{u}]$
12	b	2..	x,0,1/4	[u,0,0]	$\bar{x}+1/2, 0, 3/4$	$[\bar{u}, 0, 0]$	1/4,x,0	[0,u,0]
			3/4, $\bar{x}+1/2, 0$	$[0, \bar{u}, 0]$	0,1/4,x	[0,0,u]	0,3/4, $\bar{x}+1/2$	$[0, 0, \bar{u}]$
8	a	.3.	x,x,x	[u,u,u]	$\bar{x}+1/2, \bar{x}, \bar{x}+1/2$	$[\bar{u}, \bar{u}, \bar{u}]$	$\bar{x}, \bar{x}+1/2, \bar{x}+1/2$	$[\bar{u}, \bar{u}, \bar{u}]$
					x+1/2, $\bar{x}+1/2, \bar{x}$	$[u, \bar{u}, \bar{u}]$		

**Symmetry of Special Projections**

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,1,1] p3  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

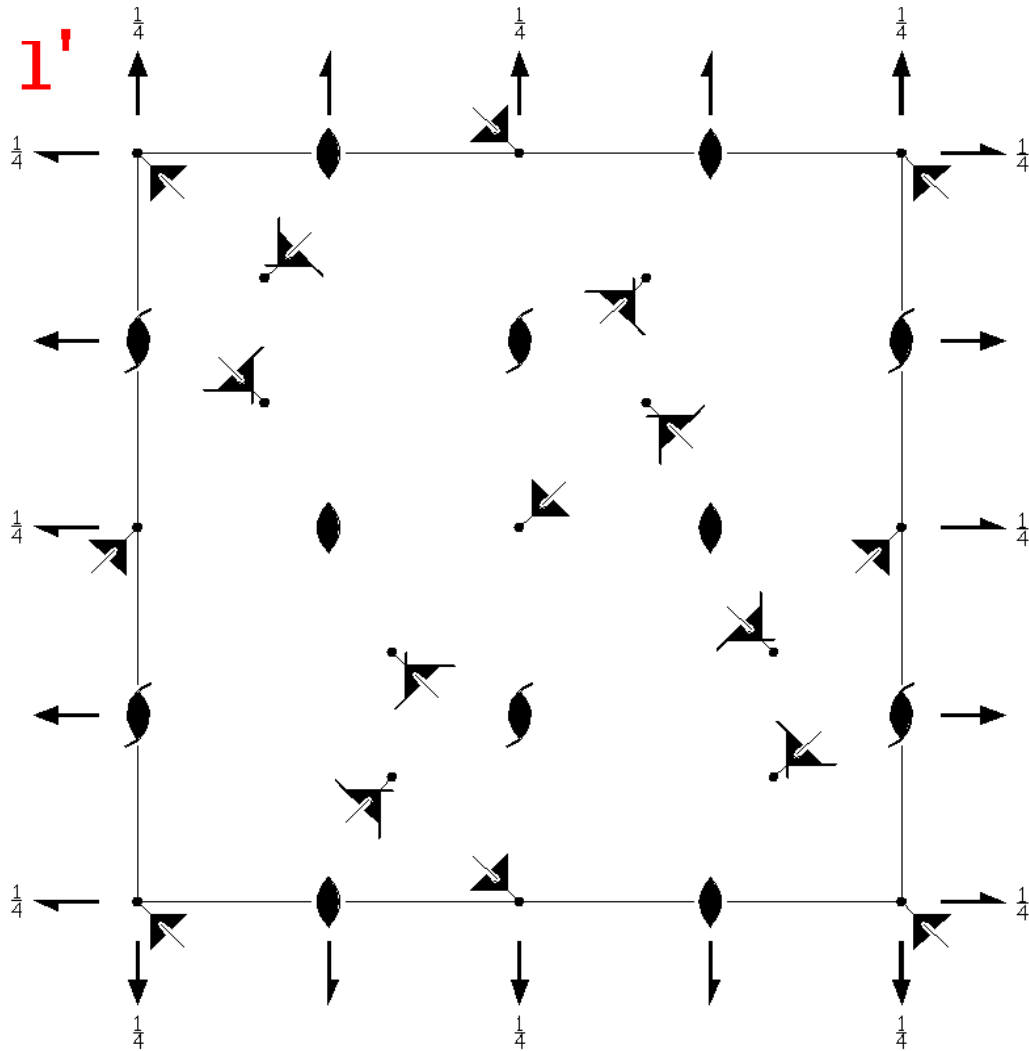
Along [1,1,0] p1m'1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x+1/4,0



$I2_131'$   
199.2.1514

$231'$   
 $I2_131'$

Cubic



**Origin** on  $31'$   $[1,1,1]$  at midpoint of three non-intersecting pairs of parallel  $2_1$  axes and of three non-intersecting pairs of parallel  $2_1$  axes

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $z \leq \min(x,y)$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $0,1/2,0$   $1/2,1/2,1/2$

### Symmetry Operations

For  $(0,0,0) + \text{set}$

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                           | (2) 2 $(0,0,1/2)$ $1/4,0,z$<br>( $2_z$   $1/2,0,1/2$ )  | (3) 2 $(0,1/2,0)$ $0,y,1/4$<br>( $2_y$   $0,1/2,1/2$ )                              | (4) 2 $(1/2,0,0)$ $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )  |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$   $0,0,0$ ) | (6) $3^+$ $\bar{x}+1/2,x,\bar{x}$<br>( $3_{\bar{xyz}}$   $1/2,1/2,0$ )                          | (7) $3^+$ $x+1/2,\bar{x}-1/2,\bar{x}$<br>( $3_{xyz}$   $1/2,0,1/2$ )                | (8) $3^+$ $\bar{x},\bar{x}+1/2,x$<br>( $3_{\bar{xyz}}$   $0,1/2,1/2$ )                          |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}$   $0,0,0$ ) | (10) $3^-$ $(-1/3,1/3,1/3)$<br>$x+1/6,\bar{x}+1/6,\bar{x}$<br>( $3_{\bar{xyz}}$   $0,1/2,1/2$ ) | (11) $3^-$ $(1/3,1/3,-1/3)$<br>$\bar{x}+1/3,x+1/6,x$<br>( $3_{xyz}$   $1/2,1/2,0$ ) | (12) $3^-$ $(1/3,-1/3,1/3)$<br>$\bar{x}-1/6,x+1/3,\bar{x}$<br>( $3_{\bar{xyz}}$   $1/2,0,1/2$ ) |

## For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) (1   1/2,1/2,1/2)	(2) 2 <sup>+</sup> 0,1/4,z (2 <sub>z</sub>   0,1/2,0)	(3) 2 <sup>+</sup> 1/4,y,0 (2 <sub>y</sub>   1/2,0,0)	(4) 2 <sup>+</sup> x,0,1/4 (2 <sub>x</sub>   0,0,1/2)
(5) 3 <sup>+</sup> (1/2,1/2,1/2) x,x,x (3 <sub>xyz</sub>   1/2,1/2,1/2)	(6) 3 <sup>+</sup> (1/6,-1/6,1/6) x-1/6,x+1/3,x (3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   0,0,1/2)	(7) 3 <sup>+</sup> (-1/6,1/6,1/6) x+1/6,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   0,1/2,0)	(8) 3 <sup>+</sup> (1/6,1/6,-1/6) x+1/3,x+1/6,x (3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2,0,0)
(9) 3 <sup>-</sup> (1/2,1/2,1/2) x,x,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,1/2)	(10) 3 <sup>-</sup> (1/6,-1/6,-1/6) x+1/6,x+1/6,x (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,0,0)	(11) 3 <sup>-</sup> (-1/6,-1/6,1/6) x+1/3,x+1/6,x (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   0,0,1/2)	(12) 3 <sup>-</sup> (-1/6,1/6,-1/6) x-1/6,x+1/3,x (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   0,1/2,0)

## For (0,0,0)' + set

(1) 1' (1   0,0,0)'	(2) 2' (0,0,1/2) 1/4,0,z (2 <sub>z</sub>   1/2,0,1/2)'	(3) 2' (0,1/2,0) 0,y,1/4 (2 <sub>y</sub>   0,1/2,1/2)'	(4) 2' (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)'
(5) 3 <sup>+</sup> ' x,x,x (3 <sub>xyz</sub>   0,0,0)'	(6) 3 <sup>+</sup> ' x+1/2,x,x (3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2,1/2,0)'	(7) 3 <sup>+</sup> ' x+1/2,x-1/2,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,0,1/2)'	(8) 3 <sup>+</sup> ' x,x+1/2,x (3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   0,1/2,1/2)'
(9) 3 <sup>-</sup> ' x,x,x (3 <sub>xyz</sub> <sup>-1</sup>   0,0,0)'	(10) 3 <sup>-</sup> ' (-1/3,1/3,1/3) x+1/6,x+1/6,x (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   0,1/2,1/2)'	(11) 3 <sup>-</sup> ' (1/3,1/3,-1/3) x+1/3,x+1/6,x (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,1/2,0)'	(12) 3 <sup>-</sup> ' (1/3,-1/3,1/3) x-1/6,x+1/3,x (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,0,1/2)'

## For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (1   1/2,1/2,1/2)'	(2) 2' 0,1/4,z (2 <sub>z</sub>   0,1/2,0)'	(3) 2' 1/4,y,0 (2 <sub>y</sub>   1/2,0,0)'	(4) 2' x,0,1/4 (2 <sub>x</sub>   0,0,1/2)'
(5) 3 <sup>+</sup> ' (1/2,1/2,1/2) x,x,x (3 <sub>xyz</sub>   1/2,1/2,1/2)'	(6) 3 <sup>+</sup> ' (1/6,-1/6,1/6) x-1/6,x+1/3,x (3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   0,0,1/2)'	(7) 3 <sup>+</sup> ' (-1/6,1/6,1/6) x+1/6,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   0,1/2,0)'	(8) 3 <sup>+</sup> ' (1/6,1/6,-1/6) x+1/3,x+1/6,x (3 <sub>x<math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>   1/2,0,0)'
(9) 3 <sup>-</sup> ' (1/2,1/2,1/2) x,x,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,1/2)'	(10) 3 <sup>-</sup> ' (1/6,-1/6,-1/6) x+1/6,x+1/6,x (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   1/2,0,0)'	(11) 3 <sup>-</sup> ' (-1/6,-1/6,1/6) x+1/3,x+1/6,x (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   0,0,1/2)'	(12) 3 <sup>-</sup> ' (-1/6,1/6,-1/6) x-1/6,x+1/3,x (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   0,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

24	c	11'	(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'
(1) x,y,z [0,0,0]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [0,0,0]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [0,0,0]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [0,0,0]	
(5) z,x,y [0,0,0]	(6) $z+1/2,\bar{x}+1/2,\bar{y}$ [0,0,0]	(7) $\bar{z}+1/2,\bar{x},y+1/2$ [0,0,0]	(8) $\bar{z},x+1/2,\bar{y}+1/2$ [0,0,0]	
(9) y,z,x [0,0,0]	(10) $\bar{y},z+1/2,\bar{x}+1/2$ [0,0,0]	(11) $y+1/2,\bar{z}+1/2,\bar{x}$ [0,0,0]	(12) $\bar{y}+1/2,\bar{z},x+1/2$ [0,0,0]	

Continued

199.2.1514

I2<sub>1</sub>3

12	b	2..1'	x,0,1/4 [0,0,0]	$\bar{x}+1/2,0,3/4$ [0,0,0]	1/4,x,0 [0,0,0]
			3/4, $\bar{x}+1/2,0$ [0,0,0]	0,1/4,x [0,0,0]	0,3/4, $\bar{x}+1/2$ [0,0,0]
8	a	.3.1'	x,x,x [0,0,0]	$\bar{x}+1/2,\bar{x},x+1/2$ [0,0,0]	$\bar{x},x+1/2,\bar{x}+1/2$ [0,0,0] $x+1/2,\bar{x}+1/2,\bar{x}$ [0,0,0]

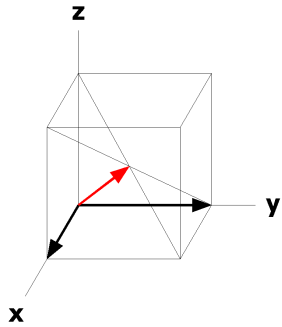
### Symmetry of Special Projections

Along [0,0,1]    c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$     $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,1,1]    p31'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$     $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

Along [1,1,0]    p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$     $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x+1/4,0

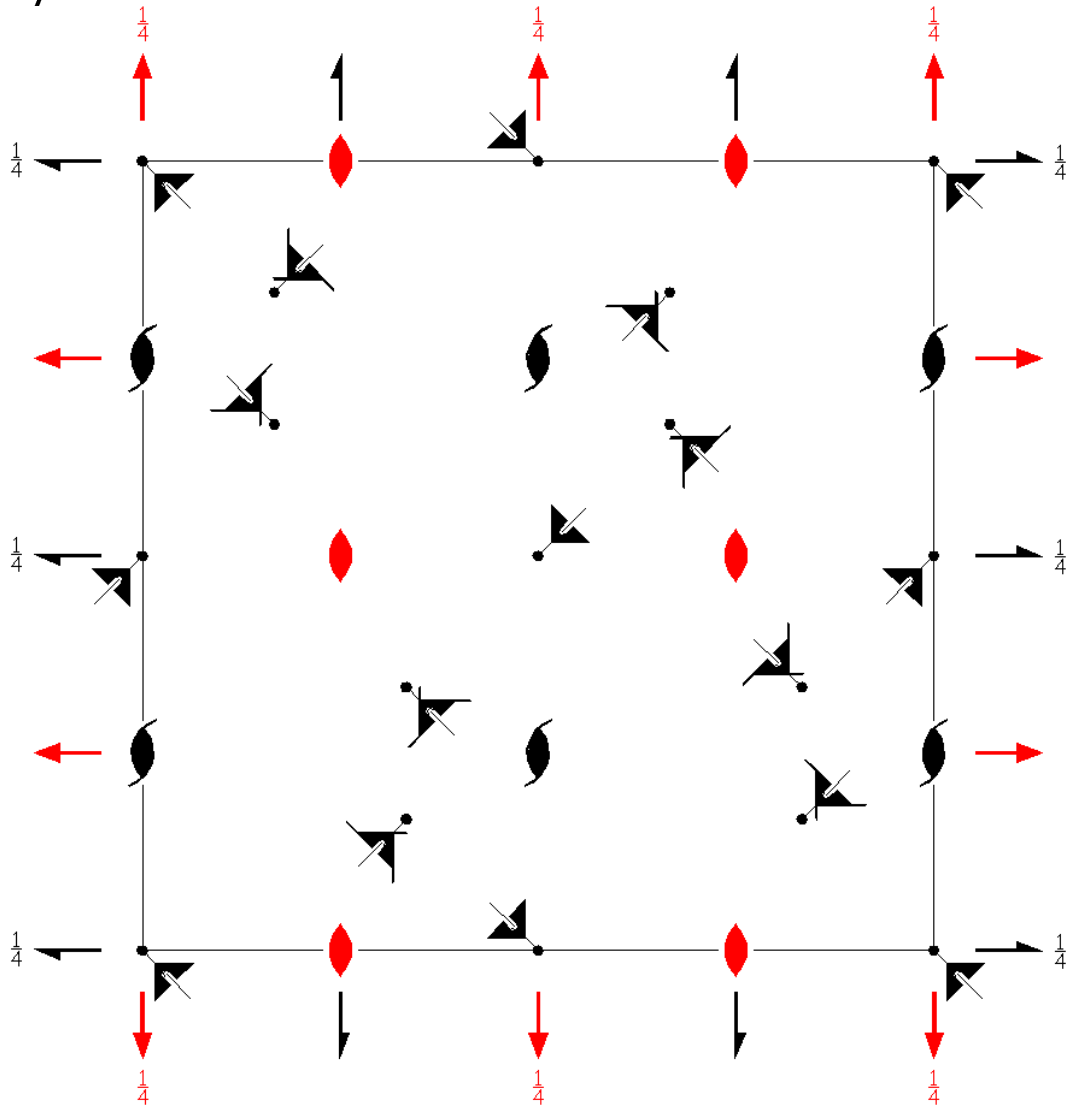




$I_{P2_13}$   
199.3.1515

$231'$   
 $I_{P2_13}$

Cubic



**Origin** on 3  $[1,1,1]$  at midpoint of three non-intersecting pairs of parallel 2 axes and of three non-intersecting pairs of parallel  $2_1$  axes

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $z \leq \min(x,y)$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $0,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                                | (2) 2 $(0,0,1/2)$ $1/4,0,z$<br>( $2_z$   $1/2,0,1/2$ )  | (3) 2 $(0,1/2,0)$ $0,y,1/4$<br>( $2_y$   $0,1/2,1/2$ )                                    | (4) 2 $(1/2,0,0)$ $x,1/4,0$<br>( $2_x$   $1/2,1/2,0$ )  |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$   $0,0,0$ )      | (6) $3^+$ $\bar{x}+1/2,x,\bar{x}$<br>( $3_{\bar{xy}z^{-1}}$   $1/2,1/2,0$ )                     | (7) $3^+$ $x+1/2,\bar{x}-1/2,\bar{x}$<br>( $3_{\bar{xyz}^{-1}}$   $1/2,0,1/2$ )           | (8) $3^+$ $\bar{x},\bar{x}+1/2,x$<br>( $3_{\bar{xy}z^{-1}}$   $0,1/2,1/2$ )                     |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz^{-1}}$   $0,0,0$ ) | (10) $3^-$ $(-1/3,1/3,1/3)$<br>$x+1/6,\bar{x}+1/6,\bar{x}$<br>( $3_{\bar{xyz}}$   $0,1/2,1/2$ ) | (11) $3^-$ $(1/3,1/3,-1/3)$<br>$\bar{x}+1/3,\bar{x}+1/6,x$<br>( $3_{xyz}$   $1/2,1/2,0$ ) | (12) $3^-$ $(1/3,-1/3,1/3)$<br>$\bar{x}-1/6,x+1/3,\bar{x}$<br>( $3_{\bar{xyz}}$   $1/2,0,1/2$ ) |

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (1   1/2,1/2,1/2)'	(2) 2' 0,1/4,z (2 <sub>z</sub>   0,1/2,0)'	(3) 2' 1/4,y,0 (2 <sub>y</sub>   1/2,0,0)'	(4) 2' x,0,1/4 (2 <sub>x</sub>   0,0,1/2)'
(5) 3 <sup>+</sup> (1/2,1/2,1/2) x,x,x (3 <sub>xyz</sub>   1/2,1/2,1/2)'	(6) 3 <sup>+</sup> (1/6,-1/6,1/6) x-1/6,x+1/3,x (3 <sub>xyz</sub> <sup>-1</sup>   0,0,1/2)'	(7) 3 <sup>+</sup> (-1/6,1/6,1/6) x+1/6,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   0,1/2,0)'	(8) 3 <sup>+</sup> (1/6,1/6,-1/6) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,0,0)'
(9) 3 <sup>-</sup> (1/2,1/2,1/2) x,x,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,1/2)'	(10) 3 <sup>-</sup> (1/6,-1/6,-1/6) x+1/6,x+1/6,x (3 <sub>xyz</sub>   1/2,0,0)'	(11) 3 <sup>-</sup> (-1/6,-1/6,1/6) x+1/3,x+1/6,x (3 <sub>xyz</sub>   0,0,1/2)'	(12) 3 <sup>-</sup> (-1/6,1/6,-1/6) x-1/6,x+1/3,x (3 <sub>xyz</sub>   0,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

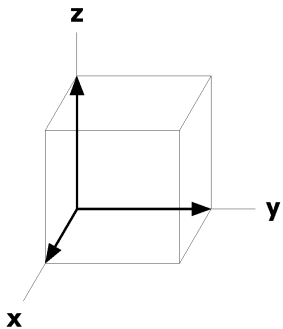
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates								
			(0,0,0) +	(1/2,1/2,1/2)' +							
24	c	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}+1/2, \bar{y}, z+1/2$	$[\bar{u}, \bar{v}, w]$	(3)	$\bar{x}, y+1/2, \bar{z}+1/2$	$[\bar{u}, v, \bar{w}]$	(4)	$x+1/2, \bar{y}+1/2, \bar{z}$	$[u, \bar{v}, \bar{w}]$
(5)	z,x,y	[w,u,v]	(6)	$z+1/2, \bar{x}+1/2, \bar{y}$	$[w, \bar{u}, \bar{v}]$	(7)	$\bar{z}+1/2, \bar{x}, y+1/2$	$[\bar{w}, \bar{u}, v]$	(8)	$\bar{z}, x+1/2, \bar{y}+1/2$	$[\bar{w}, u, \bar{v}]$
(9)	y,z,x	[v,w,u]	(10)	$\bar{y}, z+1/2, \bar{x}+1/2$	$[\bar{v}, w, \bar{u}]$	(11)	$y+1/2, \bar{z}+1/2, \bar{x}$	$[v, \bar{w}, \bar{u}]$	(12)	$\bar{y}+1/2, \bar{z}, x+1/2$	$[\bar{v}, \bar{w}, u]$
12	b	2'..	x,0,1/4	$[0, v, w]$	$\bar{x}+1/2, 0, 3/4$	$[0, \bar{v}, w]$	1/4,x,0	$[w, 0, v]$			
			3/4, $\bar{x}+1/2, 0$	$[w, 0, \bar{v}]$	0,1/4,x	$[v, w, 0]$	0,3/4, $\bar{x}+1/2$	$[\bar{v}, w, 0]$			
8	a	.3.	x,x,x	$[u, u, u]$	$\bar{x}+1/2, \bar{x}, x+1/2$	$[\bar{u}, \bar{u}, u]$	$\bar{x}, x+1/2, \bar{x}+1/2$	$[\bar{u}, u, \bar{u}]$	$x+1/2, \bar{x}+1/2, \bar{x}$	$[u, \bar{u}, \bar{u}]$	

**Symmetry of Special Projections**

Along [0,0,1] c<sub>p</sub>-2mm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,1,1] p31'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

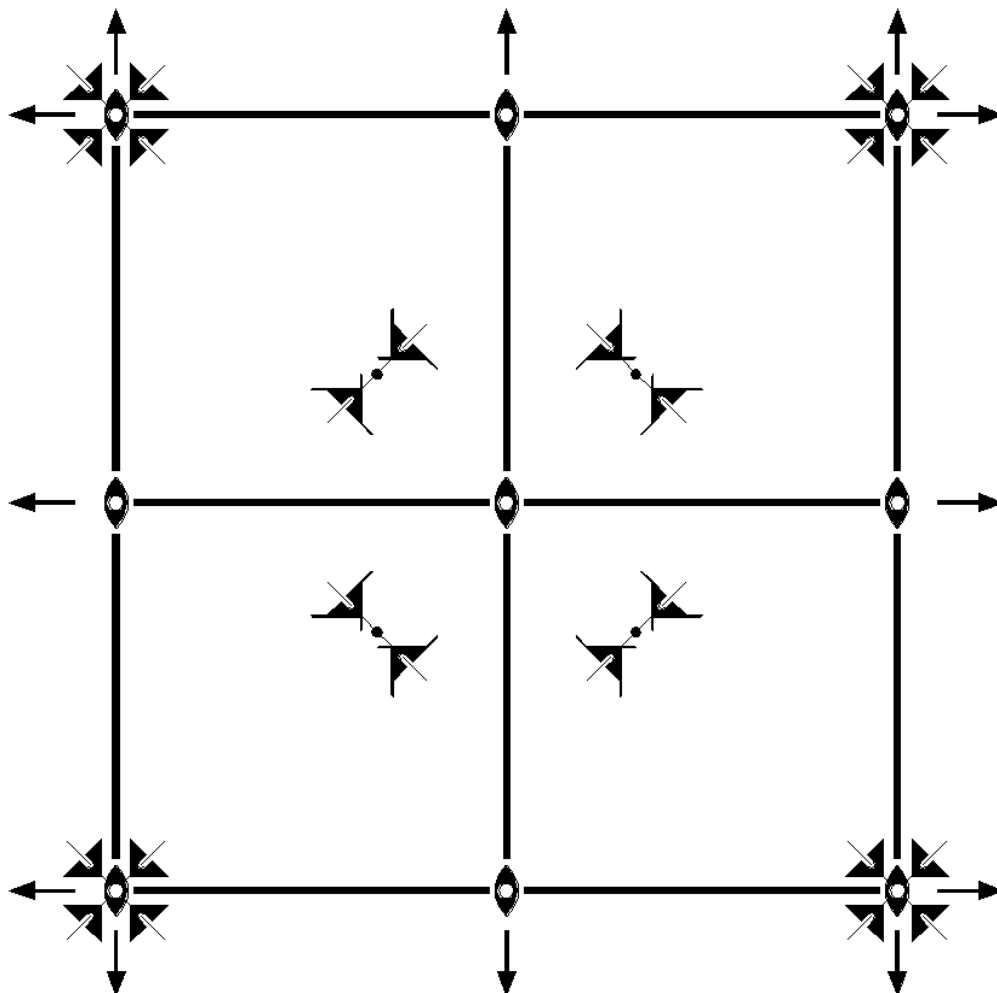
Along [1,1,0] p<sub>2b</sub>-1m1  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x+1/4,0



$Pm\bar{3}$   
200.1.1516

$m\bar{3}$   
 $P2/m\bar{3}$

Cubic



Origin at center ( $m\bar{3}$ )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $z \leq \min(x,y)$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $0,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)     | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0) | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0)              |

200.1.1516

$Pm\bar{3}$

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(14) m x,y,0 ( $m_z$  0,0,0)	(15) m x,0,z ( $m_y$  0,0,0)	(16) m 0,y,z ( $m_x$  0,0,0)
(17) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)	(18) $\bar{3}^+$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}^{-1}$  0,0,0)	(19) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}^{-1}$  0,0,0)	(20) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}^{-1}$  0,0,0)
(21) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}^{-1}$  0,0,0)	(22) $\bar{3}^-$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)	(23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)	(24) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

**Positions**

			Coordinates			
Multiplicity,	Wyckoff letter,	Site Symmetry.				
24	l	1	(1) x,y,z [u,v,w]	(2) $\bar{x}$ , $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w]	(3) $\bar{x}$ ,y, $\bar{z}$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x, $\bar{y}$ , $\bar{z}$ [u, $\bar{v}$ , $\bar{w}$ ]
			(5) z,x,y [w,u,v]	(6) z, $\bar{x}$ , $\bar{y}$ [ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ]	(7) $\bar{z}$ , $\bar{x}$ ,y [ $\bar{w}$ , $\bar{u}$ ,v]	(8) $\bar{z}$ ,x, $\bar{y}$ [ $\bar{w}$ ,u, $\bar{v}$ ]
			(9) y,z,x [v,w,u]	(10) $\bar{y}$ ,z, $\bar{x}$ [ $\bar{v}$ ,w, $\bar{u}$ ]	(11) y, $\bar{z}$ , $\bar{x}$ [v, $\bar{w}$ , $\bar{u}$ ]	(12) $\bar{y}$ , $\bar{z}$ ,x [ $\bar{v}$ , $\bar{w}$ ,u]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(14) x,y, $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ ,w]	(15) x, $\bar{y}$ ,z [ $\bar{u}$ ,v, $\bar{w}$ ]	(16) $\bar{x}$ ,y,z [u, $\bar{v}$ , $\bar{w}$ ]
			(17) $\bar{z}$ , $\bar{x}$ , $\bar{y}$ [w,u,v]	(18) $\bar{z}$ ,x,y [w, $\bar{u}$ , $\bar{v}$ ]	(19) z,x, $\bar{y}$ [ $\bar{w}$ , $\bar{u}$ ,v]	(20) z, $\bar{x}$ ,y [ $\bar{w}$ ,u, $\bar{v}$ ]
			(21) $\bar{y}$ , $\bar{z}$ , $\bar{x}$ [v,w,u]	(22) y, $\bar{z}$ ,x [ $\bar{v}$ ,w, $\bar{u}$ ]	(23) $\bar{y}$ ,z,x [v, $\bar{w}$ , $\bar{u}$ ]	(24) y,z, $\bar{x}$ [ $\bar{v}$ , $\bar{w}$ ,u]
12	k	m..	1/2,y,z [u,0,0]	1/2, $\bar{y}$ ,z [ $\bar{u}$ ,0,0]	1/2,y, $\bar{z}$ [ $\bar{u}$ ,0,0]	
			1/2, $\bar{y}$ , $\bar{z}$ [u,0,0]	z,1/2,y [0,u,0]	z,1/2, $\bar{y}$ [0, $\bar{u}$ ,0]	
			$\bar{z}$ ,1/2,y [0, $\bar{u}$ ,0]	$\bar{z}$ ,1/2, $\bar{y}$ [0,u,0]	y,z,1/2 [0,0,u]	
			$\bar{y}$ ,z,1/2 [0,0, $\bar{u}$ ]	y, $\bar{z}$ ,1/2 [0,0, $\bar{u}$ ]	$\bar{y}$ , $\bar{z}$ ,1/2 [0,0,u]	
12	j	m..	0,y,z [u,0,0]	0, $\bar{y}$ ,z [ $\bar{u}$ ,0,0]	0,y, $\bar{z}$ [ $\bar{u}$ ,0,0]	
			0, $\bar{y}$ , $\bar{z}$ [u,0,0]	z,0,y [0,u,0]	z,0, $\bar{y}$ [0, $\bar{u}$ ,0]	
			$\bar{z}$ ,0,y [0, $\bar{u}$ ,0]	$\bar{z}$ ,0, $\bar{y}$ [0,u,0]	y,z,0 [0,0,u]	
			$\bar{y}$ ,z,0 [0,0, $\bar{u}$ ]	y, $\bar{z}$ ,0 [0,0, $\bar{u}$ ]	$\bar{y}$ , $\bar{z}$ ,0 [0,0,u]	
8	i	.3.	x,x,x [u,u,u]	$\bar{x}$ , $\bar{x}$ ,x [ $\bar{u}$ , $\bar{u}$ ,u]	$\bar{x}$ ,x, $\bar{x}$ [ $\bar{u}$ ,u, $\bar{u}$ ]	x, $\bar{x}$ , $\bar{x}$ [u, $\bar{u}$ , $\bar{u}$ ]
			$\bar{x}$ , $\bar{x}$ , $\bar{x}$ [u,u,u]	x,x, $\bar{x}$ [ $\bar{u}$ , $\bar{u}$ ,u]	x, $\bar{x}$ ,x [ $\bar{u}$ ,u, $\bar{u}$ ]	$\bar{x}$ ,x,x [u, $\bar{u}$ , $\bar{u}$ ]
6	h	mm2..	x,1/2,1/2 [0,0,0]	$\bar{x}$ ,1/2,1/2 [0,0,0]	1/2,x,1/2 [0,0,0]	
			1/2, $\bar{x}$ ,1/2 [0,0,0]	1/2,1/2,x [0,0,0]	1/2,1/2, $\bar{x}$ [0,0,0]	

Continued

200.1.1516

Pm $\bar{3}$

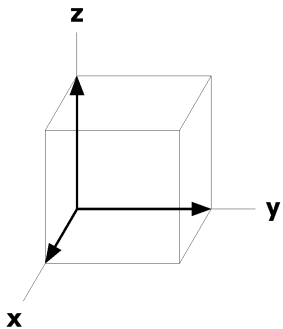
6	g	mm2..	$x, 1/2, 0 [0,0,0]$	$\bar{x}, 1/2, 0 [0,0,0]$	$0, x, 1/2 [0,0,0]$
			$0, \bar{x}, 1/2 [0,0,0]$	$1/2, 0, x [0,0,0]$	$1/2, 0, \bar{x} [0,0,0]$
6	f	mm2..	$x, 0, 1/2 [0,0,0]$	$\bar{x}, 0, 1/2 [0,0,0]$	$1/2, x, 0 [0,0,0]$
			$1/2, \bar{x}, 0 [0,0,0]$	$0, 1/2, x [0,0,0]$	$0, 1/2, \bar{x} [0,0,0]$
6	e	mm2..	$x, 0, 0 [0,0,0]$	$\bar{x}, 0, 0 [0,0,0]$	$0, x, 0 [0,0,0]$
			$0, \bar{x}, 0 [0,0,0]$	$0, 0, x [0,0,0]$	$0, 0, \bar{x} [0,0,0]$
3	d	mmm..	$1/2, 0, 0 [0,0,0]$	$0, 1/2, 0 [0,0,0]$	$0, 0, 1/2 [0,0,0]$
3	c	mmm..	$0, 1/2, 1/2 [0,0,0]$	$1/2, 0, 1/2 [0,0,0]$	$1/2, 1/2, 0 [0,0,0]$
1	b	$m\bar{3}$ .	$1/2, 1/2, 1/2 [0,0,0]$		
1	a	$m\bar{3}$ .	$0, 0, 0 [0,0,0]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p6'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x,x,x$

Along  $[1,1,0]$   $p2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,0$



$Pm\bar{3}1'$

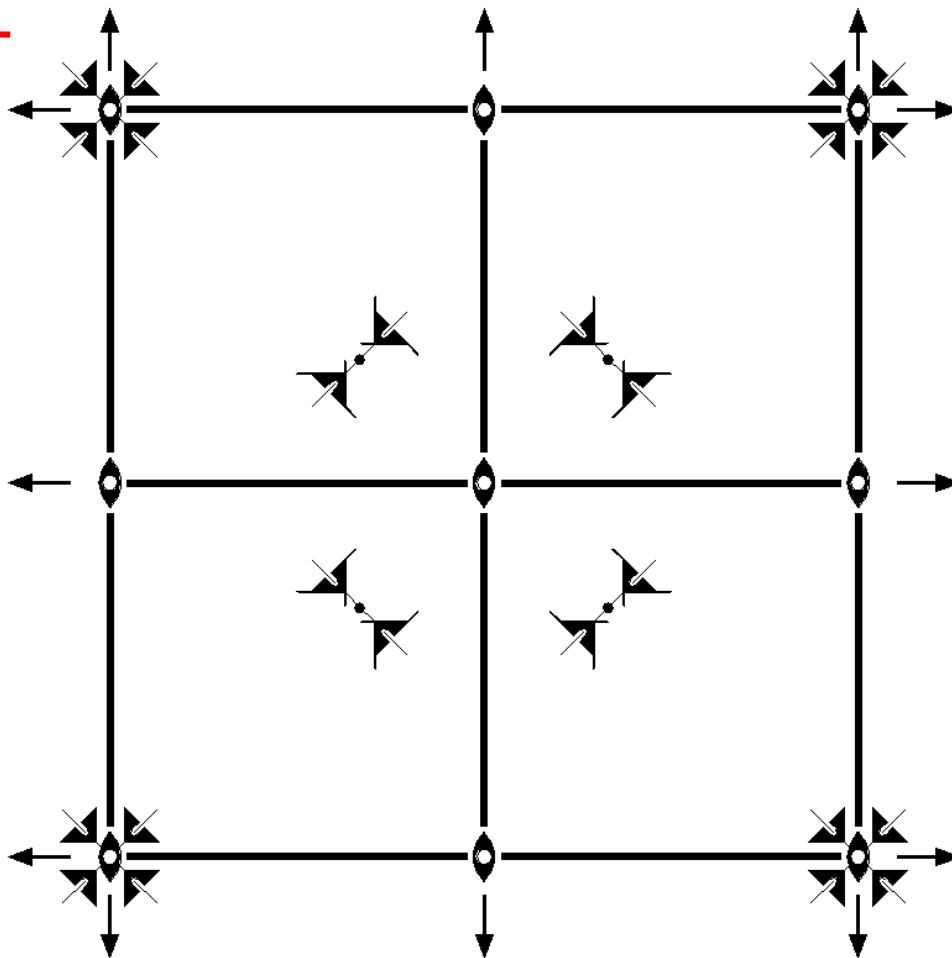
200.2.1517

$m\bar{3}1'$

$P2/m\bar{3}1'$

Cubic

1'



Origin at center ( $m\bar{3}1'$ )

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad z \leq \min(x,y)$

Vertices  $0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 0,1/2,0 \quad 1/2,1/2,1/2$

Symmetry Operations

For 1 + set

- |   |  |   |   |
|---|--|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                 | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                            | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                  |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)  | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}y\bar{z}}$  0,0,0)  |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)      | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}yz}$  0,0,0) | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{\bar{x}y\bar{z}}$  0,0,0) |

Continued

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$Pm\bar{3}1'$

- |   |  |   |  |
|---|--|---|--|
| (13) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)                     | (14) m x,y,0<br>( $m_z$  0,0,0)  | (15) m x,0,z<br>( $m_y$  0,0,0)   | (16) m 0,y,z<br>( $m_x$  0,0,0)  |
| (17) $\bar{3}^+$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$  0,0,0)      | (18) $\bar{3}^+$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,0,0) | (19) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,0,0) | (20) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,0,0) |
| (21) $\bar{3}^-$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}^{-1}$  0,0,0) | (22) $\bar{3}^-$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)     | (23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)       | (24) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)      |

For 1' + set

- |   |  |   |  |
|---|--|---|--|
| (1) 1'<br>(1 0,0,0)'  | (2) 2' 0,0,z<br>( $2_z$  0,0,0)'   | (3) 2' 0,y,0<br>( $2_y$  0,0,0)'  | (4) 2' x,0,0<br>( $2_x$  0,0,0)'   |
| (5) $3^{+'}$ x,x,x<br>( $3_{xyz}$  0,0,0)'                          | (6) $3^{+'}$ $\bar{x}$ ,x, $\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  0,0,0)'                      | (7) $3^{+'}$ x, $\bar{x}$ , $\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  0,0,0)'                      | (8) $3^{+'}$ $\bar{x}$ , $\bar{x}$ ,x<br>( $3_{x\bar{y}z}^{-1}$  0,0,0)'                     |
| (9) $3^{-'}$ x,x,x<br>( $3_{xyz}^{-1}$  0,0,0)'                     | (10) $3^{-'}$ x, $\bar{x}$ , $\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)'                         | (11) $3^{-'}$ $\bar{x}$ , $\bar{x}$ ,x<br>( $3_{x\bar{y}z}$  0,0,0)'                          | (12) $3^{-'}$ $\bar{x}$ ,x, $\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)'                          |
| (13) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)'                       | (14) m' x,y,0<br>( $m_z$  0,0,0)'  | (15) m' x,0,z<br>( $m_y$  0,0,0)'   | (16) m' 0,y,z<br>( $m_x$  0,0,0)'  |
| (17) $\bar{3}^{+'}$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$  0,0,0)'      | (18) $\bar{3}^{+'}$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,0,0)' | (19) $\bar{3}^{+'}$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,0,0)' | (20) $\bar{3}^{+'}$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,0,0)' |
| (21) $\bar{3}^{-'}$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}^{-1}$  0,0,0)' | (22) $\bar{3}^{-'}$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)'     | (23) $\bar{3}^{-'}$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)'       | (24) $\bar{3}^{-'}$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)'      |

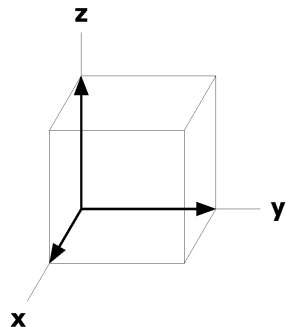
**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); 1'.

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

- |  |                                      |                                       |                                       |      |
|--|--------------------------------------|---------------------------------------|---------------------------------------|------|
| 24   | 1                                    | 11'                                   | 1 +                                   | 1' + |
| (1) x,y,z [0,0,0]                              | (2) $\bar{x}$ , $\bar{y}$ ,z [0,0,0] | (3) $\bar{x}$ ,y, $\bar{z}$ [0,0,0]   | (4) x, $\bar{y}$ , $\bar{z}$ [0,0,0]  |      |
| (5) z,x,y [0,0,0]                              | (6) z, $\bar{x}$ , $\bar{y}$ [0,0,0] | (7) $\bar{z}$ , $\bar{x}$ ,y [0,0,0]  | (8) $\bar{z}$ ,x, $\bar{y}$ [0,0,0]   |      |
| (9) y,z,x [0,0,0]                              | (10) $\bar{y}$ ,z, $\bar{x}$ [0,0,0] | (11) y, $\bar{z}$ , $\bar{x}$ [0,0,0] | (12) $\bar{y}$ , $\bar{z}$ ,x [0,0,0] |      |
| (13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [0,0,0] | (14) x,y, $\bar{z}$ [0,0,0]          | (15) x, $\bar{y}$ ,z [0,0,0]          | (16) $\bar{x}$ ,y,z [0,0,0]           |      |
| (17) $\bar{z}$ , $\bar{x}$ , $\bar{y}$ [0,0,0] | (18) $\bar{z}$ ,x,y [0,0,0]          | (19) z,x, $\bar{y}$ [0,0,0]           | (20) z, $\bar{x}$ ,y [0,0,0]          |      |
| (21) $\bar{y}$ , $\bar{z}$ , $\bar{x}$ [0,0,0] | (22) y, $\bar{z}$ ,x [0,0,0]         | (23) $\bar{y}$ ,z,x [0,0,0]           | (24) y,z, $\bar{x}$ [0,0,0]           |      |



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$Pm\bar{3}1'$

			$1/2, y, z$ [0,0,0]	$1/2, \bar{y}, z$ [0,0,0]	$1/2, y, \bar{z}$ [0,0,0]
			$1/2, \bar{y}, \bar{z}$ [0,0,0]	$z, 1/2, y$ [0,0,0]	$z, 1/2, \bar{y}$ [0,0,0]
			$\bar{z}, 1/2, y$ [0,0,0]	$\bar{z}, 1/2, \bar{y}$ [0,0,0]	$y, z, 1/2$ [0,0,0]
			$\bar{y}, z, 1/2$ [0,0,0]	$y, \bar{z}, 1/2$ [0,0,0]	$\bar{y}, \bar{z}, 1/2$ [0,0,0]
12	j	$m..1'$	$0, y, z$ [0,0,0]	$0, \bar{y}, z$ [0,0,0]	$0, y, \bar{z}$ [0,0,0]
			$0, \bar{y}, \bar{z}$ [0,0,0]	$z, 0, y$ [0,0,0]	$z, 0, \bar{y}$ [0,0,0]
			$\bar{z}, 0, y$ [0,0,0]	$\bar{z}, 0, \bar{y}$ [0,0,0]	$y, z, 0$ [0,0,0]
			$\bar{y}, z, 0$ [0,0,0]	$y, \bar{z}, 0$ [0,0,0]	$\bar{y}, \bar{z}, 0$ [0,0,0]
8	i	$.3.1'$	$x, x, x$ [0,0,0]	$\bar{x}, \bar{x}, x$ [0,0,0]	$\bar{x}, x, \bar{x}$ [0,0,0]
			$\bar{x}, \bar{x}, \bar{x}$ [0,0,0]	$x, x, \bar{x}$ [0,0,0]	$x, \bar{x}, x$ [0,0,0]
6	h	$mm2..1'$	$x, 1/2, 1/2$ [0,0,0]	$\bar{x}, 1/2, 1/2$ [0,0,0]	$1/2, x, 1/2$ [0,0,0]
			$1/2, \bar{x}, 1/2$ [0,0,0]	$1/2, 1/2, x$ [0,0,0]	$1/2, 1/2, \bar{x}$ [0,0,0]
6	g	$mm2..1'$	$x, 1/2, 0$ [0,0,0]	$\bar{x}, 1/2, 0$ [0,0,0]	$0, x, 1/2$ [0,0,0]
			$0, \bar{x}, 1/2$ [0,0,0]	$1/2, 0, x$ [0,0,0]	$1/2, 0, \bar{x}$ [0,0,0]
6	f	$mm2..1'$	$x, 0, 1/2$ [0,0,0]	$\bar{x}, 0, 1/2$ [0,0,0]	$1/2, x, 0$ [0,0,0]
			$1/2, \bar{x}, 0$ [0,0,0]	$0, 1/2, x$ [0,0,0]	$0, 1/2, \bar{x}$ [0,0,0]
6	e	$mm2..1'$	$x, 0, 0$ [0,0,0]	$\bar{x}, 0, 0$ [0,0,0]	$0, x, 0$ [0,0,0]
			$0, \bar{x}, 0$ [0,0,0]	$0, 0, x$ [0,0,0]	$0, 0, \bar{x}$ [0,0,0]
3	d	$mmm..1'$	$1/2, 0, 0$ [0,0,0]	$0, 1/2, 0$ [0,0,0]	$0, 0, 1/2$ [0,0,0]
3	c	$mmm..1'$	$0, 1/2, 1/2$ [0,0,0]	$1/2, 0, 1/2$ [0,0,0]	$1/2, 1/2, 0$ [0,0,0]
1	b	$m\bar{3}.1'$	$1/2, 1/2, 1/2$ [0,0,0]		
1	a	$m\bar{3}.1'$	$0, 0, 0$ [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1]  $p2mm1'$   
 $a^* = a$   $b^* = b$   
 Origin at 0,0,z

Along [1,1,1]  $p61'$   
 $a^* = (2a - b - c)/3$   $b^* = (-a + 2b - c)/3$   
 Origin at x,x,x

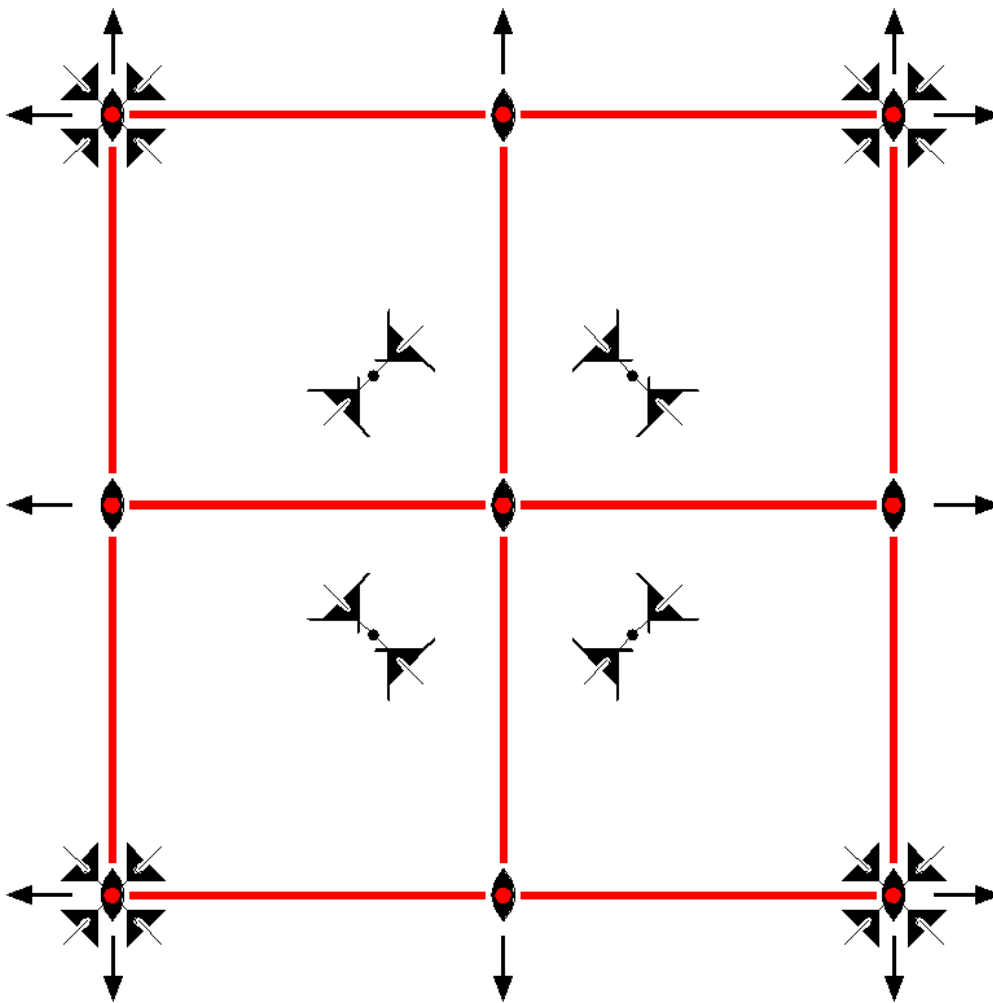
Along [1,1,0]  $p2mm1'$   
 $a^* = (-a + b)/2$   $b^* = c$   
 Origin at x,x,0

$Pm\bar{3}'$

$m\bar{3}'$

Cubic





Origin at center (m $\bar{3}$ ' )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $z \leq \min(x,y)$

Vertices 0,0,0      1/2,0,0      1/2,1/2,0      0,1/2,0      1/2,1/2,1/2

### Symmetry Operations

- |   |  |   |   |
|---|--|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ , $\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)  | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>xyz</sub>  0,0,0)                                 | (12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)               |

Continued

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Pm $\bar{3}$ '

(13) $\bar{1}'$ 0,0,0 ( $\bar{1}$  0,0,0)'	(14) m' x,y,0 (m <sub>z</sub>  0,0,0)'	(15) m' x,0,z (m <sub>y</sub>  0,0,0)'	(16) m' 0,y,z (m <sub>x</sub>  0,0,0)'
(17) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'	(18) $\bar{3}^+$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0)'	(19) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0)'	(20) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0)'
(21) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(22) $\bar{3}^-$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)'	(23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)'	(24) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.						
24	l	1	(1) x,y,z [u,v,w]	(2) $\bar{x}$ , $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w]	(3) $\bar{x}$ ,y, $\bar{z}$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x, $\bar{y}$ , $\bar{z}$ [u, $\bar{v}$ , $\bar{w}$ ]
			(5) z,x,y [w,u,v]	(6) z, $\bar{x}$ , $\bar{y}$ [ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ]	(7) $\bar{z}$ , $\bar{x}$ ,y [ $\bar{w}$ , $\bar{u}$ ,v]	(8) $\bar{z}$ ,x, $\bar{y}$ [ $\bar{w}$ ,u, $\bar{v}$ ]
			(9) y,z,x [v,w,u]	(10) $\bar{y}$ ,z, $\bar{x}$ [ $\bar{v}$ ,w, $\bar{u}$ ]	(11) y, $\bar{z}$ , $\bar{x}$ [v, $\bar{w}$ , $\bar{u}$ ]	(12) $\bar{y}$ , $\bar{z}$ ,x [ $\bar{v}$ , $\bar{w}$ ,u]
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(14) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(15) x, $\bar{y}$ ,z [u, $\bar{v}$ ,w]	(16) $\bar{x}$ ,y,z [ $\bar{u}$ ,v,w]
			(17) $\bar{z}$ , $\bar{x}$ , $\bar{y}$ [ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ]	(18) $\bar{z}$ ,x,y [ $\bar{w}$ ,u,v]	(19) z,x, $\bar{y}$ [w,u, $\bar{v}$ ]	(20) z, $\bar{x}$ ,y [w, $\bar{u}$ ,v]
			(21) $\bar{y}$ , $\bar{z}$ , $\bar{x}$ [ $\bar{v}$ , $\bar{w}$ , $\bar{u}$ ]	(22) y, $\bar{z}$ ,x [v, $\bar{w}$ ,u]	(23) $\bar{y}$ ,z,x [ $\bar{v}$ ,w,u]	(24) y,z, $\bar{x}$ [v,w, $\bar{u}$ ]
12	k	m'..	1/2,y,z [0,v,w]	1/2, $\bar{y}$ ,z [0, $\bar{v}$ ,w]	1/2,y, $\bar{z}$ [0,v, $\bar{w}$ ]	1/2,y, $\bar{z}$ [0,v, $\bar{w}$ ]
			1/2, $\bar{y}$ , $\bar{z}$ [0, $\bar{v}$ , $\bar{w}$ ]	z,1/2,y [w,0,v]	z,1/2, $\bar{y}$ [w,0, $\bar{v}$ ]	z,1/2, $\bar{y}$ [w,0, $\bar{v}$ ]
			$\bar{z}$ ,1/2,y [ $\bar{w}$ ,0,v]	$\bar{z}$ ,1/2, $\bar{y}$ [ $\bar{w}$ ,0, $\bar{v}$ ]	y,z,1/2 [v,w,0]	y,z,1/2 [v,w,0]
			$\bar{y}$ ,z,1/2 [ $\bar{v}$ ,w,0]	y, $\bar{z}$ ,1/2 [v, $\bar{w}$ ,0]	$\bar{y}$ , $\bar{z}$ ,1/2 [ $\bar{v}$ , $\bar{w}$ ,0]	$\bar{y}$ , $\bar{z}$ ,1/2 [ $\bar{v}$ , $\bar{w}$ ,0]
12	j	m'..	0,y,z [0,v,w]	0, $\bar{y}$ ,z [0, $\bar{v}$ ,w]	0,y, $\bar{z}$ [0,v, $\bar{w}$ ]	0,y, $\bar{z}$ [0,v, $\bar{w}$ ]
			0, $\bar{y}$ , $\bar{z}$ [0, $\bar{v}$ , $\bar{w}$ ]	z,0,y [w,0,v]	z,0, $\bar{y}$ [w,0, $\bar{v}$ ]	z,0, $\bar{y}$ [w,0, $\bar{v}$ ]
			$\bar{z}$ ,0,y [ $\bar{w}$ ,0,v]	$\bar{z}$ ,0, $\bar{y}$ [ $\bar{w}$ ,0, $\bar{v}$ ]	y,z,0 [v,w,0]	y,z,0 [v,w,0]
			$\bar{y}$ ,z,0 [ $\bar{v}$ ,w,0]	y, $\bar{z}$ ,0 [v, $\bar{w}$ ,0]	$\bar{y}$ , $\bar{z}$ ,0 [ $\bar{v}$ , $\bar{w}$ ,0]	$\bar{y}$ , $\bar{z}$ ,0 [ $\bar{v}$ , $\bar{w}$ ,0]
8	i	.3.	x,x,x [u,u,u]	$\bar{x}$ , $\bar{x}$ ,x [ $\bar{u}$ , $\bar{u}$ ,u]	$\bar{x}$ ,x, $\bar{x}$ [ $\bar{u}$ ,u, $\bar{u}$ ]	x, $\bar{x}$ , $\bar{x}$ [u, $\bar{u}$ , $\bar{u}$ ]
			$\bar{x}$ , $\bar{x}$ , $\bar{x}$ [ $\bar{u}$ , $\bar{u}$ , $\bar{u}$ ]	x,x, $\bar{x}$ [u,u, $\bar{u}$ ]	x, $\bar{x}$ ,x [u, $\bar{u}$ ,u]	$\bar{x}$ ,x,x [u, $\bar{u}$ ,u]
6	h	m'm'2..	x,1/2,1/2 [u,0,0]	$\bar{x}$ ,1/2,1/2 [ $\bar{u}$ ,0,0]	1/2,x,1/2 [0,u,0]	1/2,x,1/2 [0,u,0]
			1/2, $\bar{x}$ ,1/2 [0, $\bar{u}$ ,0]	1/2,1/2,x [0,0,u]	1/2,1/2, $\bar{x}$ [0,0, $\bar{u}$ ]	1/2,1/2, $\bar{x}$ [0,0, $\bar{u}$ ]

Continued

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Pm' $\bar{3}$ '

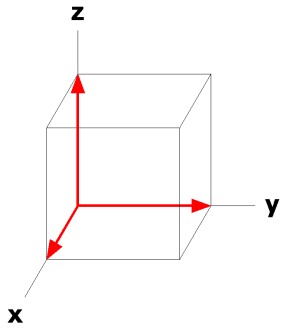
6	g	$m'm'2.. x, 1/2, 0 [u, 0, 0]$ $0, \bar{x}, 1/2 [0, \bar{u}, 0]$	$\bar{x}, 1/2, 0 [\bar{u}, 0, 0]$ $1/2, 0, x [0, 0, u]$	$0, x, 1/2 [0, u, 0]$ $1/2, 0, \bar{x} [0, 0, \bar{u}]$
6	f	$m'm'2.. x, 0, 1/2 [u, 0, 0]$ $1/2, \bar{x}, 0 [0, \bar{u}, 0]$	$\bar{x}, 0, 1/2 [\bar{u}, 0, 0]$ $0, 1/2, x [0, 0, u]$	$1/2, x, 0 [0, u, 0]$ $0, 1/2, \bar{x} [0, 0, \bar{u}]$
6	e	$m'm'2.. x, 0, 0 [u, 0, 0]$ $0, \bar{x}, 0 [0, \bar{u}, 0]$	$\bar{x}, 0, 0 [\bar{u}, 0, 0]$ $0, 0, x [0, 0, u]$	$0, x, 0 [0, u, 0]$ $0, 0, \bar{x} [0, 0, \bar{u}]$
3	d	$m'm'm'.. 1/2, 0, 0 [0, 0, 0]$	$0, 1/2, 0 [0, 0, 0]$	$0, 0, 1/2 [0, 0, 0]$
3	c	$m'm'm'.. 0, 1/2, 1/2 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$
1	b	$m'\bar{3}'.. 1/2, 1/2, 1/2 [0, 0, 0]$		
1	a	$m'\bar{3}'.. 0, 0, 0 [0, 0, 0]$		

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p2m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 1, 1]$   $p6$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

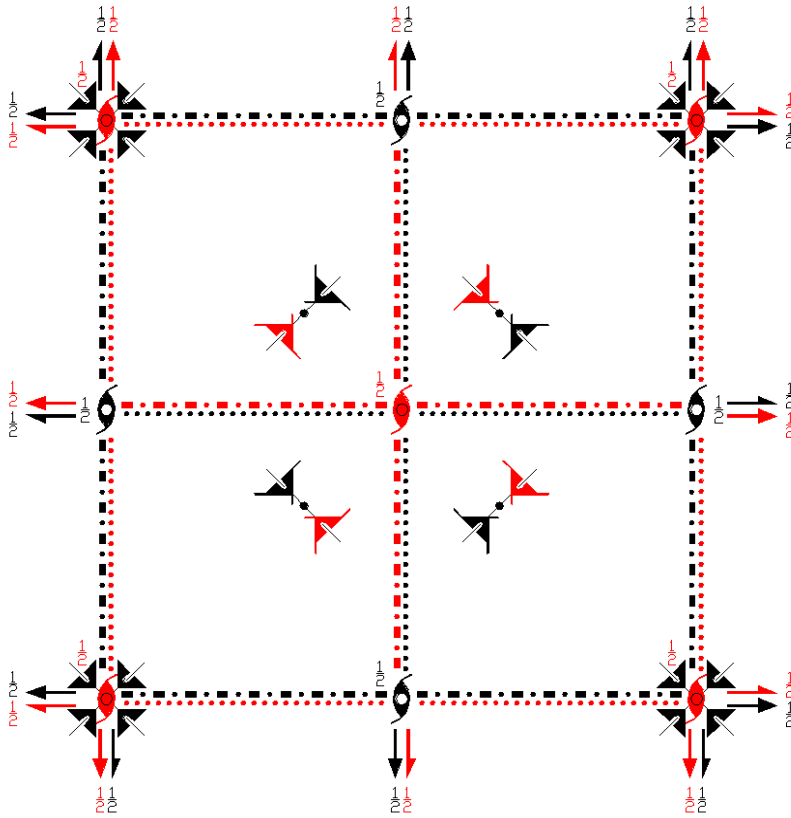
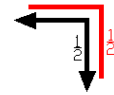
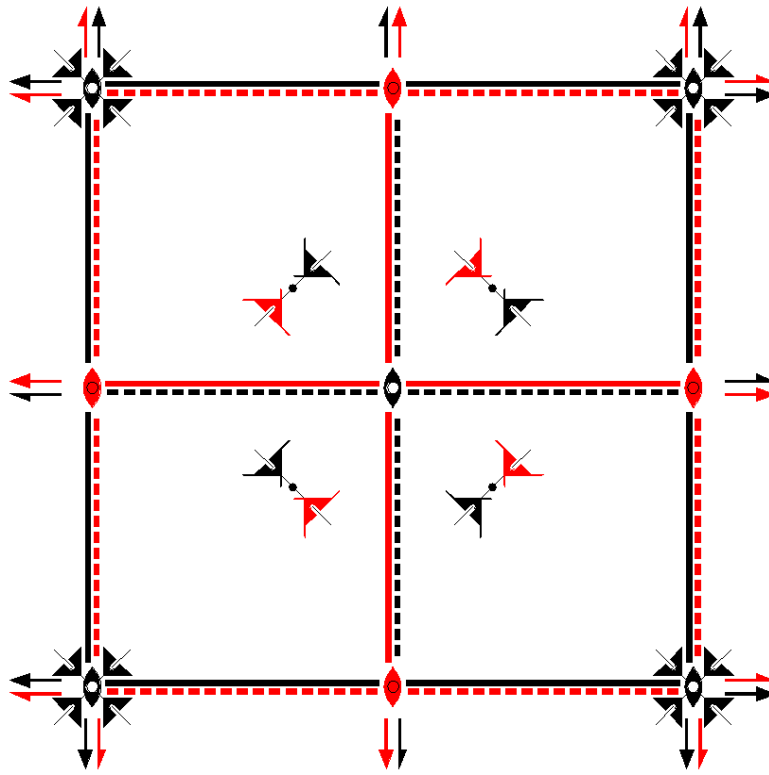
Along  $[1, 1, 0]$   $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 0$



$P_F m\bar{3}$   
200.4.1519

$m\bar{3}1'$   
 $P_F m\bar{3}$

Cubic



**Origin** at center ( $\bar{m}\bar{3}$ )**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $z \leq \min(x,y)$ 

Vertices 0,0,0      1/2,0,0      1/2,1/2,0      0,1/2,0      1/2,1/2,1/2

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |   |
|---|--|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)       | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)                                | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>x<math>\bar{y}z</math></sub>  0,0,0) | (12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub>  0,0,0)               |

Continued

200.4.1519

 $P_F \bar{m}\bar{3}$ 

- |  |   |  |   |
|--|---|--|---|
| (13) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)                              | (14) m x,y,0<br>(m <sub>z</sub>  0,0,0)   | (15) m x,0,z<br>(m <sub>y</sub>  0,0,0)  | (16) m 0,y,z<br>(m <sub>x</sub>  0,0,0)   |
| (17) $\bar{3}^+$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0) | (18) $\bar{3}^+$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$ <sup>-1</sup>  0,0,0) | (19) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0) | (20) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$ <sup>-1</sup>  0,0,0) |
| (21) $\bar{3}^-$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0) | (22) $\bar{3}^-$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)              | (23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)          | (24) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)               |

For (1,0,0)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) t' (1,0,0)<br>(1 1,0,0)'  | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'  | (3) 2' 1/2,y,0<br>(2 <sub>y</sub>  1,0,0)'  | (4) 2' (1,0,0) x,0,0<br>(2 <sub>x</sub>  1,0,0)'  |
| (5) 3 <sup>+</sup> ' (1/3,1/3,1/3)<br>x+2/3,x+1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1,0,0)' | (6) 3 <sup>+</sup> ' (1/3,-1/3,1/3)<br>x+2/3,x-1/3,x<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1,0,0)' | (7) 3 <sup>+</sup> ' (1/3,-1/3,-1/3)<br>x+2/3,x-1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1,0,0)'           | (8) 3 <sup>+</sup> ' (1/3,1/3,-1/3)<br>x+2/3,x-1/3,x<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1,0,0)' |
| (9) 3 <sup>-</sup> ' (1/3,1/3,1/3)<br>x+1/3,x-1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1,0,0)' | (10) 3 <sup>-</sup> ' (1/3,-1/3,-1/3)<br>x+1/3,x+1/3,x<br>(3 <sub>x<math>\bar{y}z</math></sub>  1,0,0)'             | (11) 3 <sup>-</sup> ' (1/3,1/3,-1/3)<br>x+1/3,x-1/3,x<br>(3 <sub>x<math>\bar{y}z</math></sub>  1,0,0)'      | (12) 3 <sup>-</sup> ' (1/3,-1/3,1/3)<br>x+1/3,x+1/3,x<br>(3 <sub>x<math>\bar{y}z</math></sub>  1,0,0)'              |
| (13) $\bar{1}$ ' 1/2,0,0<br>( $\bar{1}$ ' 1,0,0)'   | (14) a' (1,0,0) x,y,0<br>(m <sub>z</sub> ' 1,0,0)'  | (15) a' (1,0,0) x,0,z<br>(m <sub>y</sub> ' 1,0,0)'  | (16) m' 1/2,y,z<br>(m <sub>x</sub> ' 1,0,0)'  |
| (17) $\bar{3}^+$ ' x,x-1,x;<br>1/2,-1/2,1/2<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  1,0,0)'         | (18) $\bar{3}^+$ ' $\bar{x}$ ,x+1, $\bar{x}$ ;<br>1/2,1/2,1/2<br>( $\bar{3}_{x\bar{y}z}$ <sup>-1</sup>  1,0,0)'     | (19) $\bar{3}^+$ ' x, $\bar{x}$ +1, $\bar{x}$ ;<br>1/2,1/2,-1/2<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  1,0,0)' | (20) $\bar{3}^+$ ' $\bar{x}$ , $\bar{x}$ +1,x;<br>1/2,-1/2,1/2<br>( $\bar{3}_{x\bar{y}z}$ <sup>-1</sup>  1,0,0)'    |
| (21) $\bar{3}^-$ ' x+1,x+1,x;<br>1/2,1/2,-1/2<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  1,0,0)'       | (22) $\bar{3}^-$ ' x+1, $\bar{x}$ -1, $\bar{x}$ ;<br>1/2,-1/2,1/2<br>( $\bar{3}_{x\bar{y}z}$  1,0,0)'               | (23) $\bar{3}^-$ ' $\bar{x}$ +1, $\bar{x}$ +1,x;<br>1/2,1/2,1/2<br>( $\bar{3}_{x\bar{y}z}$  1,0,0)'         | (24) $\bar{3}^-$ ' $\bar{x}$ +1,x-1, $\bar{x}$ ;<br>1/2,-1/2,-1/2<br>( $\bar{3}_{x\bar{y}z}$  1,0,0)'               |

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5); (13).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates					
			(0,0,0) +	(1,0,0)' +				
48	l	1						
(1)	x,y,z	[u,v,w]	(2) $\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3) $\bar{x},y,\bar{z}$	$[\bar{u},v,\bar{w}]$	(4) $x,\bar{y},\bar{z}$	$[u,\bar{v},\bar{w}]$
(5)	z,x,y	[w,u,v]	(6) $z,\bar{x},\bar{y}$	$[w,\bar{u},\bar{v}]$	(7) $\bar{z},\bar{x},y$	$[\bar{w},\bar{u},v]$	(8) $\bar{z},x,\bar{y}$	$[\bar{w},u,\bar{v}]$
(9)	y,z,x	[v,w,u]	(10) $\bar{y},z,\bar{x}$	$[\bar{v},w,\bar{u}]$	(11) $y,\bar{z},\bar{x}$	$[v,\bar{w},\bar{u}]$	(12) $\bar{y},z,x$	$[\bar{v},w,u]$
(13)	$\bar{x},\bar{y},\bar{z}$	[u,v,w]	(14) $x,y,\bar{z}$	$[\bar{u},\bar{v},w]$	(15) $x,\bar{y},z$	$[\bar{u},v,\bar{w}]$	(16) $\bar{x},y,z$	$[u,\bar{v},\bar{w}]$
(17)	$\bar{z},\bar{x},\bar{y}$	[w,u,v]	(18) $\bar{z},x,y$	$[w,\bar{u},\bar{v}]$	(19) $z,x,\bar{y}$	$[\bar{w},\bar{u},v]$	(20) $z,\bar{x},y$	$[\bar{w},u,\bar{v}]$
(21)	$\bar{y},\bar{z},\bar{x}$	[v,w,u]	(22) $y,\bar{z},x$	$[\bar{v},w,\bar{u}]$	(23) $\bar{y},z,x$	$[v,\bar{w},\bar{u}]$	(24) $y,z,\bar{x}$	$[\bar{v},w,u]$
24	k	m'..	1/2,y,z	[0,v,w]	1/2, $\bar{y}$ ,z	[0,v, $\bar{w}$ ]	1/2,y, $\bar{z}$	[0, $\bar{v}$ ,w]
			1/2, $\bar{y}$ , $\bar{z}$	[0, $\bar{v}$ , $\bar{w}$ ]	z,1/2,y	[w,0,v]	z,1/2, $\bar{y}$	$[\bar{w},0,v]$
			$\bar{z}$ ,1/2,y	[w,0, $\bar{v}$ ]	$\bar{z}$ ,1/2, $\bar{y}$	$[\bar{w},0,\bar{v}]$	y,z,1/2	[v,w,0]
			$\bar{y}$ ,z,1/2	[v, $\bar{w}$ ,0]	$\bar{y}$ , $\bar{z}$ ,1/2	$[\bar{v},w,0]$	$\bar{y}$ , $\bar{z}$ ,1/2	$[\bar{v},\bar{w},0]$
24	j	m..	0,y,z	[u,0,0]	0, $\bar{y}$ ,z	[u,0,0]	0,y, $\bar{z}$	[u,0,0]
			0, $\bar{y}$ , $\bar{z}$	[u,0,0]	z,0,y	[0,u,0]	z,0, $\bar{y}$	[0,u,0]
			$\bar{z}$ ,0,y	[0,u,0]	$\bar{z}$ ,0, $\bar{y}$	[0,u,0]	y,z,0	[0,0,u]
			$\bar{y}$ ,z,0	[0,0,u]	$\bar{y}$ , $\bar{z}$ ,0	[0,0,u]	$\bar{y}$ , $\bar{z}$ ,0	[0,0,u]
16	i	.3.	x,x,x	[u,u,u]	$\bar{x},\bar{x},x$	$[\bar{u},\bar{u},u]$	$\bar{x},x,\bar{x}$	$[\bar{u},u,\bar{u}]$
			$\bar{x},\bar{x},\bar{x}$	[u,u,u]	x,x, $\bar{x}$	$[\bar{u},\bar{u},u]$	$\bar{x},x,x$	$[\bar{u},\bar{u},\bar{u}]$
12	h	m'm'2..	x,1/2,1/2	[u,0,0]	$\bar{x}$ ,1/2,1/2	[u,0,0]	1/2,x,1/2	[0,u,0]
			1/2, $\bar{x}$ ,1/2	[0,u,0]	1/2,1/2,x	[0,0,u]	1/2,1/2, $\bar{x}$	[0,0,u]
12	g	m'm2'..	x,1/2,0	[0,0,w]	$\bar{x}$ ,1/2,0	[0,0, $\bar{w}$ ]	0,x,1/2	[w,0,0]
			0, $\bar{x}$ ,1/2	$[\bar{w},0,0]$	1/2,0,x	[0,w,0]	1/2,0, $\bar{x}$	[0, $\bar{w}$ ,0]
12	f	mm'2'..	x,0,1/2	[0,v,0]	$\bar{x}$ ,0,1/2	[0, $\bar{v}$ ,0]	1/2,x,0	[0,0,v]
			1/2, $\bar{x}$ ,0	[0,0, $\bar{v}$ ]	0,1/2,x	[v,0,0]	0,1/2, $\bar{x}$	$[\bar{v},0,0]$
12	e	mm2'..	x,0,0	[0,0,0]	$\bar{x}$ ,0,0	[0,0,0]	0,x,0	[0,0,0]
			0, $\bar{x}$ ,0	[0,0,0]	0,0,x	[0,0,0]	0,0, $\bar{x}$	[0,0,0]

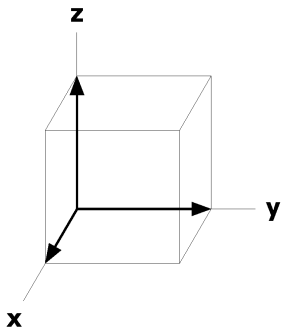
6	d	$m'mm..$ $1/2,0,0$ [0,0,0]	$0,1/2,0$ [0,0,0]	$0,0,1/2$ [0,0,0]
6	c	$mmm..$ $0,1/2,1/2$ [0,0,0]	$1/2,0,1/2$ [0,0,0]	$1/2,1/2,0$ [0,0,0]
2	b	$m'\overline{3}'$ . $1/2,1/2,1/2$ [0,0,0]		
2	a	$m'\overline{3}'$ . $0,0,0$ [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,1,1]  $p61'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

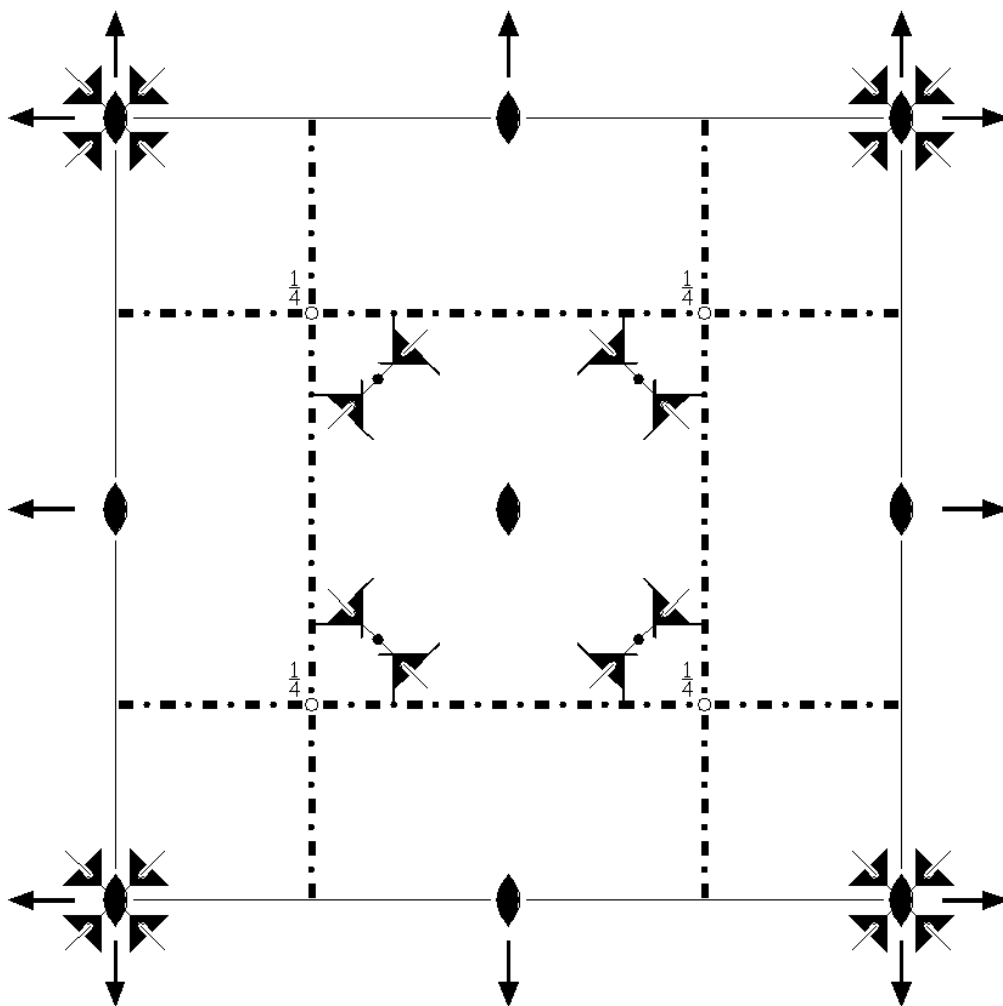
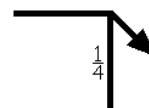
Along [1,1,0]  $p_c^- 2mm$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x-1/4, x+1/4, 0$



$Pn\bar{3}$   
201.1.1520

$m\bar{3}$   
 $P2/n\bar{3}$

Cubic



Origin at 23, at  $-1/4, -1/4, -1/4$  from center ( $\bar{3}$ )

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq \min(x, 1-x);$   $z \leq y$

Vertices  $0,0,0$   $1,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

### Symmetry Operations

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}^{-1}</math></sub>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}^{-1}</math></sub>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xyz}^{-1}</math></sub>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)                             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)                         | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)                        |



(13) $\bar{1}$ $1/4, 1/4, 1/4$ ( $\bar{1}$   $1/2, 1/2, 1/2$ )	(14) n $(1/2, 1/2, 0)$ $x, y, 1/4$ ( $m_z$   $1/2, 1/2, 1/2$ )	(15) n $(1/2, 0, 1/2)$ $x, 1/4, z$ ( $m_y$   $1/2, 1/2, 1/2$ )	(16) n $(0, 1/2, 1/2)$ $1/4, y, z$ ( $m_x$   $1/2, 1/2, 1/2$ )
(17) $\bar{3}^+$ $x, x, x;$ $1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}$   $1/2, 1/2, 1/2$ )	(18) $\bar{3}^+$ $\bar{x}-1, x+1, \bar{x};$ $-1/4, 1/4, 3/4$ ( $\bar{3}_{xyz}^{-1}$   $1/2, 1/2, 1/2$ )	(19) $\bar{3}^+$ $x, \bar{x}+1, \bar{x};$ $1/4, 3/4, -1/4$ ( $\bar{3}_{xyz}^{-1}$   $1/2, 1/2, 1/2$ )	(20) $\bar{3}^+$ $\bar{x}+1, \bar{x}, x;$ $3/4, -1/4, 1/4$ ( $\bar{3}_{xyz}^{-1}$   $1/2, 1/2, 1/2$ )
(21) $\bar{3}^-$ $x, x, x;$ $1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}^{-1}$   $1/2, 1/2, 1/2$ )	(22) $\bar{3}^-$ $x+1, \bar{x}-1, \bar{x};$ $1/4, -1/4, 3/4$ ( $\bar{3}_{xyz}$   $1/2, 1/2, 1/2$ )	(23) $\bar{3}^-$ $\bar{x}, \bar{x}+1, x;$ $-1/4, 3/4, 1/4$ ( $\bar{3}_{xyz}$   $1/2, 1/2, 1/2$ )	(24) $\bar{3}^-$ $\bar{x}+1, x, \bar{x};$ $3/4, 1/4, -1/4$ ( $\bar{3}_{xyz}$   $1/2, 1/2, 1/2$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

24 h 1

(1) $x, y, z$ [u,v,w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x, \bar{y}, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]
(5) $z, x, y$ [w,u,v]	(6) $z, \bar{x}, \bar{y}$ [ $w, \bar{u}, \bar{v}$ ]	(7) $\bar{z}, \bar{x}, y$ [ $\bar{w}, \bar{u}, v$ ]	(8) $\bar{z}, x, \bar{y}$ [ $\bar{w}, u, \bar{v}$ ]
(9) $y, z, x$ [v,w,u]	(10) $\bar{y}, z, \bar{x}$ [ $\bar{v}, w, \bar{u}$ ]	(11) $y, \bar{z}, \bar{x}$ [ $v, \bar{w}, \bar{u}$ ]	(12) $\bar{y}, \bar{z}, x$ [ $\bar{v}, \bar{w}, u$ ]

(13) $\bar{x}+1/2, \bar{y}+1/2, \bar{z}+1/2$ [u,v,w]	(14) $x+1/2, y+1/2, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(15) $x+1/2, \bar{y}+1/2, z+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(16) $\bar{x}+1/2, y+1/2, z+1/2$ [ $u, \bar{v}, \bar{w}$ ]
(17) $\bar{z}+1/2, \bar{x}+1/2, \bar{y}+1/2$ [w,u,v]	(18) $\bar{z}+1/2, x+1/2, y+1/2$ [ $w, \bar{u}, \bar{v}$ ]	(19) $z+1/2, x+1/2, \bar{y}+1/2$ [ $\bar{w}, \bar{u}, v$ ]	(20) $z+1/2, \bar{x}+1/2, y+1/2$ [ $\bar{w}, u, \bar{v}$ ]
(21) $\bar{y}+1/2, \bar{z}+1/2, \bar{x}+1/2$ [v,w,u]	(22) $y+1/2, \bar{z}+1/2, x+1/2$ [ $\bar{v}, w, \bar{u}$ ]	(23) $\bar{y}+1/2, z+1/2, x+1/2$ [ $v, \bar{w}, \bar{u}$ ]	(24) $y+1/2, z+1/2, \bar{x}+1/2$ [ $\bar{v}, \bar{w}, u$ ]

12	g	2..	$x, 1/2, 0$ [u,0,0]	$\bar{x}, 1/2, 0$ [ $\bar{u}, 0, 0$ ]	$0, x, 1/2$ [0,u,0]
			$0, \bar{x}, 1/2$ [0, $\bar{u}$ ,0]	$1/2, 0, x$ [0,0,u]	$1/2, 0, \bar{x}$ [0,0, $\bar{u}$ ]
			$\bar{x}+1/2, 0, 1/2$ [u,0,0]	$x+1/2, 0, 1/2$ [ $\bar{u}, 0, 0$ ]	$1/2, \bar{x}+1/2, 0$ [0,u,0]
			$1/2, x+1/2, 0$ [0, $\bar{u}$ ,0]	$0, 1/2, \bar{x}+1/2$ [0,0,u]	$0, 1/2, x+1/2$ [0,0, $\bar{u}$ ]
12	f	2..	$x, 0, 0$ [u,0,0]	$\bar{x}, 0, 0$ [ $\bar{u}, 0, 0$ ]	$0, x, 0$ [0,u,0]
			$0, \bar{x}, 0$ [0, $\bar{u}$ ,0]	$0, 0, x$ [0,0,u]	$0, 0, \bar{x}$ [0,0, $\bar{u}$ ]
			$\bar{x}+1/2, 1/2, 1/2$ [u,0,0]	$x+1/2, 1/2, 1/2$ [ $\bar{u}, 0, 0$ ]	$1/2, \bar{x}+1/2, 1/2$ [0,u,0]
			$1/2, x+1/2, 1/2$ [0, $\bar{u}$ ,0]	$1/2, 1/2, \bar{x}+1/2$ [0,0,u]	$1/2, 1/2, x+1/2$ [0,0, $\bar{u}$ ]
8	e	.3.	$x, x, x$ [u,u,u]	$\bar{x}, \bar{x}, x$ [ $\bar{u}, \bar{u}, u$ ]	
			$\bar{x}, x, \bar{x}$ [ $\bar{u}, u, \bar{u}$ ]	$x, \bar{x}, \bar{x}$ [u, $\bar{u}, \bar{u}$ ]	
			$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2$ [u,u,u]	$x+1/2, x+1/2, \bar{x}+1/2$ [ $\bar{u}, \bar{u}, u$ ]	
			$x+1/2, \bar{x}+1/2, x+1/2$ [ $\bar{u}, u, \bar{u}$ ]	$\bar{x}+1/2, x+1/2, x+1/2$ [u, $\bar{u}, \bar{u}$ ]	

Continued

201.1.1520

 $Pn\bar{3}$ 

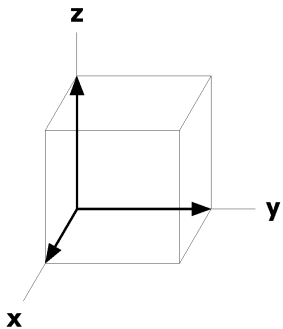
6	d	222..	0,1/2,1/2 [0,0,0] 1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0] 0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0] 0,0,1/2 [0,0,0]	
4	c	$\bar{3}$ .	3/4,3/4,3/4 [u,u,u]	1/4,1/4,3/4 [ $\bar{u}$ , $\bar{u}$ ,u]	1/4,3/4,1/4 [ $\bar{u}$ ,u, $\bar{u}$ ]	3/4,1/4,1/4 [u, $\bar{u}$ , $\bar{u}$ ]
4	b	$\bar{3}$ .	1/4,1/4,1/4 [u,u,u]	3/4,3/4,1/4 [ $\bar{u}$ , $\bar{u}$ ,u]	3/4,1/4,3/4 [ $\bar{u}$ ,u, $\bar{u}$ ]	1/4,3/4,3/4 [u, $\bar{u}$ , $\bar{u}$ ]
2	a	23.	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $c_p$ , 2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,1,1]  $p6'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

Along [1,1,0]  $p2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4

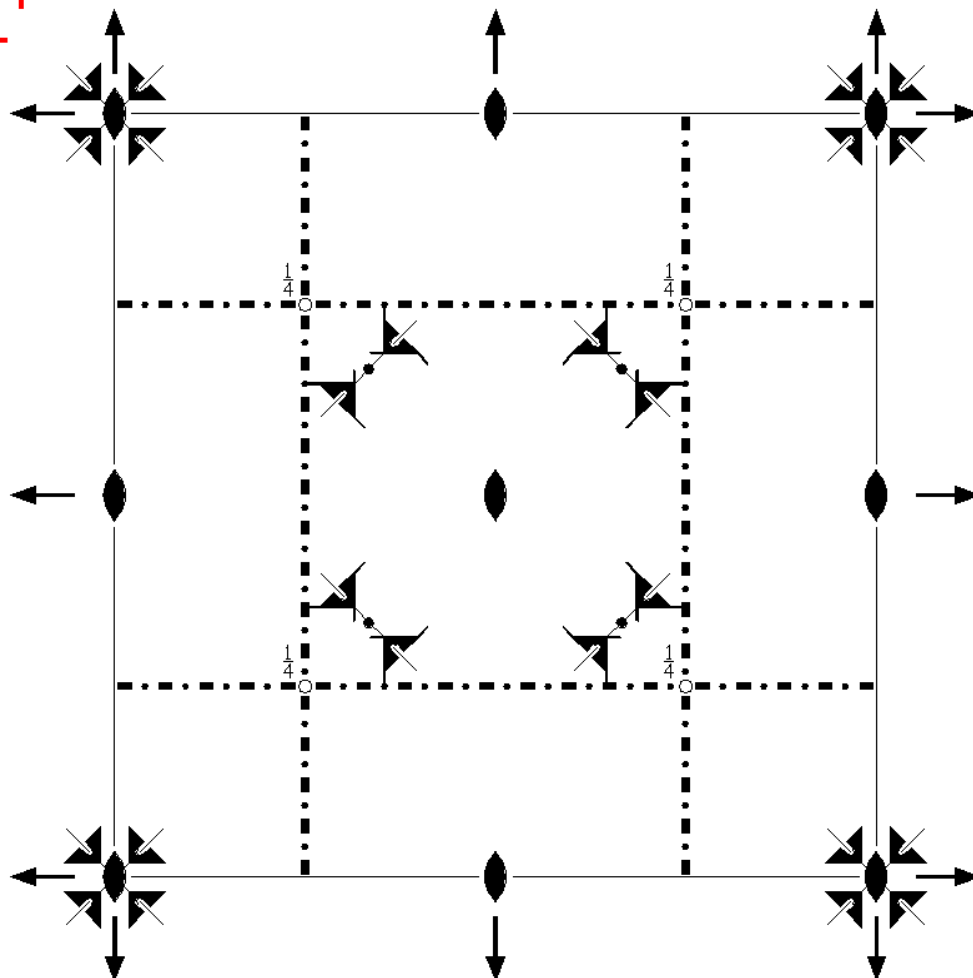


$Pn\bar{3}1'$   
201.2.1521

$m\bar{3}1'$   
 $P2/n\bar{3}1'$

Cubic

1'



Origin at  $231'$ , at  $-1/4, -1/4, -1/4$  from center ( $\bar{3}1'$ )

Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$ ;  $y \leq \min(x, 1-x)$ ;  $z \leq y$

Vertices  $0,0,0$   $1,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

### Symmetry Operations

For 1 + set

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                  | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                                  | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                 |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)        | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}y\bar{z}}$  0,0,0) |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}y\bar{z}}$  0,0,0) | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{\bar{x}yz}$  0,0,0)      |

- |   |   |  |   |
|---|---|--|---|
| (13) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$   1/2,1/2,1/2)                        | (14) n (1/2,1/2,0) x,y,1/4<br>( $m_z$   1/2,1/2,1/2)  | (15) n (1/2,0,1/2) x,1/4,z<br>( $m_y$   1/2,1/2,1/2)   | (16) n (0,1/2,1/2) 1/4,y,z<br>( $m_x$   1/2,1/2,1/2)  |
| (17) $\bar{3}^+$ x,x,x;<br>1/4,1/4,1/4<br>( $\bar{3}_{xyz}$   1/2,1/2,1/2)      | (18) $\bar{3}^+$ $\bar{x}-1,x+1,\bar{x}$ ;<br>-1/4,1/4,3/4<br>( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2) | (19) $\bar{3}^+$ x, $\bar{x}+1,\bar{x}$ ;<br>1/4,3/4,-1/4<br>( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2) | (20) $\bar{3}^+$ $\bar{x}+1,\bar{x},x$ ;<br>3/4,-1/4,1/4<br>( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2) |
| (21) $\bar{3}^-$ x,x,x;<br>1/4,1/4,1/4<br>( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2) | (22) $\bar{3}^-$ x+1, $\bar{x}-1,\bar{x}$ ;<br>1/4,-1/4,3/4<br>( $\bar{3}_{xyz}$   1/2,1/2,1/2)     | (23) $\bar{3}^-$ $\bar{x},\bar{x}+1,x$ ;<br>-1/4,3/4,1/4<br>( $\bar{3}_{xyz}$   1/2,1/2,1/2)       | (24) $\bar{3}^-$ $\bar{x}+1,x,\bar{x}$ ;<br>3/4,1/4,-1/4<br>( $\bar{3}_{xyz}$   1/2,1/2,1/2)      |

For 1' + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1'<br>(1   0,0,0)'   | (2) 2' 0,0,z<br>( $2_z$   0,0,0)'  | (3) 2' 0,y,0<br>( $2_y$   0,0,0)'   | (4) 2' x,0,0<br>( $2_x$   0,0,0)'  |
| (5) $3^{+ '}$ x,x,x<br>( $3_{xyz}$   0,0,0)'   | (6) $3^{+ '}$ $\bar{x},x,\bar{x}$<br>( $3_{xyz}^{-1}$   0,0,0)'  | (7) $3^{+ '}$ x, $\bar{x},\bar{x}$<br>( $3_{xyz}^{-1}$   0,0,0)'  | (8) $3^{+ '}$ $\bar{x},\bar{x},x$<br>( $3_{xyz}^{-1}$   0,0,0)'  |
| (9) $3^{- '}$ x,x,x<br>( $3_{xyz}^{-1}$   0,0,0)'                                    | (10) $3^{- '}$ x, $\bar{x},\bar{x}$<br>( $3_{xyz}$   0,0,0)'   | (11) $3^{- '}$ $\bar{x},\bar{x},x$<br>( $3_{xyz}$   0,0,0)'   | (12) $3^{- '}$ $\bar{x},x,\bar{x}$<br>( $3_{xyz}$   0,0,0)'  |
| (13) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$   1/2,1/2,1/2)'                          | (14) n' (1/2,1/2,0) x,y,1/4<br>( $m_z$   1/2,1/2,1/2)'   | (15) n' (1/2,0,1/2) x,1/4,z<br>( $m_y$   1/2,1/2,1/2)'  | (16) n' (0,1/2,1/2) 1/4,y,z<br>( $m_x$   1/2,1/2,1/2)'   |
| (17) $\bar{3}^{+ '}$ x,x,x;<br>1/4,1/4,1/4<br>( $\bar{3}_{xyz}$   1/2,1/2,1/2)'      | (18) $\bar{3}^{+ '}$ $\bar{x}-1,x+1,\bar{x}$ ;<br>-1/4,1/4,3/4<br>( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2)' | (19) $\bar{3}^{+ '}$ x, $\bar{x}+1,\bar{x}$ ;<br>1/4,3/4,-1/4<br>( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2)' | (20) $\bar{3}^{+ '}$ $\bar{x}+1,\bar{x},x$ ;<br>3/4,-1/4,1/4<br>( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2)' |
| (21) $\bar{3}^{- '}$ x,x,x;<br>1/4,1/4,1/4<br>( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2)' | (22) $\bar{3}^{- '}$ x+1, $\bar{x}-1,\bar{x}$ ;<br>1/4,-1/4,3/4<br>( $\bar{3}_{xyz}$   1/2,1/2,1/2)'     | (23) $\bar{3}^{- '}$ $\bar{x},\bar{x}+1,x$ ;<br>-1/4,3/4,1/4<br>( $\bar{3}_{xyz}$   1/2,1/2,1/2)'       | (24) $\bar{3}^{- '}$ $\bar{x}+1,x,\bar{x}$ ;<br>3/4,1/4,-1/4<br>( $\bar{3}_{xyz}$   1/2,1/2,1/2)'      |

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); 1'.

## Positions

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

1 +

1' +

24 h 11'

- |  |   |   |   |
|--|---|---|---|
| (1) x,y,z [0,0,0]                                  | (2) $\bar{x},\bar{y},z$ [0,0,0]         | (3) $\bar{x},y,\bar{z}$ [0,0,0]         | (4) x, $\bar{y},\bar{z}$ [0,0,0]        |
| (5) z,x,y [0,0,0]                                  | (6) z, $\bar{x},\bar{y}$ [0,0,0]        | (7) $\bar{z},\bar{x},y$ [0,0,0]         | (8) $\bar{z},x,\bar{y}$ [0,0,0]         |
| (9) y,z,x [0,0,0]                                  | (10) $\bar{y},z,\bar{x}$ [0,0,0]        | (11) y, $\bar{z},\bar{x}$ [0,0,0]       | (12) $\bar{y},\bar{z},x$ [0,0,0]        |
| (13) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [0,0,0] | (14) x+1/2,y+1/2, $\bar{z}+1/2$ [0,0,0] | (15) x+1/2, $\bar{y}+1/2,z+1/2$ [0,0,0] | (16) $\bar{x}+1/2,y+1/2,z+1/2$ [0,0,0]  |
| (17) $\bar{z}+1/2,\bar{x}+1/2,\bar{y}+1/2$ [0,0,0] | (18) $\bar{z}+1/2,x+1/2,y+1/2$ [0,0,0]  | (19) z+1/2,x+1/2, $\bar{y}+1/2$ [0,0,0] | (20) z+1/2, $\bar{x}+1/2,y+1/2$ [0,0,0] |
| (21) $\bar{y}+1/2,\bar{z}+1/2,\bar{x}+1/2$ [0,0,0] | (22) y+1/2, $\bar{z}+1/2,x+1/2$ [0,0,0] | (23) $\bar{y}+1/2,z+1/2,x+1/2$ [0,0,0]  | (24) y+1/2,z+1/2, $\bar{x}+1/2$ [0,0,0] |

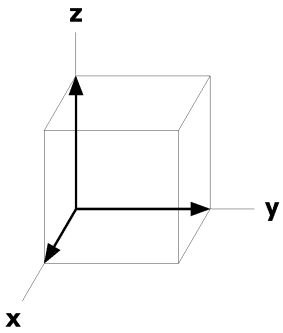
12	g	2..1'	x,1/2,0 [0,0,0]	$\bar{x}$ ,1/2,0 [0,0,0]	0,x,1/2 [0,0,0]
			0, $\bar{x}$ ,1/2 [0,0,0]	1/2,0,x [0,0,0]	1/2,0, $\bar{x}$ [0,0,0]
			$\bar{x}$ +1/2,0,1/2 [0,0,0]	x+1/2,0,1/2 [0,0,0]	1/2, $\bar{x}$ +1/2,0 [0,0,0]
			1/2,x+1/2,0 [0,0,0]	0,1/2, $\bar{x}$ +1/2 [0,0,0]	0,1/2,x+1/2 [0,0,0]
12	f	2..1'	x,0,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0]	0,x,0 [0,0,0]
			0, $\bar{x}$ ,0 [0,0,0]	0,0,x [0,0,0]	0,0, $\bar{x}$ [0,0,0]
			$\bar{x}$ +1/2,1/2,1/2 [0,0,0]	x+1/2,1/2,1/2 [0,0,0]	1/2, $\bar{x}$ +1/2,1/2 [0,0,0]
			1/2,x+1/2,1/2 [0,0,0]	1/2,1/2, $\bar{x}$ +1/2 [0,0,0]	1/2,1/2,x+1/2 [0,0,0]
8	e	.3.1'	x,x,x [0,0,0]	$\bar{x}$ , $\bar{x}$ ,x [0,0,0]	
			$\bar{x}$ ,x, $\bar{x}$ [0,0,0]	x, $\bar{x}$ , $\bar{x}$ [0,0,0]	
			$\bar{x}$ +1/2, $\bar{x}$ +1/2, $\bar{x}$ +1/2 [0,0,0]	x+1/2,x+1/2, $\bar{x}$ +1/2 [0,0,0]	
			x+1/2, $\bar{x}$ +1/2,x+1/2 [0,0,0]	$\bar{x}$ +1/2,x+1/2,x+1/2 [0,0,0]	
6	d	222..1'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
			1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	0,0,1/2 [0,0,0]
4	c	. $\bar{3}$ .1'	3/4,3/4,3/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]
					3/4,1/4,1/4 [0,0,0]
4	b	. $\bar{3}$ .1'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]
					1/4,3/4,3/4 [0,0,0]
2	a	23.1'	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,1,1] p61'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

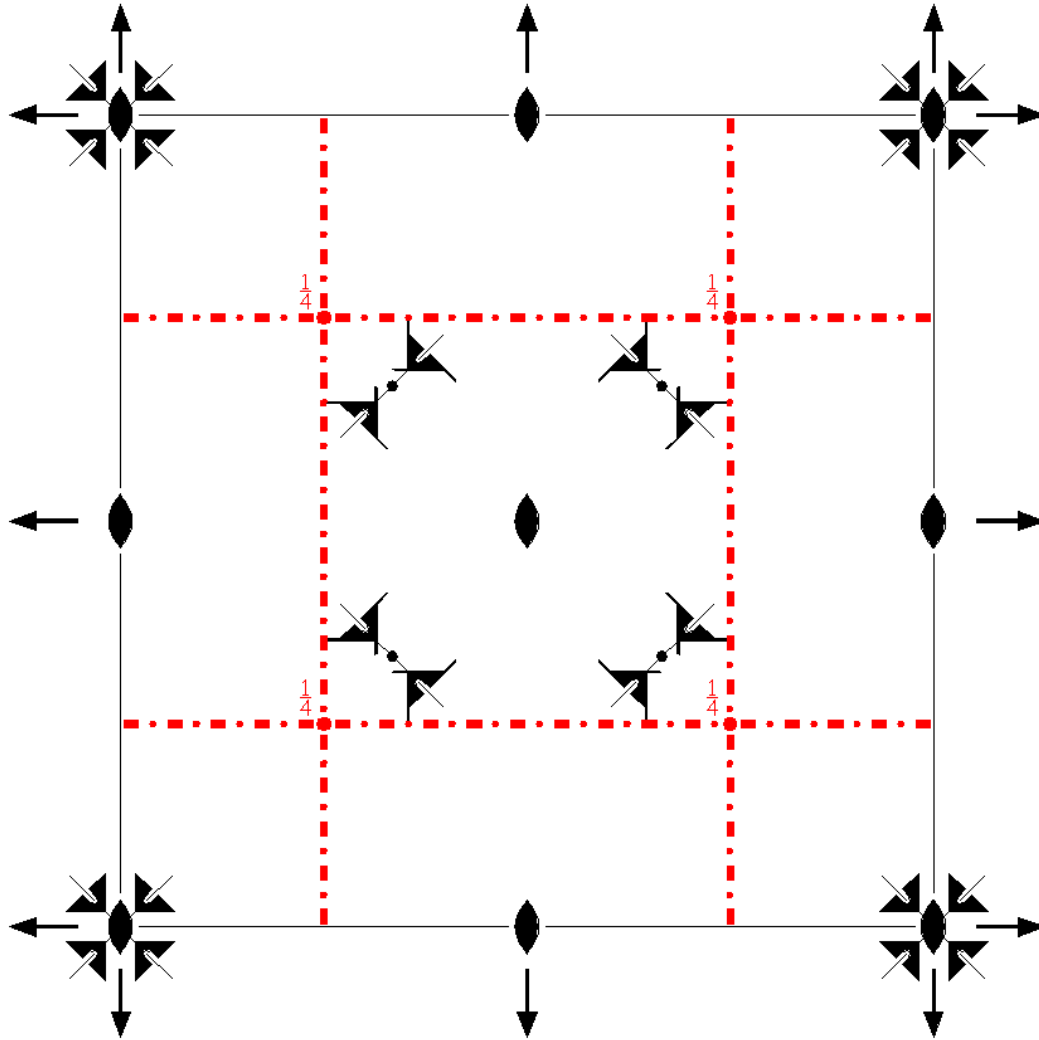
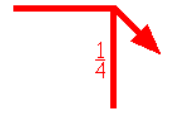
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



$Pn\bar{3}'$   
201.3.1522

$m\bar{3}'$   
 $P2/n\bar{3}'$

Cubic



Origin at 23, at  $-1/4, -1/4, -1/4$  from center ( $\bar{3}'$ )

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq \min(x, 1-x);$   $z \leq y$

Vertices  $0,0,0$   $1,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                            | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                                  | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                 |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)  | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}y\bar{z}}$  0,0,0) |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0) | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}y\bar{z}}$  0,0,0) | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{\bar{x}yz}$  0,0,0)      |

(13) $\bar{1}$ ' $1/4, 1/4, 1/4$ ( $\bar{1}$   $1/2, 1/2, 1/2$ )'	(14) n' (1/2, 1/2, 0) x, y, 1/4 ( $m_z$   $1/2, 1/2, 1/2$ )'	(15) n' (1/2, 0, 1/2) x, 1/4, z ( $m_y$   $1/2, 1/2, 1/2$ )'	(16) n' (0, 1/2, 1/2) $1/4, y, z$ ( $m_x$   $1/2, 1/2, 1/2$ )'
(17) $\bar{3}^+$ ' x, x, x; $1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}$   $1/2, 1/2, 1/2$ )'	(18) $\bar{3}^+$ ' $\bar{x}-1, x+1, \bar{x};$ $-1/4, 1/4, 3/4$ ( $\bar{3}_{xyz}^{-1}$   $1/2, 1/2, 1/2$ )'	(19) $\bar{3}^+$ ' x, $\bar{x}+1, \bar{x};$ $1/4, 3/4, -1/4$ ( $\bar{3}_{xyz}^{-1}$   $1/2, 1/2, 1/2$ )'	(20) $\bar{3}^+$ ' $\bar{x}+1, \bar{x}, x;$ $3/4, -1/4, 1/4$ ( $\bar{3}_{xyz}^{-1}$   $1/2, 1/2, 1/2$ )'
(21) $\bar{3}^-$ ' x, x, x; $1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}^{-1}$   $1/2, 1/2, 1/2$ )'	(22) $\bar{3}^-$ ' x+1, $\bar{x}-1, \bar{x};$ $1/4, -1/4, 3/4$ ( $\bar{3}_{xyz}$   $1/2, 1/2, 1/2$ )'	(23) $\bar{3}^-$ ' $\bar{x}, \bar{x}+1, x;$ $-1/4, 3/4, 1/4$ ( $\bar{3}_{xyz}$   $1/2, 1/2, 1/2$ )'	(24) $\bar{3}^-$ ' $\bar{x}+1, x, \bar{x};$ $3/4, 1/4, -1/4$ ( $\bar{3}_{xyz}$   $1/2, 1/2, 1/2$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

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(1) x, y, z [u, v, w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
(5) z, x, y [w, u, v]	(6) z, $\bar{x}, \bar{y}$ [ $w, \bar{u}, \bar{v}$ ]	(7) $\bar{z}, \bar{x}, y$ [ $\bar{w}, \bar{u}, v$ ]	(8) $\bar{z}, x, \bar{y}$ [ $\bar{w}, u, \bar{v}$ ]
(9) y, z, x [v, w, u]	(10) $\bar{y}, z, \bar{x}$ [ $\bar{v}, w, \bar{u}$ ]	(11) y, $\bar{z}, \bar{x}$ [v, $\bar{w}, \bar{u}$ ]	(12) $\bar{y}, \bar{z}, x$ [ $\bar{v}, \bar{w}, u$ ]
(13) $\bar{x}+1/2, \bar{y}+1/2, \bar{z}+1/2$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(14) x+1/2, y+1/2, $\bar{z}+1/2$ [u, v, $\bar{w}$ ]	(15) x+1/2, $\bar{y}+1/2, z+1/2$ [u, $\bar{v}, w$ ]	(16) $\bar{x}+1/2, y+1/2, z+1/2$ [ $\bar{u}, v, w$ ]
(17) $\bar{z}+1/2, \bar{x}+1/2, \bar{y}+1/2$ [ $\bar{w}, \bar{u}, \bar{v}$ ]	(18) $\bar{z}+1/2, x+1/2, y+1/2$ [ $\bar{w}, u, v$ ]	(19) z+1/2, x+1/2, $\bar{y}+1/2$ [w, u, $\bar{v}$ ]	(20) z+1/2, $\bar{x}+1/2, y+1/2$ [w, $\bar{u}, v$ ]
(21) $\bar{y}+1/2, \bar{z}+1/2, \bar{x}+1/2$ [ $\bar{v}, \bar{w}, \bar{u}$ ]	(22) y+1/2, $\bar{z}+1/2, x+1/2$ [v, $\bar{w}, u$ ]	(23) $\bar{y}+1/2, z+1/2, x+1/2$ [ $\bar{v}, w, u$ ]	(24) y+1/2, z+1/2, $\bar{x}+1/2$ [v, w, $\bar{u}$ ]

12	g	2..	x, 1/2, 0 [u, 0, 0]	$\bar{x}, 1/2, 0$ [ $\bar{u}, 0, 0$ ]	0, x, 1/2 [0, u, 0]
			0, $\bar{x}, 1/2$ [0, $\bar{u}, 0$ ]	1/2, 0, x [0, 0, u]	1/2, 0, $\bar{x}$ [0, 0, $\bar{u}$ ]
			$\bar{x}+1/2, 0, 1/2$ [ $\bar{u}, 0, 0$ ]	x+1/2, 0, 1/2 [u, 0, 0]	1/2, $\bar{x}+1/2, 0$ [0, $\bar{u}, 0$ ]
			1/2, x+1/2, 0 [0, u, 0]	0, 1/2, $\bar{x}+1/2$ [0, 0, $\bar{u}$ ]	0, 1/2, x+1/2 [0, 0, u]
12	f	2..	x, 0, 0 [u, 0, 0]	$\bar{x}, 0, 0$ [ $\bar{u}, 0, 0$ ]	0, x, 0 [0, u, 0]
			0, $\bar{x}, 0$ [0, $\bar{u}, 0$ ]	0, 0, x [0, 0, u]	0, 0, $\bar{x}$ [0, 0, $\bar{u}$ ]
			$\bar{x}+1/2, 1/2, 1/2$ [ $\bar{u}, 0, 0$ ]	x+1/2, 1/2, 1/2 [u, 0, 0]	1/2, $\bar{x}+1/2, 1/2$ [0, $\bar{u}, 0$ ]
			1/2, x+1/2, 1/2 [0, u, 0]	1/2, 1/2, $\bar{x}+1/2$ [0, 0, $\bar{u}$ ]	1/2, 1/2, x+1/2 [0, 0, u]
8	e	.3.	x, x, x [u, u, u]	$\bar{x}, \bar{x}, x$ [ $\bar{u}, \bar{u}, u$ ]	
			$\bar{x}, x, \bar{x}$ [ $\bar{u}, u, \bar{u}$ ]	x, $\bar{x}, \bar{x}$ [u, $\bar{u}, \bar{u}$ ]	

			$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2$ [ $\bar{u}, \bar{u}, \bar{u}$ ]	$x+1/2, x+1/2, \bar{x}+1/2$ [ $u, u, \bar{u}$ ]		
			$x+1/2, \bar{x}+1/2, x+1/2$ [ $u, \bar{u}, u$ ]	$\bar{x}+1/2, x+1/2, x+1/2$ [ $\bar{u}, u, u$ ]		
6	d	222..	0, 1/2, 1/2 [0, 0, 0]	1/2, 0, 1/2 [0, 0, 0]		1/2, 1/2, 0 [0, 0, 0]
			1/2, 0, 0 [0, 0, 0]	0, 1/2, 0 [0, 0, 0]		0, 0, 1/2 [0, 0, 0]
4	c	$\bar{3}$ '	3/4, 3/4, 3/4 [0, 0, 0]	1/4, 1/4, 3/4 [0, 0, 0]	1/4, 3/4, 1/4 [0, 0, 0]	3/4, 1/4, 1/4 0, 0, 0]
4	b	$\bar{3}$ '	1/4, 1/4, 1/4 [0, 0, 0]	3/4, 3/4, 1/4 [0, 0, 0]	3/4, 1/4, 3/4 [0, 0, 0]	1/4, 3/4, 3/4 [0, 0, 0]
2	a	23.	0, 0, 0 [0, 0, 0]	1/2, 1/2, 1/2 [0, 0, 0]		

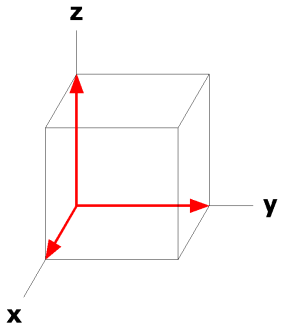
### Symmetry of Special Projections

Along [0, 0, 1]  $c2m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0, 0, z

Along [1, 1, 1]  $p6$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x, x, x

Along [1, 1, 0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x, x, 1/4

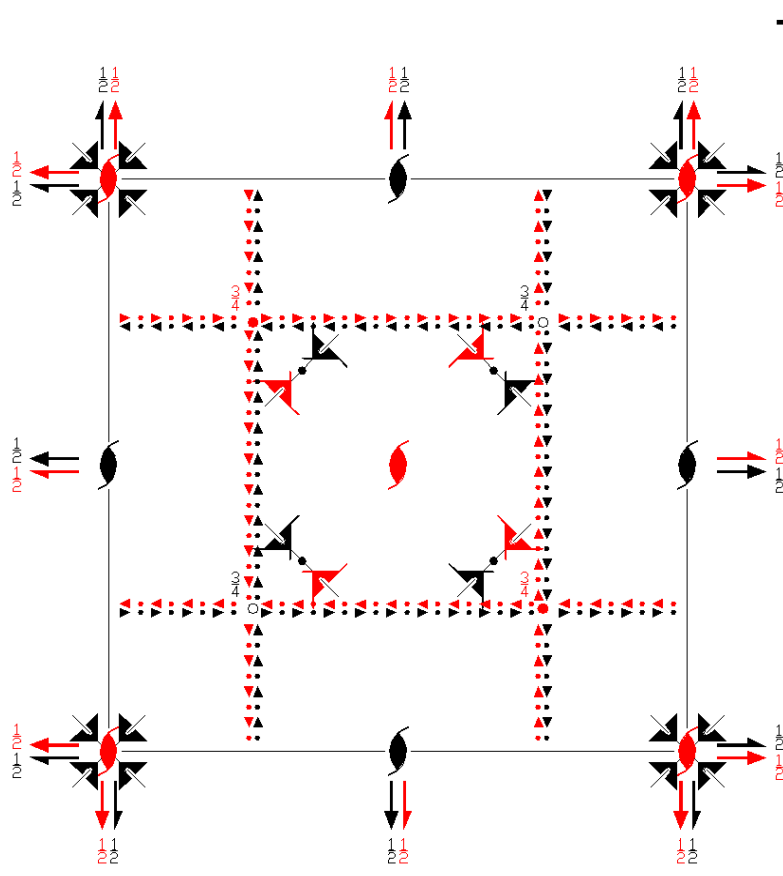
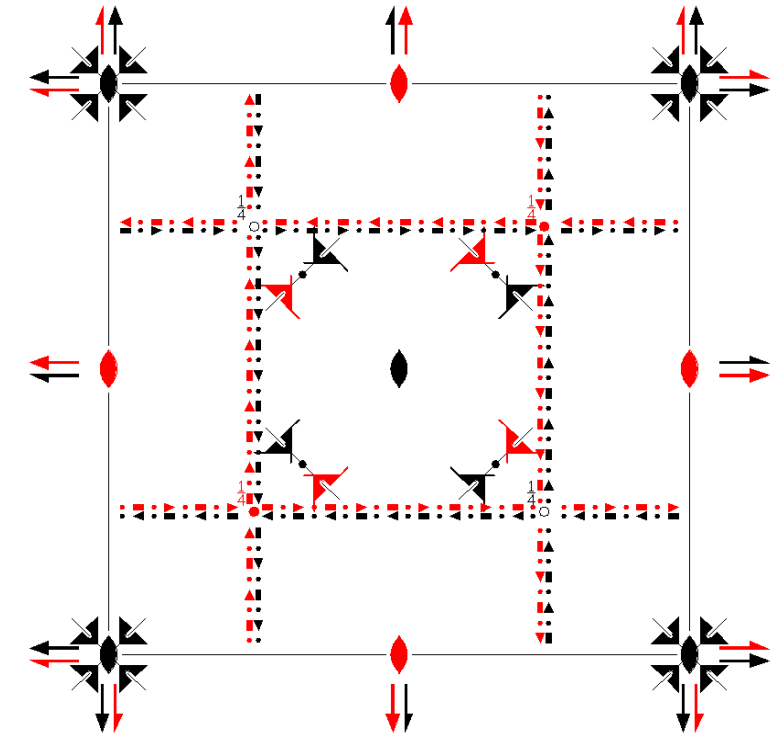
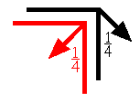




$P_F \bar{n}3$   
201.4.1523

$m\bar{3}1'$   
 $P_F 2/n\bar{3}$

Cubic



**Origin** at 23, at  $-1/4, -1/4, -1/4$  from center ( $\bar{3}$ )

<b>Asymmetric unit</b>	$0 \leq x \leq 1;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$y \leq \min(x, 1-x);$	$z \leq y$
Vertices	0,0,0	1,0,0	1/2,1/2,0	1/2,1/2,1/2	

### Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 2 0,y,0 (2 <sub>y</sub>  0,0,0)	(4) 2 x,0,0 (2 <sub>x</sub>  0,0,0)
(5) 3 <sup>+</sup> x,x,x (3 <sub>xyz</sub>  0,0,0)	(6) 3 <sup>+</sup> $\bar{x}, \bar{x}, \bar{x}$ (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>  0,0,0)	(7) 3 <sup>+</sup> $\bar{x}, \bar{x}, \bar{x}$ (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>  0,0,0)	(8) 3 <sup>+</sup> $\bar{x}, \bar{x}, \bar{x}$ (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>  0,0,0)
(9) 3 <sup>-</sup> x,x,x (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)	(10) 3 <sup>-</sup> $\bar{x}, \bar{x}, \bar{x}$ (3 <sub>xyz</sub>  0,0,0)	(11) 3 <sup>-</sup> $\bar{x}, \bar{x}, \bar{x}$ (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub>  0,0,0)	(12) 3 <sup>-</sup> $\bar{x}, \bar{x}, \bar{x}$ (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub>  0,0,0)
(13) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$  1/2,1/2,1/2)	(14) n (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>  1/2,1/2,1/2)	(15) n (1/2,0,1/2) x,1/4,z (m <sub>y</sub>  1/2,1/2,1/2)	(16) n (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1/2)
(17) 3 <sup>+</sup> x,x,x; 1/4,1/4,1/4 (3 <sub>xyz</sub>  1/2,1/2,1/2)	(18) 3 <sup>+</sup> $\bar{x}-1, \bar{x}+1, \bar{x};$ $-1/4, 1/4, 3/4$ (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1/2,1/2,1/2)	(19) 3 <sup>+</sup> $\bar{x}, \bar{x}+1, \bar{x};$ 1/4,3/4,-1/4 (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1/2,1/2,1/2)	(20) 3 <sup>+</sup> $\bar{x}+1, \bar{x}, \bar{x};$ 3/4,-1/4,1/4 (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1/2,1/2,1/2)
(21) 3 <sup>-</sup> x,x,x; 1/4,1/4,1/4 (3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2)	(22) 3 <sup>-</sup> $\bar{x}+1, \bar{x}-1, \bar{x};$ 1/4,-1/4,3/4 (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub>  1/2,1/2,1/2)	(23) 3 <sup>-</sup> $\bar{x}, \bar{x}+1, \bar{x};$ $-1/4, 3/4, 1/4$ (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub>  1/2,1/2,1/2)	(24) 3 <sup>-</sup> $\bar{x}+1, \bar{x}, \bar{x};$ 3/4,1/4,-1/4 (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub>  1/2,1/2,1/2)

For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 2' 1/2,y,0 (2 <sub>y</sub>  1,0,0)'	(4) 2' (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)'
(5) 3 <sup>+</sup> ' (1/3,1/3,1/3) x+2/3,x+1/3,x (3 <sub>xyz</sub>  1,0,0)'	(6) 3 <sup>+</sup> ' (1/3,-1/3,1/3) x+2/3,x-1/3,x (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1,0,0)'	(7) 3 <sup>+</sup> ' (1/3,-1/3,-1/3) x+2/3,x-1/3,x (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1,0,0)'	(8) 3 <sup>+</sup> ' (1/3,1/3,-1/3) x+2/3,x-1/3,x (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1,0,0)'
(9) 3 <sup>-</sup> ' (1/3,1/3,1/3) x+1/3,x-1/3,x (3 <sub>xyz</sub> <sup>-1</sup>  1,0,0)'	(10) 3 <sup>-</sup> ' (1/3,-1/3,-1/3) x+1/3,x+1/3,x (3 <sub>xyz</sub>  1,0,0)'	(11) 3 <sup>-</sup> ' (1/3,1/3,-1/3) x+1/3,x-1/3,x (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub>  1,0,0)'	(12) 3 <sup>-</sup> ' (1/3,-1/3,1/3) x+1/3,x+1/3,x (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub>  1,0,0)'
(13) $\bar{1}$ ' 3/4,1/4,1/4 ( $\bar{1}$  3/2,1/2,1/2)'	(14) n' (3/2,1/2,0) x,y,1/4 (m <sub>z</sub>  3/2,1/2,1/2)'	(15) n' (3/2,0,1/2) x,1/4,z (m <sub>y</sub>  3/2,1/2,1/2)'	(16) n' (0,1/2,1/2) 3/4,y,z (m <sub>x</sub>  3/2,1/2,1/2)'
(17) 3 <sup>+</sup> ' x,x-1,x; 3/4,1/4,3/4 (3 <sub>xyz</sub>  3/2,1/2,1/2)'	(18) 3 <sup>+</sup> ' $\bar{x}-1, \bar{x}-2, \bar{x};$ 1/4,3/4,5/4 (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>  3/2,1/2,1/2)'	(19) 3 <sup>+</sup> ' $\bar{x}, \bar{x}+2, \bar{x};$ 3/4,5/4,-3/4 (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>  3/2,1/2,1/2)'	(20) 3 <sup>+</sup> ' $\bar{x}+1, \bar{x}-1, \bar{x};$ 5/4,-3/4,-1/4 (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>  3/2,1/2,1/2)'
(21) 3 <sup>-</sup> ' x+1,x+1,x; 3/4,3/4,-1/4 (3 <sub>xyz</sub> <sup>-1</sup>  3/2,1/2,1/2)'	(22) 3 <sup>-</sup> ' $\bar{x}+2, \bar{x}-2, \bar{x};$ 3/4,-3/4,5/4 (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub>  3/2,1/2,1/2)'	(23) 3 <sup>-</sup> ' $\bar{x}+1, \bar{x}+2, \bar{x};$ 1/4,5/4,3/4 (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub>  3/2,1/2,1/2)'	(24) 3 <sup>-</sup> ' $\bar{x}+2, \bar{x}-1, \bar{x};$ 5/4,-1/4,-3/4 (3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub>  3/2,1/2,1/2)'

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5); (13).

**Positions**

**Coordinates**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

(0,0,0) + (1,0,0)' +

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(1)  $x, y, z [u, v, w]$  (2)  $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$  (3)  $\bar{x}, y, \bar{z} [\bar{u}, v, \bar{w}]$  (4)  $x, \bar{y}, \bar{z} [u, \bar{v}, \bar{w}]$   
 (5)  $z, x, y [w, u, v]$  (6)  $z, \bar{x}, \bar{y} [w, \bar{u}, \bar{v}]$  (7)  $\bar{z}, \bar{x}, y [\bar{w}, \bar{u}, v]$  (8)  $\bar{z}, x, \bar{y} [\bar{w}, u, \bar{v}]$   
 (9)  $y, z, x [v, w, u]$  (10)  $\bar{y}, z, \bar{x} [\bar{v}, w, \bar{u}]$  (11)  $y, \bar{z}, \bar{x} [v, \bar{w}, \bar{u}]$  (12)  $\bar{y}, \bar{z}, x [\bar{v}, \bar{w}, u]$

(13)  $\bar{x}+1/2, \bar{y}+1/2, \bar{z}+1/2 [u, v, w]$  (14)  $x+1/2, y+1/2, \bar{z}+1/2 [\bar{u}, \bar{v}, w]$  (15)  $x+1/2, \bar{y}+1/2, z+1/2 [\bar{u}, v, \bar{w}]$  (16)  $\bar{x}+1/2, y+1/2, z+1/2 [u, \bar{v}, \bar{w}]$   
 (17)  $\bar{z}+1/2, \bar{x}+1/2, \bar{y}+1/2 [w, u, v]$  (18)  $\bar{z}+1/2, x+1/2, y+1/2 [w, \bar{u}, \bar{v}]$  (19)  $z+1/2, x+1/2, \bar{y}+1/2 [\bar{w}, \bar{u}, v]$  (20)  $z+1/2, \bar{x}+1/2, y+1/2 [\bar{w}, u, \bar{v}]$   
 (21)  $\bar{y}+1/2, \bar{z}+1/2, \bar{x}+1/2 [v, w, u]$  (22)  $y+1/2, \bar{z}+1/2, x+1/2 [\bar{v}, w, \bar{u}]$  (23)  $\bar{y}+1/2, z+1/2, x+1/2 [v, \bar{w}, \bar{u}]$  (24)  $y+1/2, z+1/2, \bar{x}+1/2 [\bar{v}, \bar{w}, u]$

24 g 2'..  $x, 1/2, 0 [0, v, w]$   $\bar{x}, 1/2, 0 [0, v, \bar{w}]$   $0, x, 1/2 [w, 0, v]$   
 $0, \bar{x}, 1/2 [\bar{w}, 0, v]$   $1/2, 0, x [v, w, 0]$   $1/2, 0, \bar{x} [v, \bar{w}, 0]$   
 $\bar{x}+1/2, 0, 1/2 [0, v, w]$   $x+1/2, 0, 1/2 [0, v, \bar{w}]$   $1/2, \bar{x}+1/2, 0 [w, 0, v]$   
 $1/2, x+1/2, 0 [\bar{w}, 0, v]$   $0, 1/2, \bar{x}+1/2 [v, w, 0]$   $0, 1/2, x+1/2 [v, \bar{w}, 0]$

24 f 2..  $x, 0, 0 [u, 0, 0]$   $\bar{x}, 0, 0 [\bar{u}, 0, 0]$   $0, x, 0 [0, u, 0]$   
 $0, \bar{x}, 0 [0, \bar{u}, 0]$   $0, 0, x [0, 0, u]$   $0, 0, \bar{x} [0, 0, \bar{u}]$   
 $\bar{x}+1/2, 1/2, 1/2 [u, 0, 0]$   $x+1/2, 1/2, 1/2 [\bar{u}, 0, 0]$   $1/2, \bar{x}+1/2, 1/2 [0, u, 0]$   
 $1/2, x+1/2, 1/2 [0, \bar{u}, 0]$   $1/2, 1/2, \bar{x}+1/2 [0, 0, u]$   $1/2, 1/2, x+1/2 [0, 0, \bar{u}]$

16 e .3.  $x, x, x [u, u, u]$   $\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$   
 $\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$   $x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$   
 $\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [u, u, u]$   $x+1/2, x+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, u]$   
 $x+1/2, \bar{x}+1/2, x+1/2 [\bar{u}, u, \bar{u}]$   $\bar{x}+1/2, x+1/2, x+1/2 [u, \bar{u}, \bar{u}]$

12 d 22'2'..  $0, 1/2, 1/2 [u, 0, 0]$   $1/2, 0, 1/2 [0, u, 0]$   $1/2, 1/2, 0 [0, 0, u]$   
 $1/2, 0, 0 [u, 0, 0]$   $0, 1/2, 0 [0, u, 0]$   $0, 0, 1/2 [0, 0, u]$

4 c  $\bar{3}'$ .  $3/4, 3/4, 3/4 [0, 0, 0]$   $1/4, 1/4, 3/4 [0, 0, 0]$   $1/4, 3/4, 1/4 [0, 0, 0]$   $3/4, 1/4, 1/4 [0, 0, 0]$

4 b  $\bar{3}$ .  $1/4, 1/4, 1/4 [u, u, u]$   $3/4, 3/4, 1/4 [\bar{u}, \bar{u}, u]$   $3/4, 1/4, 3/4 [\bar{u}, u, \bar{u}]$   $1/4, 3/4, 3/4 [u, \bar{u}, \bar{u}]$

2 a 23.  $0, 0, 0 [0, 0, 0]$   $1/2, 1/2, 1/2 [0, 0, 0]$

Continued

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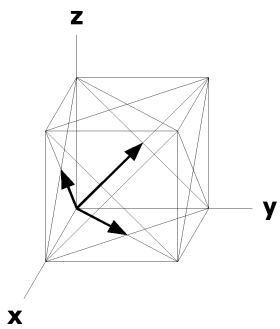
$P_{\bar{3}} n \bar{3}$

## Symmetry of Special Projections

Along  $[0,0,1]$   $c2mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at  $0,0,z$

Along  $[1,1,1]$   $p61'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
Origin at  $x,x,x$

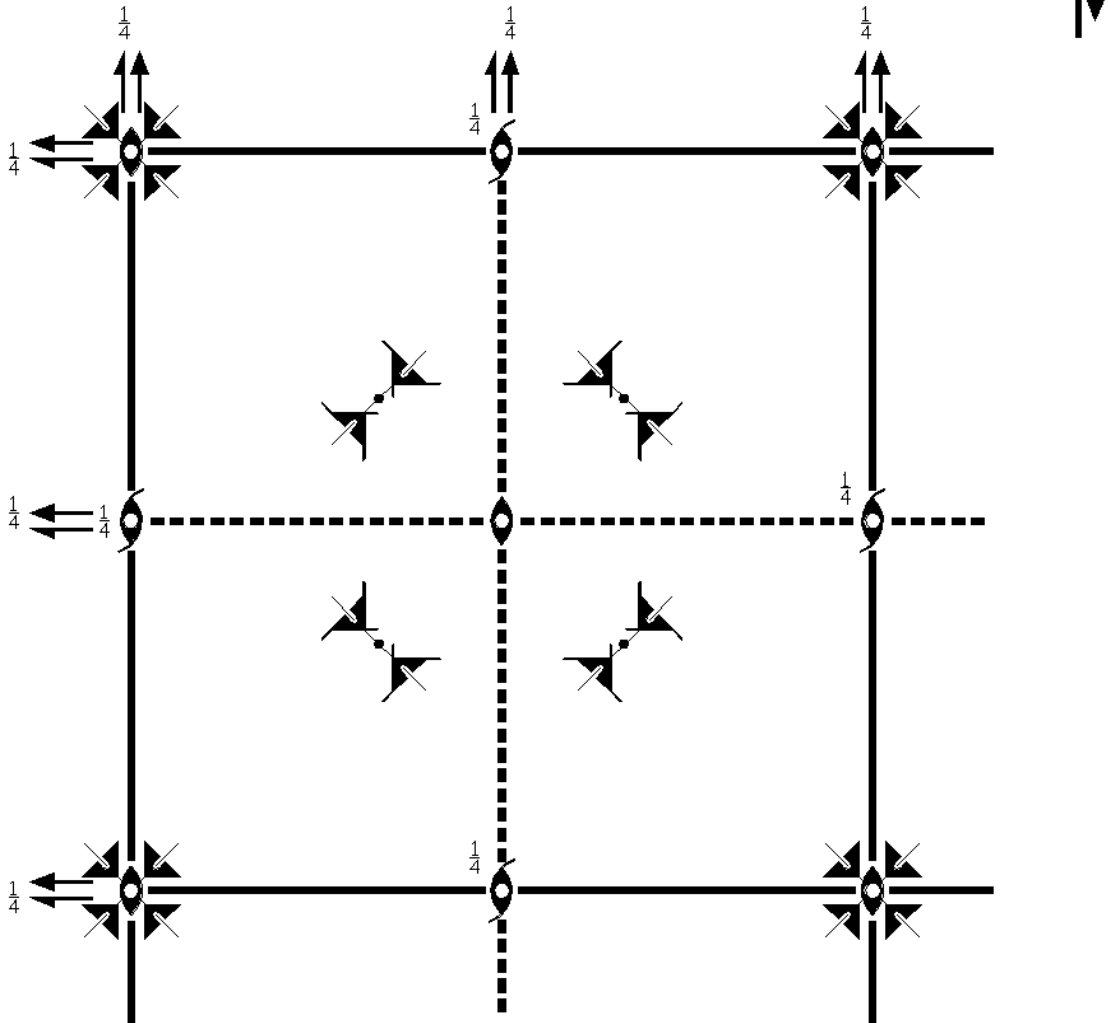
Along  $[1,1,0]$   $p_62mm$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x-1/4, x+1/4, 1/4$



$Fm\bar{3}$   
202.1.1524

$m\bar{3}$   
 $F2/m\bar{3}$

Cubic



**Origin** at center ( $m\bar{3}$ )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq x;$   $z \leq \min(1/2-x, y)$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/4,1/4,1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                  | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                                  | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                 |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)        | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}y\bar{z}}$  0,0,0) |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}y\bar{z}}$  0,0,0) | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{\bar{x}yz}$  0,0,0)      |

Continued

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$Fm\bar{3}$

- |   |  |   |  |
|---|--|---|--|
| (13) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)                     | (14) m x,y,0<br>( $m_z$  0,0,0)  | (15) m x,0,z<br>( $m_y$  0,0,0)   | (16) m 0,y,z<br>( $m_x$  0,0,0)  |
| (17) $\bar{3}^+$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$  0,0,0)      | (18) $\bar{3}^+$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,0,0) | (19) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,0,0) | (20) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,0,0) |
| (21) $\bar{3}^-$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}^{-1}$  0,0,0) | (22) $\bar{3}^-$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)     | (23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)       | (24) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)      |

For (0,1/2,1/2) + set

- |  |  |   |   |
|--|--|---|---|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2)   | (2) 2 (0,0,1/2) 0,1/4,z<br>( $2_z$  0,1/2,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>( $2_y$  0,1/2,1/2)  | (4) 2 x,1/4,1/4<br>( $2_x$  0,1/2,1/2)  |
| (5) $3^+$ (1/3,1/3,1/3)<br>x-1/3,x-1/6,x<br>( $3_{xyz}$  0,1/2,1/2)              | (6) $3^+$ $\bar{x}$ ,x+1/2, $\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  0,1/2,1/2)                                | (7) $3^+$ (-1/3,1/3,1/3)<br>x+1/3, $\bar{x}$ -1/6, $\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  0,1/2,1/2)      | (8) $3^+$ $\bar{x}$ , $\bar{x}$ +1/2,x<br>( $3_{x\bar{y}z}^{-1}$  0,1/2,1/2)                              |
| (9) $3^-$ (1/3,1/3,1/3)<br>x-1/6,x+1/6,x<br>( $3_{xyz}^{-1}$  0,1/2,1/2)         | (10) $3^-$ (-1/3,1/3,1/3)<br>x+1/6,x+1/6, $\bar{x}$<br>( $3_{x\bar{y}z}$  0,1/2,1/2)                       | (11) $3^-$ $\bar{x}$ +1/2, $\bar{x}$ +1/2,x<br>( $3_{x\bar{y}z}$  0,1/2,1/2)                            | (12) $3^-$ $\bar{x}$ -1/2,x+1/2, $\bar{x}$<br>( $3_{x\bar{y}z}$  0,1/2,1/2)                               |
| (13) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$  0,1/2,1/2)                              | (14) b (0,1/2,0) x,y,1/4<br>( $m_z$  0,1/2,1/2)  | (15) c (0,0,1/2) x,1/4,z<br>( $m_y$  0,1/2,1/2)   | (16) n (0,1/2,1/2) 0,y,z<br>( $m_x$  0,1/2,1/2)   |
| (17) $\bar{3}^+$ x,x+1/2,x;<br>0,1/2,0<br>( $\bar{3}_{xyz}$  0,1/2,1/2)          | (18) $\bar{3}^+$ $\bar{x}$ -1,x+1/2, $\bar{x}$ ;<br>-1/2,0,1/2<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,1/2,1/2) | (19) $\bar{3}^+$ x, $\bar{x}$ +1/2, $\bar{x}$ ;<br>0,1/2,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,1/2,1/2)  | (20) $\bar{3}^+$ $\bar{x}$ -1, $\bar{x}$ +1/2,x;<br>1/2,0,1/2<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,1/2,1/2) |
| (21) $\bar{3}^-$ x-1/2,x-1/2,x;<br>0,0,1/2<br>( $\bar{3}_{xyz}^{-1}$  0,1/2,1/2) | (22) $\bar{3}^-$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ;<br>0,0,1/2<br>( $\bar{3}_{x\bar{y}z}$  0,1/2,1/2)      | (23) $\bar{3}^-$ $\bar{x}$ -1/2, $\bar{x}$ +1/2,x;<br>-1/2,1/2,0<br>( $\bar{3}_{x\bar{y}z}$  0,1/2,1/2) | (24) $\bar{3}^-$ $\bar{x}$ +1/2,x+1/2, $\bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{x\bar{y}z}$  0,1/2,1/2)    |

For (1/2,0,1/2) + set

- |  |   |  |  |
|--|---|--|--|
| (1) t (1/2,0,1/2)<br>(1 1/2,0,1/2)   | (2) 2 (0,0,1/2) 1/4,0,z<br>( $2_z$  1/2,0,1/2)  | (3) 2 1/4,y,1/4<br>( $2_y$  1/2,0,1/2)   | (4) 2 (1/2,0,0) x,0,1/4<br>( $2_x$  1/2,0,1/2)   |
| (5) $3^+$ (1/3,1/3,1/3)<br>x+1/6,x-1/6,x<br>( $3_{xyz}$  1/2,0,1/2)          | (6) $3^+$ (1/3,-1/3,1/3)<br>x+1/6,x+1/6, $\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  1/2,0,1/2)                  | (7) $3^+$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  1/2,0,1/2)                             | (8) $3^+$ $\bar{x}$ +1/2, $\bar{x}$ +1/2,x<br>( $3_{x\bar{y}z}^{-1}$  1/2,0,1/2)                             |
| (9) $3^-$ (1/3,1/3,1/3)<br>x-1/6,x-1/3,x<br>( $3_{xyz}^{-1}$  1/2,0,1/2)     | (10) $3^-$ x+1/2, $\bar{x}$ , $\bar{x}$<br>( $3_{x\bar{y}z}$  1/2,0,1/2)                                  | (11) $3^-$ $\bar{x}$ +1/2, $\bar{x}$ ,x<br>( $3_{x\bar{y}z}$  1/2,0,1/2)                                     | (12) $3^-$ (1/3,-1/3,1/3)<br>x-1/6,x+1/3, $\bar{x}$<br>( $3_{x\bar{y}z}$  1/2,0,1/2)                         |
| (13) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$  1/2,0,1/2)                          | (14) a (1/2,0,0) x,y,1/4<br>( $m_z$  1/2,0,1/2)   | (15) n (1/2,0,1/2) x,0,z<br>( $m_y$  1/2,0,1/2)  | (16) c (0,0,1/2) 1/4,y,z<br>( $m_x$  1/2,0,1/2)  |
| (17) $\bar{3}^+$ x-1/2,x-1/2,x;<br>0,0,1/2<br>( $\bar{3}_{xyz}$  1/2,0,1/2)  | (18) $\bar{3}^+$ $\bar{x}$ -1/2,x+1/2, $\bar{x}$ ;<br>0,0,1/2<br>( $\bar{3}_{x\bar{y}z}^{-1}$  1/2,0,1/2) | (19) $\bar{3}^+$ x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  1/2,0,1/2) | (20) $\bar{3}^+$ $\bar{x}$ +1/2, $\bar{x}$ -1/2,x;<br>1/2,-1/2,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  1/2,0,1/2) |
| (21) $\bar{3}^-$ x+1/2,x,x;<br>1/2,0,0<br>( $\bar{3}_{xyz}^{-1}$  1/2,0,1/2) | (22) $\bar{3}^-$ x+1/2, $\bar{x}$ -1, $\bar{x}$ ;<br>0,-1/2,1/2<br>( $\bar{3}_{x\bar{y}z}$  1/2,0,1/2)    | (23) $\bar{3}^-$ $\bar{x}$ +1/2, $\bar{x}$ +1,x;<br>0,1/2,1/2<br>( $\bar{3}_{x\bar{y}z}$  1/2,0,1/2)         | (24) $\bar{3}^-$ $\bar{x}$ +1/2,x, $\bar{x}$ ;<br>1/2,0,0<br>( $\bar{3}_{x\bar{y}z}$  1/2,0,1/2)             |

Continued

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Fm $\bar{3}$

For (1/2,1/2,0) + set

(1) $t \left( \frac{1}{2}, \frac{1}{2}, 0 \right)$ $(1 \mid \frac{1}{2}, \frac{1}{2}, 0)$	(2) $2 \left( \frac{1}{4}, \frac{1}{4}, z \right)$ $(2_z \mid \frac{1}{2}, \frac{1}{2}, 0)$	(3) $2 \left( 0, \frac{1}{2}, 0 \right) \frac{1}{4}, y, 0$ $(2_y \mid \frac{1}{2}, \frac{1}{2}, 0)$	(4) $2 \left( \frac{1}{2}, 0, 0 \right) x, \frac{1}{4}, 0$ $(2_x \mid \frac{1}{2}, \frac{1}{2}, 0)$
(5) $3^+ \left( \frac{1}{3}, \frac{1}{3}, \frac{1}{3} \right)$ $x+1/6, x+1/3, x$ $(3_{xyz} \mid \frac{1}{2}, \frac{1}{2}, 0)$	(6) $3^+ \bar{x}+1/2, x, \bar{x}$ $(3_{\bar{xyz}}^{-1} \mid \frac{1}{2}, \frac{1}{2}, 0)$	(7) $3^+ x+1/2, \bar{x}, \bar{x}$ $(3_{\bar{xyz}}^{-1} \mid \frac{1}{2}, \frac{1}{2}, 0)$	(8) $3^+ \left( \frac{1}{3}, \frac{1}{3}, -\frac{1}{3} \right)$ $\bar{x}+1/6, \bar{x}+1/3, x$ $(3_{\bar{xyz}}^{-1} \mid \frac{1}{2}, \frac{1}{2}, 0)$
(9) $3^- \left( \frac{1}{3}, \frac{1}{3}, \frac{1}{3} \right)$ $x+1/3, x+1/6, x$ $(3_{xyz}^{-1} \mid \frac{1}{2}, \frac{1}{2}, 0)$	(10) $3^- x, \bar{x}+1/2, \bar{x}$ $(3_{\bar{xyz}} \mid \frac{1}{2}, \frac{1}{2}, 0)$	(11) $3^- \left( \frac{1}{3}, \frac{1}{3}, -\frac{1}{3} \right)$ $\bar{x}+1/3, \bar{x}+1/6, x$ $(3_{\bar{yz}} \mid \frac{1}{2}, \frac{1}{2}, 0)$	(12) $3^- \bar{x}, x+1/2, \bar{x}$ $(3_{\bar{yz}} \mid \frac{1}{2}, \frac{1}{2}, 0)$
(13) $\bar{1} \left( \frac{1}{4}, \frac{1}{4}, 0 \right)$ $(\bar{1} \mid \frac{1}{2}, \frac{1}{2}, 0)$	(14) $n \left( \frac{1}{2}, \frac{1}{2}, 0 \right) x, y, 0$ $(m_z \mid \frac{1}{2}, \frac{1}{2}, 0)$	(15) $a \left( \frac{1}{2}, 0, 0 \right) x, \frac{1}{4}, z$ $(m_y \mid \frac{1}{2}, \frac{1}{2}, 0)$	(16) $b \left( 0, \frac{1}{2}, 0 \right) \frac{1}{4}, y, z$ $(m_x \mid \frac{1}{2}, \frac{1}{2}, 0)$
(17) $\bar{3}^+ x+1/2, x, x;$ $\frac{1}{2}, 0, 0$ $(\bar{3}_{xyz} \mid \frac{1}{2}, \frac{1}{2}, 0)$	(18) $\bar{3}^+ \bar{x}-1/2, x+1, \bar{x};$ $0, \frac{1}{2}, \frac{1}{2}$ $(\bar{3}_{\bar{xyz}}^{-1} \mid \frac{1}{2}, \frac{1}{2}, 0)$	(19) $\bar{3}^+ x-1/2, \bar{x}+1, \bar{x};$ $0, \frac{1}{2}, -\frac{1}{2}$ $(\bar{3}_{\bar{yz}}^{-1} \mid \frac{1}{2}, \frac{1}{2}, 0)$	(20) $\bar{3}^+ \bar{x}+1/2, \bar{x}, x;$ $\frac{1}{2}, 0, 0$ $(\bar{3}_{\bar{yz}}^{-1} \mid \frac{1}{2}, \frac{1}{2}, 0)$
(21) $\bar{3}^- x, x+1/2, x;$ $0, \frac{1}{2}, 0$ $(\bar{3}_{xyz}^{-1} \mid \frac{1}{2}, \frac{1}{2}, 0)$	(22) $\bar{3}^- x+1, \bar{x}-1/2, \bar{x};$ $\frac{1}{2}, 0, \frac{1}{2}$ $(\bar{3}_{\bar{yz}} \mid \frac{1}{2}, \frac{1}{2}, 0)$	(23) $\bar{3}^- \bar{x}, \bar{x}+1/2, x;$ $0, \frac{1}{2}, 0$ $(\bar{3}_{\bar{yz}} \mid \frac{1}{2}, \frac{1}{2}, 0)$	(24) $\bar{3}^- \bar{x}+1, x-1/2, \bar{x};$ $\frac{1}{2}, 0, -\frac{1}{2}$ $(\bar{3}_{\bar{yz}} \mid \frac{1}{2}, \frac{1}{2}, 0)$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

96	i	1	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +					
(1)	x, y, z	[u, v, w]	(2)	$\bar{x}, \bar{y}, z$	[ $\bar{u}, \bar{v}, w$ ]	(3)	$\bar{x}, y, \bar{z}$	[ $\bar{u}, v, \bar{w}$ ]	(4)	$x, \bar{y}, \bar{z}$	[ $u, \bar{v}, \bar{w}$ ]
(5)	z, x, y	[w, u, v]	(6)	$\bar{z}, \bar{x}, \bar{y}$	[ $\bar{w}, \bar{u}, \bar{v}$ ]	(7)	$\bar{z}, \bar{x}, y$	[ $\bar{w}, \bar{u}, v$ ]	(8)	$\bar{z}, x, \bar{y}$	[ $\bar{w}, u, \bar{v}$ ]
(9)	y, z, x	[v, w, u]	(10)	$\bar{y}, \bar{z}, \bar{x}$	[ $\bar{v}, \bar{w}, \bar{u}$ ]	(11)	$\bar{y}, \bar{z}, x$	[ $\bar{v}, \bar{w}, u$ ]	(12)	$\bar{y}, z, \bar{x}$	[ $\bar{v}, w, \bar{u}$ ]
(13)	$\bar{x}, \bar{y}, \bar{z}$	[ $\bar{u}, \bar{v}, \bar{w}$ ]	(14)	$x, y, \bar{z}$	[ $u, v, \bar{w}$ ]	(15)	$x, \bar{y}, z$	[ $u, \bar{v}, w$ ]	(16)	$\bar{x}, y, z$	[ $u, v, \bar{w}$ ]
(17)	$\bar{z}, \bar{x}, \bar{y}$	[ $\bar{w}, \bar{u}, \bar{v}$ ]	(18)	$\bar{z}, x, y$	[ $\bar{w}, u, \bar{v}$ ]	(19)	$z, x, \bar{y}$	[ $w, u, \bar{v}$ ]	(20)	$z, \bar{x}, y$	[ $w, \bar{u}, \bar{v}$ ]
(21)	$\bar{y}, \bar{z}, \bar{x}$	[ $\bar{v}, \bar{w}, \bar{u}$ ]	(22)	$y, \bar{z}, x$	[ $v, \bar{w}, \bar{u}$ ]	(23)	$\bar{y}, z, x$	[ $\bar{v}, w, \bar{u}$ ]	(24)	$y, z, \bar{x}$	[ $v, w, \bar{u}$ ]
48	h	m..	0, y, z	[u, 0, 0]	0, $\bar{y}, z$	[ $\bar{u}, 0, 0$ ]	0, y, $\bar{z}$	[ $\bar{u}, 0, 0$ ]			
			0, $\bar{y}, \bar{z}$	[u, 0, 0]	z, 0, y	[0, u, 0]	z, 0, $\bar{y}$	[0, $\bar{u}, 0$ ]			
			$\bar{z}, 0, y$	[0, $\bar{u}, 0$ ]	$\bar{z}, 0, \bar{y}$	[0, u, 0]	y, z, 0	[0, 0, u]			
			$\bar{y}, z, 0$	[0, 0, $\bar{u}$ ]	$\bar{y}, \bar{z}, 0$	[0, 0, $\bar{u}$ ]	$\bar{y}, \bar{z}, 0$	[0, 0, u]			

Continued

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Fm $\bar{3}$

48	g	2..	x,1/4,1/4 [u,0,0]	$\bar{x},3/4,1/4 [\bar{u},0,0]$	1/4,x,1/4 [0,u,0]	
			1/4, $\bar{x},3/4 [0,\bar{u},0]$	1/4,1/4,x [0,0,u]	3/4,1/4, $\bar{x} [0,0,\bar{u}]$	
			$\bar{x},3/4,3/4 [u,0,0]$	x,1/4,3/4 [ $\bar{u},0,0]$	3/4, $\bar{x},3/4 [0,u,0]$	
			3/4,x,1/4 [0, $\bar{u},0]$	3/4,3/4, $\bar{x} [0,0,u]$	1/4,3/4,x [0,0, $\bar{u}]$	
32	f	.3.	x,x,x [u,u,u]	$\bar{x},\bar{x},x [\bar{u},\bar{u},u]$	$\bar{x},x,\bar{x} [\bar{u},u,\bar{u}]$	x, $\bar{x},\bar{x} [u,\bar{u},\bar{u}]$
			$\bar{x},\bar{x},\bar{x} [u,u,u]$	x,x, $\bar{x} [\bar{u},\bar{u},u]$	$\bar{x},\bar{x},x [\bar{u},u,\bar{u}]$	$\bar{x},x,x [u,\bar{u},\bar{u}]$
24	e	mm2..	x,0,0 [0,0,0]	$\bar{x},0,0 [0,0,0]$	0,x,0 [0,0,0]	
			0, $\bar{x},0 [0,0,0]$	0,0,x [0,0,0]	0,0, $\bar{x} [0,0,0]$	
24	d	2/m..	0,1/4,1/4 [u,0,0]	0,3/4,1/4 [ $\bar{u},0,0]$	1/4,0,1/4 [0,u,0]	
			1/4,0,3/4 [0, $\bar{u},0]$	1/4,1/4,0 [0,0,u]	3/4,1/4,0 [0,0, $\bar{u}]$	
8	c	23.	1/4,1/4,1/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]		
4	b	$m\bar{3}$ .	1/2,1/2,1/2 [0,0,0]			
4	a	$m\bar{3}$ .	0,0,0 [0,0,0]			

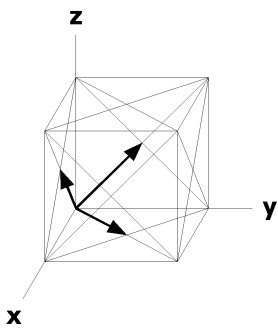
### Symmetry of Special Projections

Along [0,0,1]  $p2mm1'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,1,1]  $p6'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

Along [1,1,0]  $c2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = -(-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0





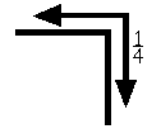
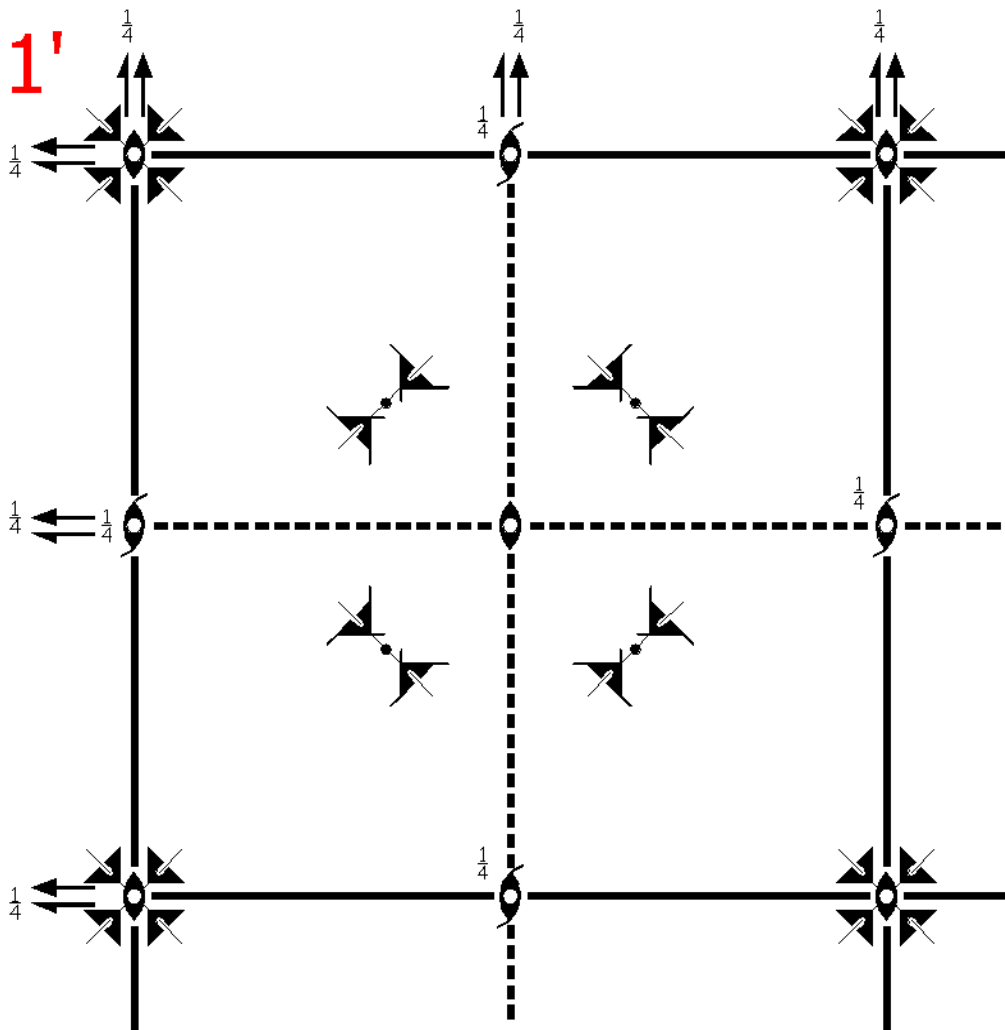
$Fm\bar{3}1'$

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$m\bar{3}1'$

$F2/m\bar{3}1'$

Cubic



Origin at center ( $m\bar{3}1'$ )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq x;$   $z \leq \min(1/2-x,y)$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/4,1/4,1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)              |

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$Fm\bar{3}1'$

- |   |  |   |  |
|---|--|---|--|
| (13) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)                     | (14) m x,y,0<br>( $m_z$  0,0,0)  | (15) m x,0,z<br>( $m_y$  0,0,0)   | (16) m 0,y,z<br>( $m_x$  0,0,0)  |
| (17) $\bar{3}^+$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$  0,0,0)      | (18) $\bar{3}^+$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,0,0) | (19) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,0,0) | (20) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,0,0) |
| (21) $\bar{3}^-$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}^{-1}$  0,0,0) | (22) $\bar{3}^-$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)     | (23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)       | (24) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)      |

For (0,1/2,1/2) + set

- |  |  |   |   |
|--|--|---|---|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2)   | (2) 2 (0,0,1/2) 0,1/4,z<br>( $2_z$  0,1/2,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>( $2_y$  0,1/2,1/2)  | (4) 2 x,1/4,1/4<br>( $2_x$  0,1/2,1/2)  |
| (5) $3^+$ (1/3,1/3,1/3)<br>x-1/3,x-1/6,x<br>( $3_{xyz}$  0,1/2,1/2)              | (6) $3^+$ $\bar{x}$ ,x+1/2, $\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  0,1/2,1/2)                                | (7) $3^+$ (-1/3,1/3,1/3)<br>x+1/3, $\bar{x}$ -1/6, $\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  0,1/2,1/2)      | (8) $3^+$ $\bar{x}$ , $\bar{x}$ +1/2,x<br>( $3_{x\bar{y}z}^{-1}$  0,1/2,1/2)                              |
| (9) $3^-$ (1/3,1/3,1/3)<br>x-1/6,x+1/6,x<br>( $3_{xyz}^{-1}$  0,1/2,1/2)         | (10) $3^-$ (-1/3,1/3,1/3)<br>x+1/6,x+1/6, $\bar{x}$<br>( $3_{x\bar{y}z}$  0,1/2,1/2)                       | (11) $3^-$ $\bar{x}$ +1/2, $\bar{x}$ +1/2,x<br>( $3_{x\bar{y}z}$  0,1/2,1/2)                            | (12) $3^-$ $\bar{x}$ -1/2,x+1/2, $\bar{x}$<br>( $3_{x\bar{y}z}$  0,1/2,1/2)                               |
| (13) $\bar{1}$ 0,1/4,1/4<br>( $\bar{1}$  0,1/2,1/2)                              | (14) b (0,1/2,0) x,y,1/4<br>( $m_z$  0,1/2,1/2)  | (15) c (0,0,1/2) x,1/4,z<br>( $m_y$  0,1/2,1/2)   | (16) n (0,1/2,1/2) 0,y,z<br>( $m_x$  0,1/2,1/2)   |
| (17) $\bar{3}^+$ x,x+1/2,x;<br>0,1/2,0<br>( $\bar{3}_{xyz}$  0,1/2,1/2)          | (18) $\bar{3}^+$ $\bar{x}$ -1,x+1/2, $\bar{x}$ ;<br>-1/2,0,1/2<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,1/2,1/2) | (19) $\bar{3}^+$ x, $\bar{x}$ +1/2, $\bar{x}$ ;<br>0,1/2,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,1/2,1/2)  | (20) $\bar{3}^+$ $\bar{x}$ -1, $\bar{x}$ +1/2,x;<br>1/2,0,1/2<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,1/2,1/2) |
| (21) $\bar{3}^-$ x-1/2,x-1/2,x;<br>0,0,1/2<br>( $\bar{3}_{xyz}^{-1}$  0,1/2,1/2) | (22) $\bar{3}^-$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ;<br>0,0,1/2<br>( $\bar{3}_{x\bar{y}z}$  0,1/2,1/2)      | (23) $\bar{3}^-$ $\bar{x}$ -1/2, $\bar{x}$ +1/2,x;<br>-1/2,1/2,0<br>( $\bar{3}_{x\bar{y}z}$  0,1/2,1/2) | (24) $\bar{3}^-$ $\bar{x}$ +1/2,x+1/2, $\bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{x\bar{y}z}$  0,1/2,1/2)    |

For (1/2,0,1/2) + set

- |  |   |  |  |
|--|---|--|--|
| (1) t (1/2,0,1/2)<br>(1 1/2,0,1/2)   | (2) 2 (0,0,1/2) 1/4,0,z<br>( $2_z$  1/2,0,1/2)  | (3) 2 1/4,y,1/4<br>( $2_y$  1/2,0,1/2)   | (4) 2 (1/2,0,0) x,0,1/4<br>( $2_x$  1/2,0,1/2)   |
| (5) $3^+$ (1/3,1/3,1/3)<br>x+1/6,x-1/6,x<br>( $3_{xyz}$  1/2,0,1/2)          | (6) $3^+$ (1/3,-1/3,1/3)<br>x+1/6,x+1/6, $\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  1/2,0,1/2)                  | (7) $3^+$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  1/2,0,1/2)                             | (8) $3^+$ $\bar{x}$ +1/2, $\bar{x}$ +1/2,x<br>( $3_{x\bar{y}z}^{-1}$  1/2,0,1/2)                             |
| (9) $3^-$ (1/3,1/3,1/3)<br>x-1/6,x-1/3,x<br>( $3_{xyz}^{-1}$  1/2,0,1/2)     | (10) $3^-$ x+1/2, $\bar{x}$ , $\bar{x}$<br>( $3_{x\bar{y}z}$  1/2,0,1/2)                                  | (11) $3^-$ $\bar{x}$ +1/2, $\bar{x}$ ,x<br>( $3_{x\bar{y}z}$  1/2,0,1/2)                                     | (12) $3^-$ (1/3,-1/3,1/3)<br>x-1/6,x+1/3, $\bar{x}$<br>( $3_{x\bar{y}z}$  1/2,0,1/2)                         |
| (13) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$  1/2,0,1/2)                          | (14) a (1/2,0,0) x,y,1/4<br>( $m_z$  1/2,0,1/2)   | (15) n (1/2,0,1/2) x,0,z<br>( $m_y$  1/2,0,1/2)  | (16) c (0,0,1/2) 1/4,y,z<br>( $m_x$  1/2,0,1/2)  |
| (17) $\bar{3}^+$ x-1/2,x-1/2,x;<br>0,0,1/2<br>( $\bar{3}_{xyz}$  1/2,0,1/2)  | (18) $\bar{3}^+$ $\bar{x}$ -1/2,x+1/2, $\bar{x}$ ;<br>0,0,1/2<br>( $\bar{3}_{x\bar{y}z}^{-1}$  1/2,0,1/2) | (19) $\bar{3}^+$ x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  1/2,0,1/2) | (20) $\bar{3}^+$ $\bar{x}$ +1/2, $\bar{x}$ -1/2,x;<br>1/2,-1/2,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  1/2,0,1/2) |
| (21) $\bar{3}^-$ x+1/2,x,x;<br>1/2,0,0<br>( $\bar{3}_{xyz}^{-1}$  1/2,0,1/2) | (22) $\bar{3}^-$ x+1/2, $\bar{x}$ -1, $\bar{x}$ ;<br>0,-1/2,1/2<br>( $\bar{3}_{x\bar{y}z}$  1/2,0,1/2)    | (23) $\bar{3}^-$ $\bar{x}$ +1/2, $\bar{x}$ +1,x;<br>0,1/2,1/2<br>( $\bar{3}_{x\bar{y}z}$  1/2,0,1/2)         | (24) $\bar{3}^-$ $\bar{x}$ +1/2,x, $\bar{x}$ ;<br>1/2,0,0<br>( $\bar{3}_{x\bar{y}z}$  1/2,0,1/2)             |

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Fm $\bar{3}1'$

For (1/2,1/2,0) + set

- |  |  |  |   |
|--|--|--|---|
| (1) $t \begin{pmatrix} 1/2, 1/2, 0 \\ (1   1/2, 1/2, 0) \end{pmatrix}$                                   | (2) $2 \begin{pmatrix} 1/4, 1/4, z \\ (2_z   1/2, 1/2, 0) \end{pmatrix}$   | (3) $2 \begin{pmatrix} (0, 1/2, 0) \quad 1/4, y, 0 \\ (2_y   1/2, 1/2, 0) \end{pmatrix}$                                       | (4) $2 \begin{pmatrix} (1/2, 0, 0) \quad x, 1/4, 0 \\ (2_x   1/2, 1/2, 0) \end{pmatrix}$                                    |
| (5) $3^+ \begin{pmatrix} 1/3, 1/3, 1/3 \\ x+1/6, x+1/3, x \\ (3_{xyz}   1/2, 1/2, 0) \end{pmatrix}$      | (6) $3^+ \begin{pmatrix} \bar{x}+1/2, x, \bar{x} \\ (3_{\bar{xyz}}^{-1}   1/2, 1/2, 0) \end{pmatrix}$                          | (7) $3^+ \begin{pmatrix} x+1/2, \bar{x}, \bar{x} \\ (3_{\bar{xyz}}^{-1}   1/2, 1/2, 0) \end{pmatrix}$                          | (8) $3^+ \begin{pmatrix} 1/3, 1/3, -1/3 \\ \bar{x}+1/6, \bar{x}+1/3, x \\ (3_{\bar{xyz}}^{-1}   1/2, 1/2, 0) \end{pmatrix}$ |
| (9) $3^- \begin{pmatrix} 1/3, 1/3, 1/3 \\ x+1/3, x+1/6, x \\ (3_{xyz}^{-1}   1/2, 1/2, 0) \end{pmatrix}$ | (10) $3^- \begin{pmatrix} x, \bar{x}+1/2, \bar{x} \\ (3_{\bar{xyz}}   1/2, 1/2, 0) \end{pmatrix}$                              | (11) $3^- \begin{pmatrix} 1/3, 1/3, -1/3 \\ \bar{x}+1/3, \bar{x}+1/6, x \\ (3_{\bar{yz}}   1/2, 1/2, 0) \end{pmatrix}$         | (12) $3^- \begin{pmatrix} \bar{x}, x+1/2, \bar{x} \\ (3_{\bar{yz}}   1/2, 1/2, 0) \end{pmatrix}$                            |
| (13) $\bar{1} \begin{pmatrix} 1/4, 1/4, 0 \\ (1   1/2, 1/2, 0) \end{pmatrix}$                            | (14) $n \begin{pmatrix} (1/2, 1/2, 0) \quad x, y, 0 \\ (m_z   1/2, 1/2, 0) \end{pmatrix}$                                      | (15) $a \begin{pmatrix} (1/2, 0, 0) \quad x, 1/4, z \\ (m_y   1/2, 1/2, 0) \end{pmatrix}$                                      | (16) $b \begin{pmatrix} (0, 1/2, 0) \quad 1/4, y, z \\ (m_x   1/2, 1/2, 0) \end{pmatrix}$                                   |
| (17) $\bar{3}^+ \begin{pmatrix} x+1/2, x, x; \\ 1/2, 0, 0 \\ (3_{xyz}   1/2, 1/2, 0) \end{pmatrix}$      | (18) $\bar{3}^+ \begin{pmatrix} \bar{x}-1/2, x+1, \bar{x}; \\ 0, 1/2, 1/2 \\ (3_{\bar{xyz}}^{-1}   1/2, 1/2, 0) \end{pmatrix}$ | (19) $\bar{3}^+ \begin{pmatrix} x-1/2, \bar{x}+1, \bar{x}; \\ 0, 1/2, -1/2 \\ (3_{\bar{yz}}^{-1}   1/2, 1/2, 0) \end{pmatrix}$ | (20) $\bar{3}^+ \begin{pmatrix} \bar{x}+1/2, \bar{x}, x; \\ 1/2, 0, 0 \\ (3_{\bar{yz}}^{-1}   1/2, 1/2, 0) \end{pmatrix}$   |
| (21) $\bar{3}^- \begin{pmatrix} x, x+1/2, x; \\ 0, 1/2, 0 \\ (3_{xyz}^{-1}   1/2, 1/2, 0) \end{pmatrix}$ | (22) $\bar{3}^- \begin{pmatrix} x+1, \bar{x}-1/2, \bar{x}; \\ 1/2, 0, 1/2 \\ (3_{\bar{yz}}   1/2, 1/2, 0) \end{pmatrix}$       | (23) $\bar{3}^- \begin{pmatrix} \bar{x}, \bar{x}+1/2, x; \\ 0, 1/2, 0 \\ (3_{\bar{yz}}   1/2, 1/2, 0) \end{pmatrix}$           | (24) $\bar{3}^- \begin{pmatrix} \bar{x}+1, x-1/2, \bar{x}; \\ 1/2, 0, -1/2 \\ (3_{\bar{yz}}   1/2, 1/2, 0) \end{pmatrix}$   |

For (0,0,0)' + set

- |   |   |  |  |
|---|---|--|--|
| (1) $1' \begin{pmatrix} 0, 0, 0 \\ (1   0, 0, 0)' \end{pmatrix}$                  | (2) $2' \begin{pmatrix} 0, 0, z \\ (2_z   0, 0, 0)'$  | (3) $2' \begin{pmatrix} 0, y, 0 \\ (2_y   0, 0, 0)'$   | (4) $2' \begin{pmatrix} x, 0, 0 \\ (2_x   0, 0, 0)'$   |
| (5) $3^{+'} \begin{pmatrix} x, x, x \\ (3_{xyz}   0, 0, 0)'$                      | (6) $3^{+'} \begin{pmatrix} \bar{x}, x, \bar{x} \\ (3_{\bar{xyz}}^{-1}   0, 0, 0)'$                 | (7) $3^{+'} \begin{pmatrix} x, \bar{x}, \bar{x} \\ (3_{\bar{yz}}^{-1}   0, 0, 0)'$                 | (8) $3^{+'} \begin{pmatrix} \bar{x}, \bar{x}, x \\ (3_{\bar{yz}}^{-1}   0, 0, 0)'$                 |
| (9) $3^{-'} \begin{pmatrix} x, x, x \\ (3_{xyz}^{-1}   0, 0, 0)'$                 | (10) $3^{-'} \begin{pmatrix} x, \bar{x}, \bar{x} \\ (3_{\bar{yz}}   0, 0, 0)'$                      | (11) $3^{-'} \begin{pmatrix} \bar{x}, \bar{x}, x \\ (3_{\bar{yz}}   0, 0, 0)'$                     | (12) $3^{-'} \begin{pmatrix} \bar{x}, x, \bar{x} \\ (3_{\bar{yz}}   0, 0, 0)'$                     |
| (13) $\bar{1}' \begin{pmatrix} 0, 0, 0 \\ (1   0, 0, 0)'$                         | (14) $m' \begin{pmatrix} x, y, 0 \\ (m_z   0, 0, 0)'$   | (15) $m' \begin{pmatrix} x, 0, z \\ (m_y   0, 0, 0)'$  | (16) $m' \begin{pmatrix} 0, y, z \\ (m_x   0, 0, 0)'$  |
| (17) $\bar{3}^{+'} \begin{pmatrix} x, x, x; 0, 0, 0 \\ (3_{xyz}   0, 0, 0)'$      | (18) $\bar{3}^{+'} \begin{pmatrix} \bar{x}, x, \bar{x}; 0, 0, 0 \\ (3_{\bar{xyz}}^{-1}   0, 0, 0)'$ | (19) $\bar{3}^{+'} \begin{pmatrix} x, \bar{x}, \bar{x}; 0, 0, 0 \\ (3_{\bar{yz}}^{-1}   0, 0, 0)'$ | (20) $\bar{3}^{+'} \begin{pmatrix} \bar{x}, \bar{x}, x; 0, 0, 0 \\ (3_{\bar{yz}}^{-1}   0, 0, 0)'$ |
| (21) $\bar{3}^{-'} \begin{pmatrix} x, x, x; 0, 0, 0 \\ (3_{xyz}^{-1}   0, 0, 0)'$ | (22) $\bar{3}^{-'} \begin{pmatrix} x, \bar{x}, \bar{x}; 0, 0, 0 \\ (3_{\bar{yz}}   0, 0, 0)'$       | (23) $\bar{3}^{-'} \begin{pmatrix} \bar{x}, \bar{x}, x; 0, 0, 0 \\ (3_{\bar{yz}}   0, 0, 0)'$      | (24) $\bar{3}^{-'} \begin{pmatrix} \bar{x}, x, \bar{x}; 0, 0, 0 \\ (3_{\bar{yz}}   0, 0, 0)'$      |

For (0,1/2,1/2)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t' \begin{pmatrix} (0, 1/2, 1/2) \\ (1   0, 1/2, 1/2)'$                                   | (2) $2' \begin{pmatrix} (0, 0, 1/2) \quad 0, 1/4, z \\ (2_z   0, 1/2, 1/2)'$                                   | (3) $2' \begin{pmatrix} (0, 1/2, 0) \quad 0, y, 1/4 \\ (2_y   0, 1/2, 1/2)'$                                       | (4) $2' \begin{pmatrix} x, 1/4, 1/4 \\ (2_x   0, 1/2, 1/2)'$                               |
| (5) $3^{+'} \begin{pmatrix} 1/3, 1/3, 1/3 \\ x-1/3, x-1/6, x \\ (3_{xyz}   0, 1/2, 1/2)'$      | (6) $3^{+'} \begin{pmatrix} \bar{x}, x+1/2, \bar{x} \\ (3_{\bar{xyz}}^{-1}   0, 1/2, 1/2)'$                    | (7) $3^{+'} \begin{pmatrix} (-1/3, 1/3, 1/3) \\ x+1/3, \bar{x}-1/6, \bar{x} \\ (3_{\bar{yz}}^{-1}   0, 1/2, 1/2)'$ | (8) $3^{+'} \begin{pmatrix} \bar{x}, \bar{x}+1/2, x \\ (3_{\bar{yz}}^{-1}   0, 1/2, 1/2)'$ |
| (9) $3^{-'} \begin{pmatrix} 1/3, 1/3, 1/3 \\ x-1/6, x+1/6, x \\ (3_{xyz}^{-1}   0, 1/2, 1/2)'$ | (10) $3^{-'} \begin{pmatrix} (-1/3, 1/3, 1/3) \\ x+1/6, \bar{x}+1/6, \bar{x} \\ (3_{\bar{yz}}   0, 1/2, 1/2)'$ | (11) $3^{-'} \begin{pmatrix} \bar{x}+1/2, \bar{x}+1/2, x \\ (3_{\bar{yz}}   0, 1/2, 1/2)'$                         | (12) $3^{-'} \begin{pmatrix} \bar{x}-1/2, x+1/2, \bar{x} \\ (3_{\bar{yz}}   0, 1/2, 1/2)'$ |

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Fm $\bar{3}1'$

- |   |  |   |   |
|---|--|---|---|
| (13) $\bar{1} \mid 0, 1/4, 1/4$<br>$(\bar{1} \mid 0, 1/2, 1/2)'$                                  | (14) $b' (0, 1/2, 0) \mid x, y, 1/4$<br>$(m_z \mid 0, 1/2, 1/2)'$  | (15) $c' (0, 0, 1/2) \mid x, 1/4, z$<br>$(m_y \mid 0, 1/2, 1/2)'$   | (16) $n' (0, 1/2, 1/2) \mid 0, y, z$<br>$(m_x \mid 0, 1/2, 1/2)'$   |
| (17) $\bar{3}^+ \mid x, x+1/2, x;$<br>$0, 1/2, 0$<br>$(\bar{3}_{xyz} \mid 0, 1/2, 1/2)'$          | (18) $\bar{3}^+ \mid \bar{x}-1, x+1/2, \bar{x};$<br>$-1/2, 0, 1/2$<br>$(\bar{3}_{xyz}^{-1} \mid 0, 1/2, 1/2)'$ | (19) $\bar{3}^+ \mid x, \bar{x}+1/2, \bar{x};$<br>$0, 1/2, 0$<br>$(\bar{3}_{xyz}^{-1} \mid 0, 1/2, 1/2)'$   | (20) $\bar{3}^+ \mid \bar{x}-1, \bar{x}+1/2, x;$<br>$1/2, 0, 1/2$<br>$(\bar{3}_{xyz}^{-1} \mid 0, 1/2, 1/2)'$ |
| (21) $\bar{3}^- \mid x-1/2, x-1/2, x;$<br>$0, 0, 1/2$<br>$(\bar{3}_{xyz}^{-1} \mid 0, 1/2, 1/2)'$ | (22) $\bar{3}^- \mid x+1/2, \bar{x}-1/2, \bar{x};$<br>$0, 0, 1/2$<br>$(\bar{3}_{xyz} \mid 0, 1/2, 1/2)'$       | (23) $\bar{3}^- \mid \bar{x}-1/2, \bar{x}+1/2, x;$<br>$-1/2, 1/2, 0$<br>$(\bar{3}_{xyz} \mid 0, 1/2, 1/2)'$ | (24) $\bar{3}^- \mid \bar{x}+1/2, x+1/2, \bar{x};$<br>$1/2, 1/2, 0$<br>$(\bar{3}_{xyz} \mid 0, 1/2, 1/2)'$    |

For (1/2, 0, 1/2)' + set

- |   |   |   |  |
|---|---|---|--|
| (1) $t' (1/2, 0, 1/2)$<br>$(1 \mid 1/2, 0, 1/2)'$   | (2) $2' (0, 0, 1/2) \mid 1/4, 0, z$<br>$(2_z \mid 1/2, 0, 1/2)'$  | (3) $2' \mid 1/4, y, 1/4$<br>$(2_y \mid 1/2, 0, 1/2)'$  | (4) $2' (1/2, 0, 0) \mid x, 0, 1/4$<br>$(2_x \mid 1/2, 0, 1/2)'$   |
| (5) $3^+ \mid (1/3, 1/3, 1/3)$<br>$x+1/6, x-1/6, x$<br>$(3_{xyz} \mid 1/2, 0, 1/2)'$          | (6) $3^+ \mid (1/3, -1/3, 1/3)$<br>$\bar{x}+1/6, x+1/6, \bar{x}$<br>$(3_{xyz}^{-1} \mid 1/2, 0, 1/2)'$        | (7) $3^+ \mid x+1/2, \bar{x}-1/2, \bar{x}$<br>$(3_{xyz}^{-1} \mid 1/2, 0, 1/2)'$                                | (8) $3^+ \mid \bar{x}+1/2, \bar{x}+1/2, x$<br>$(3_{xyz}^{-1} \mid 1/2, 0, 1/2)'$                                 |
| (9) $3^- \mid (1/3, 1/3, 1/3)$<br>$x-1/6, x-1/3, x$<br>$(3_{xyz}^{-1} \mid 1/2, 0, 1/2)'$     | (10) $3^- \mid x+1/2, \bar{x}, \bar{x}$<br>$(3_{xyz} \mid 1/2, 0, 1/2)'$                                      | (11) $3^- \mid \bar{x}+1/2, \bar{x}, x$<br>$(3_{xyz} \mid 1/2, 0, 1/2)'$  | (12) $3^- \mid (1/3, -1/3, 1/3)$<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>$(3_{xyz} \mid 1/2, 0, 1/2)'$               |
| (13) $\bar{1} \mid 1/4, 0, 1/4$<br>$(\bar{1} \mid 1/2, 0, 1/2)'$                              | (14) $a' (1/2, 0, 0) \mid x, y, 1/4$<br>$(m_z \mid 1/2, 0, 1/2)'$   | (15) $n' (1/2, 0, 1/2) \mid x, 0, z$<br>$(m_y \mid 1/2, 0, 1/2)'$   | (16) $c' (0, 0, 1/2) \mid 1/4, y, z$<br>$(m_x \mid 1/2, 0, 1/2)'$  |
| (17) $\bar{3}^+ \mid x-1/2, x-1/2, x;$<br>$0, 0, 1/2$<br>$(\bar{3}_{xyz} \mid 1/2, 0, 1/2)'$  | (18) $\bar{3}^+ \mid \bar{x}-1/2, x+1/2, \bar{x};$<br>$0, 0, 1/2$<br>$(\bar{3}_{xyz}^{-1} \mid 1/2, 0, 1/2)'$ | (19) $\bar{3}^+ \mid x+1/2, \bar{x}+1/2, \bar{x};$<br>$1/2, 1/2, 0$<br>$(\bar{3}_{xyz}^{-1} \mid 1/2, 0, 1/2)'$ | (20) $\bar{3}^+ \mid \bar{x}+1/2, \bar{x}-1/2, x;$<br>$1/2, -1/2, 0$<br>$(\bar{3}_{xyz}^{-1} \mid 1/2, 0, 1/2)'$ |
| (21) $\bar{3}^- \mid x+1/2, x, x;$<br>$1/2, 0, 0$<br>$(\bar{3}_{xyz}^{-1} \mid 1/2, 0, 1/2)'$ | (22) $\bar{3}^- \mid x+1/2, \bar{x}-1, \bar{x};$<br>$0, -1/2, 1/2$<br>$(\bar{3}_{xyz} \mid 1/2, 0, 1/2)'$     | (23) $\bar{3}^- \mid \bar{x}+1/2, \bar{x}+1, x;$<br>$0, 1/2, 1/2$<br>$(\bar{3}_{xyz} \mid 1/2, 0, 1/2)'$        | (24) $\bar{3}^- \mid \bar{x}+1/2, x, \bar{x};$<br>$1/2, 0, 0$<br>$(\bar{3}_{xyz} \mid 1/2, 0, 1/2)'$             |

For (1/2, 1/2, 0)' + set

- |   |   |  |   |
|---|---|--|---|
| (1) $t' (1/2, 1/2, 0)$<br>$(1 \mid 1/2, 1/2, 0)'$   | (2) $2' \mid 1/4, 1/4, z$<br>$(2_z \mid 1/2, 1/2, 0)'$  | (3) $2' (0, 1/2, 0) \mid 1/4, y, 0$<br>$(2_y \mid 1/2, 1/2, 0)'$   | (4) $2' (1/2, 0, 0) \mid x, 1/4, 0$<br>$(2_x \mid 1/2, 1/2, 0)'$  |
| (5) $3^+ \mid (1/3, 1/3, 1/3)$<br>$x+1/6, x+1/3, x$<br>$(3_{xyz} \mid 1/2, 1/2, 0)'$          | (6) $3^+ \mid \bar{x}+1/2, x, \bar{x}$<br>$(3_{xyz}^{-1} \mid 1/2, 1/2, 0)'$                                  | (7) $3^+ \mid x+1/2, \bar{x}, \bar{x}$<br>$(3_{xyz}^{-1} \mid 1/2, 1/2, 0)'$                                   | (8) $3^+ \mid (1/3, 1/3, -1/3)$<br>$\bar{x}+1/6, x+1/3, x$<br>$(3_{xyz}^{-1} \mid 1/2, 1/2, 0)'$          |
| (9) $3^- \mid (1/3, 1/3, 1/3)$<br>$x+1/3, x+1/6, x$<br>$(3_{xyz}^{-1} \mid 1/2, 1/2, 0)'$     | (10) $3^- \mid x, \bar{x}+1/2, \bar{x}$<br>$(3_{xyz} \mid 1/2, 1/2, 0)'$                                      | (11) $3^- \mid (1/3, 1/3, -1/3)$<br>$\bar{x}+1/3, \bar{x}+1/6, x$<br>$(3_{xyz} \mid 1/2, 1/2, 0)'$             | (12) $3^- \mid \bar{x}, x+1/2, \bar{x}$<br>$(3_{xyz} \mid 1/2, 1/2, 0)'$                                  |
| (13) $\bar{1} \mid 1/4, 1/4, 0$<br>$(\bar{1} \mid 1/2, 1/2, 0)'$                              | (14) $n' (1/2, 1/2, 0) \mid x, y, 0$<br>$(m_z \mid 1/2, 1/2, 0)'$   | (15) $a' (1/2, 0, 0) \mid x, 1/4, z$<br>$(m_y \mid 1/2, 1/2, 0)'$  | (16) $b' (0, 1/2, 0) \mid 1/4, y, z$<br>$(m_x \mid 1/2, 1/2, 0)'$   |
| (17) $\bar{3}^+ \mid x+1/2, x, x;$<br>$1/2, 0, 0$<br>$(\bar{3}_{xyz} \mid 1/2, 1/2, 0)'$      | (18) $\bar{3}^+ \mid \bar{x}-1/2, x+1, \bar{x};$<br>$0, 1/2, 1/2$<br>$(\bar{3}_{xyz}^{-1} \mid 1/2, 1/2, 0)'$ | (19) $\bar{3}^+ \mid x-1/2, \bar{x}+1, \bar{x};$<br>$0, 1/2, -1/2$<br>$(\bar{3}_{xyz}^{-1} \mid 1/2, 1/2, 0)'$ | (20) $\bar{3}^+ \mid \bar{x}+1/2, \bar{x}, x;$<br>$1/2, 0, 0$<br>$(\bar{3}_{xyz}^{-1} \mid 1/2, 1/2, 0)'$ |
| (21) $\bar{3}^- \mid x, x+1/2, x;$<br>$0, 1/2, 0$<br>$(\bar{3}_{xyz}^{-1} \mid 1/2, 1/2, 0)'$ | (22) $\bar{3}^- \mid x+1, \bar{x}-1/2, \bar{x};$<br>$1/2, 0, 1/2$<br>$(\bar{3}_{xyz} \mid 1/2, 1/2, 0)'$      | (23) $\bar{3}^- \mid \bar{x}, \bar{x}+1/2, x;$<br>$0, 1/2, 0$<br>$(\bar{3}_{xyz} \mid 1/2, 1/2, 0)'$           | (24) $\bar{3}^- \mid \bar{x}+1, x-1/2, \bar{x};$<br>$1/2, 0, -1/2$<br>$(\bar{3}_{xyz} \mid 1/2, 1/2, 0)'$ |

Continued

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Fm $\bar{3}1'$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); 1'.

**Positions**

			Coordinates			
Multiplicity, Wyckoff letter, Site Symmetry.			(0,0,0) + (0,0,0)' +	(0,1/2,1/2) + (0,1/2,1/2)' +	(1/2,0,1/2) + (1/2,0,1/2)' +	(1/2,1/2,0) + (1/2,1/2,0)' +
96	i	11'	(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{x},y,\bar{z}$ [0,0,0]	(4) x, $\bar{y},\bar{z}$ [0,0,0]
			(5) z,x,y [0,0,0]	(6) z, $\bar{x},\bar{y}$ [0,0,0]	(7) $\bar{z},\bar{x},y$ [0,0,0]	(8) $\bar{z},x,\bar{y}$ [0,0,0]
			(9) y,z,x [0,0,0]	(10) $\bar{y},z,\bar{x}$ [0,0,0]	(11) y, $\bar{z},\bar{x}$ [0,0,0]	(12) $\bar{y},\bar{z},x$ [0,0,0]
			(13) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(14) x,y, $\bar{z}$ [0,0,0]	(15) x, $\bar{y},z$ [0,0,0]	(16) $\bar{x},y,z$ [0,0,0]
			(17) $\bar{z},\bar{x},\bar{y}$ [0,0,0]	(18) $\bar{z},x,y$ [0,0,0]	(19) z,x, $\bar{y}$ [0,0,0]	(20) z, $\bar{x},y$ [0,0,0]
			(21) $\bar{y},\bar{z},\bar{x}$ [0,0,0]	(22) y, $\bar{z},x$ [0,0,0]	(23) $\bar{y},z,x$ [0,0,0]	(24) y,z, $\bar{x}$ [0,0,0]
48	h	m..1'	0,y,z [0,0,0]	0, $\bar{y},z$ [0,0,0]	0,y, $\bar{z}$ [0,0,0]	
			0, $\bar{y},\bar{z}$ [0,0,0]	z,0,y [0,0,0]	z,0, $\bar{y}$ [0,0,0]	
			$\bar{z},0,y$ [0,0,0]	$\bar{z},0,\bar{y}$ [0,0,0]	y,z,0 [0,0,0]	
			$\bar{y},z,0$ [0,0,0]	y, $\bar{z},0$ [0,0,0]	$\bar{y},\bar{z},0$ [0,0,0]	
48	g	2..1'	x,1/4,1/4 [0,0,0]	$\bar{x},3/4,1/4$ [0,0,0]	1/4,x,1/4 [0,0,0]	
			1/4, $\bar{x},3/4$ [0,0,0]	1/4,1/4,x [0,0,0]	3/4,1/4, $\bar{x}$ [0,0,0]	
			$\bar{x},3/4,3/4$ [0,0,0]	x,1/4,3/4 [0,0,0]	3/4, $\bar{x},3/4$ [0,0,0]	
			3/4,x,1/4 [0,0,0]	3/4,3/4, $\bar{x}$ [0,0,0]	1/4,3/4,x [0,0,0]	
32	f	.3.1'	x,x,x [0,0,0]	$\bar{x},\bar{x},x$ [0,0,0]	$\bar{x},x,\bar{x}$ [0,0,0]	x, $\bar{x},\bar{x}$ [0,0,0]
			$\bar{x},\bar{x},\bar{x}$ [0,0,0]	x,x, $\bar{x}$ [0,0,0]	x, $\bar{x},x$ [0,0,0]	$\bar{x},x,x$ [0,0,0]
24	e	mm2..1'	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,0 [0,0,0]	
			0, $\bar{x},0$ [0,0,0]	0,0,x [0,0,0]	0,0, $\bar{x}$ [0,0,0]	
24	d	2/m..1'	0,1/4,1/4 [0,0,0]	0,3/4,1/4 [0,0,0]	1/4,0,1/4 [0,0,0]	
			1/4,0,3/4 [0,0,0]	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]	
8	c	23.1'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]		
4	b	m $\bar{3}$ .1'	1/2,1/2,1/2 [0,0,0]			
4	a	m $\bar{3}$ .1'	0,0,0 [0,0,0]			

Continued

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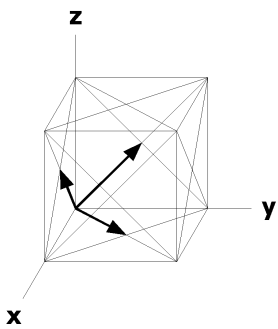
Fm $\bar{3}$ 1'

## Symmetry of Special Projections

Along  $[0,0,1]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $0,0,z$

Along  $[1,1,1]$   $p61'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
Origin at  $x,x,x$

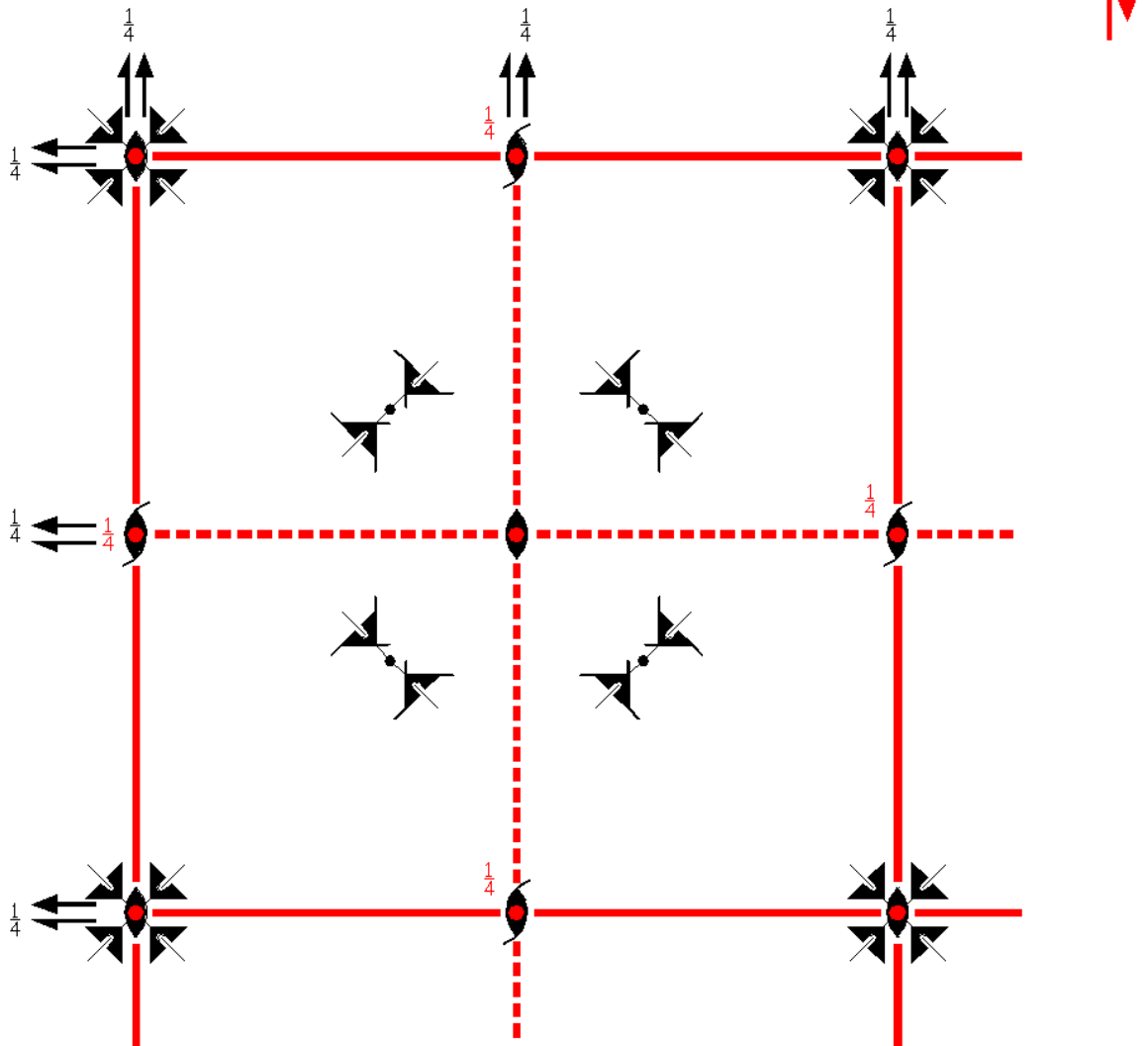
Along  $[1,1,0]$   $c2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,x,0$



$Fm\bar{3}'$   
202.3.1526

$m\bar{3}'$   
 $F2/m\bar{3}'$

Cubic



Origin at center ( $m\bar{3}'$ )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq x;$   $z \leq \min(1/2-x, y)$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/4,1/4,1/4$

**Symmetry Operations**

For  $(0,0,0) +$  set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                                | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  0,0,0) | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  0,0,0) | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}z}^{-1}$  0,0,0) |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)     | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}z}$  0,0,0)     | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)     |

- |   |  |   |  |
|---|--|---|--|
| (13) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$  0,0,0)'                              | (14) m' x,y,0<br>(m <sub>z</sub>  0,0,0)'  | (15) m' x,0,z<br>(m <sub>y</sub>  0,0,0)'   | (16) m' 0,y,z<br>(m <sub>x</sub>  0,0,0)'  |
| (17) $\bar{3}^+$ ' x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$  0,0,0)'               | (18) $\bar{3}^+$ ' $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0)' | (19) $\bar{3}^+$ ' x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0)' | (20) $\bar{3}^+$ ' $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0)' |
| (21) $\bar{3}^-$ ' x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)' | (22) $\bar{3}^-$ ' x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)'              | (23) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)'                | (24) $\bar{3}^-$ ' $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)'               |

For (0,1/2,1/2) + set

- |  |  |  |   |
|--|--|--|---|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2)   | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2 x,1/4,1/4<br>(2 <sub>x</sub>  0,1/2,1/2)  |
| (5) 3 <sup>+</sup> (1/3,1/3,1/3)<br>x-1/3,x-1/6,x<br>( $\bar{3}_{xyz}$  0,1/2,1/2)               | (6) 3 <sup>+</sup> $\bar{x}$ ,x+1/2, $\bar{x}$<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,1/2,1/2)                    | (7) 3 <sup>+</sup> (-1/3,1/3,1/3)<br>x+1/3, $\bar{x}$ -1/6, $\bar{x}$<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,1/2,1/2) | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ +1/2,x<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,1/2,1/2)                  |
| (9) 3 <sup>-</sup> (1/3,1/3,1/3)<br>x-1/6,x+1/6,x<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  0,1/2,1/2) | (10) 3 <sup>-</sup> (-1/3,1/3,1/3)<br>x+1/6, $\bar{x}$ +1/6, $\bar{x}$<br>( $\bar{3}_{x\bar{y}\bar{z}}$  0,1/2,1/2)          | (11) 3 <sup>-</sup> $\bar{x}$ +1/2, $\bar{x}$ +1/2,x<br>( $\bar{3}_{x\bar{y}\bar{z}}$  0,1/2,1/2)                                | (12) 3 <sup>-</sup> $\bar{x}$ -1/2,x+1/2, $\bar{x}$<br>( $\bar{3}_{x\bar{y}\bar{z}}$  0,1/2,1/2)                            |
| (13) $\bar{1}$ ' 0,1/4,1/4<br>( $\bar{1}$  0,1/2,1/2)'   | (14) b' (0,1/2,0) x,y,1/4<br>(m <sub>z</sub>  0,1/2,1/2)'  | (15) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)'  | (16) n' (0,1/2,1/2) 0,y,z<br>(m <sub>x</sub>  0,1/2,1/2)'   |
| (17) $\bar{3}^+$ ' x,x+1/2,x;<br>0,1/2,0<br>( $\bar{3}_{xyz}$  0,1/2,1/2)'                       | (18) $\bar{3}^+$ ' $\bar{x}$ -1,x+1/2, $\bar{x}$ ;<br>-1/2,0,1/2<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,1/2,1/2)' | (19) $\bar{3}^+$ ' x, $\bar{x}$ +1/2, $\bar{x}$ ;<br>0,1/2,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,1/2,1/2)'         | (20) $\bar{3}^+$ ' $\bar{x}$ -1, $\bar{x}$ +1/2,x;<br>1/2,0,1/2<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,1/2,1/2)' |
| (21) $\bar{3}^-$ ' x-1/2,x-1/2,x;<br>0,0,1/2<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  0,1/2,1/2)'     | (22) $\bar{3}^-$ ' x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ;<br>0,0,1/2<br>( $\bar{3}_{x\bar{y}\bar{z}}$  0,1/2,1/2)'               | (23) $\bar{3}^-$ ' $\bar{x}$ -1/2, $\bar{x}$ +1/2,x;<br>-1/2,1/2,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$  0,1/2,1/2)'                 | (24) $\bar{3}^-$ ' $\bar{x}$ +1/2,x+1/2, $\bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$  0,1/2,1/2)'             |

For (1/2,0,1/2) + set

- |  |   |  |  |
|--|---|--|--|
| (1) t (1/2,0,1/2)<br>(1 1/2,0,1/2)   | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)  | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)   | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>  1/2,0,1/2)   |
| (5) 3 <sup>+</sup> (1/3,1/3,1/3)<br>x+1/6,x-1/6,x<br>( $\bar{3}_{xyz}$  1/2,0,1/2)               | (6) 3 <sup>+</sup> (1/3,-1/3,1/3)<br>x+1/6,x+1/6, $\bar{x}$<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  1/2,0,1/2)      | (7) 3 <sup>+</sup> x+1/2, $\bar{x}$ -1/2, $\bar{x}$<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  1/2,0,1/2)                 | (8) 3 <sup>+</sup> $\bar{x}$ +1/2, $\bar{x}$ +1/2,x<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  1/2,0,1/2)                 |
| (9) 3 <sup>-</sup> (1/3,1/3,1/3)<br>x-1/6,x-1/3,x<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,0,1/2) | (10) 3 <sup>-</sup> x+1/2, $\bar{x}$ , $\bar{x}$<br>( $\bar{3}_{x\bar{y}\bar{z}}$  1/2,0,1/2)                               | (11) 3 <sup>-</sup> $\bar{x}$ +1/2, $\bar{x}$ ,x<br>( $\bar{3}_{x\bar{y}\bar{z}}$  1/2,0,1/2)                                  | (12) 3 <sup>-</sup> (1/3,-1/3,1/3)<br>$\bar{x}$ -1/6,x+1/3, $\bar{x}$<br>( $\bar{3}_{x\bar{y}\bar{z}}$  1/2,0,1/2)             |
| (13) $\bar{1}$ ' 1/4,0,1/4<br>( $\bar{1}$  1/2,0,1/2)'   | (14) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)'   | (15) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2)'  | (16) c' (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,0,1/2)'  |
| (17) $\bar{3}^+$ ' x-1/2,x-1/2,x;<br>0,0,1/2<br>( $\bar{3}_{xyz}$  1/2,0,1/2)'                   | (18) $\bar{3}^+$ ' $\bar{x}$ -1/2,x+1/2, $\bar{x}$ ;<br>0,0,1/2<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  1/2,0,1/2)' | (19) $\bar{3}^+$ ' x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  1/2,0,1/2)' | (20) $\bar{3}^+$ ' $\bar{x}$ +1/2, $\bar{x}$ -1/2,x;<br>1/2,-1/2,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  1/2,0,1/2)' |
| (21) $\bar{3}^-$ ' x+1/2,x,x;<br>1/2,0,0<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,0,1/2)'         | (22) $\bar{3}^-$ ' x+1/2, $\bar{x}$ -1, $\bar{x}$ ;<br>0,-1/2,1/2<br>( $\bar{3}_{x\bar{y}\bar{z}}$  1/2,0,1/2)'             | (23) $\bar{3}^-$ ' $\bar{x}$ +1/2, $\bar{x}$ +1,x;<br>0,1/2,1/2<br>( $\bar{3}_{x\bar{y}\bar{z}}$  1/2,0,1/2)'                  | (24) $\bar{3}^-$ ' $\bar{x}$ +1/2,x, $\bar{x}$ ;<br>1/2,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$  1/2,0,1/2)'                      |



For (1/2,1/2,0) + set

(1) $t$ (1/2,1/2,0) (1   1/2,1/2,0)	(2) $2$ 1/4,1/4,z ( $2_z$   1/2,1/2,0)	(3) $2$ (0,1/2,0) 1/4,y,0 ( $2_y$   1/2,1/2,0)	(4) $2$ (1/2,0,0) x,1/4,0 ( $2_x$   1/2,1/2,0)
(5) $3^+$ (1/3,1/3,1/3) x+1/6,x+1/3,x ( $3_{xyz}$   1/2,1/2,0)	(6) $3^+$ $\bar{x}$ +1/2,x, $\bar{x}$ ( $3_{\bar{xyz}^{-1}}$   1/2,1/2,0)	(7) $3^+$ x+1/2, $\bar{x}$ , $\bar{x}$ ( $3_{\bar{xyz}^{-1}}$   1/2,1/2,0)	(8) $3^+$ (1/3,1/3,-1/3) x+1/6, $\bar{x}$ +1/3,x ( $3_{\bar{xy}\bar{z}^{-1}}$   1/2,1/2,0)
(9) $3^-$ (1/3,1/3,1/3) x+1/3,x+1/6,x ( $3_{xyz}^{-1}$   1/2,1/2,0)	(10) $3^-$ x, $\bar{x}$ +1/2, $\bar{x}$ ( $3_{\bar{xyz}}$   1/2,1/2,0)	(11) $3^-$ (1/3,1/3,-1/3) x+1/3, $\bar{x}$ +1/6,x ( $3_{\bar{xy}\bar{z}}$   1/2,1/2,0)	(12) $3^-$ $\bar{x}$ , x+1/2, $\bar{x}$ ( $3_{\bar{xyz}}$   1/2,1/2,0)
(13) $\bar{1}$ ' 1/4,1/4,0 ( $\bar{1}$   1/2,1/2,0)'	(14) $n'$ (1/2,1/2,0) x,y,0 ( $m_z$   1/2,1/2,0)'	(15) $a'$ (1/2,0,0) x,1/4,z ( $m_y$   1/2,1/2,0)'	(16) $b'$ (0,1/2,0) 1/4,y,z ( $m_x$   1/2,1/2,0)'
(17) $\bar{3}^+$ ' x+1/2,x,x; 1/2,0,0 ( $\bar{3}_{xyz}$   1/2,1/2,0)'	(18) $\bar{3}^+$ ' $\bar{x}$ -1/2,x+1, $\bar{x}$ ; 0,1/2,1/2 ( $\bar{3}_{\bar{xyz}^{-1}}$   1/2,1/2,0)'	(19) $\bar{3}^+$ ' x-1/2, $\bar{x}$ +1, $\bar{x}$ ; 0,1/2,-1/2 ( $\bar{3}_{\bar{xyz}^{-1}}$   1/2,1/2,0)'	(20) $\bar{3}^+$ ' $\bar{x}$ +1/2, $\bar{x}$ ,x; 1/2,0,0 ( $\bar{3}_{\bar{xy}\bar{z}^{-1}}$   1/2,1/2,0)'
(21) $\bar{3}^-$ ' x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0)'	(22) $\bar{3}^-$ ' x+1, $\bar{x}$ -1/2, $\bar{x}$ ; 1/2,0,1/2 ( $\bar{3}_{\bar{xyz}}$   1/2,1/2,0)'	(23) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ +1/2,x; 0,1/2,0 ( $\bar{3}_{\bar{xy}\bar{z}}$   1/2,1/2,0)'	(24) $\bar{3}^-$ ' $\bar{x}$ +1,x-1/2, $\bar{x}$ ; 1/2,0,-1/2 ( $\bar{3}_{\bar{xyz}}$   1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

		(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
96	i 1				
(1)	x,y,z [u,v,w]	(2)	$\bar{x}$ , $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w]	(3)	$\bar{x}$ ,y, $\bar{z}$ [ $\bar{u}$ ,v, $\bar{w}$ ]
(5)	z,x,y [w,u,v]	(6)	z, $\bar{x}$ , $\bar{y}$ [ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ]	(7)	$\bar{z}$ , $\bar{x}$ ,y [ $\bar{w}$ , $\bar{u}$ ,v]
(9)	y,z,x [v,w,u]	(10)	$\bar{y}$ ,z, $\bar{x}$ [ $\bar{v}$ ,w, $\bar{u}$ ]	(11)	y, $\bar{z}$ , $\bar{x}$ [v, $\bar{w}$ , $\bar{u}$ ]
(13)	$\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(14)	x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(15)	x, $\bar{y}$ ,z [u, $\bar{v}$ ,w]
(17)	$\bar{z}$ , $\bar{x}$ , $\bar{y}$ [ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ]	(18)	$\bar{z}$ ,x,y [ $\bar{w}$ ,u,v]	(19)	z,x, $\bar{y}$ [w,u, $\bar{v}$ ]
(21)	$\bar{y}$ , $\bar{z}$ , $\bar{x}$ [ $\bar{v}$ , $\bar{w}$ , $\bar{u}$ ]	(22)	y, $\bar{z}$ ,x [v, $\bar{w}$ ,u]	(23)	$\bar{y}$ ,z,x [ $\bar{v}$ ,w,u]
48	h m'..	0,y,z [0,v,w]	0, $\bar{y}$ ,z [0, $\bar{v}$ ,w]	0,y, $\bar{z}$ [0,v, $\bar{w}$ ]	
		0, $\bar{y}$ , $\bar{z}$ [0, $\bar{v}$ , $\bar{w}$ ]	z,0,y [w,0,v]	z,0, $\bar{y}$ [w,0, $\bar{v}$ ]	
		$\bar{z}$ ,0,y [ $\bar{w}$ ,0,v]	$\bar{z}$ ,0, $\bar{y}$ [ $\bar{w}$ ,0, $\bar{v}$ ]	y,z,0 [v,w,0]	
		$\bar{y}$ ,z,0 [ $\bar{v}$ ,w,0]	y, $\bar{z}$ ,0 [v, $\bar{w}$ ,0]	$\bar{y}$ , $\bar{z}$ ,0 [ $\bar{v}$ , $\bar{w}$ ,0]	

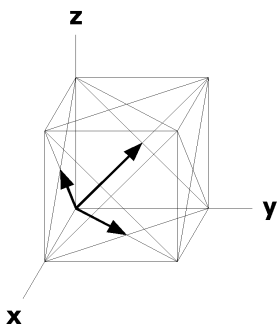
48	g	2..	x,1/4,1/4 [u,0,0]	$\bar{x}$ ,3/4,1/4 [ $\bar{u}$ ,0,0]	1/4,x,1/4 [0,u,0]
			1/4, $\bar{x}$ ,3/4 [0, $\bar{u}$ ,0]	1/4,1/4,x [0,0,u]	3/4,1/4, $\bar{x}$ [0,0, $\bar{u}$ ]
			$\bar{x}$ ,3/4,3/4 [ $\bar{u}$ ,0,0]	x,1/4,3/4 [u,0,0]	3/4, $\bar{x}$ ,3/4 [0, $\bar{u}$ ,0]
			3/4,x,1/4 [0,u,0]	3/4,3/4, $\bar{x}$ [0,0, $\bar{u}$ ]	1/4,3/4,x [0,0,u]
32	f	.3.	x,x,x [u,u,u]	$\bar{x}$ , $\bar{x}$ ,x [ $\bar{u}$ , $\bar{u}$ ,u]	$\bar{x}$ ,x, $\bar{x}$ [ $\bar{u}$ ,u, $\bar{u}$ ]
			$\bar{x}$ , $\bar{x}$ , $\bar{x}$ [ $\bar{u}$ , $\bar{u}$ , $\bar{u}$ ]	x,x, $\bar{x}$ [u,u, $\bar{u}$ ]	$\bar{x}$ ,x,x [u, $\bar{u}$ ,u]
24	e	m'm'2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0]	0,x,0 [0,u,0]
			0, $\bar{x}$ ,0 [0, $\bar{u}$ ,0]	0,0,x [0,0,u]	0,0, $\bar{x}$ [0,0, $\bar{u}$ ]
24	d	2/m'..	0,1/4,1/4 [0,0,0]	0,3/4,1/4 [0,0,0]	1/4,0,1/4 [0,0,0]
			1/4,0,3/4 [0,0,0]	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]
8	c	23.	1/4,1/4,1/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]	
4	b	m' $\bar{3}$ '.	1/2,1/2,1/2 [0,0,0]		
4	a	m' $\bar{3}$ '.	0,0,0 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p2m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,1,1] p6  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

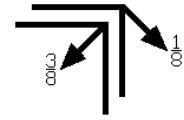
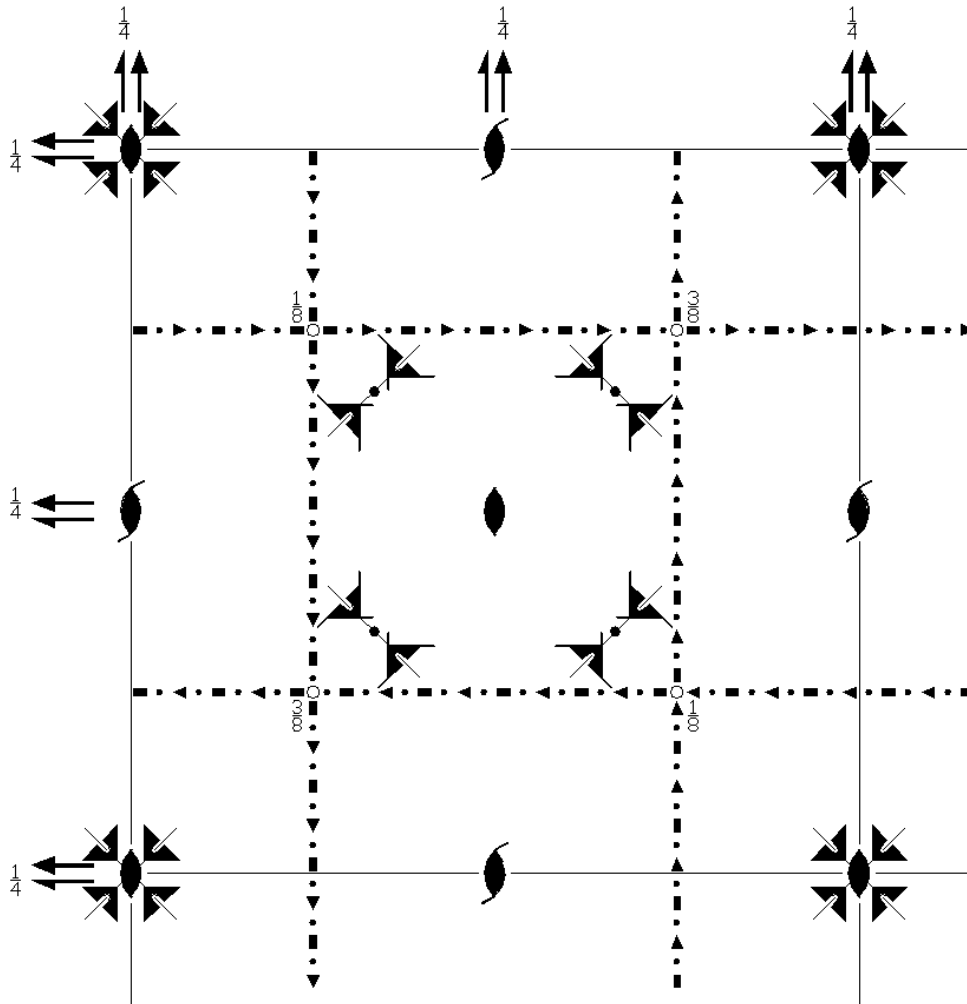
Along [1,1,0] c2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$Fd\bar{3}$   
203.1.1527

$m\bar{3}$   
 $F2/d\bar{3}$

Cubic



**Origin** at 23, at  $-1/8, -1/8, -1/8$  from center ( $\bar{3}$ )

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $-1/4 \leq z \leq 1/4$ ;  $y \leq \min(x, 1/2-x)$ ;  $-y \leq z \leq y$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/4,1/4,1/4$   $1/4,1/4,-1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                          | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                          | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                          |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{xyz}^{-1}$  0,0,0) | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{xyz}^{-1}$  0,0,0) | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{xyz}^{-1}$  0,0,0) |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{xyz}$  0,0,0)     | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{xyz}$  0,0,0)     | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{xyz}$  0,0,0)     |

- |   |   |  |   |
|---|---|--|---|
| (13) $\bar{1}$ 1/8,1/8,1/8<br>( $\bar{1}$   1/4,1/4,1/4)                        | (14) d (1/4,1/4,0) x,y,1/8<br>( $m_z$   1/4,1/4,1/4)  | (15) d (1/4,0,1/4) x,1/8,z<br>( $m_y$   1/4,1/4,1/4)   | (16) d (0,1/4,1/4) 1/8,y,z<br>( $m_x$   1/4,1/4,1/4)  |
| (17) $\bar{3}^+$ x,x,x;<br>1/8,1/8,1/8<br>( $\bar{3}_{xyz}$   1/4,1/4,1/4)      | (18) $\bar{3}^+$ $\bar{x}$ -1/2,x+1/2, $\bar{x}$ ;<br>-1/8,1/8,3/8<br>( $\bar{3}_{x\bar{y}z}^{-1}$   1/4,1/4,1/4) | (19) $\bar{3}^+$ x, $\bar{x}$ +1/2, $\bar{x}$ ;<br>1/8,3/8,-1/8<br>( $\bar{3}_{x\bar{y}z}^{-1}$   1/4,1/4,1/4) | (20) $\bar{3}^+$ $\bar{x}$ +1/2, $\bar{x}$ ,x;<br>3/8,-1/8,1/8<br>( $\bar{3}_{x\bar{y}z}^{-1}$   1/4,1/4,1/4) |
| (21) $\bar{3}^-$ x,x,x;<br>1/8,1/8,1/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,1/4,1/4) | (22) $\bar{3}^-$ x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ;<br>1/8,-1/8,3/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,1/4,1/4)      | (23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1/2, x;<br>-1/8,3/8,1/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,1/4,1/4)       | (24) $\bar{3}^-$ $\bar{x}$ +1/2, x, $\bar{x}$ ;<br>3/8,1/8,-1/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,1/4,1/4)      |

For (0,1/2,1/2) + set

- |   |   |  |   |
|---|---|--|---|
| (1) t (0,1/2,1/2)<br>(1   0,1/2,1/2)  | (2) 2 (0,0,1/2) 0,1/4,z<br>( $2_z$   0,1/2,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>( $2_y$   0,1/2,1/2)  | (4) 2 x,1/4,1/4<br>( $2_x$   0,1/2,1/2)   |
| (5) $3^+$ (1/3,1/3,1/3)<br>x-1/3,x-1/6,x<br>( $3_{xyz}$   0,1/2,1/2)                    | (6) $3^+$ $\bar{x}$ ,x+1/2, $\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$   0,1/2,1/2)                                    | (7) $3^+$ (-1/3,1/3,1/3)<br>x+1/3,x-1/6, $\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$   0,1/2,1/2)                    | (8) $3^+$ $\bar{x}$ , $\bar{x}$ +1/2,x<br>( $3_{x\bar{y}z}^{-1}$   0,1/2,1/2)                                     |
| (9) $3^-$ (1/3,1/3,1/3)<br>x-1/6,x+1/6,x<br>( $3_{xyz}^{-1}$   0,1/2,1/2)               | (10) $3^-$ (-1/3,1/3,1/3)<br>x+1/6,x+1/6, $\bar{x}$<br>( $3_{xyz}^{-1}$   0,1/2,1/2)                            | (11) $3^-$ $\bar{x}$ +1/2, $\bar{x}$ +1/2, x<br>( $3_{x\bar{y}z}$   0,1/2,1/2)                               | (12) $3^-$ $\bar{x}$ -1/2, x+1/2, $\bar{x}$<br>( $3_{x\bar{y}z}$   0,1/2,1/2)                                     |
| (13) $\bar{1}$ 1/8,3/8,3/8<br>( $\bar{1}$   1/4,3/4,3/4)                                | (14) d (1/4,3/4,0) x,y,3/8<br>( $m_z$   1/4,3/4,3/4)  | (15) d (1/4,0,3/4) x,3/8,z<br>( $m_y$   1/4,3/4,3/4)   | (16) d (0,3/4,3/4) 1/8,y,z<br>( $m_x$   1/4,3/4,3/4)  |
| (17) $\bar{3}^+$ x,x+1/2,x;<br>1/8,5/8,1/8<br>( $\bar{3}_{xyz}$   1/4,3/4,3/4)          | (18) $\bar{3}^+$ $\bar{x}$ -3/2,x+1, $\bar{x}$ ;<br>-5/8,1/8,7/8<br>( $\bar{3}_{x\bar{y}z}^{-1}$   1/4,3/4,3/4) | (19) $\bar{3}^+$ x, $\bar{x}$ +1, $\bar{x}$ ;<br>1/8,7/8,-1/8<br>( $\bar{3}_{x\bar{y}z}^{-1}$   1/4,3/4,3/4) | (20) $\bar{3}^+$ $\bar{x}$ +3/2, $\bar{x}$ +1/2,x;<br>7/8,-1/8,5/8<br>( $\bar{3}_{x\bar{y}z}^{-1}$   1/4,3/4,3/4) |
| (21) $\bar{3}^-$ x-1/2,x-1/2,x;<br>1/8,1/8,5/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,3/4,3/4) | (22) $\bar{3}^-$ x+1, $\bar{x}$ -1, $\bar{x}$ ;<br>1/8,-1/8,7/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,3/4,3/4)        | (23) $\bar{3}^-$ $\bar{x}$ -1/2, $\bar{x}$ +1, x;<br>-5/8,7/8,1/8<br>( $\bar{3}_{x\bar{y}z}$   1/4,3/4,3/4)  | (24) $\bar{3}^-$ $\bar{x}$ +1, x+1/2, $\bar{x}$ ;<br>7/8,5/8,-1/8<br>( $\bar{3}_{x\bar{y}z}$   1/4,3/4,3/4)       |

For (1/2,0,1/2) + set

- |  |   |  |   |
|--|---|--|---|
| (1) t (1/2,0,1/2)<br>(1   1/2,0,1/2)   | (2) 2 (0,0,1/2) 1/4,0,z<br>( $2_z$   1/2,0,1/2)   | (3) 2 1/4,y,1/4<br>( $2_y$   1/2,0,1/2)  | (4) 2 (1/2,0,0) x,0,1/4<br>( $2_x$   1/2,0,1/2)   |
| (5) $3^+$ (1/3,1/3,1/3)<br>x+1/6,x-1/6,x<br>( $3_{xyz}$   1/2,0,1/2)               | (6) $3^+$ (1/3,-1/3,1/3)<br>x+1/6,x+1/6, $\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$   1/2,0,1/2)                     | (7) $3^+$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$   1/2,0,1/2)                                | (8) $3^+$ $\bar{x}$ +1/2, $\bar{x}$ +1/2,x<br>( $3_{x\bar{y}z}^{-1}$   1/2,0,1/2)                               |
| (9) $3^-$ (1/3,1/3,1/3)<br>x-1/6,x-1/3,x<br>( $3_{xyz}^{-1}$   1/2,0,1/2)          | (10) $3^-$ x+1/2, $\bar{x}$ , $\bar{x}$<br>( $3_{x\bar{y}z}$   1/2,0,1/2)                                     | (11) $3^-$ $\bar{x}$ +1/2, $\bar{x}$ , x<br>( $3_{x\bar{y}z}$   1/2,0,1/2)                                       | (12) $3^-$ (1/3,-1/3,1/3)<br>$\bar{x}$ -1/6, x+1/3, $\bar{x}$<br>( $3_{x\bar{y}z}$   1/2,0,1/2)                 |
| (13) $\bar{1}$ 3/8,1/8,3/8<br>( $\bar{1}$   3/4,1/4,3/4)                           | (14) d (3/4,1/4,0) x,y,3/8<br>( $m_z$   3/4,1/4,3/4)  | (15) d (3/4,0,3/4) x,1/8,z<br>( $m_y$   3/4,1/4,3/4)   | (16) d (0,1/4,3/4) 3/8,y,z<br>( $m_x$   3/4,1/4,3/4)  |
| (17) $\bar{3}^+$ x-1/2,x-1/2,x;<br>1/8,1/8,5/8<br>( $\bar{3}_{xyz}$   3/4,1/4,3/4) | (18) $\bar{3}^+$ $\bar{x}$ -1,x+1, $\bar{x}$ ;<br>-1/8,1/8,7/8<br>( $\bar{3}_{x\bar{y}z}^{-1}$   3/4,1/4,3/4) | (19) $\bar{3}^+$ x+1/2, $\bar{x}$ +1, $\bar{x}$ ;<br>5/8,7/8,-1/8<br>( $\bar{3}_{x\bar{y}z}^{-1}$   3/4,1/4,3/4) | (20) $\bar{3}^+$ $\bar{x}$ +1, $\bar{x}$ -1/2,x;<br>7/8,-5/8,1/8<br>( $\bar{3}_{x\bar{y}z}^{-1}$   3/4,1/4,3/4) |

$$(21) \bar{3}^- \quad x+1/2, x, x; \\ 5/8, 1/8, 1/8 \\ (\bar{3}_{xyz}^{-1} | 3/4, 1/4, 3/4)$$

$$(22) \bar{3}^- \quad x+1, \bar{x}-3/2, \bar{x}; \\ 1/8, -5/8, 7/8 \\ (\bar{3}_{xyz} | 3/4, 1/4, 3/4)$$

$$(23) \bar{3}^- \quad \bar{x}+1/2, \bar{x}+3/2, x; \\ -1/8, 7/8, 5/8 \\ (\bar{3}_{xyz} | 3/4, 1/4, 3/4)$$

$$(24) \bar{3}^- \quad \bar{x}+1, x, \bar{x}; \\ 7/8, 1/8, -1/8 \\ (\bar{3}_{xyz} | 3/4, 1/4, 3/4)$$

For (1/2, 1/2, 0) + set

$$(1) t \quad (1/2, 1/2, 0) \\ (1 | 1/2, 1/2, 0)$$

$$(2) 2 \quad 1/4, 1/4, z \\ (2_z | 1/2, 1/2, 0)$$

$$(3) 2 \quad (0, 1/2, 0) \quad 1/4, y, 0 \\ (2_y | 1/2, 1/2, 0)$$

$$(4) 2 \quad (1/2, 0, 0) \quad x, 1/4, 0 \\ (2_x | 1/2, 1/2, 0)$$

$$(5) 3^+ \quad (1/3, 1/3, 1/3) \\ x+1/6, x+1/3, x \\ (3_{xyz} | 1/2, 1/2, 0)$$

$$(6) 3^+ \quad \bar{x}+1/2, x, \bar{x} \\ (3_{xyz}^{-1} | 1/2, 1/2, 0)$$

$$(7) 3^+ \quad x+1/2, \bar{x}, \bar{x} \\ (3_{xyz}^{-1} | 1/2, 1/2, 0)$$

$$(8) 3^+ \quad (1/3, 1/3, -1/3) \\ x+1/6, x+1/3, x \\ (3_{xyz}^{-1} | 1/2, 1/2, 0)$$

$$(9) 3^- \quad (1/3, 1/3, 1/3) \\ x+1/3, x+1/6, x \\ (3_{xyz}^{-1} | 1/2, 1/2, 0)$$

$$(10) 3^- \quad x, \bar{x}+1/2, \bar{x} \\ (3_{xyz} | 1/2, 1/2, 0)$$

$$(11) 3^- \quad (1/3, 1/3, -1/3) \\ x+1/3, x+1/6, x \\ (3_{xyz} | 1/2, 1/2, 0)$$

$$(12) 3^- \quad \bar{x}, x+1/2, \bar{x} \\ (3_{xyz} | 1/2, 1/2, 0)$$

$$(13) \bar{1} \quad 3/8, 3/8, 1/8 \\ (\bar{1} | 3/4, 3/4, 1/4)$$

$$(14) d \quad (3/4, 3/4, 0) \quad x, y, 1/8 \\ (m_z | 3/4, 3/4, 1/4)$$

$$(15) d \quad (3/4, 0, 1/4) \quad x, 3/8, z \\ (m_y | 3/4, 3/4, 1/4)$$

$$(16) d \quad (0, 3/4, 1/4) \quad 3/8, y, z \\ (m_x | 3/4, 3/4, 1/4)$$

$$(17) \bar{3}^+ \quad x+1/2, x, x; \\ 5/8, 1/8, 1/8 \\ (\bar{3}_{xyz} | 3/4, 3/4, 1/4)$$

$$(18) \bar{3}^+ \quad \bar{x}-1, x+3/2, \bar{x}; \\ -1/8, 5/8, 7/8 \\ (\bar{3}_{xyz}^{-1} | 3/4, 3/4, 1/4)$$

$$(19) \bar{3}^+ \quad x-1/2, \bar{x}+3/2, \bar{x}; \\ 1/8, 7/8, -5/8 \\ (\bar{3}_{xyz}^{-1} | 3/4, 3/4, 1/4)$$

$$(20) \bar{3}^+ \quad \bar{x}+1, \bar{x}, x; \\ 7/8, -1/8, 1/8 \\ (\bar{3}_{xyz}^{-1} | 3/4, 3/4, 1/4)$$

$$(21) \bar{3}^- \quad x, x+1/2, x; \\ 1/8, 5/8, 1/8 \\ (\bar{3}_{xyz}^{-1} | 3/4, 3/4, 1/4)$$

$$(22) \bar{3}^- \quad x+3/2, \bar{x}-1, \bar{x}; \\ 5/8, -1/8, 7/8 \\ (\bar{3}_{xyz} | 3/4, 3/4, 1/4)$$

$$(23) \bar{3}^- \quad \bar{x}, \bar{x}+1, x; \\ -1/8, 7/8, 1/8 \\ (\bar{3}_{xyz} | 3/4, 3/4, 1/4)$$

$$(24) \bar{3}^- \quad \bar{x}+3/2, x-1/2, \bar{x}; \\ 7/8, 1/8, -5/8 \\ (\bar{3}_{xyz} | 3/4, 3/4, 1/4)$$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

## Positions

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

96      g      1

(0,0,0) +      (0,1/2,1/2) +      (1/2,0,1/2) +      (1/2,1/2,0) +

(1) x, y, z [u, v, w]

(2)  $\bar{x}, \bar{y}, z$  [ $\bar{u}, \bar{v}, w$ ]

(3)  $\bar{x}, y, \bar{z}$  [ $\bar{u}, v, \bar{w}$ ]

(4) x,  $\bar{y}, \bar{z}$  [u,  $\bar{v}, \bar{w}$ ]

(5) z, x, y [w, u, v]

(6) z,  $\bar{x}, \bar{y}$  [w,  $\bar{u}, \bar{v}$ ]

(7)  $\bar{z}, x, y$  [ $\bar{w}, u, v$ ]

(8)  $\bar{z}, x, \bar{y}$  [ $\bar{w}, u, \bar{v}$ ]

(9) y, z, x [v, w, u]

(10)  $\bar{y}, z, \bar{x}$  [ $\bar{v}, w, \bar{u}$ ]

(11) y,  $\bar{z}, \bar{x}$  [v,  $\bar{w}, \bar{u}$ ]

(12)  $\bar{y}, \bar{z}, x$  [ $\bar{v}, \bar{w}, u$ ]

(13)  $\bar{x}+1/4, \bar{y}+1/4, \bar{z}+1/4$  [u, v, w] (14)  $x+1/4, y+1/4, \bar{z}+1/4$  [ $\bar{u}, \bar{v}, w$ ] (15)  $x+1/4, \bar{y}+1/4, z+1/4$  [ $\bar{u}, v, \bar{w}$ ] (16)  $\bar{x}+1/4, y+1/4, z+1/4$  [u,  $\bar{v}, \bar{w}$ ]

(17)  $\bar{z}+1/4, \bar{x}+1/4, \bar{y}+1/4$  [w, u, v] (18)  $\bar{z}+1/4, x+1/4, y+1/4$  [w,  $\bar{u}, \bar{v}$ ] (19)  $z+1/4, x+1/4, \bar{y}+1/4$  [ $\bar{w}, u, v$ ] (20)  $z+1/4, \bar{x}+1/4, y+1/4$  [ $\bar{w}, u, \bar{v}$ ]

(21)  $\bar{y}+1/4, \bar{z}+1/4, \bar{x}+1/4$  [v, w, u] (22)  $y+1/4, \bar{z}+1/4, x+1/4$  [ $\bar{v}, w, \bar{u}$ ] (23)  $\bar{y}+1/4, z+1/4, x+1/4$  [v,  $\bar{w}, \bar{u}$ ] (24)  $y+1/4, z+1/4, \bar{x}+1/4$  [ $\bar{v}, \bar{w}, u$ ]

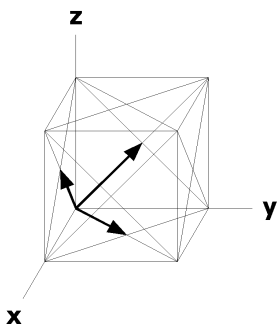
48	f	2..	x,0,0 [u,0,0] 0, $\bar{x}$ ,0 [0, $\bar{u}$ ,0] $\bar{x}+1/4,1/4,1/4$ [u,0,0] 1/4,x+1/4,1/4 [0, $\bar{u}$ ,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ] 0,0,x [0,0,u] x+1/4,1/4,1/4 [ $\bar{u},0,0$ ] 1/4,1/4, $\bar{x}+1/4$ [0,0,u]	0,x,0 [0,u,0] 0,0, $\bar{x}$ [0,0, $\bar{u}$ ] 1/4, $\bar{x}+1/4,1/4$ [0,u,0] 1/4,1/4,x+1/4 [0,0, $\bar{u}$ ]	
32	e	.3.	x,x,x [u,u,u] $\bar{x},x,\bar{x}$ [ $\bar{u},u,\bar{u}$ ] $\bar{x}+1/4,\bar{x}+1/4,\bar{x}+1/4$ [u,u,u] x+1/4, $\bar{x}+1/4,x+1/4$ [ $\bar{u},u,\bar{u}$ ]	$\bar{x},\bar{x},x$ [ $\bar{u},\bar{u},u$ ] x, $\bar{x},\bar{x}$ [u, $\bar{u},\bar{u}$ ] x+1/4,x+1/4, $\bar{x}+1/4$ [ $\bar{u},\bar{u},u$ ] $\bar{x}+1/4,x+1/4,x+1/4$ [u, $\bar{u},\bar{u}$ ]		
16	d	$\bar{3}$ .	5/8,5/8,5/8 [u,u,u]	3/8,3/8,5/8 [ $\bar{u},\bar{u},u$ ]	3/8,5/8,3/8 [ $\bar{u},u,\bar{u}$ ]	5/8,3/8,3/8 [u, $\bar{u},\bar{u}$ ]
16	c	$\bar{3}$ .	1/8,1/8,1/8 [u,u,u]	7/8,7/8,1/8 [ $\bar{u},\bar{u},u$ ]	7/8,1/8,7/8 [ $\bar{u},u,\bar{u}$ ]	1/8,7/8,7/8 [u, $\bar{u},\bar{u}$ ]
8	b	23.	1/2,1/2,1/2 [0,0,0]	3/4,3/4,3/4 [0,0,0]		
8	a	23.	0,0,0 [0,0,0]	1/4,1/4,1/4 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1]  $c_p-2m'm'$   
 $a^* = a/2$   $b^* = b/2$   
 Origin at 0,0,z

Along [1,1,1]  $p6'$   
 $a^* = (2a - b - c)/6$   $b^* = (-a + 2b - c)/6$   
 Origin at x,x,x

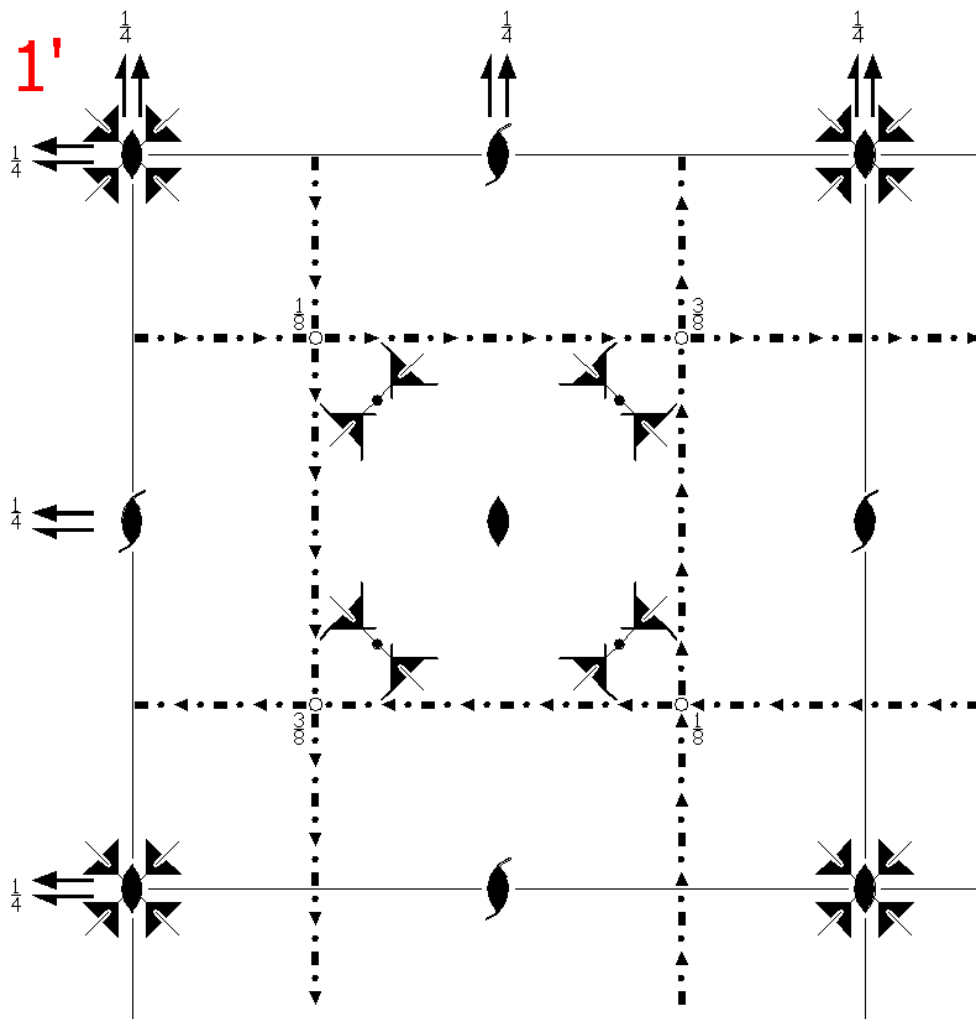
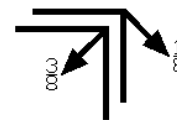
Along [1,1,0]  $c2'mm'$   
 $a^* = c$   $b^* = -(-a + b)/2$   
 Origin at x,x,1/8



$Fd\bar{3}1'$   
203.2.1528

$m\bar{3}1'$   
 $F2/d\bar{3}1'$

Cubic



**Origin** at  $231'$ , at  $-1/8, -1/8, -1/8$  from center ( $\bar{3}1'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $-1/4 \leq z \leq 1/4$ ;  $y \leq \min(x, 1/2-x)$ ;  $-y \leq z \leq y$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/4,1/4,1/4$   $1/4,1/4,-1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                            | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                                  | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                  |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{xy\bar{z}}$  0,0,0)  | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}\bar{y}z}$  0,0,0)  |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{xy\bar{z}}$  0,0,0) | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{\bar{x}\bar{y}z}$  0,0,0) |

- |   |   |  |   |
|---|---|--|---|
| (13) $\bar{1}$ 1/8,1/8,1/8<br>( $\bar{1}$   1/4,1/4,1/4)                        | (14) d (1/4,1/4,0) x,y,1/8<br>( $m_z$   1/4,1/4,1/4)  | (15) d (1/4,0,1/4) x,1/8,z<br>( $m_y$   1/4,1/4,1/4)   | (16) d (0,1/4,1/4) 1/8,y,z<br>( $m_x$   1/4,1/4,1/4)  |
| (17) $\bar{3}^+$ x,x,x;<br>1/8,1/8,1/8<br>( $\bar{3}_{xyz}$   1/4,1/4,1/4)      | (18) $\bar{3}^+$ $\bar{x}$ -1/2,x+1/2, $\bar{x}$ ;<br>-1/8,1/8,3/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,1/4,1/4) | (19) $\bar{3}^+$ x, $\bar{x}$ +1/2, $\bar{x}$ ;<br>1/8,3/8,-1/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,1/4,1/4) | (20) $\bar{3}^+$ $\bar{x}$ +1/2, $\bar{x}$ ,x;<br>3/8,-1/8,1/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,1/4,1/4) |
| (21) $\bar{3}^-$ x,x,x;<br>1/8,1/8,1/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,1/4,1/4) | (22) $\bar{3}^-$ x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ;<br>1/8,-1/8,3/8<br>( $\bar{3}_{xyz}$   1/4,1/4,1/4)     | (23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1/2, x;<br>-1/8,3/8,1/8<br>( $\bar{3}_{xyz}$   1/4,1/4,1/4)      | (24) $\bar{3}^-$ $\bar{x}$ +1/2, x, $\bar{x}$ ;<br>3/8,1/8,-1/8<br>( $\bar{3}_{xyz}$   1/4,1/4,1/4)     |

For (0,1/2,1/2) + set

- |   |   |  |   |
|---|---|--|---|
| (1) t (0,1/2,1/2)<br>(1   0,1/2,1/2)  | (2) 2 (0,0,1/2) 0,1/4,z<br>( $2_z$   0,1/2,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>( $2_y$   0,1/2,1/2)  | (4) 2 x,1/4,1/4<br>( $2_x$   0,1/2,1/2)   |
| (5) $3^+$ (1/3,1/3,1/3)<br>x-1/3,x-1/6,x<br>( $3_{xyz}$   0,1/2,1/2)                    | (6) $3^+$ $\bar{x}$ ,x+1/2, $\bar{x}$<br>( $3_{xyz}^{-1}$   0,1/2,1/2)                                    | (7) $3^+$ (-1/3,1/3,1/3)<br>x+1/3,x-1/6, $\bar{x}$<br>( $3_{xyz}^{-1}$   0,1/2,1/2)                    | (8) $3^+$ $\bar{x}$ , $\bar{x}$ +1/2,x<br>( $3_{xyz}^{-1}$   0,1/2,1/2)                                     |
| (9) $3^-$ (1/3,1/3,1/3)<br>x-1/6,x+1/6,x<br>( $3_{xyz}^{-1}$   0,1/2,1/2)               | (10) $3^-$ (-1/3,1/3,1/3)<br>x+1/6,x+1/6, $\bar{x}$<br>( $3_{xyz}$   0,1/2,1/2)                           | (11) $3^-$ $\bar{x}$ +1/2, $\bar{x}$ +1/2, x<br>( $3_{xyz}$   0,1/2,1/2)                               | (12) $3^-$ $\bar{x}$ -1/2, x+1/2, $\bar{x}$<br>( $3_{xyz}$   0,1/2,1/2)                                     |
| (13) $\bar{1}$ 1/8,3/8,3/8<br>( $\bar{1}$   1/4,3/4,3/4)                                | (14) d (1/4,3/4,0) x,y,3/8<br>( $m_z$   1/4,3/4,3/4)  | (15) d (1/4,0,3/4) x,3/8,z<br>( $m_y$   1/4,3/4,3/4)   | (16) d (0,3/4,3/4) 1/8,y,z<br>( $m_x$   1/4,3/4,3/4)  |
| (17) $\bar{3}^+$ x,x+1/2,x;<br>1/8,5/8,1/8<br>( $\bar{3}_{xyz}$   1/4,3/4,3/4)          | (18) $\bar{3}^+$ $\bar{x}$ -3/2,x+1, $\bar{x}$ ;<br>-5/8,1/8,7/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,3/4,3/4) | (19) $\bar{3}^+$ x, $\bar{x}$ +1, $\bar{x}$ ;<br>1/8,7/8,-1/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,3/4,3/4) | (20) $\bar{3}^+$ $\bar{x}$ +3/2, $\bar{x}$ +1/2,x;<br>7/8,-1/8,5/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,3/4,3/4) |
| (21) $\bar{3}^-$ x-1/2,x-1/2,x;<br>1/8,1/8,5/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,3/4,3/4) | (22) $\bar{3}^-$ x+1, $\bar{x}$ -1, $\bar{x}$ ;<br>1/8,-1/8,7/8<br>( $\bar{3}_{xyz}$   1/4,3/4,3/4)       | (23) $\bar{3}^-$ $\bar{x}$ -1/2, $\bar{x}$ +1, x;<br>-5/8,7/8,1/8<br>( $\bar{3}_{xyz}$   1/4,3/4,3/4)  | (24) $\bar{3}^-$ $\bar{x}$ +1, x+1/2, $\bar{x}$ ;<br>7/8,5/8,-1/8<br>( $\bar{3}_{xyz}$   1/4,3/4,3/4)       |

For (1/2,0,1/2) + set

- |   |   |  |   |
|---|---|--|---|
| (1) t (1/2,0,1/2)<br>(1   1/2,0,1/2)  | (2) 2 (0,0,1/2) 1/4,0,z<br>( $2_z$   1/2,0,1/2)   | (3) 2 1/4,y,1/4<br>( $2_y$   1/2,0,1/2)  | (4) 2 (1/2,0,0) x,0,1/4<br>( $2_x$   1/2,0,1/2)   |
| (5) $3^+$ (1/3,1/3,1/3)<br>x+1/6,x-1/6,x<br>( $3_{xyz}$   1/2,0,1/2)                | (6) $3^+$ (1/3,-1/3,1/3)<br>x+1/6,x+1/6, $\bar{x}$<br>( $3_{xyz}^{-1}$   1/2,0,1/2)                     | (7) $3^+$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$<br>( $3_{xyz}^{-1}$   1/2,0,1/2)                                | (8) $3^+$ $\bar{x}$ +1/2, $\bar{x}$ +1/2,x<br>( $3_{xyz}^{-1}$   1/2,0,1/2)                               |
| (9) $3^-$ (1/3,1/3,1/3)<br>x-1/6,x-1/3,x<br>( $3_{xyz}^{-1}$   1/2,0,1/2)           | (10) $3^-$ x+1/2, $\bar{x}$ , $\bar{x}$<br>( $3_{xyz}$   1/2,0,1/2)                                     | (11) $3^-$ $\bar{x}$ +1/2, $\bar{x}$ , x<br>( $3_{xyz}$   1/2,0,1/2)                                       | (12) $3^-$ (1/3,-1/3,1/3)<br>$\bar{x}$ -1/6, x+1/3, $\bar{x}$<br>( $3_{xyz}$   1/2,0,1/2)                 |
| (13) $\bar{1}$ 3/8,1/8,3/8<br>( $\bar{1}$   3/4,1/4,3/4)                            | (14) d (3/4,1/4,0) x,y,3/8<br>( $m_z$   3/4,1/4,3/4)  | (15) d (3/4,0,3/4) x,1/8,z<br>( $m_y$   3/4,1/4,3/4)   | (16) d (0,1/4,3/4) 3/8,y,z<br>( $m_x$   3/4,1/4,3/4)  |
| (17) $\bar{3}^+$ x-1/2,x-1/2,x;<br>1/8,1/8,5/8<br>( $\bar{3}_{xyz}$   3/4,1/4,3/4)  | (18) $\bar{3}^+$ $\bar{x}$ -1,x+1, $\bar{x}$ ;<br>-1/8,1/8,7/8<br>( $\bar{3}_{xyz}^{-1}$   3/4,1/4,3/4) | (19) $\bar{3}^+$ x+1/2, $\bar{x}$ +1, $\bar{x}$ ;<br>5/8,7/8,-1/8<br>( $\bar{3}_{xyz}^{-1}$   3/4,1/4,3/4) | (20) $\bar{3}^+$ $\bar{x}$ +1, $\bar{x}$ -1/2,x;<br>7/8,-5/8,1/8<br>( $\bar{3}_{xyz}^{-1}$   3/4,1/4,3/4) |
| (21) $\bar{3}^-$ x+1/2,x,x;<br>5/8,1/8,1/8<br>( $\bar{3}_{xyz}^{-1}$   3/4,1/4,3/4) | (22) $\bar{3}^-$ x+1, $\bar{x}$ -3/2, $\bar{x}$ ;<br>1/8,-5/8,7/8<br>( $\bar{3}_{xyz}$   3/4,1/4,3/4)   | (23) $\bar{3}^-$ $\bar{x}$ +1/2, $\bar{x}$ +3/2, x;<br>-1/8,7/8,5/7<br>( $\bar{3}_{xyz}$   3/4,1/4,3/4)    | (24) $\bar{3}^-$ $\bar{x}$ +1, x, $\bar{x}$ ;<br>7/8,1/8,-1/8<br>( $\bar{3}_{xyz}$   3/4,1/4,3/4)         |



## For (1/2,1/2,0) + set

- |   |  |  |   |
|---|--|--|---|
| (1) $t$ (1/2,1/2,0)<br>(1   1/2,1/2,0)  | (2) $2$ 1/4,1/4,z<br>( $z$   1/2,1/2,0)  | (3) $2$ (0,1/2,0) 1/4,y,0<br>( $y$   1/2,1/2,0)  | (4) $2$ (1/2,0,0) $x$ ,1/4,0<br>( $x$   1/2,1/2,0)  |
| (5) $3^+$ (1/3,1/3,1/3)<br>$x+1/6,x+1/3,x$<br>( $3_{xyz}$   1/2,1/2,0)                | (6) $3^+$ $\bar{x}+1/2,x,\bar{x}$<br>( $3_{xyz}^{-1}$   1/2,1/2,0)                                   | (7) $3^+$ $x+1/2,\bar{x},\bar{x}$<br>( $3_{xyz}^{-1}$   1/2,1/2,0)                                     | (8) $3^+$ (1/3,1/3,-1/3)<br>$\bar{x}+1/6,\bar{x}+1/3,x$<br>( $3_{xyz}^{-1}$   1/2,1/2,0)          |
| (9) $3^-$ (1/3,1/3,1/3)<br>$x+1/3,x+1/6,x$<br>( $3_{xyz}^{-1}$   1/2,1/2,0)           | (10) $3^-$ $x,\bar{x}+1/2,\bar{x}$<br>( $3_{xyz}$   1/2,1/2,0)                                       | (11) $3^-$ (1/3,1/3,-1/3)<br>$\bar{x}+1/3,\bar{x}+1/6,x$<br>( $3_{xyz}$   1/2,1/2,0)                   | (12) $3^-$ $\bar{x},x+1/2,\bar{x}$<br>( $3_{xyz}$   1/2,1/2,0)                                    |
| (13) $\bar{1}$ 3/8,3/8,1/8<br>( $\bar{1}$   3/4,3/4,1/4)                              | (14) $d$ (3/4,3/4,0) $x,y,1/8$<br>( $m_z$   3/4,3/4,1/4)   | (15) $d$ (3/4,0,1/4) $x,3/8,z$<br>( $m_y$   3/4,3/4,1/4)   | (16) $d$ (0,3/4,1/4) 3/8,y,z<br>( $m_x$   3/4,3/4,1/4)  |
| (17) $\bar{3}^+$ $x+1/2,x,x;$<br>5/8,1/8,1/8<br>( $\bar{3}_{xyz}$   3/4,3/4,1/4)      | (18) $\bar{3}^+$ $\bar{x}-1,x+3/2,\bar{x};$<br>-1/8,5/8,7/8<br>( $\bar{3}_{xyz}^{-1}$   3/4,3/4,1/4) | (19) $\bar{3}^+$ $x-1/2,\bar{x}+3/2,\bar{x};$<br>1/8,7/8,-5/8<br>( $\bar{3}_{xyz}^{-1}$   3/4,3/4,1/4) | (20) $\bar{3}^+$ $\bar{x}+1,\bar{x},x;$<br>7/8,-1/8,1/8<br>( $\bar{3}_{xyz}^{-1}$   3/4,3/4,1/4)  |
| (21) $\bar{3}^-$ $x,x+1/2,x;$<br>1/8,5/8,1/8<br>( $\bar{3}_{xyz}^{-1}$   3/4,3/4,1/4) | (22) $\bar{3}^-$ $x+3/2,\bar{x}-1,\bar{x};$<br>5/8,-1/8,7/8<br>( $\bar{3}_{xyz}$   3/4,3/4,1/4)      | (23) $\bar{3}^-$ $\bar{x},\bar{x}+1,x;$<br>-1/8,7/8,1/8<br>( $\bar{3}_{xyz}$   3/4,3/4,1/4)            | (24) $\bar{3}^-$ $\bar{x}+3/2,x-1/2,\bar{x};$<br>7/8,1/8,-5/8<br>( $\bar{3}_{xyz}$   3/4,3/4,1/4) |

## For (0,0,0)' + set

- |  |   |   |   |
|--|---|---|---|
| (1) $1'$<br>(1   0,0,0)'   | (2) $2'$ 0,0,z<br>( $z$   0,0,0)'   | (3) $2'$ 0,y,0<br>( $y$   0,0,0)'   | (4) $2'$ $x,0,0$<br>( $x$   0,0,0)'   |
| (5) $3^+$ ' $x,x,x$<br>( $3_{xyz}$   0,0,0)'   | (6) $3^+$ ' $\bar{x},x,\bar{x}$<br>( $3_{xyz}^{-1}$   0,0,0)'   | (7) $3^+$ ' $x,\bar{x},\bar{x}$<br>( $3_{xyz}^{-1}$   0,0,0)'   | (8) $3^+$ ' $\bar{x},\bar{x},x$<br>( $3_{xyz}^{-1}$   0,0,0)'   |
| (9) $3^-$ ' $x,x,x$<br>( $3_{xyz}^{-1}$   0,0,0)'                                    | (10) $3^-$ ' $x,\bar{x},\bar{x}$<br>( $3_{xyz}$   0,0,0)'   | (11) $3^-$ ' $\bar{x},\bar{x},x$<br>( $3_{xyz}$   0,0,0)'   | (12) $3^-$ ' $\bar{x},x,\bar{x}$<br>( $3_{xyz}$   0,0,0)'   |
| (13) $\bar{1}'$ 1/8,1/8,1/8<br>( $\bar{1}'$   1/4,1/4,1/4)'                          | (14) $d'$ (1/4,1/4,0) $x,y,1/8$<br>( $m_z$   1/4,1/4,1/4)'  | (15) $d'$ (1/4,0,1/4) $x,1/8,z$<br>( $m_y$   1/4,1/4,1/4)'  | (16) $d'$ (0,1/4,1/4) 1/8,y,z<br>( $m_x$   1/4,1/4,1/4)'  |
| (17) $\bar{3}^+$ ' $x,x,x;$<br>1/8,1/8,1/8<br>( $\bar{3}_{xyz}$   1/4,1/4,1/4)'      | (18) $\bar{3}^+$ ' $\bar{x}-1/2,x+1/2,\bar{x};$<br>-1/8,1/8,3/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,1/4,1/4)' | (19) $\bar{3}^+$ ' $x,\bar{x}+1/2,\bar{x};$<br>1/8,3/8,-1/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,1/4,1/4)' | (20) $\bar{3}^+$ ' $\bar{x}+1/2,\bar{x},x;$<br>3/8,-1/8,1/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,1/4,1/4)' |
| (21) $\bar{3}^-$ ' $x,x,x;$<br>1/8,1/8,1/8<br>( $\bar{3}_{xyz}^{-1}$   1/4,1/4,1/4)' | (22) $\bar{3}^-$ ' $x+1/2,\bar{x}+1/2,\bar{x};$<br>1/8,-1/8,3/8<br>( $\bar{3}_{xyz}$   1/4,1/4,1/4)'      | (23) $\bar{3}^-$ ' $\bar{x},\bar{x}+1/2,x;$<br>-1/8,3/8,1/8<br>( $\bar{3}_{xyz}$   1/4,1/4,1/4)'      | (24) $\bar{3}^-$ ' $\bar{x}+1/2,x,\bar{x};$<br>3/8,1/8,-1/8<br>( $\bar{3}_{xyz}$   1/4,1/4,1/4)'      |

## For (0,1/2,1/2)' + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t'$ (0,1/2,1/2)<br>(1   0,1/2,1/2)'                                       | (2) $2'$ (0,0,1/2) 0,1/4,z<br>( $z$   0,1/2,1/2)'   | (3) $2'$ (0,1/2,0) 0,y,1/4<br>( $y$   0,1/2,1/2)'   | (4) $2'$ $x,1/4,1/4$<br>( $x$   0,1/2,1/2)'                           |
| (5) $3^+$ ' (1/3,1/3,1/3)<br>$x-1/3,x-1/6,x$<br>( $3_{xyz}$   0,1/2,1/2)'      | (6) $3^+$ ' $\bar{x},x+1/2,\bar{x}$<br>( $3_{xyz}^{-1}$   0,1/2,1/2)'                         | (7) $3^+$ ' (-1/3,1/3,1/3)<br>$\bar{x}+1/3,x-1/6,\bar{x}$<br>( $3_{xyz}^{-1}$   0,1/2,1/2)' | (8) $3^+$ ' $\bar{x},\bar{x}+1/2,x$<br>( $3_{xyz}^{-1}$   0,1/2,1/2)' |
| (9) $3^-$ ' (1/3,1/3,1/3)<br>$x-1/6,x+1/6,x$<br>( $3_{xyz}^{-1}$   0,1/2,1/2)' | (10) $3^-$ ' (-1/3,1/3,1/3)<br>$\bar{x}+1/6,\bar{x}+1/6,\bar{x}$<br>( $3_{xyz}$   0,1/2,1/2)' | (11) $3^-$ ' $\bar{x}+1/2,\bar{x}+1/2,x$<br>( $3_{xyz}$   0,1/2,1/2)'                       | (12) $3^-$ ' $\bar{x}-1/2,x+1/2,\bar{x}$<br>( $3_{xyz}$   0,1/2,1/2)' |

- |   |  |  |  |
|---|--|--|--|
| (13) $\bar{1} \mid 1/8, 3/8, 3/8$<br>$(\bar{1} \mid 1/4, 3/4, 3/4)'$                                    | (14) $d' \mid (1/4, 3/4, 0) \ x, y, 3/8$<br>$(m_z \mid 1/4, 3/4, 3/4)'$  | (15) $d' \mid (1/4, 0, 3/4) \ x, 3/8, z$<br>$(m_y \mid 1/4, 3/4, 3/4)'$  | (16) $d' \mid (0, 3/4, 3/4) \ 1/8, y, z$<br>$(m_x \mid 1/4, 3/4, 3/4)'$  |
| (17) $\bar{3}^+ \mid x, x+1/2, x;$<br>$1/8, 5/8, 1/8$<br>$(\bar{3}_{xyz} \mid 1/4, 3/4, 3/4)'$          | (18) $\bar{3}^+ \mid \bar{x}-3/2, x+1, \bar{x};$<br>$-5/8, 1/8, 7/8$<br>$(\bar{3}_{x\bar{y}\bar{z}}^{-1} \mid 1/4, 3/4, 3/4)'$ | (19) $\bar{3}^+ \mid x, \bar{x}+1, \bar{x};$<br>$1/8, 7/8, -1/8$<br>$(\bar{3}_{x\bar{y}\bar{z}}^{-1} \mid 1/4, 3/4, 3/4)'$ | (20) $\bar{3}^+ \mid \bar{x}+3/2, \bar{x}+1/2, x;$<br>$7/8, -1/8, 5/8$<br>$(\bar{3}_{x\bar{y}\bar{z}}^{-1} \mid 1/4, 3/4, 3/4)'$ |
| (21) $\bar{3}^- \mid x-1/2, x-1/2, x;$<br>$1/8, 1/8, 5/8$<br>$(\bar{3}_{xyz}^{-1} \mid 1/4, 3/4, 3/4)'$ | (22) $\bar{3}^- \mid x+1, \bar{x}-1, \bar{x};$<br>$1/8, -1/8, 7/8$<br>$(\bar{3}_{xyz} \mid 1/4, 3/4, 3/4)'$                    | (23) $\bar{3}^- \mid \bar{x}-1/2, \bar{x}+1, x;$<br>$-5/8, 7/8, 1/8$<br>$(\bar{3}_{xyz} \mid 1/4, 3/4, 3/4)'$              | (24) $\bar{3}^- \mid \bar{x}+1, x+1/2, \bar{x};$<br>$7/8, 5/8, -1/8$<br>$(\bar{3}_{x\bar{y}\bar{z}} \mid 1/4, 3/4, 3/4)'$        |

For (1/2, 0, 1/2)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t' \mid (1/2, 0, 1/2)$<br>$(1 \mid 1/2, 0, 1/2)'$  | (2) $2' \mid (0, 0, 1/2) \ 1/4, 0, z$<br>$(2_z \mid 1/2, 0, 1/2)'$   | (3) $2' \mid 1/4, y, 1/4$<br>$(2_y \mid 1/2, 0, 1/2)'$   | (4) $2' \mid (1/2, 0, 0) \ x, 0, 1/4$<br>$(2_x \mid 1/2, 0, 1/2)'$   |
| (5) $3^+ \mid (1/3, 1/3, 1/3)$<br>$x+1/6, x-1/6, x$<br>$(3_{xyz} \mid 1/2, 0, 1/2)'$                | (6) $3^+ \mid (1/3, -1/3, 1/3)$<br>$x+1/6, x+1/6, \bar{x}$<br>$(3_{x\bar{y}\bar{z}}^{-1} \mid 1/2, 0, 1/2)'$                 | (7) $3^+ \mid x+1/2, \bar{x}-1/2, \bar{x}$<br>$(3_{x\bar{y}\bar{z}}^{-1} \mid 1/2, 0, 1/2)'$                                   | (8) $3^+ \mid \bar{x}+1/2, \bar{x}+1/2, x$<br>$(3_{x\bar{y}\bar{z}}^{-1} \mid 1/2, 0, 1/2)'$                                   |
| (9) $3^- \mid (1/3, 1/3, 1/3)$<br>$x-1/6, x-1/3, x$<br>$(3_{xyz}^{-1} \mid 1/2, 0, 1/2)'$           | (10) $3^- \mid x+1/2, \bar{x}, \bar{x}$<br>$(3_{xyz} \mid 1/2, 0, 1/2)'$   | (11) $3^- \mid \bar{x}+1/2, \bar{x}, x$<br>$(3_{x\bar{y}\bar{z}} \mid 1/2, 0, 1/2)'$   | (12) $3^- \mid (1/3, -1/3, 1/3)$<br>$x-1/6, x+1/3, \bar{x}$<br>$(3_{x\bar{y}\bar{z}} \mid 1/2, 0, 1/2)'$                       |
| (13) $\bar{1} \mid 3/8, 1/8, 3/8$<br>$(\bar{1} \mid 3/4, 1/4, 3/4)'$                                | (14) $d' \mid (3/4, 1/4, 0) \ x, y, 3/8$<br>$(m_z \mid 3/4, 1/4, 3/4)'$  | (15) $d' \mid (3/4, 0, 3/4) \ x, 1/8, z$<br>$(m_y \mid 3/4, 1/4, 3/4)'$  | (16) $d' \mid (0, 1/4, 3/4) \ 3/8, y, z$<br>$(m_x \mid 3/4, 1/4, 3/4)'$  |
| (17) $\bar{3}^+ \mid x-1/2, x-1/2, x;$<br>$1/8, 1/8, 5/8$<br>$(\bar{3}_{xyz} \mid 3/4, 1/4, 3/4)'$  | (18) $\bar{3}^+ \mid \bar{x}-1, x+1, \bar{x};$<br>$-1/8, 1/8, 7/8$<br>$(\bar{3}_{x\bar{y}\bar{z}}^{-1} \mid 3/4, 1/4, 3/4)'$ | (19) $\bar{3}^+ \mid x+1/2, \bar{x}+1, \bar{x};$<br>$5/8, 7/8, -1/8$<br>$(\bar{3}_{x\bar{y}\bar{z}}^{-1} \mid 3/4, 1/4, 3/4)'$ | (20) $\bar{3}^+ \mid \bar{x}+1, \bar{x}-1/2, x;$<br>$7/8, -5/8, 1/8$<br>$(\bar{3}_{x\bar{y}\bar{z}}^{-1} \mid 3/4, 1/4, 3/4)'$ |
| (21) $\bar{3}^- \mid x+1/2, x, x;$<br>$5/8, 1/8, 1/8$<br>$(\bar{3}_{xyz}^{-1} \mid 3/4, 1/4, 3/4)'$ | (22) $\bar{3}^- \mid x+1, \bar{x}-3/2, \bar{x};$<br>$1/8, -5/8, 7/8$<br>$(\bar{3}_{xyz} \mid 3/4, 1/4, 3/4)'$                | (23) $\bar{3}^- \mid \bar{x}+1/2, \bar{x}+3/2, x;$<br>$-1/8, 7/8, 5/7$<br>$(\bar{3}_{x\bar{y}\bar{z}} \mid 3/4, 1/4, 3/4)'$    | (24) $\bar{3}^- \mid \bar{x}+1, x, \bar{x};$<br>$7/8, 1/8, -1/8$<br>$(\bar{3}_{x\bar{y}\bar{z}} \mid 3/4, 1/4, 3/4)'$          |

For (1/2, 1/2, 0)' + set

- |   |  |  |   |
|---|--|--|---|
| (1) $t' \mid (1/2, 1/2, 0)$<br>$(1 \mid 1/2, 1/2, 0)'$  | (2) $2' \mid 1/4, 1/4, z$<br>$(2_z \mid 1/2, 1/2, 0)'$   | (3) $2' \mid (0, 1/2, 0) \ 1/4, y, 0$<br>$(2_y \mid 1/2, 1/2, 0)'$   | (4) $2' \mid (1/2, 0, 0) \ x, 1/4, 0$<br>$(2_x \mid 1/2, 1/2, 0)'$  |
| (5) $3^+ \mid (1/3, 1/3, 1/3)$<br>$x+1/6, x+1/3, x$<br>$(3_{xyz} \mid 1/2, 1/2, 0)'$                | (6) $3^+ \mid \bar{x}+1/2, x, \bar{x}$<br>$(3_{x\bar{y}\bar{z}}^{-1} \mid 1/2, 1/2, 0)'$                                       | (7) $3^+ \mid x+1/2, \bar{x}, \bar{x}$<br>$(3_{x\bar{y}\bar{z}}^{-1} \mid 1/2, 1/2, 0)'$   | (8) $3^+ \mid (1/3, 1/3, -1/3)$<br>$x+1/6, x+1/3, x$<br>$(3_{x\bar{y}\bar{z}}^{-1} \mid 1/2, 1/2, 0)'$                      |
| (9) $3^- \mid (1/3, 1/3, 1/3)$<br>$x+1/3, x+1/6, x$<br>$(3_{xyz}^{-1} \mid 1/2, 1/2, 0)'$           | (10) $3^- \mid x, \bar{x}+1/2, \bar{x}$<br>$(3_{xyz} \mid 1/2, 1/2, 0)'$   | (11) $3^- \mid (1/3, 1/3, -1/3)$<br>$x+1/3, x+1/6, x$<br>$(3_{x\bar{y}\bar{z}} \mid 1/2, 1/2, 0)'$                               | (12) $3^- \mid \bar{x}, x+1/2, \bar{x}$<br>$(3_{x\bar{y}\bar{z}} \mid 1/2, 1/2, 0)'$  |
| (13) $\bar{1} \mid 3/8, 3/8, 1/8$<br>$(\bar{1} \mid 3/4, 3/4, 1/4)'$                                | (14) $d' \mid (3/4, 3/4, 0) \ x, y, 1/8$<br>$(m_z \mid 3/4, 3/4, 1/4)'$  | (15) $d' \mid (3/4, 0, 1/4) \ x, 3/8, z$<br>$(m_y \mid 3/4, 3/4, 1/4)'$  | (16) $d' \mid (0, 3/4, 1/4) \ 3/8, y, z$<br>$(m_x \mid 3/4, 3/4, 1/4)'$   |
| (17) $\bar{3}^+ \mid x+1/2, x, x;$<br>$5/8, 1/8, 1/8$<br>$(\bar{3}_{xyz} \mid 3/4, 3/4, 1/4)'$      | (18) $\bar{3}^+ \mid \bar{x}-1, x+3/2, \bar{x};$<br>$-1/8, 5/8, 7/8$<br>$(\bar{3}_{x\bar{y}\bar{z}}^{-1} \mid 3/4, 3/4, 1/4)'$ | (19) $\bar{3}^+ \mid x-1/2, \bar{x}+3/2, \bar{x};$<br>$1/8, 7/8, -5/8$<br>$(\bar{3}_{x\bar{y}\bar{z}}^{-1} \mid 3/4, 3/4, 1/4)'$ | (20) $\bar{3}^+ \mid \bar{x}+1, \bar{x}, x;$<br>$7/8, -1/8, 1/8$<br>$(\bar{3}_{x\bar{y}\bar{z}}^{-1} \mid 3/4, 3/4, 1/4)'$  |
| (21) $\bar{3}^- \mid x, x+1/2, x;$<br>$1/8, 5/8, 1/8$<br>$(\bar{3}_{xyz}^{-1} \mid 3/4, 3/4, 1/4)'$ | (22) $\bar{3}^- \mid x+3/2, \bar{x}-1, \bar{x};$<br>$5/8, -1/8, 7/8$<br>$(\bar{3}_{xyz} \mid 3/4, 3/4, 1/4)'$                  | (23) $\bar{3}^- \mid \bar{x}, \bar{x}+1, x;$<br>$-1/8, 7/8, 1/8$<br>$(\bar{3}_{x\bar{y}\bar{z}} \mid 3/4, 3/4, 1/4)'$            | (24) $\bar{3}^- \mid \bar{x}+3/2, x-1/2, \bar{x};$<br>$7/8, 1/8, -5/8$<br>$(\bar{3}_{x\bar{y}\bar{z}} \mid 3/4, 3/4, 1/4)'$ |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); 1'.

### Positions

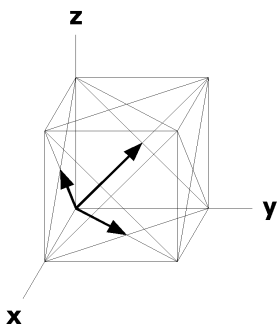
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates								
			(0,0,0) + (0,0,0)' +	(0,1/2,1/2) + (0,1/2,1/2)' +	(1/2,0,1/2) + (1/2,0,1/2)' +	(1/2,1/2,0) + (1/2,1/2,0)' +					
96	g	11'									
(1)	x,y,z	[0,0,0]	(2)	$\bar{x},\bar{y},z$	[0,0,0]	(3)	$\bar{x},y,\bar{z}$	[0,0,0]	(4)	$x,\bar{y},\bar{z}$	[0,0,0]
(5)	z,x,y	[0,0,0]	(6)	$z,\bar{x},\bar{y}$	[0,0,0]	(7)	$\bar{z},\bar{x},y$	[0,0,0]	(8)	$\bar{z},x,\bar{y}$	[0,0,0]
(9)	y,z,x	[0,0,0]	(10)	$\bar{y},z,\bar{x}$	[0,0,0]	(11)	$y,\bar{z},\bar{x}$	[0,0,0]	(12)	$\bar{y},\bar{z},x$	[0,0,0]
(13)	$\bar{x}+1/4,\bar{y}+1/4,\bar{z}+1/4$	[0,0,0]	(14)	$x+1/4,y+1/4,\bar{z}+1/4$	[0,0,0]	(15)	$x+1/4,\bar{y}+1/4,z+1/4$	[0,0,0]	(16)	$\bar{x}+1/4,y+1/4,z+1/4$	[0,0,0]
(17)	$\bar{z}+1/4,\bar{x}+1/4,\bar{y}+1/4$	[0,0,0]	(18)	$\bar{z}+1/4,x+1/4,y+1/4$	[0,0,0]	(19)	$z+1/4,x+1/4,\bar{y}+1/4$	[0,0,0]	(20)	$z+1/4,\bar{x}+1/4,y+1/4$	[0,0,0]
(21)	$\bar{y}+1/4,\bar{z}+1/4,\bar{x}+1/4$	[0,0,0]	(22)	$y+1/4,\bar{z}+1/4,x+1/4$	[0,0,0]	(23)	$\bar{y}+1/4,z+1/4,x+1/4$	[0,0,0]	(24)	$y+1/4,z+1/4,\bar{x}+1/4$	[0,0,0]
48	f	2..1'	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,0 [0,0,0]						
			0, $\bar{x}$ ,0 [0,0,0]	0,0,x [0,0,0]	0,0, $\bar{x}$ [0,0,0]						
			$\bar{x}+1/4,1/4,1/4$ [0,0,0]	$x+1/4,1/4,1/4$ [0,0,0]	$1/4,\bar{x}+1/4,1/4$ [0,0,0]						
			$1/4,x+1/4,1/4$ [0,0,0]	$1/4,1/4,\bar{x}+1/4$ [0,0,0]	$1/4,1/4,x+1/4$ [0,0,0]						
32	e	.3.1'	x,x,x [0,0,0]	$\bar{x},\bar{x},x$ [0,0,0]							
			$\bar{x},x,\bar{x}$ [0,0,0]	$x,\bar{x},\bar{x}$ [0,0,0]							
			$\bar{x}+1/4,\bar{x}+1/4,\bar{x}+1/4$ [0,0,0]	$x+1/4,x+1/4,\bar{x}+1/4$ [0,0,0]							
			$x+1/4,\bar{x}+1/4,x+1/4$ [0,0,0]	$\bar{x}+1/4,x+1/4,x+1/4$ [0,0,0]							
16	d	$\bar{3}.1'$	5/8,5/8,5/8 [0,0,0]	3/8,3/8,5/8 [0,0,0]	3/8,5/8,3/8 [0,0,0]	5/8,3/8,3/8 [0,0,0]					
16	c	$\bar{3}.1'$	1/8,1/8,1/8 [0,0,0]	7/8,7/8,1/8 [0,0,0]	7/8,1/8,7/8 [0,0,0]	1/8,7/8,7/8 [0,0,0]					
8	b	23.1'	1/2,1/2,1/2 [0,0,0]	3/4,3/4,3/4 [0,0,0]							
8	a	23.1'	0,0,0 [0,0,0]	1/4,1/4,1/4 [0,0,0]							

### Symmetry of Special Projections

Along [0,0,1]  $c2mm1'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,1,1]  $p61'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

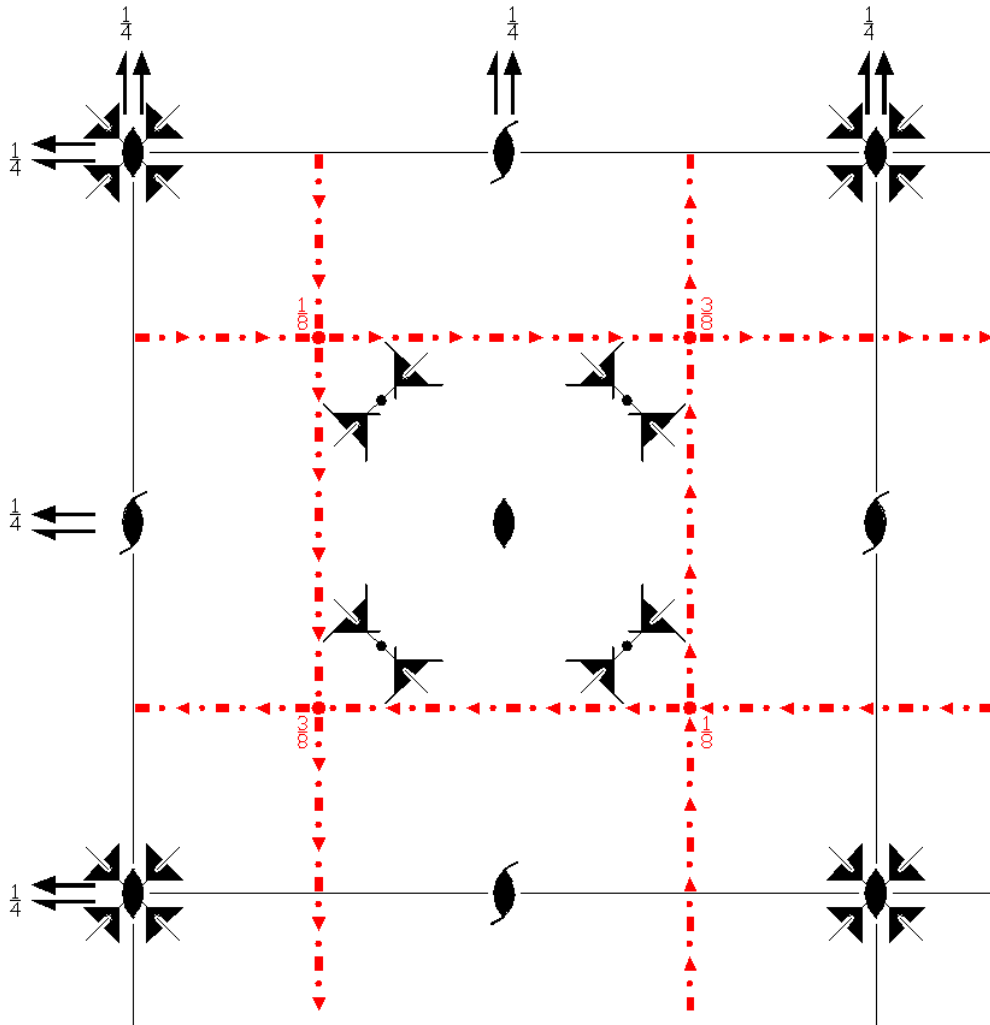
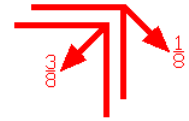
Along [1,1,0]  $c2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/8



$Fd\bar{3}'$   
203.3.1529

$m\bar{3}'$   
 $F2/d\bar{3}'$

Cubic



**Origin** at 23, at  $-1/8, -1/8, -1/8$  from center ( $\bar{3}'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $-1/4 \leq z \leq 1/4$ ;  $y \leq \min(x, 1/2-x)$ ;  $-y \leq z \leq y$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/4,1/4,1/4$   $1/4,1/4,-1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                  | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                                  | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                  |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) |

- |   |  |  |  |
|---|--|--|--|
| (13) $\bar{1} \mid 1/8, 1/8, 1/8$<br>$(\bar{1} \mid 1/4, 1/4, 1/4)'$                            | (14) $d' (1/4, 1/4, 0) \ x, y, 1/8$<br>$(m_z \mid 1/4, 1/4, 1/4)'$   | (15) $d' (1/4, 0, 1/4) \ x, 1/8, z$<br>$(m_y \mid 1/4, 1/4, 1/4)'$   | (16) $d' (0, 1/4, 1/4) \ 1/8, y, z$<br>$(m_x \mid 1/4, 1/4, 1/4)'$   |
| (17) $\bar{3}^+ \mid x, x, x;$<br>$1/8, 1/8, 1/8$<br>$(\bar{3}_{xyz} \mid 1/4, 1/4, 1/4)'$      | (18) $\bar{3}^+ \mid \bar{x} - 1/2, x + 1/2, \bar{x};$<br>$-1/8, 1/8, 3/8$<br>$(\bar{3}_{xyz}^{-1} \mid 1/4, 1/4, 1/4)'$ | (19) $\bar{3}^+ \mid x, \bar{x} + 1/2, \bar{x};$<br>$1/8, 3/8, -1/8$<br>$(\bar{3}_{xyz}^{-1} \mid 1/4, 1/4, 1/4)'$ | (20) $\bar{3}^+ \mid \bar{x} + 1/2, \bar{x}, x;$<br>$3/8, -1/8, 1/8$<br>$(\bar{3}_{xyz}^{-1} \mid 1/4, 1/4, 1/4)'$ |
| (21) $\bar{3}^- \mid x, x, x;$<br>$1/8, 1/8, 1/8$<br>$(\bar{3}_{xyz}^{-1} \mid 1/4, 1/4, 1/4)'$ | (22) $\bar{3}^- \mid x + 1/2, \bar{x} + 1/2, \bar{x};$<br>$1/8, -1/8, 3/8$<br>$(\bar{3}_{xyz} \mid 1/4, 1/4, 1/4)'$      | (23) $\bar{3}^- \mid \bar{x}, \bar{x} + 1/2, x;$<br>$-1/8, 3/8, 1/8$<br>$(\bar{3}_{xyz} \mid 1/4, 1/4, 1/4)'$      | (24) $\bar{3}^- \mid \bar{x} + 1/2, x, \bar{x};$<br>$3/8, 1/8, -1/8$<br>$(\bar{3}_{xyz} \mid 1/4, 1/4, 1/4)'$      |

For (0, 1/2, 1/2) + set

- |   |  |   |  |
|---|--|---|--|
| (1) $t (0, 1/2, 1/2)$<br>$(1 \mid 0, 1/2, 1/2)$   | (2) $2 (0, 0, 1/2) \ 0, 1/4, z$<br>$(2_z \mid 0, 1/2, 1/2)$  | (3) $2 (0, 1/2, 0) \ 0, y, 1/4$<br>$(2_y \mid 0, 1/2, 1/2)$   | (4) $2 \ x, 1/4, 1/4$<br>$(2_x \mid 0, 1/2, 1/2)$  |
| (5) $3^+ (1/3, 1/3, 1/3)$<br>$x - 1/3, x - 1/6, x$<br>$(3_{xyz} \mid 0, 1/2, 1/2)$                          | (6) $3^+ \ \bar{x}, x + 1/2, \bar{x}$<br>$(3_{xyz}^{-1} \mid 0, 1/2, 1/2)$   | (7) $3^+ (-1/3, 1/3, 1/3)$<br>$x + 1/3, x - 1/6, \bar{x}$<br>$(3_{xyz}^{-1} \mid 0, 1/2, 1/2)$                    | (8) $3^+ \ \bar{x}, \bar{x} + 1/2, x$<br>$(3_{xyz}^{-1} \mid 0, 1/2, 1/2)$   |
| (9) $3^- (1/3, 1/3, 1/3)$<br>$x - 1/6, x + 1/6, x$<br>$(3_{xyz}^{-1} \mid 0, 1/2, 1/2)$                     | (10) $3^- (-1/3, 1/3, 1/3)$<br>$x + 1/6, x + 1/6, \bar{x}$<br>$(3_{xyz} \mid 0, 1/2, 1/2)$                             | (11) $3^- \ \bar{x} + 1/2, \bar{x} + 1/2, x$<br>$(3_{xyz} \mid 0, 1/2, 1/2)$                                      | (12) $3^- \ \bar{x} - 1/2, x + 1/2, \bar{x}$<br>$(3_{xyz} \mid 0, 1/2, 1/2)$   |
| (13) $\bar{1} \mid 1/8, 3/8, 3/8$<br>$(\bar{1} \mid 1/4, 3/4, 3/4)'$  | (14) $d' (1/4, 3/4, 0) \ x, y, 3/8$<br>$(m_z \mid 1/4, 3/4, 3/4)'$   | (15) $d' (1/4, 0, 3/4) \ x, 3/8, z$<br>$(m_y \mid 1/4, 3/4, 3/4)'$  | (16) $d' (0, 3/4, 3/4) \ 1/8, y, z$<br>$(m_x \mid 1/4, 3/4, 3/4)'$   |
| (17) $\bar{3}^+ \mid x, x + 1/2, x;$<br>$1/8, 5/8, 1/8$<br>$(\bar{3}_{xyz} \mid 1/4, 3/4, 3/4)'$            | (18) $\bar{3}^+ \mid \bar{x} - 3/2, x + 1, \bar{x};$<br>$-5/8, 1/8, 7/8$<br>$(\bar{3}_{xyz}^{-1} \mid 1/4, 3/4, 3/4)'$ | (19) $\bar{3}^+ \mid x, \bar{x} + 1, \bar{x};$<br>$1/8, 7/8, -1/8$<br>$(\bar{3}_{xyz}^{-1} \mid 1/4, 3/4, 3/4)'$  | (20) $\bar{3}^+ \mid \bar{x} + 3/2, \bar{x} + 1/2, x;$<br>$7/8, -1/8, 5/8$<br>$(\bar{3}_{xyz}^{-1} \mid 1/4, 3/4, 3/4)'$ |
| (21) $\bar{3}^- \mid x - 1/2, x - 1/2, x;$<br>$1/8, 1/8, 5/8$<br>$(\bar{3}_{xyz}^{-1} \mid 1/4, 3/4, 3/4)'$ | (22) $\bar{3}^- \mid x + 1, \bar{x} - 1, \bar{x};$<br>$1/8, -1/8, 7/8$<br>$(\bar{3}_{xyz} \mid 1/4, 3/4, 3/4)'$        | (23) $\bar{3}^- \mid \bar{x} - 1/2, \bar{x} + 1, x;$<br>$-5/8, 7/8, 1/8$<br>$(\bar{3}_{xyz} \mid 1/4, 3/4, 3/4)'$ | (24) $\bar{3}^- \mid \bar{x} + 1, x + 1/2, \bar{x};$<br>$7/8, 5/8, -1/8$<br>$(\bar{3}_{xyz} \mid 1/4, 3/4, 3/4)'$        |

For (1/2, 0, 1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t (1/2, 0, 1/2)$<br>$(1 \mid 1/2, 0, 1/2)$  | (2) $2 (0, 0, 1/2) \ 1/4, 0, z$<br>$(2_z \mid 1/2, 0, 1/2)$  | (3) $2 \ 1/4, y, 1/4$<br>$(2_y \mid 1/2, 0, 1/2)$  | (4) $2 (1/2, 0, 0) \ x, 0, 1/4$<br>$(2_x \mid 1/2, 0, 1/2)$  |
| (5) $3^+ (1/3, 1/3, 1/3)$<br>$x + 1/6, x - 1/6, x$<br>$(3_{xyz} \mid 1/2, 0, 1/2)$                     | (6) $3^+ (1/3, -1/3, 1/3)$<br>$x + 1/6, x + 1/6, \bar{x}$<br>$(3_{xyz}^{-1} \mid 1/2, 0, 1/2)$                       | (7) $3^+ \ x + 1/2, \bar{x} - 1/2, \bar{x}$<br>$(3_{xyz}^{-1} \mid 1/2, 0, 1/2)$                                       | (8) $3^+ \ \bar{x} + 1/2, \bar{x} + 1/2, x$<br>$(3_{xyz}^{-1} \mid 1/2, 0, 1/2)$                                       |
| (9) $3^- (1/3, 1/3, 1/3)$<br>$x - 1/6, x - 1/3, x$<br>$(3_{xyz}^{-1} \mid 1/2, 0, 1/2)$                | (10) $3^- \ x + 1/2, \bar{x}, \bar{x}$<br>$(3_{xyz} \mid 1/2, 0, 1/2)$   | (11) $3^- \ \bar{x} + 1/2, \bar{x}, x$<br>$(3_{xyz} \mid 1/2, 0, 1/2)$   | (12) $3^- (1/3, -1/3, 1/3)$<br>$\bar{x} - 1/6, x + 1/3, \bar{x}$<br>$(3_{xyz} \mid 1/2, 0, 1/2)$                       |
| (13) $\bar{1} \mid 3/8, 1/8, 3/8$<br>$(\bar{1} \mid 3/4, 1/4, 3/4)'$                                   | (14) $d' (3/4, 1/4, 0) \ x, y, 3/8$<br>$(m_z \mid 3/4, 1/4, 3/4)'$   | (15) $d' (3/4, 0, 3/4) \ x, 1/8, z$<br>$(m_y \mid 3/4, 1/4, 3/4)'$   | (16) $d' (0, 1/4, 3/4) \ 3/8, y, z$<br>$(m_x \mid 3/4, 1/4, 3/4)'$   |
| (17) $\bar{3}^+ \mid x - 1/2, x - 1/2, x;$<br>$1/8, 1/8, 5/8$<br>$(\bar{3}_{xyz} \mid 3/4, 1/4, 3/4)'$ | (18) $\bar{3}^+ \mid \bar{x} - 1, x + 1, \bar{x};$<br>$-1/8, 1/8, 7/8$<br>$(\bar{3}_{xyz}^{-1} \mid 3/4, 1/4, 3/4)'$ | (19) $\bar{3}^+ \mid x + 1/2, \bar{x} + 1, \bar{x};$<br>$5/8, 7/8, -1/8$<br>$(\bar{3}_{xyz}^{-1} \mid 3/4, 1/4, 3/4)'$ | (20) $\bar{3}^+ \mid \bar{x} + 1, \bar{x} - 1/2, x;$<br>$7/8, -5/8, 1/8$<br>$(\bar{3}_{xyz}^{-1} \mid 3/4, 1/4, 3/4)'$ |
| (21) $\bar{3}^- \mid x + 1/2, x, x;$<br>$5/8, 1/8, 1/8$<br>$(\bar{3}_{xyz}^{-1} \mid 3/4, 1/4, 3/4)'$  | (22) $\bar{3}^- \mid x + 1, \bar{x} - 3/2, \bar{x};$<br>$1/8, -5/8, 7/8$<br>$(\bar{3}_{xyz} \mid 3/4, 1/4, 3/4)'$    | (23) $\bar{3}^- \mid \bar{x} + 1/2, \bar{x} + 3/2, x;$<br>$-1/8, 7/8, 5/7$<br>$(\bar{3}_{xyz} \mid 3/4, 1/4, 3/4)'$    | (24) $\bar{3}^- \mid \bar{x} + 1, x, \bar{x};$<br>$7/8, 1/8, -1/8$<br>$(\bar{3}_{xyz} \mid 3/4, 1/4, 3/4)'$            |

For (1/2,1/2,0) + set

(1) $t$ (1/2,1/2,0) (1   1/2,1/2,0)	(2) $2$ 1/4,1/4,z ( $2_z$   1/2,1/2,0)	(3) $2$ (0,1/2,0) 1/4,y,0 ( $2_y$   1/2,1/2,0)	(4) $2$ (1/2,0,0) x,1/4,0 ( $2_x$   1/2,1/2,0)
(5) $3^+$ (1/3,1/3,1/3) x+1/6,x+1/3,x ( $3_{xyz}$   1/2,1/2,0)	(6) $3^+$ $\bar{x}$ +1/2,x, $\bar{x}$ ( $3_{\bar{xyz}}$   1/2,1/2,0)	(7) $3^+$ x+1/2, $\bar{x}$ , $\bar{x}$ ( $3_{\bar{xyz}}$   1/2,1/2,0)	(8) $3^+$ (1/3,1/3,-1/3) x+1/6, $\bar{x}$ +1/3,x ( $3_{\bar{xyz}}$   1/2,1/2,0)
(9) $3^-$ (1/3,1/3,1/3) x+1/3,x+1/6,x ( $3_{xyz}$   1/2,1/2,0)	(10) $3^-$ x, $\bar{x}$ +1/2, $\bar{x}$ ( $3_{\bar{xyz}}$   1/2,1/2,0)	(11) $3^-$ (1/3,1/3,-1/3) x+1/3, $\bar{x}$ +1/6,x ( $3_{\bar{xyz}}$   1/2,1/2,0)	(12) $3^-$ $\bar{x}$ ,x+1/2, $\bar{x}$ ( $3_{\bar{xyz}}$   1/2,1/2,0)
(13) $\bar{1}$ ' 3/8,3/8,1/8 ( $1$   3/4,3/4,1/4)'	(14) $d'$ (3/4,3/4,0) x,y,1/8 ( $m_z$   3/4,3/4,1/4)'	(15) $d'$ (3/4,0,1/4) x,3/8,z ( $m_y$   3/4,3/4,1/4)'	(16) $d'$ (0,3/4,1/4) 3/8,y,z ( $m_x$   3/4,3/4,1/4)'
(17) $\bar{3}^+$ ' x+1/2,x,x; 5/8,1/8,1/8 ( $\bar{3}_{xyz}$   3/4,3/4,1/4)'	(18) $\bar{3}^+$ ' $\bar{x}$ -1,x+3/2, $\bar{x}$ ; -1/8,5/8,7/8 ( $\bar{3}_{\bar{xyz}}$   3/4,3/4,1/4)'	(19) $\bar{3}^+$ ' x-1/2, $\bar{x}$ +3/2, $\bar{x}$ ; 1/8,7/8,-5/8 ( $\bar{3}_{\bar{xyz}}$   3/4,3/4,1/4)'	(20) $\bar{3}^+$ ' $\bar{x}$ +1, $\bar{x}$ ,x; 7/8,-1/8,1/8 ( $\bar{3}_{\bar{xyz}}$   3/4,3/4,1/4)'
(21) $\bar{3}^-$ ' x,x+1/2,x; 1/8,5/8,1/8 ( $\bar{3}_{xyz}$   3/4,3/4,1/4)'	(22) $\bar{3}^-$ ' x+3/2, $\bar{x}$ -1, $\bar{x}$ ; 5/8,-1/8,7/8 ( $\bar{3}_{\bar{xyz}}$   3/4,3/4,1/4)'	(23) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ +1,x; -1/8,7/8,1/8 ( $\bar{3}_{\bar{yz}}$   3/4,3/4,1/4)'	(24) $\bar{3}^-$ ' $\bar{x}$ +3/2,x-1/2, $\bar{x}$ ; 7/8,1/8,-5/8 ( $\bar{3}_{\bar{yz}}$   3/4,3/4,1/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

96	g	1	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +					
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}$ , $\bar{y}$ ,z	[ $\bar{u}$ , $\bar{v}$ ,w]	(3)	$\bar{x}$ ,y, $\bar{z}$	[ $\bar{u}$ ,v, $\bar{w}$ ]	(4)	x, $\bar{y}$ , $\bar{z}$	[u, $\bar{v}$ , $\bar{w}$ ]
(5)	z,x,y	[w,u,v]	(6)	z, $\bar{x}$ , $\bar{y}$	[w, $\bar{u}$ , $\bar{v}$ ]	(7)	$\bar{z}$ , $\bar{x}$ ,y	[ $\bar{w}$ , $\bar{u}$ ,v]	(8)	$\bar{z}$ ,x,y	[ $\bar{w}$ ,u,v]
(9)	y,z,x	[v,w,u]	(10)	$\bar{y}$ ,z, $\bar{x}$	[ $\bar{v}$ ,w, $\bar{u}$ ]	(11)	y, $\bar{z}$ , $\bar{x}$	[v, $\bar{w}$ , $\bar{u}$ ]	(12)	$\bar{y}$ , $\bar{z}$ ,x	[ $\bar{v}$ , $\bar{w}$ ,u]
(13)	$\bar{x}$ +1/4, $\bar{y}$ +1/4, $\bar{z}$ +1/4	[ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(14)	x+1/4,y+1/4, $\bar{z}$ +1/4	[u,v, $\bar{w}$ ]	(15)	x+1/4, $\bar{y}$ +1/4,z+1/4	[u, $\bar{v}$ ,w]	(16)	$\bar{x}$ +1/4,y+1/4,z+1/4	[ $\bar{u}$ ,v,w]
(17)	$\bar{z}$ +1/4, $\bar{x}$ +1/4, $\bar{y}$ +1/4	[ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ]	(18)	$\bar{z}$ +1/4,x+1/4,y+1/4	[ $\bar{w}$ ,u,v]	(19)	z+1/4,x+1/4, $\bar{y}$ +1/4	[w,u, $\bar{v}$ ]	(20)	z+1/4, $\bar{x}$ +1/4,y+1/4	[w, $\bar{u}$ ,v]
(21)	$\bar{y}$ +1/4, $\bar{z}$ +1/4, $\bar{x}$ +1/4	[ $\bar{v}$ , $\bar{w}$ , $\bar{u}$ ]	(22)	y+1/4, $\bar{z}$ +1/4,x+1/4	[v, $\bar{w}$ ,u]	(23)	$\bar{y}$ +1/4,z+1/4,x+1/4	[ $\bar{v}$ ,w,u]	(24)	y+1/4,z+1/4, $\bar{x}$ +1/4	[v,w, $\bar{u}$ ]
48	f	2..	x,0,0	[u,0,0]	$\bar{x}$ ,0,0	[ $\bar{u}$ ,0,0]	0,x,0	[0,u,0]	0,0, $\bar{x}$	[0,0, $\bar{u}$ ]	
			0, $\bar{x}$ ,0	[0, $\bar{u}$ ,0]	0,0,x	[0,0,u]	0,0, $\bar{x}$	[0,0, $\bar{u}$ ]			
			$\bar{x}$ +1/4,1/4,1/4	[ $\bar{u}$ ,0,0]	x+1/4,1/4,1/4	[u,0,0]	1/4, $\bar{x}$ +1/4,1/4	[0, $\bar{u}$ ,0]			
			1/4,x+1/4,1/4	[0,u,0]	1/4,1/4, $\bar{x}$ +1/4	[0,0, $\bar{u}$ ]	1/4,1/4,x+1/4	[0,0,u]			

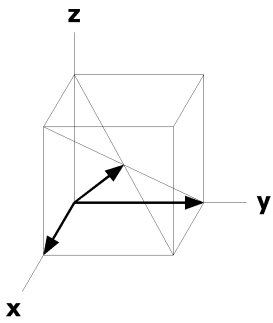
32	e	.3.	$x, x, x [u, u, u]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$		
			$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$		
			$\bar{x}+1/4, \bar{x}+1/4, \bar{x}+1/4 [\bar{u}, \bar{u}, \bar{u}]$	$x+1/4, x+1/4, \bar{x}+1/4 [u, u, \bar{u}]$		
			$x+1/4, \bar{x}+1/4, x+1/4 [u, \bar{u}, u]$	$\bar{x}+1/4, x+1/4, x+1/4 [\bar{u}, u, u]$		
16	d	$\bar{3}$ '	$5/8, 5/8, 5/8 [0, 0, 0]$	$3/8, 3/8, 5/8 [0, 0, 0]$	$3/8, 5/8, 3/8 [0, 0, 0]$	$5/8, 3/8, 3/8 [0, 0, 0]$
16	c	$\bar{3}$ '	$1/8, 1/8, 1/8 [0, 0, 0]$	$7/8, 7/8, 1/8 [0, 0, 0]$	$7/8, 1/8, 7/8 [0, 0, 0]$	$1/8, 7/8, 7/8 [0, 0, 0]$
8	b	23.	$1/2, 1/2, 1/2 [0, 0, 0]$	$3/4, 3/4, 3/4 [0, 0, 0]$		
8	a	23.	$0, 0, 0 [0, 0, 0]$	$1/4, 1/4, 1/4 [0, 0, 0]$		

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $c2m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $0, 0, z$

Along  $[1, 1, 1]$   $p6$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at  $x, x, x$

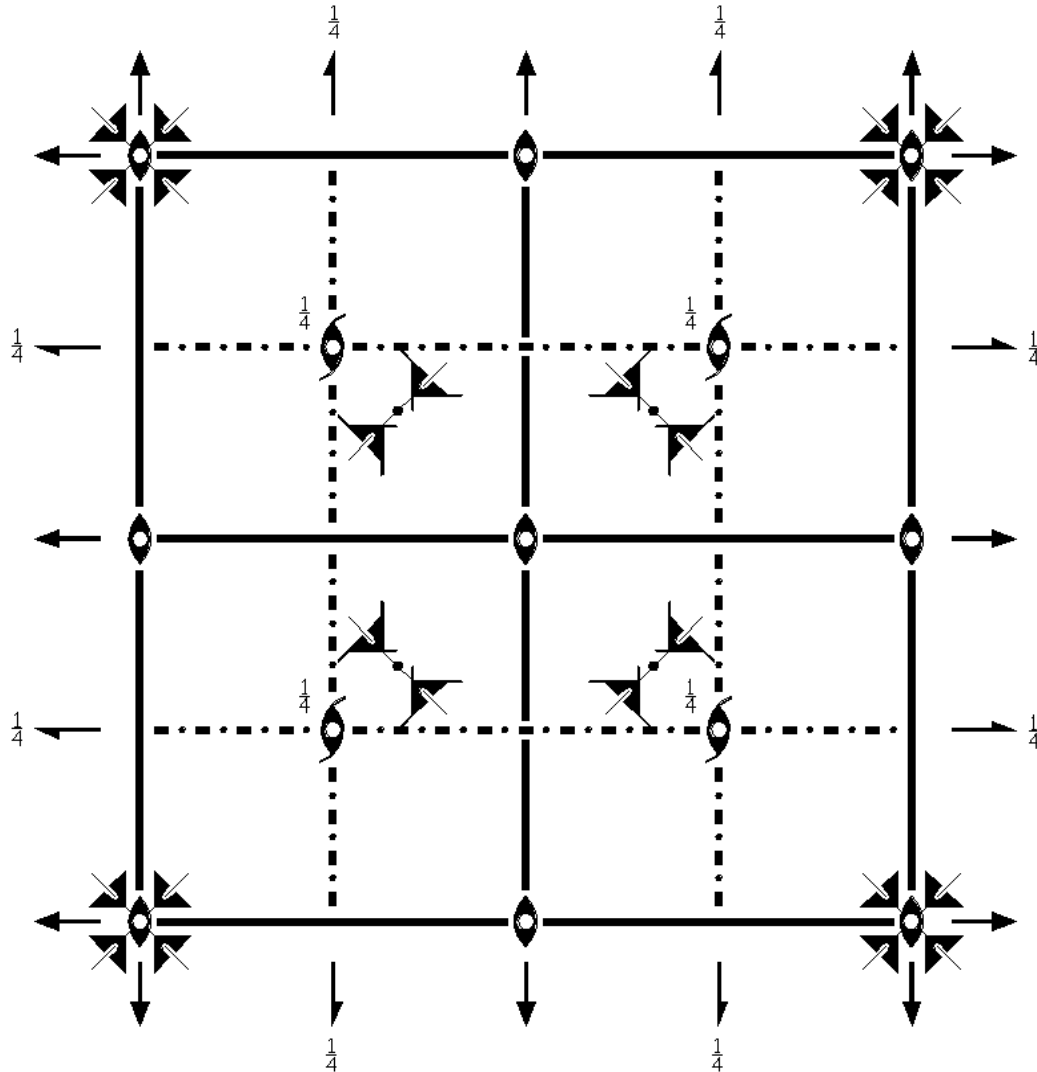
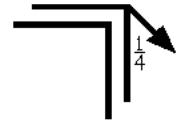
Along  $[1, 1, 0]$   $c2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 1/8$



$Im\bar{3}$   
204.1.1530

$m\bar{3}$   
 $I2/m\bar{3}$

Cubic



Origin at center ( $m\bar{3}$ )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq x;$   $z \leq y$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                          | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  0,0,0) | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{xyz}^{-1}$  0,0,0) | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}z}^{-1}$  0,0,0) |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)     | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{xyz}$  0,0,0)     | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)     |

204.1.1530

$Im\bar{3}$

Continued



- |  |   |  |   |
|--|---|--|---|
| (13) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)                              | (14) m x,y,0<br>( $m_z$  0,0,0)   | (15) m x,0,z<br>( $m_y$  0,0,0)  | (16) m 0,y,z<br>( $m_x$  0,0,0)   |
| (17) $\bar{3}^+$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$  0,0,0)               | (18) $\bar{3}^+$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0) | (19) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0) | (20) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0) |
| (21) $\bar{3}^-$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0) | (22) $\bar{3}^-$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)              | (23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)                | (24) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)               |

For (1/2,1/2,1/2) + set

- |   |   |  |   |
|---|---|--|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)  | (2) 2 (0,0,1/2) 1/4,1/4,z<br>( $2_z$  1/2,1/2,1/2)  | (3) 2 (0,1/2,0) 1/4,y,1/4<br>( $2_y$  1/2,1/2,1/2)   | (4) 2 (1/2,0,0) x,1/4,1/4<br>( $2_x$  1/2,1/2,1/2)  |
| (5) $3^+$ (1/2,1/2,1/2) x,x,x<br>( $3_{xyz}$  1/2,1/2,1/2)                              | (6) $3^+$ (1/6,-1/6,1/6)<br>x+1/3,x+1/3, $\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$ <sup>-1</sup>  1/2,1/2,1/2)                   | (7) $3^+$ (-1/6,1/6,1/6)<br>x+2/3, $\bar{x}$ -1/3, $\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$ <sup>-1</sup>  1/2,1/2,1/2)        | (8) $3^+$ (1/6,1/6,-1/6)<br>x+1/3, $\bar{x}$ +2/3,x<br>( $3_{x\bar{y}\bar{z}}$ <sup>-1</sup>  1/2,1/2,1/2)                |
| (9) $3^-$ (1/2,1/2,1/2) x,x,x<br>( $3_{xyz}$ <sup>-1</sup>  1/2,1/2,1/2)                | (10) $3^-$ (-1/6,1/6,1/6)<br>x+1/3, $\bar{x}$ +1/3, $\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  1/2,1/2,1/2)                      | (11) $3^-$ (1/6,1/6,-1/6)<br>x+2/3, $\bar{x}$ +1/3,x<br>( $3_{x\bar{y}\bar{z}}$  1/2,1/2,1/2)                              | (12) $3^-$ (1/6,-1/6,1/6)<br>x-1/3,x+2/3, $\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  1/2,1/2,1/2)                              |
| (13) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)                                 | (14) n (1/2,1/2,0) x,y,1/4<br>( $m_z$  1/2,1/2,1/2)   | (15) n (1/2,0,1/2) x,1/4,z<br>( $m_y$  1/2,1/2,1/2)  | (16) n (0,1/2,1/2) 1/4,y,z<br>( $m_x$  1/2,1/2,1/2)   |
| (17) $\bar{3}^+$ x,x,x;<br>1/4,1/4,1/4<br>( $\bar{3}_{xyz}$  1/2,1/2,1/2)               | (18) $\bar{3}^+$ $\bar{x}$ -1,x+1, $\bar{x}$ ;<br>-1/4,1/4,3/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  1/2,1/2,1/2) | (19) $\bar{3}^+$ x, $\bar{x}$ +1, $\bar{x}$ ;<br>1/4,3/4,-1/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  1/2,1/2,1/2) | (20) $\bar{3}^+$ $\bar{x}$ +1, $\bar{x}$ ,x;<br>3/4,-1/4,1/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  1/2,1/2,1/2) |
| (21) $\bar{3}^-$ x,x,x;<br>1/4,1/4,1/4<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,1/2,1/2) | (22) $\bar{3}^-$ x+1, $\bar{x}$ -1, $\bar{x}$ ;<br>1/4,-1/4,3/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$  1/2,1/2,1/2)              | (23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1,x;<br>-1/4,3/4,1/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$  1/2,1/2,1/2)                | (24) $\bar{3}^-$ $\bar{x}$ +1,x, $\bar{x}$ ;<br>3/4,1/4,-1/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$  1/2,1/2,1/2)               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

48 h 1

(0,0,0) + (1/2,1/2,1/2) +

- |  |  |   |   |
|--|--|---|---|
| (1) x,y,z [u,v,w]                              | (2) $\bar{x}$ , $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w]           | (3) $\bar{x}$ ,y, $\bar{z}$ [ $\bar{u}$ ,v, $\bar{w}$ ]   | (4) x, $\bar{y}$ , $\bar{z}$ [u, $\bar{v}$ , $\bar{w}$ ]  |
| (5) z,x,y [w,u,v]                              | (6) z, $\bar{x}$ , $\bar{y}$ [ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ] | (7) $\bar{z}$ , $\bar{x}$ ,y [ $\bar{w}$ , $\bar{u}$ ,v]  | (8) $\bar{z}$ ,x, $\bar{y}$ [ $\bar{w}$ ,u, $\bar{v}$ ]   |
| (9) y,z,x [v,w,u]                              | (10) $\bar{y}$ ,z, $\bar{x}$ [ $\bar{v}$ ,w, $\bar{u}$ ]           | (11) y, $\bar{z}$ , $\bar{x}$ [v, $\bar{w}$ , $\bar{u}$ ] | (12) $\bar{y}$ , $\bar{z}$ ,x [ $\bar{v}$ , $\bar{w}$ ,u] |
| (13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w] | (14) x,y, $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]          | (15) x, $\bar{y}$ ,z [u,v, $\bar{w}$ ]                    | (16) $\bar{x}$ ,y,z [u, $\bar{v}$ , $\bar{w}$ ]           |
| (17) $\bar{z}$ , $\bar{x}$ , $\bar{y}$ [w,u,v] | (18) $\bar{z}$ ,x,y [ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ]          | (19) z,x, $\bar{y}$ [ $\bar{w}$ , $\bar{u}$ ,v]           | (20) z, $\bar{x}$ ,y [ $\bar{w}$ ,u, $\bar{v}$ ]          |
| (21) $\bar{y}$ , $\bar{z}$ , $\bar{x}$ [v,w,u] | (22) y, $\bar{z}$ ,x [ $\bar{v}$ , $\bar{w}$ , $\bar{u}$ ]         | (23) $\bar{y}$ ,z,x [v, $\bar{w}$ , $\bar{u}$ ]           | (24) y,z, $\bar{x}$ [ $\bar{v}$ , $\bar{w}$ ,u]           |

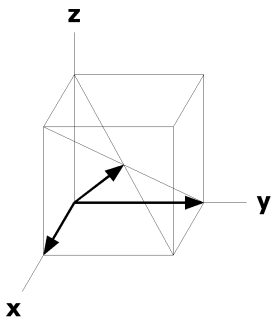
24	g	m..	0,y,z [u,0,0] 0, $\bar{y}$ , $\bar{z}$ [u,0,0] $\bar{z}$ ,0,y [0, $\bar{u}$ ,0] $\bar{y}$ ,z,0 [0,0, $\bar{u}$ ]	0, $\bar{y}$ ,z [ $\bar{u}$ ,0,0] z,0,y [0,u,0] $\bar{z}$ ,0, $\bar{y}$ [0,u,0] y, $\bar{z}$ ,0 [0,0, $\bar{u}$ ]	0,y, $\bar{z}$ [ $\bar{u}$ ,0,0] z,0, $\bar{y}$ [0, $\bar{u}$ ,0] y,z,0 [0,0,u] $\bar{y}$ , $\bar{z}$ ,0 [0,0,u]	
16	f	.3.	x,x,x [u,u,u] $\bar{x}$ , $\bar{x}$ , $\bar{x}$ [u,u,u]	$\bar{x}$ , $\bar{x}$ ,x [ $\bar{u}$ , $\bar{u}$ ,u] x,x, $\bar{x}$ [ $\bar{u}$ , $\bar{u}$ ,u]	$\bar{x}$ ,x, $\bar{x}$ [ $\bar{u}$ ,u, $\bar{u}$ ] x, $\bar{x}$ ,x [ $\bar{u}$ ,u, $\bar{u}$ ]	x, $\bar{x}$ , $\bar{x}$ [u, $\bar{u}$ , $\bar{u}$ ] $\bar{x}$ ,x,x [u, $\bar{u}$ , $\bar{u}$ ]
12	e	mm2..	x,0,1/2 [0,0,0] 1/2, $\bar{x}$ ,0 [0,0,0]	$\bar{x}$ ,0,1/2 [0,0,0] 0,1/2,x [0,0,0]	1/2,x,0 [0,0,0] 0,1/2, $\bar{x}$ [0,0,0]	
12	d	mm2..	x,0,0 [0,0,0] 0, $\bar{x}$ ,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0] 0,0,x [0,0,0]	0,x,0 [0,0,0] 0,0, $\bar{x}$ [0,0,0]	
8	c	. $\bar{3}$ .	1/4,1/4,1/4 [u,u,u]	3/4,3/4,1/4 [ $\bar{u}$ , $\bar{u}$ ,u]	3/4,1/4,3/4 [ $\bar{u}$ ,u, $\bar{u}$ ]	1/4,3/4,3/4 [u, $\bar{u}$ , $\bar{u}$ ]
6	b	mmm..	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	
2	a	m $\bar{3}$ .	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,1,1] p6'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

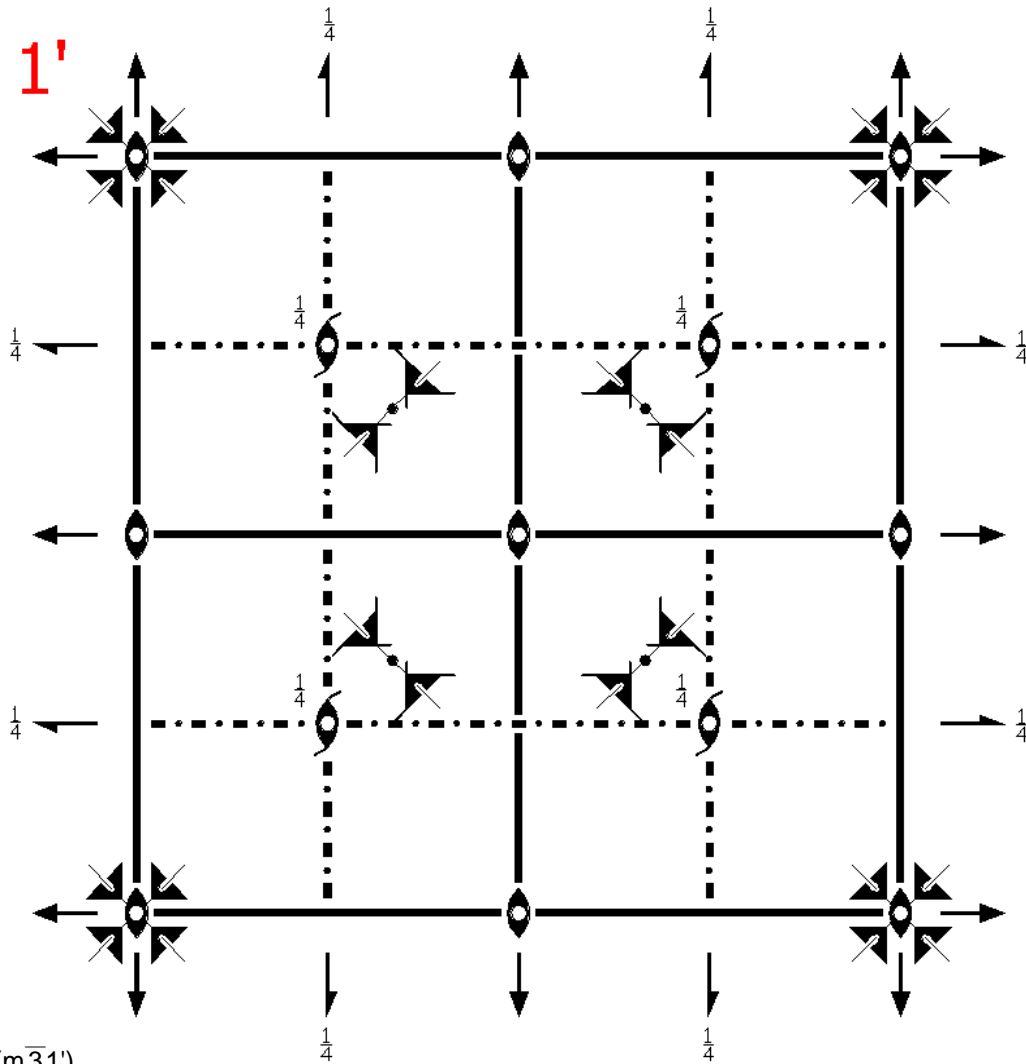
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$Im\bar{3}1'$   
204.2.1531

$m\bar{3}1'$   
 $I2/m\bar{3}1'$

Cubic



Origin at center ( $m\bar{3}1'$ )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq x;$   $z \leq y$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

### Symmetry Operations

For (0,0,0) + set

- |   |  |   |  |
|---|--|---|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)                   | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)                                  | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)                    |

Continued

204.2.1531

$Im\bar{3}1'$

- |  |  |  |  |
|--|--|--|--|
| (13) $\bar{1} \ 0,0,0$<br>( $\bar{1} \mid 0,0,0$ )                     | (14) $m \ x,y,0$<br>( $m_z \mid 0,0,0$ )   | (15) $m \ x,0,z$<br>( $m_y \mid 0,0,0$ )   | (16) $m \ 0,y,z$<br>( $m_x \mid 0,0,0$ )   |
| (17) $\bar{3}^+ \ x,x,x; 0,0,0$<br>( $\bar{3}_{xyz} \mid 0,0,0$ )      | (18) $\bar{3}^+ \ \bar{x},\bar{x},\bar{x}; 0,0,0$<br>( $\bar{3}_{\bar{xyz}}^{-1} \mid 0,0,0$ ) | (19) $\bar{3}^+ \ x,\bar{x},\bar{x}; 0,0,0$<br>( $\bar{3}_{\bar{xyz}}^{-1} \mid 0,0,0$ ) | (20) $\bar{3}^+ \ \bar{x},\bar{x},x; 0,0,0$<br>( $\bar{3}_{\bar{xyz}}^{-1} \mid 0,0,0$ ) |
| (21) $\bar{3}^- \ x,x,x; 0,0,0$<br>( $\bar{3}_{xyz}^{-1} \mid 0,0,0$ ) | (22) $\bar{3}^- \ x,\bar{x},\bar{x}; 0,0,0$<br>( $\bar{3}_{\bar{xyz}} \mid 0,0,0$ )            | (23) $\bar{3}^- \ \bar{x},\bar{x},x; 0,0,0$<br>( $\bar{3}_{\bar{xyz}} \mid 0,0,0$ )      | (24) $\bar{3}^- \ \bar{x},x,\bar{x}; 0,0,0$<br>( $\bar{3}_{\bar{xyz}} \mid 0,0,0$ )      |

For (1/2,1/2,1/2) + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t \ (1/2, 1/2, 1/2)$<br>( $1 \mid 1/2, 1/2, 1/2$ )                                     | (2) $2 \ (0,0,1/2) \ 1/4,1/4,z$<br>( $2_z \mid 1/2, 1/2, 1/2$ )  | (3) $2 \ (0,1/2,0) \ 1/4,y,1/4$<br>( $2_y \mid 1/2, 1/2, 1/2$ )  | (4) $2 \ (1/2,0,0) \ x,1/4,1/4$<br>( $2_x \mid 1/2, 1/2, 1/2$ )  |
| (5) $3^+ \ (1/2, 1/2, 1/2) \ x,x,x$<br>( $3_{xyz} \mid 1/2, 1/2, 1/2$ )                     | (6) $3^+ \ (1/6, -1/6, 1/6)$<br>$\bar{x}+1/3, \bar{x}+1/3, \bar{x}$<br>( $3_{\bar{xyz}}^{-1} \mid 1/2, 1/2, 1/2$ )         | (7) $3^+ \ (-1/6, 1/6, 1/6)$<br>$x+2/3, \bar{x}-1/3, \bar{x}$<br>( $3_{\bar{xyz}}^{-1} \mid 1/2, 1/2, 1/2$ )       | (8) $3^+ \ (1/6, 1/6, -1/6)$<br>$\bar{x}+1/3, \bar{x}+2/3, x$<br>( $3_{\bar{xyz}}^{-1} \mid 1/2, 1/2, 1/2$ )       |
| (9) $3^- \ (1/2, 1/2, 1/2) \ x,x,x$<br>( $3_{xyz}^{-1} \mid 1/2, 1/2, 1/2$ )                | (10) $3^- \ (-1/6, 1/6, 1/6)$<br>$x+1/3, \bar{x}+1/3, \bar{x}$<br>( $3_{\bar{xyz}} \mid 1/2, 1/2, 1/2$ )                   | (11) $3^- \ (1/6, 1/6, -1/6)$<br>$\bar{x}+2/3, \bar{x}+1/3, x$<br>( $3_{\bar{xyz}} \mid 1/2, 1/2, 1/2$ )           | (12) $3^- \ (1/6, -1/6, 1/6)$<br>$\bar{x}-1/3, x+2/3, \bar{x}$<br>( $3_{\bar{xyz}} \mid 1/2, 1/2, 1/2$ )           |
| (13) $\bar{1} \ 1/4, 1/4, 1/4$<br>( $\bar{1} \mid 1/2, 1/2, 1/2$ )                          | (14) $n \ (1/2, 1/2, 0) \ x,y,1/4$<br>( $m_z \mid 1/2, 1/2, 1/2$ )   | (15) $n \ (1/2, 0, 1/2) \ x,1/4,z$<br>( $m_y \mid 1/2, 1/2, 1/2$ )   | (16) $n \ (0, 1/2, 1/2) \ 1/4,y,z$<br>( $m_x \mid 1/2, 1/2, 1/2$ )   |
| (17) $\bar{3}^+ \ x,x,x;$<br>$1/4, 1/4, 1/4$<br>( $\bar{3}_{xyz} \mid 1/2, 1/2, 1/2$ )      | (18) $\bar{3}^+ \ \bar{x}-1, \bar{x}+1, \bar{x};$<br>$-1/4, 1/4, 3/4$<br>( $\bar{3}_{\bar{xyz}}^{-1} \mid 1/2, 1/2, 1/2$ ) | (19) $\bar{3}^+ \ x, \bar{x}+1, \bar{x};$<br>$1/4, 3/4, -1/4$<br>( $\bar{3}_{\bar{xyz}}^{-1} \mid 1/2, 1/2, 1/2$ ) | (20) $\bar{3}^+ \ \bar{x}+1, \bar{x}, x;$<br>$3/4, -1/4, 1/4$<br>( $\bar{3}_{\bar{xyz}}^{-1} \mid 1/2, 1/2, 1/2$ ) |
| (21) $\bar{3}^- \ x,x,x;$<br>$1/4, 1/4, 1/4$<br>( $\bar{3}_{xyz}^{-1} \mid 1/2, 1/2, 1/2$ ) | (22) $\bar{3}^- \ x+1, \bar{x}-1, \bar{x};$<br>$1/4, -1/4, 3/4$<br>( $\bar{3}_{\bar{xyz}} \mid 1/2, 1/2, 1/2$ )            | (23) $\bar{3}^- \ \bar{x}, \bar{x}+1, x;$<br>$-1/4, 3/4, 1/4$<br>( $\bar{3}_{\bar{xyz}} \mid 1/2, 1/2, 1/2$ )      | (24) $\bar{3}^- \ \bar{x}+1, x, \bar{x};$<br>$3/4, 1/4, -1/4$<br>( $\bar{3}_{\bar{xyz}} \mid 1/2, 1/2, 1/2$ )      |

For (0,0,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $1'$<br>( $1 \mid 0,0,0$ )'  | (2) $2' \ 0,0,z$<br>( $2_z \mid 0,0,0$ )'  | (3) $2' \ 0,y,0$<br>( $2_y \mid 0,0,0$ )'  | (4) $2' \ x,0,0$<br>( $2_x \mid 0,0,0$ )'  |
| (5) $3^{+'} \ x,x,x$<br>( $3_{xyz} \mid 0,0,0$ )'                          | (6) $3^{+'} \ \bar{x},\bar{x},\bar{x}$<br>( $3_{\bar{xyz}}^{-1} \mid 0,0,0$ )'                     | (7) $3^{+'} \ x,\bar{x},\bar{x}$<br>( $3_{\bar{xyz}}^{-1} \mid 0,0,0$ )'                     | (8) $3^{+'} \ \bar{x},\bar{x},x$<br>( $3_{\bar{xyz}}^{-1} \mid 0,0,0$ )'                     |
| (9) $3^{-'} \ x,x,x$<br>( $3_{xyz}^{-1} \mid 0,0,0$ )'                     | (10) $3^{-'} \ x,\bar{x},\bar{x}$<br>( $3_{\bar{xyz}} \mid 0,0,0$ )'                               | (11) $3^{-'} \ \bar{x},\bar{x},x$<br>( $3_{\bar{xyz}} \mid 0,0,0$ )'                         | (12) $3^{-'} \ \bar{x},x,\bar{x}$<br>( $3_{\bar{xyz}} \mid 0,0,0$ )'                         |
| (13) $\bar{1}' \ 0,0,0$<br>( $\bar{1} \mid 0,0,0$ )'                       | (14) $m' \ x,y,0$<br>( $m_z \mid 0,0,0$ )'   | (15) $m' \ x,0,z$<br>( $m_y \mid 0,0,0$ )'   | (16) $m' \ 0,y,z$<br>( $m_x \mid 0,0,0$ )'   |
| (17) $\bar{3}^{+'} \ x,x,x; 0,0,0$<br>( $\bar{3}_{xyz} \mid 0,0,0$ )'      | (18) $\bar{3}^{+'} \ \bar{x},\bar{x},\bar{x}; 0,0,0$<br>( $\bar{3}_{\bar{xyz}}^{-1} \mid 0,0,0$ )' | (19) $\bar{3}^{+'} \ x,\bar{x},\bar{x}; 0,0,0$<br>( $\bar{3}_{\bar{xyz}}^{-1} \mid 0,0,0$ )' | (20) $\bar{3}^{+'} \ \bar{x},\bar{x},x; 0,0,0$<br>( $\bar{3}_{\bar{xyz}}^{-1} \mid 0,0,0$ )' |
| (21) $\bar{3}^{-'} \ x,x,x; 0,0,0$<br>( $\bar{3}_{xyz}^{-1} \mid 0,0,0$ )' | (22) $\bar{3}^{-'} \ x,\bar{x},\bar{x}; 0,0,0$<br>( $\bar{3}_{\bar{xyz}} \mid 0,0,0$ )'            | (23) $\bar{3}^{-'} \ \bar{x},\bar{x},x; 0,0,0$<br>( $\bar{3}_{\bar{xyz}} \mid 0,0,0$ )'      | (24) $\bar{3}^{-'} \ \bar{x},x,\bar{x}; 0,0,0$<br>( $\bar{3}_{\bar{xyz}} \mid 0,0,0$ )'      |

Continued

204.2.1531

Im  $\bar{3}1'$

For (1/2,1/2,1/2)' + set

(1) $t' (1/2, 1/2, 1/2)$ (1   1/2, 1/2, 1/2)'	(2) $2' (0, 0, 1/2) \quad 1/4, 1/4, z$ ( $2_z$   1/2, 1/2, 1/2)'	(3) $2' (0, 1/2, 0) \quad 1/4, y, 1/4$ ( $2_y$   1/2, 1/2, 1/2)'	(4) $2' (1/2, 0, 0) \quad x, 1/4, 1/4$ ( $2_x$   1/2, 1/2, 1/2)'
(5) $3^+ ' (1/2, 1/2, 1/2) \quad x, x, x$ ( $3_{xyz}$   1/2, 1/2, 1/2)'	(6) $3^+ ' (1/6, -1/6, 1/6) \quad \bar{x}$ $\bar{x}+1/3, \bar{x}+1/3, \bar{x}$ ( $3_{\bar{xyz}}$   1/2, 1/2, 1/2)'	(7) $3^+ ' (-1/6, 1/6, 1/6) \quad \bar{x}$ $\bar{x}+2/3, \bar{x}-1/3, \bar{x}$ ( $3_{\bar{xyz}}$   1/2, 1/2, 1/2)'	(8) $3^+ ' (1/6, 1/6, -1/6) \quad \bar{x}$ $\bar{x}+1/3, \bar{x}+2/3, \bar{x}$ ( $3_{\bar{xyz}}$   1/2, 1/2, 1/2)'
(9) $3^- ' (1/2, 1/2, 1/2) \quad x, x, x$ ( $3_{xyz}$   1/2, 1/2, 1/2)'	(10) $3^- ' (-1/6, 1/6, 1/6) \quad \bar{x}$ $\bar{x}+1/3, \bar{x}+1/3, \bar{x}$ ( $3_{\bar{xyz}}$   1/2, 1/2, 1/2)'	(11) $3^- ' (1/6, 1/6, -1/6) \quad \bar{x}$ $\bar{x}+2/3, \bar{x}+1/3, \bar{x}$ ( $3_{\bar{xyz}}$   1/2, 1/2, 1/2)'	(12) $3^- ' (1/6, -1/6, 1/6) \quad \bar{x}$ $\bar{x}-1/3, \bar{x}+2/3, \bar{x}$ ( $3_{\bar{xyz}}$   1/2, 1/2, 1/2)'
(13) $\bar{1}' \quad 1/4, 1/4, 1/4$ ( $\bar{1}$   1/2, 1/2, 1/2)'	(14) $n' (1/2, 1/2, 0) \quad x, y, 1/4$ ( $m_z$   1/2, 1/2, 1/2)'	(15) $n' (1/2, 0, 1/2) \quad x, 1/4, z$ ( $m_y$   1/2, 1/2, 1/2)'	(16) $n' (0, 1/2, 1/2) \quad 1/4, y, z$ ( $m_x$   1/2, 1/2, 1/2)'
(17) $\bar{3}^+ ' \quad x, x, x;$ $1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}$   1/2, 1/2, 1/2)'	(18) $\bar{3}^+ ' \quad \bar{x}-1, \bar{x}+1, \bar{x};$ $-1/4, 1/4, 3/4$ ( $\bar{3}_{\bar{xyz}}$   1/2, 1/2, 1/2)'	(19) $\bar{3}^+ ' \quad x, \bar{x}+1, \bar{x};$ $1/4, 3/4, -1/4$ ( $\bar{3}_{\bar{xyz}}$   1/2, 1/2, 1/2)'	(20) $\bar{3}^+ ' \quad \bar{x}+1, \bar{x}, \bar{x};$ $3/4, -1/4, 1/4$ ( $\bar{3}_{\bar{xyz}}$   1/2, 1/2, 1/2)'
(21) $\bar{3}^- ' \quad x, x, x;$ $1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}$   1/2, 1/2, 1/2)'	(22) $\bar{3}^- ' \quad \bar{x}+1, \bar{x}-1, \bar{x};$ $1/4, -1/4, 3/4$ ( $\bar{3}_{\bar{xyz}}$   1/2, 1/2, 1/2)'	(23) $\bar{3}^- ' \quad \bar{x}, \bar{x}+1, \bar{x};$ $-1/4, 3/4, 1/4$ ( $\bar{3}_{\bar{xyz}}$   1/2, 1/2, 1/2)'	(24) $\bar{3}^- ' \quad \bar{x}+1, \bar{x}, \bar{x};$ $3/4, 1/4, -1/4$ ( $\bar{3}_{\bar{xyz}}$   1/2, 1/2, 1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (1/2,1/2,1/2) +  
(0,0,0)' + (1/2,1/2,1/2)'

48 h 11'

(1) $x, y, z$ [0,0,0]	(2) $\bar{x}, \bar{y}, z$ [0,0,0]	(3) $\bar{x}, y, \bar{z}$ [0,0,0]	(4) $x, \bar{y}, \bar{z}$ [0,0,0]
(5) $z, x, y$ [0,0,0]	(6) $z, \bar{x}, \bar{y}$ [0,0,0]	(7) $\bar{z}, \bar{x}, y$ [0,0,0]	(8) $\bar{z}, x, \bar{y}$ [0,0,0]
(9) $y, z, x$ [0,0,0]	(10) $\bar{y}, z, \bar{x}$ [0,0,0]	(11) $y, \bar{z}, \bar{x}$ [0,0,0]	(12) $\bar{y}, \bar{z}, x$ [0,0,0]
(13) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]	(14) $x, y, \bar{z}$ [0,0,0]	(15) $x, \bar{y}, z$ [0,0,0]	(16) $\bar{x}, y, z$ [0,0,0]
(17) $\bar{z}, \bar{x}, \bar{y}$ [0,0,0]	(18) $\bar{z}, x, y$ [0,0,0]	(19) $z, x, \bar{y}$ [0,0,0]	(20) $z, \bar{x}, y$ [0,0,0]
(21) $\bar{y}, \bar{z}, \bar{x}$ [0,0,0]	(22) $y, \bar{z}, x$ [0,0,0]	(23) $\bar{y}, z, x$ [0,0,0]	(24) $y, z, \bar{x}$ [0,0,0]

24 g m..1'	$0, y, z$ [0,0,0]	$0, \bar{y}, z$ [0,0,0]	$0, y, \bar{z}$ [0,0,0]
	$0, \bar{y}, \bar{z}$ [0,0,0]	$z, 0, y$ [0,0,0]	$z, 0, \bar{y}$ [0,0,0]
	$\bar{z}, 0, y$ [0,0,0]	$\bar{z}, 0, \bar{y}$ [0,0,0]	$y, z, 0$ [0,0,0]
	$\bar{y}, z, 0$ [0,0,0]	$y, \bar{z}, 0$ [0,0,0]	$\bar{y}, \bar{z}, 0$ [0,0,0]

Continued

204.2.1531

Im $\bar{3}1'$

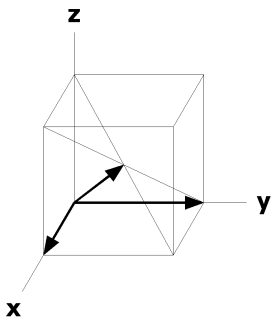
16	f	.3.1'	$x, x, x [0,0,0]$	$\bar{x}, \bar{x}, x [0,0,0]$	$\bar{x}, x, \bar{x} [0,0,0]$	$x, \bar{x}, \bar{x} [0,0,0]$
			$\bar{x}, \bar{x}, \bar{x} [0,0,0]$	$x, x, \bar{x} [0,0,0]$	$x, \bar{x}, x [0,0,0]$	$\bar{x}, x, x [0,0,0]$
12	e	mm2..1'	$x, 0, 1/2 [0,0,0]$	$\bar{x}, 0, 1/2 [0,0,0]$	$1/2, x, 0 [0,0,0]$	$1/2, x, 0 [0,0,0]$
			$1/2, \bar{x}, 0 [0,0,0]$	$0, 1/2, x [0,0,0]$	$0, 1/2, \bar{x} [0,0,0]$	$0, 1/2, \bar{x} [0,0,0]$
12	d	mm2..1'	$x, 0, 0 [0,0,0]$	$\bar{x}, 0, 0 [0,0,0]$	$0, x, 0 [0,0,0]$	$0, x, 0 [0,0,0]$
			$0, \bar{x}, 0 [0,0,0]$	$0, 0, x [0,0,0]$	$0, 0, \bar{x} [0,0,0]$	$0, 0, \bar{x} [0,0,0]$
8	c	. $\bar{3}$ .1'	$1/4, 1/4, 1/4 [0,0,0]$	$3/4, 3/4, 1/4 [0,0,0]$	$3/4, 1/4, 3/4 [0,0,0]$	$1/4, 3/4, 3/4 [0,0,0]$
6	b	mmm..1'	$0, 1/2, 1/2 [0,0,0]$	$1/2, 0, 1/2 [0,0,0]$	$1/2, 1/2, 0 [0,0,0]$	$1/2, 1/2, 0 [0,0,0]$
2	a	m $\bar{3}$ .1'	$0, 0, 0 [0,0,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $c2mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p61'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x,x,x$

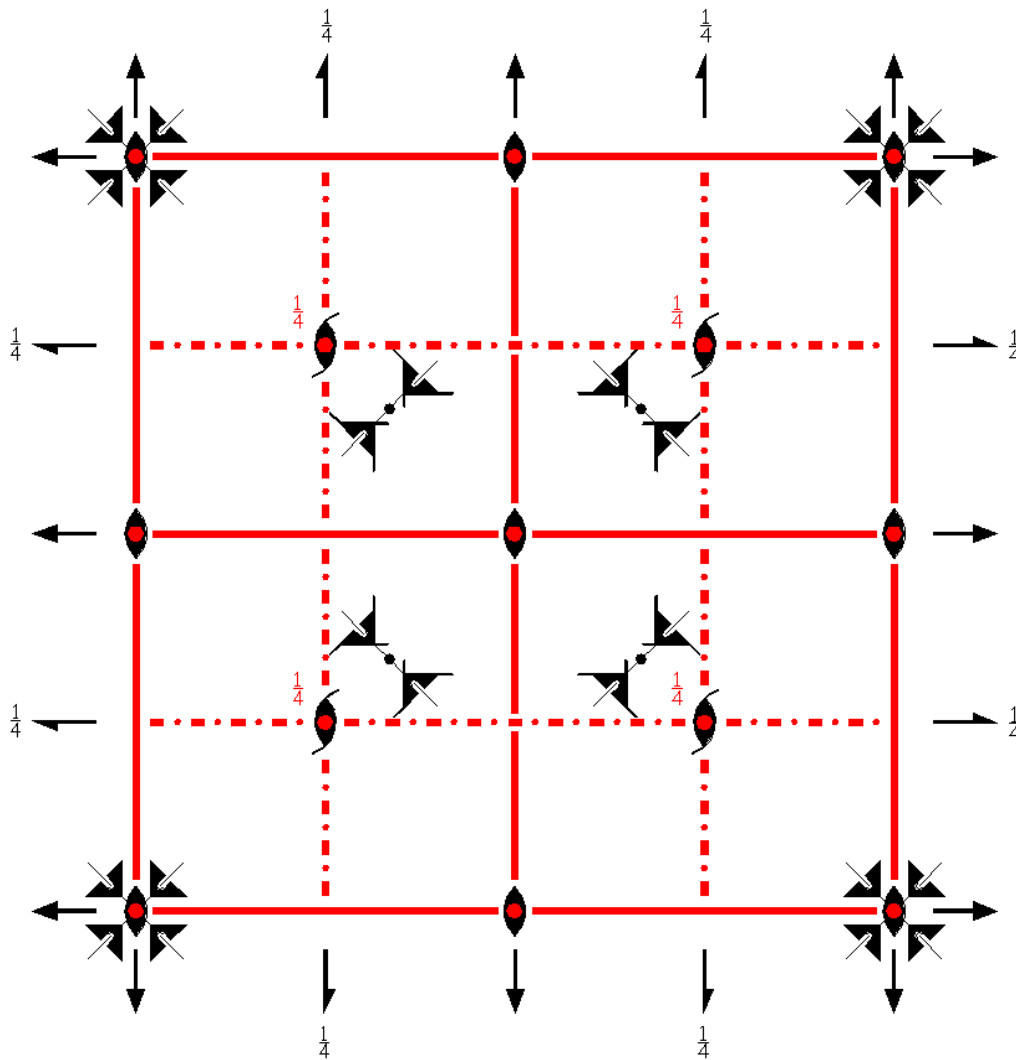
Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



$Im\bar{3}'$   
204.3.1532

$m\bar{3}'$   
 $I2/m\bar{3}'$

Cubic



Origin at center ( $m\bar{3}'$ )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq x;$   $z \leq y$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)              |

Continued

204.3.1532

$Im\bar{3}'$

- |  |   |  |   |
|--|---|--|---|
| (13) $\bar{1}'$ 0,0,0<br>( $\bar{1}$  0,0,0)'                    | (14) $m'$ x,y,0<br>( $m_z$  0,0,0)'   | (15) $m'$ x,0,z<br>( $m_y$  0,0,0)'  | (16) $m'$ 0,y,z<br>( $m_x$  0,0,0)'   |
| (17) $\bar{3}^+$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$  0,0,0)'      | (18) $\bar{3}^+$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,0,0)' | (19) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,0,0)' | (20) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}z}^{-1}$  0,0,0)' |
| (21) $\bar{3}^-$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}^{-1}$  0,0,0)' | (22) $\bar{3}^-$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)'     | (23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)'       | (24) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}z}$  0,0,0)'      |

For (1/2,1/2,1/2) + set

- |   |   |  |   |
|---|---|--|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)  | (2) 2 (0,0,1/2) 1/4,1/4,z<br>( $2_z$  1/2,1/2,1/2)  | (3) 2 (0,1/2,0) 1/4,y,1/4<br>( $2_y$  1/2,1/2,1/2)   | (4) 2 (1/2,0,0) x,1/4,1/4<br>( $2_x$  1/2,1/2,1/2)  |
| (5) $3^+$ (1/2,1/2,1/2) x,x,x<br>( $3_{xyz}$  1/2,1/2,1/2)                      | (6) $3^+$ (1/6,-1/6,1/6)<br>$\bar{x}+1/3, \bar{x}+1/3, \bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  1/2,1/2,1/2)           | (7) $3^+$ (-1/6,1/6,1/6)<br>$\bar{x}+2/3, \bar{x}-1/3, \bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  1/2,1/2,1/2)    | (8) $3^+$ (1/6,1/6,-1/6)<br>$\bar{x}+1/3, \bar{x}+2/3, \bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  1/2,1/2,1/2)         |
| (9) $3^-$ (1/2,1/2,1/2) x,x,x<br>( $3_{xyz}^{-1}$  1/2,1/2,1/2)                 | (10) $3^-$ (-1/6,1/6,1/6)<br>$\bar{x}+1/3, \bar{x}+1/3, \bar{x}$<br>( $3_{x\bar{y}z}$  1/2,1/2,1/2)               | (11) $3^-$ (1/6,1/6,-1/6)<br>$\bar{x}+2/3, \bar{x}+1/3, \bar{x}$<br>( $3_{x\bar{y}z}$  1/2,1/2,1/2)        | (12) $3^-$ (1/6,-1/6,1/6)<br>$\bar{x}-1/3, \bar{x}+2/3, \bar{x}$<br>( $3_{x\bar{y}z}$  1/2,1/2,1/2)             |
| (13) $\bar{1}'$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)'                       | (14) $n'$ (1/2,1/2,0) x,y,1/4<br>( $m_z$  1/2,1/2,1/2)'   | (15) $n'$ (1/2,0,1/2) x,1/4,z<br>( $m_y$  1/2,1/2,1/2)'  | (16) $n'$ (0,1/2,1/2) 1/4,y,z<br>( $m_x$  1/2,1/2,1/2)'   |
| (17) $\bar{3}^+$ x,x,x;<br>1/4,1/4,1/4<br>( $\bar{3}_{xyz}$  1/2,1/2,1/2)'      | (18) $\bar{3}^+$ $\bar{x}-1, \bar{x}+1, \bar{x}$ ;<br>-1/4,1/4,3/4<br>( $\bar{3}_{x\bar{y}z}^{-1}$  1/2,1/2,1/2)' | (19) $\bar{3}^+$ x, $\bar{x}+1, \bar{x}$ ;<br>1/4,3/4,-1/4<br>( $\bar{3}_{x\bar{y}z}^{-1}$  1/2,1/2,1/2)'  | (20) $\bar{3}^+$ $\bar{x}+1, \bar{x}, \bar{x}$ ;<br>3/4,-1/4,1/4<br>( $\bar{3}_{x\bar{y}z}^{-1}$  1/2,1/2,1/2)' |
| (21) $\bar{3}^-$ x,x,x;<br>1/4,1/4,1/4<br>( $\bar{3}_{xyz}^{-1}$  1/2,1/2,1/2)' | (22) $\bar{3}^-$ $\bar{x}+1, \bar{x}-1, \bar{x}$ ;<br>1/4,-1/4,3/4<br>( $\bar{3}_{x\bar{y}z}$  1/2,1/2,1/2)'      | (23) $\bar{3}^-$ $\bar{x}, \bar{x}+1, \bar{x}$ ;<br>-1/4,3/4,1/4<br>( $\bar{3}_{x\bar{y}z}$  1/2,1/2,1/2)' | (24) $\bar{3}^-$ $\bar{x}+1, \bar{x}, \bar{x}$ ;<br>3/4,1/4,-1/4<br>( $\bar{3}_{x\bar{y}z}$  1/2,1/2,1/2)'      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

48 h 1

(0,0,0) + (1/2,1/2,1/2) +

- |  |  |   |  |
|--|--|---|--|
| (1) x,y,z [u,v,w]  | (2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]  | (3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ] | (4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]   |
| (5) z,x,y [w,u,v]  | (6) z, $\bar{x}, \bar{y}$ [w, $\bar{u}, \bar{v}$ ]   | (7) $\bar{z}, \bar{x}, y$ [ $\bar{w}, \bar{u}, v$ ] | (8) $\bar{z}, x, \bar{y}$ [ $\bar{w}, u, \bar{v}$ ]  |
| (9) y,z,x [v,w,u]  | (10) $\bar{y}, z, \bar{x}$ [ $\bar{v}, w, \bar{u}$ ] | (11) y, $\bar{z}, \bar{x}$ [v, $\bar{w}, \bar{u}$ ] | (12) $\bar{y}, \bar{z}, x$ [ $\bar{v}, \bar{w}, u$ ] |
| (13) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ] | (14) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]                | (15) x, $\bar{y}, z$ [u, $\bar{v}, w$ ]             | (16) $\bar{x}, y, z$ [ $\bar{u}, v, w$ ]             |
| (17) $\bar{z}, \bar{x}, \bar{y}$ [ $\bar{w}, \bar{u}, \bar{v}$ ] | (18) $\bar{z}, x, y$ [ $\bar{w}, u, v$ ]             | (19) z,x, $\bar{y}$ [w,u, $\bar{v}$ ]               | (20) z, $\bar{x}, y$ [w, $\bar{u}, v$ ]              |
| (21) $\bar{y}, \bar{z}, \bar{x}$ [ $\bar{v}, \bar{w}, \bar{u}$ ] | (22) y, $\bar{z}, x$ [v, $\bar{w}, u$ ]              | (23) $\bar{y}, z, x$ [ $\bar{v}, w, u$ ]            | (24) y,z, $\bar{x}$ [v,w, $\bar{u}$ ]                |



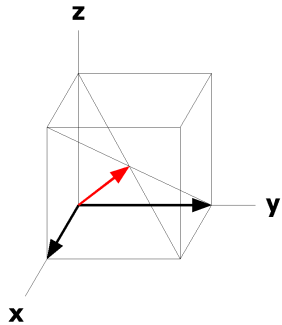
24	g	m' $\bar{3}$ '	0,y,z [0,v,w] 0, $\bar{y}$ , $\bar{z}$ [0, $\bar{v}$ , $\bar{w}$ ] $\bar{z}$ ,0,y [ $\bar{w}$ ,0,v] $\bar{y}$ ,z,0 [ $\bar{v}$ , w,0]	0, $\bar{y}$ ,z [0, $\bar{v}$ ,w] z,0,y [w,0,v] $\bar{z}$ ,0, $\bar{y}$ [ $\bar{w}$ ,0, $\bar{v}$ ] y, $\bar{z}$ ,0 [v, $\bar{w}$ ,0]	0,y, $\bar{z}$ [0,v, $\bar{w}$ ] z,0, $\bar{y}$ [w,0, $\bar{v}$ ] y,z,0 [v,w,0] $\bar{y}$ , $\bar{z}$ ,0 [ $\bar{v}$ , $\bar{w}$ ,0]
16	f	.3.	x,x,x [u,u,u] $\bar{x}$ , $\bar{x}$ , $\bar{x}$ [ $\bar{u}$ , $\bar{u}$ , $\bar{u}$ ]	$\bar{x}$ , $\bar{x}$ ,x [ $\bar{u}$ , $\bar{u}$ ,u] x,x, $\bar{x}$ [u,u, $\bar{u}$ ]	$\bar{x}$ ,x, $\bar{x}$ [ $\bar{u}$ ,u, $\bar{u}$ ] x, $\bar{x}$ ,x [u, $\bar{u}$ ,u] x, $\bar{x}$ ,x [u, $\bar{u}$ ,u] $\bar{x}$ ,x,x [ $\bar{u}$ ,u,u]
12	e	m'm' $\bar{2}$ '	x,0,1/2 [u,0,0] 1/2, $\bar{x}$ ,0 [0, $\bar{u}$ ,0]	$\bar{x}$ ,0,1/2 [ $\bar{u}$ ,0,0] 0,1/2,x [0,0,u]	1/2,x,0 [0,u,0] 0,1/2, $\bar{x}$ [0,0, $\bar{u}$ ]
12	d	m'm' $\bar{2}$ '	x,0,0 [u,0,0] 0, $\bar{x}$ ,0 [0, $\bar{u}$ ,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0] 0,0,x [0,0,u]	0,x,0 [0,u,0] 0,0, $\bar{x}$ [0,0, $\bar{u}$ ]
8	c	$\bar{3}$ '	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]
6	b	m'm'm' $\bar{3}$ '	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
2	a	m' $\bar{3}$ '	0,0,0 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] c2m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,1,1] p6  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

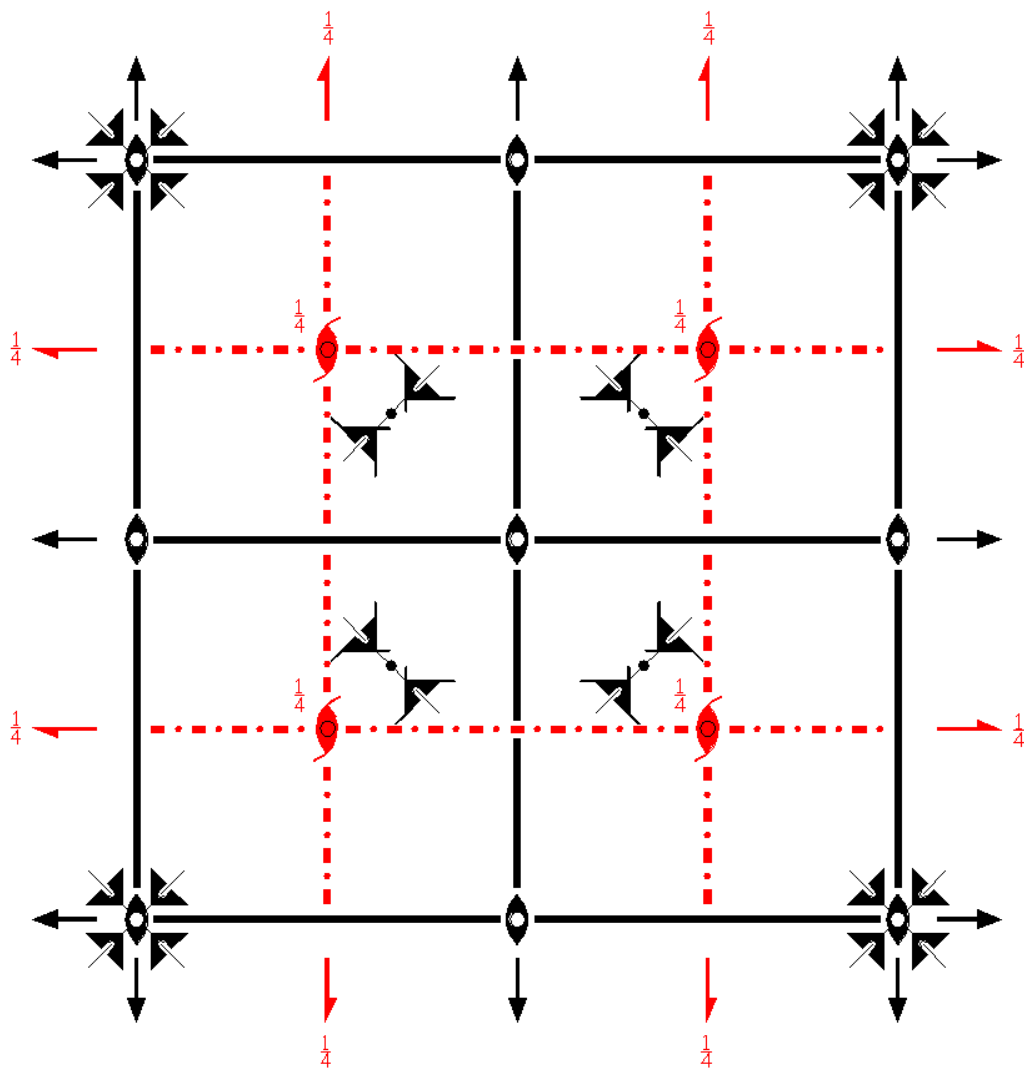
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I_p \bar{m}\bar{3}$   
204.4.1533

$m\bar{3}1'$   
 $I_p 2/m\bar{3}$

Cubic



Origin at center ( $m\bar{3}$ )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq x;$   $z \leq y$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)     | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0) | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0)              |

Continued

204.4.1533

$I_p \bar{m}\bar{3}$

- |   |   |   |  |
|---|---|---|--|
| (13) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0)                | (14) m x,y,0<br>( $m_z$   0,0,0)  | (15) m x,0,z<br>( $m_y$   0,0,0)  | (16) m 0,y,z<br>( $m_x$   0,0,0)   |
| (17) $\bar{3}^+$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$   0,0,0) | (18) $\bar{3}^+$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$   0,0,0)  | (19) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$   0,0,0) | (20) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$   0,0,0) |
| (21) $\bar{3}^-$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$   0,0,0) | (22) $\bar{3}^-$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$   0,0,0) | (23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$   0,0,0)  | (24) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$   0,0,0) |

For (1/2,1/2,1/2)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) t' (1/2,1/2,1/2)<br>( $\bar{1}$   1/2,1/2,1/2)'                         | (2) 2' (0,0,1/2) 1/4,1/4,z<br>( $2_z$   1/2,1/2,1/2)'   | (3) 2' (0,1/2,0) 1/4,y,1/4<br>( $2_y$   1/2,1/2,1/2)'   | (4) 2' (1/2,0,0) x,1/4,1/4<br>( $2_x$   1/2,1/2,1/2)'   |
| (5) $3^+$ (1/2,1/2,1/2) x,x,x<br>( $3_{xyz}$   1/2,1/2,1/2)'                | (6) $3^+$ (1/6,-1/6,1/6)<br>$\bar{x}+1/3, \bar{x}+1/3, \bar{x}$<br>( $3_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)'          | (7) $3^+$ (-1/6,1/6,1/6)<br>$x+2/3, \bar{x}-1/3, \bar{x}$<br>( $3_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)'              | (8) $3^+$ (1/6,1/6,-1/6)<br>$\bar{x}+1/3, \bar{x}+2/3, \bar{x}$<br>( $3_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)'        |
| (9) $3^-$ (1/2,1/2,1/2) x,x,x<br>( $3_{xyz}$   1/2,1/2,1/2)'                | (10) $3^-$ (-1/6,1/6,1/6)<br>$x+1/3, \bar{x}+1/3, \bar{x}$<br>( $3_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)'               | (11) $3^-$ (1/6,1/6,-1/6)<br>$\bar{x}+2/3, \bar{x}+1/3, \bar{x}$<br>( $3_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)'       | (12) $3^-$ (1/6,-1/6,1/6)<br>$\bar{x}-1/3, \bar{x}+2/3, \bar{x}$<br>( $3_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)'       |
| (13) $\bar{1}$ ' 1/4,1/4,1/4<br>( $\bar{1}$   1/2,1/2,1/2)'                 | (14) n' (1/2,1/2,0) x,y,1/4<br>( $m_z$   1/2,1/2,1/2)'  | (15) n' (1/2,0,1/2) x,1/4,z<br>( $m_y$   1/2,1/2,1/2)'  | (16) n' (0,1/2,1/2) 1/4,y,z<br>( $m_x$   1/2,1/2,1/2)'  |
| (17) $\bar{3}^+$ x,x,x;<br>1/4,1/4,1/4<br>( $\bar{3}_{xyz}$   1/2,1/2,1/2)' | (18) $\bar{3}^+$ $\bar{x}-1, \bar{x}+1, \bar{x}$ ;<br>-1/4,1/4,3/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)' | (19) $\bar{3}^+$ x, $\bar{x}+1, \bar{x}$ ;<br>1/4,3/4,-1/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)'       | (20) $\bar{3}^+$ $\bar{x}+1, \bar{x}, \bar{x}$ ;<br>3/4,-1/4,1/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)' |
| (21) $\bar{3}^-$ x,x,x;<br>1/4,1/4,1/4<br>( $\bar{3}_{xyz}$   1/2,1/2,1/2)' | (22) $\bar{3}^-$ x+1, $\bar{x}-1, \bar{x}$ ;<br>1/4,-1/4,3/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)'       | (23) $\bar{3}^-$ $\bar{x}, \bar{x}+1, \bar{x}$ ;<br>-1/4,3/4,1/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)' | (24) $\bar{3}^-$ $\bar{x}+1, \bar{x}, \bar{x}$ ;<br>3/4,1/4,-1/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)' |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

48 h 1

(0,0,0) + (1/2,1/2,1/2)' +

- |  |  |  |  |
|--|--|--|--|
| (1) x,y,z [u,v,w]  | (2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]  | (3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]  | (4) x, $\bar{y}, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]  |
| (5) z,x,y [w,u,v]  | (6) z, $\bar{x}, \bar{y}$ [ $w, \bar{u}, \bar{v}$ ]  | (7) $\bar{z}, \bar{x}, y$ [ $\bar{w}, \bar{u}, v$ ]  | (8) $\bar{z}, x, \bar{y}$ [ $\bar{w}, u, \bar{v}$ ]  |
| (9) y,z,x [v,w,u]  | (10) $\bar{y}, z, \bar{x}$ [ $\bar{v}, w, \bar{u}$ ] | (11) y, $\bar{z}, \bar{x}$ [ $v, \bar{w}, \bar{u}$ ] | (12) $\bar{y}, \bar{z}, x$ [ $\bar{v}, \bar{w}, u$ ] |
| (13) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ] | (14) x,y, $\bar{z}$ [ $\bar{u}, \bar{v}, w$ ]        | (15) x, $\bar{y}, z$ [ $\bar{u}, v, \bar{w}$ ]       | (16) $\bar{x}, y, z$ [ $u, \bar{v}, \bar{w}$ ]       |
| (17) $\bar{z}, \bar{x}, \bar{y}$ [ $\bar{w}, \bar{u}, \bar{v}$ ] | (18) $\bar{z}, x, y$ [ $\bar{w}, \bar{u}, v$ ]       | (19) z,x, $\bar{y}$ [ $\bar{w}, \bar{u}, v$ ]        | (20) z, $\bar{x}, y$ [ $\bar{w}, \bar{u}, \bar{v}$ ] |
| (21) $\bar{y}, \bar{z}, \bar{x}$ [ $\bar{v}, \bar{w}, \bar{u}$ ] | (22) y, $\bar{z}, \bar{x}$ [ $\bar{v}, w, \bar{u}$ ] | (23) $\bar{y}, z, x$ [ $\bar{v}, \bar{w}, \bar{u}$ ] | (24) y,z, $\bar{x}$ [ $\bar{v}, \bar{w}, u$ ]        |

Continued

204.4.1533

$I_p m \bar{3}$

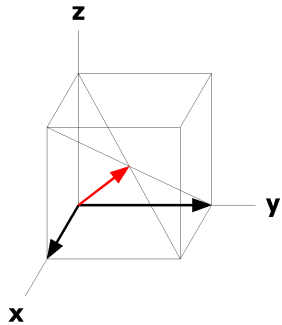
24	g	m..	0,y,z [u,0,0]	$0,\bar{y},z [\bar{u},0,0]$	$0,y,\bar{z} [\bar{u},0,0]$
			$0,\bar{y},\bar{z} [u,0,0]$	$z,0,y [0,u,0]$	$z,0,\bar{y} [0,\bar{u},0]$
			$\bar{z},0,y [0,\bar{u},0]$	$\bar{z},0,\bar{y} [0,u,0]$	$y,z,0 [0,0,u]$
			$\bar{y},z,0 [0,0,\bar{u}]$	$y,\bar{z},0 [0,0,\bar{u}]$	$\bar{y},\bar{z},0 [0,0,u]$
16	f	.3.	x,x,x [u,u,u]	$\bar{x},\bar{x},x [\bar{u},\bar{u},u]$	$\bar{x},x,\bar{x} [\bar{u},u,\bar{u}]$
			$\bar{x},\bar{x},\bar{x} [u,u,u]$	$x,x,\bar{x} [\bar{u},\bar{u},u]$	$\bar{x},x,x [u,\bar{u},\bar{u}]$
12	e	mm2..	x,0,1/2 [0,0,0]	$\bar{x},0,1/2 [0,0,0]$	1/2,x,0 [0,0,0]
			1/2, $\bar{x}$ ,0 [0,0,0]	0,1/2,x [0,0,0]	0,1/2, $\bar{x}$ [0,0,0]
12	d	mm2..	x,0,0 [0,0,0]	$\bar{x},0,0 [0,0,0]$	0,x,0 [0,0,0]
			0, $\bar{x}$ ,0 [0,0,0]	0,0,x [0,0,0]	0,0, $\bar{x}$ [0,0,0]
8	c	$\bar{3}$ .	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]
			1/4,3/4,3/4 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
6	b	mmm..	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
2	a	$m\bar{3}$ .	0,0,0 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1]  $c2mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,1,1]  $p61'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

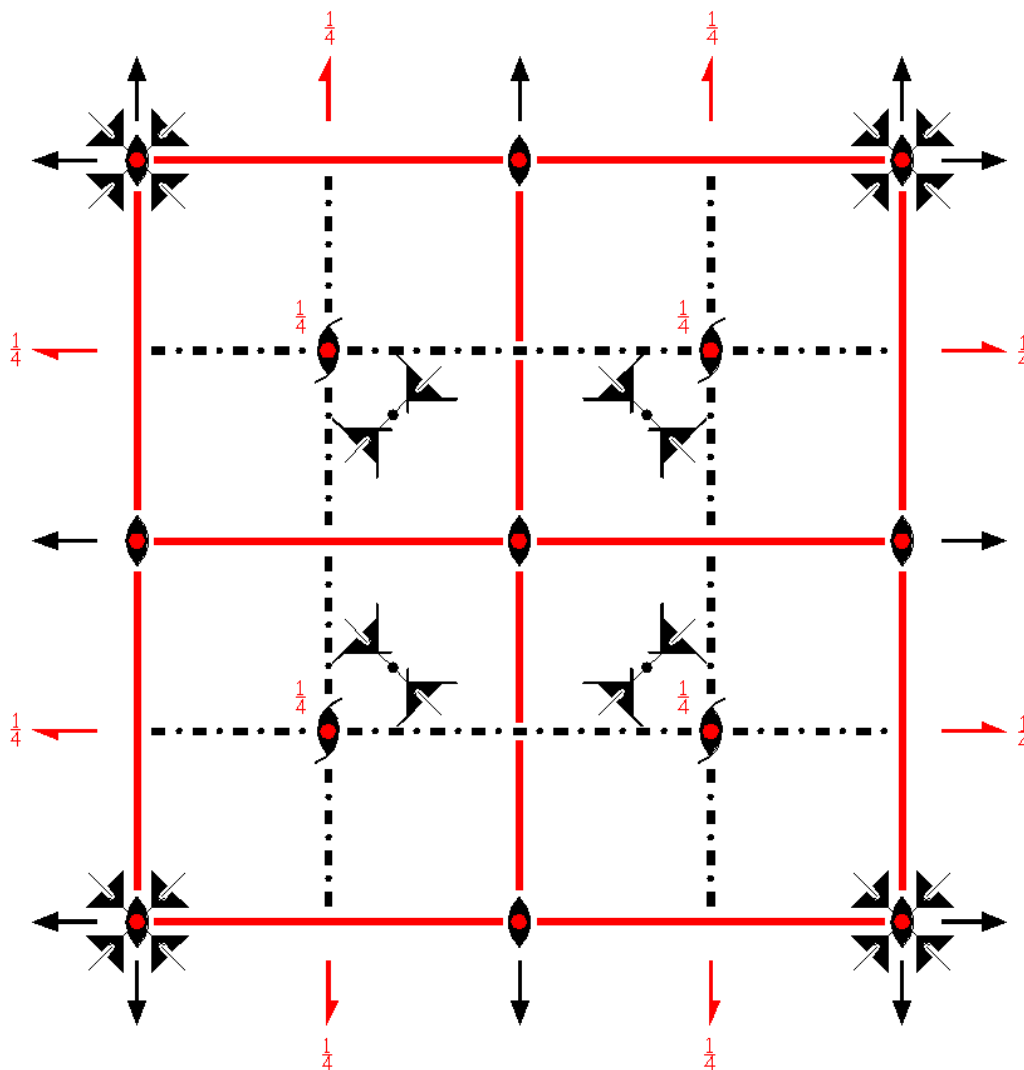
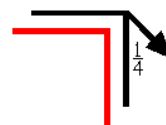
Along [1,1,0]  $p_{2a}2mm$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at x-1/4,x+1/4,0



$I_P m\bar{3}'$   
204.5.1534

$m\bar{3}1'$   
 $I_P 2/m\bar{3}'$

Cubic



**Origin** at center ( $m\bar{3}'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq x;$   $z \leq y$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)                                       |

204.5.1534

$I_P m\bar{3}'$

- |  |  |  |   |
|--|--|--|---|
| (13) $\bar{1}^-$ 0,0,0<br>( $\bar{1}$   0,0,0)'              | (14) $m'$ x,y,0<br>( $m_z$   0,0,0)'   | (15) $m'$ x,0,z<br>( $m_y$   0,0,0)'   | (16) $m'$ 0,y,z<br>( $m_x$   0,0,0)'  |
| (17) $\bar{3}^+$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$   0,0,0)' | (18) $\bar{3}^+$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$   0,0,0)'  | (19) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$   0,0,0)' | (20) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$   0,0,0)' |
| (21) $\bar{3}^-$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$   0,0,0)' | (22) $\bar{3}^-$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$   0,0,0)' | (23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$   0,0,0)'  | (24) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0<br>( $\bar{3}_{x\bar{y}\bar{z}}$   0,0,0)' |

For (1/2,1/2,1/2)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t'$ (1/2,1/2,1/2)<br>( $\bar{1}$   1/2,1/2,1/2)'                      | (2) $2'$ (0,0,1/2) 1/4,1/4,z<br>( $2_z$   1/2,1/2,1/2)'  | (3) $2'$ (0,1/2,0) 1/4,y,1/4<br>( $2_y$   1/2,1/2,1/2)'  | (4) $2'$ (1/2,0,0) x,1/4,1/4<br>( $2_x$   1/2,1/2,1/2)'  |
| (5) $3^+$ (1/2,1/2,1/2) x,x,x<br>( $3_{xyz}$   1/2,1/2,1/2)'               | (6) $3^+$ (1/6,-1/6,1/6)<br>$\bar{x}+1/3, \bar{x}+1/3, \bar{x}$<br>( $3_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)'         | (7) $3^+$ (-1/6,1/6,1/6)<br>$x+2/3, \bar{x}-1/3, \bar{x}$<br>( $3_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)'             | (8) $3^+$ (1/6,1/6,-1/6)<br>$\bar{x}+1/3, \bar{x}+2/3, \bar{x}$<br>( $3_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)'       |
| (9) $3^-$ (1/2,1/2,1/2) x,x,x<br>( $3_{xyz}$   1/2,1/2,1/2)'               | (10) $3^-$ (-1/6,1/6,1/6)<br>$x+1/3, \bar{x}+1/3, \bar{x}$<br>( $3_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)'              | (11) $3^-$ (1/6,1/6,-1/6)<br>$\bar{x}+2/3, \bar{x}+1/3, \bar{x}$<br>( $3_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)'      | (12) $3^-$ (1/6,-1/6,1/6)<br>$\bar{x}-1/3, \bar{x}+2/3, \bar{x}$<br>( $3_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)'      |
| (13) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$   1/2,1/2,1/2)                   | (14) $n$ (1/2,1/2,0) x,y,1/4<br>( $m_z$   1/2,1/2,1/2)   | (15) $n$ (1/2,0,1/2) x,1/4,z<br>( $m_y$   1/2,1/2,1/2)   | (16) $n$ (0,1/2,1/2) 1/4,y,z<br>( $m_x$   1/2,1/2,1/2)   |
| (17) $\bar{3}^+$ x,x,x;<br>1/4,1/4,1/4<br>( $\bar{3}_{xyz}$   1/2,1/2,1/2) | (18) $\bar{3}^+$ $\bar{x}-1, \bar{x}+1, \bar{x}$ ;<br>-1/4,1/4,3/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$   1/2,1/2,1/2) | (19) $\bar{3}^+$ x, $\bar{x}+1, \bar{x}$ ;<br>1/4,3/4,-1/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)       | (20) $\bar{3}^+$ $\bar{x}+1, \bar{x}, \bar{x}$ ;<br>3/4,-1/4,1/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$   1/2,1/2,1/2) |
| (21) $\bar{3}^-$ x,x,x;<br>1/4,1/4,1/4<br>( $\bar{3}_{xyz}$   1/2,1/2,1/2) | (22) $\bar{3}^-$ $x+1, \bar{x}-1, \bar{x}$ ;<br>1/4,-1/4,3/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)       | (23) $\bar{3}^-$ $\bar{x}, \bar{x}+1, \bar{x}$ ;<br>-1/4,3/4,1/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$   1/2,1/2,1/2) | (24) $\bar{3}^-$ $\bar{x}+1, \bar{x}, \bar{x}$ ;<br>3/4,1/4,-1/4<br>( $\bar{3}_{x\bar{y}\bar{z}}$   1/2,1/2,1/2) |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

48 h 1

(0,0,0) + (1/2,1/2,1/2)' +

- |  |  |  |  |
|--|--|--|--|
| (1) x,y,z [u,v,w]  | (2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]  | (3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]  | (4) x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]   |
| (5) z,x,y [w,u,v]  | (6) z, $\bar{x}, \bar{y}$ [w, $\bar{u}, \bar{v}$ ]   | (7) $\bar{z}, \bar{x}, y$ [ $\bar{w}, \bar{u}, v$ ]  | (8) $\bar{z}, x, \bar{y}$ [ $\bar{w}, u, \bar{v}$ ]  |
| (9) y,z,x [v,w,u]  | (10) $\bar{y}, z, \bar{x}$ [ $\bar{v}, w, \bar{u}$ ] | (11) y, $\bar{z}, \bar{x}$ [v, $\bar{w}, \bar{u}$ ]  | (12) $\bar{y}, \bar{z}, x$ [ $\bar{v}, \bar{w}, u$ ] |
| (13) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ] | (14) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]                | (15) x, $\bar{y}, z$ [u, $\bar{v}, w$ ]              | (16) $\bar{x}, y, z$ [ $\bar{u}, v, w$ ]             |
| (17) $\bar{z}, \bar{x}, \bar{y}$ [ $\bar{w}, \bar{u}, \bar{v}$ ] | (18) $\bar{z}, x, y$ [ $\bar{w}, u, v$ ]             | (19) z,x, $\bar{y}$ [w,u, $\bar{v}$ ]                | (20) z, $\bar{x}, y$ [w, $\bar{u}, \bar{v}$ ]        |
| (21) $\bar{y}, \bar{z}, \bar{x}$ [ $\bar{v}, \bar{w}, \bar{u}$ ] | (22) y, $\bar{z}, \bar{x}$ [v, $\bar{w}, \bar{u}$ ]  | (23) $\bar{y}, z, \bar{x}$ [ $\bar{v}, w, \bar{u}$ ] | (24) y,z, $\bar{x}$ [v,w, $\bar{u}$ ]                |

Continued

204.5.1534

$I_p m \bar{3}'$

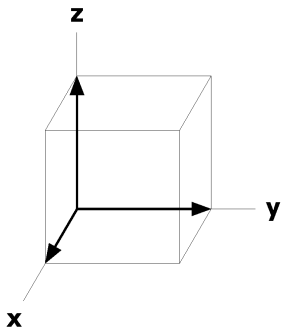
24	g	$m'..$	$0,y,z [0,v,w]$	$0,\bar{y},z [0,\bar{v},w]$	$0,y,\bar{z} [0,v,\bar{w}]$
			$0,\bar{y},\bar{z} [0,\bar{v},\bar{w}]$	$z,0,y [w,0,v]$	$z,0,\bar{y} [w,0,\bar{v}]$
			$\bar{z},0,y [\bar{w},0,v]$	$\bar{z},0,\bar{y} [\bar{w},0,\bar{v}]$	$y,z,0 [v,w,0]$
			$\bar{y},z,0 [\bar{v}, w,0]$	$y,\bar{z},0 [v, \bar{w},0]$	$\bar{y},\bar{z},0 [\bar{v},\bar{w},0]$
16	f	$.3.$	$x,x,x [u,u,u]$	$\bar{x},\bar{x},x [\bar{u},\bar{u},u]$	$\bar{x},x,\bar{x} [\bar{u},u,\bar{u}]$
			$\bar{x},\bar{x},\bar{x} [\bar{u},\bar{u},\bar{u}]$	$x,x,\bar{x} [u,u,\bar{u}]$	$\bar{x},x,x [\bar{u},u,u]$
12	e	$m'm'2..$	$x,0,1/2 [u,0,0]$	$\bar{x},0,1/2 [\bar{u},0,0]$	$1/2,x,0 [0,u,0]$
			$1/2, \bar{x},0 [0,\bar{u},0]$	$0,1/2,x [0,0,u]$	$0,1/2,\bar{x} [0,0,\bar{u}]$
12	d	$m'm'2..$	$x,0,0 [u,0,0]$	$\bar{x},0,0 [\bar{u},0,0]$	$0,x,0 [0,u,0]$
			$0,\bar{x},0 [0,\bar{u},0]$	$0,0,x [0,0,u]$	$0,0,\bar{x} [0,0,\bar{u}]$
8	c	$.\bar{3}.$	$1/4,1/4,1/4 [u,u,u]$	$3/4,3/4,1/4 [\bar{u},\bar{u},u]$	$3/4,1/4,3/4 [\bar{u},u,\bar{u}]$
					$1/4,3/4,3/4 [u,\bar{u},\bar{u}]$
6	b	$m'm'm'..$	$0,1/2,1/2 [0,0,0]$	$1/2,0,1/2 [0,0,0]$	$1/2,1/2,0 [0,0,0]$
2	a	$m'\bar{3}'.$	$0,0,0 [0,0,0]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $c_p, 2m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p61'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x,x,x$

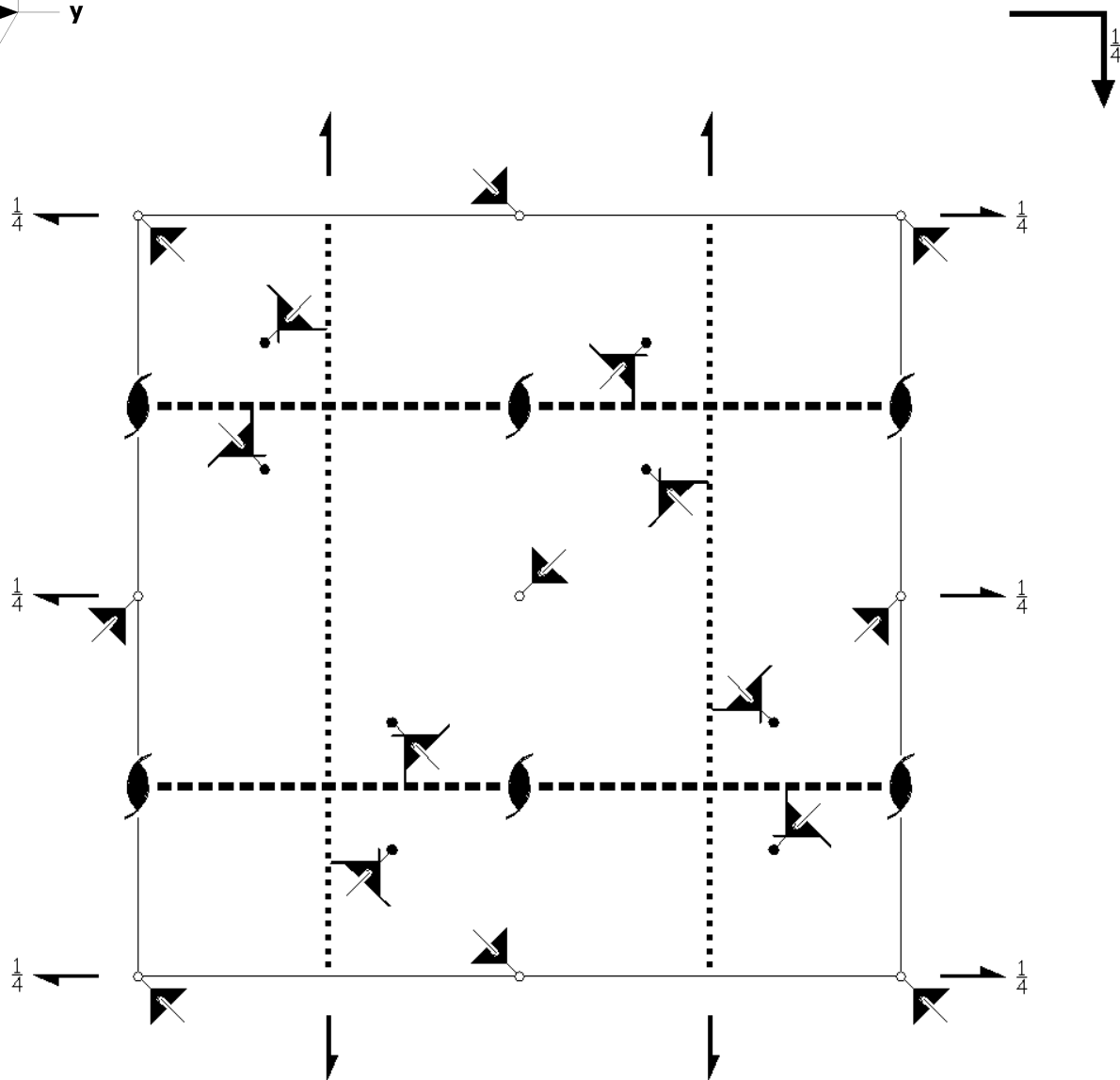
Along  $[1,1,0]$   $p_{2a}, 2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



$\text{Pa}\bar{3}$   
205.1.1535

$m\bar{3}$   
 $\text{P2}_1/\text{a}\bar{3}$

Cubic



Origin at center ( $\bar{3}$ )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $z \leq \min(x,y)$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $0,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}+1/2, \bar{x}, \bar{x}$<br>(3 <sub><math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1/2,1/2,0)          | (7) 3 <sup>+</sup> $\bar{x}+1/2, \bar{x}-1/2, \bar{x}$<br>(3 <sub><math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1/2,0,1/2)      | (8) 3 <sup>+</sup> $\bar{x}, \bar{x}+1/2, \bar{x}$<br>(3 <sub><math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  0,1/2,1/2)          |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> (-1/3,1/3,1/3)<br>$\bar{x}+1/6, \bar{x}+1/6, \bar{x}$<br>(3 <sub><math>\bar{y}\bar{z}</math></sub>  0,1/2,1/2) | (11) 3 <sup>-</sup> (1/3,1/3,-1/3)<br>$\bar{x}+1/3, \bar{x}+1/6, \bar{x}$<br>(3 <sub><math>\bar{y}\bar{z}</math></sub>  1/2,1/2,0) | (12) 3 <sup>-</sup> (1/3,-1/3,1/3)<br>$\bar{x}-1/6, \bar{x}+1/3, \bar{x}$<br>(3 <sub><math>\bar{y}\bar{z}</math></sub>  1/2,0,1/2) |



(13) $\bar{1}$ 0,0,0 ( $\bar{1}$   0,0,0)	(14) a (1/2,0,0) x,y,1/4 ( $m_z$   1/2,0,1/2)	(15) c (0,0,1/2) x,1/4,z ( $m_y$   0,1/2,1/2)	(16) b (0,1/2,0) 1/4,y,z ( $m_x$   1/2,1/2,0)
(17) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$   0,0,0)	(18) $\bar{3}^+$ $\bar{x}$ -1/2,x+1, $\bar{x}$ ; 0,1/2,1/2 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0)	(19) $\bar{3}^+$ x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ; 1/2,1/2,0 ( $\bar{3}_{xyz}^{-1}$   1/2,0,1/2)	(20) $\bar{3}^+$ $\bar{x}$ +1, $\bar{x}$ +1/2,x; 1/2,0,1/2 ( $\bar{3}_{xyz}^{-1}$   0,1/2,1/2)
(21) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}^{-1}$   0,0,0)	(22) $\bar{3}^-$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ; 0,0,1/2 ( $\bar{3}_{xyz}$   0,1/2,1/2)	(23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1/2, x; 0,1/2,0 ( $\bar{3}_{xyz}$   1/2,1/2,0)	(24) $\bar{3}^-$ $\bar{x}$ +1/2, x, $\bar{x}$ ; 1/2,0,0 ( $\bar{3}_{xyz}$   1/2,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

24 d 1

(1) x,y,z [u,v,w]	(2) $\bar{x}$ +1/2, $\bar{y}$ ,z+1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(3) $\bar{x}$ ,y+1/2, $\bar{z}$ +1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x+1/2, $\bar{y}$ +1/2, $\bar{z}$ [u, $\bar{v}$ , $\bar{w}$ ]
(5) z,x,y [w,u,v]	(6) z+1/2, $\bar{x}$ +1/2, $\bar{y}$ [w, $\bar{u}$ , $\bar{v}$ ]	(7) $\bar{z}$ +1/2, $\bar{x}$ ,y+1/2 [ $\bar{w}$ , $\bar{u}$ ,v]	(8) $\bar{z}$ ,x+1/2, $\bar{y}$ +1/2 [ $\bar{w}$ ,u, $\bar{v}$ ]
(9) y,z,x [v,w,u]	(10) $\bar{y}$ ,z+1/2, $\bar{x}$ +1/2 [ $\bar{v}$ ,w, $\bar{u}$ ]	(11) y+1/2, $\bar{z}$ +1/2, $\bar{x}$ [v, $\bar{w}$ , $\bar{u}$ ]	(12) $\bar{y}$ +1/2, $\bar{z}$ ,x+1/2 [ $\bar{v}$ , $\bar{w}$ ,u]
(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(14) x+1/2,y, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(15) x, $\bar{y}$ +1/2,z+1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	(16) $\bar{x}$ +1/2,y+1/2,z [u, $\bar{v}$ , $\bar{w}$ ]
(17) $\bar{z}$ , $\bar{x}$ , $\bar{y}$ [w,u,v]	(18) $\bar{z}$ +1/2,x+1/2,y [w, $\bar{u}$ , $\bar{v}$ ]	(19) z+1/2,x, $\bar{y}$ +1/2 [ $\bar{w}$ , $\bar{u}$ ,v]	(20) z, $\bar{x}$ +1/2,y+1/2 [ $\bar{w}$ ,u, $\bar{v}$ ]
(21) $\bar{y}$ , $\bar{z}$ , $\bar{x}$ [v,w,u]	(22) y, $\bar{z}$ +1/2,x+1/2 [ $\bar{v}$ ,w, $\bar{u}$ ]	(23) $\bar{y}$ +1/2,z+1/2,x [v, $\bar{w}$ , $\bar{u}$ ]	(24) y+1/2,z, $\bar{x}$ +1/2 [ $\bar{v}$ , $\bar{w}$ ,u]

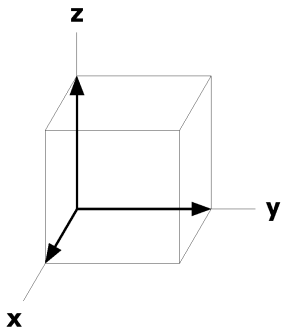
8	c	.3.	x,x,x [u,u,u]	$\bar{x}$ +1/2, $\bar{x}$ ,x+1/2 [ $\bar{u}$ , $\bar{u}$ ,u]	$\bar{x}$ ,x+1/2, $\bar{x}$ +1/2 [ $\bar{u}$ ,u, $\bar{u}$ ]	x+1/2, $\bar{x}$ +1/2, $\bar{x}$ [u, $\bar{u}$ , $\bar{u}$ ]
			$\bar{x}$ , $\bar{x}$ , $\bar{x}$ [u,u,u]	x+1/2,x, $\bar{x}$ +1/2 [ $\bar{u}$ , $\bar{u}$ ,u]	x, $\bar{x}$ +1/2,x+1/2 [ $\bar{u}$ ,u, $\bar{u}$ ]	$\bar{x}$ ,+1/2 x+1/2,x [u, $\bar{u}$ , $\bar{u}$ ]
4	b	. $\bar{3}$ .	1/2,1/2,1/2 [u,u,u]	0,1/2,0 [ $\bar{u}$ , $\bar{u}$ ,u]	1/2,0,0 [ $\bar{u}$ ,u, $\bar{u}$ ]	0,0,1/2 [u, $\bar{u}$ , $\bar{u}$ ]
4	a	. $\bar{3}$ .	0,0,0 [u,u,u]	1/2,0,1/2 [ $\bar{u}$ , $\bar{u}$ ,u]	0,1/2,1/2 [ $\bar{u}$ ,u, $\bar{u}$ ]	1/2,1/2,0 [u, $\bar{u}$ , $\bar{u}$ ]

### Symmetry of Special Projections

Along [0,0,1]  $p_{2b} \cdot 2mg$   
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = -\mathbf{a}/2$   
 Origin at 0,0,z

Along [1,1,1]  $p6'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

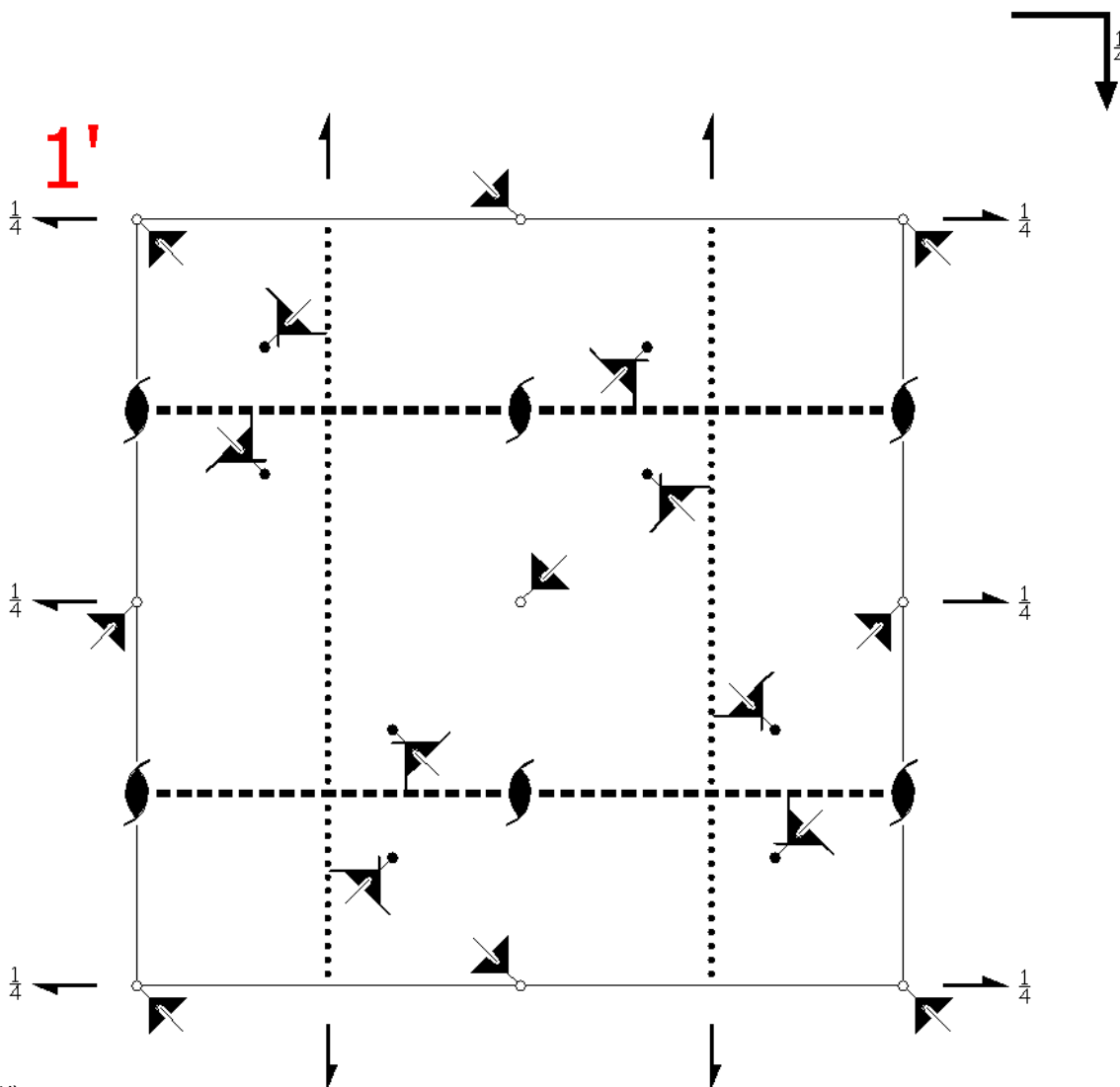
Along [1,1,0]  $p2'gg'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$\text{Pa}\bar{3}1'$   
205.2.1536

$m\bar{3}1'$   
 $\text{P2}_1/\text{a}\bar{3}1'$

Cubic



Origin at center ( $\bar{3}1'$ )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $z \leq \min(x,y)$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $0,1/2,0$   $1/2,1/2,1/2$

### Symmetry Operations

For 1 + set

- |   |  |   |  |
|---|--|---|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)                                       | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)  | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) 3 <sup>+</sup> $\bar{x},x,x$<br>(3 <sub>xyz</sub>  0,0,0)         | (6) 3 <sup>+</sup> $\bar{x}+1/2,x,\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0)    | (7) 3 <sup>+</sup> $\bar{x}+1/2,\bar{x}-1/2,\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) | (8) 3 <sup>+</sup> $\bar{x},\bar{x}+1/2,x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)          |
| (9) 3 <sup>-</sup> $x,x,x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> (-1/3,1/3,1/3)<br>$x+1/6,x+1/6,\bar{x}$<br>(3 <sub>xyz</sub>  0,1/2,1/2) | (11) 3 <sup>-</sup> (1/3,1/3,-1/3)<br>$\bar{x}+1/3,\bar{x}+1/6,x$<br>(3 <sub>xyz</sub>  1/2,1/2,0)  | (12) 3 <sup>-</sup> (1/3,-1/3,1/3)<br>$\bar{x}-1/6,x+1/3,\bar{x}$<br>(3 <sub>xyz</sub>  1/2,0,1/2) |

Continued

205.2.1536

$\text{Pa}\bar{3}1'$

- |   |  |   |  |
|---|--|---|--|
| (13) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0)                        | (14) a (1/2,0,0) x,y,1/4<br>( $m_z$   1/2,0,1/2)   | (15) c (0,0,1/2) x,1/4,z<br>( $m_y$   0,1/2,1/2)  | (16) b (0,1/2,0) 1/4,y,z<br>( $m_x$   1/2,1/2,0)   |
| (17) $\bar{3}^+$ x,x,x;<br>0,0,0<br>( $\bar{3}_{xyz}$   0,0,0)      | (18) $\bar{3}^+$ $\bar{x}$ -1/2,x+1, $\bar{x}$ ;<br>0,1/2,1/2<br>( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0) | (19) $\bar{3}^+$ x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{xyz}^{-1}$   1/2,0,1/2) | (20) $\bar{3}^+$ $\bar{x}$ +1, $\bar{x}$ +1/2,x;<br>1/2,0,1/2<br>( $\bar{3}_{xyz}^{-1}$   0,1/2,1/2) |
| (21) $\bar{3}^-$ x,x,x;<br>0,0,0<br>( $\bar{3}_{xyz}^{-1}$   0,0,0) | (22) $\bar{3}^-$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ;<br>0,0,1/2<br>( $\bar{3}_{xyz}$   0,1/2,1/2)     | (23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1/2, x;<br>0,1/2,0<br>( $\bar{3}_{xyz}$   1/2,1/2,0)            | (24) $\bar{3}^-$ $\bar{x}$ +1/2, x, $\bar{x}$ ;<br>1/2,0,0<br>( $\bar{3}_{xyz}$   1/2,0,1/2)         |

For 1' + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1'<br>(1   0,0,0)'   | (2) 2' (0,0,1/2) 1/4,0,z<br>( $2_z$   1/2,0,1/2)'  | (3) 2' (0,1/2,0) 0,y,1/4<br>( $2_y$   0,1/2,1/2)'   | (4) 2' (1/2,0,0) x,1/4,0<br>( $2_x$   1/2,1/2,0)'  |
| (5) $3^{+'}$ x,x,x<br>( $3_{xyz}$   0,0,0)'                              | (6) $3^{+'}$ $\bar{x}$ +1/2,x, $\bar{x}$<br>( $3_{xyz}^{-1}$   1/2,1/2,0)'                               | (7) $3^{+'}$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$<br>( $3_{xyz}^{-1}$   1/2,0,1/2)'                             | (8) $3^{+'}$ $\bar{x}$ , $\bar{x}$ +1/2,x<br>( $3_{xyz}^{-1}$   0,1/2,1/2)'                              |
| (9) $3^{-'}$ x,x,x<br>( $3_{xyz}^{-1}$   0,0,0)'                         | (10) $3^{-'}$ (-1/3,1/3,1/3)<br>x+1/6, $\bar{x}$ +1/6, $\bar{x}$<br>( $3_{xyz}$   0,1/2,1/2)'            | (11) $3^{-'}$ (1/3,1/3,-1/3)<br>x+1/3, $\bar{x}$ +1/6, x<br>( $3_{xyz}$   1/2,1/2,0)'                       | (12) $3^{-'}$ (1/3,-1/3,1/3)<br>x-1/6, x+1/3, $\bar{x}$<br>( $3_{xyz}$   1/2,0,1/2)'                     |
| (13) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$   0,0,0)'                          | (14) a' (1/2,0,0) x,y,1/4<br>( $m_z$   1/2,0,1/2)'   | (15) c' (0,0,1/2) x,1/4,z<br>( $m_y$   0,1/2,1/2)'  | (16) b' (0,1/2,0) 1/4,y,z<br>( $m_x$   1/2,1/2,0)'   |
| (17) $\bar{3}^{+'}$ x,x,x;<br>0,0,0'<br>( $\bar{3}_{xyz}$   0,0,0)'      | (18) $\bar{3}^{+'}$ $\bar{x}$ -1/2,x+1, $\bar{x}$ ;<br>0,1/2,1/2<br>( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0)' | (19) $\bar{3}^{+'}$ x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{xyz}^{-1}$   1/2,0,1/2)' | (20) $\bar{3}^{+'}$ $\bar{x}$ +1, $\bar{x}$ +1/2,x;<br>1/2,0,1/2<br>( $\bar{3}_{xyz}^{-1}$   0,1/2,1/2)' |
| (21) $\bar{3}^{-'}$ x,x,x;<br>0,0,0'<br>( $\bar{3}_{xyz}^{-1}$   0,0,0)' | (22) $\bar{3}^{-'}$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ;<br>0,0,1/2<br>( $\bar{3}_{xyz}$   0,1/2,1/2)'     | (23) $\bar{3}^{-'}$ $\bar{x}$ , $\bar{x}$ +1/2, x;<br>0,1/2,0<br>( $\bar{3}_{xyz}$   1/2,1/2,0)'            | (24) $\bar{3}^{-'}$ $\bar{x}$ +1/2, x, $\bar{x}$ ;<br>1/2,0,0<br>( $\bar{3}_{xyz}$   1/2,0,1/2)'         |

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); 1'.

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates								
			1 +	1 +							
24	d	11'									
(1)	x,y,z	[0,0,0]	(2)	$\bar{x}$ +1/2, $\bar{y}$ ,z+1/2	[0,0,0]	(3)	$\bar{x}$ ,y+1/2, $\bar{z}$ +1/2	[0,0,0]	(4)	x+1/2, $\bar{y}$ +1/2, $\bar{z}$	[0,0,0]
(5)	z,x,y	[0,0,0]	(6)	z+1/2, $\bar{x}$ +1/2, $\bar{y}$	[0,0,0]	(7)	$\bar{z}$ +1/2, $\bar{x}$ ,y+1/2	[0,0,0]	(8)	$\bar{z}$ ,x+1/2, $\bar{y}$ +1/2	[0,0,0]
(9)	y,z,x	[0,0,0]	(10)	$\bar{y}$ ,z+1/2, $\bar{x}$ +1/2	[0,0,0]	(11)	y+1/2, $\bar{z}$ +1/2, $\bar{x}$	[0,0,0]	(12)	$\bar{y}$ +1/2, $\bar{z}$ ,x+1/2	[0,0,0]
(13)	$\bar{x}$ , $\bar{y}$ , $\bar{z}$	[0,0,0]	(14)	x+1/2,y, $\bar{z}$ +1/2	[0,0,0]	(15)	x, $\bar{y}$ +1/2,z+1/2	[0,0,0]	(16)	$\bar{x}$ +1/2,y+1/2,z	[0,0,0]
(17)	$\bar{z}$ , $\bar{x}$ , $\bar{y}$	[0,0,0]	(18)	$\bar{z}$ +1/2,x+1/2,y	[0,0,0]	(19)	z+1/2,x, $\bar{y}$ +1/2	[0,0,0]	(20)	z, $\bar{x}$ +1/2,y+1/2	[0,0,0]
(21)	$\bar{y}$ , $\bar{z}$ , $\bar{x}$	[0,0,0]	(22)	y, $\bar{z}$ +1/2,x+1/2	[0,0,0]	(23)	$\bar{y}$ +1/2,z+1/2,x	[0,0,0]	(24)	y+1/2,z, $\bar{x}$ +1/2	[0,0,0]

Continued

205.2.1536

Pa $\bar{3}$ 1'

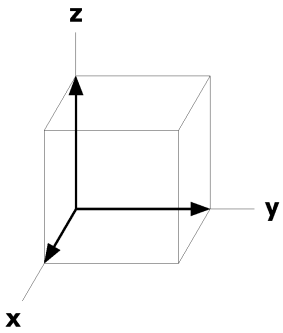
8	c	.3.1'	x,x,x [0,0,0]	$\bar{x}+1/2, \bar{x}, \bar{x}+1/2$ [0,0,0]	$\bar{x}, \bar{x}+1/2, \bar{x}+1/2$ [0,0,0]	$x+1/2, \bar{x}+1/2, \bar{x}$ [0,0,0]
			$\bar{x}, \bar{x}, \bar{x}$ [0,0,0]	$x+1/2, x, \bar{x}+1/2$ [0,0,0]	$x, \bar{x}+1/2, x+1/2$ [0,0,0]	$\bar{x}, +1/2, x+1/2, x$ [0,0,0]
4	b	$\bar{3}.1'$	1/2,1/2,1/2 [0,0,0]	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]	0,0,1/2 [0,0,0]
4	a	$\bar{3}.1'$	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p2mg1'  
 $\mathbf{a}^* = \mathbf{b}$   $\mathbf{b}^* = -\mathbf{a}/2$   
 Origin at 0,0,z

Along [1,1,1] p61'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

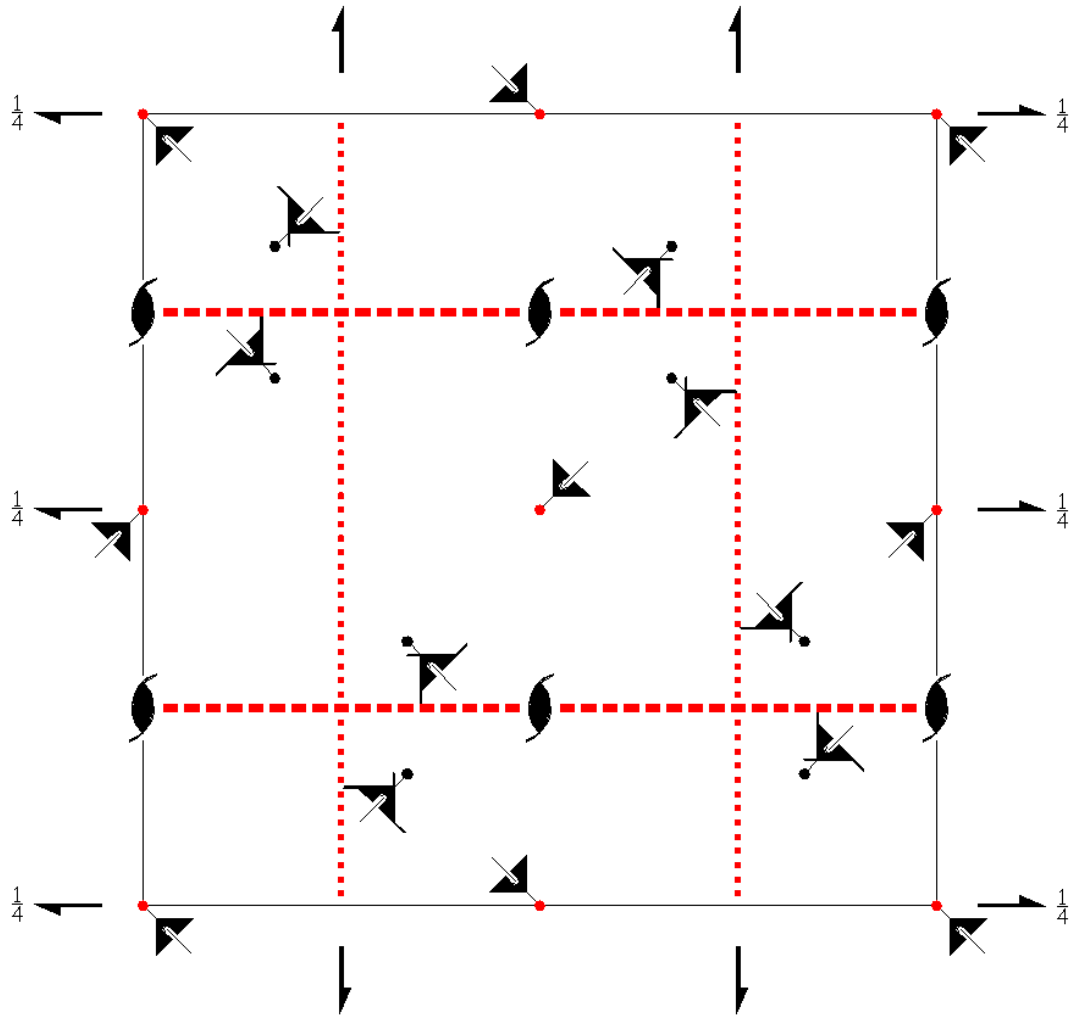
Along [1,1,0] p2gg1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$Pa\bar{3}'$   
205.3.1537

$m'\bar{3}'$   
 $P2_1/a'\bar{3}'$

Cubic



Origin at center ( $\bar{3}'$ )

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $z \leq \min(x,y)$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $0,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

- |   |  |   |  |
|---|--|---|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)  | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}+1/2,x,\bar{x}$<br>(3 <sub><math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1/2,1/2,0)    | (7) 3 <sup>+</sup> $x+1/2,\bar{x}-1/2,\bar{x}$<br>(3 <sub><math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  1/2,0,1/2) | (8) 3 <sup>+</sup> $\bar{x},\bar{x}+1/2,x$<br>(3 <sub><math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  0,1/2,1/2)    |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> (-1/3,1/3,1/3)<br>$x+1/6,x+1/6,\bar{x}$<br>(3 <sub><math>\bar{y}\bar{z}</math></sub>  0,1/2,1/2) | (11) 3 <sup>-</sup> (1/3,1/3,-1/3)<br>$x+1/3,x+1/6,x$<br>(3 <sub><math>\bar{y}\bar{z}</math></sub>  1/2,1/2,0)        | (12) 3 <sup>-</sup> (1/3,-1/3,1/3)<br>$x-1/6,x+1/3,\bar{x}$<br>(3 <sub><math>\bar{y}\bar{z}</math></sub>  1/2,0,1/2) |

(13) $\bar{1}$ ' 0,0,0 ( $\bar{1}$  0,0,0)'	(14) a' (1/2,0,0) x,y,1/4 ( $m_z$  1/2,0,1/2)'	(15) c' (0,0,1/2) x,1/4,z ( $m_y$  0,1/2,1/2)'	(16) b' (0,1/2,0) 1/4,y,z ( $m_x$  1/2,1/2,0)'
(17) $\bar{3}^+$ ' x,x,x; 0,0,0' ( $\bar{3}_{xyz}$  0,0,0)'	(18) $\bar{3}^+$ ' $\bar{x}$ -1/2,x+1, $\bar{x}$ ; 0,1/2,1/2 ( $\bar{3}_{xyz}^{-1}$  1/2,1/2,0)'	(19) $\bar{3}^+$ ' x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ; 1/2,1/2,0 ( $\bar{3}_{xyz}^{-1}$  1/2,0,1/2)'	(20) $\bar{3}^+$ ' $\bar{x}$ +1, $\bar{x}$ +1/2,x; 1/2,0,1/2 ( $\bar{3}_{xyz}^{-1}$  0,1/2,1/2)'
(21) $\bar{3}^-$ ' x,x,x; 0,0,0 ( $\bar{3}_{xyz}^{-1}$  0,0,0)'	(22) $\bar{3}^-$ ' x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ; 0,0,1/2 ( $\bar{3}_{xyz}$  0,1/2,1/2)'	(23) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ +1/2, x; 0,1/2,0 ( $\bar{3}_{xyz}$  1/2,1/2,0)'	(24) $\bar{3}^-$ ' $\bar{x}$ +1/2, x, $\bar{x}$ ; 1/2,0,0 ( $\bar{3}_{xyz}$  1/2,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

24 d 1

(1) x,y,z [u,v,w]	(2) $\bar{x}$ +1/2, $\bar{y}$ ,z+1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(3) $\bar{x}$ ,y+1/2, $\bar{z}$ +1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x+1/2, $\bar{y}$ +1/2, $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]
(5) z,x,y [w,u,v]	(6) z+1/2, $\bar{x}$ +1/2, $\bar{y}$ [w, $\bar{u}$ , $\bar{v}$ ]	(7) $\bar{z}$ +1/2, $\bar{x}$ ,y+1/2 [ $\bar{w}$ , $\bar{u}$ ,v]	(8) $\bar{z}$ ,x+1/2, $\bar{y}$ +1/2 [ $\bar{w}$ ,u, $\bar{v}$ ]
(9) y,z,x [v,w,u]	(10) $\bar{y}$ ,z+1/2, $\bar{x}$ +1/2 [ $\bar{v}$ ,w, $\bar{u}$ ]	(11) y+1/2, $\bar{z}$ +1/2, $\bar{x}$ [v, $\bar{w}$ , $\bar{u}$ ]	(12) $\bar{y}$ +1/2, $\bar{z}$ ,x+1/2 [ $\bar{v}$ , $\bar{w}$ ,u]
(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(14) x+1/2,y, $\bar{z}$ +1/2 [u,v, $\bar{w}$ ]	(15) x, $\bar{y}$ +1/2,z+1/2 [u, $\bar{v}$ ,w]	(16) $\bar{x}$ +1/2,y+1/2,z [ $\bar{u}$ ,v,w]
(17) $\bar{z}$ , $\bar{x}$ , $\bar{y}$ [ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ]	(18) $\bar{z}$ +1/2,x+1/2,y [ $\bar{w}$ ,u,v]	(19) z+1/2,x, $\bar{y}$ +1/2 [w,u, $\bar{v}$ ]	(20) z, $\bar{x}$ +1/2,y+1/2 [w, $\bar{u}$ , $\bar{v}$ ]
(21) $\bar{y}$ , $\bar{z}$ , $\bar{x}$ [ $\bar{v}$ , $\bar{w}$ , $\bar{u}$ ]	(22) y, $\bar{z}$ +1/2,x+1/2 [v, $\bar{w}$ ,u]	(23) $\bar{y}$ +1/2,z+1/2,x [ $\bar{v}$ ,w,u]	(24) y+1/2,z, $\bar{x}$ +1/2 [v,w, $\bar{u}$ ]

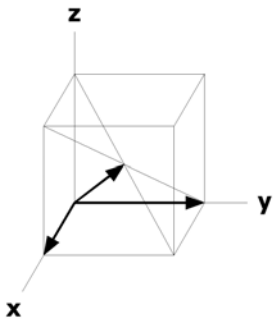
8 c .3.	x,x,x [u,u,u]	$\bar{x}$ +1/2, $\bar{x}$ ,x+1/2 [ $\bar{u}$ , $\bar{u}$ ,u]	$\bar{x}$ ,x+1/2, $\bar{x}$ +1/2 [ $\bar{u}$ ,u, $\bar{u}$ ]	x+1/2, $\bar{x}$ +1/2, $\bar{x}$ [u, $\bar{u}$ , $\bar{u}$ ]
	$\bar{x}$ , $\bar{x}$ , $\bar{x}$ [ $\bar{u}$ , $\bar{u}$ , $\bar{u}$ ]	x+1/2,x, $\bar{x}$ +1/2 [u,u, $\bar{u}$ ]	x, $\bar{x}$ +1/2,x+1/2 [u, $\bar{u}$ ,u]	$\bar{x}$ ,+1/2 x+1/2,x [ $\bar{u}$ ,u,u]
4 b . $\bar{3}$ '.	1/2,1/2,1/2 [0,0,0]	0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]	0,0,1/2 [0,0,0]
4 a . $\bar{3}$ '.	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p2m'g'  
a\* = b b\* = -a/2  
Origin at 0,0,z

Along [1,1,1] p6  
a\* = (2a - b - c)/3 b\* = (-a + 2b - c)/3  
Origin at x,x,x

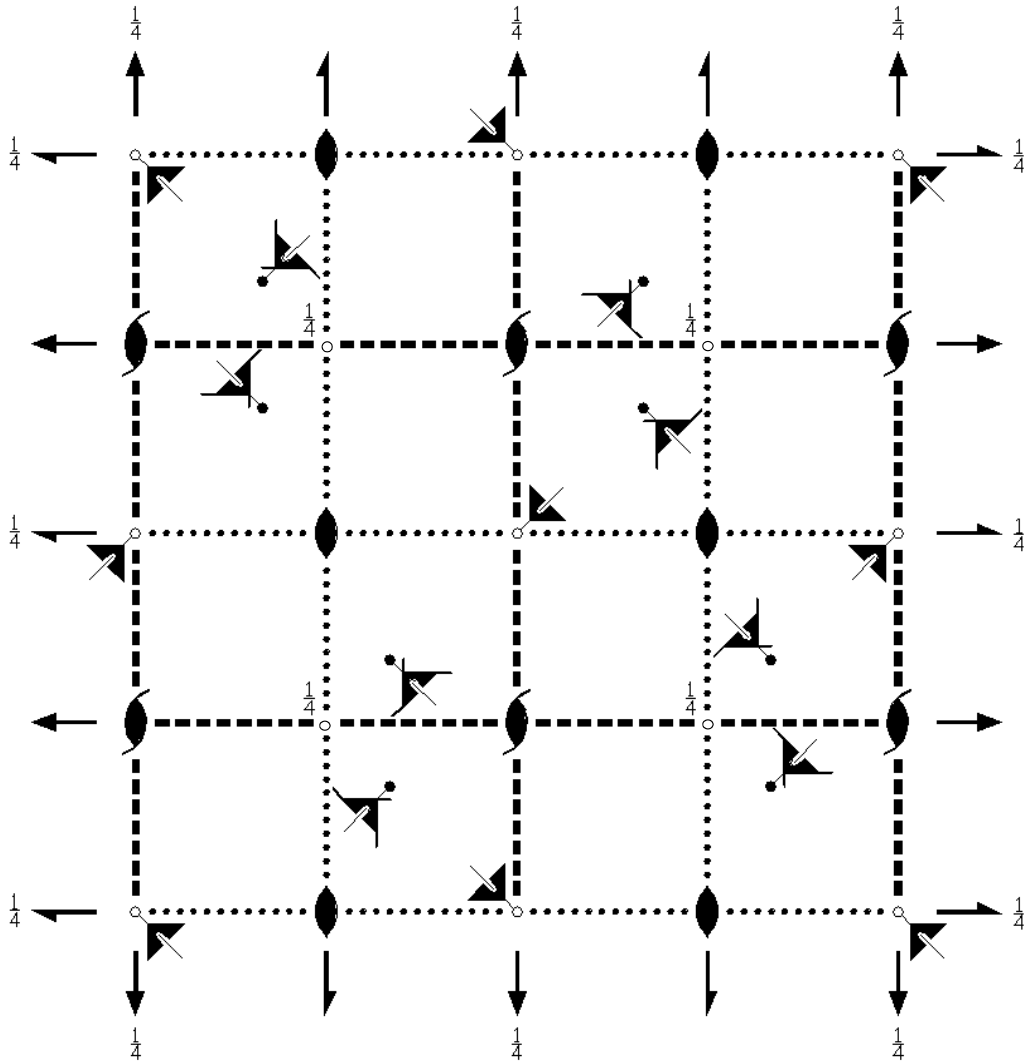
Along [1,1,0] p2g'g'  
a\* = (-a + b)/2 b\* = c  
Origin at x,x,0



la $\bar{3}$   
206.1.1538

m $\bar{3}$   
I $2_1/a\bar{3}$

Cubic



Origin at center ( $\bar{3}$ )

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$ ;  $z \leq \min(x,y)$

Vertices 0,0,0    1/2,0,0    1/2,1/2,0    0,1/2,0    1/2,1/2,1/2

**Symmetry Operations**

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1*0,0,0)  | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub> *1/2,0,1/2)  | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub> *0,1/2,1/2)                                   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub> *1/2,1/2,0)                                   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub> *0,0,0)               | (6) 3 <sup>+</sup> &+1/2,x,&<br>(3 <sub>x&amp;z</sub> *1/2,1/2,0)                                   | (7) 3 <sup>+</sup> x+1/2,&-1/2,&<br>(3 <sub>&amp;y<sub>z</sub></sub> *1/2,0,1/2)         | (8) 3 <sup>+</sup> &,&+1/2,x<br>(3 <sub>xy&amp;</sub> *0,1/2,1/2)                        |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup> *0,0,0) | (10) 3 <sup>-</sup> (-1/3,1/3,1/3)<br>x+1/6,&+1/6,&<br>(3 <sub>&amp;y<sub>z</sub></sub> *0,1/2,1/2) | (11) 3 <sup>-</sup> (1/3,1/3,-1/3)<br>&+1/3,&+1/6,x<br>(3 <sub>xy&amp;</sub> *1/2,1/2,0) | (12) 3 <sup>-</sup> (1/3,-1/3,1/3)<br>&-1/6,x+1/3,&<br>(3 <sub>x&amp;z</sub> *1/2,0,1/2) |

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$   0,0,0)	(14) a (1/2,0,0) x,y,1/4 ( $m_z$   1/2,0,1/2)	(15) c (0,0,1/2) x,1/4,z ( $m_y$   0,1/2,1/2)	(16) b (0,1/2,0) 1/4,y,z ( $m_x$   1/2,1/2,0)
(17) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$   0,0,0)	(18) $\bar{3}^+$ $\bar{x}$ -1/2,x+1, $\bar{x}$ ; 0,1/2,1/2 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0)	(19) $\bar{3}^+$ x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ; 1/2,1/2,0 ( $\bar{3}_{xyz}^{-1}$   1/2,0,1/2)	(20) $\bar{3}^+$ $\bar{x}$ +1, $\bar{x}$ +1/2,x; 1/2,0,1/2 ( $\bar{3}_{xyz}^{-1}$   0,1/2,1/2)
(21) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}^{-1}$   0,0,0)	(22) $\bar{3}^-$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ; 0,0,1/2 ( $\bar{3}_{xyz}$   0,1/2,1/2)	(23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1/2, x; 0,1/2,0 ( $\bar{3}_{xyz}$   1/2,1/2,0)	(24) $\bar{3}^-$ $\bar{x}$ +1/2, x, $\bar{x}$ ; 1/2,0,0 ( $\bar{3}_{xyz}$   1/2,0,1/2)

For (1/2,1/2,1/2) + set

(1) 1 (1   1/2,1/2,1/2)	(2) 2 0,1/4,z ( $2_z$   0,1/2,0)	(3) 2 1/4,y,0 ( $2_y$   1/2,0,0)	(4) 2 x,0,1/4 ( $2_x$   0,0,1/2)
(5) $3^+$ (1/2,1/2,1/2) x,x,x ( $3_{xyz}$   1/2,1/2,1/2)	(6) $3^+$ (1/6,-1/6,1/6) x-1/6,x+1/3, $\bar{x}$ ( $3_{xyz}^{-1}$   0,0,1/2)	(7) $3^+$ (-1/6,1/6,1/6) x+1/6, $\bar{x}$ +1/6, $\bar{x}$ ( $3_{xyz}^{-1}$   0,1/2,0)	(8) $3^+$ (1/6,1/6,-1/6) x+1/3, $\bar{x}$ +1/6,x ( $3_{xyz}^{-1}$   1/2,0,0)
(9) $3^-$ (1/2,1/2,1/2) x,x,x ( $3_{xyz}^{-1}$   1/2,1/2,1/2)	(10) $3^-$ (1/6,-1/6,-1/6) x+1/6, $\bar{x}$ +1/6, $\bar{x}$ ( $3_{xyz}$   1/2,0,0)	(11) $3^-$ (-1/6,-1/6,1/6) x+1/3, $\bar{x}$ +1/6, x ( $3_{xyz}$   0,0,1/2)	(12) $3^-$ (-1/6,1/6,-1/6) x-1/6, x+1/3, $\bar{x}$ ( $3_{xyz}$   0,1/2,0)
(13) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)	(14) b (0,1/2,0) x,y,0 ( $m_z$   0,1/2,0)	(15) a (1/2,0,0) x,0,z ( $m_y$   1/2,0,0)	(16) c (0,0,1/2) 0,y,z ( $m_x$   0,0,1/2)
(17) $\bar{3}^+$ x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}$   1/2,1/2,1/2)	(18) $\bar{3}^+$ $\bar{x}$ -1/2,x, $\bar{x}$ ; -1/4,-1/4,1/4 ( $\bar{3}_{xyz}^{-1}$   0,0,1/2)	(19) $\bar{3}^+$ x-1/2, $\bar{x}$ +1/2, $\bar{x}$ ; -1/4,1/4,-1/4 ( $\bar{3}_{xyz}^{-1}$   0,1/2,0)	(20) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ -1/2,x; 1/4,-1/4,-1/4 ( $\bar{3}_{xyz}^{-1}$   1/2,0,0)
(21) $\bar{3}^-$ x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2)	(22) $\bar{3}^-$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ; 1/4,-1/4,1/4 ( $\bar{3}_{xyz}$   1/2,0,0)	(23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1/2, x; -1/4,1/4,1/4 ( $\bar{3}_{xyz}$   0,0,1/2)	(24) $\bar{3}^-$ $\bar{x}$ +1/2, x, $\bar{x}$ ; 1/4,1/4,-1/4 ( $\bar{3}_{xyz}$   0,1/2,0)

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).

## Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
48 e 1				
(1) x,y,z [u,v,w]	(2) $\bar{x}$ +1/2, $\bar{y}$ ,z+1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(3) $\bar{x}$ ,y+1/2, $\bar{z}$ +1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x+1/2, $\bar{y}$ +1/2, $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	
(5) z,x,y [w,u,v]	(6) z+1/2, $\bar{x}$ +1/2, $\bar{y}$ [w, $\bar{u}$ , $\bar{v}$ ]	(7) $\bar{z}$ +1/2, $\bar{x}$ ,y+1/2 [ $\bar{w}$ , $\bar{u}$ ,v]	(8) $\bar{z}$ ,x+1/2, $\bar{y}$ +1/2 [ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ]	
(9) y,z,x [v,w,u]	(10) $\bar{y}$ ,z+1/2, $\bar{x}$ +1/2 [ $\bar{v}$ ,w, $\bar{u}$ ]	(11) y+1/2, $\bar{z}$ +1/2, $\bar{x}$ [v, $\bar{w}$ , $\bar{u}$ ]	(12) $\bar{y}$ +1/2, $\bar{z}$ ,x+1/2 [ $\bar{v}$ , $\bar{w}$ ,u]	
(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(14) x+1/2,y, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(15) x, $\bar{y}$ +1/2,z+1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	(16) $\bar{x}$ +1/2,y+1/2,z [u, $\bar{v}$ , $\bar{w}$ ]	
(17) $\bar{z}$ , $\bar{x}$ , $\bar{y}$ [w,u,v]	(18) $\bar{z}$ +1/2,x+1/2,y [w, $\bar{u}$ , $\bar{v}$ ]	(19) z+1/2,x, $\bar{y}$ +1/2 [ $\bar{w}$ , $\bar{u}$ ,v]	(20) z, $\bar{x}$ +1/2,y+1/2 [ $\bar{w}$ ,u, $\bar{v}$ ]	
(21) $\bar{y}$ , $\bar{z}$ , $\bar{x}$ [v,w,u]	(22) y, $\bar{z}$ +1/2,x+1/2 [ $\bar{v}$ ,w, $\bar{u}$ ]	(23) $\bar{y}$ +1/2,z+1/2,x [v, $\bar{w}$ , $\bar{u}$ ]	(24) y+1/2,z, $\bar{x}$ +1/2 [ $\bar{v}$ , $\bar{w}$ ,u]	



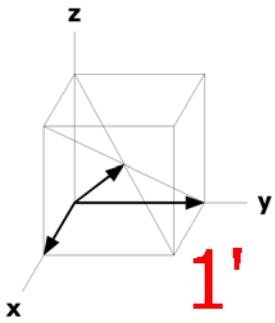
24	d	2..	x,0,1/4 [u,0,0]	$\bar{x}+1/2,0,3/4 [\bar{u},0,0]$	1/4,x,0 [0,u,0]	3/4, $\bar{x}+1/2,0 [0,\bar{u},0]$
			0,1/4,x [0,0,u]	0,3/4, $\bar{x}+1/2 [0,0,\bar{u}]$	$\bar{x},0,3/4 [u,0,0]$	x+1/2,0,1/4 [ $\bar{u},0,0]$
			3/4, $\bar{x},0 [0,u,0]$	1/4,x+1/2,0 [0, $\bar{u},0]$	0,3/4, $\bar{x} [0,0,u]$	0,1/4,x+1/2 [0,0, $\bar{u}]$
16	c	.3.	x,x,x [u,u,u]	$\bar{x}+1/2,\bar{x},x+1/2 [\bar{u},\bar{u},u]$	$\bar{x},x+1/2,\bar{x}+1/2 [\bar{u},u,\bar{u}]$	x+1/2, $\bar{x}+1/2,\bar{x} [u,\bar{u},\bar{u}]$
			$\bar{x},\bar{x},\bar{x} [u,u,u]$	x+1/2,x, $\bar{x}+1/2 [\bar{u},\bar{u},u]$	x, $\bar{x}+1/2,x+1/2 [\bar{u},u,\bar{u}]$	$\bar{x},+1/2 x+1/2,x [u,\bar{u},\bar{u}]$
8	b	$\bar{3}$ .	1/4,1/4,1/4 [u,u,u]	1/4,3/4,3/4 [ $\bar{u},\bar{u},u]$	3/4,3/4,1/4 [ $\bar{u},u,\bar{u}]$	3/4,1/4,3/4 [u, $\bar{u},\bar{u}]$
8	a	$\bar{3}$ .	0,0,0 [u,u,u]	1/2,0,1/2 [ $\bar{u},\bar{u},u]$	0,1/2,1/2 [ $\bar{u},u,\bar{u}]$	1/2,1/2,0 [u, $\bar{u},\bar{u}]$

### Symmetry of Special Projections

Along [0,0,1]  $p_c^* 2mm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,1/4,z

Along [1,1,1]  $p6'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

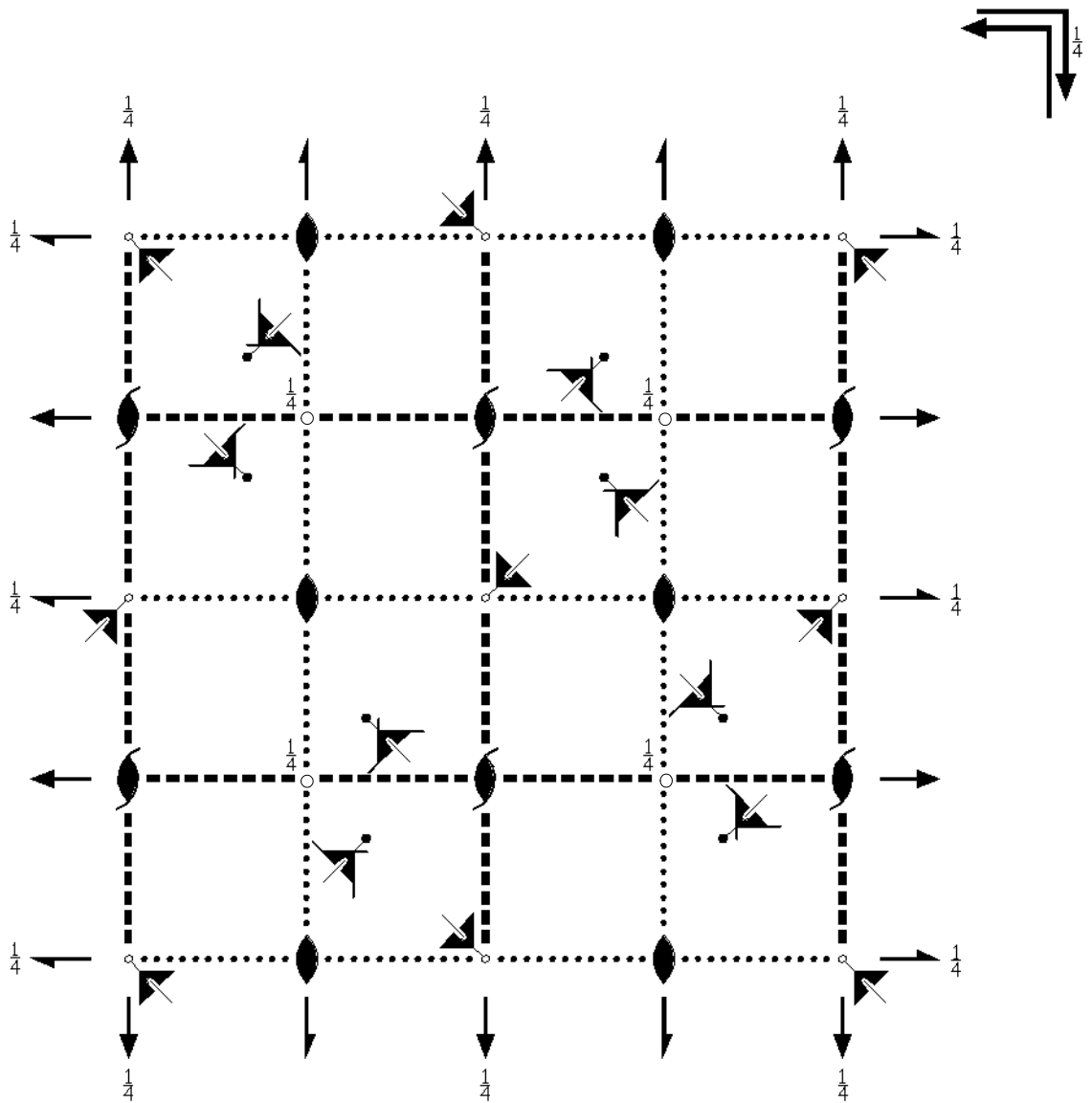
Along [1,1,0]  $p2'mg'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$la\bar{1}'$   
206.2.1539

$m\bar{1}'$   
 $I2_1/a\bar{1}'$

Cubic



Origin at cent

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $z \leq \min(x,y)$

Vertices 0,0,0    1/2,0,0    1/2,1/2,0    0,1/2,0    1/2,1/2,1/2

**Symmetry Operations**

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>( $1^*0,0,0$ )                     | (2) 2 (0,0,1/2) $1/4,0,z$<br>( $2_z^*1/2,0,1/2$ )   | (3) 2 (0,1/2,0) $0,y,1/4$<br>( $2_y^*0,1/2,1/2$ )  | (4) 2 (1/2,0,0) $x,1/4,0$<br>( $2_x^*1/2,1/2,0$ )  |
| (5) $3^+$ x,x,x<br>( $3_{xyz}^*0,0,0$ )     | (6) $3^+$ $\bar{x}+1/2,x,\bar{z}$<br>( $3_{x\bar{z}}^{-1*1/2,1/2,0}$ )                          | (7) $3^+$ $x+1/2,\bar{z}-1/2,\bar{y}$<br>( $3_{\bar{y}\bar{z}}^{-1*1/2,0,1/2}$ )           | (8) $3^+$ $\bar{z},\bar{z}+1/2,x$<br>( $3_{xy\bar{z}}^{-1*0,1/2,1/2}$ )                          |
| (9) $3^-$ x,x,x<br>( $3_{xyz}^{-1*0,0,0}$ ) | (10) $3^-$ (-1/3,1/3,1/3)<br>$x+1/6,\bar{z}+1/6,\bar{y}$<br>( $3_{\bar{y}\bar{z}}^*0,1/2,1/2$ ) | (11) $3^-$ (1/3,1/3,-1/3)<br>$\bar{z}+1/3,\bar{y}+1/6,x$<br>( $3_{xy\bar{z}}^*1/2,1/2,0$ ) | (12) $3^-$ (1/3,-1/3,1/3)<br>$\bar{z}-1/6,x+1/3,\bar{y}$<br>( $3_{x\bar{y}\bar{z}}^*1/2,0,1/2$ ) |

- |   |  |   |  |
|---|--|---|--|
| (13) $\bar{1}$ 0,0,0<br>( $\bar{1}$   0,0,0)                        | (14) a (1/2,0,0) x,y,1/4<br>( $m_z$   1/2,0,1/2)   | (15) c (0,0,1/2) x,1/4,z<br>( $m_y$   0,1/2,1/2)  | (16) b (0,1/2,0) 1/4,y,z<br>( $m_x$   1/2,1/2,0)   |
| (17) $\bar{3}^+$ x,x,x;<br>0,0,0<br>( $\bar{3}_{xyz}$   0,0,0)      | (18) $\bar{3}^+$ $\bar{x}$ -1/2,x+1, $\bar{x}$ ;<br>0,1/2,1/2<br>( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0) | (19) $\bar{3}^+$ x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{xyz}^{-1}$   1/2,0,1/2) | (20) $\bar{3}^+$ $\bar{x}$ +1, $\bar{x}$ +1/2,x;<br>1/2,0,1/2<br>( $\bar{3}_{xyz}^{-1}$   0,1/2,1/2) |
| (21) $\bar{3}^-$ x,x,x;<br>0,0,0<br>( $\bar{3}_{xyz}^{-1}$   0,0,0) | (22) $\bar{3}^-$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ;<br>0,0,1/2<br>( $\bar{3}_{xyz}$   0,1/2,1/2)     | (23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1/2, x;<br>0,1/2,0<br>( $\bar{3}_{xyz}$   1/2,1/2,0)            | (24) $\bar{3}^-$ $\bar{x}$ +1/2, x, $\bar{x}$ ;<br>1/2,0,0<br>( $\bar{3}_{xyz}$   1/2,0,1/2)         |

For (1/2,1/2,1/2) + set

- |   |  |   |  |
|---|--|---|--|
| (1) 1<br>(1   1/2,1/2,1/2)  | (2) 2 0,1/4,z<br>( $2_z$   0,1/2,0)  | (3) 2 1/4,y,0<br>( $2_y$   1/2,0,0)   | (4) 2 x,0,1/4<br>( $2_x$   0,0,1/2)  |
| (5) $3^+$ (1/2,1/2,1/2) x,x,x<br>( $3_{xyz}$   1/2,1/2,1/2)                     | (6) $3^+$ (1/6,-1/6,1/6)<br>$\bar{x}$ -1/6,x+1/3, $\bar{x}$<br>( $3_{xyz}^{-1}$   0,0,1/2)           | (7) $3^+$ (-1/6,1/6,1/6)<br>x+1/6, $\bar{x}$ +1/6, $\bar{x}$<br>( $3_{xyz}^{-1}$   0,1/2,0)               | (8) $3^+$ (1/6,1/6,-1/6)<br>$\bar{x}$ +1/3, $\bar{x}$ +1/6,x<br>( $3_{xyz}^{-1}$   1/2,0,0)          |
| (9) $3^-$ (1/2,1/2,1/2) x,x,x<br>( $3_{xyz}^{-1}$   1/2,1/2,1/2)                | (10) $3^-$ (1/6,-1/6,-1/6)<br>x+1/6, $\bar{x}$ +1/6, $\bar{x}$<br>( $3_{xyz}$   1/2,0,0)             | (11) $3^-$ (-1/6,-1/6,1/6)<br>x+1/3, $\bar{x}$ +1/6, x<br>( $3_{xyz}$   0,0,1/2)                          | (12) $3^-$ (-1/6,1/6,-1/6)<br>$\bar{x}$ -1/6, x+1/3, $\bar{x}$<br>( $3_{xyz}$   0,1/2,0)             |
| (13) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$   1/2,1/2,1/2)                        | (14) b (0,1/2,0) x,y,0<br>( $m_z$   0,1/2,0)   | (15) a (1/2,0,0) x,0,z<br>( $m_y$   1/2,0,0)  | (16) c (0,0,1/2) 0,y,z<br>( $m_x$   0,0,1/2)   |
| (17) $\bar{3}^+$ x,x,x;<br>1/4,1/4,1/4<br>( $\bar{3}_{xyz}$   1/2,1/2,1/2)      | (18) $\bar{3}^+$ $\bar{x}$ -1/2,x, $\bar{x}$ ;<br>-1/4,-1/4,1/4<br>( $\bar{3}_{xyz}^{-1}$   0,0,1/2) | (19) $\bar{3}^+$ x-1/2, $\bar{x}$ +1/2, $\bar{x}$ ;<br>-1/4,1/4,-1/4<br>( $\bar{3}_{xyz}^{-1}$   0,1/2,0) | (20) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ -1/2,x;<br>1/4,-1/4,-1/4<br>( $\bar{3}_{xyz}^{-1}$   1/2,0,0) |
| (21) $\bar{3}^-$ x,x,x;<br>1/4,1/4,1/4<br>( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2) | (22) $\bar{3}^-$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ;<br>1/4,-1/4,1/4<br>( $\bar{3}_{xyz}$   1/2,0,0)  | (23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1/2, x;<br>-1/4,1/4,1/4<br>( $\bar{3}_{xyz}$   0,0,1/2)           | (24) $\bar{3}^-$ $\bar{x}$ +1/2, x, $\bar{x}$ ;<br>1/4,1/4,-1/4<br>( $\bar{3}_{xyz}$   0,1/2,0)      |

For (0,0,0)' + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1'<br>(1   0,0,0)'  | (2) 2' (0,0,1/2) 1/4,0,z<br>( $2_z$   1/2,0,1/2)'   | (3) 2' (0,1/2,0) 0,y,1/4<br>( $2_y$   0,1/2,1/2)'  | (4) 2' (1/2,0,0) x,1/4,0<br>( $2_x$   1/2,1/2,0)'   |
| (5) $3^+$ ' x,x,x<br>( $3_{xyz}$   0,0,0)'                              | (6) $3^+$ ' $\bar{x}$ +1/2,x, $\bar{x}$<br>( $3_{xyz}^{-1}$   1/2,1/2,0)'                               | (7) $3^+$ ' x+1/2, $\bar{x}$ -1/2, $\bar{x}$<br>( $3_{xyz}^{-1}$   1/2,0,1/2)'                             | (8) $3^+$ ' $\bar{x}$ , $\bar{x}$ +1/2,x<br>( $3_{xyz}^{-1}$   0,1/2,1/2)'                              |
| (9) $3^-$ ' x,x,x<br>( $3_{xyz}^{-1}$   0,0,0)'                         | (10) $3^-$ ' (-1/3,1/3,1/3)<br>x+1/6, $\bar{x}$ +1/6, $\bar{x}$<br>( $3_{xyz}$   0,1/2,1/2)'            | (11) $3^-$ ' (1/3,1/3,-1/3)<br>x+1/3, $\bar{x}$ +1/6, x<br>( $3_{xyz}$   1/2,1/2,0)'                       | (12) $3^-$ ' (1/3,-1/3,1/3)<br>x-1/6, x+1/3, $\bar{x}$<br>( $3_{xyz}$   1/2,0,1/2)'                     |
| (13) $\bar{1}$ ' 0,0,0<br>( $\bar{1}$   0,0,0)'                         | (14) a' (1/2,0,0) x,y,1/4<br>( $m_z$   1/2,0,1/2)'  | (15) c' (0,0,1/2) x,1/4,z<br>( $m_y$   0,1/2,1/2)'   | (16) b' (0,1/2,0) 1/4,y,z<br>( $m_x$   1/2,1/2,0)'  |
| (17) $\bar{3}^+$ ' x,x,x;<br>0,0,0'<br>( $\bar{3}_{xyz}$   0,0,0)'      | (18) $\bar{3}^+$ ' $\bar{x}$ -1/2,x+1, $\bar{x}$ ;<br>0,1/2,1/2<br>( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0)' | (19) $\bar{3}^+$ ' x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{xyz}^{-1}$   1/2,0,1/2)' | (20) $\bar{3}^+$ ' $\bar{x}$ +1, $\bar{x}$ +1/2,x;<br>1/2,0,1/2<br>( $\bar{3}_{xyz}^{-1}$   0,1/2,1/2)' |
| (21) $\bar{3}^-$ ' x,x,x;<br>0,0,0'<br>( $\bar{3}_{xyz}^{-1}$   0,0,0)' | (22) $\bar{3}^-$ ' x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ;<br>0,0,1/2<br>( $\bar{3}_{xyz}$   0,1/2,1/2)'     | (23) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ +1/2, x;<br>0,1/2,0<br>( $\bar{3}_{xyz}$   1/2,1/2,0)'            | (24) $\bar{3}^-$ ' $\bar{x}$ +1/2, x, $\bar{x}$ ;<br>1/2,0,0<br>( $\bar{3}_{xyz}$   1/2,0,1/2)'         |

For (1/2,1/2,1/2)' + set

(1) 1' (1   1/2,1/2,1/2)'	(2) 2' 0,1/4,z (2 <sub>z</sub>   0,1/2,0)'	(3) 2' 1/4,y,0 (2 <sub>y</sub>   1/2,0,0)'	(4) 2' x,0,1/4 (2 <sub>x</sub>   0,0,1/2)'
(5) 3 <sup>+</sup> ' (1/2,1/2,1/2) x,x,x (3 <sub>xyz</sub>   1/2,1/2,1/2)'	(6) 3 <sup>+</sup> ' (1/6,-1/6,1/6) x-1/6,x+1/3,x (3 <sub>xyz</sub> <sup>-1</sup>   0,0,1/2)'	(7) 3 <sup>+</sup> ' (-1/6,1/6,1/6) x+1/6,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   0,1/2,0)'	(8) 3 <sup>+</sup> ' (1/6,1/6,-1/6) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,0,0)'
(9) 3 <sup>-</sup> ' (1/2,1/2,1/2) x,x,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,1/2)'	(10) 3 <sup>-</sup> ' (1/6,-1/6,-1/6) x+1/6,x+1/6,x (3 <sub>xyz</sub>   1/2,0,0)'	(11) 3 <sup>-</sup> ' (-1/6,-1/6,1/6) x+1/3,x+1/6,x (3 <sub>xyz</sub>   0,0,1/2)'	(12) 3 <sup>-</sup> ' (-1/6,1/6,-1/6) x-1/6,x+1/3,x (3 <sub>xyz</sub>   0,1/2,0)'
(13) $\bar{1}$ ' 1/4,1/4,1/4 (1   1/2,1/2,1/2)'	(14) b' (0,1/2,0) x,y,0 (m <sub>z</sub>   0,1/2,0)'	(15) a' (1/2,0,0) x,0,z (m <sub>y</sub>   1/2,0,0)'	(16) c' (0,0,1/2) 0,y,z (m <sub>x</sub>   0,0,1/2)'
(17) $\bar{3}^+$ ' x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}$   1/2,1/2,1/2)'	(18) $\bar{3}^+$ ' x-1/2,x,x; -1/4,-1/4,1/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>   0,0,1/2)'	(19) $\bar{3}^+$ ' x-1/2,x+1/2,x; -1/4,1/4,-1/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>   0,1/2,0)'	(20) $\bar{3}^+$ ' x,x-1/2,x; 1/4,-1/4,-1/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,0,0)'
(21) $\bar{3}^-$ ' x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,1/2)'	(22) $\bar{3}^-$ ' x+1/2,x-1/2,x; 1/4,-1/4,1/4 ( $\bar{3}_{xyz}$   1/2,0,0)'	(23) $\bar{3}^-$ ' x,x+1/2,x; -1/4,1/4,1/4 ( $\bar{3}_{xyz}$   0,0,1/2)'	(24) $\bar{3}^-$ ' x+1/2,x,x; 1/4,1/4,-1/4 ( $\bar{3}_{xyz}$   0,1/2,0)'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); 1'.

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

(0,0,0) + (1/2,1/2,1/2) +  
(0,0,0)' + (1/2,1/2,1/2)'

48 e 11'	(1) x,y,z [0,0,0]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [0,0,0]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [0,0,0]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [0,0,0]
	(5) z,x,y [0,0,0]	(6) $z+1/2,\bar{x}+1/2,\bar{y}$ [0,0,0]	(7) $\bar{z}+1/2,\bar{x},y+1/2$ [0,0,0]	(8) $\bar{z},x+1/2,\bar{y}+1/2$ [0,0,0]
	(9) y,z,x [0,0,0]	(10) $\bar{y},z+1/2,\bar{x}+1/2$ [0,0,0]	(11) $y+1/2,\bar{z}+1/2,\bar{x}$ [0,0,0]	(12) $\bar{y}+1/2,\bar{z},x+1/2$ [0,0,0]
	(13) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(14) $x+1/2,y,\bar{z}+1/2$ [0,0,0]	(15) $x,\bar{y}+1/2,z+1/2$ [0,0,0]	(16) $\bar{x}+1/2,y+1/2,z$ [0,0,0]
	(17) $\bar{z},\bar{x},\bar{y}$ [0,0,0]	(18) $\bar{z}+1/2,x+1/2,y$ [0,0,0]	(19) $z+1/2,x,\bar{y}+1/2$ [0,0,0]	(20) $z,\bar{x}+1/2,y+1/2$ [0,0,0]
	(21) $\bar{y},\bar{z},\bar{x}$ [0,0,0]	(22) $y,\bar{z}+1/2,x+1/2$ [0,0,0]	(23) $\bar{y}+1/2,z+1/2,x$ [0,0,0]	(24) $y+1/2,z,\bar{x}+1/2$ [0,0,0]
24 d 2..1'	x,0,1/4 [0,0,0]	$\bar{x}+1/2,0,3/4$ [0,0,0]	1/4,x,0 [0,0,0]	3/4, $\bar{x}+1/2,0$ [0,0,0]
	0,1/4,x [0,0,0]	0,3/4, $\bar{x}+1/2$ [0,0,0]	$\bar{x},0,3/4$ [0,0,0]	$x+1/2,0,1/4$ [0,0,0]
	3/4, $\bar{x},0$ [0,0,0]	1/4, $x+1/2,0$ [0,0,0]	0,3/4, $\bar{x}$ [0,0,0]	0,1/4, $x+1/2$ [0,0,0]
8 c .3.1'	x,x,x [0,0,0]	$\bar{x}+1/2,\bar{x},x+1/2$ [0,0,0]	$\bar{x},x+1/2,\bar{x}+1/2$ [0,0,0]	$x+1/2,\bar{x}+1/2,\bar{x}$ [0,0,0]
	$\bar{x},\bar{x},\bar{x}$ [0,0,0]	$x+1/2,x,\bar{x}+1/2$ [0,0,0]	$x,\bar{x}+1/2,x+1/2$ [0,0,0]	$\bar{x},+1/2 x+1/2,x$ [0,0,0]

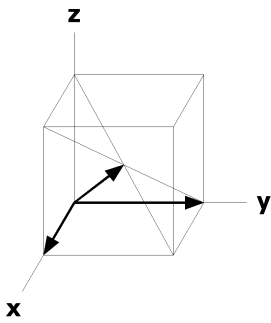
4	b	$\bar{3}.1'$	$1/4, 1/4, 1/4 [0,0,0]$	$1/4, 3/4, 3/4 [0,0,0]$	$3/4, 3/4, 1/4 [0,0,0]$	$3/4, 1/4, 3/4 [0,0,0]$
4	a	$\bar{3}.1'$	$0,0,0 [0,0,0]$	$1/2, 0, 1/2 [0,0,0]$	$0, 1/2, 1/2 [0,0,0]$	$1/2, 1/2, 0 [0,0,0]$

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p2mm1'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p61'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x,x,x$

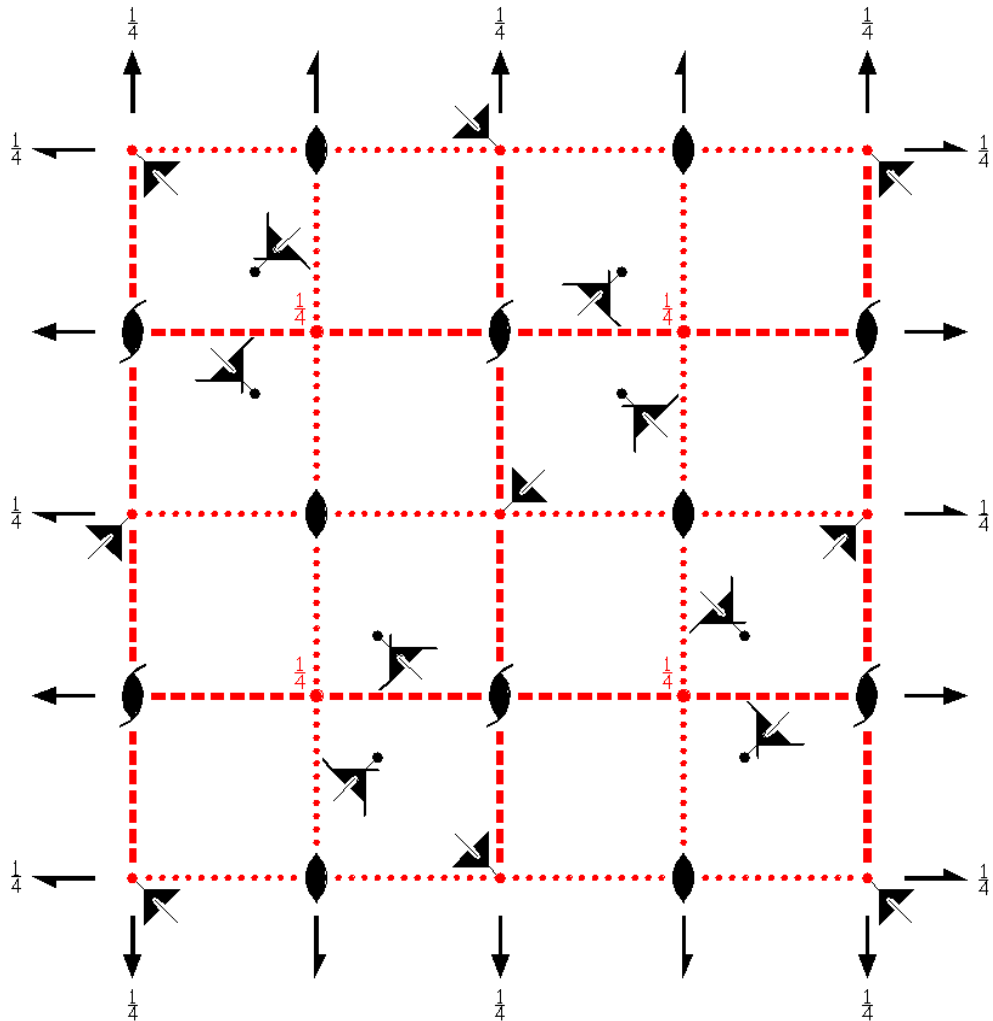
Along  $[1,1,0]$   $p2mg1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



$la\bar{3}'$   
206.3.1540

$m'\bar{3}'$   
 $I2_1/a'\bar{3}'$

Cubic



Origin at center ( $\bar{3}'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; z \leq \min(x,y)$

Vertices 0,0,0    1/2,0,0    1/2,1/2,0    0,1/2,0    1/2,1/2,1/2

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |   |
|---|--|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}+1/2, \bar{x}, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,1/2,0) | (7) 3 <sup>+</sup> $\bar{x}+1/2, \bar{x}-1/2, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,0,1/2) | (8) 3 <sup>+</sup> $\bar{x}, \bar{x}+1/2, \bar{x}$<br>(3 <sub><math>\bar{yz}</math></sub> <sup>-1</sup>  0,1/2,1/2) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> (-1/3,1/3,1/3)<br>x+1/6, x+1/6, x<br>(3 <sub><math>\bar{xyz}</math></sub>  0,1/2,1/2)            | (11) 3 <sup>-</sup> (1/3,1/3,-1/3)<br>x+1/3, x+1/6, x<br>(3 <sub><math>\bar{yz}</math></sub>  1/2,1/2,0)                 | (12) 3 <sup>-</sup> (1/3,-1/3,1/3)<br>x-1/6, x+1/3, x<br>(3 <sub><math>\bar{yz}</math></sub>  1/2,0,1/2)            |

(13) $\bar{1}$ ' 0,0,0 ( $\bar{1}$   0,0,0)'	(14) a' (1/2,0,0) x,y,1/4 ( $m_z$   1/2,0,1/2)'	(15) c' (0,0,1/2) x,1/4,z ( $m_y$   0,1/2,1/2)'	(16) b' (0,1/2,0) 1/4,y,z ( $m_x$   1/2,1/2,0)'
(17) $\bar{3}^+$ ' x,x,x; 0,0,0' ( $\bar{3}_{xyz}$   0,0,0)	(18) $\bar{3}^+$ ' $\bar{x}$ -1/2,x+1, $\bar{x}$ ; 0,1/2,1/2 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0)'	(19) $\bar{3}^+$ ' x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ; 1/2,1/2,0 ( $\bar{3}_{xyz}^{-1}$   1/2,0,1/2)'	(20) $\bar{3}^+$ ' $\bar{x}$ +1, $\bar{x}$ +1/2,x; 1/2,0,1/2 ( $\bar{3}_{xyz}^{-1}$   0,1/2,1/2)'
(21) $\bar{3}^-$ ' x,x,x; 0,0,0 ( $\bar{3}_{xyz}^{-1}$   0,0,0)'	(22) $\bar{3}^-$ ' x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ; 0,0,1/2 ( $\bar{3}_{xyz}$   0,1/2,1/2)'	(23) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ +1/2, x; 0,1/2,0 ( $\bar{3}_{xyz}$   1/2,1/2,0)'	(24) $\bar{3}^-$ ' $\bar{x}$ +1/2, x, $\bar{x}$ ; 1/2,0,0 ( $\bar{3}_{xyz}$   1/2,0,1/2)'

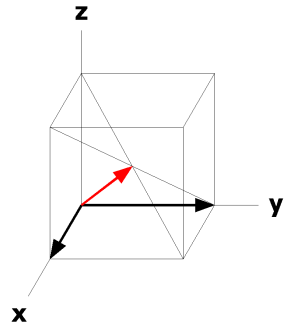
For (1/2,1/2,1/2) + set

(1) 1 (1   1/2,1/2,1/2)	(2) 2 0,1/4,z ( $2_z$   0,1/2,0)	(3) 2 1/4,y,0 ( $2_y$   1/2,0,0)	(4) 2 x,0,1/4 ( $2_x$   0,0,1/2)
(5) $3^+$ (1/2,1/2,1/2) x,x,x ( $3_{xyz}$   1/2,1/2,1/2)	(6) $3^+$ (1/6,-1/6,1/6) $\bar{x}$ -1/6,x+1/3, $\bar{x}$ ( $3_{xyz}^{-1}$   0,0,1/2)	(7) $3^+$ (-1/6,1/6,1/6) x+1/6, $\bar{x}$ +1/6, $\bar{x}$ ( $3_{xyz}^{-1}$   0,1/2,0)	(8) $3^+$ (1/6,1/6,-1/6) $\bar{x}$ +1/3, $\bar{x}$ +1/6,x ( $3_{xyz}^{-1}$   1/2,0,0)
(9) $3^-$ (1/2,1/2,1/2) x,x,x ( $3_{xyz}^{-1}$   1/2,1/2,1/2)	(10) $3^-$ (1/6,-1/6,-1/6) x+1/6, $\bar{x}$ +1/6, $\bar{x}$ ( $3_{xyz}$   1/2,0,0)	(11) $3^-$ (-1/6,-1/6,1/6) $\bar{x}$ +1/3, $\bar{x}$ +1/6, x ( $3_{xyz}$   0,0,1/2)	(12) $3^-$ (-1/6,1/6,-1/6) $\bar{x}$ -1/6, x+1/3, $\bar{x}$ ( $3_{xyz}$   0,1/2,0)
(13) $\bar{1}$ ' 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)'	(14) b' (0,1/2,0) x,y,0 ( $m_z$   0,1/2,0)'	(15) a' (1/2,0,0) x,0,z ( $m_y$   1/2,0,0)'	(16) c' (0,0,1/2) 0,y,z ( $m_x$   0,0,1/2)'
(17) $\bar{3}^+$ ' x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}$   1/2,1/2,1/2)'	(18) $\bar{3}^+$ ' $\bar{x}$ -1/2,x, $\bar{x}$ ; -1/4,-1/4,1/4 ( $\bar{3}_{xyz}^{-1}$   0,0,1/2)'	(19) $\bar{3}^+$ ' x-1/2, $\bar{x}$ +1/2, $\bar{x}$ ; -1/4,1/4,-1/4 ( $\bar{3}_{xyz}^{-1}$   0,1/2,0)'	(20) $\bar{3}^+$ ' $\bar{x}$ , $\bar{x}$ -1/2,x; 1/4,-1/4,-1/4 ( $\bar{3}_{xyz}^{-1}$   1/2,0,0)'
(21) $\bar{3}^-$ ' x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2)'	(22) $\bar{3}^-$ ' x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ; 1/4,-1/4,1/4 ( $\bar{3}_{xyz}$   1/2,0,0)'	(23) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ +1/2, x; -1/4,1/4,1/4 ( $\bar{3}_{xyz}$   0,0,1/2)'	(24) $\bar{3}^-$ ' $\bar{x}$ +1/2, x, $\bar{x}$ ; 1/4,1/4,-1/4 ( $\bar{3}_{xyz}$   0,1/2,0)'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).

## Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2) +		
48 e 1				
(1) x,y,z [u,v,w]	(2) $\bar{x}$ +1/2, $\bar{y}$ ,z+1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(3) $\bar{x}$ ,y+1/2, $\bar{z}$ +1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x+1/2, $\bar{y}$ +1/2, $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	
(5) z,x,y [w,u,v]	(6) z+1/2, $\bar{x}$ +1/2, $\bar{y}$ [w, $\bar{u}$ , $\bar{v}$ ]	(7) $\bar{z}$ +1/2, $\bar{x}$ ,y+1/2 [ $\bar{w}$ , $\bar{u}$ ,v]	(8) $\bar{z}$ ,x+1/2, $\bar{y}$ +1/2 [ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ]	
(9) y,z,x [v,w,u]	(10) $\bar{y}$ ,z+1/2, $\bar{x}$ +1/2 [ $\bar{v}$ ,w, $\bar{u}$ ]	(11) y+1/2, $\bar{z}$ +1/2, $\bar{x}$ [v, $\bar{w}$ , $\bar{u}$ ]	(12) $\bar{y}$ +1/2, $\bar{z}$ ,x+1/2 [ $\bar{v}$ , $\bar{w}$ ,u]	
(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(14) x+1/2,y, $\bar{z}$ +1/2 [u,v, $\bar{w}$ ]	(15) x, $\bar{y}$ +1/2,z+1/2 [u, $\bar{v}$ ,w]	(16) $\bar{x}$ +1/2,y+1/2,z [ $\bar{u}$ ,v,w]	
(17) $\bar{z}$ , $\bar{x}$ , $\bar{y}$ [ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ]	(18) $\bar{z}$ +1/2,x+1/2,y [ $\bar{w}$ ,u,v]	(19) z+1/2,x, $\bar{y}$ +1/2 [w,u, $\bar{v}$ ]	(20) z, $\bar{x}$ +1/2,y+1/2 [w, $\bar{u}$ , $\bar{v}$ ]	
(21) $\bar{y}$ , $\bar{z}$ , $\bar{x}$ [ $\bar{v}$ , $\bar{w}$ , $\bar{u}$ ]	(22) y, $\bar{z}$ +1/2,x+1/2 [v, $\bar{w}$ ,u]	(23) $\bar{y}$ +1/2,z+1/2,x [ $\bar{v}$ ,w,u]	(24) y+1/2,z, $\bar{x}$ +1/2 [v,w, $\bar{u}$ ]	



206.3.1540

$Ia\bar{3}'$

			$x, 0, 1/4 [u, 0, 0]$	$\bar{x}+1/2, 0, 3/4 [\bar{u}, 0, 0]$	$1/4, x, 0 [0, u, 0]$	$3/4, \bar{x}+1/2, 0 [0, \bar{u}, 0]$
			$0, 1/4, x [0, 0, u]$	$0, 3/4, \bar{x}+1/2 [0, 0, \bar{u}]$	$\bar{x}, 0, 3/4 [\bar{u}, 0, 0]$	$x+1/2, 0, 1/4 [u, 0, 0]$
			$3/4, \bar{x}, 0 [0, \bar{u}, 0]$	$1/4, x+1/2, 0 [0, u, 0]$	$0, 3/4, \bar{x} [0, 0, \bar{u}]$	$0, 1/4, x+1/2 [0, 0, u]$
8	c	.3.	$x, x, x [u, u, u]$	$\bar{x}+1/2, \bar{x}, x+1/2 [\bar{u}, \bar{u}, u]$	$\bar{x}, x+1/2, \bar{x}+1/2 [\bar{u}, u, \bar{u}]$	$x+1/2, \bar{x}+1/2, \bar{x} [u, \bar{u}, \bar{u}]$
			$\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$	$x+1/2, x, \bar{x}+1/2 [u, u, \bar{u}]$	$x, \bar{x}+1/2, x+1/2 [u, \bar{u}, u]$	$\bar{x}, +1/2, x+1/2, x [\bar{u}, u, u]$
4	b	. $\bar{3}'$ .	$1/4, 1/4, 1/4 [0, 0, 0]$	$1/4, 3/4, 3/4 [0, 0, 0]$	$3/4, 3/4, 1/4 [0, 0, 0]$	$3/4, 1/4, 3/4 [0, 0, 0]$
4	a	. $\bar{3}'$ .	$0, 0, 0 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p2m'm'$   
 $a^* = a/2$   $b^* = b/2$   
 Origin at  $0, 0, z$

Along  $[1, 1, 1]$   $p6$   
 $a^* = (2a - b - c)/3$   $b^* = (-a + 2b - c)/3$   
 Origin at  $x, x, x$

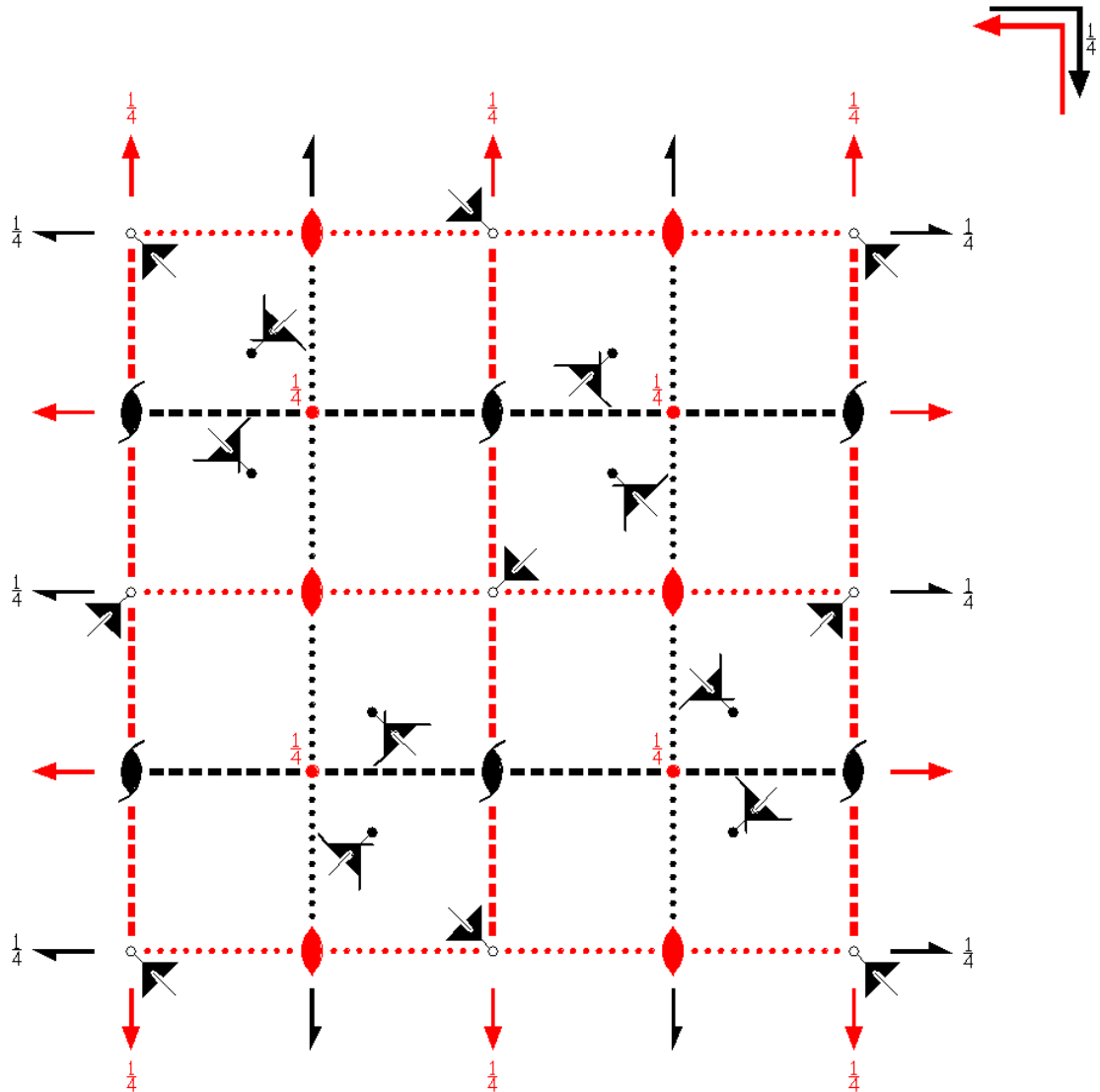
Along  $[1, 1, 0]$   $p2m'g'$   
 $a^* = (-a + b)/2$   $b^* = c/2$   
 Origin at  $x, x, 0$

$I_p a\bar{3}$

$m\bar{3}1'$

Cubic





Origin at center ( $\bar{3}$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; z \leq \min(x,y)$

Vertices  $0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 0,1/2,0 \quad 1/2,1/2,1/2$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}+1/2,x,\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,1/2,0)      | (7) 3 <sup>+</sup> $x+1/2,\bar{x}-1/2,\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2)            | (8) 3 <sup>+</sup> $\bar{x},\bar{x}+1/2,x$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,1/2,1/2)                    |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> (-1/3,1/3,1/3)<br>x+1/6, x+1/6, $\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub>  0,1/2,1/2) | (11) 3 <sup>-</sup> (1/3,1/3,-1/3)<br>x+1/3, x+1/6, x<br>(3 <sub><math>\bar{y}z</math></sub>  1/2,1/2,0) | (12) 3 <sup>-</sup> (1/3,-1/3,1/3)<br>x-1/6, x+1/3, $\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,0,1/2) |

Continued

(13) $\bar{1}$ 0,0,0 ( $\bar{1}$   0,0,0)	(14) a (1/2,0,0) x,y,1/4 ( $m_z$   1/2,0,1/2)	(15) c (0,0,1/2) x,1/4,z ( $m_y$   0,1/2,1/2)	(16) b (0,1/2,0) 1/4,y,z ( $m_x$   1/2,1/2,0)
(17) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$   0,0,0)	(18) $\bar{3}^+$ $\bar{x}$ -1/2,x+1, $\bar{x}$ ; 0,1/2,1/2 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0)	(19) $\bar{3}^+$ x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ; 1/2,1/2,0 ( $\bar{3}_{xyz}^{-1}$   1/2,0,1/2)	(20) $\bar{3}^+$ $\bar{x}$ +1, $\bar{x}$ +1/2,x; 1/2,0,1/2 ( $\bar{3}_{xyz}^{-1}$   0,1/2,1/2)
(21) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}^{-1}$   0,0,0)	(22) $\bar{3}^-$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ; 0,0,1/2 ( $\bar{3}_{xyz}$   0,1/2,1/2)	(23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1/2, x; 0,1/2,0 ( $\bar{3}_{xyz}$   1/2,1/2,0)	(24) $\bar{3}^-$ $\bar{x}$ +1/2, x, $\bar{x}$ ; 1/2,0,0 ( $\bar{3}_{xyz}$   1/2,0,1/2)

For (1/2,1/2,1/2)' + set

(1) 1' (1   1/2,1/2,1/2)'	(2) 2' 0,1/4,z ( $2_z$   0,1/2,0)'	(3) 2' 1/4,y,0 ( $2_y$   1/2,0,0)'	(4) 2' x,0,1/4 ( $2_x$   0,0,1/2)'
(5) $3^{+'}$ (1/2,1/2,1/2) x,x,x ( $3_{xyz}$   1/2,1/2,1/2)'	(6) $3^{+'}$ (1/6,-1/6,1/6) x-1/6,x+1/3, $\bar{x}$ ( $3_{xyz}^{-1}$   0,0,1/2)'	(7) $3^{+'}$ (-1/6,1/6,1/6) x+1/6, $\bar{x}$ +1/6, $\bar{x}$ ( $3_{xyz}^{-1}$   0,1/2,0)'	(8) $3^{+'}$ (1/6,1/6,-1/6) x+1/3, $\bar{x}$ +1/6,x ( $3_{xyz}^{-1}$   1/2,0,0)'
(9) $3^{-'}$ (1/2,1/2,1/2) x,x,x ( $3_{xyz}^{-1}$   1/2,1/2,1/2)'	(10) $3^{-'}$ (1/6,-1/6,-1/6) x+1/6, $\bar{x}$ +1/6, $\bar{x}$ ( $3_{xyz}$   1/2,0,0)'	(11) $3^{-'}$ (-1/6,-1/6,1/6) x+1/3, $\bar{x}$ +1/6, x ( $3_{xyz}$   0,0,1/2)'	(12) $3^{-'}$ (-1/6,1/6,-1/6) x-1/6, x+1/3, $\bar{x}$ ( $3_{xyz}$   0,1/2,0)'
(13) $\bar{1}'$ 1/4,1/4,1/4 ( $\bar{1}$   1/2,1/2,1/2)'	(14) b' (0,1/2,0) x,y,0 ( $m_z$   0,1/2,0)'	(15) a' (1/2,0,0) x,0,z ( $m_y$   1/2,0,0)'	(16) c' (0,0,1/2) 0,y,z ( $m_x$   0,0,1/2)'
(17) $\bar{3}^{+'}$ x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}$   1/2,1/2,1/2)'	(18) $\bar{3}^{+'}$ $\bar{x}$ -1/2,x, $\bar{x}$ ; -1/4,-1/4,1/4 ( $\bar{3}_{xyz}^{-1}$   0,0,1/2)'	(19) $\bar{3}^{+'}$ x-1/2, $\bar{x}$ +1/2, $\bar{x}$ ; -1/4,1/4,-1/4 ( $\bar{3}_{xyz}^{-1}$   0,1/2,0)'	(20) $\bar{3}^{+'}$ $\bar{x}$ , $\bar{x}$ -1/2,x; 1/4,-1/4,-1/4 ( $\bar{3}_{xyz}^{-1}$   1/2,0,0)'
(21) $\bar{3}^{-'}$ x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2)'	(22) $\bar{3}^{-'}$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ; 1/4,-1/4,1/4 ( $\bar{3}_{xyz}$   1/2,0,0)'	(23) $\bar{3}^{-'}$ $\bar{x}$ , $\bar{x}$ +1/2, x; -1/4,1/4,1/4 ( $\bar{3}_{xyz}$   0,0,1/2)'	(24) $\bar{3}^{-'}$ $\bar{x}$ +1/2, x, $\bar{x}$ ; 1/4,1/4,-1/4 ( $\bar{3}_{xyz}$   0,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

48	e	1	(0,0,0) +	(1/2,1/2,1/2)' +
(1) x,y,z [u,v,w]	(2) $\bar{x}$ +1/2, $\bar{y}$ ,z+1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(3) $\bar{x}$ ,y+1/2, $\bar{z}$ +1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x+1/2, $\bar{y}$ +1/2, $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	
(5) z,x,y [w,u,v]	(6) z+1/2, $\bar{x}$ +1/2, $\bar{y}$ [w, $\bar{u}$ , $\bar{v}$ ]	(7) $\bar{z}$ +1/2, $\bar{x}$ ,y+1/2 [ $\bar{w}$ , $\bar{u}$ ,v]	(8) $\bar{z}$ ,x+1/2, $\bar{y}$ +1/2 [ $\bar{w}$ ,u, $\bar{v}$ ]	
(9) y,z,x [v,w,u]	(10) $\bar{y}$ ,z+1/2, $\bar{x}$ +1/2 [ $\bar{v}$ ,w, $\bar{u}$ ]	(11) y+1/2, $\bar{z}$ +1/2, $\bar{x}$ [v, $\bar{w}$ , $\bar{u}$ ]	(12) $\bar{y}$ +1/2, $\bar{z}$ ,x+1/2 [ $\bar{v}$ , $\bar{w}$ ,u]	
(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [u,v,w]	(14) x+1/2,y, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(15) x, $\bar{y}$ +1/2,z+1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	(16) $\bar{x}$ +1/2,y+1/2,z [u, $\bar{v}$ , $\bar{w}$ ]	
(17) $\bar{z}$ , $\bar{x}$ , $\bar{y}$ [w,u,v]	(18) $\bar{z}$ +1/2,x+1/2,y [w, $\bar{u}$ , $\bar{v}$ ]	(19) z+1/2,x, $\bar{y}$ +1/2 [ $\bar{w}$ , $\bar{u}$ ,v]	(20) z, $\bar{x}$ +1/2,y+1/2 [ $\bar{w}$ ,u, $\bar{v}$ ]	
(21) $\bar{y}$ , $\bar{z}$ , $\bar{x}$ [v,w,u]	(22) y, $\bar{z}$ +1/2,x+1/2 [ $\bar{v}$ ,w, $\bar{u}$ ]	(23) $\bar{y}$ +1/2,z+1/2,x [v, $\bar{w}$ , $\bar{u}$ ]	(24) y+1/2,z, $\bar{x}$ +1/2 [ $\bar{v}$ , $\bar{w}$ ,u]	

Continued

206.4.1541

$I_p a\bar{3}$

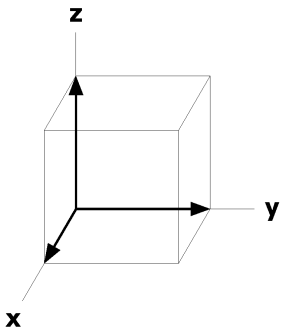
24	d	2..	x,0,1/4 [u,0,0] 0,1/4,x [0,0,u] 3/4, $\bar{x}$ ,0 [0,u,0]	$\bar{x}+1/2,0,3/4 [\bar{u},0,0]$ 0,3/4, $\bar{x}+1/2 [0,0,\bar{u}]$ 1/4,x+1/2,0 [0, $\bar{u}$ ,0]	1/4,x,0 [0,u,0] $\bar{x},0,3/4 [u,0,0]$ 0,3/4, $\bar{x} [0,0,u]$	3/4, $\bar{x}+1/2,0 [0,\bar{u},0]$ x+1/2,0,1/4 [ $\bar{u},0,0]$ 0,1/4,x+1/2 [0,0, $\bar{u}$ ]
8	c	.3.	x,x,x [u,u,u] $\bar{x},\bar{x},\bar{x} [u,u,u]$	$\bar{x}+1/2,\bar{x},x+1/2 [\bar{u},\bar{u},u]$ x+1/2,x, $\bar{x}+1/2 [\bar{u},\bar{u},u]$	$\bar{x},x+1/2,\bar{x}+1/2 [\bar{u},u,\bar{u}]$ x, $\bar{x}+1/2,x+1/2 [\bar{u},u,\bar{u}]$	x+1/2, $\bar{x}+1/2,\bar{x} [u,\bar{u},\bar{u}]$ $\bar{x},+1/2 x+1/2,x [u,\bar{u},\bar{u}]$
4	b	. $\bar{3}$ .	1/4,1/4,1/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]
4	a	. $\bar{3}$ .	0,0,0 [u,u,u]	1/2,0,1/2 [ $\bar{u},\bar{u},u]$	0,1/2,1/2 [ $\bar{u},u,\bar{u}$ ]	1/2,1/2,0 [u, $\bar{u},\bar{u}$ ]

### Symmetry of Special Projections

Along [0,0,1]  $p_{2a}$ -2mm  
 $\mathbf{a}^* = \mathbf{b}/2$   $\mathbf{b}^* = -\mathbf{a}/2$   
 Origin at 0,0,z

Along [1,1,1]  $p_{61}$ '  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

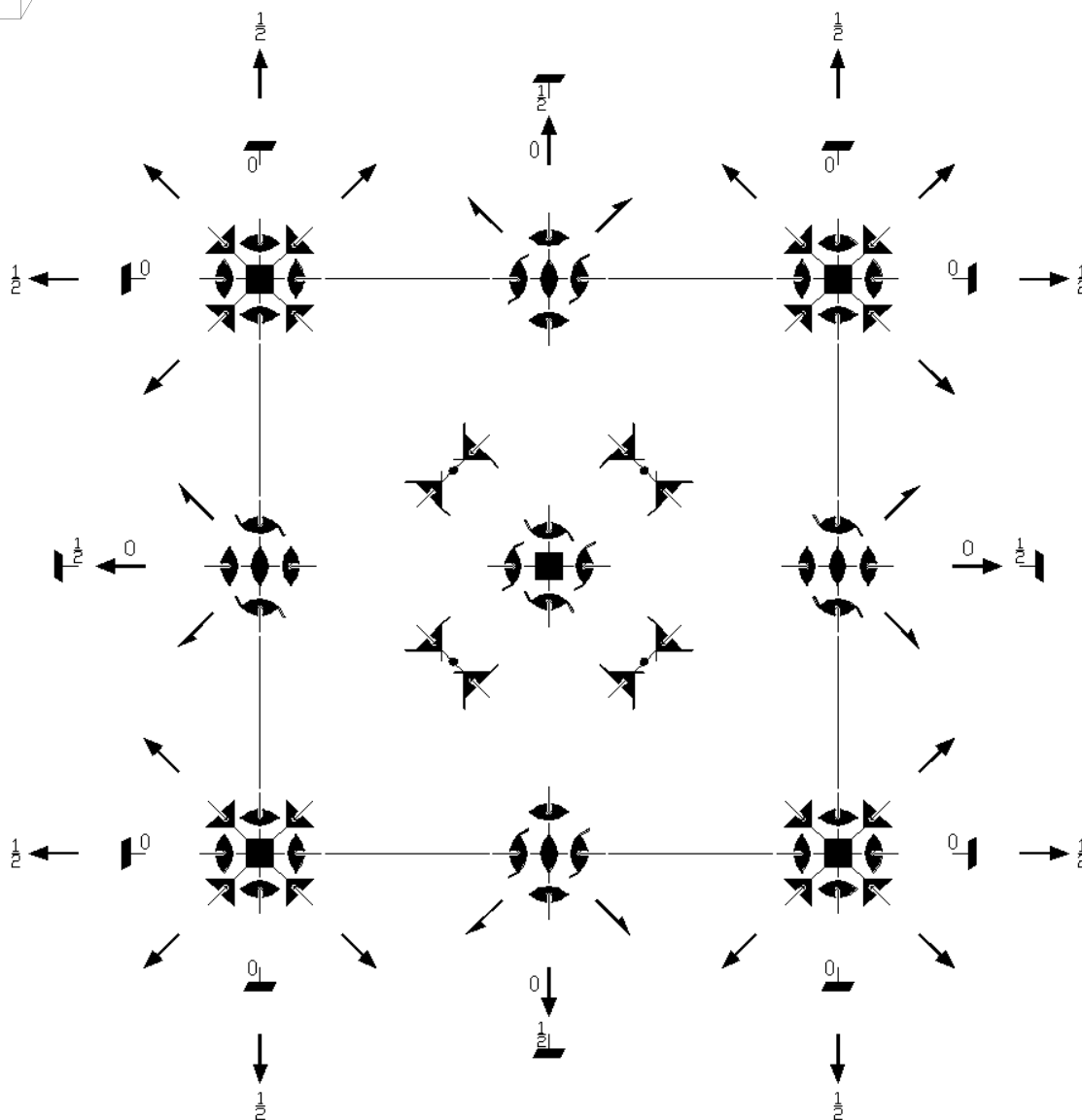
Along [1,1,0]  $p_{2b}$ -2mg  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



P432  
207.1.1542

432  
P432

Cubic



Origin at 432

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq \min(x, 1-x);$   $z \leq y$

Vertices  $0,0,0$   $1,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> $x,\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)       | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> $x,\bar{x},\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)                                | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xy<math>\bar{z}</math></sub>  0,0,0) | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0)              |

(13) $2_{xy}^- x,x,0$ ( $2_{xy}^-   0,0,0$ )	(14) $2_{\bar{xy}} x,\bar{x},0$ ( $2_{\bar{xy}}   0,0,0$ )	(15) $4_z^- 0,0,z$ ( $4_z^-   0,0,0$ )	(16) $4_z^+ 0,0,z$ ( $4_z^+   0,0,0$ )
(17) $4_x^- x,0,0$ ( $4_x^-   0,0,0$ )	(18) $2_{yz} 0,y,y$ ( $2_{yz}   0,0,0$ )	(19) $2_{\bar{yz}} 0,y,\bar{y}$ ( $2_{\bar{yz}}   0,0,0$ )	(20) $4_x^+ x,0,0$ ( $4_x^+   0,0,0$ )
(21) $4_y^+ 0,y,0$ ( $4_y^+   0,0,0$ )	(22) $2_{xz} x,0,x$ ( $2_{xz}   0,0,0$ )	(23) $4_y^- 0,y,0$ ( $4_y^-   0,0,0$ )	(24) $2_{\bar{xz}} \bar{x},0,x$ ( $2_{\bar{xz}}   0,0,0$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

24	k	1									
(1)	$x,y,z$	[u,v,w]	(2)	$\bar{x},\bar{y},z$	[ $\bar{u},\bar{v},w$ ]	(3)	$\bar{x},y,\bar{z}$	[ $\bar{u},v,\bar{w}$ ]	(4)	$x,\bar{y},\bar{z}$	[ $u,\bar{v},\bar{w}$ ]
(5)	$z,x,y$	[w,u,v]	(6)	$z,\bar{x},\bar{y}$	[ $w,\bar{u},\bar{v}$ ]	(7)	$\bar{z},\bar{x},y$	[ $\bar{w},\bar{u},v$ ]	(8)	$\bar{z},x,\bar{y}$	[ $\bar{w},u,\bar{v}$ ]
(9)	$y,z,x$	[v,w,u]	(10)	$\bar{y},z,\bar{x}$	[ $\bar{v},w,\bar{u}$ ]	(11)	$y,\bar{z},\bar{x}$	[ $v,\bar{w},\bar{u}$ ]	(12)	$\bar{y},\bar{z},x$	[ $\bar{v},\bar{w},u$ ]
(13)	$y,x,\bar{z}$	[v,u, $\bar{w}$ ]	(14)	$\bar{y},\bar{x},\bar{z}$	[ $\bar{v},\bar{u},\bar{w}$ ]	(15)	$y,\bar{x},z$	[v, $\bar{u},w$ ]	(16)	$\bar{y},x,z$	[ $\bar{v},u,w$ ]
(17)	$x,z,\bar{y}$	[u,w, $\bar{v}$ ]	(18)	$\bar{x},z,y$	[ $\bar{u},w,v$ ]	(19)	$\bar{x},\bar{z},\bar{y}$	[ $\bar{u},\bar{w},\bar{v}$ ]	(20)	$x,\bar{z},y$	[u, $\bar{w},v$ ]
(21)	$z,y,\bar{x}$	[w,v, $\bar{u}$ ]	(22)	$z,\bar{y},x$	[ $w,\bar{v},u$ ]	(23)	$\bar{z},y,x$	[ $\bar{w},v,u$ ]	(24)	$\bar{z},\bar{y},\bar{x}$	[ $\bar{w},\bar{v},\bar{u}$ ]
12	j	..2	$1/2,y,y$	[0,v,v]	$1/2,\bar{y},y$	[0, $\bar{v},v$ ]	$1/2,y,\bar{y}$	[0,v, $\bar{v}$ ]	$1/2,\bar{y},\bar{y}$	[0, $\bar{v},\bar{v}$ ]	
			$y,1/2,y$	[v,0,v]	$y,1/2,\bar{y}$	[v,0, $\bar{v}$ ]	$\bar{y},1/2,y$	[ $\bar{v},0,v$ ]	$\bar{y},1/2,\bar{y}$	[ $\bar{v},0,\bar{v}$ ]	
			$y,y,1/2$	[v,v,0]	$\bar{y},y,1/2$	[ $\bar{v},v,0$ ]	$y,\bar{y},1/2$	[v, $\bar{v},0$ ]	$\bar{y},\bar{y},1/2$	[ $\bar{v},\bar{v},0$ ]	
12	i	..2	$0,y,y$	[0,v,v]	$0,\bar{y},y$	[0, $\bar{v},v$ ]	$0,y,\bar{y}$	[0,v, $\bar{v}$ ]	$0,\bar{y},\bar{y}$	[0, $\bar{v},\bar{v}$ ]	
			$y,0,y$	[v,0,v]	$y,0,\bar{y}$	[v,0, $\bar{v}$ ]	$\bar{y},0,y$	[ $\bar{v},0,v$ ]	$\bar{y},0,\bar{y}$	[ $\bar{v},0,\bar{v}$ ]	
			$y,y,0$	[v,v,0]	$\bar{y},y,0$	[ $\bar{v},v,0$ ]	$y,\bar{y},0$	[v, $\bar{v},0$ ]	$\bar{y},\bar{y},0$	[ $\bar{v},\bar{v},0$ ]	
12	h	2..	$x,1/2,0$	[u,0,0]	$\bar{x},1/2,0$	[ $\bar{u},0,0$ ]	$0,x,1/2$	[0,u,0]	$0,\bar{x},1/2$	[0, $\bar{u},0$ ]	
			$1/2,0,x$	[0,0,u]	$1/2,0,\bar{x}$	[0,0, $\bar{u}$ ]	$1/2,x,0$	[0,u,0]	$1/2,\bar{x},0$	[0, $\bar{u},0$ ]	
			$x,0,1/2$	[u,0,0]	$\bar{x},0,1/2$	[ $\bar{u},0,0$ ]	$0,1/2,\bar{x}$	[0,0, $\bar{u}$ ]	$0,1/2,x$	[0,0,u]	
8	g	.3.	$x,x,x$	[u,u,u]	$\bar{x},\bar{x},x$	[ $\bar{u},\bar{u},u$ ]	$\bar{x},x,\bar{x}$	[ $\bar{u},u,\bar{u}$ ]	$x,\bar{x},\bar{x}$	[u, $\bar{u},\bar{u}$ ]	
			$x,x,\bar{x}$	[u,u, $\bar{u}$ ]	$\bar{x},\bar{x},\bar{x}$	[ $\bar{u},\bar{u},\bar{u}$ ]	$x,\bar{x},x$	[u, $\bar{u},u$ ]	$\bar{x},x,x$	[ $\bar{u},u,u$ ]	
6	f	4..	$x,1/2,1/2$	[u,0,0]	$\bar{x},1/2,1/2$	[ $\bar{u},0,0$ ]	$1/2,x,1/2$	[0,u,0]	$1/2,1/2,\bar{x}$	[0,0, $\bar{u}$ ]	
			$1/2,\bar{x},1/2$	[0, $\bar{u},0$ ]	$1/2,1/2,x$	[0,0,u]					

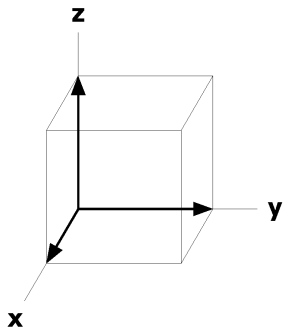
6	e	4..	$x,0,0 [u,0,0]$ $0,\bar{x},0 [0,\bar{u},0]$	$\bar{x},0,0 [\bar{u},0,0]$ $0,0,x [0,0,u]$	$0,x,0 [0,u,0]$ $0,0,\bar{x} [0,0,\bar{u}]$
3	d	42.2	$1/2,0,0 [0,0,0]$	$0,1/2,0 [0,0,0]$	$0,0,1/2 [0,0,0]$
3	c	42.2	$0,1/2,1/2 [0,0,0]$	$1/2,0,1/2 [0,0,0]$	$1/2,1/2,0 [0,0,0]$
1	b	432	$1/2,1/2,1/2 [0,0,0]$		
1	a	432	$0,0,0 [0,0,0]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p3m'1$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x,x,x$

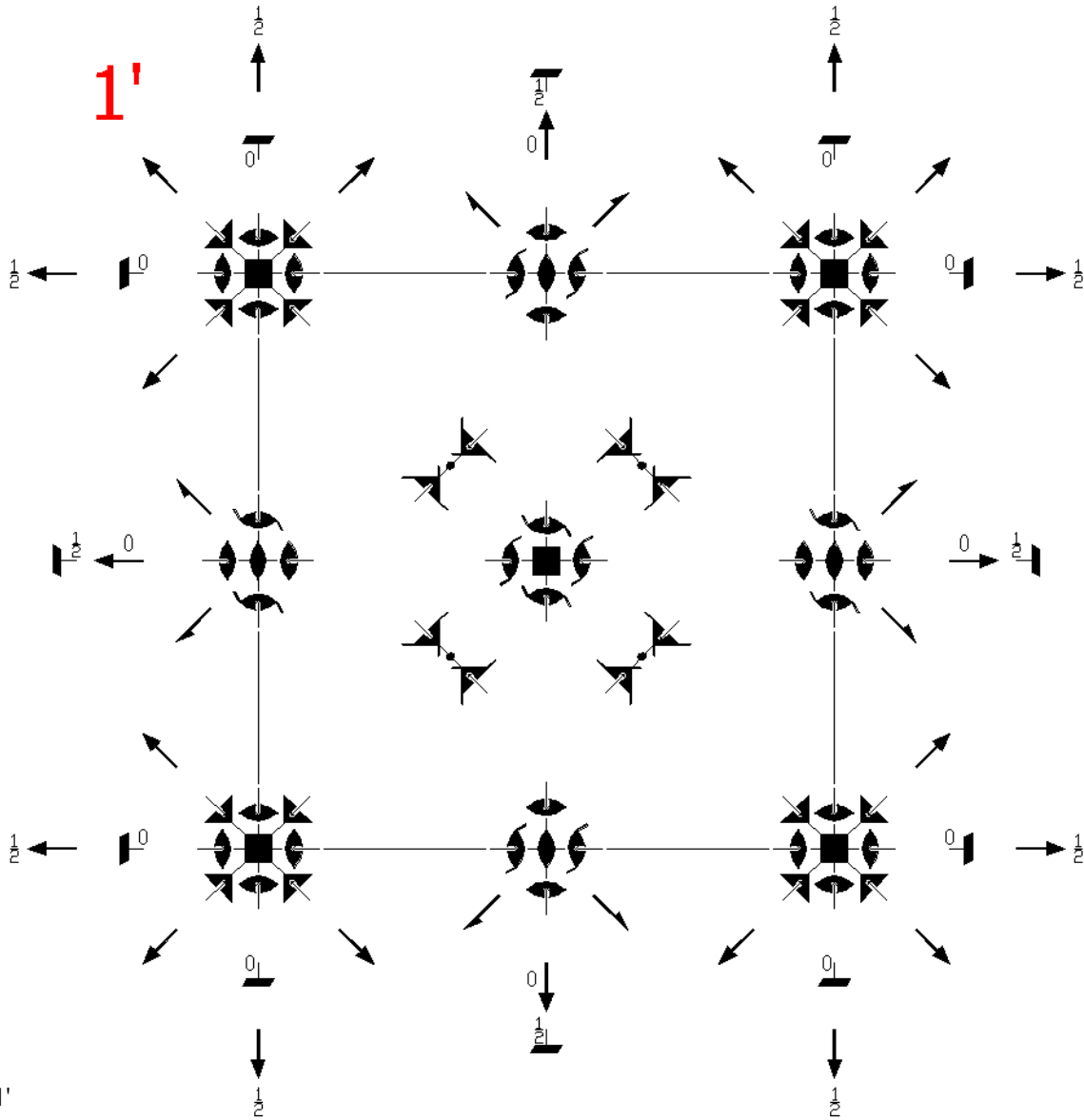
Along  $[1,1,0]$   $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$



P4321'  
207.2.1543

4321'  
P4321'

Cubic



Origin at 4321'

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq \min(x, 1-x);$   $z \leq y$

Vertices  $0,0,0$   $1,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

For 1 + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)     | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)                               | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0) | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0)              |

(13) $2^- x,x,0$ ( $2_{xy} 0,0,0$ )	(14) $2^- x,\bar{x},0$ ( $2_{\bar{xy}} 0,0,0$ )	(15) $4^- 0,0,z$ ( $4_z^{-1} 0,0,0$ )	(16) $4^+ 0,0,z$ ( $4_z 0,0,0$ )
(17) $4^- x,0,0$ ( $4_x^{-1} 0,0,0$ )	(18) $2^- 0,y,y$ ( $2_{yz} 0,0,0$ )	(19) $2^- 0,y,\bar{y}$ ( $2_{\bar{yz}} 0,0,0$ )	(20) $4^+ x,0,0$ ( $4_x 0,0,0$ )
(21) $4^+ 0,y,0$ ( $4_y 0,0,0$ )	(22) $2^- x,0,x$ ( $2_{xz} 0,0,0$ )	(23) $4^- 0,y,0$ ( $4_y^{-1} 0,0,0$ )	(24) $2^- \bar{x},0,x$ ( $2_{\bar{xz}} 0,0,0$ )

For 1' + set

(1) $1'$ ( $1 0,0,0$ )'	(2) $2'$ $0,0,z$ ( $2_z 0,0,0$ )'	(3) $2'$ $0,y,0$ ( $2_y 0,0,0$ )'	(4) $2'$ $x,0,0$ ( $2_x 0,0,0$ )'
(5) $3^+ x,x,x$ ( $3_{xyz} 0,0,0$ )'	(6) $3^+ \bar{x},x,\bar{x}$ ( $3_{\bar{xyz}}^{-1} 0,0,0$ )'	(7) $3^+ x,\bar{x},\bar{x}$ ( $3_{\bar{xyz}}^{-1} 0,0,0$ )'	(8) $3^+ \bar{x},\bar{x},x$ ( $3_{\bar{yz}}^{-1} 0,0,0$ )'
(9) $3^- x,x,x$ ( $3_{xyz}^{-1} 0,0,0$ )'	(10) $3^- x,\bar{x},\bar{x}$ ( $3_{\bar{xyz}} 0,0,0$ )'	(11) $3^- \bar{x},\bar{x},x$ ( $3_{\bar{yz}} 0,0,0$ )'	(12) $3^- \bar{x},x,\bar{x}$ ( $3_{xyz} 0,0,0$ )'
(13) $2'$ $x,x,0$ ( $2_{xy} 0,0,0$ )'	(14) $2'$ $x,\bar{x},0$ ( $2_{\bar{xy}} 0,0,0$ )'	(15) $4^- 0,0,z$ ( $4_z^{-1} 0,0,0$ )'	(16) $4^+ 0,0,z$ ( $4_z 0,0,0$ )'
(17) $4^- x,0,0$ ( $4_x^{-1} 0,0,0$ )'	(18) $2'$ $0,y,y$ ( $2_{yz} 0,0,0$ )'	(19) $2'$ $0,y,\bar{y}$ ( $2_{\bar{yz}} 0,0,0$ )'	(20) $4^+ x,0,0$ ( $4_x 0,0,0$ )'
(21) $4^+ 0,y,0$ ( $4_y 0,0,0$ )'	(22) $2'$ $x,0,x$ ( $2_{xz} 0,0,0$ )'	(23) $4^- 0,y,0$ ( $4_y^{-1} 0,0,0$ )'	(24) $2'$ $\bar{x},0,x$ ( $2_{\bar{xz}} 0,0,0$ )'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); 1'.

## Positions

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates			
			1 +		1' +	
24	k	11'	(1) $x,y,z$ [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{x},y,\bar{z}$ [0,0,0]	(4) $x,\bar{y},\bar{z}$ [0,0,0]
			(5) $z,x,y$ [0,0,0]	(6) $z,\bar{x},\bar{y}$ [0,0,0]	(7) $\bar{z},\bar{x},y$ [0,0,0]	(8) $\bar{z},x,\bar{y}$ [0,0,0]
			(9) $y,z,x$ [0,0,0]	(10) $\bar{y},z,\bar{x}$ [0,0,0]	(11) $y,\bar{z},\bar{x}$ [0,0,0]	(12) $\bar{y},\bar{z},x$ [0,0,0]
			(13) $y,x,\bar{z}$ [0,0,0]	(14) $\bar{y},\bar{x},\bar{z}$ [0,0,0]	(15) $y,\bar{x},z$ [0,0,0]	(16) $\bar{y},x,z$ [0,0,0]
			(17) $x,z,\bar{y}$ [0,0,0]	(18) $\bar{x},z,y$ [0,0,0]	(19) $\bar{x},\bar{z},\bar{y}$ [0,0,0]	(20) $x,\bar{z},y$ [0,0,0]
			(21) $z,y,\bar{x}$ [0,0,0]	(22) $z,\bar{y},x$ [0,0,0]	(23) $\bar{z},y,x$ [0,0,0]	(24) $\bar{z},\bar{y},\bar{x}$ [0,0,0]
12	j	..21'	$1/2,y,y$ [0,0,0]	$1/2,\bar{y},y$ [0,0,0]	$1/2,y,\bar{y}$ [0,0,0]	$1/2,\bar{y},\bar{y}$ [0,0,0]
			$y,1/2,y$ [0,0,0]	$y,1/2,\bar{y}$ [0,0,0]	$\bar{y},1/2,y$ [0,0,0]	$\bar{y},1/2,\bar{y}$ [0,0,0]
			$y,y,1/2$ [0,0,0]	$\bar{y},y,1/2$ [0,0,0]	$y,\bar{y},1/2$ [0,0,0]	$\bar{y},\bar{y},1/2$ [0,0,0]



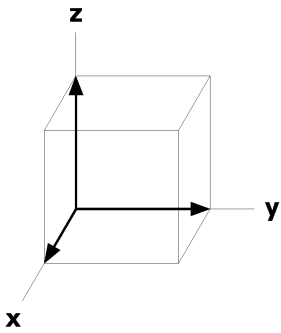
12	i	..21'	0,y,y [0,0,0]	$0,\bar{y},y$ [0,0,0]	$0,y,\bar{y}$ [0,0,0]	$0,\bar{y},\bar{y}$ [0,0,0]
			y,0,y [0,0,0]	$y,0,\bar{y}$ [0,0,0]	$\bar{y},0,y$ [0,0,0]	$\bar{y},0,\bar{y}$ [0,0,0]
			y,y,0 [0,0,0]	$\bar{y},y,0$ [0,0,0]	$y,\bar{y},0$ [0,0,0]	$\bar{y},\bar{y},0$ [0,0,0]
12	h	2..1'	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]	$0,x,1/2$ [0,0,0]	$0,\bar{x},1/2$ [0,0,0]
			1/2,0,x [0,0,0]	$1/2,0,\bar{x}$ [0,0,0]	$1/2,x,0$ [0,0,0]	$1/2,\bar{x},0$ [0,0,0]
			x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]	$0,1/2,\bar{x}$ [0,0,0]	$0,1/2,x$ [0,0,0]
8	g	.3.1'	x,x,x [0,0,0]	$\bar{x},\bar{x},x$ [0,0,0]	$\bar{x},x,\bar{x}$ [0,0,0]	$x,\bar{x},\bar{x}$ [0,0,0]
			x,x, $\bar{x}$ [0,0,0]	$\bar{x},\bar{x},\bar{x}$ [0,0,0]	$x,\bar{x},x$ [0,0,0]	$\bar{x},x,x$ [0,0,0]
6	f	4..1'	x,1/2,1/2 [0,0,0]	$\bar{x},1/2,1/2$ [0,0,0]	$1/2,x,1/2$ [0,0,0]	
			$1/2,\bar{x},1/2$ [0,0,0]	$1/2,1/2,x$ [0,0,0]	$1/2,1/2,\bar{x}$ [0,0,0]	
6	e	4..1'	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	$0,x,0$ [0,0,0]	
			$0,\bar{x},0$ [0,0,0]	$0,0,x$ [0,0,0]	$0,0,\bar{x}$ [0,0,0]	
3	d	42.21'	1/2,0,0 [0,0,0]	$0,1/2,0$ [0,0,0]	$0,0,1/2$ [0,0,0]	
3	c	42.21'	0,1/2,1/2 [0,0,0]	$1/2,0,1/2$ [0,0,0]	$1/2,1/2,0$ [0,0,0]	
1	b	4321'	$1/2,1/2,1/2$ [0,0,0]			
1	a	4321'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,1,1] p3m11'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

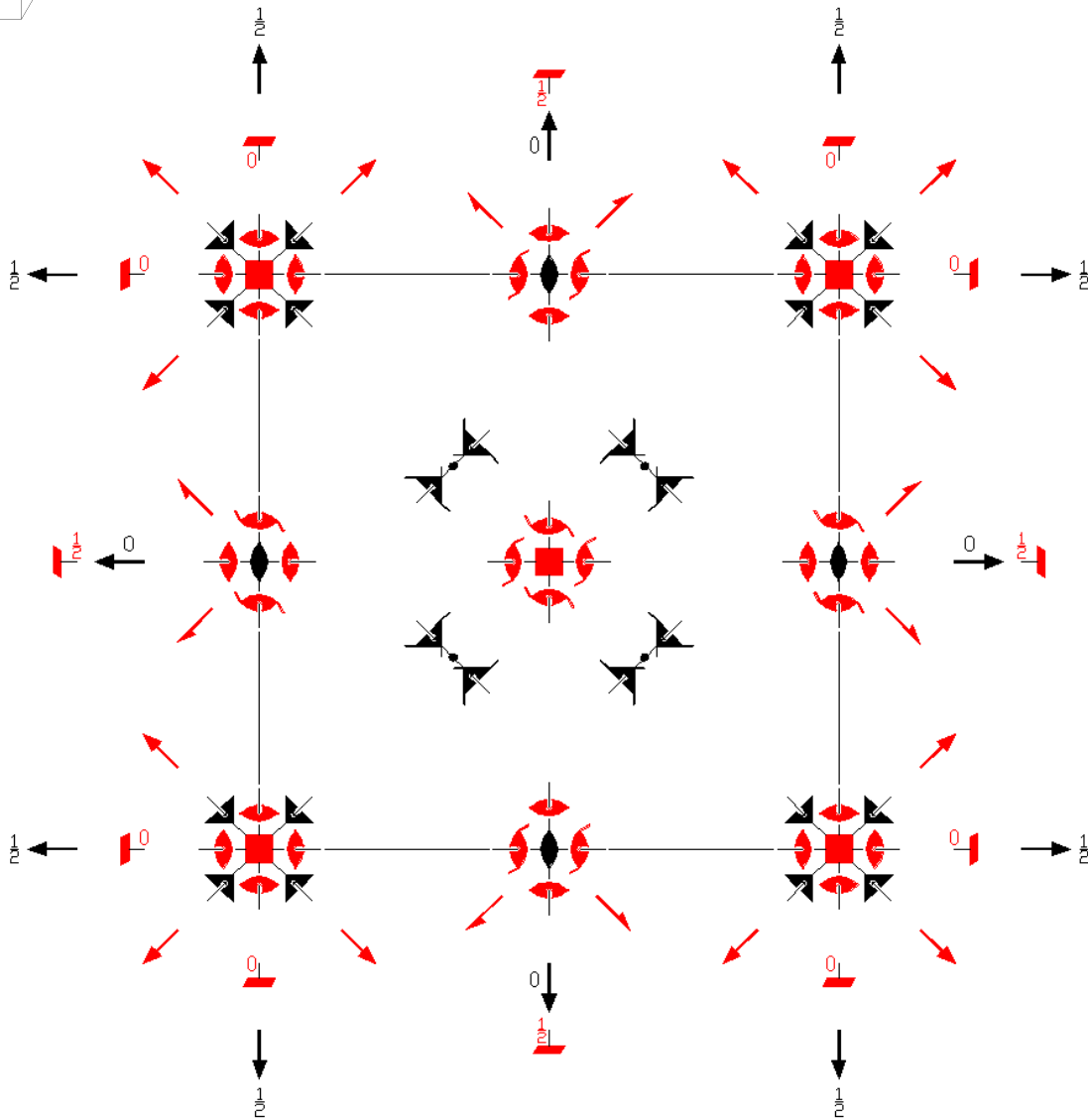
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



P4'32'  
207.3.1544

4'32'  
P4'32'

Cubic



Origin at 4'32'

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq \min(x, 1-x);$   $z \leq y$

Vertices  $0,0,0$   $1,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)     | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)                               | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0) | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0)              |

(13) $2' \begin{matrix} x,x,0 \\ (2_{xy} 0,0,0)' \end{matrix}$	(14) $2' \begin{matrix} x,\bar{x},0 \\ (2_{\bar{xy}} 0,0,0)' \end{matrix}$	(15) $4^{-1} \begin{matrix} 0,0,z \\ (4_z^{-1} 0,0,0)' \end{matrix}$	(16) $4^{+1} \begin{matrix} 0,0,z \\ (4_z 0,0,0)' \end{matrix}$
(17) $4^{-1} \begin{matrix} x,0,0 \\ (4_x^{-1} 0,0,0)' \end{matrix}$	(18) $2' \begin{matrix} 0,y,y \\ (2_{yz} 0,0,0)' \end{matrix}$	(19) $2' \begin{matrix} 0,y,\bar{y} \\ (2_{\bar{yz}} 0,0,0)' \end{matrix}$	(20) $4^{+1} \begin{matrix} x,0,0 \\ (4_x 0,0,0)' \end{matrix}$
(21) $4^{+1} \begin{matrix} 0,y,0 \\ (4_y 0,0,0)' \end{matrix}$	(22) $2' \begin{matrix} x,0,x \\ (2_{xz} 0,0,0)' \end{matrix}$	(23) $4^{-1} \begin{matrix} 0,y,0 \\ (4_y^{-1} 0,0,0)' \end{matrix}$	(24) $2' \begin{matrix} \bar{x},0,x \\ (2_{\bar{xz}} 0,0,0)' \end{matrix}$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

24	k	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{x},y,\bar{z}$	$[\bar{u},v,\bar{w}]$	(4)	x, $\bar{y},\bar{z}$	$[u,\bar{v},\bar{w}]$
(5)	z,x,y	[w,u,v]	(6)	$z,\bar{x},\bar{y}$	$[w,\bar{u},\bar{v}]$	(7)	$\bar{z},\bar{x},y$	$[\bar{w},\bar{u},v]$	(8)	$\bar{z},x,\bar{y}$	$[\bar{w},u,\bar{v}]$
(9)	y,z,x	[v,w,u]	(10)	$\bar{y},z,\bar{x}$	$[\bar{v},w,\bar{u}]$	(11)	$y,\bar{z},\bar{x}$	$[v,\bar{w},\bar{u}]$	(12)	$\bar{y},z,x$	$[\bar{v},w,u]$
(13)	y,x, $\bar{z}$	$[\bar{v},\bar{u},w]$	(14)	$\bar{y},\bar{x},\bar{z}$	$[v,u,w]$	(15)	$y,\bar{x},z$	$[\bar{v},u,\bar{w}]$	(16)	$\bar{y},x,z$	$[v,\bar{u},\bar{w}]$
(17)	x,z, $\bar{y}$	$[\bar{u},\bar{w},v]$	(18)	$\bar{x},z,y$	$[u,\bar{w},\bar{v}]$	(19)	$\bar{x},\bar{z},\bar{y}$	$[u,w,v]$	(20)	x, $\bar{z},y$	$[\bar{u},w,\bar{v}]$
(21)	z,y, $\bar{x}$	$[\bar{w},\bar{v},u]$	(22)	$z,\bar{y},x$	$[\bar{w},v,\bar{u}]$	(23)	$\bar{z},y,x$	$[w,\bar{v},\bar{u}]$	(24)	$\bar{z},\bar{y},\bar{x}$	$[w,v,u]$
12	j	..2'	1/2,y,y	$[u,v,\bar{v}]$	1/2, $\bar{y},y$	$[\bar{u},\bar{v},\bar{v}]$	1/2,y, $\bar{y}$	$[\bar{u},v,v]$	1/2, $\bar{y},\bar{y}$	$[u,\bar{v},v]$	
			y,1/2,y	$[\bar{v},u,v]$	y,1/2, $\bar{y}$	$[\bar{v},\bar{u},\bar{v}]$	$\bar{y},1/2,y$	$[v,\bar{u},v]$	$\bar{y},1/2,\bar{y}$	$[v,u,\bar{v}]$	
			y,y,1/2	$[v,\bar{v},u]$	$\bar{y},y,1/2$	$[\bar{v},\bar{v},\bar{u}]$	$y,\bar{y},1/2$	$[v,v,\bar{u}]$	$\bar{y},\bar{y},1/2$	$[\bar{v},v,u]$	
12	i	..2'	0,y,y	$[u,v,\bar{v}]$	0, $\bar{y},y$	$[\bar{u},\bar{v},\bar{v}]$	0,y, $\bar{y}$	$[\bar{u},v,v]$	0, $\bar{y},\bar{y}$	$[u,\bar{v},v]$	
			y,0,y	$[\bar{v},u,v]$	y,0, $\bar{y}$	$[\bar{v},\bar{u},\bar{v}]$	$\bar{y},0,y$	$[v,\bar{u},v]$	$\bar{y},0,\bar{y}$	$[v,u,\bar{v}]$	
			y,y,0	$[v,\bar{v},u]$	$\bar{y},y,0$	$[\bar{v},\bar{v},\bar{u}]$	$y,\bar{y},0$	$[v,v,\bar{u}]$	$\bar{y},\bar{y},0$	$[\bar{v},v,u]$	
12	h	2..	x,1/2,0	$[u,0,0]$	$\bar{x},1/2,0$	$[\bar{u},0,0]$	0,x,1/2	$[0,u,0]$	0, $\bar{x},1/2$	$[0,\bar{u},0]$	
			1/2,0,x	$[0,0,u]$	1/2,0, $\bar{x}$	$[0,0,\bar{u}]$	1/2,x,0	$[0,\bar{u},0]$	1/2, $\bar{x},0$	$[0,u,0]$	
			x,0,1/2	$[\bar{u},0,0]$	$\bar{x},0,1/2$	$[u,0,0]$	0,1/2, $\bar{x}$	$[0,0,u]$	0,1/2,x	$[0,0,\bar{u}]$	
8	g	.3.	x,x,x	$[u,u,u]$	$\bar{x},\bar{x},x$	$[\bar{u},\bar{u},u]$	$\bar{x},x,\bar{x}$	$[\bar{u},u,\bar{u}]$	x, $\bar{x},\bar{x}$	$[u,\bar{u},\bar{u}]$	
			x,x, $\bar{x}$	$[\bar{u},\bar{u},u]$	$\bar{x},\bar{x},\bar{x}$	$[u,u,u]$	x, $\bar{x},x$	$[\bar{u},u,\bar{u}]$	$\bar{x},x,x$	$[u,\bar{u},\bar{u}]$	
6	f	4'..	x,1/2,1/2	$[0,0,0]$	$\bar{x},1/2,1/2$	$[0,0,0]$	1/2,x,1/2	$[0,0,0]$	1/2,1/2, $\bar{x}$	$[0,0,0]$	
			1/2, $\bar{x},1/2$	$[0,0,0]$	1/2,1/2,x	$[0,0,0]$					

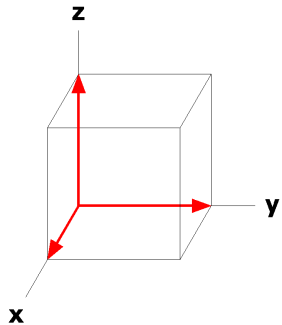
6	e	4'..	$x,0,0 [0,0,0]$ $0,\bar{x},0 [0,0,0]$	$\bar{x},0,0 [0,0,0]$ $0,0,x [0,0,0]$	$0,x,0 [0,0,0]$ $0,0,\bar{x} [0,0,0]$
3	d	4'2.2'	$1/2,0,0 [0,0,0]$	$0,1/2,0 [0,0,0]$	$0,0,1/2 [0,0,0]$
3	c	4'2.2'	$0,1/2,1/2 [0,0,0]$	$1/2,0,1/2 [0,0,0]$	$1/2,1/2,0 [0,0,0]$
1	b	4'32'	$1/2,1/2,1/2 [0,0,0]$		
1	a	4'32'	$0,0,0 [0,0,0]$		

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4'm'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p3m1$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x,x,x$

Along  $[1,1,0]$   $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$



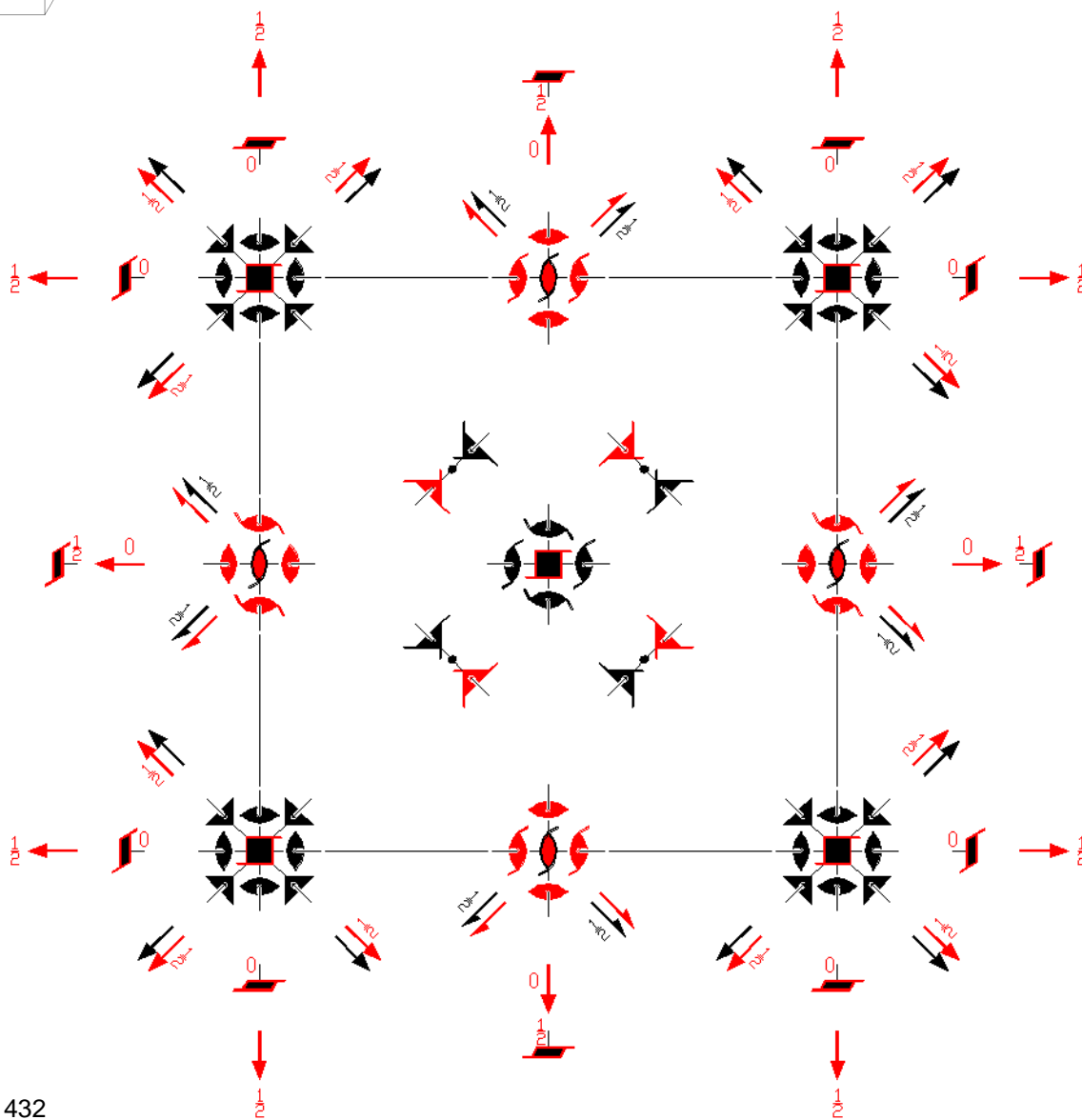
P<sub>F</sub> 432

207.4.1545

4321'

P<sub>F</sub> 432

Cubic



Origin at 432

Asymmetric unit  $0 \leq x \leq 1;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq \min(x, 1-x);$   $z \leq y$

Vertices  $0,0,0$   $1,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)              | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub>xyz<sup>-1</sup></sub>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz<sup>-1</sup></sub>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz<sup>-1</sup></sub>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz<sup>-1</sup></sub>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)            | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)              | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)             |

- |  |  |  |  |
|--|--|--|--|
| (13) $2^- \ x, x, 0$<br>( $2_{xy}   0, 0, 0$ )   | (14) $2^- \ x, \bar{x}, 0$<br>( $2_{\bar{xy}}   0, 0, 0$ ) | (15) $4^- \ 0, 0, z$<br>( $4_z^{-1}   0, 0, 0$ )           | (16) $4^+ \ 0, 0, z$<br>( $4_z   0, 0, 0$ )                |
| (17) $4^- \ x, 0, 0$<br>( $4_x^{-1}   0, 0, 0$ ) | (18) $2^- \ 0, y, y$<br>( $2_{yz}   0, 0, 0$ )             | (19) $2^- \ 0, y, \bar{y}$<br>( $2_{\bar{yz}}   0, 0, 0$ ) | (20) $4^+ \ x, 0, 0$<br>( $4_x   0, 0, 0$ )                |
| (21) $4^+ \ 0, y, 0$<br>( $4_y   0, 0, 0$ )      | (22) $2^- \ x, 0, x$<br>( $2_{xz}   0, 0, 0$ )             | (23) $4^- \ 0, y, 0$<br>( $4_y^{-1}   0, 0, 0$ )           | (24) $2^- \ \bar{x}, 0, x$<br>( $2_{\bar{xz}}   0, 0, 0$ ) |

For (1,0,0)<sup>l</sup> + set

- |  |  |  |   |
|--|--|--|---|
| (1) $t' \ (1, 0, 0)$<br>( $1   1, 0, 0$ )'   | (2) $2' \ 1/2, 0, z$<br>( $2_z   1, 0, 0$ )'   | (3) $2' \ 1/2, y, 0$<br>( $2_y   1, 0, 0$ )'   | (4) $2' \ (1, 0, 0) \ x, 0, 0$<br>( $2_x   1, 0, 0$ )'  |
| (5) $3^{+'} \ (1/3, 1/3, 1/3)$<br>$x+2/3, x+1/3, x$<br>( $3_{xyz}   1, 0, 0$ )'      | (6) $3^{+'} \ (1/3, -1/3, 1/3)$<br>$x+2/3, x-1/3, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   1, 0, 0$ )'    | (7) $3^{+'} \ (1/3, -1/3, -1/3)$<br>$x+2/3, \bar{x}-1/3, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   1, 0, 0$ )' | (8) $3^{+'} \ (1/3, 1/3, -1/3)$<br>$\bar{x}+2/3, \bar{x}-1/3, x$<br>( $3_{\bar{xyz}}^{-1}   1, 0, 0$ )' |
| (9) $3^{-'} \ (1/3, 1/3, 1/3)$<br>$x+1/3, x-1/3, x$<br>( $3_{xyz}^{-1}   1, 0, 0$ )' | (10) $3^{-'} \ (1/3, -1/3, -1/3)$<br>$x+1/3, \bar{x}+1/3, \bar{x}$<br>( $3_{\bar{xyz}}   1, 0, 0$ )' | (11) $3^{-'} \ (1/3, 1/3, -1/3)$<br>$\bar{x}+1/3, \bar{x}-1/3, x$<br>( $3_{\bar{xyz}}   1, 0, 0$ )'      | (12) $3^{-'} \ (1/3, -1/3, 1/3)$<br>$x+1/3, x+1/3, \bar{x}$<br>( $3_{\bar{xyz}}   1, 0, 0$ )'           |
| (13) $2' \ (1/2, 1/2, 0) \ x+1, x+1/2, 0$<br>( $2_{xy}   1, 0, 0$ )'                 | (14) $2' \ (-1/2, 1/2, 0) \ x+1, \bar{x}-1/2, 0$<br>( $2_{\bar{xy}}   1, 0, 0$ )'                    | (15) $4^{-'} \ 1/2, -1/2, z$<br>( $4_z^{-1}   1, 0, 0$ )'  | (16) $4^{+'} \ 1/2, 1/2, z$<br>( $4_z   1, 0, 0$ )'   |
| (17) $4^{-'} \ (1, 0, 0) \ x, 0, 0$<br>( $4_x^{-1}   1, 0, 0$ )'                     | (18) $2' \ 1/2, y, y$<br>( $2_{yz}   1, 0, 0$ )'   | (19) $2' \ 1/2, y, \bar{y}$<br>( $2_{\bar{yz}}   1, 0, 0$ )'   | (20) $4^{+'} \ (1, 0, 0) \ x, 0, 0$<br>( $4_x   1, 0, 0$ )'   |
| (21) $4^{+'} \ 1/2, y, -1/2$<br>( $4_y   1, 0, 0$ )'                                 | (22) $2' \ (1/2, 0, 1/2) \ x+1/2, 0, x$<br>( $2_{xz}   1, 0, 0$ )'                                   | (23) $4^{-'} \ 1/2, y, 1/2$<br>( $4_y^{-1}   1, 0, 0$ )'   | (24) $2' \ \bar{x}+1/2, 0, x$<br>( $2_{\bar{xz}}   1, 0, 0$ )'  |

Generators selected (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5); (13).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

			(0,0,0) +	(1,0,0) <sup>l</sup> +							
48	k	1									
(1)	x, y, z	[u, v, w]	(2)	$\bar{x}, \bar{y}, z$	[ $\bar{u}, \bar{v}, w$ ]	(3)	$\bar{x}, y, \bar{z}$	[ $\bar{u}, v, \bar{w}$ ]	(4)	$x, \bar{y}, \bar{z}$	[ $u, \bar{v}, \bar{w}$ ]
(5)	z, x, y	[w, u, v]	(6)	$z, \bar{x}, \bar{y}$	[ $w, \bar{u}, \bar{v}$ ]	(7)	$\bar{z}, \bar{x}, y$	[ $\bar{w}, \bar{u}, v$ ]	(8)	$\bar{z}, x, \bar{y}$	[ $\bar{w}, u, \bar{v}$ ]
(9)	y, z, x	[v, w, u]	(10)	$\bar{y}, z, \bar{x}$	[ $\bar{v}, w, \bar{u}$ ]	(11)	$y, \bar{z}, \bar{x}$	[ $v, \bar{w}, \bar{u}$ ]	(12)	$\bar{y}, \bar{z}, x$	[ $\bar{v}, \bar{w}, u$ ]
(13)	y, x, $\bar{z}$	[v, u, $\bar{w}$ ]	(14)	$\bar{y}, \bar{x}, \bar{z}$	[ $\bar{v}, \bar{u}, \bar{w}$ ]	(15)	$y, \bar{x}, z$	[ $v, \bar{u}, w$ ]	(16)	$\bar{y}, x, z$	[ $\bar{v}, u, w$ ]
(17)	x, z, $\bar{y}$	[u, w, $\bar{v}$ ]	(18)	$\bar{x}, z, y$	[ $\bar{u}, w, v$ ]	(19)	$\bar{x}, \bar{z}, \bar{y}$	[ $\bar{u}, \bar{w}, \bar{v}$ ]	(20)	$x, \bar{z}, y$	[ $u, \bar{w}, v$ ]
(21)	z, y, $\bar{x}$	[w, v, $\bar{u}$ ]	(22)	$z, \bar{y}, x$	[ $w, \bar{v}, u$ ]	(23)	$\bar{z}, y, x$	[ $\bar{w}, v, u$ ]	(24)	$\bar{z}, \bar{y}, \bar{x}$	[ $\bar{w}, \bar{v}, \bar{u}$ ]

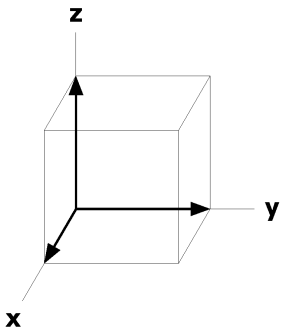
24	j	..2'	1/2,y,y [u,v, $\bar{v}$ ] y,1/2,y [ $\bar{v}$ ,u,v] y,y,1/2 [v, $\bar{v}$ ,u]	1/2, $\bar{y}$ ,y [u,v,v] y,1/2, $\bar{y}$ [v,u,v] $\bar{y}$ ,y,1/2 [v,v,u]	1/2,y, $\bar{y}$ [u, $\bar{v}$ , $\bar{v}$ ] $\bar{y}$ ,1/2,y [ $\bar{v}$ ,u, $\bar{v}$ ] y, $\bar{y}$ ,1/2 [ $\bar{v}$ , $\bar{v}$ ,u]	1/2, $\bar{y}$ , $\bar{y}$ [u, $\bar{v}$ ,v] $\bar{y}$ ,1/2, $\bar{y}$ [v,u, $\bar{v}$ ] $\bar{y}$ , $\bar{y}$ ,1/2 [ $\bar{v}$ ,v,u]
24	i	..2	0,y,y [0,v,v] y,0,y [v,0,v] y,y,0 [v,v,0]	0, $\bar{y}$ ,y [0, $\bar{v}$ ,v] y,0, $\bar{y}$ [v,0, $\bar{v}$ ] $\bar{y}$ ,y,0 [ $\bar{v}$ ,v,0]	0,y, $\bar{y}$ [0,v, $\bar{v}$ ] $\bar{y}$ ,0,y [v,0,v] y, $\bar{y}$ ,0 [v, $\bar{v}$ ,0]	0, $\bar{y}$ , $\bar{y}$ [0, $\bar{v}$ , $\bar{v}$ ] $\bar{y}$ ,0, $\bar{y}$ [v,0, $\bar{v}$ ] $\bar{y}$ , $\bar{y}$ ,0 [ $\bar{v}$ , $\bar{v}$ ,0]
24	h	2'..	x,1/2,0 [0,v,w] 1/2,0,x [v,w,0] x,0,1/2 [0, $\bar{w}$ ,v]	$\bar{x}$ ,1/2,0 [0,v, $\bar{w}$ ] 1/2,0, $\bar{x}$ [v, $\bar{w}$ ,0] $\bar{x}$ ,0,1/2 [0,w,v]	0,x,1/2 [w,0,v] 1/2,x,0 [v,0, $\bar{w}$ ] 0,1/2, $\bar{x}$ [w,v,0]	0, $\bar{x}$ ,1/2 [ $\bar{w}$ ,0,v] 1/2, $\bar{x}$ ,0 [v,0,w] 0,1/2,x [ $\bar{w}$ ,v,0]
16	g	.3.	x,x,x [u,u,u] x,x, $\bar{x}$ [u,u, $\bar{u}$ ]	$\bar{x}$ , $\bar{x}$ ,x [ $\bar{u}$ , $\bar{u}$ ,u] $\bar{x}$ , $\bar{x}$ , $\bar{x}$ [ $\bar{u}$ , $\bar{u}$ , $\bar{u}$ ]	$\bar{x}$ ,x, $\bar{x}$ [ $\bar{u}$ ,u, $\bar{u}$ ] x, $\bar{x}$ ,x [u, $\bar{u}$ ,u]	x, $\bar{x}$ , $\bar{x}$ [u, $\bar{u}$ , $\bar{u}$ ] $\bar{x}$ ,x,x [ $\bar{u}$ ,u,u]
12	f	4'..	x,1/2,1/2 [0,0,0] 1/2, $\bar{x}$ ,1/2 [0,0,0]	$\bar{x}$ ,1/2,1/2 [0,0,0] 1/2,1/2,x [0,0,0]	1/2,x,1/2 [0,0,0] 1/2,1/2, $\bar{x}$ [0,0,0]	
12	e	4..	x,0,0 [u,0,0] 0, $\bar{x}$ ,0 [0, $\bar{u}$ ,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0] 0,0,x [0,0,u]	0,x,0 [0,u,0] 0,0, $\bar{x}$ [0,0, $\bar{u}$ ]	
6	d	42'.2'	1/2,0,0 [u,0,0]	0,1/2,0 [0,u,0]	0,0,1/2 [0,0,u]	
6	c	4'2'.2	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	
2	b	4'32'	1/2,1/2,1/2 [0,0,0]			
2	a	432	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,1,1] p3m11'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

Along [1,1,0] p<sub>c</sub>-2mm  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x-1/4,x+1/4,1/2



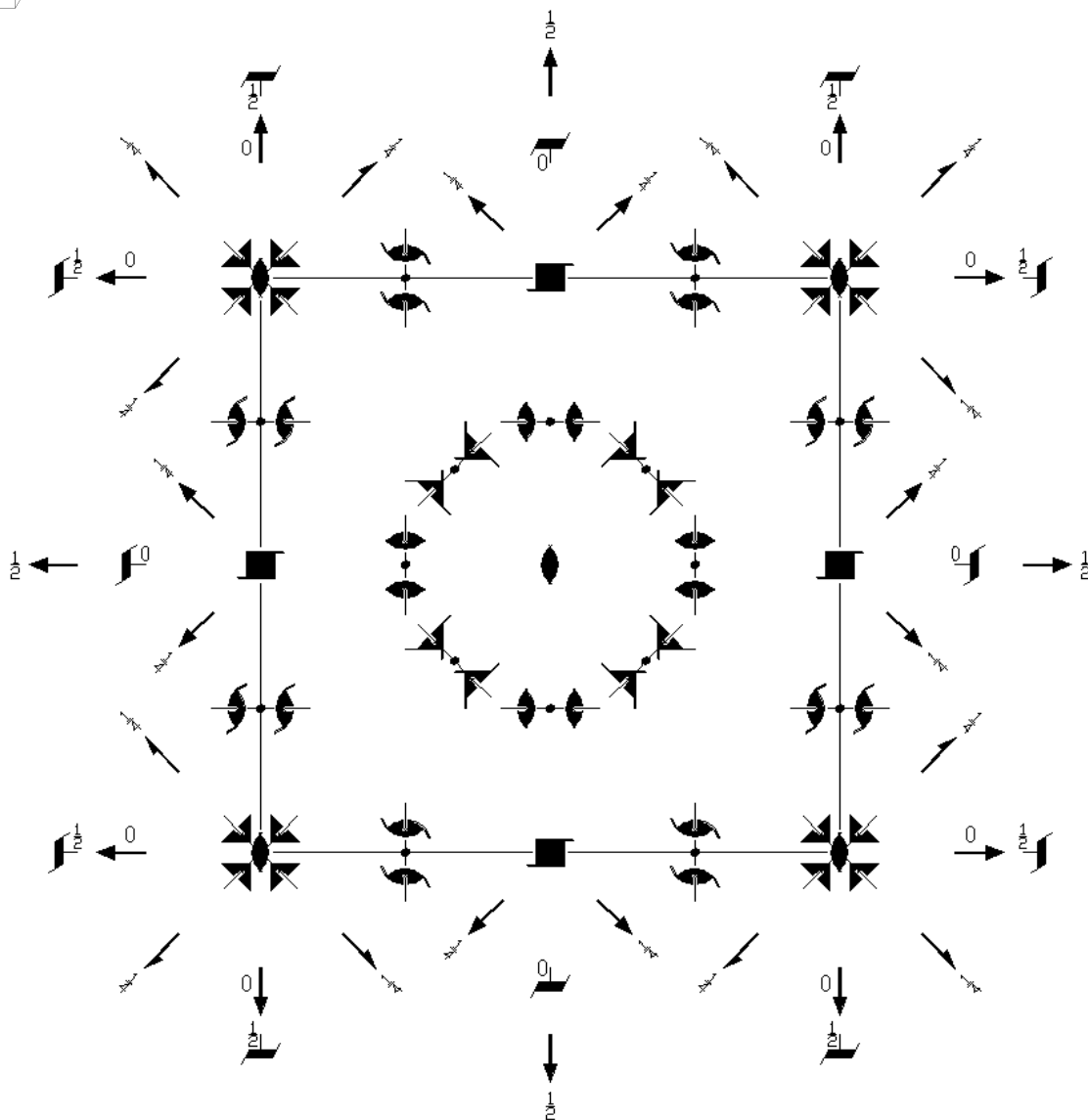
P4<sub>2</sub>32

432

Cubic

208.1.1546

P4<sub>2</sub>32



Origin at 23

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $-1/4 \leq z \leq 1/4;$   $\max(-x, x-1/2, -y, y-1/2) \leq z \leq \min(x, 1/2-x, y, 1/2-y)$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $0,1/2,0$   $1/4,1/4,1/4$   $1/4,1/4,-1/4$

**Symmetry Operations**

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)     | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)                               | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0) | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0)              |



(13) $2 \begin{pmatrix} 1/2, 1/2, 0 \\ 2_{xy}   1/2, 1/2, 1/2 \end{pmatrix} x, x, 1/4$	(14) $2 \begin{pmatrix} x, \bar{x}+1/2, 1/4 \\ 2_{\bar{xy}}   1/2, 1/2, 1/2 \end{pmatrix}$	(15) $4^- \begin{pmatrix} 0, 0, 1/2 \\ 4_z^{-1}   1/2, 1/2, 1/2 \end{pmatrix} 1/2, 0, z$	(16) $4^+ \begin{pmatrix} 0, 0, 1/2 \\ 4_z   1/2, 1/2, 1/2 \end{pmatrix} 0, 1/2, z$
(17) $4^- \begin{pmatrix} 1/2, 0, 0 \\ 4_x^{-1}   1/2, 1/2, 1/2 \end{pmatrix} x, 1/2, 0$	(18) $2 \begin{pmatrix} 0, 1/2, 1/2 \\ 2_{yz}   1/2, 1/2, 1/2 \end{pmatrix} 1/4, y, y$	(19) $2 \begin{pmatrix} 1/4, y+1/2, \bar{y} \\ 2_{\bar{yz}}   1/2, 1/2, 1/2 \end{pmatrix}$	(20) $4^+ \begin{pmatrix} 1/2, 0, 0 \\ 4_x   1/2, 1/2, 1/2 \end{pmatrix} x, 0, 1/2$
(21) $4^+ \begin{pmatrix} 0, 1/2, 0 \\ 4_y   1/2, 1/2, 1/2 \end{pmatrix} 1/2, y, 0$	(22) $2 \begin{pmatrix} 1/2, 0, 1/2 \\ 2_{xz}   1/2, 1/2, 1/2 \end{pmatrix} x, 1/4, x$	(23) $4^- \begin{pmatrix} 0, 1/2, 0 \\ 4_y^{-1}   1/2, 1/2, 1/2 \end{pmatrix} 0, y, 1/2$	(24) $2 \begin{pmatrix} \bar{x}+1/2, 1/4, x \\ 2_{\bar{xz}}   1/2, 1/2, 1/2 \end{pmatrix}$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

24 m 1

(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{x}, y, \bar{z} [\bar{u}, v, \bar{w}]$	(4) $x, \bar{y}, \bar{z} [u, \bar{v}, \bar{w}]$
(5) $z, x, y [w, u, v]$	(6) $z, \bar{x}, \bar{y} [w, \bar{u}, \bar{v}]$	(7) $\bar{z}, \bar{x}, y [\bar{w}, \bar{u}, v]$	(8) $\bar{z}, x, \bar{y} [\bar{w}, u, \bar{v}]$
(9) $y, z, x [v, w, u]$	(10) $\bar{y}, z, \bar{x} [\bar{v}, w, \bar{u}]$	(11) $y, \bar{z}, \bar{x} [v, \bar{w}, \bar{u}]$	(12) $\bar{y}, \bar{z}, x [\bar{v}, \bar{w}, u]$
(13) $y+1/2, x+1/2, \bar{z}+1/2 [v, u, \bar{w}]$	(14) $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2 [\bar{v}, \bar{u}, \bar{w}]$	(15) $y+1/2, \bar{x}+1/2, z+1/2 [v, \bar{u}, w]$	(16) $\bar{y}+1/2, x+1/2, z+1/2 [\bar{v}, u, w]$
(17) $x+1/2, z+1/2, \bar{y}+1/2 [u, w, \bar{v}]$	(18) $\bar{x}+1/2, z+1/2, y+1/2 [\bar{u}, w, v]$	(19) $\bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2 [\bar{u}, \bar{w}, \bar{v}]$	(20) $x+1/2, \bar{z}+1/2, y+1/2 [u, \bar{w}, v]$
(21) $z+1/2, y+1/2, \bar{x}+1/2 [w, v, \bar{u}]$	(22) $z+1/2, \bar{y}+1/2, x+1/2 [w, \bar{v}, u]$	(23) $\bar{z}+1/2, y+1/2, x+1/2 [\bar{w}, v, u]$	(24) $\bar{z}+1/2, \bar{y}+1/2, \bar{x}+1/2 [\bar{w}, \bar{v}, \bar{u}]$

12	l	..2	$1/4, y, y+1/2 [0, v, v]$	$3/4, \bar{y}, y+1/2 [0, \bar{v}, v]$	$3/4, y, \bar{y}+1/2 [0, v, \bar{v}]$	$1/4, \bar{y}, \bar{y}+1/2 [0, \bar{v}, \bar{v}]$
			$y+1/2, 1/4, y [v, 0, v]$	$y+1/2, 3/4, \bar{y} [v, 0, \bar{v}]$	$\bar{y}+1/2, 3/4, y [\bar{v}, 0, v]$	$\bar{y}+1/2, 1/4, \bar{y} [\bar{v}, 0, \bar{v}]$
			$y, y+1/2, 1/4 [v, v, 0]$	$\bar{y}, y+1/2, 3/4 [\bar{v}, v, 0]$	$y, \bar{y}+1/2, 3/4 [v, \bar{v}, 0]$	$\bar{y}, \bar{y}+1/2, 1/4 [\bar{v}, \bar{v}, 0]$
12	k	..2	$1/4, y, \bar{y}+1/2 [0, \bar{v}, v]$	$3/4, \bar{y}, \bar{y}+1/2 [0, v, v]$	$3/4, y, y+1/2 [0, \bar{v}, \bar{v}]$	$1/4, \bar{y}, y+1/2 [0, v, \bar{v}]$
			$\bar{y}+1/2, 1/4, y [v, 0, \bar{v}]$	$\bar{y}+1/2, 3/4, \bar{y} [v, 0, v]$	$y+1/2, 3/4, y [\bar{v}, 0, \bar{v}]$	$y+1/2, 1/4, \bar{y} [\bar{v}, 0, v]$
			$y, \bar{y}+1/2, 1/4 [\bar{v}, v, 0]$	$\bar{y}, \bar{y}+1/2, 3/4 [v, v, 0]$	$y, y+1/2, 3/4 [\bar{v}, \bar{v}, 0]$	$\bar{y}, y+1/2, 1/4 [v, \bar{v}, 0]$
12	j	2..	$x, 1/2, 0 [u, 0, 0]$	$\bar{x}, 1/2, 0 [\bar{u}, 0, 0]$	$0, x, 1/2 [0, u, 0]$	$0, \bar{x}, 1/2 [0, \bar{u}, 0]$
			$1/2, 0, x [0, 0, u]$	$1/2, 0, \bar{x} [0, 0, \bar{u}]$	$0, x+1/2, 1/2 [0, u, 0]$	$0, \bar{x}+1/2, 1/2 [0, \bar{u}, 0]$
			$x+1/2, 1/2, 0 [u, 0, 0]$	$\bar{x}+1/2, 1/2, 0 [\bar{u}, 0, 0]$	$1/2, 0, \bar{x}+1/2 [0, 0, \bar{u}]$	$1/2, 0, x+1/2 [0, 0, u]$
12	i	2..	$x, 0, 1/2 [u, 0, 0]$	$\bar{x}, 0, 1/2 [\bar{u}, 0, 0]$	$1/2, x, 0 [0, u, 0]$	$1/2, \bar{x}, 0 [0, \bar{u}, 0]$
			$0, 1/2, x [0, 0, u]$	$0, 1/2, \bar{x} [0, 0, \bar{u}]$	$1/2, x+1/2, 0 [0, u, 0]$	$1/2, \bar{x}+1/2, 0 [0, \bar{u}, 0]$
			$x+1/2, 0, 1/2 [u, 0, 0]$	$\bar{x}+1/2, 0, 1/2 [\bar{u}, 0, 0]$	$0, 1/2, \bar{x}+1/2 [0, 0, \bar{u}]$	$0, 1/2, x+1/2 [0, 0, u]$

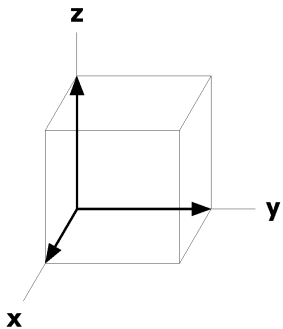
12	h	2..	x,0,0 [u,0,0] 0,0,x [0,0,u] x+1/2,1/2,1/2 [u,0,0]	$\bar{x},0,0 [\bar{u},0,0]$ 0,0, $\bar{x}$ [0,0, $\bar{u}$ ] $\bar{x}+1/2,1/2,1/2 [\bar{u},0,0]$	0,x,0 [0,u,0] 1/2,x+1/2,1/2 [0,u,0] 1/2,1/2, $\bar{x}+1/2$ [0,0, $\bar{u}$ ]	0, $\bar{x},0 [0,\bar{u},0]$ 1/2, $\bar{x}+1/2,1/2 [0,\bar{u},0]$ 1/2,1/2,x+1/2 [0,0,u]
8	g	.3.	x,x,x [u,u,u] $\bar{x},x,\bar{x} [\bar{u},u,\bar{u}]$ x+1/2,x+1/2, $\bar{x}+1/2$ [u,u, $\bar{u}$ ] x+1/2, $\bar{x}+1/2,x+1/2$ [u, $\bar{u},u$ ]	$\bar{x},\bar{x},x [\bar{u},\bar{u},u]$ x, $\bar{x},\bar{x} [u,\bar{u},\bar{u}]$ $\bar{x}+1/2,\bar{x}+1/2,\bar{x}+1/2 [\bar{u},\bar{u},\bar{u}]$ $\bar{x}+1/2,x+1/2,x+1/2 [\bar{u},u,u]$		
6	f	2.22	1/4,1/2,0 [0,0,0] 0,3/4,1/2 [0,0,0]	3/4,1/2,0 [0,0,0] 1/2,0,1/4 [0,0,0]	0,1/4,1/2 [0,0,0] 1/2,0,3/4 [0,0,0]	
6	e	2.22	1/4,0,1/2 [0,0,0] 1/2,3/4,0 [0,0,0]	3/4,0,1/2 [0,0,0] 0,1/2,1/4 [0,0,0]	1/2,1/4,0 [0,0,0] 0,1/2,3/4 [0,0,0]	
6	d	222..	0,1/2,1/2 [0,0,0] 0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0] 1/2,0,0 [0,0,0]	1/2,1/2,0 [0,0,0] 0,0,1/2 [0,0,0]	
4	c	.32	3/4,3/4,3/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
4	b	.32	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]
2	a	23.	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,1,1] p3m'1  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

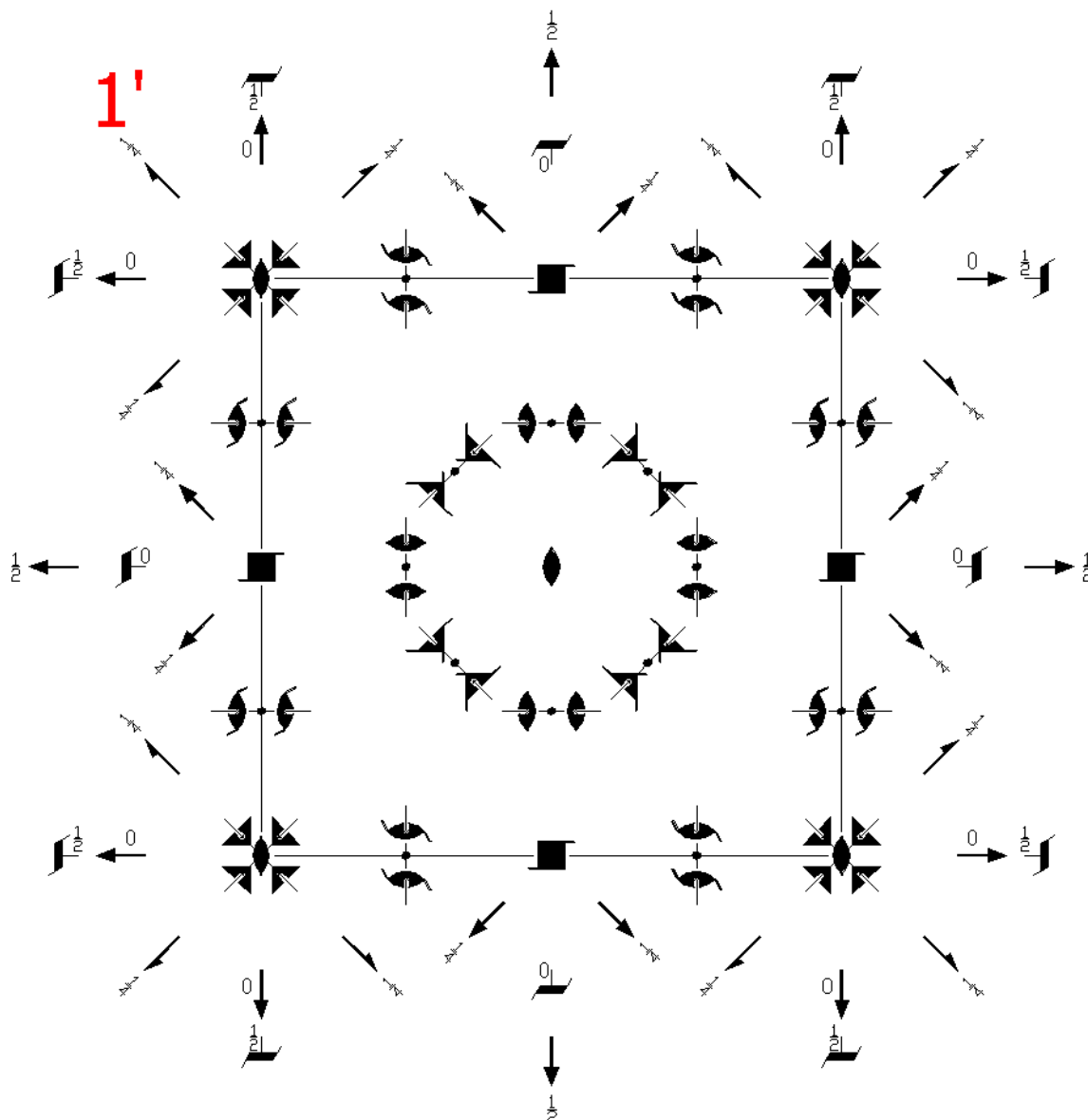
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



$P4_2 321'$   
208.2.1547

$4321'$   
 $P4_2 321'$

Cubic



Origin at  $231'$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $-1/4 \leq z \leq 1/4;$   $\max(-x, x-1/2, -y, y-1/2) \leq z \leq \min(x, 1/2-x, y, 1/2-y)$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $0,1/2,0$   $1/4,1/4,1/4$   $1/4,1/4,-1/4$

**Symmetry Operations**

For 1 + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                                | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  0,0,0) | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  0,0,0) | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}z}^{-1}$  0,0,0) |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)     | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}z}$  0,0,0)     | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)     |

(13) 2 (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)	(14) 2 x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)	(15) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)	(16) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)
(17) 4 <sup>-</sup> (1/2,0,0) x,1/2,0 (4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,1/2)	(18) 2 (0,1/2,1/2) 1/4,y,y (2 <sub>yz</sub>  1/2,1/2,1/2)	(19) 2 1/4,y+1/2, $\bar{y}$ (2 <sub>yz</sub>  1/2,1/2,1/2)	(20) 4 <sup>+</sup> (1/2,0,0) x,0,1/2 (4 <sub>x</sub>  1/2,1/2,1/2)
(21) 4 <sup>+</sup> (0,1/2,0) 1/2,y,0 (4 <sub>y</sub>  1/2,1/2,1/2)	(22) 2 (1/2,0,1/2) x,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)	(23) 4 <sup>-</sup> (0,1/2,0) 0,y,1/2 (4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,1/2)	(24) 2 $\bar{x}$ +1/2,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)

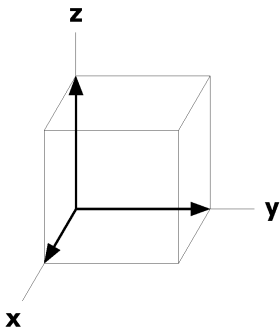
## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(4) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'
(5) 3 <sup>+</sup> x,x,x (3 <sub>xyz</sub>  0,0,0)'	(6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)'	(7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)'	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)'
(9) 3 <sup>-</sup> x,x,x (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)'	(10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub>  0,0,0)'	(11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x (3 <sub>xyz</sub>  0,0,0)'	(12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$ (3 <sub>xyz</sub>  0,0,0)'
(13) 2' (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(14) 2' x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(15) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(16) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)'
(17) 4 <sup>-</sup> (1/2,0,0) x,1/2,0 (4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(18) 2' (0,1/2,1/2) 1/4,y,y (2 <sub>yz</sub>  1/2,1/2,1/2)'	(19) 2' 1/4,y+1/2, $\bar{y}$ (2 <sub>yz</sub>  1/2,1/2,1/2)'	(20) 4 <sup>+</sup> (1/2,0,0) x,0,1/2 (4 <sub>x</sub>  1/2,1/2,1/2)'
(21) 4 <sup>+</sup> (0,1/2,0) 1/2,y,0 (4 <sub>y</sub>  1/2,1/2,1/2)'	(22) 2' (1/2,0,1/2) x,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)'	(23) 4 <sup>-</sup> (0,1/2,0) 0,y,1/2 (4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(24) 2' $\bar{x}$ +1/2,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); 1'.

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates								
			1 +	1' +							
24	m	11'									
(1)	x,y,z	[0,0,0]	(2)	$\bar{x}$ , $\bar{y}$ ,z	[0,0,0]	(3)	$\bar{x}$ ,y, $\bar{z}$	[0,0,0]	(4)	x, $\bar{y}$ , $\bar{z}$	[0,0,0]
(5)	z,x,y	[0,0,0]	(6)	z, $\bar{x}$ , $\bar{y}$	[0,0,0]	(7)	$\bar{z}$ , $\bar{x}$ ,y	[0,0,0]	(8)	$\bar{z}$ ,x, $\bar{y}$	[0,0,0]
(9)	y,z,x	[0,0,0]	(10)	$\bar{y}$ ,z, $\bar{x}$	[0,0,0]	(11)	y, $\bar{z}$ , $\bar{x}$	[0,0,0]	(12)	$\bar{y}$ , $\bar{z}$ ,x	[0,0,0]
(13)	y+1/2,x+1/2, $\bar{z}$ +1/2	[0,0,0]	(14)	$\bar{y}$ +1/2, $\bar{x}$ +1/2, $\bar{z}$ +1/2	[0,0,0]	(15)	y+1/2, $\bar{x}$ +1/2,z+1/2	[0,0,0]	(16)	$\bar{y}$ +1/2,x+1/2,z+1/2	[0,0,0]
(17)	x+1/2,z+1/2, $\bar{y}$ +1/2	[0,0,0]	(18)	$\bar{x}$ +1/2,z+1/2,y+1/2	[0,0,0]	(19)	$\bar{x}$ +1/2, $\bar{z}$ +1/2, $\bar{y}$ +1/2	[0,0,0]	(20)	x+1/2, $\bar{z}$ +1/2,y+1/2	[0,0,0]
(21)	z+1/2,y+1/2, $\bar{x}$ +1/2	[0,0,0]	(22)	z+1/2, $\bar{y}$ +1/2,x+1/2	[0,0,0]	(23)	$\bar{z}$ +1/2,y+1/2,x+1/2	[0,0,0]	(24)	$\bar{z}$ +1/2, $\bar{y}$ +1/2, $\bar{x}$ +1/2	[0,0,0]
12	l	..21'	1/4,y,y+1/2	[0,0,0]	3/4, $\bar{y}$ ,y+1/2	[0,0,0]	3/4,y, $\bar{y}$ +1/2	[0,0,0]	1/4, $\bar{y}$ , $\bar{y}$ +1/2	[0,0,0]	
			y+1/2,1/4,y	[0,0,0]	y+1/2,3/4, $\bar{y}$	[0,0,0]	$\bar{y}$ +1/2,3/4,y	[0,0,0]	$\bar{y}$ +1/2,1/4, $\bar{y}$	[0,0,0]	
			y,y+1/2,1/4	[0,0,0]	$\bar{y}$ ,y+1/2,3/4	[0,0,0]	y, $\bar{y}$ +1/2,3/4	[0,0,0]	$\bar{y}$ , $\bar{y}$ +1/2,1/4	[0,0,0]	



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P4<sub>2</sub> 321'

			$1/4, y, \bar{y}+1/2 [0,0,0]$	$3/4, \bar{y}, \bar{y}+1/2 [0,0,0]$	$3/4, y, y+1/2 [0,0,0]$	$1/4, \bar{y}, y+1/2 [0,0,0]$
			$\bar{y}+1/2, 1/4, y [0,0,0]$	$\bar{y}+1/2, 3/4, \bar{y} [0,0,0]$	$y+1/2, 3/4, y [0,0,0]$	$y+1/2, 1/4, \bar{y} [0,0,0]$
			$y, \bar{y}+1/2, 1/4 [0,0,0]$	$\bar{y}, \bar{y}+1/2, 3/4 [0,0,0]$	$y, y+1/2, 3/4 [0,0,0]$	$\bar{y}, y+1/2, 1/4 [0,0,0]$
12	j	2..1'	$x, 1/2, 0 [0,0,0]$	$\bar{x}, 1/2, 0 [0,0,0]$	$0, x, 1/2 [0,0,0]$	$0, \bar{x}, 1/2 [0,0,0]$
			$1/2, 0, x [0,0,0]$	$1/2, 0, \bar{x} [0,0,0]$	$0, x+1/2, 1/2 [0,0,0]$	$0, \bar{x}+1/2, 1/2 [0,0,0]$
			$x+1/2, 1/2, 0 [0,0,0]$	$\bar{x}+1/2, 1/2, 0 [0,0,0]$	$1/2, 0, \bar{x}+1/2 [0,0,0]$	$1/2, 0, x+1/2 [0,0,0]$
12	i	2..1'	$x, 0, 1/2 [0,0,0]$	$\bar{x}, 0, 1/2 [0,0,0]$	$1/2, x, 0 [0,0,0]$	$1/2, \bar{x}, 0 [0,0,0]$
			$0, 1/2, x [0,0,0]$	$0, 1/2, \bar{x} [0,0,0]$	$1/2, x+1/2, 0 [0,0,0]$	$1/2, \bar{x}+1/2, 0 [0,0,0]$
			$x+1/2, 0, 1/2 [0,0,0]$	$\bar{x}+1/2, 0, 1/2 [0,0,0]$	$0, 1/2, \bar{x}+1/2 [0,0,0]$	$0, 1/2, x+1/2 [0,0,0]$
12	h	2..1'	$x, 0, 0 [0,0,0]$	$\bar{x}, 0, 0 [0,0,0]$	$0, x, 0 [0,0,0]$	$0, \bar{x}, 0 [0,0,0]$
			$0, 0, x [0,0,0]$	$0, 0, \bar{x} [0,0,0]$	$1/2, x+1/2, 1/2 [0,0,0]$	$1/2, \bar{x}+1/2, 1/2 [0,0,0]$
			$x+1/2, 1/2, 1/2 [0,0,0]$	$\bar{x}+1/2, 1/2, 1/2 [0,0,0]$	$1/2, 1/2, \bar{x}+1/2 [0,0,0]$	$1/2, 1/2, x+1/2 [0,0,0]$
8	g	.3.1'	$x, x, x [0,0,0]$	$\bar{x}, \bar{x}, x [0,0,0]$		
			$\bar{x}, x, \bar{x} [0,0,0]$	$x, \bar{x}, \bar{x} [0,0,0]$		
			$x+1/2, x+1/2, \bar{x}+1/2 [0,0,0]$	$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [0,0,0]$		
			$x+1/2, \bar{x}+1/2, x+1/2 [0,0,0]$	$\bar{x}+1/2, x+1/2, x+1/2 [0,0,0]$		
6	f	2.221'	$1/4, 1/2, 0 [0,0,0]$	$3/4, 1/2, 0 [0,0,0]$	$0, 1/4, 1/2 [0,0,0]$	
			$0, 3/4, 1/2 [0,0,0]$	$1/2, 0, 1/4 [0,0,0]$	$1/2, 0, 3/4 [0,0,0]$	
6	e	2.221'	$1/4, 0, 1/2 [0,0,0]$	$3/4, 0, 1/2 [0,0,0]$	$1/2, 1/4, 0 [0,0,0]$	
			$1/2, 3/4, 0 [0,0,0]$	$0, 1/2, 1/4 [0,0,0]$	$0, 1/2, 3/4 [0,0,0]$	
6	d	222..1'	$0, 1/2, 1/2 [0,0,0]$	$1/2, 0, 1/2 [0,0,0]$	$1/2, 1/2, 0 [0,0,0]$	
			$0, 1/2, 0 [0,0,0]$	$1/2, 0, 0 [0,0,0]$	$0, 0, 1/2 [0,0,0]$	
4	c	.321'	$3/4, 3/4, 3/4 [0,0,0]$	$1/4, 1/4, 3/4 [0,0,0]$	$1/4, 3/4, 1/4 [0,0,0]$	$3/4, 1/4, 1/4 [0,0,0]$
4	b	.321'	$1/4, 1/4, 1/4 [0,0,0]$	$3/4, 3/4, 1/4 [0,0,0]$	$3/4, 1/4, 3/4 [0,0,0]$	$1/4, 3/4, 3/4 [0,0,0]$
2	a	23.1'	$0, 0, 0 [0,0,0]$	$1/2, 1/2, 1/2 [0,0,0]$		

### Symmetry of Special Projections

Along  $[0,0,1]$  p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 1/2, z$

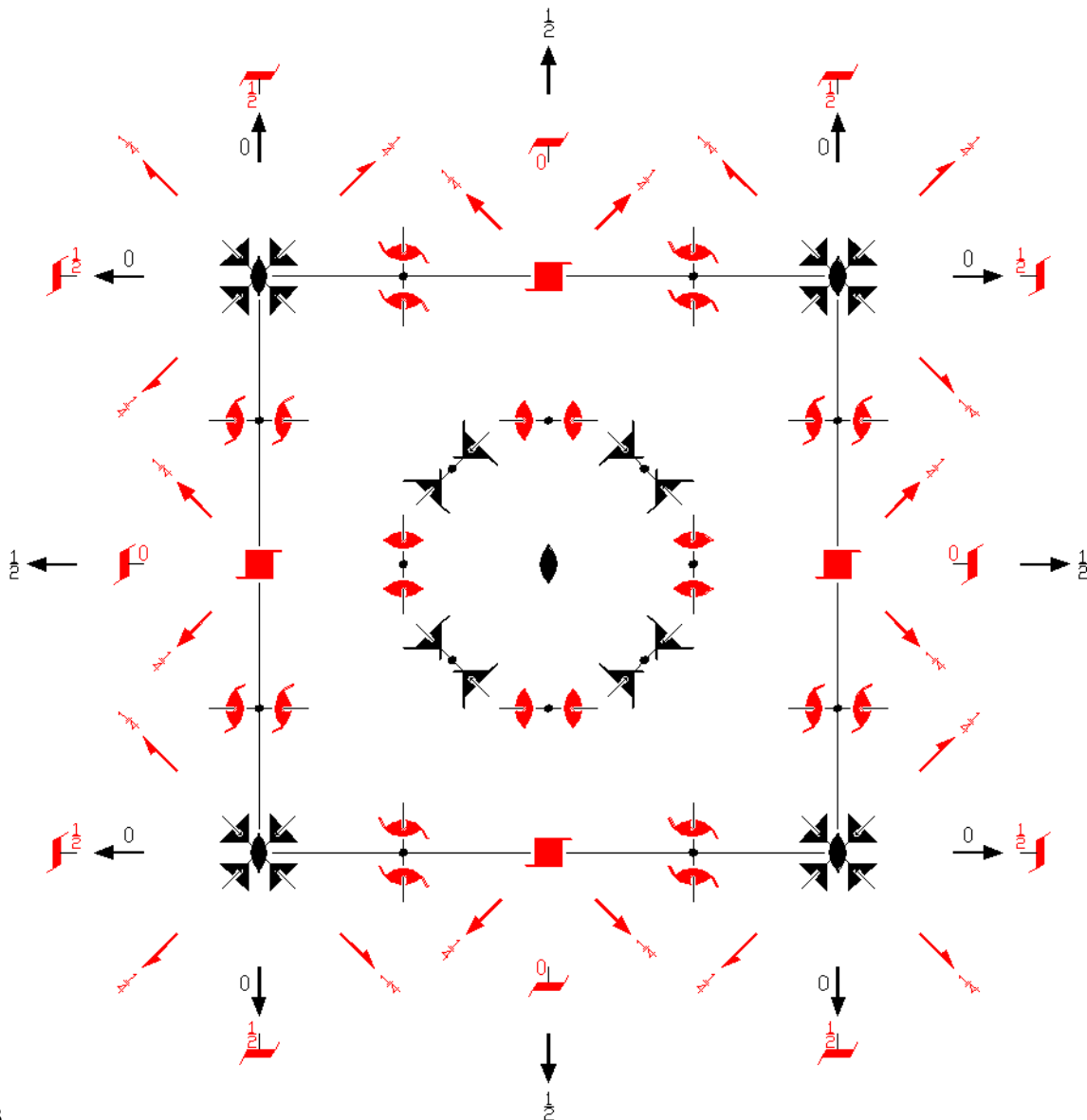
Along  $[1,1,1]$  p3m11'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

Along  $[1,1,0]$  p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 1/4$

P4<sub>2</sub>' 32'

4'32'

Cubic



Origin at 23

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $-1/4 \leq z \leq 1/4;$   $\max(-x, x-1/2, -y, y-1/2) \leq z \leq \min(x, 1/2-x, y, 1/2-y)$

Vertices 0,0,0      1/2,0,0      1/2,1/2,0      0,1/2,0      1/4,1/4,1/4      1/4,1/4,-1/4

**Symmetry Operations**

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)                               | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>xyz</sub>  0,0,0)              | (12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0)               |

Continued

(13) $2' (1/2, 1/2, 0) \quad x, x, 1/4$ $(2_{xy}   1/2, 1/2, 1/2)'$	(14) $2' \quad x, \bar{x}+1/2, 1/4$ $(2_{\bar{xy}}   1/2, 1/2, 1/2)'$	(15) $4' (0, 0, 1/2) \quad 1/2, 0, z$ $(4_z^{-1}   1/2, 1/2, 1/2)'$	(16) $4^+ (0, 0, 1/2) \quad 0, 1/2, z$ $(4_z   1/2, 1/2, 1/2)'$
(17) $4' (1/2, 0, 0) \quad x, 1/2, 0$ $(4_x^{-1}   1/2, 1/2, 1/2)'$	(18) $2' (0, 1/2, 1/2) \quad 1/4, y, y$ $(2_{yz}   1/2, 1/2, 1/2)'$	(19) $2' \quad 1/4, y+1/2, \bar{y}$ $(2_{\bar{yz}}   1/2, 1/2, 1/2)'$	(20) $4^+ (1/2, 0, 0) \quad x, 0, 1/2$ $(4_x   1/2, 1/2, 1/2)'$
(21) $4^+ (0, 1/2, 0) \quad 1/2, y, 0$ $(4_y   1/2, 1/2, 1/2)'$	(22) $2' (1/2, 0, 1/2) \quad x, 1/4, x$ $(2_{xz}   1/2, 1/2, 1/2)'$	(23) $4' (0, 1/2, 0) \quad 0, y, 1/2$ $(4_y^{-1}   1/2, 1/2, 1/2)'$	(24) $2' \quad \bar{x}+1/2, 1/4, x$ $(2_{\bar{xz}}   1/2, 1/2, 1/2)'$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

24 m 1

(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{x}, y, \bar{z} [\bar{u}, v, \bar{w}]$	(4) $x, \bar{y}, \bar{z} [u, \bar{v}, \bar{w}]$	
(5) $z, x, y [w, u, v]$	(6) $z, \bar{x}, \bar{y} [w, \bar{u}, \bar{v}]$	(7) $\bar{z}, \bar{x}, y [\bar{w}, \bar{u}, v]$	(8) $\bar{z}, x, \bar{y} [\bar{w}, u, \bar{v}]$	
(9) $y, z, x [v, w, u]$	(10) $\bar{y}, z, \bar{x} [\bar{v}, w, \bar{u}]$	(11) $y, \bar{z}, \bar{x} [v, \bar{w}, \bar{u}]$	(12) $\bar{y}, \bar{z}, x [\bar{v}, \bar{w}, u]$	
(13) $y+1/2, x+1/2, \bar{z}+1/2 [\bar{v}, \bar{u}, w]$	(14) $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2 [v, u, w]$	(15) $y+1/2, \bar{x}+1/2, z+1/2 [\bar{v}, u, \bar{w}]$	(16) $\bar{y}+1/2, x+1/2, z+1/2 [v, \bar{u}, \bar{w}]$	
(17) $x+1/2, z+1/2, \bar{y}+1/2 [\bar{u}, \bar{w}, v]$	(18) $\bar{x}+1/2, z+1/2, y+1/2 [u, \bar{w}, \bar{v}]$	(19) $\bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2 [u, w, v]$	(20) $x+1/2, \bar{z}+1/2, y+1/2 [\bar{u}, w, \bar{v}]$	
(21) $z+1/2, y+1/2, \bar{x}+1/2 [\bar{w}, \bar{v}, u]$	(22) $z+1/2, \bar{y}+1/2, x+1/2 [\bar{w}, v, \bar{u}]$	(23) $\bar{z}+1/2, y+1/2, x+1/2 [w, \bar{v}, \bar{u}]$	(24) $\bar{z}+1/2, \bar{y}+1/2, \bar{x}+1/2 [w, v, u]$	
12 l ..2'	$1/4, y, y+1/2 [u, v, \bar{v}]$	$3/4, \bar{y}, y+1/2 [\bar{u}, \bar{v}, \bar{v}]$	$3/4, y, \bar{y}+1/2 [\bar{u}, v, v]$	$1/4, \bar{y}, \bar{y}+1/2 [u, \bar{v}, v]$
	$y+1/2, 1/4, y [\bar{v}, u, v]$	$y+1/2, 3/4, \bar{y} [\bar{v}, \bar{u}, \bar{v}]$	$\bar{y}+1/2, 3/4, y [v, \bar{u}, v]$	$\bar{y}+1/2, 1/4, \bar{y} [v, u, \bar{v}]$
	$y, y+1/2, 1/4 [v, \bar{v}, u]$	$\bar{y}, y+1/2, 3/4 [\bar{v}, \bar{v}, \bar{u}]$	$y, \bar{y}+1/2, 3/4 [v, v, \bar{u}]$	$\bar{y}, \bar{y}+1/2, 1/4 [\bar{v}, v, u]$
12 k ..2'	$1/4, y, \bar{y}+1/2 [u, v, v]$	$3/4, \bar{y}, \bar{y}+1/2 [\bar{u}, \bar{v}, v]$	$3/4, y, y+1/2 [\bar{u}, v, \bar{v}]$	$1/4, \bar{y}, y+1/2 [u, \bar{v}, \bar{v}]$
	$\bar{y}+1/2, 1/4, y [v, u, v]$	$\bar{y}+1/2, 3/4, \bar{y} [v, \bar{u}, \bar{v}]$	$y+1/2, 3/4, y [\bar{v}, \bar{u}, v]$	$y+1/2, 1/4, \bar{y} [\bar{v}, u, \bar{v}]$
	$y, \bar{y}+1/2, 1/4 [v, v, u]$	$\bar{y}, \bar{y}+1/2, 3/4 [\bar{v}, v, \bar{u}]$	$y, y+1/2, 3/4 [v, \bar{v}, \bar{u}]$	$\bar{y}, y+1/2, 1/4 [\bar{v}, \bar{v}, u]$
12 j 2..	$x, 1/2, 0 [u, 0, 0]$	$\bar{x}, 1/2, 0 [\bar{u}, 0, 0]$	$0, x, 1/2 [0, u, 0]$	$0, \bar{x}, 1/2 [0, \bar{u}, 0]$
	$1/2, 0, x [0, 0, u]$	$1/2, 0, \bar{x} [0, 0, \bar{u}]$	$0, x+1/2, 1/2 [0, \bar{u}, 0]$	$0, \bar{x}+1/2, 1/2 [0, u, 0]$
	$x+1/2, 1/2, 0 [\bar{u}, 0, 0]$	$\bar{x}+1/2, 1/2, 0 [u, 0, 0]$	$1/2, 0, \bar{x}+1/2 [0, 0, u]$	$1/2, 0, x+1/2 [0, 0, \bar{u}]$
12 i 2..	$x, 0, 1/2 [u, 0, 0]$	$\bar{x}, 0, 1/2 [\bar{u}, 0, 0]$	$1/2, x, 0 [0, u, 0]$	$1/2, \bar{x}, 0 [0, \bar{u}, 0]$
	$0, 1/2, x [0, 0, u]$	$0, 1/2, \bar{x} [0, 0, \bar{u}]$	$1/2, x+1/2, 0 [0, \bar{u}, 0]$	$1/2, \bar{x}+1/2, 0 [0, u, 0]$
	$x+1/2, 0, 1/2 [\bar{u}, 0, 0]$	$\bar{x}+1/2, 0, 1/2 [u, 0, 0]$	$0, 1/2, \bar{x}+1/2 [0, 0, u]$	$0, 1/2, x+1/2 [0, 0, \bar{u}]$

12	h	2..	x,0,0 [u,0,0] 0,0,x [0,0,u] x+1/2,1/2,1/2 [ $\bar{u}$ ,0,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0] 0,0, $\bar{x}$ [0,0, $\bar{u}$ ] $\bar{x}$ +1/2,1/2,1/2 [u,0,0]	0,x,0 [0,u,0] 1/2,x+1/2,1/2 [0, $\bar{u}$ ,0] 1/2,1/2, $\bar{x}$ +1/2 [0,0,u]	0, $\bar{x}$ ,0 [0, $\bar{u}$ ,0] 1/2, $\bar{x}$ +1/2,1/2 [0,u,0] 1/2,1/2,x+1/2 [0,0, $\bar{u}$ ]
8	g	.3.	x,x,x [u,u,u] $\bar{x}$ , $\bar{x}$ , $\bar{x}$ [ $\bar{u}$ ,u, $\bar{u}$ ] x+1/2,x+1/2, $\bar{x}$ +1/2 [ $\bar{u}$ , $\bar{u}$ ,u] x+1/2, $\bar{x}$ +1/2,x+1/2 [ $\bar{u}$ ,u, $\bar{u}$ ]	$\bar{x}$ , $\bar{x}$ ,x [ $\bar{u}$ , $\bar{u}$ ,u] x, $\bar{x}$ , $\bar{x}$ [u, $\bar{u}$ , $\bar{u}$ ] $\bar{x}$ +1/2, $\bar{x}$ +1/2, $\bar{x}$ +1/2 [u,u,u] $\bar{x}$ +1/2,x+1/2,x+1/2 [u, $\bar{u}$ , $\bar{u}$ ]		
6	f	2.2'2'	1/4,1/2,0 [u,0,0] 0,3/4,1/2 [0, $\bar{u}$ ,0]	3/4,1/2,0 [ $\bar{u}$ ,0,0] 1/2,0,1/4 [0,0,u]	0,1/4,1/2 [0,u,0] 1/2,0,3/4 [0,0, $\bar{u}$ ]	
6	e	2.2'2'	1/4,0,1/2 [u,0,0] 1/2,3/4,0 [0, $\bar{u}$ ,0]	3/4,0,1/2 [ $\bar{u}$ ,0,0] 0,1/2,1/4 [0,0,u]	1/2,1/4,0 [0,u,0] 0,1/2,3/4 [0,0, $\bar{u}$ ]	
6	d	222..	0,1/2,1/2 [0,0,0] 0,1/2,0 [0,0,0]	1/2,0,1/2 [0,0,0] 1/2,0,0 [0,0,0]	1/2,1/2,0 [0,0,0] 0,0,1/2 [0,0,0]	
4	c	.32'	3/4,3/4,3/4 [u,u,u]	1/4,1/4,3/4 [ $\bar{u}$ , $\bar{u}$ ,u]	1/4,3/4,1/4 [ $\bar{u}$ ,u, $\bar{u}$ ]	3/4,1/4,1/4 [u, $\bar{u}$ , $\bar{u}$ ]
4	b	.32'	1/4,1/4,1/4 [u,u,u]	3/4,3/4,1/4 [ $\bar{u}$ , $\bar{u}$ ,u]	3/4,1/4,3/4 [ $\bar{u}$ ,u, $\bar{u}$ ]	1/4,3/4,3/4 [u, $\bar{u}$ , $\bar{u}$ ]
2	a	23.	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

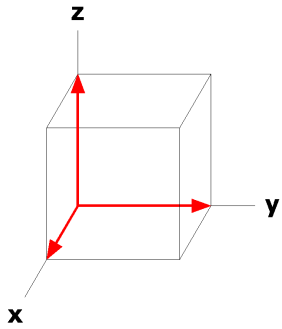
### Symmetry of Special Projections

Along [0,0,1] p4'm'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,1,1] p3m1  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = -(-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4





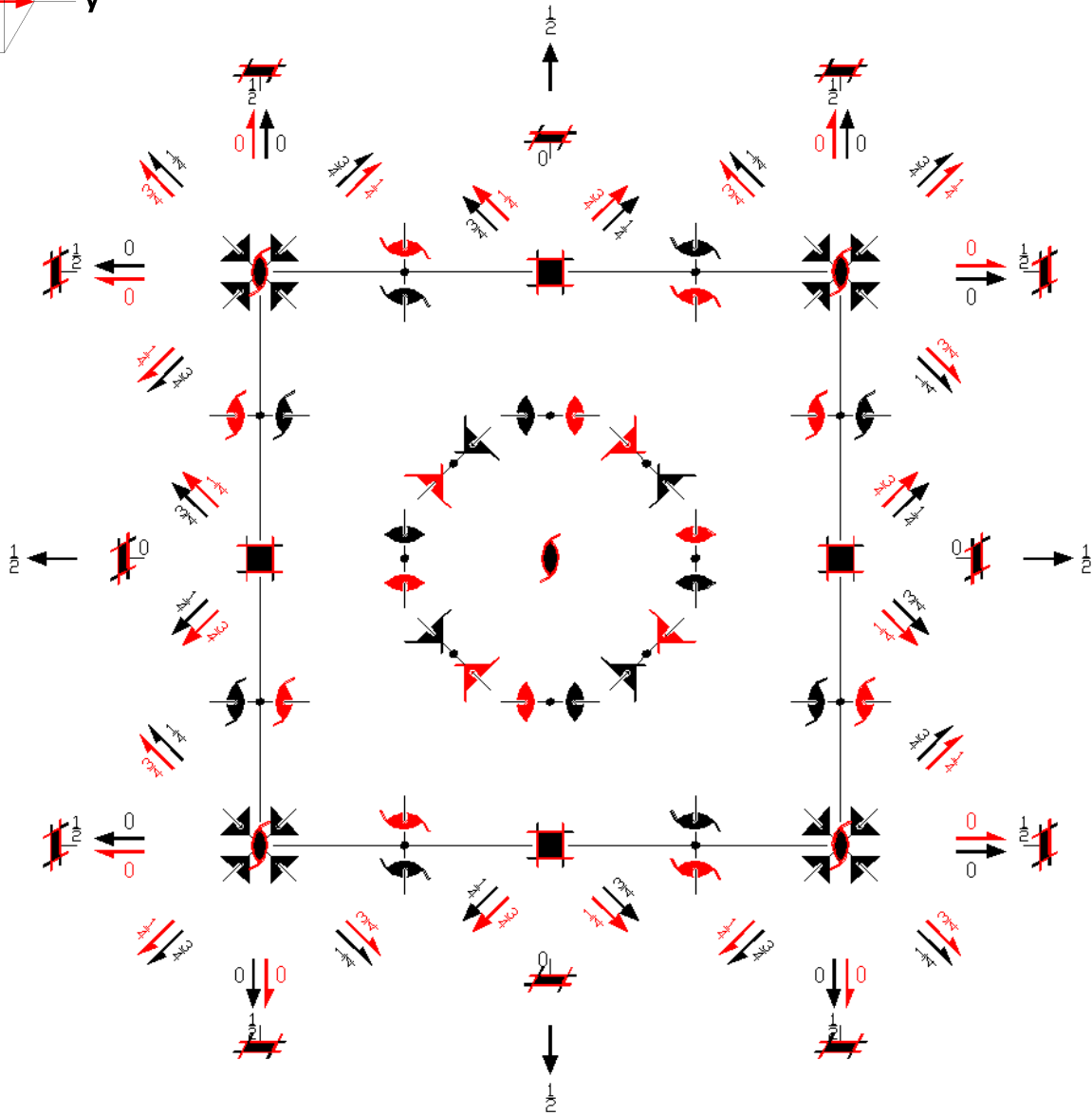
$P_F 4_2 32$

4321'

Cubic

208.4.1549

$P_F 4_2 32$



Origin at 23

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $-1/4 \leq z \leq 1/4;$   $\max(-x, x-1/2, -y, y-1/2) \leq z \leq \min(x, 1/2-x, y, 1/2-y)$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $0,1/2,0$   $1/4,1/4,1/4$   $1/4,1/4,-1/4$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0)              |

- |  |  |  |  |
|--|--|--|--|
| (13) $2 (1/2, 1/2, 0) \quad x, x, 1/4$<br>$(2_{xy}   1/2, 1/2, 1/2)$   | (14) $2 \quad x, \bar{x}+1/2, 1/4$<br>$(2_{\bar{xy}}   1/2, 1/2, 1/2)$ | (15) $4^- (0, 0, 1/2) \quad 1/2, 0, z$<br>$(4_z^{-1}   1/2, 1/2, 1/2)$ | (16) $4^+ (0, 0, 1/2) \quad 0, 1/2, z$<br>$(4_z   1/2, 1/2, 1/2)$      |
| (17) $4^- (1/2, 0, 0) \quad x, 1/2, 0$<br>$(4_x^{-1}   1/2, 1/2, 1/2)$ | (18) $2 (0, 1/2, 1/2) \quad 1/4, y, y$<br>$(2_{yz}   1/2, 1/2, 1/2)$   | (19) $2 \quad 1/4, y+1/2, \bar{y}$<br>$(2_{\bar{yz}}   1/2, 1/2, 1/2)$ | (20) $4^+ (1/2, 0, 0) \quad x, 0, 1/2$<br>$(4_x   1/2, 1/2, 1/2)$      |
| (21) $4^+ (0, 1/2, 0) \quad 1/2, y, 0$<br>$(4_y   1/2, 1/2, 1/2)$      | (22) $2 (1/2, 0, 1/2) \quad x, 1/4, x$<br>$(2_{xz}   1/2, 1/2, 1/2)$   | (23) $4^- (0, 1/2, 0) \quad 0, y, 1/2$<br>$(4_y^{-1}   1/2, 1/2, 1/2)$ | (24) $2 \quad \bar{x}+1/2, 1/4, x$<br>$(2_{\bar{xz}}   1/2, 1/2, 1/2)$ |

For (1,0,0)<sup>l</sup> + set

- |   |   |   |  |
|---|---|---|--|
| (1) $t^l (1, 0, 0)$<br>$(1   1, 0, 0)^l$  | (2) $2^l \quad 1/2, 0, z$<br>$(2_z   1, 0, 0)^l$  | (3) $2^l \quad 1/2, y, 0$<br>$(2_y   1, 0, 0)^l$  | (4) $2^l (1, 0, 0) \quad x, 0, 0$<br>$(2_x   1, 0, 0)^l$   |
| (5) $3^{+l} (1/3, 1/3, 1/3)$<br>$x+2/3, x+1/3, x$<br>$(3_{xyz}   1, 0, 0)^l$      | (6) $3^{+l} (1/3, -1/3, 1/3)$<br>$\bar{x}+2/3, x-1/3, \bar{x}$<br>$(3_{\bar{xyz}}^{-1}   1, 0, 0)^l$    | (7) $3^{+l} (1/3, -1/3, -1/3)$<br>$x+2/3, \bar{x}-1/3, \bar{x}$<br>$(3_{\bar{xyz}}^{-1}   1, 0, 0)^l$ | (8) $3^{+l} (1/3, 1/3, -1/3)$<br>$\bar{x}+2/3, \bar{x}-1/3, x$<br>$(3_{x\bar{y}z}^{-1}   1, 0, 0)^l$ |
| (9) $3^{-l} (1/3, 1/3, 1/3)$<br>$x+1/3, x-1/3, x$<br>$(3_{xyz}^{-1}   1, 0, 0)^l$ | (10) $3^{-l} (1/3, -1/3, -1/3)$<br>$\bar{x}+1/3, \bar{x}+1/3, \bar{x}$<br>$(3_{\bar{xyz}}   1, 0, 0)^l$ | (11) $3^{-l} (1/3, 1/3, -1/3)$<br>$\bar{x}+1/3, \bar{x}-1/3, x$<br>$(3_{x\bar{y}z}   1, 0, 0)^l$      | (12) $3^{-l} (1/3, -1/3, 1/3)$<br>$\bar{x}+1/3, x+1/3, \bar{x}$<br>$(3_{x\bar{y}z}   1, 0, 0)^l$     |
| (13) $2^l \quad x+1/2, x, 1/4$<br>$(2_{xy}   3/2, 1/2, 1/2)^l$                    | (14) $2^l (1/2, 1/2, 0) \quad x, \bar{x}, 1/4$<br>$(2_{\bar{xy}}   3/2, 1/2, 1/2)^l$                    | (15) $4^- (0, 0, 1/2) \quad 1, -1/2, z$<br>$(4_z^{-1}   3/2, 1/2, 1/2)^l$                             | (16) $4^+ (0, 0, 1/2) \quad 1/2, 1, z$<br>$(4_z   3/2, 1/2, 1/2)^l$                                  |
| (17) $4^- (3/2, 0, 0) \quad x, 1/2, 0$<br>$(4_x^{-1}   3/2, 1/2, 1/2)^l$          | (18) $2^l (0, 1/2, 1/2) \quad 3/4, y, y$<br>$(2_{yz}   3/2, 1/2, 1/2)^l$                                | (19) $2^l \quad 3/4, y+1/2, \bar{y}$<br>$(2_{\bar{yz}}   3/2, 1/2, 1/2)^l$                            | (20) $4^+ (3/2, 0, 0) \quad x, 0, 1/2$<br>$(4_x   3/2, 1/2, 1/2)^l$                                  |
| (21) $4^+ (0, 1/2, 0) \quad 1, y, -1/2$<br>$(4_y   3/2, 1/2, 1/2)^l$              | (22) $2^l \quad x+1/2, 1/4, x$<br>$(2_{xz}   3/2, 1/2, 1/2)^l$  | (23) $4^- (0, 1/2, 0) \quad 1/2, y, 1$<br>$(4_y^{-1}   3/2, 1/2, 1/2)^l$                              | (24) $2^l (1/2, 0, -1/2) \quad \bar{x}+1, 1/4, x$<br>$(2_{\bar{xz}}   3/2, 1/2, 1/2)^l$              |

Generators selected (1); t<sup>l</sup>(1,0,0); t<sup>l</sup>(0,1,0); t<sup>l</sup>(0,0,1); (2); (3); (5); (13).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

- |  |  |  |  |                        |
|--|--|--|--|------------------------|
| 48   | m  | 1  | (0,0,0) +  | (1,0,0) <sup>l</sup> + |
| (1) x, y, z [u, v, w]                                | (2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]                          | (3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]                          | (4) $x, \bar{y}, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]                          |                        |
| (5) z, x, y [w, u, v]                                | (6) $z, \bar{x}, \bar{y}$ [ $w, \bar{u}, \bar{v}$ ]                          | (7) $\bar{z}, \bar{x}, y$ [ $\bar{w}, \bar{u}, v$ ]                          | (8) $\bar{z}, x, \bar{y}$ [ $\bar{w}, u, \bar{v}$ ]                          |                        |
| (9) y, z, x [v, w, u]                                | (10) $\bar{y}, z, \bar{x}$ [ $\bar{v}, w, \bar{u}$ ]                         | (11) $y, \bar{z}, \bar{x}$ [ $v, \bar{w}, \bar{u}$ ]                         | (12) $\bar{y}, \bar{z}, x$ [ $\bar{v}, \bar{w}, u$ ]                         |                        |
| (13) $y+1/2, x+1/2, \bar{z}+1/2$ [ $v, u, \bar{w}$ ] | (14) $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2$ [ $\bar{v}, \bar{u}, \bar{w}$ ] | (15) $y+1/2, \bar{x}+1/2, z+1/2$ [ $v, \bar{u}, w$ ]                         | (16) $\bar{y}+1/2, x+1/2, z+1/2$ [ $\bar{v}, u, w$ ]                         |                        |
| (17) $x+1/2, z+1/2, \bar{y}+1/2$ [ $u, w, \bar{v}$ ] | (18) $\bar{x}+1/2, z+1/2, y+1/2$ [ $\bar{u}, w, v$ ]                         | (19) $\bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2$ [ $\bar{u}, \bar{w}, \bar{v}$ ] | (20) $x+1/2, \bar{z}+1/2, y+1/2$ [ $u, \bar{w}, v$ ]                         |                        |
| (21) $z+1/2, y+1/2, \bar{x}+1/2$ [ $w, v, \bar{u}$ ] | (22) $z+1/2, \bar{y}+1/2, x+1/2$ [ $w, \bar{v}, u$ ]                         | (23) $\bar{z}+1/2, y+1/2, x+1/2$ [ $\bar{w}, v, u$ ]                         | (24) $\bar{z}+1/2, \bar{y}+1/2, \bar{x}+1/2$ [ $\bar{w}, \bar{v}, \bar{u}$ ] |                        |

24	l	..2'	1/4,y,y+1/2 [u,v,v̄] y+1/2,1/4,y [v̄,u,v] y,y+1/2,1/4 [v,v̄,u]	3/4,ȳ,y+1/2 [u,v,v] y+1/2,3/4,ȳ [v,u,v] ȳ,y+1/2,3/4 [v,v,u]	3/4,y,ȳ+1/2 [ū,v,v] ȳ+1/2,3/4,y [v,ū,v] y,ȳ+1/2,3/4 [v,v,ū]	1/4,ȳ,ȳ+1/2 [ū,v,v̄] ȳ+1/2,1/4,ȳ [v̄,ū,v] ȳ,ȳ+1/2,1/4 [v,v̄,ū]
24	k	..2	1/4,y,ȳ+1/2 [0,v̄,v] ȳ+1/2,1/4,y [v,0,v̄] y,ȳ+1/2,1/4 [v̄,v,0]	3/4,ȳ,ȳ+1/2 [0,v̄,v̄] ȳ+1/2,3/4,ȳ [v̄,0,v̄] ȳ,ȳ+1/2,3/4 [v̄,v̄,0]	3/4,y,y+1/2 [0,v̄,v̄] y+1/2,3/4,y [v̄,0,v̄] y,y+1/2,3/4 [v̄,v̄,0]	1/4,ȳ,y+1/2 [0,v̄,v] y+1/2,1/4,ȳ [v,0,v̄] ȳ,y+1/2,1/4 [v̄,v,0]
24	j	2'..	x,1/2,0 [0,v,w] 1/2,0,x [v,w,0] x+1/2,1/2,0 [0,w,v̄]	x̄,1/2,0 [0,v,w̄] 1/2,0,x̄ [v,w̄,0] x̄+1/2,1/2,0 [0,w̄,v̄]	0,x,1/2 [w,0,v] 0,x+1/2,1/2 [v,0,w̄] 1/2,0,x̄+1/2 [w,v,0]	0,x̄,1/2 [w̄,0,v] 0,x̄+1/2,1/2 [v,0,w] 1/2,0,x+1/2 [w̄,v,0]
24	i	2'..	x,0,1/2 [0,v,w] 0,1/2,x [v,w,0] x+1/2,0,1/2 [0,w̄,v]	x̄,0,1/2 [0,v̄,w] 0,1/2,x̄ [v̄,w,0] x̄+1/2,0,1/2 [0,w̄,v̄]	1/2,x,0 [w,0,v] 1/2,x+1/2,0 [v,0,w̄] 0,1/2,x̄+1/2 [w̄,v̄,0]	1/2,x̄,0 [w,0,v̄] 1/2,x̄+1/2,0 [v̄,0,w̄] 0,1/2,x+1/2 [w,v̄,0]
24	h	2..	x,0,0 [u,0,0] 0,0,x [0,0,u] x+1/2,1/2,1/2 [u,0,0]	x̄,0,0 [ū,0,0] 0,0,x̄ [0,0,ū] x̄+1/2,1/2,1/2 [ū,0,0]	0,x,0 [0,u,0] 1/2,x+1/2,1/2 [0,u,0] 1/2,1/2,x̄+1/2 [0,0,ū]	0,x̄,0 [0,ū,0] 1/2,x̄+1/2,1/2 [0,ū,0] 1/2,1/2,x+1/2 [0,0,u]
16	g	.3.	x,x,x [u,u,u] x+1/2,x+1/2,x̄+1/2 [u,u,ū] x+1/2,x̄+1/2,x+1/2 [u,ū,u]	x̄,x̄,x̄ [ū,ū,ū] x̄+1/2,x̄+1/2,x̄+1/2 [ū,ū,ū] x̄+1/2,x+1/2,x+1/2 [ū,u,u]		
12	f	2'.2'2	1/4,1/2,0 [0,v̄,v] 0,3/4,1/2 [v,0,v]	3/4,1/2,0 [0,v,v] 1/2,0,1/4 [v̄,v,0]	0,1/4,1/2 [v,0,v̄] 1/2,0,3/4 [v,v,0]	
12	e	2'.2'2	1/4,0,1/2 [0,v̄,v] 1/2,3/4,0 [v̄,0,v̄]	3/4,0,1/2 [0,v̄,v̄] 0,1/2,1/4 [v̄,v,0]	1/2,1/4,0 [v,0,v̄] 0,1/2,3/4 [v̄,v̄,0]	
12	d	22'2'..	0,1/2,1/2 [u,0,0] 0,1/2,0 [0,ū,0]	1/2,0,1/2 [0,u,0] 1/2,0,0 [ū,0,0]	1/2,1/2,0 [0,0,u] 0,0,1/2 [0,0,ū]	
8	c	.32'	3/4,3/4,3/4 [u,u,u]	1/4,1/4,3/4 [ū,ū,u]	1/4,3/4,1/4 [ū,u,ū]	3/4,1/4,1/4 [u,ū,ū]
8	b	.32	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]
4	a	23.	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'

$$\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}$$

Origin at 0,1/2,z

Along [1,1,1] p3m11'

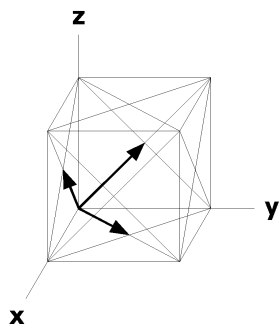
$$\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3 \quad \mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$$

Origin at x,x,x

Along [1,1,0] p<sub>c</sub>-2mm

$$\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}$$

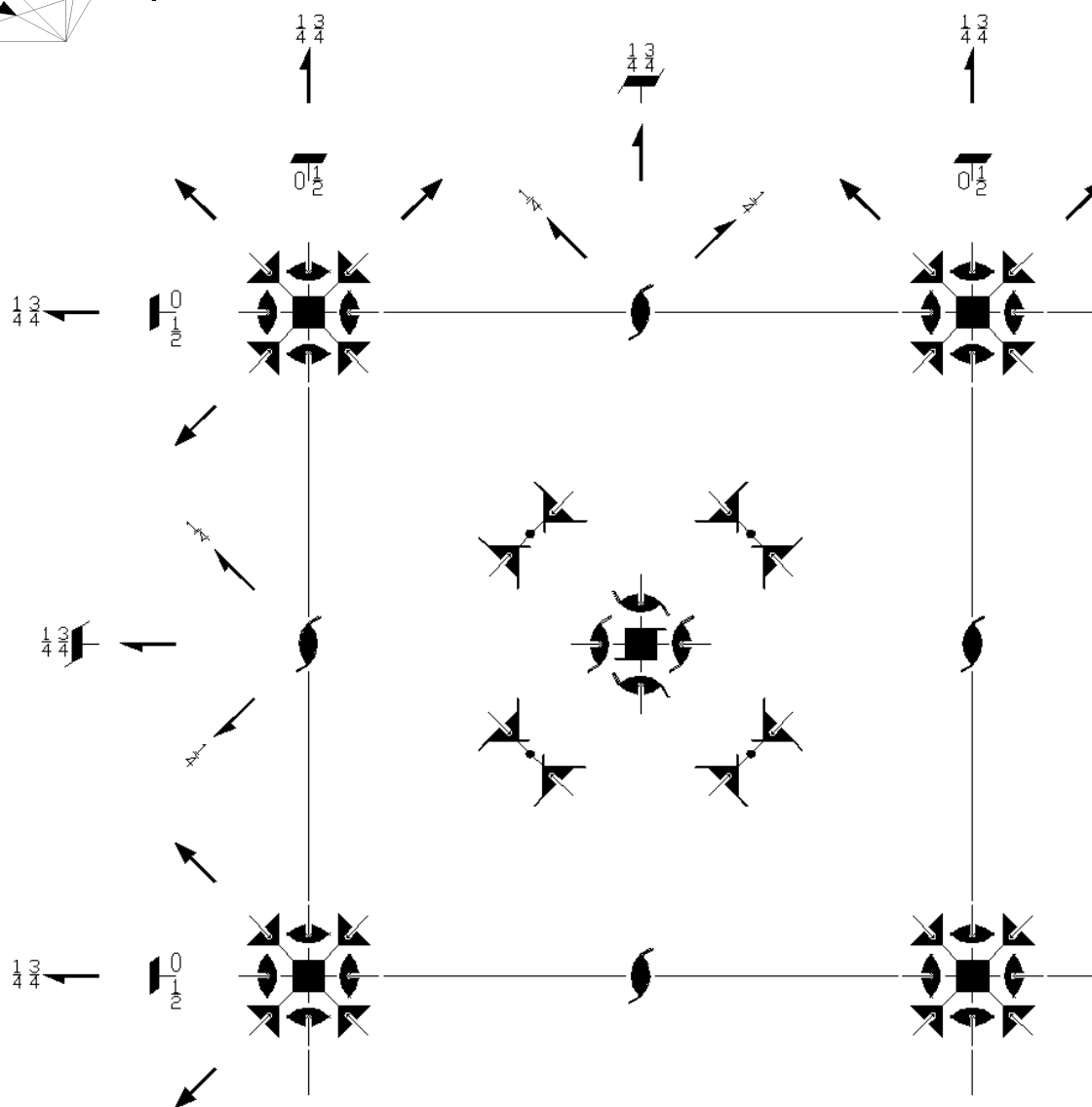
Origin at x-1/4,x+1/4,3/4



F432  
209.1.1550

432  
F432

Cubic



Origin at 432

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $-1/4 \leq z \leq 1/4$ ;  $y \leq \min(x, 1/2-x)$ ;  $-y \leq z \leq y$

Vertices 0,0,0      1/2,0,0      1/4,1/4,1/4      1/4,1/4,-1/4

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)              | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub>xyz<sup>-1</sup></sub>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz<sup>-1</sup></sub>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>xyz<sup>-1</sup></sub>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz<sup>-1</sup></sub>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)            | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>xyz</sub>  0,0,0)             | (12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)              |

- |   |   |   |   |
|---|---|---|---|
| (13) $2 \begin{array}{c} x,x,0 \\ (2_{xy} 0,0,0) \end{array}$     | (14) $2 \begin{array}{c} x,\bar{x},0 \\ (2_{xy} 0,0,0) \end{array}$ | (15) $4^- \begin{array}{c} 0,0,z \\ (4_z^{-1} 0,0,0) \end{array}$   | (16) $4^+ \begin{array}{c} 0,0,z \\ (4_z 0,0,0) \end{array}$        |
| (17) $4^- \begin{array}{c} x,0,0 \\ (4_x^{-1} 0,0,0) \end{array}$ | (18) $2 \begin{array}{c} 0,y,y \\ (2_{yz} 0,0,0) \end{array}$       | (19) $2 \begin{array}{c} 0,y,\bar{y} \\ (2_{yz} 0,0,0) \end{array}$ | (20) $4^+ \begin{array}{c} x,0,0 \\ (4_x 0,0,0) \end{array}$        |
| (21) $4^+ \begin{array}{c} 0,y,0 \\ (4_y 0,0,0) \end{array}$      | (22) $2 \begin{array}{c} x,0,x \\ (2_{xz} 0,0,0) \end{array}$       | (23) $4^- \begin{array}{c} 0,y,0 \\ (4_y^{-1} 0,0,0) \end{array}$   | (24) $2 \begin{array}{c} \bar{x},0,x \\ (2_{xz} 0,0,0) \end{array}$ |

For (0,1/2,1/2) + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t \begin{array}{c} (0,1/2,1/2) \\ (1 0,1/2,1/2) \end{array}$                                 | (2) $2 \begin{array}{c} (0,0,1/2) \quad 0,1/4,z \\ (2_z 0,1/2,1/2) \end{array}$                            | (3) $2 \begin{array}{c} (0,1/2,0) \quad 0,y,1/4 \\ (2_y 0,1/2,1/2) \end{array}$                                      | (4) $2 \begin{array}{c} x,1/4,1/4 \\ (2_x 0,1/2,1/2) \end{array}$                              |
| (5) $3^+ \begin{array}{c} (1/3,1/3,1/3) \\ x-1/3,x-1/6,x \\ (3_{xyz} 0,1/2,1/2) \end{array}$      | (6) $3^+ \begin{array}{c} \bar{x},x+1/2,\bar{x} \\ (3_{x\bar{y}z}^{-1} 0,1/2,1/2) \end{array}$             | (7) $3^+ \begin{array}{c} (-1/3,1/3,1/3) \\ x+1/3,\bar{x}-1/6,\bar{x} \\ (3_{x\bar{y}z}^{-1} 0,1/2,1/2) \end{array}$ | (8) $3^+ \begin{array}{c} \bar{x},\bar{x}+1/2,x \\ (3_{x\bar{y}z}^{-1} 0,1/2,1/2) \end{array}$ |
| (9) $3^- \begin{array}{c} (1/3,1/3,1/3) \\ x-1/6,x+1/6,x \\ (3_{xyz}^{-1} 0,1/2,1/2) \end{array}$ | (10) $3^- \begin{array}{c} (-1/3,1/3,1/3) \\ x+1/6,\bar{x}+1/6,\bar{x} \\ (3_{xyz} 0,1/2,1/2) \end{array}$ | (11) $3^- \begin{array}{c} \bar{x}+1/2,\bar{x}+1/2,x \\ (3_{x\bar{y}z} 0,1/2,1/2) \end{array}$                       | (12) $3^- \begin{array}{c} \bar{x}-1/2,x+1/2,\bar{x} \\ (3_{x\bar{y}z} 0,1/2,1/2) \end{array}$ |
| (13) $2 \begin{array}{c} (1/4,1/4,0) \quad x,x+1/4,1/4 \\ (2_{xy} 0,1/2,1/2) \end{array}$         | (14) $2 \begin{array}{c} (-1/4,1/4,0) \quad x,\bar{x}+1/4,1/4 \\ (2_{xy} 0,1/2,1/2) \end{array}$           | (15) $4^- \begin{array}{c} (0,0,1/2) \quad 1/4,1/4,z \\ (4_z^{-1} 0,1/2,1/2) \end{array}$                            | (16) $4^+ \begin{array}{c} (0,0,1/2) \quad -1/4,1/4,z \\ (4_z 0,1/2,1/2) \end{array}$          |
| (17) $4^- \begin{array}{c} x,1/2,0 \\ (4_x^{-1} 0,1/2,1/2) \end{array}$                           | (18) $2 \begin{array}{c} (0,1/2,1/2) \quad 0,y,y \\ (2_{yz} 0,1/2,1/2) \end{array}$                        | (19) $2 \begin{array}{c} 0,y+1/2,\bar{y} \\ (2_{yz} 0,1/2,1/2) \end{array}$  | (20) $4^+ \begin{array}{c} x,0,1/2 \\ (4_x 0,1/2,1/2) \end{array}$                             |
| (21) $4^+ \begin{array}{c} (0,1/2,0) \quad 1/4,y,1/4 \\ (4_y 0,1/2,1/2) \end{array}$              | (22) $2 \begin{array}{c} (1/4,0,1/4) \quad x-1/4,1/4,x \\ (2_{xz} 0,1/2,1/2) \end{array}$                  | (23) $4^- \begin{array}{c} (0,1/2,0) \quad -1/4,y,1/4 \\ (4_y^{-1} 0,1/2,1/2) \end{array}$                           | (24) $2 \begin{array}{c} (-1/4,0,1/4)\bar{x}+1/4,1/4,x \\ (2_{xz} 0,1/2,1/2) \end{array}$      |

For (1/2,0,1/2) + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t \begin{array}{c} (1/2,0,1/2) \\ (1 1/2,0,1/2) \end{array}$                                 | (2) $2 \begin{array}{c} (0,0,1/2) \quad 1/4,0,z \\ (2_z 1/2,0,1/2) \end{array}$                                      | (3) $2 \begin{array}{c} 1/4,y,1/4 \\ (2_y 1/2,0,1/2) \end{array}$                                  | (4) $2 \begin{array}{c} (1/2,0,0) \quad x,0,1/4 \\ (2_x 1/2,0,1/2) \end{array}$                                  |
| (5) $3^+ \begin{array}{c} (1/3,1/3,1/3) \\ x+1/6,x-1/6,x \\ (3_{xyz} 1/2,0,1/2) \end{array}$      | (6) $3^+ \begin{array}{c} (1/3,-1/3,1/3) \\ \bar{x}+1/6,x+1/6,\bar{x} \\ (3_{x\bar{y}z}^{-1} 1/2,0,1/2) \end{array}$ | (7) $3^+ \begin{array}{c} x+1/2,\bar{x}-1/2,\bar{x} \\ (3_{x\bar{y}z}^{-1} 1/2,0,1/2) \end{array}$ | (8) $3^+ \begin{array}{c} \bar{x}+1/2,\bar{x}+1/2,x \\ (3_{x\bar{y}z}^{-1} 1/2,0,1/2) \end{array}$               |
| (9) $3^- \begin{array}{c} (1/3,1/3,1/3) \\ x-1/6,x-1/3,x \\ (3_{xyz}^{-1} 1/2,0,1/2) \end{array}$ | (10) $3^- \begin{array}{c} x+1/2,\bar{x},\bar{x} \\ (3_{x\bar{y}z} 1/2,0,1/2) \end{array}$                           | (11) $3^- \begin{array}{c} \bar{x}+1/2,\bar{x},x \\ (3_{x\bar{y}z} 1/2,0,1/2) \end{array}$         | (12) $3^- \begin{array}{c} (1/3,-1/3,1/3) \\ \bar{x}-1/6,x+1/3,\bar{x} \\ (3_{x\bar{y}z} 1/2,0,1/2) \end{array}$ |
| (13) $2 \begin{array}{c} (1/4,1/4,0) \quad x,x-1/4,1/4 \\ (2_{xy} 1/2,0,1/2) \end{array}$         | (14) $2 \begin{array}{c} (1/4,-1/4,0) \quad x,\bar{x}+1/4,1/4 \\ (2_{xy} 1/2,0,1/2) \end{array}$                     | (15) $4^- \begin{array}{c} (0,0,1/2) \quad 1/4,-1/4,z \\ (4_z^{-1} 1/2,0,1/2) \end{array}$         | (16) $4^+ \begin{array}{c} (0,0,1/2) \quad 1/4,1/4,z \\ (4_z 1/2,0,1/2) \end{array}$                             |
| (17) $4^- \begin{array}{c} (1/2,0,0) \quad x,1/4,1/4 \\ (4_x^{-1} 1/2,0,1/2) \end{array}$         | (18) $2 \begin{array}{c} (0,1/4,1/4) \quad 1/4,y-1/4,y \\ (2_{yz} 1/2,0,1/2) \end{array}$                            | (19) $2 \begin{array}{c} (0,-1/4,1/4) \quad 1/4,y+1/4,\bar{y} \\ (2_{yz} 1/2,0,1/2) \end{array}$   | (20) $4^+ \begin{array}{c} (1/2,0,0) \quad x,-1/4,1/4 \\ (4_x 1/2,0,1/2) \end{array}$                            |
| (21) $4^+ \begin{array}{c} 1/2,y,0 \\ (4_y 1/2,0,1/2) \end{array}$                                | (22) $2 \begin{array}{c} (1/2,0,1/2) \quad x,0,x \\ (2_{xz} 1/2,0,1/2) \end{array}$                                  | (23) $4^- \begin{array}{c} 0,y,1/2 \\ (4_y^{-1} 1/2,0,1/2) \end{array}$                            | (24) $2 \begin{array}{c} \bar{x}+1/2,0,x \\ (2_{xz} 1/2,0,1/2) \end{array}$                                      |

## For (1/2,1/2,0) + set

(1) $t(1/2,1/2,0)$ (1   1/2,1/2,0)	(2) $2(1/4,1/4,z)$ (2 <sub>z</sub>   1/2,1/2,0)	(3) $2(0,1/2,0) 1/4,y,0$ (2 <sub>y</sub>   1/2,1/2,0)	(4) $2(1/2,0,0) x,1/4,0$ (2 <sub>x</sub>   1/2,1/2,0)
(5) $3^+(1/3,1/3,1/3)$ $x+1/6,x+1/3,x$ (3 <sub>xyz</sub>   1/2,1/2,0)	(6) $3^+ \bar{x}+1/2,x,\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(7) $3^+ x+1/2,\bar{x},\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(8) $3^+(1/3,1/3,-1/3)$ $\bar{x}+1/6,\bar{x}+1/3,x$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)
(9) $3^-(1/3,1/3,1/3)$ $x+1/3,x+1/6,x$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) $3^- x,\bar{x}+1/2,\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)	(11) $3^-(1/3,1/3,-1/3)$ $\bar{x}+1/3,\bar{x}+1/6,x$ (3 <sub>xyz</sub>   1/2,1/2,0)	(12) $3^- \bar{x},x+1/2,\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)
(13) $2(1/2,1/2,0) x,x,0$ (2 <sub>xy</sub>   1/2,1/2,0)	(14) $2(x,\bar{x}+1/2,0)$ (2 <sub>xy</sub>   1/2,1/2,0)	(15) $4^-(1/2,0,z)$ (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,0)	(16) $4^+ 0,1/2,z$ (4 <sub>z</sub>   1/2,1/2,0)
(17) $4^-(1/2,0,0) x,1/4,-1/4$ (4 <sub>x</sub> <sup>-1</sup>   1/2,1/2,0)	(18) $2(0,1/4,1/4) 1/4,y+1/4,y$ (2 <sub>yz</sub>   1/2,1/2,0)	(19) $2(0,1/4,-1/4) 1/4,y+1/4,\bar{y}$ (2 <sub>yz</sub>   1/2,1/2,0)	(20) $4^+(1/2,0,0) x,1/4,1/4$ (4 <sub>x</sub>   1/2,1/2,0)
(21) $4^+(0,1/2,0) 1/4,y,-1/4$ (4 <sub>y</sub>   1/2,1/2,0)	(22) $2(1/4,0,1/4) x+1/4,1/4,x$ (2 <sub>xz</sub>   1/2,1/2,0)	(23) $4^-(0,1/2,0) 1/4,y,1/4$ (4 <sub>y</sub> <sup>-1</sup>   1/2,1/2,0)	(24) $2(1/4,0,-1/4)\bar{x}+1/4,1/4,x$ (2 <sub>xz</sub>   1/2,1/2,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

		(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
96	j 1				
(1)	$x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $\bar{x},y,\bar{z} [\bar{u},v,\bar{w}]$	(4) $x,\bar{y},\bar{z} [u,\bar{v},\bar{w}]$	
(5)	$z,x,y [w,u,v]$	(6) $z,\bar{x},\bar{y} [w,\bar{u},\bar{v}]$	(7) $\bar{z},\bar{x},y [\bar{w},\bar{u},v]$	(8) $\bar{z},x,\bar{y} [\bar{w},u,\bar{v}]$	
(9)	$y,z,x [v,w,u]$	(10) $\bar{y},z,\bar{x} [\bar{v},w,\bar{u}]$	(11) $y,\bar{z},\bar{x} [v,\bar{w},\bar{u}]$	(12) $\bar{y},\bar{z},x [\bar{v},\bar{w},u]$	
(13)	$y,x,\bar{z} [v,u,\bar{w}]$	(14) $\bar{y},\bar{x},\bar{z} [\bar{v},\bar{u},\bar{w}]$	(15) $y,\bar{x},z [v,\bar{u},w]$	(16) $\bar{y},x,z [\bar{v},u,w]$	
(17)	$x,z,\bar{y} [u,w,\bar{v}]$	(18) $\bar{x},z,y [\bar{u},w,v]$	(19) $\bar{x},\bar{z},\bar{y} [\bar{u},\bar{w},\bar{v}]$	(20) $x,\bar{z},y [u,\bar{w},v]$	
(21)	$z,y,\bar{x} [w,v,\bar{u}]$	(22) $z,\bar{y},x [w,\bar{v},u]$	(23) $\bar{z},y,x [\bar{w},v,u]$	(24) $\bar{z},\bar{y},\bar{x} [\bar{w},\bar{v},\bar{u}]$	
48	i 2..	$x,1/4,1/4 [u,0,0]$	$\bar{x},3/4,1/4 [\bar{u},0,0]$	$1/4,x,1/4 [0,u,0]$	$1/4,\bar{x},3/4 [0,\bar{u},0]$
		$1/4,1/4,x [0,0,u]$	$3/4,1/4,\bar{x} [0,0,\bar{u}]$	$1/4,x,3/4 [0,u,0]$	$3/4,\bar{x},3/4 [0,\bar{u},0]$
		$x,1/4,3/4 [u,0,0]$	$\bar{x},1/4,1/4 [\bar{u},0,0]$	$1/4,1/4,\bar{x} [0,0,\bar{u}]$	$1/4,3/4,x [0,0,u]$
48	h ..2	$1/2,y,y [0,v,v]$	$1/2,\bar{y},y [0,\bar{v},v]$	$1/2,y,\bar{y} [0,v,\bar{v}]$	$1/2,\bar{y},\bar{y} [0,\bar{v},\bar{v}]$
		$y,1/2,y [v,0,v]$	$y,1/2,\bar{y} [v,0,\bar{v}]$	$\bar{y},1/2,y [\bar{v},0,v]$	$\bar{y},1/2,\bar{y} [\bar{v},0,\bar{v}]$
		$y,y,1/2 [v,v,0]$	$\bar{y},y,1/2 [\bar{v},v,0]$	$y,\bar{y},1/2 [v,\bar{v},0]$	$\bar{y},\bar{y},1/2 [\bar{v},\bar{v},0]$

48	g	..2	0,y,y [0,v,v] y,0,y [v,0,v] y,y,0 [v,v,0]	$0,\bar{y},y$ [0, $\bar{v}$ ,v] $y,0,\bar{y}$ [v,0, $\bar{v}$ ] $\bar{y},y,0$ [ $\bar{v}$ ,v,0]	0,y, $\bar{y}$ [0,v, $\bar{v}$ ] $\bar{y},0,y$ [ $\bar{v}$ ,0,v] y, $\bar{y},0$ [v, $\bar{v}$ ,0]	0, $\bar{y},\bar{y}$ [0, $\bar{v},\bar{v}$ ] $\bar{y},0,\bar{y}$ [ $\bar{v},0,\bar{v}$ ] $\bar{y},\bar{y},0$ [ $\bar{v},\bar{v},0$ ]
32	f	.3.	x,x,x [u,u,u] x,x, $\bar{x}$ [u,u, $\bar{u}$ ]	$\bar{x},\bar{x},x$ [ $\bar{u},\bar{u},u$ ] $\bar{x},\bar{x},\bar{x}$ [ $\bar{u},\bar{u},\bar{u}$ ]	$\bar{x},x,\bar{x}$ [ $\bar{u},u,\bar{u}$ ] x, $\bar{x},x$ [u, $\bar{u},u$ ]	x, $\bar{x},\bar{x}$ [u, $\bar{u},\bar{u}$ ] $\bar{x},x,x$ [ $\bar{u},u,u$ ]
24	e	4..	x,0,0 [u,0,0] 0, $\bar{x}$ ,0 [0, $\bar{u}$ ,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ] 0,0,x [0,0,u]	0,x,0 [0,u,0] 0,0, $\bar{x}$ [0,0, $\bar{u}$ ]	
24	d	2.22	0,1/4,1/4 [0,0,0] 1/4,0,3/4 [0,0,0]	0,3/4,1/4 [0,0,0] 1/4,1/4,0 [0,0,0]	1/4,0,1/4 [0,0,0] 3/4,1/4,0 [0,0,0]	
8	c	23.	1/4,1/4,1/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]		
4	b	432	1/2,1/2,1/2 [0,0,0]			
4	a	432	0,0,0 [0,0,0]			

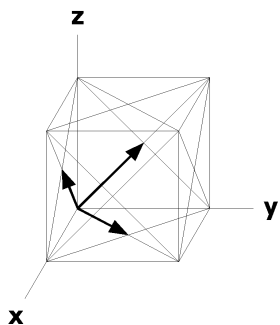
### Symmetry of Special Projections

Along [0,0,1]  $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,1,1]  $p3m'1$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

Along [1,1,0]  $c2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0

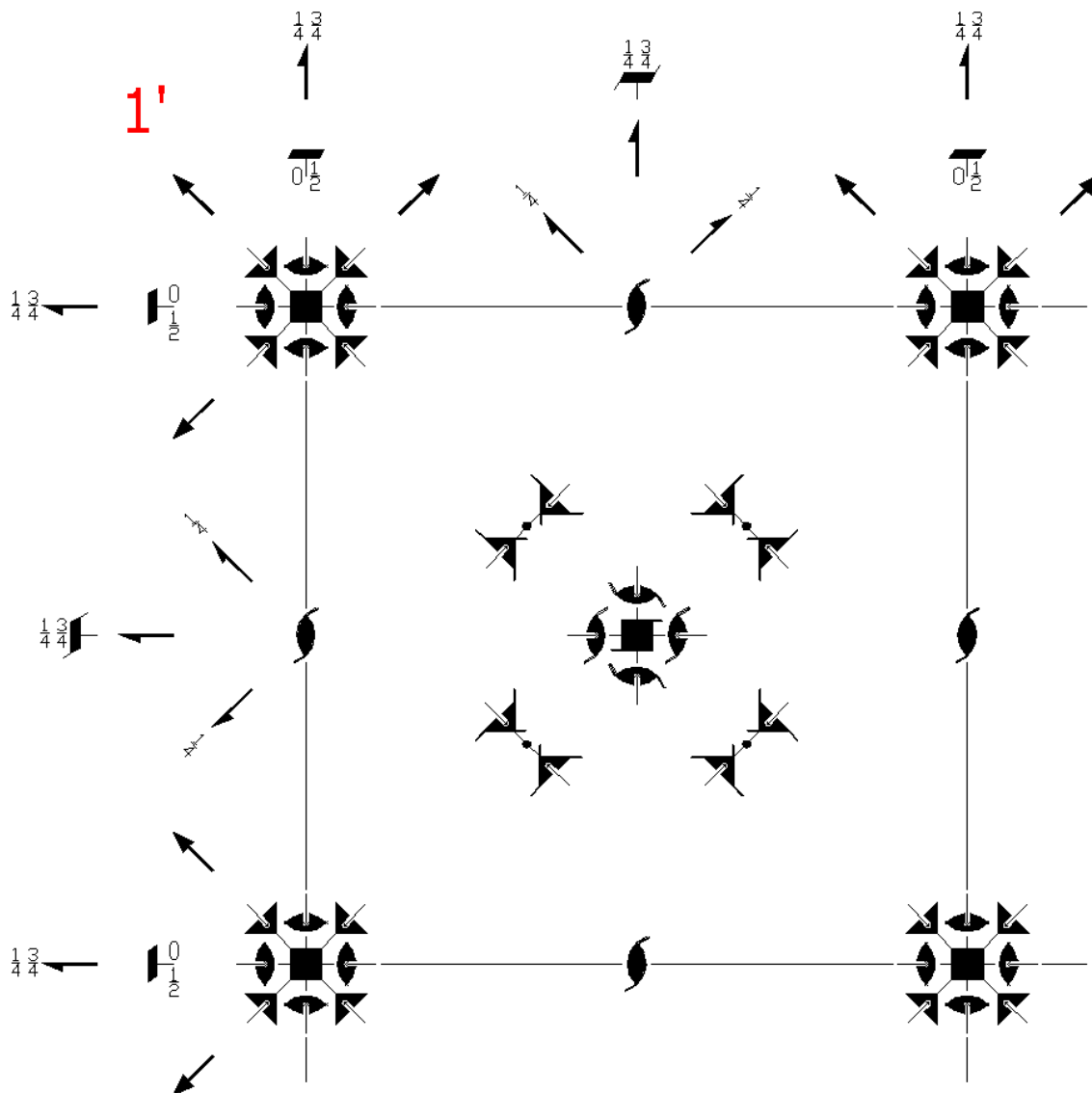




F4321'  
209.2.1551

4321'  
F4321'

Cubic



Origin at 4321'

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/4;$   $-1/4 \leq z \leq 1/4;$   $y \leq \min(x, 1/2-x);$   $-y \leq z \leq y$

Vertices  $0,0,0$   $1/2,0,0$   $1/4,1/4,1/4$   $1/4,1/4,-1/4$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)              |

- |   |   |   |   |
|---|---|---|---|
| (13) $2 \begin{array}{c} x,x,0 \\ (2_{xy} 0,0,0) \end{array}$     | (14) $2 \begin{array}{c} x,\bar{x},0 \\ (2_{xy} 0,0,0) \end{array}$ | (15) $4^- \begin{array}{c} 0,0,z \\ (4_z^{-1} 0,0,0) \end{array}$   | (16) $4^+ \begin{array}{c} 0,0,z \\ (4_z 0,0,0) \end{array}$        |
| (17) $4^- \begin{array}{c} x,0,0 \\ (4_x^{-1} 0,0,0) \end{array}$ | (18) $2 \begin{array}{c} 0,y,y \\ (2_{yz} 0,0,0) \end{array}$       | (19) $2 \begin{array}{c} 0,y,\bar{y} \\ (2_{yz} 0,0,0) \end{array}$ | (20) $4^+ \begin{array}{c} x,0,0 \\ (4_x 0,0,0) \end{array}$        |
| (21) $4^+ \begin{array}{c} 0,y,0 \\ (4_y 0,0,0) \end{array}$      | (22) $2 \begin{array}{c} x,0,x \\ (2_{xz} 0,0,0) \end{array}$       | (23) $4^- \begin{array}{c} 0,y,0 \\ (4_y^{-1} 0,0,0) \end{array}$   | (24) $2 \begin{array}{c} \bar{x},0,x \\ (2_{xz} 0,0,0) \end{array}$ |

For (0,1/2,1/2) + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t \begin{array}{c} (0,1/2,1/2) \\ (1 0,1/2,1/2) \end{array}$                                 | (2) $2 \begin{array}{c} (0,0,1/2) \quad 0,1/4,z \\ (2_z 0,1/2,1/2) \end{array}$                            | (3) $2 \begin{array}{c} (0,1/2,0) \quad 0,y,1/4 \\ (2_y 0,1/2,1/2) \end{array}$                                      | (4) $2 \begin{array}{c} x,1/4,1/4 \\ (2_x 0,1/2,1/2) \end{array}$                                |
| (5) $3^+ \begin{array}{c} (1/3,1/3,1/3) \\ x-1/3,x-1/6,x \\ (3_{xyz} 0,1/2,1/2) \end{array}$      | (6) $3^+ \begin{array}{c} \bar{x},x+1/2,\bar{x} \\ (3_{x\bar{y}z}^{-1} 0,1/2,1/2) \end{array}$             | (7) $3^+ \begin{array}{c} (-1/3,1/3,1/3) \\ x+1/3,\bar{x}-1/6,\bar{x} \\ (3_{x\bar{y}z}^{-1} 0,1/2,1/2) \end{array}$ | (8) $3^+ \begin{array}{c} \bar{x},\bar{x}+1/2,x \\ (3_{x\bar{y}z}^{-1} 0,1/2,1/2) \end{array}$   |
| (9) $3^- \begin{array}{c} (1/3,1/3,1/3) \\ x-1/6,x+1/6,x \\ (3_{xyz}^{-1} 0,1/2,1/2) \end{array}$ | (10) $3^- \begin{array}{c} (-1/3,1/3,1/3) \\ x+1/6,\bar{x}+1/6,\bar{x} \\ (3_{xyz} 0,1/2,1/2) \end{array}$ | (11) $3^- \begin{array}{c} \bar{x}+1/2,\bar{x}+1/2,x \\ (3_{x\bar{y}z} 0,1/2,1/2) \end{array}$                       | (12) $3^- \begin{array}{c} \bar{x}-1/2,x+1/2,\bar{x} \\ (3_{x\bar{y}z} 0,1/2,1/2) \end{array}$   |
| (13) $2 \begin{array}{c} (1/4,1/4,0) \quad x,x+1/4,1/4 \\ (2_{xy} 0,1/2,1/2) \end{array}$         | (14) $2 \begin{array}{c} (-1/4,1/4,0) \quad x,\bar{x}+1/4,1/4 \\ (2_{xy} 0,1/2,1/2) \end{array}$           | (15) $4^- \begin{array}{c} (0,0,1/2) \quad 1/4,1/4,z \\ (4_z^{-1} 0,1/2,1/2) \end{array}$                            | (16) $4^+ \begin{array}{c} (0,0,1/2) \quad -1/4,1/4,z \\ (4_z 0,1/2,1/2) \end{array}$            |
| (17) $4^- \begin{array}{c} x,1/2,0 \\ (4_x^{-1} 0,1/2,1/2) \end{array}$                           | (18) $2 \begin{array}{c} (0,1/2,1/2) \quad 0,y,y \\ (2_{yz} 0,1/2,1/2) \end{array}$                        | (19) $2 \begin{array}{c} 0,y+1/2,\bar{y} \\ (2_{yz} 0,1/2,1/2) \end{array}$  | (20) $4^+ \begin{array}{c} x,0,1/2 \\ (4_x 0,1/2,1/2) \end{array}$                               |
| (21) $4^+ \begin{array}{c} (0,1/2,0) \quad 1/4,y,1/4 \\ (4_y 0,1/2,1/2) \end{array}$              | (22) $2 \begin{array}{c} (1/4,0,1/4) \quad x-1/4,1/4,x \\ (2_{xz} 0,1/2,1/2) \end{array}$                  | (23) $4^- \begin{array}{c} (0,1/2,0) \quad -1/4,y,1/4 \\ (4_y^{-1} 0,1/2,1/2) \end{array}$                           | (24) $2 \begin{array}{c} (-1/4,0,1/4) \quad \bar{x}+1/4,1/4,x \\ (2_{xz} 0,1/2,1/2) \end{array}$ |

For (1/2,0,1/2) + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t \begin{array}{c} (1/2,0,1/2) \\ (1 1/2,0,1/2) \end{array}$                                 | (2) $2 \begin{array}{c} (0,0,1/2) \quad 1/4,0,z \\ (2_z 1/2,0,1/2) \end{array}$                                      | (3) $2 \begin{array}{c} 1/4,y,1/4 \\ (2_y 1/2,0,1/2) \end{array}$                                  | (4) $2 \begin{array}{c} (1/2,0,0) \quad x,0,1/4 \\ (2_x 1/2,0,1/2) \end{array}$                                  |
| (5) $3^+ \begin{array}{c} (1/3,1/3,1/3) \\ x+1/6,x-1/6,x \\ (3_{xyz} 1/2,0,1/2) \end{array}$      | (6) $3^+ \begin{array}{c} (1/3,-1/3,1/3) \\ \bar{x}+1/6,x+1/6,\bar{x} \\ (3_{x\bar{y}z}^{-1} 1/2,0,1/2) \end{array}$ | (7) $3^+ \begin{array}{c} x+1/2,\bar{x}-1/2,\bar{x} \\ (3_{x\bar{y}z}^{-1} 1/2,0,1/2) \end{array}$ | (8) $3^+ \begin{array}{c} \bar{x}+1/2,\bar{x}+1/2,x \\ (3_{x\bar{y}z}^{-1} 1/2,0,1/2) \end{array}$               |
| (9) $3^- \begin{array}{c} (1/3,1/3,1/3) \\ x-1/6,x-1/3,x \\ (3_{xyz}^{-1} 1/2,0,1/2) \end{array}$ | (10) $3^- \begin{array}{c} x+1/2,\bar{x},\bar{x} \\ (3_{x\bar{y}z} 1/2,0,1/2) \end{array}$                           | (11) $3^- \begin{array}{c} \bar{x}+1/2,\bar{x},x \\ (3_{x\bar{y}z} 1/2,0,1/2) \end{array}$         | (12) $3^- \begin{array}{c} (1/3,-1/3,1/3) \\ \bar{x}-1/6,x+1/3,\bar{x} \\ (3_{x\bar{y}z} 1/2,0,1/2) \end{array}$ |
| (13) $2 \begin{array}{c} (1/4,1/4,0) \quad x,x-1/4,1/4 \\ (2_{xy} 1/2,0,1/2) \end{array}$         | (14) $2 \begin{array}{c} (1/4,-1/4,0) \quad x,\bar{x}+1/4,1/4 \\ (2_{xy} 1/2,0,1/2) \end{array}$                     | (15) $4^- \begin{array}{c} (0,0,1/2) \quad 1/4,-1/4,z \\ (4_z^{-1} 1/2,0,1/2) \end{array}$         | (16) $4^+ \begin{array}{c} (0,0,1/2) \quad 1/4,1/4,z \\ (4_z 1/2,0,1/2) \end{array}$                             |
| (17) $4^- \begin{array}{c} (1/2,0,0) \quad x,1/4,1/4 \\ (4_x^{-1} 1/2,0,1/2) \end{array}$         | (18) $2 \begin{array}{c} (0,1/4,1/4) \quad 1/4,y-1/4,y \\ (2_{yz} 1/2,0,1/2) \end{array}$                            | (19) $2 \begin{array}{c} (0,-1/4,1/4) \quad 1/4,y+1/4,\bar{y} \\ (2_{yz} 1/2,0,1/2) \end{array}$   | (20) $4^+ \begin{array}{c} (1/2,0,0) \quad x,-1/4,1/4 \\ (4_x 1/2,0,1/2) \end{array}$                            |
| (21) $4^+ \begin{array}{c} 1/2,y,0 \\ (4_y 1/2,0,1/2) \end{array}$                                | (22) $2 \begin{array}{c} (1/2,0,1/2) \quad x,0,x \\ (2_{xz} 1/2,0,1/2) \end{array}$                                  | (23) $4^- \begin{array}{c} 0,y,1/2 \\ (4_y^{-1} 1/2,0,1/2) \end{array}$                            | (24) $2 \begin{array}{c} \bar{x}+1/2,0,x \\ (2_{xz} 1/2,0,1/2) \end{array}$                                      |

## For (1/2,1/2,0) + set

- |  |   |  |  |
|--|---|--|--|
| (1) $t \begin{pmatrix} 1/2, 1/2, 0 \\ 1   1/2, 1/2, 0 \end{pmatrix}$   | (2) $2 \begin{pmatrix} 1/4, 1/4, z \\ 2_z   1/2, 1/2, 0 \end{pmatrix}$  | (3) $2 \begin{pmatrix} 0, 1/2, 0 \\ 2_y   1/2, 1/2, 0 \end{pmatrix} \begin{matrix} 1/4, y, 0 \\ \end{matrix}$                        | (4) $2 \begin{pmatrix} 1/2, 0, 0 \\ 2_x   1/2, 1/2, 0 \end{pmatrix} \begin{matrix} x, 1/4, 0 \\ \end{matrix}$                        |
| (5) $3^+ \begin{pmatrix} 1/3, 1/3, 1/3 \\ x+1/6, x+1/3, x \\ 3_{xyz}   1/2, 1/2, 0 \end{pmatrix}$                        | (6) $3^+ \begin{pmatrix} \bar{x}+1/2, x, \bar{x} \\ 3_{\bar{xyz}}^{-1}   1/2, 1/2, 0 \end{pmatrix}$                     | (7) $3^+ \begin{pmatrix} x+1/2, \bar{x}, \bar{x} \\ 3_{\bar{xyz}}^{-1}   1/2, 1/2, 0 \end{pmatrix}$                                  | (8) $3^+ \begin{pmatrix} 1/3, 1/3, -1/3 \\ \bar{x}+1/6, \bar{x}+1/3, x \\ 3_{\bar{xyz}}^{-1}   1/2, 1/2, 0 \end{pmatrix}$            |
| (9) $3^- \begin{pmatrix} 1/3, 1/3, 1/3 \\ x+1/3, x+1/6, x \\ 3_{xyz}^{-1}   1/2, 1/2, 0 \end{pmatrix}$                   | (10) $3^- \begin{pmatrix} x, \bar{x}+1/2, \bar{x} \\ 3_{\bar{xyz}}   1/2, 1/2, 0 \end{pmatrix}$                         | (11) $3^- \begin{pmatrix} 1/3, 1/3, -1/3 \\ \bar{x}+1/3, \bar{x}+1/6, x \\ 3_{\bar{xyz}}   1/2, 1/2, 0 \end{pmatrix}$                | (12) $3^- \begin{pmatrix} \bar{x}, x+1/2, \bar{x} \\ 3_{\bar{xyz}}   1/2, 1/2, 0 \end{pmatrix}$                                      |
| (13) $2 \begin{pmatrix} 1/2, 1/2, 0 \\ 2_{xy}   1/2, 1/2, 0 \end{pmatrix} \begin{matrix} x, x, 0 \\ \end{matrix}$        | (14) $2 \begin{pmatrix} x, \bar{x}+1/2, 0 \\ 2_{\bar{xy}}   1/2, 1/2, 0 \end{pmatrix}$                                  | (15) $4^- \begin{pmatrix} 1/2, 0, z \\ 4_z^{-1}   1/2, 1/2, 0 \end{pmatrix}$   | (16) $4^+ \begin{pmatrix} 0, 1/2, z \\ 4_z   1/2, 1/2, 0 \end{pmatrix}$  |
| (17) $4^- \begin{pmatrix} 1/2, 0, 0 \\ 4_x^{-1}   1/2, 1/2, 0 \end{pmatrix} \begin{matrix} x, 1/4, -1/4 \\ \end{matrix}$ | (18) $2 \begin{pmatrix} 0, 1/4, 1/4 \\ 2_{yz}   1/2, 1/2, 0 \end{pmatrix} \begin{matrix} 1/4, y+1/4, y \\ \end{matrix}$ | (19) $2 \begin{pmatrix} 0, 1/4, -1/4 \\ 2_{\bar{yz}}   1/2, 1/2, 0 \end{pmatrix} \begin{matrix} 1/4, y+1/4, \bar{y} \\ \end{matrix}$ | (20) $4^+ \begin{pmatrix} 1/2, 0, 0 \\ 4_x   1/2, 1/2, 0 \end{pmatrix} \begin{matrix} x, 1/4, 1/4 \\ \end{matrix}$                   |
| (21) $4^+ \begin{pmatrix} 0, 1/2, 0 \\ 4_y   1/2, 1/2, 0 \end{pmatrix} \begin{matrix} 1/4, y, -1/4 \\ \end{matrix}$      | (22) $2 \begin{pmatrix} 1/4, 0, 1/4 \\ 2_{xz}   1/2, 1/2, 0 \end{pmatrix} \begin{matrix} x+1/4, 1/4, x \\ \end{matrix}$ | (23) $4^- \begin{pmatrix} 0, 1/2, 0 \\ 4_y^{-1}   1/2, 1/2, 0 \end{pmatrix} \begin{matrix} 1/4, y, 1/4 \\ \end{matrix}$              | (24) $2 \begin{pmatrix} 1/4, 0, -1/4 \\ 2_{\bar{xz}}   1/2, 1/2, 0 \end{pmatrix} \begin{matrix} \bar{x}+1/4, 1/4, x \\ \end{matrix}$ |

## For (0,0,0)' + set

- |   |   |   |  |
|---|---|---|--|
| (1) $1' \begin{pmatrix} 0, 0, 0 \\ 1   0, 0, 0 \end{pmatrix}'$                | (2) $2' \begin{pmatrix} 0, 0, z \\ 2_z   0, 0, 0 \end{pmatrix}'$                                | (3) $2' \begin{pmatrix} 0, y, 0 \\ 2_y   0, 0, 0 \end{pmatrix}'$                                | (4) $2' \begin{pmatrix} x, 0, 0 \\ 2_x   0, 0, 0 \end{pmatrix}'$                               |
| (5) $3^{+'} \begin{pmatrix} x, x, x \\ 3_{xyz}   0, 0, 0 \end{pmatrix}'$      | (6) $3^{+'} \begin{pmatrix} \bar{x}, x, \bar{x} \\ 3_{\bar{xyz}}^{-1}   0, 0, 0 \end{pmatrix}'$ | (7) $3^{+'} \begin{pmatrix} x, \bar{x}, \bar{x} \\ 3_{\bar{xyz}}^{-1}   0, 0, 0 \end{pmatrix}'$ | (8) $3^{+'} \begin{pmatrix} \bar{x}, \bar{x}, x \\ 3_{\bar{yz}}^{-1}   0, 0, 0 \end{pmatrix}'$ |
| (9) $3^{-'} \begin{pmatrix} x, x, x \\ 3_{xyz}^{-1}   0, 0, 0 \end{pmatrix}'$ | (10) $3^{-'} \begin{pmatrix} x, \bar{x}, \bar{x} \\ 3_{\bar{xyz}}   0, 0, 0 \end{pmatrix}'$     | (11) $3^{-'} \begin{pmatrix} \bar{x}, \bar{x}, x \\ 3_{\bar{yz}}   0, 0, 0 \end{pmatrix}'$      | (12) $3^{-'} \begin{pmatrix} \bar{x}, x, \bar{x} \\ 3_{\bar{xyz}}   0, 0, 0 \end{pmatrix}'$    |
| (13) $2' \begin{pmatrix} x, x, 0 \\ 2_{xy}   0, 0, 0 \end{pmatrix}'$          | (14) $2' \begin{pmatrix} x, \bar{x}, 0 \\ 2_{\bar{xy}}   0, 0, 0 \end{pmatrix}'$                | (15) $4^{-'} \begin{pmatrix} 0, 0, z \\ 4_z^{-1}   0, 0, 0 \end{pmatrix}'$                      | (16) $4^{+'} \begin{pmatrix} 0, 0, z \\ 4_z   0, 0, 0 \end{pmatrix}'$                          |
| (17) $4^{-'} \begin{pmatrix} x, 0, 0 \\ 4_x^{-1}   0, 0, 0 \end{pmatrix}'$    | (18) $2' \begin{pmatrix} 0, y, y \\ 2_{yz}   0, 0, 0 \end{pmatrix}'$                            | (19) $2' \begin{pmatrix} 0, y, \bar{y} \\ 2_{\bar{yz}}   0, 0, 0 \end{pmatrix}'$                | (20) $4^{+'} \begin{pmatrix} x, 0, 0 \\ 4_x   0, 0, 0 \end{pmatrix}'$                          |
| (21) $4^{+'} \begin{pmatrix} 0, y, 0 \\ 4_y   0, 0, 0 \end{pmatrix}'$         | (22) $2' \begin{pmatrix} x, 0, x \\ 2_{xz}   0, 0, 0 \end{pmatrix}'$                            | (23) $4^{-'} \begin{pmatrix} 0, y, 0 \\ 4_y^{-1}   0, 0, 0 \end{pmatrix}'$                      | (24) $2' \begin{pmatrix} \bar{x}, 0, x \\ 2_{\bar{xz}}   0, 0, 0 \end{pmatrix}'$               |

## For (0,1/2,1/2)' + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t' \begin{pmatrix} 0, 1/2, 1/2 \\ 1   0, 1/2, 1/2 \end{pmatrix}'$                                     | (2) $2' \begin{pmatrix} 0, 0, 1/2 \\ 2_z   0, 1/2, 1/2 \end{pmatrix}' \begin{matrix} 0, 1/4, z \\ \end{matrix}$           | (3) $2' \begin{pmatrix} 0, 1/2, 0 \\ 2_y   0, 1/2, 1/2 \end{pmatrix}' \begin{matrix} 0, y, 1/4 \\ \end{matrix}$               | (4) $2' \begin{pmatrix} x, 1/4, 1/4 \\ 2_x   0, 1/2, 1/2 \end{pmatrix}'$                                |
| (5) $3^{+'} \begin{pmatrix} 1/3, 1/3, 1/3 \\ x-1/3, x-1/6, x \\ 3_{xyz}   0, 1/2, 1/2 \end{pmatrix}'$      | (6) $3^{+'} \begin{pmatrix} \bar{x}, x+1/2, \bar{x} \\ 3_{\bar{xyz}}^{-1}   0, 1/2, 1/2 \end{pmatrix}'$                   | (7) $3^{+'} \begin{pmatrix} -1/3, 1/3, 1/3 \\ x+1/3, \bar{x}-1/6, \bar{x} \\ 3_{\bar{xyz}}^{-1}   0, 1/2, 1/2 \end{pmatrix}'$ | (8) $3^{+'} \begin{pmatrix} \bar{x}, \bar{x}+1/2, x \\ 3_{\bar{yz}}^{-1}   0, 1/2, 1/2 \end{pmatrix}'$  |
| (9) $3^{-'} \begin{pmatrix} 1/3, 1/3, 1/3 \\ x-1/6, x+1/6, x \\ 3_{xyz}^{-1}   0, 1/2, 1/2 \end{pmatrix}'$ | (10) $3^{-'} \begin{pmatrix} -1/3, 1/3, 1/3 \\ x+1/6, \bar{x}+1/6, \bar{x} \\ 3_{\bar{xyz}}   0, 1/2, 1/2 \end{pmatrix}'$ | (11) $3^{-'} \begin{pmatrix} \bar{x}+1/2, \bar{x}+1/2, x \\ 3_{\bar{yz}}   0, 1/2, 1/2 \end{pmatrix}'$                        | (12) $3^{-'} \begin{pmatrix} \bar{x}-1/2, x+1/2, \bar{x} \\ 3_{\bar{xyz}}   0, 1/2, 1/2 \end{pmatrix}'$ |

- (13)  $2' (1/4, 1/4, 0) \quad x, x+1/4, 1/4$     (14)  $2' (-1/4, 1/4, 0) \quad x, \bar{x}+1/4, 1/4$     (15)  $4^{-1} (0, 0, 1/2) \quad 1/4, 1/4, z$     (16)  $4^{+1} (0, 0, 1/2) \quad -1/4, 1/4, z$   
 $(2_{xy} | 0, 1/2, 1/2)'$      $(2_{\bar{xy}} | 0, 1/2, 1/2)'$      $(4_z^{-1} | 0, 1/2, 1/2)'$      $(4_z | 0, 1/2, 1/2)'$
- (17)  $4^{-1} \quad x, 1/2, 0$     (18)  $2' (0, 1/2, 1/2) \quad 0, y, y$     (19)  $2' \quad 0, y+1/2, \bar{y}$     (20)  $4^{+1} \quad x, 0, 1/2$   
 $(4_x^{-1} | 0, 1/2, 1/2)'$      $(2_{yz} | 0, 1/2, 1/2)'$      $(2_{\bar{yz}} | 0, 1/2, 1/2)'$      $(4_x | 0, 1/2, 1/2)'$
- (21)  $4^{+1} (0, 1/2, 0) \quad 1/4, y, 1/4$     (22)  $2' (1/4, 0, 1/4) \quad x-1/4, 1/4, x$     (23)  $4^{-1} (0, 1/2, 0) \quad -1/4, y, 1/4$     (24)  $2' (-1/4, 0, 1/4) \quad \bar{x}+1/4, 1/4, x$   
 $(4_y | 0, 1/2, 1/2)'$      $(2_{xz} | 0, 1/2, 1/2)'$      $(4_y^{-1} | 0, 1/2, 1/2)'$      $(2_{\bar{xz}} | 0, 1/2, 1/2)'$

For  $(1/2, 0, 1/2)' + \text{set}$ 

- (1)  $t' (1/2, 0, 1/2)$     (2)  $2' (0, 0, 1/2) \quad 1/4, 0, z$     (3)  $2' \quad 1/4, y, 1/4$     (4)  $2' (1/2, 0, 0) \quad x, 0, 1/4$   
 $(1 | 1/2, 0, 1/2)'$      $(2_z | 1/2, 0, 1/2)'$      $(2_y | 1/2, 0, 1/2)'$      $(2_x | 1/2, 0, 1/2)'$
- (5)  $3^{+1} (1/3, 1/3, 1/3)$     (6)  $3^{+1} (1/3, -1/3, 1/3)$     (7)  $3^{+1} \quad x+1/2, \bar{x}-1/2, \bar{x}$     (8)  $3^{+1} \quad \bar{x}+1/2, \bar{x}+1/2, x$   
 $x+1/6, x-1/6, x$      $\bar{x}+1/6, x+1/6, \bar{x}$      $(3_{\bar{xyz}}^{-1} | 1/2, 0, 1/2)'$      $(3_{xyz}^{-1} | 1/2, 0, 1/2)'$
- (9)  $3^{-1} (1/3, 1/3, 1/3)$     (10)  $3^{-1} \quad x+1/2, \bar{x}, \bar{x}$     (11)  $3^{-1} \quad \bar{x}+1/2, \bar{x}, x$     (12)  $3^{-1} (1/3, -1/3, 1/3)$   
 $x-1/6, x-1/3, x$      $(3_{\bar{xyz}} | 1/2, 0, 1/2)'$      $(3_{xyz} | 1/2, 0, 1/2)'$      $\bar{x}-1/6, x+1/3, \bar{x}$   
 $(3_{xyz}^{-1} | 1/2, 0, 1/2)'$      $(3_{\bar{xyz}} | 1/2, 0, 1/2)'$      $(3_{xyz} | 1/2, 0, 1/2)'$
- (13)  $2' (1/4, 1/4, 0) \quad x, x-1/4, 1/4$     (14)  $2' (1/4, -1/4, 0) \quad x, \bar{x}+1/4, 1/4$     (15)  $4^{-1} (0, 0, 1/2) \quad 1/4, -1/4, z$     (16)  $4^{+1} (0, 0, 1/2) \quad 1/4, 1/4, z$   
 $(2_{xy} | 1/2, 0, 1/2)'$      $(2_{\bar{xy}} | 1/2, 0, 1/2)'$      $(4_z^{-1} | 1/2, 0, 1/2)'$      $(4_z | 1/2, 0, 1/2)'$
- (17)  $4^{-1} (1/2, 0, 0) \quad x, 1/4, 1/4$     (18)  $2' (0, 1/4, 1/4) \quad 1/4, y-1/4, y$     (19)  $2' (0, -1/4, 1/4) \quad 1/4, y+1/4, \bar{y}$     (20)  $4^{+1} (1/2, 0, 0) \quad x, -1/4, 1/4$   
 $(4_x^{-1} | 1/2, 0, 1/2)'$      $(2_{yz} | 1/2, 0, 1/2)'$      $(2_{\bar{yz}} | 1/2, 0, 1/2)'$      $(4_x | 1/2, 0, 1/2)'$
- (21)  $4^{+1} \quad 1/2, y, 0$     (22)  $2' (1/2, 0, 1/2) \quad x, 0, x$     (23)  $4^{-1} \quad 0, y, 1/2$     (24)  $2' \quad \bar{x}+1/2, 0, x$   
 $(4_y | 1/2, 0, 1/2)'$      $(2_{xz} | 1/2, 0, 1/2)'$      $(4_y^{-1} | 1/2, 0, 1/2)'$      $(2_{\bar{xz}} | 1/2, 0, 1/2)'$

For  $(1/2, 1/2, 0)' + \text{set}$ 

- (1)  $t' (1/2, 1/2, 0)$     (2)  $2' \quad 1/4, 1/4, z$     (3)  $2' (0, 1/2, 0) \quad 1/4, y, 0$     (4)  $2' (1/2, 0, 0) \quad x, 1/4, 0$   
 $(1 | 1/2, 1/2, 0)'$      $(2_z | 1/2, 1/2, 0)'$      $(2_y | 1/2, 1/2, 0)'$      $(2_x | 1/2, 1/2, 0)'$
- (5)  $3^{+1} (1/3, 1/3, 1/3)$     (6)  $3^{+1} \quad \bar{x}+1/2, x, \bar{x}$     (7)  $3^{+1} \quad x+1/2, \bar{x}, \bar{x}$     (8)  $3^{+1} (1/3, 1/3, -1/3)$   
 $x+1/6, x+1/3, x$      $(3_{\bar{xyz}}^{-1} | 1/2, 1/2, 0)'$      $(3_{xyz}^{-1} | 1/2, 1/2, 0)'$      $\bar{x}+1/6, x+1/3, x$   
 $(3_{xyz} | 1/2, 1/2, 0)'$      $(3_{\bar{xyz}} | 1/2, 1/2, 0)'$      $(3_{xyz} | 1/2, 1/2, 0)'$
- (9)  $3^{-1} (1/3, 1/3, 1/3)$     (10)  $3^{-1} \quad x, \bar{x}+1/2, \bar{x}$     (11)  $3^{-1} (1/3, 1/3, -1/3)$     (12)  $3^{-1} \quad \bar{x}, x+1/2, \bar{x}$   
 $x+1/3, x+1/6, x$      $(3_{\bar{xyz}}^{-1} | 1/2, 1/2, 0)'$      $\bar{x}+1/3, x+1/6, x$      $(3_{\bar{xyz}} | 1/2, 1/2, 0)'$   
 $(3_{xyz}^{-1} | 1/2, 1/2, 0)'$      $(3_{\bar{xyz}} | 1/2, 1/2, 0)'$      $(3_{xyz} | 1/2, 1/2, 0)'$
- (13)  $2' (1/2, 1/2, 0) \quad x, x, 0$     (14)  $2' \quad x, \bar{x}+1/2, 0$     (15)  $4^{-1} \quad 1/2, 0, z$     (16)  $4^{+1} \quad 0, 1/2, z$   
 $(2_{xy} | 1/2, 1/2, 0)'$      $(2_{\bar{xy}} | 1/2, 1/2, 0)'$      $(4_z^{-1} | 1/2, 1/2, 0)'$      $(4_z | 1/2, 1/2, 0)'$
- (17)  $4^{-1} (1/2, 0, 0) \quad x, 1/4, -1/4$     (18)  $2' (0, 1/4, 1/4) \quad 1/4, y+1/4, y$     (19)  $2' (0, 1/4, -1/4) \quad 1/4, y+1/4, \bar{y}$     (20)  $4^{+1} (1/2, 0, 0) \quad x, 1/4, 1/4$   
 $(4_x^{-1} | 1/2, 1/2, 0)'$      $(2_{yz} | 1/2, 1/2, 0)'$      $(2_{\bar{yz}} | 1/2, 1/2, 0)'$      $(4_x | 1/2, 1/2, 0)'$
- (21)  $4^{+1} (0, 1/2, 0) \quad 1/4, y, -1/4$     (22)  $2' (1/4, 0, 1/4) \quad x+1/4, 1/4, x$     (23)  $4^{-1} (0, 1/2, 0) \quad 1/4, y, 1/4$     (24)  $2' (1/4, 0, -1/4) \quad \bar{x}+1/4, 1/4, x$   
 $(4_y | 1/2, 1/2, 0)'$      $(2_{xz} | 1/2, 1/2, 0)'$      $(4_y^{-1} | 1/2, 1/2, 0)'$      $(2_{\bar{xz}} | 1/2, 1/2, 0)'$

Generators selected (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ;  $t(0, 1/2, 1/2)$ ;  $t(1/2, 0, 1/2)$ ; (2); (3); (5); (13); 1'.

## Positions

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

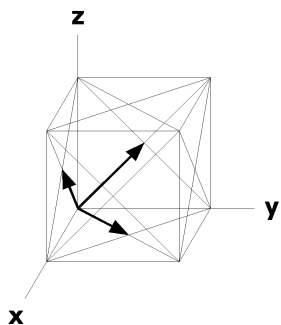
			(0,0,0) + (0,0,0)' +	(0,1/2,1/2) + (0,1/2,1/2)' +	(1/2,0,1/2) + (1/2,0,1/2)' +	(1/2,1/2,0) + (1/2,1/2,0)' +					
96	j	11'									
(1)	x,y,z	[0,0,0]	(2)	$\bar{x}, \bar{y}, z$	[0,0,0]	(3)	$\bar{x}, y, \bar{z}$	[0,0,0]	(4)	x, $\bar{y}, \bar{z}$	[0,0,0]
(5)	z,x,y	[0,0,0]	(6)	z, $\bar{x}, \bar{y}$	[0,0,0]	(7)	$\bar{z}, \bar{x}, y$	[0,0,0]	(8)	$\bar{z}, x, \bar{y}$	[0,0,0]
(9)	y,z,x	[0,0,0]	(10)	$\bar{y}, z, \bar{x}$	[0,0,0]	(11)	y, $\bar{z}, \bar{x}$	[0,0,0]	(12)	$\bar{y}, \bar{z}, x$	[0,0,0]
(13)	y,x, $\bar{z}$	[0,0,0]	(14)	$\bar{y}, \bar{x}, \bar{z}$	[0,0,0]	(15)	y, $\bar{x}, z$	[0,0,0]	(16)	$\bar{y}, x, z$	[0,0,0]
(17)	x,z, $\bar{y}$	[0,0,0]	(18)	$\bar{x}, z, y$	[0,0,0]	(19)	$\bar{x}, \bar{z}, \bar{y}$	[0,0,0]	(20)	x, $\bar{z}, y$	[0,0,0]
(21)	z,y, $\bar{x}$	[0,0,0]	(22)	z, $\bar{y}, x$	[0,0,0]	(23)	$\bar{z}, y, x$	[0,0,0]	(24)	$\bar{z}, \bar{y}, \bar{x}$	[0,0,0]
48	i	2..1'	x,1/4,1/4 [0,0,0]	$\bar{x}, 3/4, 1/4$ [0,0,0]	1/4,x,1/4 [0,0,0]	1/4, $\bar{x}, 3/4$ [0,0,0]					
			1/4,1/4,x [0,0,0]	3/4,1/4, $\bar{x}$ [0,0,0]	1/4,x,3/4 [0,0,0]	3/4, $\bar{x}, 3/4$ [0,0,0]					
			x,1/4,3/4 [0,0,0]	$\bar{x}, 1/4, 1/4$ [0,0,0]	1/4,1/4, $\bar{x}$ [0,0,0]	1/4,3/4,x [0,0,0]					
48	h	..21'	1/2,y,y [0,0,0]	1/2, $\bar{y}, y$ [0,0,0]	1/2,y, $\bar{y}$ [0,0,0]	1/2, $\bar{y}, \bar{y}$ [0,0,0]					
			y,1/2,y [0,0,0]	y,1/2, $\bar{y}$ [0,0,0]	$\bar{y}, 1/2, y$ [0,0,0]	$\bar{y}, 1/2, \bar{y}$ [0,0,0]					
			y,y,1/2 [0,0,0]	$\bar{y}, y, 1/2$ [0,0,0]	y, $\bar{y}, 1/2$ [0,0,0]	$\bar{y}, \bar{y}, 1/2$ [0,0,0]					
48	g	..21'	0,y,y [0,0,0]	0, $\bar{y}, y$ [0,0,0]	0,y, $\bar{y}$ [0,0,0]	0, $\bar{y}, \bar{y}$ [0,0,0]					
			y,0,y [0,0,0]	y,0, $\bar{y}$ [0,0,0]	$\bar{y}, 0, y$ [0,0,0]	$\bar{y}, 0, \bar{y}$ [0,0,0]					
			y,y,0 [0,0,0]	$\bar{y}, y, 0$ [0,0,0]	y, $\bar{y}, 0$ [0,0,0]	$\bar{y}, \bar{y}, 0$ [0,0,0]					
32	f	.3.1'	x,x,x [0,0,0]	$\bar{x}, \bar{x}, x$ [0,0,0]	$\bar{x}, x, \bar{x}$ [0,0,0]	x, $\bar{x}, \bar{x}$ [0,0,0]					
			x,x, $\bar{x}$ [0,0,0]	$\bar{x}, \bar{x}, \bar{x}$ [0,0,0]	x, $\bar{x}, x$ [0,0,0]	$\bar{x}, x, x$ [0,0,0]					
24	e	4..1'	x,0,0 [0,0,0]	$\bar{x}, 0, 0$ [0,0,0]	0,x,0 [0,0,0]						
			0, $\bar{x}, 0$ [0,0,0]	0,0,x [0,0,0]	0,0, $\bar{x}$ [0,0,0]						
24	d	2.221'	0,1/4,1/4 [0,0,0]	0,3/4,1/4 [0,0,0]	1/4,0,1/4 [0,0,0]						
			1/4,0,3/4 [0,0,0]	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]						
8	c	23.1'	1/4,1/4,1/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]							
4	b	4321'	1/2,1/2,1/2 [0,0,0]								
4	a	4321'	0,0,0 [0,0,0]								

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $0,0,z$

Along  $[1,1,1]$   $p3m11'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
Origin at  $x,x,x$

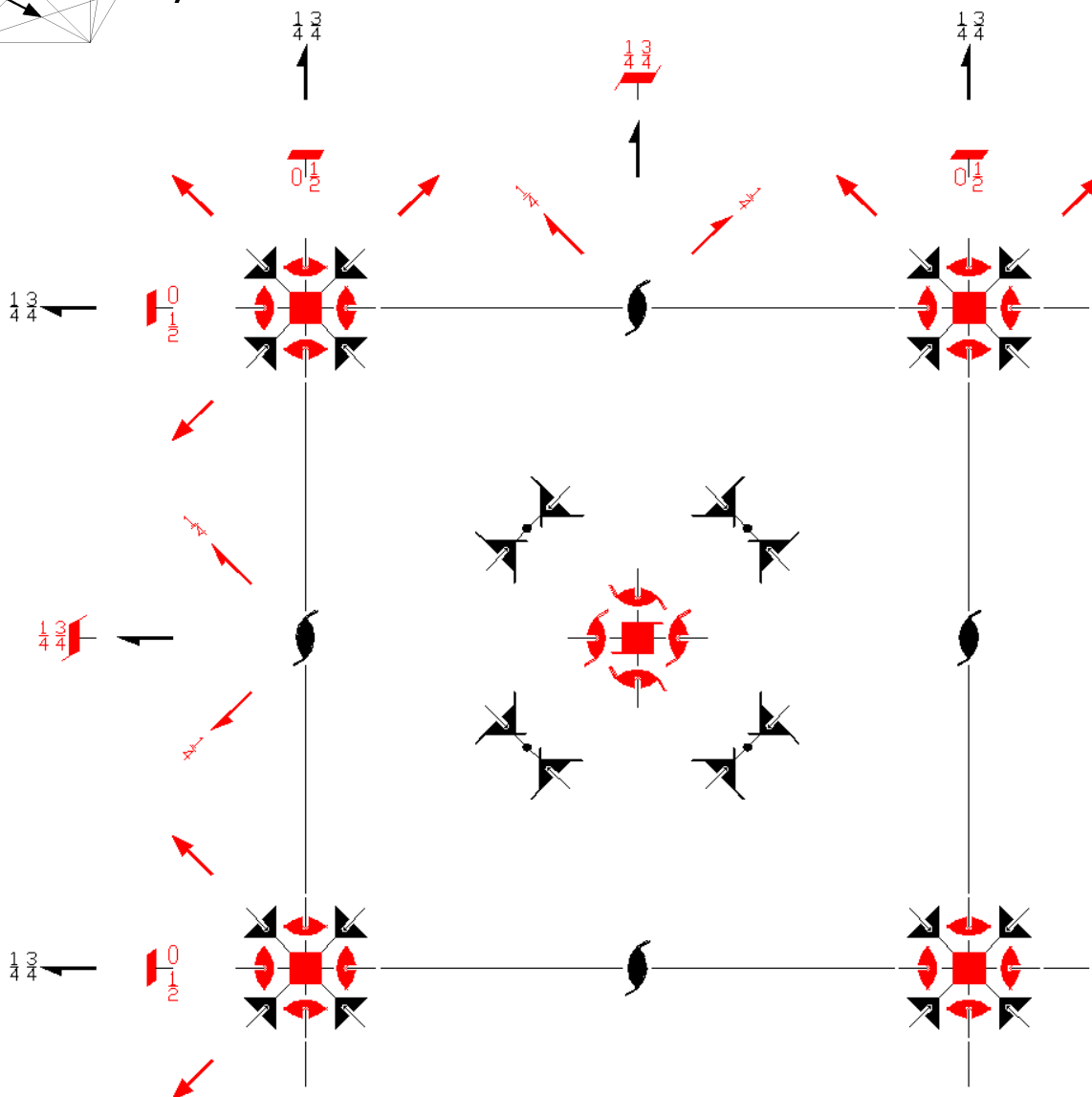
Along  $[1,1,0]$   $c2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at  $x,x,0$



F4'32'  
209.3.1552

4'32'  
F4'32'

Cubic



Origin at 4'32'

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/4;$   $-1/4 \leq z \leq 1/4;$   $y \leq \min(x, 1/2-x);$   $-y \leq z \leq y$

Vertices  $0,0,0$   $1/2,0,0$   $1/4,1/4,1/4$   $1/4,1/4,-1/4$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)              | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub>xyz<sup>-1</sup></sub>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz<sup>-1</sup></sub>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz<sup>-1</sup></sub>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz<sup>-1</sup></sub>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)            | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)              | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)             |

(13) $2' \begin{matrix} x,x,0 \\ (2_{xy} 0,0,0)' \end{matrix}$	(14) $2' \begin{matrix} x,\bar{x},0 \\ (2_{xy} 0,0,0)' \end{matrix}$	(15) $4^{-1} \begin{matrix} 0,0,z \\ (4_z^{-1} 0,0,0)' \end{matrix}$	(16) $4^{+1} \begin{matrix} 0,0,z \\ (4_z 0,0,0)' \end{matrix}$
(17) $4^{-1} \begin{matrix} x,0,0 \\ (4_x^{-1} 0,0,0)' \end{matrix}$	(18) $2' \begin{matrix} 0,y,y \\ (2_{yz} 0,0,0)' \end{matrix}$	(19) $2' \begin{matrix} 0,y,\bar{y} \\ (2_{yz} 0,0,0)' \end{matrix}$	(20) $4^{+1} \begin{matrix} x,0,0 \\ (4_x 0,0,0)' \end{matrix}$
(21) $4^{+1} \begin{matrix} 0,y,0 \\ (4_y 0,0,0)' \end{matrix}$	(22) $2' \begin{matrix} x,0,x \\ (2_{xz} 0,0,0)' \end{matrix}$	(23) $4^{-1} \begin{matrix} 0,y,0 \\ (4_y^{-1} 0,0,0)' \end{matrix}$	(24) $2' \begin{matrix} \bar{x},0,x \\ (2_{xz} 0,0,0)' \end{matrix}$

For (0,1/2,1/2) + set

(1) $t \begin{matrix} (0,1/2,1/2) \\ (1 0,1/2,1/2) \end{matrix}$	(2) $2 \begin{matrix} (0,0,1/2) \quad 0,1/4,z \\ (2_z 0,1/2,1/2) \end{matrix}$	(3) $2 \begin{matrix} (0,1/2,0) \quad 0,y,1/4 \\ (2_y 0,1/2,1/2) \end{matrix}$	(4) $2 \begin{matrix} x,1/4,1/4 \\ (2_x 0,1/2,1/2) \end{matrix}$
(5) $3^{+} \begin{matrix} (1/3,1/3,1/3) \\ x-1/3,x-1/6,x \\ (3_{xyz} 0,1/2,1/2) \end{matrix}$	(6) $3^{+} \begin{matrix} \bar{x},x+1/2,\bar{x} \\ (3_{xyz}^{-1} 0,1/2,1/2) \end{matrix}$	(7) $3^{+} \begin{matrix} (-1/3,1/3,1/3) \\ x+1/3,\bar{x}-1/6,\bar{x} \\ (3_{xyz}^{-1} 0,1/2,1/2) \end{matrix}$	(8) $3^{+} \begin{matrix} \bar{x},\bar{x}+1/2,x \\ (3_{xyz}^{-1} 0,1/2,1/2) \end{matrix}$
(9) $3^{-} \begin{matrix} (1/3,1/3,1/3) \\ x-1/6,x+1/6,x \\ (3_{xyz}^{-1} 0,1/2,1/2) \end{matrix}$	(10) $3^{-} \begin{matrix} (-1/3,1/3,1/3) \\ x+1/6,\bar{x}+1/6,\bar{x} \\ (3_{xyz} 0,1/2,1/2) \end{matrix}$	(11) $3^{-} \begin{matrix} \bar{x}+1/2,\bar{x}+1/2,x \\ (3_{xyz} 0,1/2,1/2) \end{matrix}$	(12) $3^{-} \begin{matrix} \bar{x}-1/2,x+1/2,\bar{x} \\ (3_{xyz} 0,1/2,1/2) \end{matrix}$
(13) $2' \begin{matrix} (1/4,1/4,0) \quad x,x+1/4,1/4 \\ (2_{xy} 0,1/2,1/2)' \end{matrix}$	(14) $2' \begin{matrix} (-1/4,1/4,0) \quad x,\bar{x}+1/4,1/4 \\ (2_{xy} 0,1/2,1/2)' \end{matrix}$	(15) $4^{-1} \begin{matrix} (0,0,1/2) \quad 1/4,1/4,z \\ (4_z^{-1} 0,1/2,1/2)' \end{matrix}$	(16) $4^{+1} \begin{matrix} (0,0,1/2) \quad -1/4,1/4,z \\ (4_z 0,1/2,1/2)' \end{matrix}$
(17) $4^{-1} \begin{matrix} x,1/2,0 \\ (4_x^{-1} 0,1/2,1/2)' \end{matrix}$	(18) $2' \begin{matrix} (0,1/2,1/2) \quad 0,y,y \\ (2_{yz} 0,1/2,1/2)' \end{matrix}$	(19) $2' \begin{matrix} 0,y+1/2,\bar{y} \\ (2_{yz} 0,1/2,1/2)' \end{matrix}$	(20) $4^{+1} \begin{matrix} x,0,1/2 \\ (4_x 0,1/2,1/2)' \end{matrix}$
(21) $4^{+1} \begin{matrix} (0,1/2,0) \quad 1/4,y,1/4 \\ (4_y 0,1/2,1/2)' \end{matrix}$	(22) $2' \begin{matrix} (1/4,0,1/4) \quad x-1/4,1/4,x \\ (2_{xz} 0,1/2,1/2)' \end{matrix}$	(23) $4^{-1} \begin{matrix} (0,1/2,0) \quad -1/4,y,1/4 \\ (4_y^{-1} 0,1/2,1/2)' \end{matrix}$	(24) $2' \begin{matrix} (-1/4,0,1/4) \quad \bar{x}+1/4,1/4,x \\ (2_{xz} 0,1/2,1/2)' \end{matrix}$

For (1/2,0,1/2) + set

(1) $t \begin{matrix} (1/2,0,1/2) \\ (1 1/2,0,1/2) \end{matrix}$	(2) $2 \begin{matrix} (0,0,1/2) \quad 1/4,0,z \\ (2_z 1/2,0,1/2) \end{matrix}$	(3) $2 \begin{matrix} 1/4,y,1/4 \\ (2_y 1/2,0,1/2) \end{matrix}$	(4) $2 \begin{matrix} (1/2,0,0) \quad x,0,1/4 \\ (2_x 1/2,0,1/2) \end{matrix}$
(5) $3^{+} \begin{matrix} (1/3,1/3,1/3) \\ x+1/6,x-1/6,x \\ (3_{xyz} 1/2,0,1/2) \end{matrix}$	(6) $3^{+} \begin{matrix} (1/3,-1/3,1/3) \\ \bar{x}+1/6,x+1/6,\bar{x} \\ (3_{xyz}^{-1} 1/2,0,1/2) \end{matrix}$	(7) $3^{+} \begin{matrix} x+1/2,\bar{x}-1/2,\bar{x} \\ (3_{xyz}^{-1} 1/2,0,1/2) \end{matrix}$	(8) $3^{+} \begin{matrix} \bar{x}+1/2,\bar{x}+1/2,x \\ (3_{xyz}^{-1} 1/2,0,1/2) \end{matrix}$
(9) $3^{-} \begin{matrix} (1/3,1/3,1/3) \\ x-1/6,x-1/3,x \\ (3_{xyz}^{-1} 1/2,0,1/2) \end{matrix}$	(10) $3^{-} \begin{matrix} x+1/2,\bar{x},\bar{x} \\ (3_{xyz} 1/2,0,1/2) \end{matrix}$	(11) $3^{-} \begin{matrix} \bar{x}+1/2,\bar{x},x \\ (3_{xyz} 1/2,0,1/2) \end{matrix}$	(12) $3^{-} \begin{matrix} (1/3,-1/3,1/3) \\ \bar{x}-1/6,x+1/3,\bar{x} \\ (3_{xyz} 1/2,0,1/2) \end{matrix}$
(13) $2' \begin{matrix} (1/4,1/4,0) \quad x,x-1/4,1/4 \\ (2_{xy} 1/2,0,1/2)' \end{matrix}$	(14) $2' \begin{matrix} (1/4,-1/4,0) \quad x,\bar{x}+1/4,1/4 \\ (2_{xy} 1/2,0,1/2)' \end{matrix}$	(15) $4^{-1} \begin{matrix} (0,0,1/2) \quad 1/4,-1/4,z \\ (4_z^{-1} 1/2,0,1/2)' \end{matrix}$	(16) $4^{+1} \begin{matrix} (0,0,1/2) \quad 1/4,1/4,z \\ (4_z 1/2,0,1/2)' \end{matrix}$
(17) $4^{-1} \begin{matrix} (1/2,0,0) \quad x,1/4,1/4 \\ (4_x^{-1} 1/2,0,1/2)' \end{matrix}$	(18) $2' \begin{matrix} (0,1/4,1/4) \quad 1/4,y-1/4,y \\ (2_{yz} 1/2,0,1/2)' \end{matrix}$	(19) $2' \begin{matrix} (0,-1/4,1/4) \quad 1/4,y+1/4,\bar{y} \\ (2_{yz} 1/2,0,1/2)' \end{matrix}$	(20) $4^{+1} \begin{matrix} (1/2,0,0) \quad x,-1/4,1/4 \\ (4_x 1/2,0,1/2)' \end{matrix}$
(21) $4^{+1} \begin{matrix} 1/2,y,0 \\ (4_y 1/2,0,1/2)' \end{matrix}$	(22) $2' \begin{matrix} (1/2,0,1/2) \quad x,0,x \\ (2_{xz} 1/2,0,1/2)' \end{matrix}$	(23) $4^{-1} \begin{matrix} 0,y,1/2 \\ (4_y^{-1} 1/2,0,1/2)' \end{matrix}$	(24) $2' \begin{matrix} \bar{x}+1/2,0,x \\ (2_{xz} 1/2,0,1/2)' \end{matrix}$



For (1/2,1/2,0) + set

(1) $t(1/2,1/2,0)$ (1   1/2,1/2,0)	(2) $2(1/4,1/4,z)$ (2 <sub>z</sub>   1/2,1/2,0)	(3) $2(0,1/2,0) 1/4,y,0$ (2 <sub>y</sub>   1/2,1/2,0)	(4) $2(1/2,0,0) x,1/4,0$ (2 <sub>x</sub>   1/2,1/2,0)
(5) $3^+(1/3,1/3,1/3)$ $x+1/6,x+1/3,x$ (3 <sub>xyz</sub>   1/2,1/2,0)	(6) $3^+ \bar{x}+1/2,x,\bar{x}$ (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>   1/2,1/2,0)	(7) $3^+ x+1/2,\bar{x},\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(8) $3^+(1/3,1/3,-1/3)$ $\bar{x}+1/6,\bar{x}+1/3,x$ (3 <sub><math>\bar{yz}</math></sub> <sup>-1</sup>   1/2,1/2,0)
(9) $3^-(1/3,1/3,1/3)$ $x+1/3,x+1/6,x$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) $3^- x,\bar{x}+1/2,\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)	(11) $3^-(1/3,1/3,-1/3)$ $\bar{x}+1/3,\bar{x}+1/6,x$ (3 <sub><math>\bar{yz}</math></sub>   1/2,1/2,0)	(12) $3^- \bar{x},x+1/2,\bar{x}$ (3 <sub><math>\bar{yz}</math></sub>   1/2,1/2,0)
(13) $2'(1/2,1/2,0) x,x,0$ (2 <sub>xy</sub>   1/2,1/2,0)'	(14) $2' x,\bar{x}+1/2,0$ (2 <sub>xy</sub>   1/2,1/2,0)'	(15) $4^- ' 1/2,0,z$ (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,0)'	(16) $4^+ ' 0,1/2,z$ (4 <sub>z</sub>   1/2,1/2,0)'
(17) $4^- '(1/2,0,0) x,1/4,-1/4$ (4 <sub>x</sub> <sup>-1</sup>   1/2,1/2,0)'	(18) $2'(0,1/4,1/4) 1/4,y+1/4,y$ (2 <sub>yz</sub>   1/2,1/2,0)'	(19) $2'(0,1/4,-1/4) 1/4,y+1/4,\bar{y}$ (2 <sub>yz</sub>   1/2,1/2,0)'	(20) $4^+ '(1/2,0,0) x,1/4,1/4$ (4 <sub>x</sub>   1/2,1/2,0)'
(21) $4^+ '(0,1/2,0) 1/4,y,-1/4$ (4 <sub>y</sub>   1/2,1/2,0)'	(22) $2'(1/4,0,1/4) x+1/4,1/4,x$ (2 <sub>xz</sub>   1/2,1/2,0)'	(23) $4^- '(0,1/2,0) 1/4,y,1/4$ (4 <sub>y</sub> <sup>-1</sup>   1/2,1/2,0)'	(24) $2'(1/4,0,-1/4)\bar{x}+1/4,1/4,x$ (2 <sub>xz</sub>   1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

		(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
96	j	1			
(1)	x,y,z	[u,v,w]	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
(5)	z,x,y	[w,u,v]	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
(9)	y,z,x	[v,w,u]	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
(13)	y,x, $\bar{z}$	[ $\bar{v},\bar{u},w$ ]	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$
(17)	x,z, $\bar{y}$	[ $\bar{u},\bar{w},v$ ]	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$
(21)	z,y, $\bar{x}$	[ $\bar{w},\bar{v},u$ ]	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$
48	i	2..	$x,1/4,1/4$	$\bar{x},3/4,1/4$	$1/4,x,1/4$
			[u,0,0]	[ $\bar{u},0,0$ ]	[0,u,0]
			$1/4,1/4,x$	$3/4,1/4,\bar{x}$	$1/4,x,3/4$
			[0,0,u]	[0,0, $\bar{u}$ ]	[0, $\bar{u},0$ ]
			$x,1/4,3/4$	$\bar{x},1/4,1/4$	$1/4,1/4,\bar{x}$
			[ $\bar{u},0,0$ ]	[u,0,0]	[0,0,u]
48	h	..2'	$1/2,y,y$	$1/2,\bar{y},y$	$1/2,y,\bar{y}$
			[u,v, $\bar{v}$ ]	[ $\bar{u},\bar{v},\bar{v}$ ]	[u,v,v]
			$y,1/2,y$	$y,1/2,\bar{y}$	$\bar{y},1/2,y$
			[ $\bar{v},u,v$ ]	[ $\bar{v},\bar{u},\bar{v}$ ]	[v,u,v]
			$y,y,1/2$	$\bar{y},y,1/2$	$y,\bar{y},1/2$
			[v, $\bar{v},u$ ]	[ $\bar{v},\bar{v},\bar{u}$ ]	[v,v, $\bar{u}$ ]

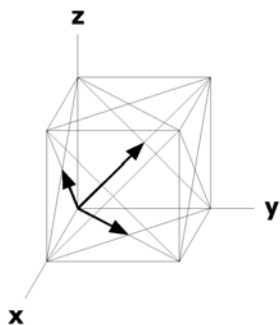
48	g	..2'	0,y,y [u,v, $\bar{v}$ ] y,0,y [ $\bar{v}$ ,u,v] y,y,0 [v, $\bar{v}$ ,u]	0, $\bar{y}$ ,y [ $\bar{u}$ , $\bar{v}$ , $\bar{v}$ ] y,0, $\bar{y}$ [ $\bar{v}$ , $\bar{u}$ , $\bar{v}$ ] $\bar{y}$ ,y,0 [ $\bar{v}$ , $\bar{v}$ , $\bar{u}$ ]	0,y, $\bar{y}$ [ $\bar{u}$ ,v,v] $\bar{y}$ ,0,y [v, $\bar{u}$ ,v] y, $\bar{y}$ ,0 [v,v, $\bar{u}$ ]	0, $\bar{y}$ , $\bar{y}$ [u, $\bar{v}$ ,v] $\bar{y}$ ,0, $\bar{y}$ [v,u, $\bar{v}$ ] $\bar{y}$ , $\bar{y}$ ,0 [ $\bar{v}$ ,v,u]
32	f	.3.	x,x,x [u,u,u] x,x, $\bar{x}$ [ $\bar{u}$ , $\bar{u}$ ,u]	$\bar{x}$ , $\bar{x}$ ,x [ $\bar{u}$ , $\bar{u}$ ,u] $\bar{x}$ , $\bar{x}$ , $\bar{x}$ [u,u,u]	$\bar{x}$ ,x, $\bar{x}$ [ $\bar{u}$ ,u, $\bar{u}$ ] x, $\bar{x}$ ,x [ $\bar{u}$ ,u, $\bar{u}$ ]	x, $\bar{x}$ , $\bar{x}$ [u, $\bar{u}$ , $\bar{u}$ ] $\bar{x}$ ,x,x [u, $\bar{u}$ , $\bar{u}$ ]
24	e	4..	x,0,0 [u,0,0] 0, $\bar{x}$ ,0 [0, $\bar{u}$ ,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0] 0,0,x [0,0,u]	0,x,0 [0,u,0] 0,0, $\bar{x}$ [0,0, $\bar{u}$ ]	
24	d	2.2'2'	0,1/4,1/4 [u,0,0] 1/4,0,3/4 [0, $\bar{u}$ ,0]	0,3/4,1/4 [ $\bar{u}$ ,0,0] 1/4,1/4,0 [0,0,u]	1/4,0,1/4 [0,u,0] 3/4,1/4,0 [0,0, $\bar{u}$ ]	
8	c	23.	1/4,1/4,1/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]		
4	b	4'32'	1/2,1/2,1/2 [0,0,0]			
4	a	4'32'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1]  $p4'm'm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,1,1]  $p3m1$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

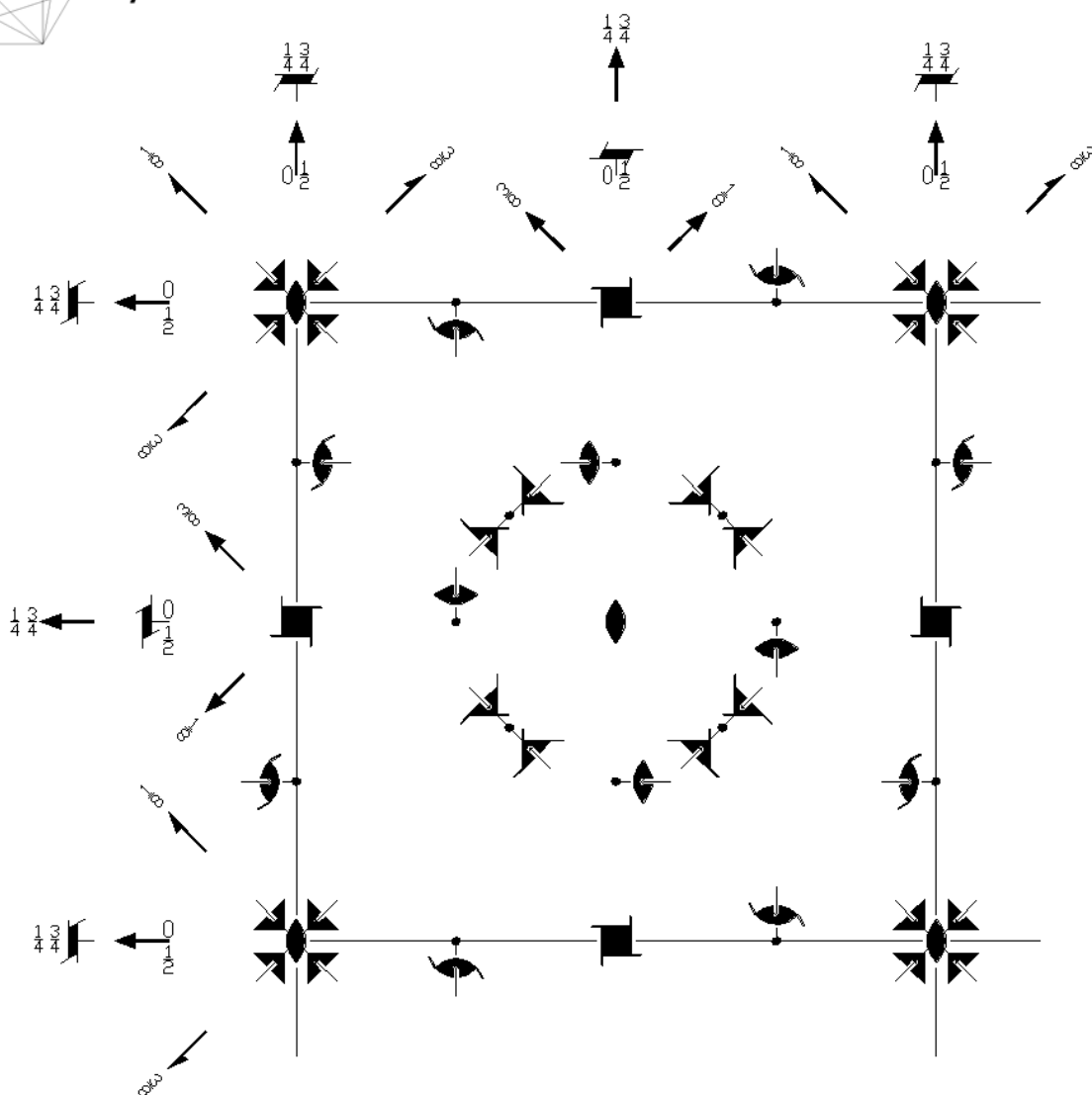
Along [1,1,0]  $c2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



F4<sub>1</sub>32  
210.1.1553

432  
F4<sub>1</sub>32

Cubic



Origin at 23

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $-1/8 \leq y \leq 1/8$ ;  $-1/8 \leq z \leq 1/8$ ;  $y \leq \min(x, 1/2-x)$ ;  $-y \leq z \leq \min(x, 1/2-x)$

**Vertices**  
 $0,0,0$        $1/8, 1/8, 1/8$        $1/8, 1/8, -1/8$        $1/8, -1/8, 1/8$   
 $1/2, 0, 0$        $3/8, 1/8, 1/8$        $3/8, 1/8, -1/8$        $3/8, -1/8, 1/8$

### Symmetry Operations

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)  | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)  | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>  1/2,0,1/2)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> (1/3,-1/3,1/3)<br>$\bar{x}+1/6, \bar{x}+1/6, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) | (7) 3 <sup>+</sup> (-1/3,1/3,1/3)<br>$x+1/3, \bar{x}-1/6, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2) | (8) 3 <sup>+</sup> (1/3,1/3,-1/3)<br>$\bar{x}+1/6, \bar{x}+1/3, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x}+1/2, \bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub>  1/2,1/2,0)                       | (11) 3 <sup>-</sup> $\bar{x}+1/2, \bar{x}, x$<br>(3 <sub>xyz</sub>  1/2,0,1/2)                                    | (12) 3 <sup>-</sup> $\bar{x}-1/2, x+1/2, \bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub>  0,1/2,1/2)                   |

- |  |  |  |  |
|--|--|--|--|
| (13) $2 (1/2, 1/2, 0) \ x, x-1/4, 3/8$<br>( $2_{xy}   3/4, 1/4, 3/4$ ) | (14) $2 \ x, \bar{x}+1/4, 1/8$<br>( $2_{\bar{xy}}   1/4, 1/4, 1/4$ )   | (15) $4^- (0, 0, 3/4) \ 1/2, 1/4, z$<br>( $4_z^{-1}   1/4, 3/4, 3/4$ ) | (16) $4^+ (0, 0, 1/4) \ 0, 3/4, z$<br>( $4_z   3/4, 3/4, 1/4$ )      |
| (17) $4^- (3/4, 0, 0) \ x, 1/2, 1/4$<br>( $4_x^{-1}   3/4, 1/4, 3/4$ ) | (18) $2 (0, 1/2, 1/2) \ 3/8, y+1/4, y$<br>( $2_{yz}   3/4, 3/4, 1/4$ ) | (19) $2 \ 1/8, y+1/4, \bar{y}$<br>( $2_{\bar{yz}}   1/4, 1/4, 1/4$ )   | (20) $4^+ (1/4, 0, 0) \ x, 0, 3/4$<br>( $4_x   1/4, 3/4, 3/4$ )      |
| (21) $4^+ (0, 1/4, 0) \ 3/4, y, 0$<br>( $4_y   3/4, 1/4, 3/4$ )        | (22) $2 (1/2, 0, 1/2) \ x-1/4, 3/8, x$<br>( $2_{xz}   1/4, 3/4, 3/4$ ) | (23) $4^- (0, 3/4, 0) \ 1/4, y, 1/2$<br>( $4_y^{-1}   3/4, 3/4, 1/4$ ) | (24) $2 \ \bar{x}+1/4, 1/8, x$<br>( $2_{\bar{xz}}   1/4, 1/4, 1/4$ ) |

For (0, 1/2, 1/2) + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t (0, 1/2, 1/2)$<br>( $1   0, 1/2, 1/2$ )                                     | (2) $2 \ 0, 0, z$<br>( $2_z   0, 0, 0$ )  | (3) $2 \ 1/4, y, 1/4$<br>( $2_y   1/2, 0, 1/2$ )  | (4) $2 (1/2, 0, 0) \ x, 1/4, 0$<br>( $2_x   1/2, 1/2, 0$ )                          |
| (5) $3^+ (1/3, 1/3, 1/3)$<br>$x-1/3, x-1/6, x$<br>( $3_{xyz}   0, 1/2, 1/2$ )      | (6) $3^+ \ \bar{x}+1/2, x, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   1/2, 1/2, 0$ )       | (7) $3^+ \ x, \bar{x}, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   0, 0, 0$ )                       | (8) $3^+ \ \bar{x}+1/2, \bar{x}+1/2, x$<br>( $3_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ )   |
| (9) $3^- (1/3, 1/3, 1/3)$<br>$x-1/6, x+1/6, x$<br>( $3_{xyz}^{-1}   0, 1/2, 1/2$ ) | (10) $3^- \ x+1/2, \bar{x}, \bar{x}$<br>( $3_{\bar{xyz}}   1/2, 0, 1/2$ )           | (11) $3^- (1/3, 1/3, -1/3)$<br>$\bar{x}+1/3, \bar{x}+1/6, x$<br>( $3_{xyz}   1/2, 1/2, 0$ ) | (12) $3^- \ \bar{x}, x, \bar{x}$<br>( $3_{\bar{xyz}}   0, 0, 0$ )                   |
| (13) $2 (3/4, 3/4, 0) \ x, x, 1/8$<br>( $2_{xy}   3/4, 3/4, 1/4$ )                 | (14) $2 (-1/4, 1/4, 0) \ x, \bar{x}+1/2, 3/8$<br>( $2_{\bar{xy}}   1/4, 3/4, 3/4$ ) | (15) $4^- (0, 0, 1/4) \ 1/4, 0, z$<br>( $4_z^{-1}   1/4, 1/4, 1/4$ )                        | (16) $4^+ (0, 0, 3/4) \ 1/4, 1/2, z$<br>( $4_z   3/4, 1/4, 3/4$ )                   |
| (17) $4^- (3/4, 0, 0) \ x, 1/2, -1/4$<br>( $4_x^{-1}   3/4, 3/4, 1/4$ )            | (18) $2 (0, 1/2, 1/2) \ 3/8, y-1/4, y$<br>( $2_{yz}   3/4, 1/4, 3/4$ )              | (19) $2 \ 1/8, y+3/4, \bar{y}$<br>( $2_{\bar{yz}}   1/4, 3/4, 3/4$ )                        | (20) $4^+ (1/4, 0, 0) \ x, 0, 1/4$<br>( $4_x   1/4, 1/4, 1/4$ )                     |
| (21) $4^+ (0, 3/4, 0) \ 1/2, y, -1/4$<br>( $4_y   3/4, 3/4, 1/4$ )                 | (22) $2 (1/4, 0, 1/4) \ x, 1/8, x$<br>( $2_{xz}   1/4, 1/4, 1/4$ )                  | (23) $4^- (0, 1/4, 0) \ 0, y, 3/4$<br>( $4_y^{-1}   3/4, 1/4, 3/4$ )                        | (24) $2 (-1/4, 0, 1/4) \ \bar{x}+1/2, 3/8, x$<br>( $2_{\bar{xz}}   1/4, 3/4, 3/4$ ) |

For (1/2, 0, 1/2) + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t (1/2, 0, 1/2)$<br>( $1   1/2, 0, 1/2$ )                                     | (2) $2 \ 1/4, 1/4, z$<br>( $2_z   1/2, 1/2, 0$ )  | (3) $2 (0, 1/2, 0) \ 0, y, 1/4$<br>( $2_y   0, 1/2, 1/2$ )                          | (4) $2 \ x, 0, 0$<br>( $2_x   0, 0, 0$ )                                      |
| (5) $3^+ (1/3, 1/3, 1/3)$<br>$x+1/6, x-1/6, x$<br>( $3_{xyz}   1/2, 0, 1/2$ )      | (6) $3^+ \ \bar{x}, x, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   0, 0, 0$ )                       | (7) $3^+ \ x+1/2, \bar{x}, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   1/2, 1/2, 0$ )       | (8) $3^+ \ \bar{x}, \bar{x}+1/2, x$<br>( $3_{\bar{xyz}}^{-1}   0, 1/2, 1/2$ ) |
| (9) $3^- (1/3, 1/3, 1/3)$<br>$x-1/6, x-1/3, x$<br>( $3_{xyz}^{-1}   1/2, 0, 1/2$ ) | (10) $3^- (-1/3, 1/3, 1/3)$<br>$x+1/6, x+1/6, \bar{x}$<br>( $3_{\bar{xyz}}   0, 1/2, 1/2$ ) | (11) $3^- \ \bar{x}, \bar{x}, x$<br>( $3_{xyz}   0, 0, 0$ )                         | (12) $3^- \ \bar{x}, x+1/2, \bar{x}$<br>( $3_{\bar{xyz}}   1/2, 1/2, 0$ )     |
| (13) $2 (1/4, 1/4, 0) \ x, x, 1/8$<br>( $2_{xy}   1/4, 1/4, 1/4$ )                 | (14) $2 (1/4, -1/4, 0) \ x, \bar{x}+1/2, 3/8$<br>( $2_{\bar{xy}}   3/4, 1/4, 3/4$ )         | (15) $4^- (0, 0, 1/4) \ 3/4, 0, z$<br>( $4_z^{-1}   3/4, 3/4, 1/4$ )                | (16) $4^+ (0, 0, 3/4) \ -1/4, 1/2, z$<br>( $4_z   1/4, 3/4, 3/4$ )            |
| (17) $4^- (1/4, 0, 0) \ x, 1/4, 0$<br>( $4_x^{-1}   1/4, 1/4, 1/4$ )               | (18) $2 (0, 3/4, 3/4) \ 1/8, y, y$<br>( $2_{yz}   1/4, 3/4, 3/4$ )                          | (19) $2 (0, -1/4, 1/4) \ 3/8, y+1/2, \bar{y}$<br>( $2_{\bar{yz}}   3/4, 1/4, 3/4$ ) | (20) $4^+ (3/4, 0, 0) \ x, 1/4, 1/2$<br>( $4_x   3/4, 3/4, 1/4$ )             |
| (21) $4^+ (0, 1/4, 0) \ 1/4, y, 0$<br>( $4_y   1/4, 1/4, 1/4$ )                    | (22) $2 (1/2, 0, 1/2) \ x+1/4, 3/8, x$<br>( $2_{xz}   3/4, 3/4, 1/4$ )                      | (23) $4^- (0, 3/4, 0) \ -1/4, y, 1/2$<br>( $4_y^{-1}   1/4, 3/4, 3/4$ )             | (24) $2 \ \bar{x}+3/4, 1/8, x$<br>( $2_{\bar{xz}}   3/4, 1/4, 3/4$ )          |

For (1/2,1/2,0) + set

(1) $t(1/2, 1/2, 0)$ (1   1/2, 1/2, 0)	(2) $2(0, 0, 1/2) \quad 1/4, 0, z$ (2 <sub>z</sub>   1/2, 0, 1/2)	(3) $2(0, y, 0)$ (2 <sub>y</sub>   0, 0, 0)	(4) $2(x, 1/4, 1/4)$ (2 <sub>x</sub>   0, 1/2, 1/2)
(5) $3^+(1/3, 1/3, 1/3)$ $x+1/6, x+1/3, x$ (3 <sub>xyz</sub>   1/2, 1/2, 0)	(6) $3^+ \bar{x}, x+1/2, \bar{x}$ (3 <sub>xy<math>\bar{z}</math></sub> <sup>-1</sup>   0, 1/2, 1/2)	(7) $3^+ x+1/2, \bar{x}-1/2, \bar{x}$ (3 <sub>xy<math>\bar{z}</math></sub> <sup>-1</sup>   1/2, 0, 1/2)	(8) $3^+ \bar{x}, \bar{x}, x$ (3 <sub>xy<math>\bar{z}</math></sub> <sup>-1</sup>   0, 0, 0)
(9) $3^-(1/3, 1/3, 1/3)$ $x+1/3, x+1/6, x$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2, 1/2, 0)	(10) $3^- x, \bar{x}, \bar{x}$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   0, 0, 0)	(11) $3^- \bar{x}+1/2, \bar{x}+1/2, x$ (3 <sub>x<math>\bar{y}\bar{z}</math></sub>   0, 1/2, 1/2)	(12) $3^- (1/3, -1/3, 1/3)$ $\bar{x}-1/6, x+1/3, \bar{x}$ (3 <sub>xy<math>\bar{z}</math></sub>   1/2, 0, 1/2)
(13) $2(1/2, 1/2, 0) \quad x, x+1/4, 3/8$ (2 <sub>xy</sub>   1/4, 3/4, 3/4)	(14) $2(x, \bar{x}+3/4, 1/8)$ (2 <sub>xy</sub>   3/4, 3/4, 1/4)	(15) $4^-(0, 0, 3/4) \quad 1/2, -1/4, z$ (4 <sub>z</sub> <sup>-1</sup>   3/4, 1/4, 3/4)	(16) $4^+(0, 0, 1/4) \quad 0, 1/4, z$ (4 <sub>z</sub>   1/4, 1/4, 1/4)
(17) $4^-(1/4, 0, 0) \quad x, 3/4, 0$ (4 <sub>x</sub> <sup>-1</sup>   1/4, 3/4, 3/4)	(18) $2(0, 1/4, 1/4) \quad 1/8, y, y$ (2 <sub>yz</sub>   1/4, 1/4, 1/4)	(19) $2(0, 1/4, -1/4) \quad 3/8, y+1/2, \bar{y}$ (2 <sub>yz</sub>   3/4, 3/4, 1/4)	(20) $4^+(3/4, 0, 0) \quad x, -1/4, 1/2$ (4 <sub>x</sub>   3/4, 1/4, 3/4)
(21) $4^+(0, 3/4, 0) \quad 1/2, y, 1/4$ (4 <sub>y</sub>   1/4, 3/4, 3/4)	(22) $2(3/4, 0, 3/4) \quad x, 1/8, x$ (2 <sub>xz</sub>   3/4, 1/4, 3/4)	(23) $4^-(0, 1/4, 0) \quad 0, y, 1/4$ (4 <sub>y</sub> <sup>-1</sup>   1/4, 1/4, 1/4)	(24) $2(1/4, 0, -1/4) \quad \bar{x}+1/2, 3/8, x$ (2 <sub>xz</sub>   3/4, 3/4, 1/4)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

96	h	1	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +					
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}, \bar{y}+1/2, z+1/2$	$[\bar{u}, \bar{v}, w]$	(3)	$\bar{x}+1/2, y+1/2, \bar{z}$	$[\bar{u}, v, \bar{w}]$	(4)	$x+1/2, \bar{y}, \bar{z}+1/2$	$[u, \bar{v}, \bar{w}]$
(5)	z,x,y	[w,u,v]	(6)	$z+1/2, \bar{x}, \bar{y}+1/2$	$[w, \bar{u}, \bar{v}]$	(7)	$\bar{z}, \bar{x}+1/2, y+1/2$	$[\bar{w}, \bar{u}, v]$	(8)	$\bar{z}+1/2, x+1/2, \bar{y}$	$[\bar{w}, u, \bar{v}]$
(9)	y,z,x	[v,w,u]	(10)	$\bar{y}+1/2, z+1/2, \bar{x}$	$[\bar{v}, w, \bar{u}]$	(11)	$y+1/2, \bar{z}, \bar{x}+1/2$	$[v, \bar{w}, \bar{u}]$	(12)	$\bar{y}, \bar{z}+1/2, x+1/2$	$[\bar{v}, \bar{w}, u]$
(13)	$y+3/4, x+1/4, \bar{z}+3/4$	$[v, u, \bar{w}]$	(14)	$\bar{y}+1/4, \bar{x}+1/4, \bar{z}+1/4$	$[\bar{v}, \bar{u}, \bar{w}]$	(15)	$y+1/4, \bar{x}+3/4, z+3/4$	$[v, \bar{u}, w]$	(16)	$\bar{y}+3/4, x+3/4, z+1/4$	$[\bar{v}, u, w]$
(17)	$x+3/4, z+1/4, \bar{y}+3/4$	$[u, w, \bar{v}]$	(18)	$\bar{x}+3/4, z+3/4, y+1/4$	$[\bar{u}, w, v]$	(19)	$\bar{x}+1/4, \bar{z}+1/4, \bar{y}+1/4$	$[\bar{u}, \bar{w}, \bar{v}]$	(20)	$x+1/4, \bar{z}+3/4, y+3/4$	$[u, \bar{w}, v]$
(21)	$z+3/4, y+1/4, \bar{x}+3/4$	$[w, v, \bar{u}]$	(22)	$z+1/4, \bar{y}+3/4, x+3/4$	$[w, \bar{v}, u]$	(23)	$\bar{z}+3/4, y+3/4, x+1/4$	$[\bar{w}, v, u]$	(24)	$\bar{z}+1/4, \bar{y}+1/4, \bar{x}+1/4$	$[\bar{w}, \bar{v}, \bar{u}]$
48	g	..2	$1/8, y, \bar{y}+1/4$	$[0, v, \bar{v}]$	$7/8, \bar{y}+1/2, \bar{y}+3/4$	$[0, \bar{v}, \bar{v}]$	$3/8, y+1/2, y+3/4$	$[0, v, v]$	$5/8, \bar{y}, y+1/4$	$[0, \bar{v}, v]$	
			$\bar{y}+1/4, 1/8, y$	$[\bar{v}, 0, v]$	$\bar{y}+3/4, 7/8, \bar{y}+1/2$	$[\bar{v}, 0, \bar{v}]$	$y+3/4, 3/8, y+1/2$	$[v, 0, v]$	$y+1/4, 5/8, \bar{y}$	$[v, 0, \bar{v}]$	
			$y, \bar{y}+1/4, 1/8$	$[v, \bar{v}, 0]$	$\bar{y}+1/2, \bar{y}+3/4, 7/8$	$[\bar{v}, \bar{v}, 0]$	$y+1/2, y+3/4, 3/8$	$[v, v, 0]$	$\bar{y}, y+1/4, 5/8$	$[\bar{v}, v, 0]$	
48	f	2..	$x, 0, 0$	$[u, 0, 0]$	$\bar{x}, 1/2, 1/2$	$[\bar{u}, 0, 0]$	$0, x, 0$	$[0, u, 0]$	$1/2, \bar{x}, 1/2$	$[0, \bar{u}, 0]$	
			$0, 0, x$	$[0, 0, u]$	$1/2, 1/2, \bar{x}$	$[0, 0, \bar{u}]$	$3/4, x+1/4, 3/4$	$[0, u, 0]$	$1/4, \bar{x}+1/4, 1/4$	$[0, \bar{u}, 0]$	
			$x+3/4, 1/4, 3/4$	$[u, 0, 0]$	$\bar{x}+3/4, 3/4, 1/4$	$[\bar{u}, 0, 0]$	$3/4, 1/4, \bar{x}+3/4$	$[0, 0, \bar{u}]$	$1/4, 3/4, x+3/4$	$[0, 0, u]$	

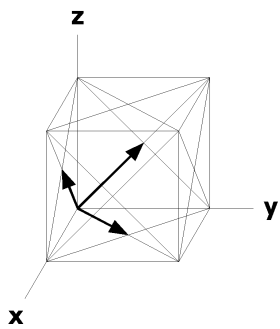
32	e	.3.	$x, x, x [u, u, u]$		$\bar{x}, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, \bar{u}]$	
			$\bar{x}+1/2, \bar{x}+1/2, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$		$x+1/2, \bar{x}, \bar{x}+1/2 [u, \bar{u}, \bar{u}]$	
			$x+3/4, x+1/4, \bar{x}+3/4 [u, u, \bar{u}]$		$\bar{x}+1/4, \bar{x}+1/4, \bar{x}+1/4 [\bar{u}, \bar{u}, \bar{u}]$	
			$x+1/4, \bar{x}+3/4, x+3/4 [u, \bar{u}, \bar{u}]$		$\bar{x}+3/4, x+3/4, x+1/4 [\bar{u}, u, \bar{u}]$	
16	d	.32	$5/8, 5/8, 5/8 [0, 0, 0]$	$3/8, 7/8, 1/8 [0, 0, 0]$	$7/8, 1/8, 3/8 [0, 0, 0]$	$1/8, 3/8, 7/8 [0, 0, 0]$
16	c	.32	$1/8, 1/8, 1/8 [0, 0, 0]$	$7/8, 3/8, 5/8 [0, 0, 0]$	$3/8, 5/8, 7/8 [0, 0, 0]$	$5/8, 7/8, 3/8 [0, 0, 0]$
8	b	23.	$1/2, 1/2, 1/2 [0, 0, 0]$		$1/4, 3/4, 1/4 [0, 0, 0]$	
8	a	23.	$0, 0, 0 [0, 0, 0]$		$3/4, 1/4, 3/4 [0, 0, 0]$	

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $1/4, 0, z$

Along  $[1, 1, 1]$   $p3m'1$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at  $x, x, x$

Along  $[1, 1, 0]$   $c2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 1/8$



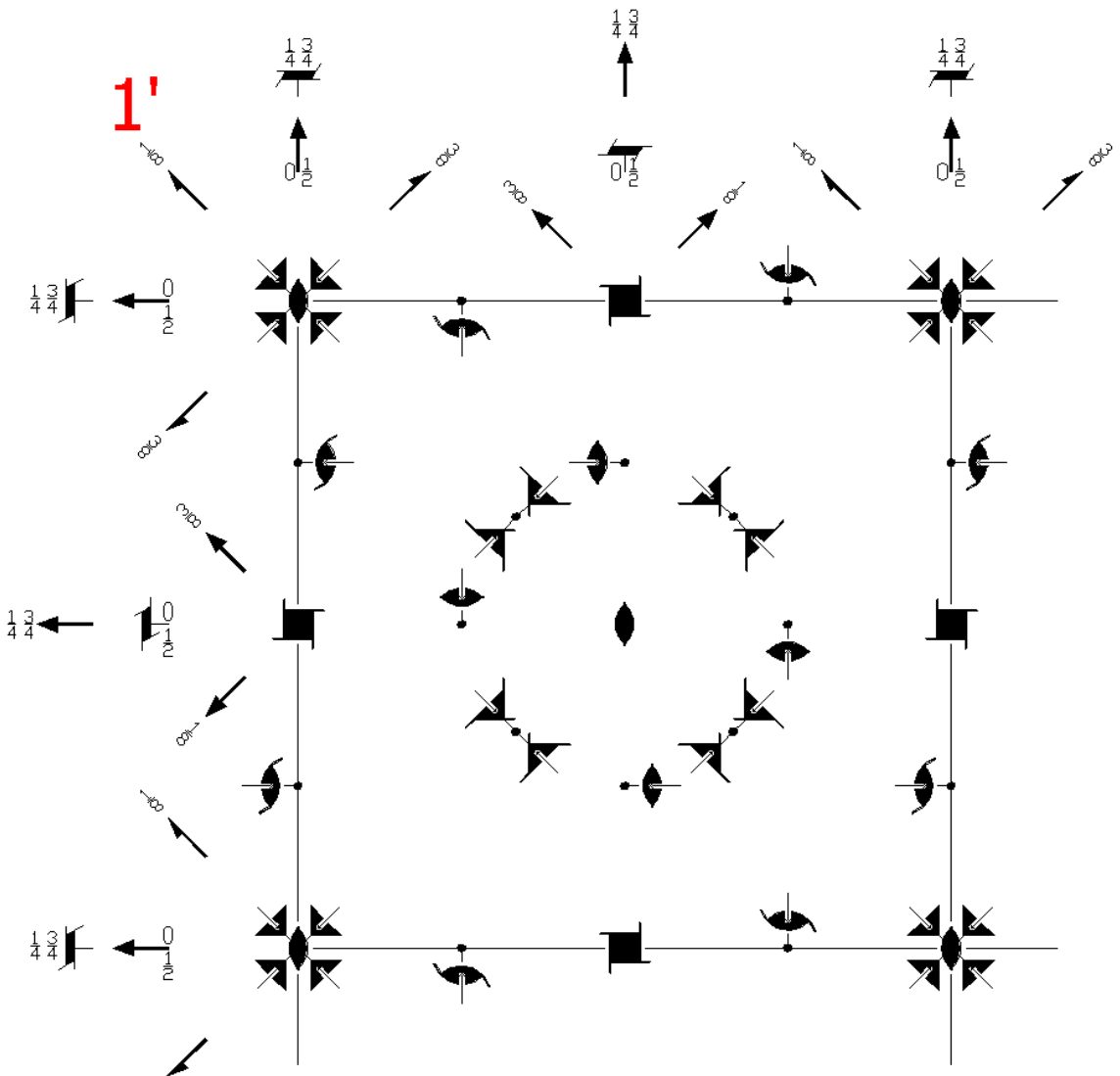
F4<sub>1</sub>321'

4321'

Cubic

210.2.1554

F4<sub>1</sub>321'



Origin at 231'

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $-1/8 \leq y \leq 1/8;$   $-1/8 \leq z \leq 1/8;$   $y \leq \min(x, 1/2-x);$   $-y \leq z \leq \min(x, 1/2-x)$

**Vertices**  $0,0,0$   $1/8,1/8,1/8$   $1/8,1/8,-1/8$   $1/8,-1/8,1/8$   
 $1/2,0,0$   $3/8,1/8,1/8$   $3/8,1/8,-1/8$   $3/8,-1/8,1/8$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |   |  |
|---|--|---|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)   | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)  | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>  1/2,0,1/2)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> (1/3,-1/3,1/3)<br>x+1/6,x+1/6,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) | (7) 3 <sup>+</sup> (-1/3,1/3,1/3)<br>x+1/3,x̄-1/6,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2) | (8) 3 <sup>+</sup> (1/3,1/3,-1/3)<br>x+1/6,x+1/3,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x,x̄+1/2,x̄<br>(3 <sub>xyz</sub>  1/2,1/2,0)                                   | (11) 3 <sup>-</sup> x̄+1/2,x̄,x<br>(3 <sub>xyz</sub>  1/2,0,1/2)                                    | (12) 3 <sup>-</sup> x̄-1/2,x+1/2,x̄<br>(3 <sub>xyz</sub>  0,1/2,1/2)                               |

- |  |  |  |   |
|--|--|--|---|
| (13) $2 (1/2, 1/2, 0) \quad x, x-1/4, 3/8$<br>$(2_{xy}   3/4, 1/4, 3/4)$ | (14) $2 \quad x, \bar{x}+1/4, 1/8$<br>$(2_{xy}   1/4, 1/4, 1/4)$         | (15) $4^- (0, 0, 3/4) \quad 1/2, 1/4, z$<br>$(4_z^{-1}   1/4, 3/4, 3/4)$ | (16) $4^+ (0, 0, 1/4) \quad 0, 3/4, z$<br>$(4_z   3/4, 3/4, 1/4)$ |
| (17) $4^- (3/4, 0, 0) \quad x, 1/2, 1/4$<br>$(4_x^{-1}   3/4, 1/4, 3/4)$ | (18) $2 (0, 1/2, 1/2) \quad 3/8, y+1/4, y$<br>$(2_{yz}   3/4, 3/4, 1/4)$ | (19) $2 \quad 1/8, y+1/4, \bar{y}$<br>$(2_{yz}   1/4, 1/4, 1/4)$         | (20) $4^+ (1/4, 0, 0) \quad x, 0, 3/4$<br>$(4_x   1/4, 3/4, 3/4)$ |
| (21) $4^+ (0, 1/4, 0) \quad 3/4, y, 0$<br>$(4_y   3/4, 1/4, 3/4)$        | (22) $2 (1/2, 0, 1/2) \quad x-1/4, 3/8, x$<br>$(2_{xz}   1/4, 3/4, 3/4)$ | (23) $4^- (0, 3/4, 0) \quad 1/4, y, 1/2$<br>$(4_y^{-1}   3/4, 3/4, 1/4)$ | (24) $2 \quad \bar{x}+1/4, 1/8, x$<br>$(2_{xz}   1/4, 1/4, 1/4)$  |

For (0, 1/2, 1/2) + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t (0, 1/2, 1/2)$<br>$(1   0, 1/2, 1/2)$                                     | (2) $2 \quad 0, 0, z$<br>$(2_z   0, 0, 0)$                                      | (3) $2 \quad 1/4, y, 1/4$<br>$(2_y   1/2, 0, 1/2)$  | (4) $2 (1/2, 0, 0) \quad x, 1/4, 0$<br>$(2_x   1/2, 1/2, 0)$                    |
| (5) $3^+ (1/3, 1/3, 1/3)$<br>$x-1/3, x-1/6, x$<br>$(3_{xyz}   0, 1/2, 1/2)$      | (6) $3^+ \quad \bar{x}+1/2, x, \bar{x}$<br>$(3_{xyz}^{-1}   1/2, 1/2, 0)$       | (7) $3^+ \quad x, \bar{x}, \bar{x}$<br>$(3_{xyz}^{-1}   0, 0, 0)$                         | (8) $3^+ \quad \bar{x}+1/2, \bar{x}+1/2, x$<br>$(3_{xyz}^{-1}   1/2, 0, 1/2)$   |
| (9) $3^- (1/3, 1/3, 1/3)$<br>$x-1/6, x+1/6, x$<br>$(3_{xyz}^{-1}   0, 1/2, 1/2)$ | (10) $3^- \quad x+1/2, \bar{x}, \bar{x}$<br>$(3_{xyz}   1/2, 0, 1/2)$           | (11) $3^- (1/3, 1/3, -1/3)$<br>$\bar{x}+1/3, \bar{x}+1/6, x$<br>$(3_{xyz}   1/2, 1/2, 0)$ | (12) $3^- \quad \bar{x}, x, \bar{x}$<br>$(3_{xyz}   0, 0, 0)$                   |
| (13) $2 (3/4, 3/4, 0) \quad x, x, 1/8$<br>$(2_{xy}   3/4, 3/4, 1/4)$             | (14) $2 (-1/4, 1/4, 0) \quad x, \bar{x}+1/2, 3/8$<br>$(2_{xy}   1/4, 3/4, 3/4)$ | (15) $4^- (0, 0, 1/4) \quad 1/4, 0, z$<br>$(4_z^{-1}   1/4, 1/4, 1/4)$                    | (16) $4^+ (0, 0, 3/4) \quad 1/4, 1/2, z$<br>$(4_z   3/4, 1/4, 3/4)$             |
| (17) $4^- (3/4, 0, 0) \quad x, 1/2, -1/4$<br>$(4_x^{-1}   3/4, 3/4, 1/4)$        | (18) $2 (0, 1/2, 1/2) \quad 3/8, y-1/4, y$<br>$(2_{yz}   3/4, 1/4, 3/4)$        | (19) $2 \quad 1/8, y+3/4, \bar{y}$<br>$(2_{yz}   1/4, 3/4, 3/4)$                          | (20) $4^+ (1/4, 0, 0) \quad x, 0, 1/4$<br>$(4_x   1/4, 1/4, 1/4)$               |
| (21) $4^+ (0, 3/4, 0) \quad 1/2, y, -1/4$<br>$(4_y   3/4, 3/4, 1/4)$             | (22) $2 (1/4, 0, 1/4) \quad x, 1/8, x$<br>$(2_{xz}   1/4, 1/4, 1/4)$            | (23) $4^- (0, 1/4, 0) \quad 0, y, 3/4$<br>$(4_y^{-1}   3/4, 1/4, 3/4)$                    | (24) $2 (-1/4, 0, 1/4) \quad \bar{x}+1/2, 3/8, x$<br>$(2_{xz}   1/4, 3/4, 3/4)$ |

For (1/2, 0, 1/2) + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t (1/2, 0, 1/2)$<br>$(1   1/2, 0, 1/2)$                                     | (2) $2 \quad 1/4, 1/4, z$<br>$(2_z   1/2, 1/2, 0)$                                  | (3) $2 (0, 1/2, 0) \quad 0, y, 1/4$<br>$(2_y   0, 1/2, 1/2)$                    | (4) $2 \quad x, 0, 0$<br>$(2_x   0, 0, 0)$                                |
| (5) $3^+ (1/3, 1/3, 1/3)$<br>$x+1/6, x-1/6, x$<br>$(3_{xyz}   1/2, 0, 1/2)$      | (6) $3^+ \quad \bar{x}, x, \bar{x}$<br>$(3_{xyz}^{-1}   0, 0, 0)$                   | (7) $3^+ \quad x+1/2, \bar{x}, \bar{x}$<br>$(3_{xyz}^{-1}   1/2, 1/2, 0)$       | (8) $3^+ \quad \bar{x}, \bar{x}+1/2, x$<br>$(3_{xyz}^{-1}   0, 1/2, 1/2)$ |
| (9) $3^- (1/3, 1/3, 1/3)$<br>$x-1/6, x-1/3, x$<br>$(3_{xyz}^{-1}   1/2, 0, 1/2)$ | (10) $3^- (-1/3, 1/3, 1/3)$<br>$x+1/6, x+1/6, \bar{x}$<br>$(3_{xyz}   0, 1/2, 1/2)$ | (11) $3^- \quad \bar{x}, \bar{x}, x$<br>$(3_{xyz}   0, 0, 0)$                   | (12) $3^- \quad \bar{x}, x+1/2, \bar{x}$<br>$(3_{xyz}   1/2, 1/2, 0)$     |
| (13) $2 (1/4, 1/4, 0) \quad x, x, 1/8$<br>$(2_{xy}   1/4, 1/4, 1/4)$             | (14) $2 (1/4, -1/4, 0) \quad x, \bar{x}+1/2, 3/8$<br>$(2_{xy}   3/4, 1/4, 3/4)$     | (15) $4^- (0, 0, 1/4) \quad 3/4, 0, z$<br>$(4_z^{-1}   3/4, 3/4, 1/4)$          | (16) $4^+ (0, 0, 3/4) \quad -1/4, 1/2, z$<br>$(4_z   1/4, 3/4, 3/4)$      |
| (17) $4^- (1/4, 0, 0) \quad x, 1/4, 0$<br>$(4_x^{-1}   1/4, 1/4, 1/4)$           | (18) $2 (0, 3/4, 3/4) \quad 1/8, y, y$<br>$(2_{yz}   1/4, 3/4, 3/4)$                | (19) $2 (0, -1/4, 1/4) \quad 3/8, y+1/2, \bar{y}$<br>$(2_{yz}   3/4, 1/4, 3/4)$ | (20) $4^+ (3/4, 0, 0) \quad x, 1/4, 1/2$<br>$(4_x   3/4, 3/4, 1/4)$       |
| (21) $4^+ (0, 1/4, 0) \quad 1/4, y, 0$<br>$(4_y   1/4, 1/4, 1/4)$                | (22) $2 (1/2, 0, 1/2) \quad x+1/4, 3/8, x$<br>$(2_{xz}   3/4, 3/4, 1/4)$            | (23) $4^- (0, 3/4, 0) \quad -1/4, y, 1/2$<br>$(4_y^{-1}   1/4, 3/4, 3/4)$       | (24) $2 \quad \bar{x}+3/4, 1/8, x$<br>$(2_{xz}   3/4, 1/4, 3/4)$          |



## For (1/2,1/2,0) + set

- |  |   |  |  |
|--|---|--|--|
| (1) $t$ (1/2,1/2,0)<br>(1   1/2,1/2,0)   | (2) $2$ (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>   1/2,0,1/2)                             | (3) $2$ 0,y,0<br>(2 <sub>y</sub>   0,0,0)  | (4) $2$ x,1/4,1/4<br>(2 <sub>x</sub>   0,1/2,1/2)  |
| (5) $3^+$ (1/3,1/3,1/3)<br>x+1/6,x+1/3,x<br>(3 <sub>xyz</sub>   1/2,1/2,0)               | (6) $3^+$ $\bar{x}$ ,x+1/2, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   0,1/2,1/2) | (7) $3^+$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,0,1/2) | (8) $3^+$ $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   0,0,0)                 |
| (9) $3^-$ (1/3,1/3,1/3)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0) | (10) $3^-$ x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub>   0,0,0)                     | (11) $3^-$ $\bar{x}$ +1/2, $\bar{x}$ +1/2,x<br>(3 <sub>xyz</sub>   0,1/2,1/2)              | (12) $3^-$ (1/3,-1/3,1/3)<br>$\bar{x}$ -1/6,x+1/3, $\bar{x}$<br>(3 <sub>xyz</sub>   1/2,0,1/2) |
| (13) $2$ (1/2,1/2,0) x,x+1/4,3/8<br>(2 <sub>xy</sub>   1/4,3/4,3/4)                      | (14) $2$ x, $\bar{x}$ +3/4,1/8<br>(2 <sub>xy</sub>   3/4,3/4,1/4)                     | (15) $4^-$ (0,0,3/4) 1/2,-1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>   3/4,1/4,3/4)            | (16) $4^+$ (0,0,1/4) 0,1/4,z<br>(4 <sub>z</sub>   1/4,1/4,1/4)                                 |
| (17) $4^-$ (1/4,0,0) x,3/4,0<br>(4 <sub>x</sub> <sup>-1</sup>   1/4,3/4,3/4)             | (18) $2$ (0,1/4,1/4) 1/8,y,y<br>(2 <sub>yz</sub>   1/4,1/4,1/4)                       | (19) $2$ (0,1/4,-1/4) 3/8,y+1/2, $\bar{y}$<br>(2 <sub>yz</sub>   3/4,3/4,1/4)              | (20) $4^+$ (3/4,0,0) x,-1/4,1/2<br>(4 <sub>x</sub>   3/4,1/4,3/4)                              |
| (21) $4^+$ (0,3/4,0) 1/2,y,1/4<br>(4 <sub>y</sub>   1/4,3/4,3/4)                         | (22) $2$ (3/4,0,3/4) x,1/8,x<br>(2 <sub>xz</sub>   3/4,1/4,3/4)                       | (23) $4^-$ (0,1/4,0) 0,y,1/4<br>(4 <sub>y</sub> <sup>-1</sup>   1/4,1/4,1/4)               | (24) $2$ (1/4,0,-1/4) $\bar{x}$ +1/2,3/8,x<br>(2 <sub>xz</sub>   3/4,3/4,1/4)                  |

## For (0,0,0)' + set

- |   |  |   |   |
|---|--|---|---|
| (1) $1'$<br>(1   0,0,0)'  | (2) $2'$ (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>   0,1/2,1/2)'  | (3) $2'$ (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)'   | (4) $2'$ (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>   1/2,0,1/2)'   |
| (5) $3^+$ ' x,x,x<br>(3 <sub>xyz</sub>   0,0,0)'                                  | (6) $3^+$ ' (1/3,-1/3,1/3)<br>$\bar{x}$ +1/6,x+1/6, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,0,1/2)' | (7) $3^+$ ' (-1/3,1/3,1/3)<br>x+1/3, $\bar{x}$ -1/6, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   0,1/2,1/2)' | (8) $3^+$ ' (1/3,1/3,-1/3)<br>$\bar{x}$ +1/6, $\bar{x}$ +1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)' |
| (9) $3^-$ ' x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   0,0,0)'                    | (10) $3^-$ ' x, $\bar{x}$ +1/2, $\bar{x}$<br>(3 <sub>xyz</sub>   1/2,1/2,0)'                                   | (11) $3^-$ ' $\bar{x}$ +1/2, $\bar{x}$ ,x<br>(3 <sub>xyz</sub>   1/2,0,1/2)'                                    | (12) $3^-$ ' $\bar{x}$ -1/2,x+1/2, $\bar{x}$<br>(3 <sub>xyz</sub>   0,1/2,1/2)'                                 |
| (13) $2'$ (1/2,1/2,0) x,x-1/4,3/8<br>(2 <sub>xy</sub>   3/4,1/4,3/4)'             | (14) $2'$ x, $\bar{x}$ +1/4,1/8<br>(2 <sub>xy</sub>   1/4,1/4,1/4)'  | (15) $4^-$ ' (0,0,3/4) 1/2,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>   1/4,3/4,3/4)'                               | (16) $4^+$ ' (0,0,1/4) 0,3/4,z<br>(4 <sub>z</sub>   3/4,3/4,1/4)'   |
| (17) $4^-$ ' (3/4,0,0) x,1/2,1/4<br>(4 <sub>x</sub> <sup>-1</sup>   3/4,1/4,3/4)' | (18) $2'$ (0,1/2,1/2) 3/8,y+1/4,y<br>(2 <sub>yz</sub>   3/4,3/4,1/4)'  | (19) $2'$ 1/8,y+1/4, $\bar{y}$<br>(2 <sub>yz</sub>   1/4,1/4,1/4)'  | (20) $4^+$ ' (1/4,0,0) x,0,3/4<br>(4 <sub>x</sub>   1/4,3/4,3/4)'   |
| (21) $4^+$ ' (0,1/4,0) 3/4,y,0<br>(4 <sub>y</sub>   3/4,1/4,3/4)'                 | (22) $2'$ (1/2,0,1/2) x-1/4,3/8,x<br>(2 <sub>xz</sub>   1/4,3/4,3/4)'  | (23) $4^-$ ' (0,3/4,0) 1/4,y,1/2<br>(4 <sub>y</sub> <sup>-1</sup>   3/4,3/4,1/4)'                               | (24) $2'$ $\bar{x}$ +1/4,1/8,x<br>(2 <sub>xz</sub>   1/4,1/4,1/4)'  |

## For (0,1/2,1/2)' + set

- |   |  |   |   |
|---|--|---|---|
| (1) $t'$ (0,1/2,1/2)<br>(1   0,1/2,1/2)'  | (2) $2'$ 0,0,z<br>(2 <sub>z</sub>   0,0,0)'  | (3) $2'$ 1/4,y,1/4<br>(2 <sub>y</sub>   1/2,0,1/2)'                                       | (4) $2'$ (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)'                                   |
| (5) $3^+$ ' (1/3,1/3,1/3)<br>x-1/3,x-1/6,x<br>(3 <sub>xyz</sub>   0,1/2,1/2)'               | (6) $3^+$ ' $\bar{x}$ +1/2,x, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)' | (7) $3^+$ ' x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   0,0,0)'         | (8) $3^+$ ' $\bar{x}$ +1/2, $\bar{x}$ +1/2,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,0,1/2)' |
| (9) $3^-$ ' (1/3,1/3,1/3)<br>x-1/6,x+1/6,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   0,1/2,1/2)' | (10) $3^-$ ' x+1/2, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub>   1/2,0,1/2)'             | (11) $3^-$ ' (1/3,1/3,-1/3)<br>x+1/3, $\bar{x}$ +1/6,x<br>(3 <sub>xyz</sub>   1/2,1/2,0)' | (12) $3^-$ ' $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub>xyz</sub>   0,0,0)'                           |

- |   |   |  |   |
|---|---|--|---|
| (13) $2' (3/4, 3/4, 0) \ x, x, 1/8$<br>$(2_{xy}   3/4, 3/4, 1/4)'$        | (14) $2' (-1/4, 1/4, 0) \ x, \bar{x} + 1/2, 3/8$<br>$(2_{\bar{xy}}   1/4, 3/4, 3/4)'$ | (15) $4^{-1} (0, 0, 1/4) \ 1/4, 0, z$<br>$(4_z^{-1}   1/4, 1/4, 1/4)'$ | (16) $4^{+1} (0, 0, 3/4) \ 1/4, 1/2, z$<br>$(4_z   3/4, 1/4, 3/4)'$                   |
| (17) $4^{-1} (3/4, 0, 0) \ x, 1/2, -1/4$<br>$(4_x^{-1}   3/4, 3/4, 1/4)'$ | (18) $2' (0, 1/2, 1/2) \ 3/8, y - 1/4, y$<br>$(2_{yz}   3/4, 1/4, 3/4)'$              | (19) $2' \ 1/8, y + 3/4, \bar{y}$<br>$(2_{\bar{yz}}   1/4, 3/4, 3/4)'$ | (20) $4^{+1} (1/4, 0, 0) \ x, 0, 1/4$<br>$(4_x   1/4, 1/4, 1/4)'$                     |
| (21) $4^{+1} (0, 3/4, 0) \ 1/2, y, -1/4$<br>$(4_y   3/4, 3/4, 1/4)'$      | (22) $2' (1/4, 0, 1/4) \ x, 1/8, x$<br>$(2_{xz}   1/4, 1/4, 1/4)'$                    | (23) $4^{-1} (0, 1/4, 0) \ 0, y, 3/4$<br>$(4_y^{-1}   3/4, 1/4, 3/4)'$ | (24) $2' (-1/4, 0, 1/4) \ \bar{x} + 1/2, 3/8, x$<br>$(2_{\bar{xz}}   1/4, 3/4, 3/4)'$ |

For  $(1/2, 0, 1/2)'$  + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t' (1/2, 0, 1/2)$<br>$(1   1/2, 0, 1/2)'$   | (2) $2' \ 1/4, 1/4, z$<br>$(2_z   1/2, 1/2, 0)'$  | (3) $2' (0, 1/2, 0) \ 0, y, 1/4$<br>$(2_y   0, 1/2, 1/2)'$                            | (4) $2' \ x, 0, 0$<br>$(2_x   0, 0, 0)'$  |
| (5) $3^{+1} (1/3, 1/3, 1/3)$<br>$x + 1/6, x - 1/6, x$<br>$(3_{xyz}   1/2, 0, 1/2)'$      | (6) $3^{+1} \ \bar{x}, x, \bar{x}$<br>$(3_{\bar{xyz}}^{-1}   0, 0, 0)'$                                 | (7) $3^{+1} \ x + 1/2, \bar{x}, \bar{x}$<br>$(3_{\bar{xyz}}^{-1}   1/2, 1/2, 0)'$     | (8) $3^{+1} \ \bar{x}, \bar{x} + 1/2, x$<br>$(3_{\bar{xyz}}^{-1}   0, 1/2, 1/2)'$ |
| (9) $3^{-1} (1/3, 1/3, 1/3)$<br>$x - 1/6, x - 1/3, x$<br>$(3_{xyz}^{-1}   1/2, 0, 1/2)'$ | (10) $3^{-1} (-1/3, 1/3, 1/3)$<br>$x + 1/6, \bar{x} + 1/6, \bar{x}$<br>$(3_{\bar{xyz}}   0, 1/2, 1/2)'$ | (11) $3^{-1} \ \bar{x}, \bar{x}, x$<br>$(3_{\bar{xyz}}   0, 0, 0)'$                   | (12) $3^{-1} \ \bar{x}, x + 1/2, \bar{x}$<br>$(3_{\bar{xyz}}   1/2, 1/2, 0)'$     |
| (13) $2' (1/4, 1/4, 0) \ x, x, 1/8$<br>$(2_{xy}   1/4, 1/4, 1/4)'$                       | (14) $2' (1/4, -1/4, 0) \ x, \bar{x} + 1/2, 3/8$<br>$(2_{\bar{xy}}   3/4, 1/4, 3/4)'$                   | (15) $4^{-1} (0, 0, 1/4) \ 3/4, 0, z$<br>$(4_z^{-1}   3/4, 3/4, 1/4)'$                | (16) $4^{+1} (0, 0, 3/4) \ -1/4, 1/2, z$<br>$(4_z   1/4, 3/4, 3/4)'$              |
| (17) $4^{-1} (1/4, 0, 0) \ x, 1/4, 0$<br>$(4_x^{-1}   1/4, 1/4, 1/4)'$                   | (18) $2' (0, 3/4, 3/4) \ 1/8, y, y$<br>$(2_{yz}   1/4, 3/4, 3/4)'$                                      | (19) $2' (0, -1/4, 1/4) \ 3/8, y + 1/2, \bar{y}$<br>$(2_{\bar{yz}}   3/4, 1/4, 3/4)'$ | (20) $4^{+1} (3/4, 0, 0) \ x, 1/4, 1/2$<br>$(4_x   3/4, 3/4, 1/4)'$               |
| (21) $4^{+1} (0, 1/4, 0) \ 1/4, y, 0$<br>$(4_y   1/4, 1/4, 1/4)'$                        | (22) $2' (1/2, 0, 1/2) \ x + 1/4, 3/8, x$<br>$(2_{xz}   3/4, 3/4, 1/4)'$                                | (23) $4^{-1} (0, 3/4, 0) \ -1/4, y, 1/2$<br>$(4_y^{-1}   1/4, 3/4, 3/4)'$             | (24) $2' \ \bar{x} + 3/4, 1/8, x$<br>$(2_{\bar{xz}}   3/4, 1/4, 3/4)'$            |

For  $(1/2, 1/2, 0)'$  + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t' (1/2, 1/2, 0)$<br>$(1   1/2, 1/2, 0)'$   | (2) $2' (0, 0, 1/2) \ 1/4, 0, z$<br>$(2_z   1/2, 0, 1/2)'$                        | (3) $2' \ 0, y, 0$<br>$(2_y   0, 0, 0)'$  | (4) $2' \ x, 1/4, 1/4$<br>$(2_x   0, 1/2, 1/2)'$  |
| (5) $3^{+1} (1/3, 1/3, 1/3)$<br>$x + 1/6, x + 1/3, x$<br>$(3_{xyz}   1/2, 1/2, 0)'$      | (6) $3^{+1} \ \bar{x}, x + 1/2, \bar{x}$<br>$(3_{\bar{xyz}}^{-1}   0, 1/2, 1/2)'$ | (7) $3^{+1} \ x + 1/2, \bar{x} - 1/2, \bar{x}$<br>$(3_{\bar{xyz}}^{-1}   1/2, 0, 1/2)'$ | (8) $3^{+1} \ \bar{x}, \bar{x}, x$<br>$(3_{\bar{xyz}}^{-1}   0, 0, 0)'$                     |
| (9) $3^{-1} (1/3, 1/3, 1/3)$<br>$x + 1/3, x + 1/6, x$<br>$(3_{xyz}^{-1}   1/2, 1/2, 0)'$ | (10) $3^{-1} \ x, \bar{x}, \bar{x}$<br>$(3_{\bar{xyz}}   0, 0, 0)'$               | (11) $3^{-1} \ \bar{x} + 1/2, \bar{x} + 1/2, x$<br>$(3_{\bar{xyz}}   0, 1/2, 1/2)'$     | (12) $3^{-1} (1/3, -1/3, 1/3)$<br>$x - 1/6, x + 1/3, x$<br>$(3_{\bar{xyz}}   1/2, 0, 1/2)'$ |
| (13) $2' (1/2, 1/2, 0) \ x, x + 1/4, 3/8$<br>$(2_{xy}   1/4, 3/4, 3/4)'$                 | (14) $2' \ x, \bar{x} + 3/4, 1/8$<br>$(2_{\bar{xy}}   3/4, 3/4, 1/4)'$            | (15) $4^{-1} (0, 0, 3/4) \ 1/2, -1/4, z$<br>$(4_z^{-1}   3/4, 1/4, 3/4)'$               | (16) $4^{+1} (0, 0, 1/4) \ 0, 1/4, z$<br>$(4_z   1/4, 1/4, 1/4)'$                           |
| (17) $4^{-1} (1/4, 0, 0) \ x, 3/4, 0$<br>$(4_x^{-1}   1/4, 3/4, 3/4)'$                   | (18) $2' (0, 1/4, 1/4) \ 1/8, y, y$<br>$(2_{yz}   1/4, 1/4, 1/4)'$                | (19) $2' (0, 1/4, -1/4) \ 3/8, y + 1/2, \bar{y}$<br>$(2_{\bar{yz}}   3/4, 3/4, 1/4)'$   | (20) $4^{+1} (3/4, 0, 0) \ x, -1/4, 1/2$<br>$(4_x   3/4, 1/4, 3/4)'$                        |
| (21) $4^{+1} (0, 3/4, 0) \ 1/2, y, 1/4$<br>$(4_y   1/4, 3/4, 3/4)'$                      | (22) $2' (3/4, 0, 3/4) \ x, 1/8, x$<br>$(2_{xz}   3/4, 1/4, 3/4)'$                | (23) $4^{-1} (0, 1/4, 0) \ 0, y, 1/4$<br>$(4_y^{-1}   1/4, 1/4, 1/4)'$                  | (24) $2' (1/4, 0, -1/4) \ \bar{x} + 1/2, 3/8, x$<br>$(2_{\bar{xz}}   3/4, 3/4, 1/4)'$       |

**Generators selected** (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ;  $t(0, 1/2, 1/2)$ ;  $t(1/2, 0, 1/2)$ ; (2); (3); (5); (13): 1'.

## Positions

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

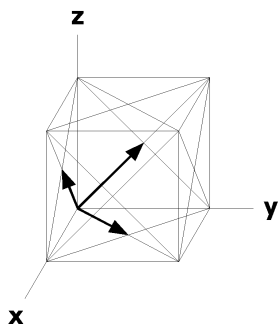
			(0,0,0) + (0,0,0)' +	(0,1/2,1/2) + (0,1/2,1/2)' +	(1/2,0,1/2) + (1/2,0,1/2)' +	(1/2,1/2,0) + (1/2,1/2,0)' +				
96	h	11'								
(1)	x,y,z	[0,0,0]	(2) $\bar{x}, \bar{y} + 1/2, z + 1/2$	[0,0,0]	(3) $\bar{x} + 1/2, y + 1/2, \bar{z}$	[0,0,0]	(4) $x + 1/2, \bar{y}, \bar{z} + 1/2$	[0,0,0]		
(5)	z,x,y	[0,0,0]	(6) $z + 1/2, \bar{x}, \bar{y} + 1/2$	[0,0,0]	(7) $\bar{z}, \bar{x} + 1/2, y + 1/2$	[0,0,0]	(8) $\bar{z} + 1/2, x + 1/2, \bar{y}$	[0,0,0]		
(9)	y,z,x	[0,0,0]	(10) $\bar{y} + 1/2, z + 1/2, \bar{x}$	[0,0,0]	(11) $y + 1/2, \bar{z}, \bar{x} + 1/2$	[0,0,0]	(12) $\bar{y}, \bar{z} + 1/2, x + 1/2$	[0,0,0]		
(13)	$y + 3/4, x + 1/4, \bar{z} + 3/4$	[0,0,0]	(14) $\bar{y} + 1/4, \bar{x} + 1/4, \bar{z} + 1/4$	[0,0,0]	(15) $y + 1/4, \bar{x} + 3/4, z + 3/4$	[0,0,0]	(16) $\bar{y} + 3/4, x + 3/4, z + 1/4$	[0,0,0]		
(17)	$x + 3/4, z + 1/4, \bar{y} + 3/4$	[0,0,0]	(18) $\bar{x} + 3/4, z + 3/4, y + 1/4$	[0,0,0]	(19) $\bar{x} + 1/4, \bar{z} + 1/4, \bar{y} + 1/4$	[0,0,0]	(20) $x + 1/4, \bar{z} + 3/4, y + 3/4$	[0,0,0]		
(21)	$z + 3/4, y + 1/4, \bar{x} + 3/4$	[0,0,0]	(22) $z + 1/4, \bar{y} + 3/4, x + 3/4$	[0,0,0]	(23) $\bar{z} + 3/4, y + 3/4, x + 1/4$	[0,0,0]	(24) $\bar{z} + 1/4, \bar{y} + 1/4, \bar{x} + 1/4$	[0,0,0]		
48	g	..21'	$1/8, \bar{y}, \bar{y} + 1/4$	[0,0,0]	$7/8, \bar{y} + 1/2, \bar{y} + 3/4$	[0,0,0]	$3/8, y + 1/2, y + 3/4$	[0,0,0]	$5/8, \bar{y}, y + 1/4$	[0,0,0]
			$\bar{y} + 1/4, 1/8, y$	[0,0,0]	$\bar{y} + 3/4, 7/8, \bar{y} + 1/2$	[0,0,0]	$y + 3/4, 3/8, y + 1/2$	[0,0,0]	$y + 1/4, 5/8, \bar{y}$	[0,0,0]
			$y, \bar{y} + 1/4, 1/8$	[0,0,0]	$\bar{y} + 1/2, \bar{y} + 3/4, 7/8$	[0,0,0]	$y + 1/2, y + 3/4, 3/8$	[0,0,0]	$\bar{y}, y + 1/4, 5/8$	[0,0,0]
48	f	2..1'	x,0,0	[0,0,0]	$\bar{x}, 1/2, 1/2$	[0,0,0]	0,x,0	[0,0,0]	$1/2, \bar{x}, 1/2$	[0,0,0]
			0,0,x	[0,0,0]	$1/2, 1/2, \bar{x}$	[0,0,0]	$3/4, x + 1/4, 3/4$	[0,0,0]	$1/4, \bar{x} + 1/4, 1/4$	[0,0,0]
			$x + 3/4, 1/4, 3/4$	[0,0,0]	$\bar{x} + 3/4, 3/4, 1/4$	[0,0,0]	$3/4, 1/4, \bar{x} + 3/4$	[0,0,0]	$1/4, 3/4, x + 3/4$	[0,0,0]
32	e	.3.1'	x,x,x	[0,0,0]		$\bar{x}, \bar{x} + 1/2, x + 1/2$	[0,0,0]			
			$\bar{x} + 1/2, x + 1/2, \bar{x}$	[0,0,0]		$x + 1/2, \bar{x}, \bar{x} + 1/2$	[0,0,0]			
			$x + 3/4, x + 1/4, \bar{x} + 3/4$	[0,0,0]		$\bar{x} + 1/4, \bar{x} + 1/4, \bar{x} + 1/4$	[0,0,0]			
			$x + 1/4, \bar{x} + 3/4, x + 3/4$	[0,0,0]		$\bar{x} + 3/4, x + 3/4, x + 1/4$	[0,0,0]			
16	d	.321'	$5/8, 5/8, 5/8$	[0,0,0]	$3/8, 7/8, 1/8$	[0,0,0]	$7/8, 1/8, 3/8$	[0,0,0]	$1/8, 3/8, 7/8$	[0,0,0]
16	c	.321'	$1/8, 1/8, 1/8$	[0,0,0]	$7/8, 3/8, 5/8$	[0,0,0]	$3/8, 5/8, 7/8$	[0,0,0]	$5/8, 7/8, 3/8$	[0,0,0]
8	b	23.1'	$1/2, 1/2, 1/2$	[0,0,0]		$1/4, 3/4, 1/4$	[0,0,0]			
8	a	23.1'	0,0,0	[0,0,0]		$3/4, 1/4, 3/4$	[0,0,0]			

## Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,0,z

Along [1,1,1] p3m11'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

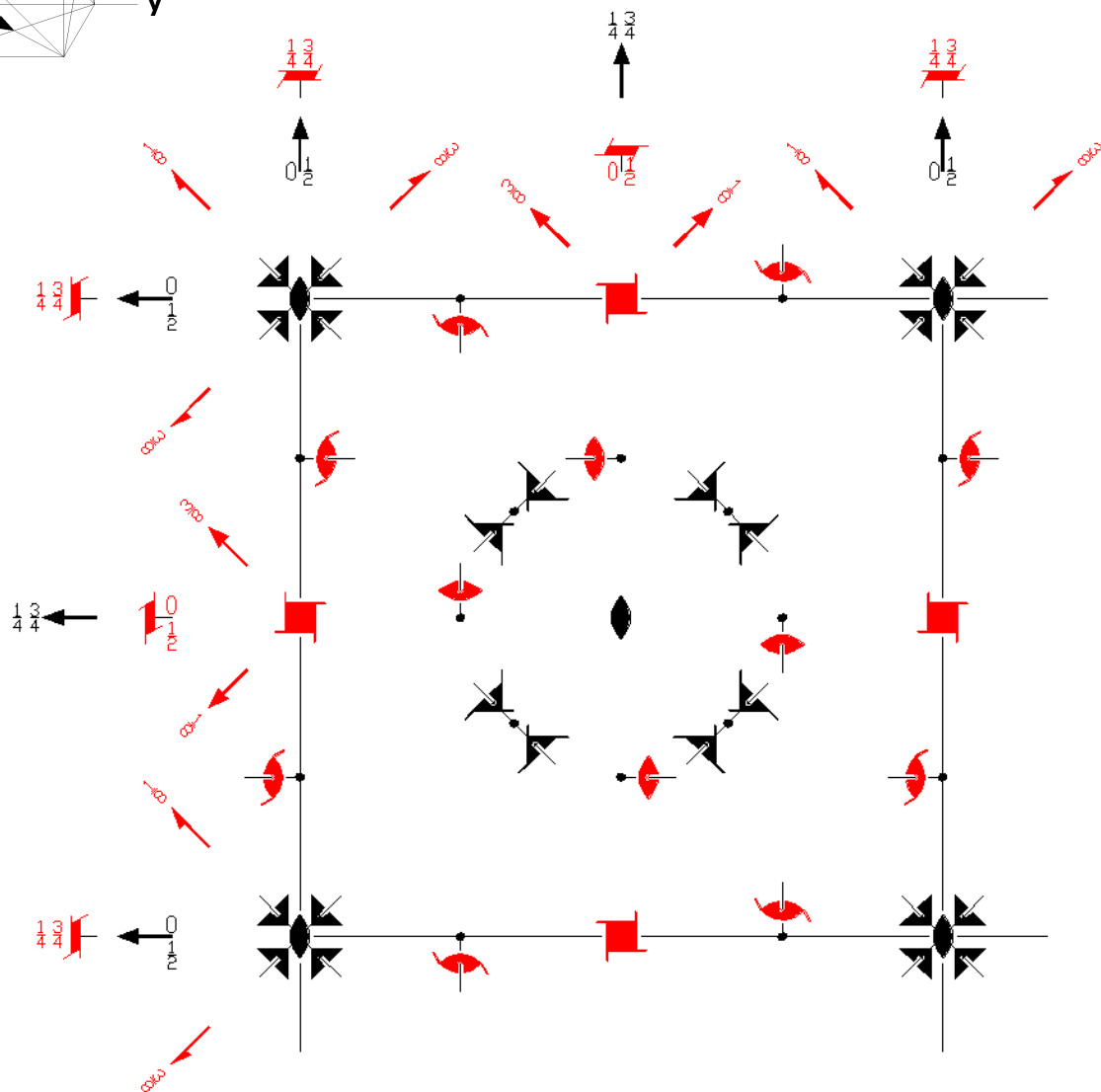
Along [1,1,0] c2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/8



F4<sub>1</sub>'32'  
210.3.1555

4'32'  
F4<sub>1</sub>'32'

Cubic



Origin at 23

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $-1/8 \leq y \leq 1/8$ ;  $-1/8 \leq z \leq 1/8$ ;  $y \leq \min(x, 1/2-x)$ ;  $-y \leq z \leq \min(x, 1/2-x)$

**Vertices**  $0,0,0$   $1/8,1/8,1/8$   $1/8,1/8,-1/8$   $1/8,-1/8,1/8$   
 $1/2,0,0$   $3/8,1/8,1/8$   $3/8,1/8,-1/8$   $3/8,-1/8,1/8$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |   |  |
|---|--|---|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)   | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)  | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>  1/2,0,1/2)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> (1/3,-1/3,1/3)<br>x+1/6,x+1/6,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) | (7) 3 <sup>+</sup> (-1/3,1/3,1/3)<br>x+1/3,x̄-1/6,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2) | (8) 3 <sup>+</sup> (1/3,1/3,-1/3)<br>x+1/6,x+1/3,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x,x̄+1/2,x̄<br>(3 <sub>xyz</sub>  1/2,1/2,0)                                   | (11) 3 <sup>-</sup> x̄+1/2,x̄,x<br>(3 <sub>xyz</sub>  1/2,0,1/2)                                    | (12) 3 <sup>-</sup> x̄-1/2,x+1/2,x̄<br>(3 <sub>xyz</sub>  0,1/2,1/2)                               |

- |   |  |   |   |
|---|--|---|---|
| (13) 2' (1/2,1/2,0) x,x-1/4,3/8<br>(2 <sub>xy</sub>  3/4,1/4,3/4)'                        | (14) 2' x, $\bar{x}$ +1/4,1/8<br>(2 <sub>xy</sub>  1/4,1/4,1/4)'   | (15) 4 <sup>-</sup> ' (0,0,3/4) 1/2,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/4,3/4,3/4)' | (16) 4 <sup>+</sup> ' (0,0,1/4) 0,3/4,z<br>(4 <sub>z</sub>  3/4,3/4,1/4)' |
| (17) 4 <sup>-</sup> ' (3/4,0,0) x,1/2,1/4<br>(4 <sub>x</sub> <sup>-1</sup>  3/4,1/4,3/4)' | (18) 2' (0,1/2,1/2) 3/8,y+1/4,y<br>(2 <sub>yz</sub>  3/4,3/4,1/4)' | (19) 2' 1/8,y+1/4, $\bar{y}$<br>(2 <sub>yz</sub>  1/4,1/4,1/4)'                           | (20) 4 <sup>+</sup> ' (1/4,0,0) x,0,3/4<br>(4 <sub>x</sub>  1/4,3/4,3/4)' |
| (21) 4 <sup>+</sup> ' (0,1/4,0) 3/4,y,0<br>(4 <sub>y</sub>  3/4,1/4,3/4)'                 | (22) 2' (1/2,0,1/2) x-1/4,3/8,x<br>(2 <sub>xz</sub>  1/4,3/4,3/4)' | (23) 4 <sup>-</sup> ' (0,3/4,0) 1/4,y,1/2<br>(4 <sub>y</sub> <sup>-1</sup>  3/4,3/4,1/4)' | (24) 2' $\bar{x}$ +1/4,1/8,x<br>(2 <sub>xz</sub>  1/4,1/4,1/4)'           |

For (0,1/2,1/2) + set

- |  |   |   |  |
|--|---|---|--|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)  | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) 3 <sup>+</sup> (1/3,1/3,1/3)<br>x-1/3,x-1/6,x<br>(3 <sub>xyz</sub>  0,1/2,1/2)               | (6) 3 <sup>+</sup> $\bar{x}$ +1/2,x, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0) | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)                  | (8) 3 <sup>+</sup> $\bar{x}$ +1/2, $\bar{x}$ +1/2,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) |
| (9) 3 <sup>-</sup> (1/3,1/3,1/3)<br>x-1/6,x+1/6,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2) | (10) 3 <sup>-</sup> x+1/2, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub>  1/2,0,1/2)             | (11) 3 <sup>-</sup> (1/3,1/3,-1/3)<br>$\bar{x}$ +1/3, $\bar{x}$ +1/6,x<br>(3 <sub>xyz</sub>  1/2,1/2,0) | (12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)                           |
| (13) 2' (3/4,3/4,0) x,x,1/8<br>(2 <sub>xy</sub>  3/4,3/4,1/4)'                                   | (14) 2' (-1/4,1/4,0) x, $\bar{x}$ +1/2,3/8<br>(2 <sub>xy</sub>  1/4,3/4,3/4)'                 | (15) 4 <sup>-</sup> ' (0,0,1/4) 1/4,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/4,1/4,1/4)'                 | (16) 4 <sup>+</sup> ' (0,0,3/4) 1/4,1/2,z<br>(4 <sub>z</sub>  3/4,1/4,3/4)'                        |
| (17) 4 <sup>-</sup> ' (3/4,0,0) x,1/2,-1/4<br>(4 <sub>x</sub> <sup>-1</sup>  3/4,3/4,1/4)'       | (18) 2' (0,1/2,1/2) 3/8,y-1/4,y<br>(2 <sub>yz</sub>  3/4,1/4,3/4)'                            | (19) 2' 1/8,y+3/4, $\bar{y}$<br>(2 <sub>yz</sub>  1/4,3/4,3/4)'   | (20) 4 <sup>+</sup> ' (1/4,0,0) x,0,1/4<br>(4 <sub>x</sub>  1/4,1/4,1/4)'                          |
| (21) 4 <sup>+</sup> ' (0,3/4,0) 1/2,y,-1/4<br>(4 <sub>y</sub>  3/4,3/4,1/4)'                     | (22) 2' (1/4,0,1/4) x,1/8,x<br>(2 <sub>xz</sub>  1/4,1/4,1/4)'                                | (23) 4 <sup>-</sup> ' (0,1/4,0) 0,y,3/4<br>(4 <sub>y</sub> <sup>-1</sup>  3/4,1/4,3/4)'                 | (24) 2' (-1/4,0,1/4) $\bar{x}$ +1/2,3/8,x<br>(2 <sub>xz</sub>  1/4,3/4,3/4)'                       |

For (1/2,0,1/2) + set

- |  |   |  |  |
|--|---|--|--|
| (1) t (1/2,0,1/2)<br>(1 1/2,0,1/2)   | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)  | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> (1/3,1/3,1/3)<br>x+1/6,x-1/6,x<br>(3 <sub>xyz</sub>  1/2,0,1/2)               | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)         | (7) 3 <sup>+</sup> x+1/2, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0) | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ +1/2,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2) |
| (9) 3 <sup>-</sup> (1/3,1/3,1/3)<br>x-1/6,x-1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) | (10) 3 <sup>-</sup> (-1/3,1/3,1/3)<br>x+1/6,x+1/6, $\bar{x}$<br>(3 <sub>xyz</sub>  0,1/2,1/2) | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>xyz</sub>  0,0,0)                      | (12) 3 <sup>-</sup> $\bar{x}$ ,x+1/2, $\bar{x}$<br>(3 <sub>xyz</sub>  1/2,1/2,0)               |
| (13) 2' (1/4,1/4,0) x,x,1/8<br>(2 <sub>xy</sub>  1/4,1/4,1/4)'                                   | (14) 2' (1/4,-1/4,0) x, $\bar{x}$ +1/2,3/8<br>(2 <sub>xy</sub>  3/4,1/4,3/4)'                 | (15) 4 <sup>-</sup> ' (0,0,1/4) 3/4,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  3/4,3/4,1/4)'        | (16) 4 <sup>+</sup> ' (0,0,3/4) -1/4,1/2,z<br>(4 <sub>z</sub>  1/4,3/4,3/4)'                   |
| (17) 4 <sup>-</sup> ' (1/4,0,0) x,1/4,0<br>(4 <sub>x</sub> <sup>-1</sup>  1/4,1/4,1/4)'          | (18) 2' (0,3/4,3/4) 1/8,y,y<br>(2 <sub>yz</sub>  1/4,3/4,3/4)'                                | (19) 2' (0,-1/4,1/4) 3/8,y+1/2, $\bar{y}$<br>(2 <sub>yz</sub>  3/4,1/4,3/4)'                   | (20) 4 <sup>+</sup> ' (3/4,0,0) x,1/4,1/2<br>(4 <sub>x</sub>  3/4,3/4,1/4)'                    |
| (21) 4 <sup>+</sup> ' (0,1/4,0) 1/4,y,0<br>(4 <sub>y</sub>  1/4,1/4,1/4)'                        | (22) 2' (1/2,0,1/2) x+1/4,3/8,x<br>(2 <sub>xz</sub>  3/4,3/4,1/4)'                            | (23) 4 <sup>-</sup> ' (0,3/4,0) -1/4,y,1/2<br>(4 <sub>y</sub> <sup>-1</sup>  1/4,3/4,3/4)'     | (24) 2' $\bar{x}$ +3/4,1/8,x<br>(2 <sub>xz</sub>  3/4,1/4,3/4)'                                |

For (1/2,1/2,0) + set

(1) $t(1/2,1/2,0)$ (1 1/2,1/2,0)	(2) $2(0,0,1/2) \quad 1/4,0,z$ (2 <sub>z</sub>  1/2,0,1/2)	(3) $2 \quad 0,y,0$ (2 <sub>y</sub>  0,0,0)	(4) $2 \quad x,1/4,1/4$ (2 <sub>x</sub>  0,1/2,1/2)
(5) $3^+ (1/3,1/3,1/3)$ $x+1/6,x+1/3,x$ (3 <sub>xyz</sub>  1/2,1/2,0)	(6) $3^+ \quad \bar{x},x+1/2,\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(7) $3^+ \quad x+1/2,\bar{x}-1/2,\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2)	(8) $3^+ \quad \bar{x},\bar{x},x$ (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)
(9) $3^- (1/3,1/3,1/3)$ $x+1/3,x+1/6,x$ (3 <sub>xy</sub> <sup>-1</sup>  1/2,1/2,0)	(10) $3^- \quad x,\bar{x},\bar{x}$ (3 <sub>xyz</sub>  0,0,0)	(11) $3^- \quad \bar{x}+1/2,\bar{x}+1/2,x$ (3 <sub>xyz</sub>  0,1/2,1/2)	(12) $3^- (1/3,-1/3,1/3)$ $\bar{x}-1/6,x+1/3,\bar{x}$ (3 <sub>xyz</sub>  1/2,0,1/2)
(13) $2' (1/2,1/2,0) \quad x,x+1/4,3/8$ (2 <sub>xy</sub>  1/4,3/4,3/4)'	(14) $2' \quad x,\bar{x}+3/4,1/8$ (2 <sub>xy</sub>  3/4,3/4,1/4)'	(15) $4^- (0,0,3/4) \quad 1/2,-1/4,z$ (4 <sub>z</sub> <sup>-1</sup>  3/4,1/4,3/4)'	(16) $4^+ (0,0,1/4) \quad 0,1/4,z$ (4 <sub>z</sub>  1/4,1/4,1/4)'
(17) $4^- (1/4,0,0) \quad x,3/4,0$ (4 <sub>x</sub> <sup>-1</sup>  1/4,3/4,3/4)'	(18) $2' (0,1/4,1/4) \quad 1/8,y,y$ (2 <sub>yz</sub>  1/4,1/4,1/4)'	(19) $2' (0,1/4,-1/4) \quad 3/8,y+1/2,\bar{y}$ (2 <sub>yz</sub>  3/4,3/4,1/4)'	(20) $4^+ (3/4,0,0) \quad x,-1/4,1/2$ (4 <sub>x</sub>  3/4,1/4,3/4)'
(21) $4^+ (0,3/4,0) \quad 1/2,y,1/4$ (4 <sub>y</sub>  1/4,3/4,3/4)'	(22) $2' (3/4,0,3/4) \quad x,1/8,x$ (2 <sub>xz</sub>  3/4,1/4,3/4)'	(23) $4^- (0,1/4,0) \quad 0,y,1/4$ (4 <sub>y</sub> <sup>-1</sup>  1/4,1/4,1/4)'	(24) $2' (1/4,0,-1/4) \quad \bar{x}+1/2,3/8,x$ (2 <sub>xz</sub>  3/4,3/4,1/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

96	h	1	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +					
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y}+1/2,z+1/2$	$[\bar{u},\bar{v},w]$	(3)	$\bar{x}+1/2,y+1/2,\bar{z}$	$[\bar{u},v,\bar{w}]$	(4)	$x+1/2,\bar{y},\bar{z}+1/2$	$[u,\bar{v},\bar{w}]$
(5)	z,x,y	[w,u,v]	(6)	$z+1/2,\bar{x},\bar{y}+1/2$	$[w,\bar{u},\bar{v}]$	(7)	$\bar{z},\bar{x}+1/2,y+1/2$	$[\bar{w},\bar{u},v]$	(8)	$\bar{z}+1/2,x+1/2,\bar{y}$	$[\bar{w},u,\bar{v}]$
(9)	y,z,x	[v,w,u]	(10)	$\bar{y}+1/2,z+1/2,\bar{x}$	$[\bar{v},w,\bar{u}]$	(11)	$y+1/2,\bar{z},\bar{x}+1/2$	$[v,\bar{w},\bar{u}]$	(12)	$\bar{y},\bar{z}+1/2,x+1/2$	$[\bar{v},\bar{w},u]$
(13)	$y+3/4,x+1/4,\bar{z}+3/4$	$[\bar{v},\bar{u},w]$	(14)	$\bar{y}+1/4,\bar{x}+1/4,\bar{z}+1/4$	$[v,u,w]$	(15)	$y+1/4,\bar{x}+3/4,z+3/4$	$[\bar{v},u,\bar{w}]$	(16)	$\bar{y}+3/4,x+3/4,z+1/4$	$[v,\bar{u},\bar{w}]$
(17)	$x+3/4,z+1/4,\bar{y}+3/4$	$[\bar{u},\bar{w},v]$	(18)	$\bar{x}+3/4,z+3/4,y+1/4$	$[u,\bar{w},\bar{v}]$	(19)	$\bar{x}+1/4,\bar{z}+1/4,\bar{y}+1/4$	$[u,w,v]$	(20)	$x+1/4,\bar{z}+3/4,y+3/4$	$[\bar{u},w,\bar{v}]$
(21)	$z+3/4,y+1/4,\bar{x}+3/4$	$[\bar{w},\bar{v},u]$	(22)	$z+1/4,\bar{y}+3/4,x+3/4$	$[\bar{w},v,\bar{u}]$	(23)	$\bar{z}+3/4,y+3/4,x+1/4$	$[w,\bar{v},\bar{u}]$	(24)	$\bar{z}+1/4,\bar{y}+1/4,\bar{x}+1/4$	$[w,v,u]$
48	g	..2'	$1/8,y,\bar{y}+1/4$	$[u,v,v]$	$7/8,\bar{y}+1/2,\bar{y}+3/4$	$[\bar{u},\bar{v},v]$	$3/8,y+1/2,y+3/4$	$[\bar{u},v,\bar{v}]$	$5/8,\bar{y},y+1/4$	$[u,\bar{v},\bar{v}]$	
			$\bar{y}+1/4,1/8,y$	$[v,u,v]$	$\bar{y}+3/4,7/8,\bar{y}+1/2$	$[v,\bar{u},\bar{v}]$	$y+3/4,3/8,y+1/2$	$[\bar{v},\bar{u},v]$	$y+1/4,5/8,\bar{y}$	$[\bar{v},u,\bar{v}]$	
			$y,\bar{y}+1/4,1/8$	$[v,v,u]$	$\bar{y}+1/2,\bar{y}+3/4,7/8$	$[\bar{v},v,\bar{u}]$	$y+1/2,y+3/4,3/8$	$[v,\bar{v},\bar{u}]$	$\bar{y},y+1/4,5/8$	$[\bar{v},\bar{v},u]$	
48	f	2..	$x,0,0$	$[u,0,0]$	$\bar{x},1/2,1/2$	$[\bar{u},0,0]$	$0,x,0$	$[0,u,0]$	$1/2,\bar{x},1/2$	$[0,\bar{u},0]$	
			$0,0,x$	$[0,0,u]$	$1/2,1/2,\bar{x}$	$[0,0,\bar{u}]$	$3/4,x+1/4,3/4$	$[0,\bar{u},0]$	$1/4,\bar{x}+1/4,1/4$	$[0,u,0]$	
			$x+3/4,1/4,3/4$	$[\bar{u},0,0]$	$\bar{x}+3/4,3/4,1/4$	$[u,0,0]$	$3/4,1/4,\bar{x}+3/4$	$[0,0,u]$	$1/4,3/4,x+3/4$	$[0,0,\bar{u}]$	

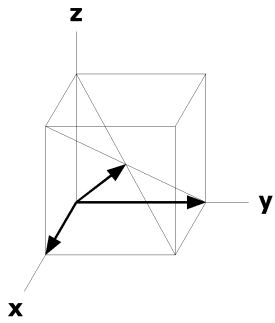
32	e	.3.	$x, x, x [u, u, u]$		$\bar{x}, \bar{x}+1/2, x+1/2 [\bar{u}, \bar{u}, u]$	
			$\bar{x}+1/2, x+1/2, \bar{x} [\bar{u}, u, \bar{u}]$		$x+1/2, \bar{x}, \bar{x}+1/2 [u, \bar{u}, \bar{u}]$	
			$x+3/4, x+1/4, \bar{x}+3/4 [\bar{u}, \bar{u}, u]$		$\bar{x}+1/4, \bar{x}+1/4, \bar{x}+1/4 [u, u, u]$	
			$x+1/4, \bar{x}+3/4, x+3/4 [\bar{u}, u, \bar{u}]$		$\bar{x}+3/4, x+3/4, x+1/4 [u, \bar{u}, \bar{u}]$	
16	d	.32'	$5/8, 5/8, 5/8 [u, u, u]$	$3/8, 7/8, 1/8 [\bar{u}, \bar{u}, u]$	$7/8, 1/8, 3/8 [\bar{u}, u, \bar{u}]$	$1/8, 3/8, 7/8 [u, \bar{u}, \bar{u}]$
16	c	.32'	$1/8, 1/8, 1/8 [u, u, u]$	$7/8, 3/8, 5/8 [\bar{u}, \bar{u}, u]$	$3/8, 5/8, 7/8 [\bar{u}, u, \bar{u}]$	$5/8, 7/8, 3/8 [u, \bar{u}, \bar{u}]$
8	b	23.	$1/2, 1/2, 1/2 [0, 0, 0]$		$1/4, 3/4, 1/4 [0, 0, 0]$	
8	a	23.	$0, 0, 0 [0, 0, 0]$		$3/4, 1/4, 3/4 [0, 0, 0]$	

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p4'm'm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $1/4, 0, z$

Along  $[1, 1, 1]$   $p3m1$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at  $x, x, x$

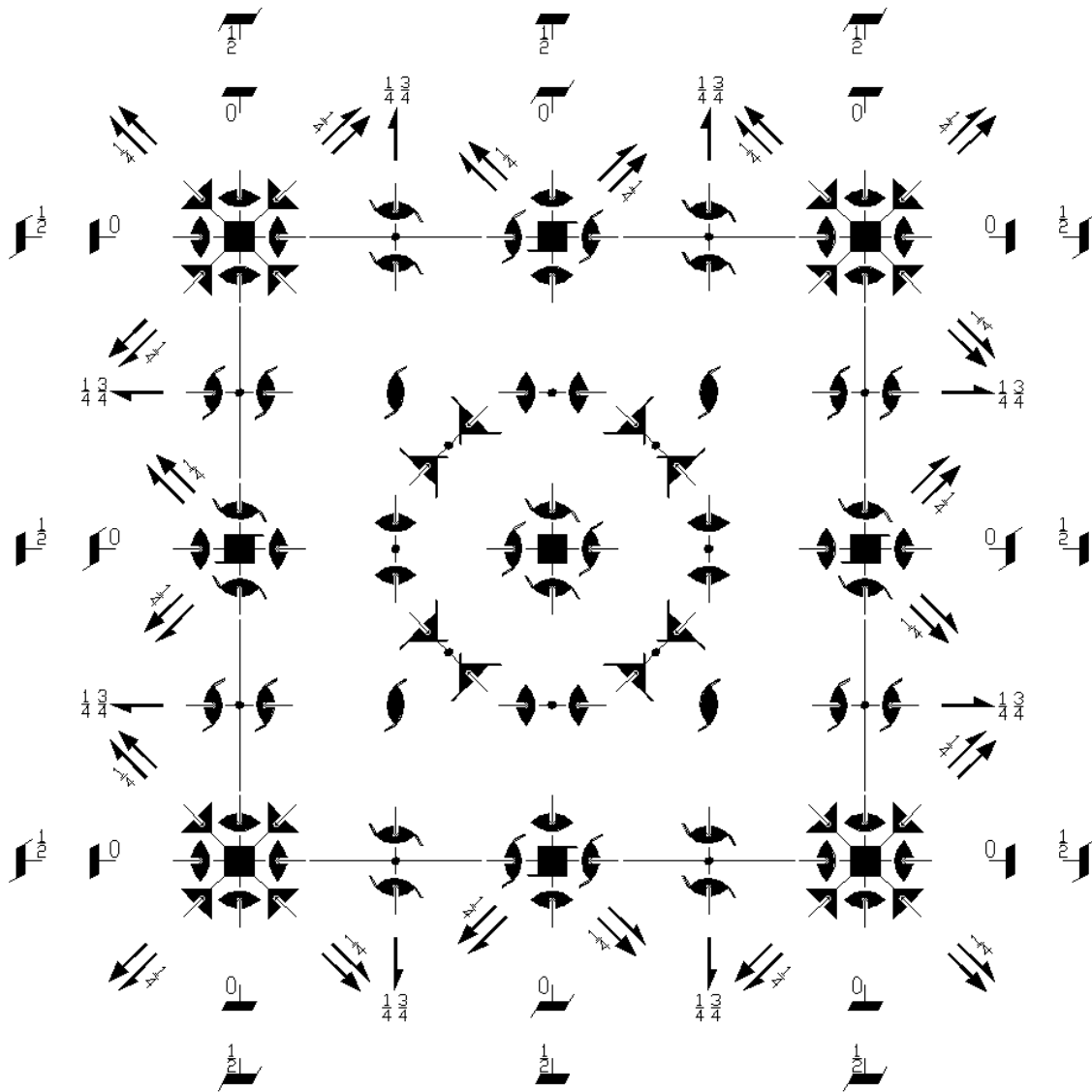
Along  $[1, 1, 0]$   $c2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = -(-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x, x, 1/8$



I432  
211.1.1556

432  
I432

Cubic



Origin at 432

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/4;$   $z \leq \min(x, 1/2-x, y, 1/2-y)$

**Vertices** 0,0,0      1/2,0,0      1/2,1/2,0      0,1/2,0      1/4,1/4,1/4

**Symmetry Operations**

For (0,0,0) + set

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                         | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)    | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)     | (12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)      |



(13) $2^- \ x,x,0$ ( $2_{xy} 0,0,0$ )	(14) $2^- \ x,\bar{x},0$ ( $2_{\bar{xy}} 0,0,0$ )	(15) $4^- \ 0,0,z$ ( $4_z^{-1} 0,0,0$ )	(16) $4^+ \ 0,0,z$ ( $4_z 0,0,0$ )
(17) $4^- \ x,0,0$ ( $4_x^{-1} 0,0,0$ )	(18) $2^- \ 0,y,y$ ( $2_{yz} 0,0,0$ )	(19) $2^- \ 0,y,\bar{y}$ ( $2_{\bar{yz}} 0,0,0$ )	(20) $4^+ \ x,0,0$ ( $4_x 0,0,0$ )
(21) $4^+ \ 0,y,0$ ( $4_y 0,0,0$ )	(22) $2^- \ x,0,x$ ( $2_{xz} 0,0,0$ )	(23) $4^- \ 0,y,0$ ( $4_y^{-1} 0,0,0$ )	(24) $2^- \ \bar{x},0,x$ ( $2_{\bar{xz}} 0,0,0$ )

For (1/2,1/2,1/2) + set

(1) $t \ (1/2,1/2,1/2)$ ( $1 1/2,1/2,1/2$ )	(2) $2 \ (0,0,1/2) \ 1/4,1/4,z$ ( $2_z 1/2,1/2,1/2$ )	(3) $2 \ (0,1/2,0) \ 1/4,y,1/4$ ( $2_y 1/2,1/2,1/2$ )	(4) $2 \ (1/2,0,0) \ x,1/4,1/4$ ( $2_x 1/2,1/2,1/2$ )
(5) $3^+ \ (1/2,1/2,1/2) \ x,x,x$ ( $3_{xyz} 1/2,1/2,1/2$ )	(6) $3^+ \ (1/6,-1/6,1/6)$ $\quad \quad \quad \bar{x}+1/3,\bar{x}+1/3,\bar{x}$ ( $3_{\bar{xyz}}^{-1} 1/2,1/2,1/2$ )	(7) $3^+ \ (-1/6,1/6,1/6)$ $\quad \quad \quad \bar{x}+2/3,\bar{x}-1/3,\bar{x}$ ( $3_{\bar{xyz}}^{-1} 1/2,1/2,1/2$ )	(8) $3^+ \ (1/6,1/6,-1/6)$ $\quad \quad \quad \bar{x}+1/3,\bar{x}+2/3,\bar{x}$ ( $3_{\bar{xyz}}^{-1} 1/2,1/2,1/2$ )
(9) $3^- \ (1/2,1/2,1/2) \ x,x,x$ ( $3_{xyz}^{-1} 1/2,1/2,1/2$ )	(10) $3^- \ (-1/6,1/6,1/6)$ $\quad \quad \quad \bar{x}+1/3,\bar{x}+1/3,\bar{x}$ ( $3_{\bar{xyz}} 1/2,1/2,1/2$ )	(11) $3^- \ (1/6,1/6,-1/6)$ $\quad \quad \quad \bar{x}+2/3,\bar{x}+1/3,\bar{x}$ ( $3_{\bar{xyz}} 1/2,1/2,1/2$ )	(12) $3^- \ (1/6,-1/6,1/6)$ $\quad \quad \quad \bar{x}-1/3,\bar{x}+2/3,\bar{x}$ ( $3_{\bar{xyz}} 1/2,1/2,1/2$ )
(13) $2 \ (1/2,1/2,0) \ x,x,1/4$ ( $2_{xy} 1/2,1/2,1/2$ )	(14) $2^- \ x,\bar{x}+1/2,1/4$ ( $2_{\bar{xy}} 1/2,1/2,1/2$ )	(15) $4^- \ (0,0,1/2) \ 1/2,0,z$ ( $4_z^{-1} 1/2,1/2,1/2$ )	(16) $4^+ \ (0,0,1/2) \ 0,1/2,z$ ( $4_z 1/2,1/2,1/2$ )
(17) $4^- \ (1/2,0,0) \ x,1/2,0$ ( $4_x^{-1} 1/2,1/2,1/2$ )	(18) $2 \ (0,1/2,1/2) \ 1/4,y,y$ ( $2_{yz} 1/2,1/2,1/2$ )	(19) $2^- \ 1/4,y+1/2,\bar{y}$ ( $2_{\bar{yz}} 1/2,1/2,1/2$ )	(20) $4^+ \ (1/2,0,0) \ x,0,1/2$ ( $4_x 1/2,1/2,1/2$ )
(21) $4^+ \ (0,1/2,0) \ 1/2,y,0$ ( $4_y 1/2,1/2,1/2$ )	(22) $2 \ (1/2,0,1/2) \ x,1/4,x$ ( $2_{xz} 1/2,1/2,1/2$ )	(23) $4^- \ (0,1/2,0) \ 0,y,1/2$ ( $4_y^{-1} 1/2,1/2,1/2$ )	(24) $2^- \ \bar{x}+1/2,1/4,x$ ( $2_{\bar{xz}} 1/2,1/2,1/2$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).**Positions**Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) +      (1/2,1/2,1/2) +

48	j	1									
(1)	$x,y,z$	[u,v,w]	(2)	$\bar{x},\bar{y},z$	[ $\bar{u},\bar{v},w$ ]	(3)	$\bar{x},y,\bar{z}$	[ $\bar{u},v,\bar{w}$ ]	(4)	$x,\bar{y},\bar{z}$	[ $u,\bar{v},\bar{w}$ ]
(5)	$z,x,y$	[w,u,v]	(6)	$z,\bar{x},\bar{y}$	[ $w,\bar{u},\bar{v}$ ]	(7)	$\bar{z},\bar{x},y$	[ $\bar{w},\bar{u},v$ ]	(8)	$\bar{z},x,\bar{y}$	[ $\bar{w},u,\bar{v}$ ]
(9)	$y,z,x$	[v,w,u]	(10)	$\bar{y},z,\bar{x}$	[ $\bar{v},w,\bar{u}$ ]	(11)	$y,\bar{z},\bar{x}$	[ $v,\bar{w},\bar{u}$ ]	(12)	$\bar{y},\bar{z},x$	[ $\bar{v},\bar{w},u$ ]
(13)	$y,x,\bar{z}$	[v,u, $\bar{w}$ ]	(14)	$\bar{y},\bar{x},\bar{z}$	[ $\bar{v},\bar{u},\bar{w}$ ]	(15)	$y,\bar{x},z$	[ $v,\bar{u},w$ ]	(16)	$\bar{y},x,z$	[ $\bar{v},u,w$ ]
(17)	$x,z,\bar{y}$	[u,w, $\bar{v}$ ]	(18)	$\bar{x},z,y$	[ $\bar{u},w,v$ ]	(19)	$\bar{x},\bar{z},\bar{y}$	[ $\bar{u},\bar{w},\bar{v}$ ]	(20)	$x,\bar{z},y$	[ $u,\bar{w},v$ ]
(21)	$z,y,\bar{x}$	[w,v, $\bar{u}$ ]	(22)	$z,\bar{y},x$	[ $w,\bar{v},u$ ]	(23)	$\bar{z},y,x$	[ $\bar{w},v,u$ ]	(24)	$\bar{z},\bar{y},\bar{x}$	[ $\bar{w},\bar{v},\bar{u}$ ]

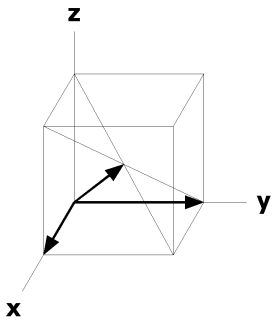
24	i	..2	$1/4, y, \bar{y} + 1/2 [0, \bar{v}, v]$ $\bar{y} + 1/2, 1/4, y [v, 0, \bar{v}]$ $y, \bar{y} + 1/2, 1/4 [\bar{v}, v, 0]$	$3/4, \bar{y}, \bar{y} + 1/2 [0, v, v]$ $\bar{y} + 1/2, 3/4, \bar{y} [v, 0, v]$ $\bar{y}, \bar{y} + 1/2, 3/4 [v, v, 0]$	$3/4, y, y + 1/2 [\bar{v}, \bar{v}, 0]$ $y + 1/2, 3/4, y [\bar{v}, 0, \bar{v}]$ $y, y + 1/2, 3/4 [\bar{v}, \bar{v}, 0]$	$1/4, \bar{y}, y + 1/2 [0, v, \bar{v}]$ $y + 1/2, 1/4, \bar{y} [\bar{v}, 0, v]$ $\bar{y}, y + 1/2, 1/4 [v, \bar{v}, 0]$
24	h	..2	$0, y, y [0, v, v]$ $y, 0, y [v, 0, v]$ $y, y, 0 [v, v, 0]$	$0, \bar{y}, y [0, \bar{v}, v]$ $y, 0, \bar{y} [v, 0, \bar{v}]$ $\bar{y}, y, 0 [\bar{v}, v, 0]$	$0, y, \bar{y} [0, v, \bar{v}]$ $\bar{y}, 0, y [\bar{v}, 0, v]$ $y, \bar{y}, 0 [v, \bar{v}, 0]$	$0, \bar{y}, \bar{y} [0, \bar{v}, \bar{v}]$ $\bar{y}, 0, \bar{y} [\bar{v}, 0, \bar{v}]$ $\bar{y}, \bar{y}, 0 [\bar{v}, \bar{v}, 0]$
24	g	2..	$x, 1/2, 0 [u, 0, 0]$ $1/2, 0, x [0, 0, u]$ $x, 0, 1/2 [u, 0, 0]$	$\bar{x}, 1/2, 0 [\bar{u}, 0, 0]$ $1/2, 0, \bar{x} [0, 0, \bar{u}]$ $\bar{x}, 0, 1/2 [\bar{u}, 0, 0]$	$0, x, 1/2 [0, u, 0]$ $1/2, x, 0 [0, u, 0]$ $0, 1/2, \bar{x} [0, 0, \bar{u}]$	$0, \bar{x}, 1/2 [0, \bar{u}, 0]$ $1/2, \bar{x}, 0 [0, \bar{u}, 0]$ $0, 1/2, x [0, 0, u]$
16	f	.3.	$x, x, x [u, u, u]$ $x, x, \bar{x} [u, u, \bar{u}]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$ $\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$	$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$ $x, \bar{x}, x [u, \bar{u}, u]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$ $\bar{x}, x, x [\bar{u}, u, u]$
12	e	4..	$x, 0, 0 [u, 0, 0]$ $0, \bar{x}, 0 [0, \bar{u}, 0]$	$\bar{x}, 0, 0 [\bar{u}, 0, 0]$ $0, 0, x [0, 0, u]$	$0, x, 0 [0, u, 0]$ $0, 0, \bar{x} [0, 0, \bar{u}]$	
12	d	2.22	$1/4, 1/2, 0 [0, 0, 0]$ $0, 3/4, 1/2 [0, 0, 0]$	$3/4, 1/2, 0 [0, 0, 0]$ $1/2, 0, 1/4 [0, 0, 0]$	$0, 1/4, 1/2 [0, 0, 0]$ $1/2, 0, 3/4 [0, 0, 0]$	
8	c	.32	$1/4, 1/4, 1/4 [0, 0, 0]$	$3/4, 3/4, 1/4 [0, 0, 0]$	$3/4, 1/4, 3/4 [0, 0, 0]$	$1/4, 3/4, 3/4 [0, 0, 0]$
6	b	42.2	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$	
2	a	432	$0, 0, 0 [0, 0, 0]$			

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0, 0, z$

Along  $[1, 1, 1]$   $p3m'1$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

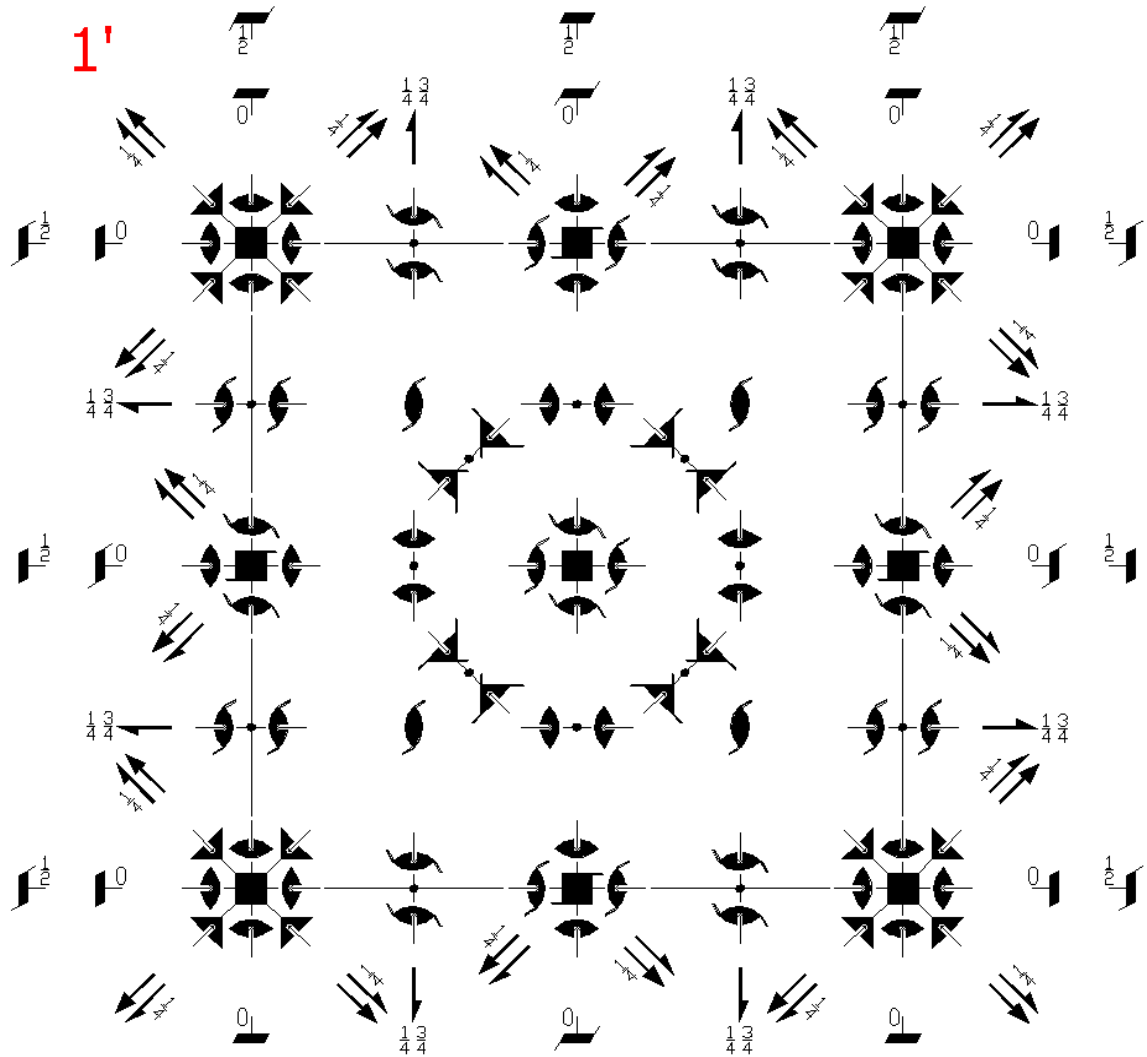
Along  $[1, 1, 0]$   $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, x, 0$



I4321'  
211.2.1557

4321'  
I4321'

Cubic



Origin at 432

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $z \leq \min(x, 1/2-x, y, 1/2-y)$

Vertices 0,0,0    1/2,0,0    1/2,1/2,0    0,1/2,0    1/4,1/4,1/4

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |   |
|---|--|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)             | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)                                      | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0) | (12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)               |

(13) $2^- \ x, x, 0$ ( $2_{xy}   0, 0, 0$ )	(14) $2^- \ x, \bar{x}, 0$ ( $2_{\bar{xy}}   0, 0, 0$ )	(15) $4^- \ 0, 0, z$ ( $4_z^{-1}   0, 0, 0$ )	(16) $4^+ \ 0, 0, z$ ( $4_z   0, 0, 0$ )
(17) $4^- \ x, 0, 0$ ( $4_x^{-1}   0, 0, 0$ )	(18) $2^- \ 0, y, y$ ( $2_{yz}   0, 0, 0$ )	(19) $2^- \ 0, y, \bar{y}$ ( $2_{\bar{yz}}   0, 0, 0$ )	(20) $4^+ \ x, 0, 0$ ( $4_x   0, 0, 0$ )
(21) $4^+ \ 0, y, 0$ ( $4_y   0, 0, 0$ )	(22) $2^- \ x, 0, x$ ( $2_{xz}   0, 0, 0$ )	(23) $4^- \ 0, y, 0$ ( $4_y^{-1}   0, 0, 0$ )	(24) $2^- \ \bar{x}, 0, x$ ( $2_{\bar{xz}}   0, 0, 0$ )

## For (1/2, 1/2, 1/2) + set

(1) $t \ (1/2, 1/2, 1/2)$ ( $1   1/2, 1/2, 1/2$ )	(2) $2^- \ (0, 0, 1/2) \ 1/4, 1/4, z$ ( $2_z   1/2, 1/2, 1/2$ )	(3) $2^- \ (0, 1/2, 0) \ 1/4, y, 1/4$ ( $2_y   1/2, 1/2, 1/2$ )	(4) $2^- \ (1/2, 0, 0) \ x, 1/4, 1/4$ ( $2_x   1/2, 1/2, 1/2$ )
(5) $3^+ \ (1/2, 1/2, 1/2) \ x, x, x$ ( $3_{xyz}   1/2, 1/2, 1/2$ )	(6) $3^+ \ (1/6, -1/6, 1/6)$ $\quad \quad \quad \bar{x} + 1/3, \bar{x} + 1/3, \bar{x}$ ( $3_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2$ )	(7) $3^+ \ (-1/6, 1/6, 1/6)$ $\quad \quad \quad \bar{x} + 2/3, \bar{x} - 1/3, \bar{x}$ ( $3_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2$ )	(8) $3^+ \ (1/6, 1/6, -1/6)$ $\quad \quad \quad \bar{x} + 1/3, \bar{x} + 2/3, \bar{x}$ ( $3_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2$ )
(9) $3^- \ (1/2, 1/2, 1/2) \ x, x, x$ ( $3_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(10) $3^- \ (-1/6, 1/6, 1/6)$ $\quad \quad \quad \bar{x} + 1/3, \bar{x} + 1/3, \bar{x}$ ( $3_{\bar{xyz}}   1/2, 1/2, 1/2$ )	(11) $3^- \ (1/6, 1/6, -1/6)$ $\quad \quad \quad \bar{x} + 2/3, \bar{x} + 1/3, \bar{x}$ ( $3_{\bar{xyz}}   1/2, 1/2, 1/2$ )	(12) $3^- \ (1/6, -1/6, 1/6)$ $\quad \quad \quad \bar{x} - 1/3, \bar{x} + 2/3, \bar{x}$ ( $3_{\bar{xyz}}   1/2, 1/2, 1/2$ )
(13) $2^- \ (1/2, 1/2, 0) \ x, x, 1/4$ ( $2_{xy}   1/2, 1/2, 1/2$ )	(14) $2^- \ x, \bar{x} + 1/2, 1/4$ ( $2_{\bar{xy}}   1/2, 1/2, 1/2$ )	(15) $4^- \ (0, 0, 1/2) \ 1/2, 0, z$ ( $4_z^{-1}   1/2, 1/2, 1/2$ )	(16) $4^+ \ (0, 0, 1/2) \ 0, 1/2, z$ ( $4_z   1/2, 1/2, 1/2$ )
(17) $4^- \ (1/2, 0, 0) \ x, 1/2, 0$ ( $4_x^{-1}   1/2, 1/2, 1/2$ )	(18) $2^- \ (0, 1/2, 1/2) \ 1/4, y, y$ ( $2_{yz}   1/2, 1/2, 1/2$ )	(19) $2^- \ 1/4, y + 1/2, \bar{y}$ ( $2_{\bar{yz}}   1/2, 1/2, 1/2$ )	(20) $4^+ \ (1/2, 0, 0) \ x, 0, 1/2$ ( $4_x   1/2, 1/2, 1/2$ )
(21) $4^+ \ (0, 1/2, 0) \ 1/2, y, 0$ ( $4_y   1/2, 1/2, 1/2$ )	(22) $2^- \ (1/2, 0, 1/2) \ x, 1/4, x$ ( $2_{xz}   1/2, 1/2, 1/2$ )	(23) $4^- \ (0, 1/2, 0) \ 0, y, 1/2$ ( $4_y^{-1}   1/2, 1/2, 1/2$ )	(24) $2^- \ \bar{x} + 1/2, 1/4, x$ ( $2_{\bar{xz}}   1/2, 1/2, 1/2$ )

## For (0, 0, 0)' + set

(1) $1'$ ( $1   0, 0, 0$ )'	(2) $2'$ $0, 0, z$ ( $2_z   0, 0, 0$ )'	(3) $2'$ $0, y, 0$ ( $2_y   0, 0, 0$ )'	(4) $2'$ $x, 0, 0$ ( $2_x   0, 0, 0$ )'
(5) $3^+ \ x, x, x$ ( $3_{xyz}   0, 0, 0$ )'	(6) $3^+ \ \bar{x}, \bar{x}, \bar{x}$ ( $3_{\bar{xyz}}^{-1}   0, 0, 0$ )'	(7) $3^+ \ x, \bar{x}, \bar{x}$ ( $3_{\bar{xyz}}^{-1}   0, 0, 0$ )'	(8) $3^+ \ \bar{x}, \bar{x}, x$ ( $3_{\bar{xyz}}^{-1}   0, 0, 0$ )'
(9) $3^- \ x, x, x$ ( $3_{xyz}^{-1}   0, 0, 0$ )'	(10) $3^- \ x, \bar{x}, \bar{x}$ ( $3_{\bar{xyz}}   0, 0, 0$ )'	(11) $3^- \ \bar{x}, \bar{x}, x$ ( $3_{\bar{xyz}}   0, 0, 0$ )'	(12) $3^- \ \bar{x}, x, \bar{x}$ ( $3_{\bar{xyz}}   0, 0, 0$ )'
(13) $2'$ $x, x, 0$ ( $2_{xy}   0, 0, 0$ )'	(14) $2'$ $x, \bar{x}, 0$ ( $2_{\bar{xy}}   0, 0, 0$ )'	(15) $4^- \ 0, 0, z$ ( $4_z^{-1}   0, 0, 0$ )'	(16) $4^+ \ 0, 0, z$ ( $4_z   0, 0, 0$ )'
(17) $4^- \ x, 0, 0$ ( $4_x^{-1}   0, 0, 0$ )'	(18) $2'$ $0, y, y$ ( $2_{yz}   0, 0, 0$ )'	(19) $2'$ $0, y, \bar{y}$ ( $2_{\bar{yz}}   0, 0, 0$ )'	(20) $4^+ \ x, 0, 0$ ( $4_x   0, 0, 0$ )'
(21) $4^+ \ 0, y, 0$ ( $4_y   0, 0, 0$ )'	(22) $2'$ $x, 0, x$ ( $2_{xz}   0, 0, 0$ )'	(23) $4^- \ 0, y, 0$ ( $4_y^{-1}   0, 0, 0$ )'	(24) $2'$ $\bar{x}, 0, x$ ( $2_{\bar{xz}}   0, 0, 0$ )'

For (1/2,1/2,1/2)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t' (1/2, 1/2, 1/2)$<br>(1   1/2, 1/2, 1/2)'   | (2) $2' (0, 0, 1/2) \quad 1/4, 1/4, z$<br>(2 <sub>z</sub>   1/2, 1/2, 1/2)'  | (3) $2' (0, 1/2, 0) \quad 1/4, y, 1/4$<br>(2 <sub>y</sub>   1/2, 1/2, 1/2)'  | (4) $2' (1/2, 0, 0) \quad x, 1/4, 1/4$<br>(2 <sub>x</sub>   1/2, 1/2, 1/2)'  |
| (5) $3^{+} (1/2, 1/2, 1/2) \quad x, x, x$<br>(3 <sub>xyz</sub>   1/2, 1/2, 1/2)'               | (6) $3^{+} (1/6, -1/6, 1/6)$<br>$\bar{x} + 1/3, \bar{x} + 1/3, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2, 1/2, 1/2)' | (7) $3^{+} (-1/6, 1/6, 1/6)$<br>$\bar{x} + 2/3, \bar{x} - 1/3, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2, 1/2, 1/2)' | (8) $3^{+} (1/6, 1/6, -1/6)$<br>$\bar{x} + 1/3, \bar{x} + 2/3, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2, 1/2, 1/2)' |
| (9) $3^{-} (1/2, 1/2, 1/2) \quad x, x, x$<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2, 1/2, 1/2)' | (10) $3^{-} (-1/6, 1/6, 1/6)$<br>$\bar{x} + 1/3, \bar{x} + 1/3, \bar{x}$<br>(3 <sub>xyz</sub>   1/2, 1/2, 1/2)'              | (11) $3^{-} (1/6, 1/6, -1/6)$<br>$\bar{x} + 2/3, \bar{x} + 1/3, \bar{x}$<br>(3 <sub>xyz</sub>   1/2, 1/2, 1/2)'              | (12) $3^{-} (1/6, -1/6, 1/6)$<br>$\bar{x} - 1/3, \bar{x} + 2/3, \bar{x}$<br>(3 <sub>xyz</sub>   1/2, 1/2, 1/2)'              |
| (13) $2' (1/2, 1/2, 0) \quad x, x, 1/4$<br>(2 <sub>xy</sub>   1/2, 1/2, 1/2)'                  | (14) $2' \quad \bar{x}, \bar{x} + 1/2, 1/4$<br>(2 <sub>xy</sub>   1/2, 1/2, 1/2)'  | (15) $4^{-} (0, 0, 1/2) \quad 1/2, 0, z$<br>(4 <sub>z</sub> <sup>-1</sup>   1/2, 1/2, 1/2)'                                  | (16) $4^{+} (0, 0, 1/2) \quad 0, 1/2, z$<br>(4 <sub>z</sub>   1/2, 1/2, 1/2)'  |
| (17) $4^{-} (1/2, 0, 0) \quad x, 1/2, 0$<br>(4 <sub>x</sub> <sup>-1</sup>   1/2, 1/2, 1/2)'    | (18) $2' (0, 1/2, 1/2) \quad 1/4, y, y$<br>(2 <sub>yz</sub>   1/2, 1/2, 1/2)'  | (19) $2' \quad 1/4, y + 1/2, \bar{y}$<br>(2 <sub>yz</sub>   1/2, 1/2, 1/2)'  | (20) $4^{+} (1/2, 0, 0) \quad x, 0, 1/2$<br>(4 <sub>x</sub>   1/2, 1/2, 1/2)'  |
| (21) $4^{+} (0, 1/2, 0) \quad 1/2, y, 0$<br>(4 <sub>y</sub>   1/2, 1/2, 1/2)'                  | (22) $2' (1/2, 0, 1/2) \quad x, 1/4, x$<br>(2 <sub>xz</sub>   1/2, 1/2, 1/2)'  | (23) $4^{-} (0, 1/2, 0) \quad 0, y, 1/2$<br>(4 <sub>y</sub> <sup>-1</sup>   1/2, 1/2, 1/2)'                                  | (24) $2' \quad \bar{x} + 1/2, 1/4, x$<br>(2 <sub>xz</sub>   1/2, 1/2, 1/2)'  |

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); 1'.

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (1/2,1/2,1/2) +  
(0,0,0)' + (1/2,1/2,1/2)' +

48 j 11'

- |                                |  |  |  |
|--------------------------------|--|--|--|
| (1) $x, y, z [0, 0, 0]$        | (2) $\bar{x}, \bar{y}, z [0, 0, 0]$        | (3) $\bar{x}, y, \bar{z} [0, 0, 0]$        | (4) $x, \bar{y}, \bar{z} [0, 0, 0]$        |
| (5) $z, x, y [0, 0, 0]$        | (6) $z, \bar{x}, \bar{y} [0, 0, 0]$        | (7) $\bar{z}, \bar{x}, y [0, 0, 0]$        | (8) $\bar{z}, x, \bar{y} [0, 0, 0]$        |
| (9) $y, z, x [0, 0, 0]$        | (10) $\bar{y}, z, \bar{x} [0, 0, 0]$       | (11) $y, \bar{z}, \bar{x} [0, 0, 0]$       | (12) $\bar{y}, \bar{z}, x [0, 0, 0]$       |
| (13) $y, x, \bar{z} [0, 0, 0]$ | (14) $\bar{y}, \bar{x}, \bar{z} [0, 0, 0]$ | (15) $y, \bar{x}, z [0, 0, 0]$             | (16) $\bar{y}, x, z [0, 0, 0]$             |
| (17) $x, z, \bar{y} [0, 0, 0]$ | (18) $\bar{x}, z, y [0, 0, 0]$             | (19) $\bar{x}, \bar{z}, \bar{y} [0, 0, 0]$ | (20) $x, \bar{z}, y [0, 0, 0]$             |
| (21) $z, y, \bar{x} [0, 0, 0]$ | (22) $z, \bar{y}, x [0, 0, 0]$             | (23) $\bar{z}, y, x [0, 0, 0]$             | (24) $\bar{z}, \bar{y}, \bar{x} [0, 0, 0]$ |
- 
- |    |   |       |   |   |                             |                                   |
|----|---|-------|---|---|-----------------------------|-----------------------------------|
| 24 | i | ..21' | $1/4, \bar{y}, \bar{y} + 1/2 [0, 0, 0]$ | $3/4, \bar{y}, \bar{y} + 1/2 [0, 0, 0]$ | $3/4, y, y + 1/2 [0, 0, 0]$ | $1/4, \bar{y}, y + 1/2 [0, 0, 0]$ |
|    |   |       | $\bar{y} + 1/2, 1/4, y [0, 0, 0]$       | $\bar{y} + 1/2, 3/4, \bar{y} [0, 0, 0]$ | $y + 1/2, 3/4, y [0, 0, 0]$ | $y + 1/2, 1/4, \bar{y} [0, 0, 0]$ |
|    |   |       | $y, \bar{y} + 1/2, 1/4 [0, 0, 0]$       | $\bar{y}, \bar{y} + 1/2, 3/4 [0, 0, 0]$ | $y, y + 1/2, 3/4 [0, 0, 0]$ | $\bar{y}, y + 1/2, 1/4 [0, 0, 0]$ |

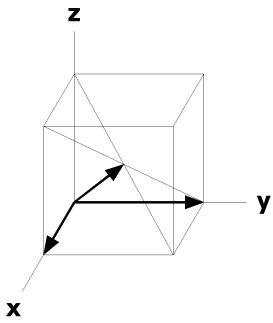
24	h	..21'	0,y,y [0,0,0]	$0,\bar{y},y$ [0,0,0]	$0,y,\bar{y}$ [0,0,0]	$0,\bar{y},\bar{y}$ [0,0,0]
			y,0,y [0,0,0]	$y,0,\bar{y}$ [0,0,0]	$\bar{y},0,y$ [0,0,0]	$\bar{y},0,\bar{y}$ [0,0,0]
			y,y,0 [0,0,0]	$\bar{y},y,0$ [0,0,0]	$y,\bar{y},0$ [0,0,0]	$\bar{y},\bar{y},0$ [0,0,0]
24	g	2..1'	x,1/2,0 [0,0,0]	$\bar{x},1/2,0$ [0,0,0]	0,x,1/2 [0,0,0]	$0,\bar{x},1/2$ [0,0,0]
			1/2,0,x [0,0,0]	$1/2,0,\bar{x}$ [0,0,0]	1/2,x,0 [0,0,0]	$1/2,\bar{x},0$ [0,0,0]
			x,0,1/2 [0,0,0]	$\bar{x},0,1/2$ [0,0,0]	0,1/2, $\bar{x}$ [0,0,0]	0,1/2,x [0,0,0]
16	f	.3.1'	x,x,x [0,0,0]	$\bar{x},\bar{x},x$ [0,0,0]	$\bar{x},x,\bar{x}$ [0,0,0]	$x,\bar{x},\bar{x}$ [0,0,0]
			x,x, $\bar{x}$ [0,0,0]	$\bar{x},\bar{x},\bar{x}$ [0,0,0]	$x,\bar{x},x$ [0,0,0]	$\bar{x},x,x$ [0,0,0]
12	e	4..1'	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,0 [0,0,0]	
			$0,\bar{x},0$ [0,0,0]	0,0,x [0,0,0]	$0,0,\bar{x}$ [0,0,0]	
12	d	2.221'	1/4,1/2,0 [0,0,0]	3/4,1/2,0 [0,0,0]	0,1/4,1/2 [0,0,0]	
			0,3/4,1/2 [0,0,0]	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]	
8	c	.321'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]
6	b	42.21'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	
2	a	4321'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,1,1] p3m11'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

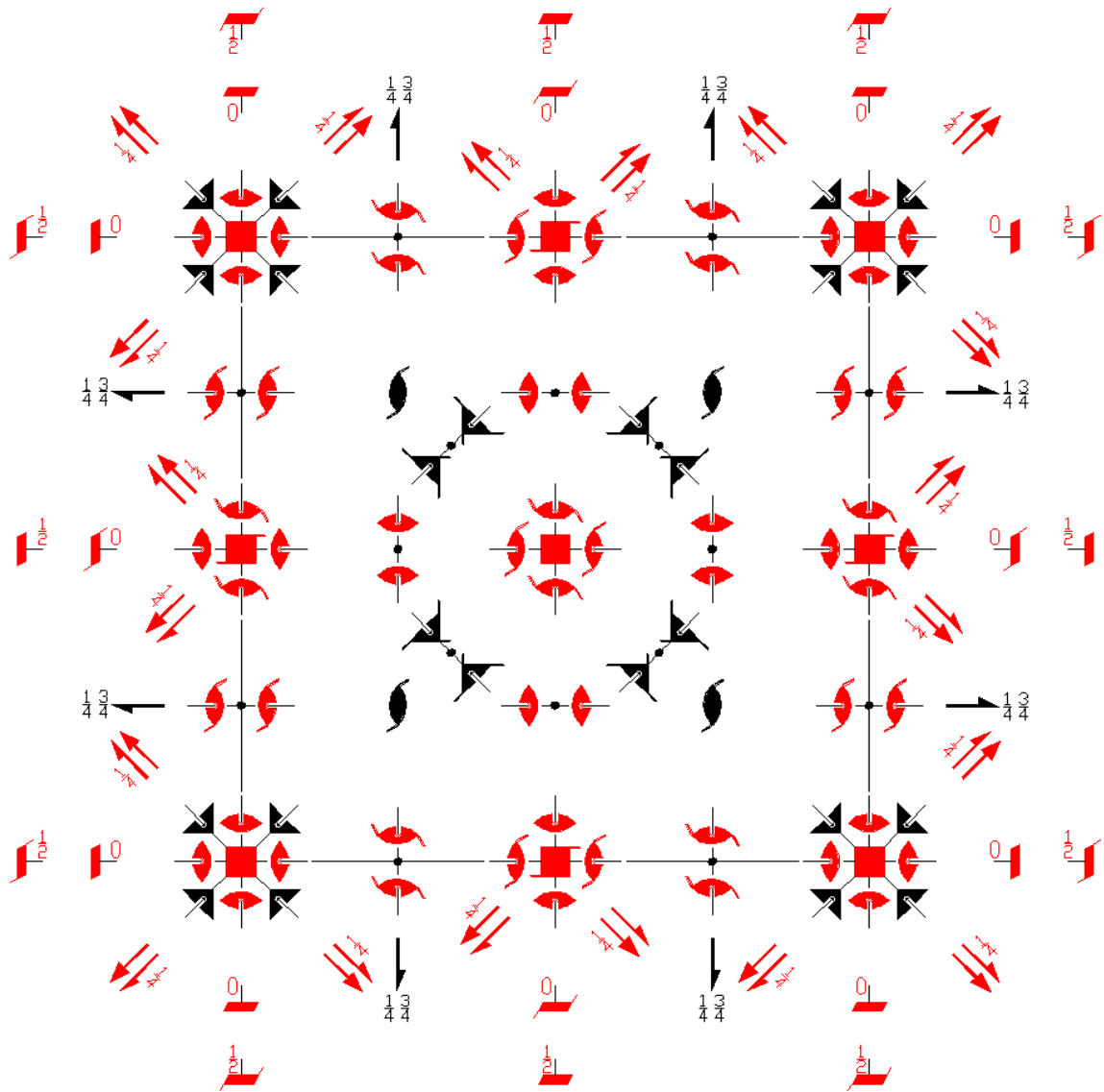
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



14'32'  
211.3.1558

4'32'  
14'32'

Cubic



Origin at 4'32'

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $z \leq \min(x, 1/2-x, y, 1/2-y)$

Vertices 0,0,0    1/2,0,0    1/2,1/2,0    0,1/2,0    1/4,1/4,1/4

### Symmetry Operations

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)              |

(13) $2' \ x, x, 0$ $(2_{xy}   0, 0, 0)'$	(14) $2' \ x, \bar{x}, 0$ $(2_{\bar{xy}}   0, 0, 0)'$	(15) $4' \ 0, 0, z$ $(4_z^{-1}   0, 0, 0)'$	(16) $4^+ \ 0, 0, z$ $(4_z   0, 0, 0)'$
(17) $4' \ x, 0, 0$ $(4_x^{-1}   0, 0, 0)'$	(18) $2' \ 0, y, y$ $(2_{yz}   0, 0, 0)'$	(19) $2' \ 0, y, \bar{y}$ $(2_{\bar{yz}}   0, 0, 0)'$	(20) $4^+ \ x, 0, 0$ $(4_x   0, 0, 0)'$
(21) $4^+ \ 0, y, 0$ $(4_y   0, 0, 0)'$	(22) $2' \ x, 0, x$ $(2_{xz}   0, 0, 0)'$	(23) $4' \ 0, y, 0$ $(4_y^{-1}   0, 0, 0)'$	(24) $2' \ \bar{x}, 0, x$ $(2_{\bar{xz}}   0, 0, 0)'$
For (1/2, 1/2, 1/2) + set			
(1) $t \ (1/2, 1/2, 1/2)$ $(1   1/2, 1/2, 1/2)$	(2) $2 \ (0, 0, 1/2) \ 1/4, 1/4, z$ $(2_z   1/2, 1/2, 1/2)$	(3) $2 \ (0, 1/2, 0) \ 1/4, y, 1/4$ $(2_y   1/2, 1/2, 1/2)$	(4) $2 \ (1/2, 0, 0) \ x, 1/4, 1/4$ $(2_x   1/2, 1/2, 1/2)$
(5) $3^+ \ (1/2, 1/2, 1/2) \ x, x, x$ $(3_{xyz}   1/2, 1/2, 1/2)$	(6) $3^+ \ (1/6, -1/6, 1/6)$ $\quad \quad \quad \bar{x} + 1/3, \bar{x} + 1/3, \bar{x}$ $(3_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2)$	(7) $3^+ \ (-1/6, 1/6, 1/6)$ $\quad \quad \quad \bar{x} + 2/3, \bar{x} - 1/3, \bar{x}$ $(3_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2)$	(8) $3^+ \ (1/6, 1/6, -1/6)$ $\quad \quad \quad \bar{x} + 1/3, \bar{x} + 2/3, \bar{x}$ $(3_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2)$
(9) $3^- \ (1/2, 1/2, 1/2) \ x, x, x$ $(3_{xyz}^{-1}   1/2, 1/2, 1/2)$	(10) $3^- \ (-1/6, 1/6, 1/6)$ $\quad \quad \quad \bar{x} + 1/3, \bar{x} + 1/3, \bar{x}$ $(3_{\bar{xyz}}   1/2, 1/2, 1/2)$	(11) $3^- \ (1/6, 1/6, -1/6)$ $\quad \quad \quad \bar{x} + 2/3, \bar{x} + 1/3, \bar{x}$ $(3_{\bar{xyz}}   1/2, 1/2, 1/2)$	(12) $3^- \ (1/6, -1/6, 1/6)$ $\quad \quad \quad \bar{x} - 1/3, \bar{x} + 2/3, \bar{x}$ $(3_{\bar{xyz}}   1/2, 1/2, 1/2)$
(13) $2' \ (1/2, 1/2, 0) \ x, x, 1/4$ $(2_{xy}   1/2, 1/2, 1/2)'$	(14) $2' \ x, \bar{x} + 1/2, 1/4$ $(2_{\bar{xy}}   1/2, 1/2, 1/2)'$	(15) $4' \ (0, 0, 1/2) \ 1/2, 0, z$ $(4_z^{-1}   1/2, 1/2, 1/2)'$	(16) $4^+ \ (0, 0, 1/2) \ 0, 1/2, z$ $(4_z   1/2, 1/2, 1/2)'$
(17) $4' \ (1/2, 0, 0) \ x, 1/2, 0$ $(4_x^{-1}   1/2, 1/2, 1/2)'$	(18) $2' \ (0, 1/2, 1/2) \ 1/4, y, y$ $(2_{yz}   1/2, 1/2, 1/2)'$	(19) $2' \ 1/4, y + 1/2, \bar{y}$ $(2_{\bar{yz}}   1/2, 1/2, 1/2)'$	(20) $4^+ \ (1/2, 0, 0) \ x, 0, 1/2$ $(4_x   1/2, 1/2, 1/2)'$
(21) $4^+ \ (0, 1/2, 0) \ 1/2, y, 0$ $(4_y   1/2, 1/2, 1/2)'$	(22) $2' \ (1/2, 0, 1/2) \ x, 1/4, x$ $(2_{xz}   1/2, 1/2, 1/2)'$	(23) $4' \ (0, 1/2, 0) \ 0, y, 1/2$ $(4_y^{-1}   1/2, 1/2, 1/2)'$	(24) $2' \ \bar{x} + 1/2, 1/4, x$ $(2_{\bar{xz}}   1/2, 1/2, 1/2)'$

**Generators selected** (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ;  $t(1/2, 1/2, 1/2)$ ; (2); (3); (5); (13).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0, 0, 0) +      (1/2, 1/2, 1/2) +

48	j	1									
(1)	$x, y, z$	$[u, v, w]$	(2)	$\bar{x}, \bar{y}, z$	$[\bar{u}, \bar{v}, w]$	(3)	$\bar{x}, y, z$	$[\bar{u}, v, w]$	(4)	$x, \bar{y}, z$	$[u, \bar{v}, w]$
(5)	$z, x, y$	$[w, u, v]$	(6)	$z, \bar{x}, \bar{y}$	$[w, \bar{u}, \bar{v}]$	(7)	$\bar{z}, \bar{x}, y$	$[\bar{w}, \bar{u}, v]$	(8)	$\bar{z}, x, \bar{y}$	$[\bar{w}, u, \bar{v}]$
(9)	$y, z, x$	$[v, w, u]$	(10)	$\bar{y}, z, \bar{x}$	$[\bar{v}, w, \bar{u}]$	(11)	$y, \bar{z}, \bar{x}$	$[v, \bar{w}, \bar{u}]$	(12)	$\bar{y}, z, x$	$[\bar{v}, w, u]$
(13)	$y, x, z$	$[\bar{v}, \bar{u}, w]$	(14)	$\bar{y}, \bar{x}, z$	$[\bar{v}, u, w]$	(15)	$y, \bar{x}, z$	$[\bar{v}, u, \bar{w}]$	(16)	$\bar{y}, x, z$	$[v, \bar{u}, \bar{w}]$
(17)	$x, z, \bar{y}$	$[\bar{u}, \bar{w}, v]$	(18)	$\bar{x}, z, y$	$[u, \bar{w}, \bar{v}]$	(19)	$\bar{x}, z, \bar{y}$	$[u, w, v]$	(20)	$x, z, y$	$[\bar{u}, w, \bar{v}]$
(21)	$z, y, \bar{x}$	$[\bar{w}, \bar{v}, u]$	(22)	$z, \bar{y}, x$	$[\bar{w}, v, \bar{u}]$	(23)	$\bar{z}, y, x$	$[w, \bar{v}, \bar{u}]$	(24)	$\bar{z}, y, \bar{x}$	$[w, v, u]$



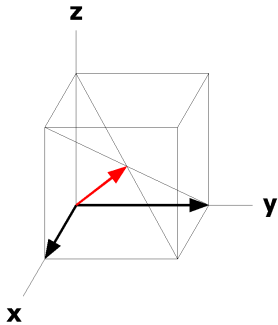
24	i	..2'	$1/4, y, \bar{y} + 1/2 [u, v, v]$ $\bar{y} + 1/2, 1/4, y [v, u, v]$ $y, \bar{y} + 1/2, 1/4 [v, v, u]$	$3/4, \bar{y}, \bar{y} + 1/2 [\bar{u}, \bar{v}, v]$ $\bar{y} + 1/2, 3/4, \bar{y} [v, \bar{u}, \bar{v}]$ $\bar{y}, \bar{y} + 1/2, 3/4 [v, \bar{v}, \bar{u}]$	$3/4, y, y + 1/2 [\bar{u}, v, \bar{v}]$ $y + 1/2, 3/4, y [v, \bar{u}, v]$ $y, y + 1/2, 3/4 [v, \bar{v}, \bar{u}]$	$1/4, \bar{y}, y + 1/2 [u, \bar{v}, \bar{v}]$ $y + 1/2, 1/4, \bar{y} [v, u, \bar{v}]$ $\bar{y}, y + 1/2, 1/4 [v, \bar{v}, u]$
24	h	..2'	$0, y, y [u, v, \bar{v}]$ $y, 0, y [v, u, \bar{v}]$ $y, y, 0 [v, \bar{v}, u]$	$0, \bar{y}, y [\bar{u}, \bar{v}, \bar{v}]$ $y, 0, \bar{y} [v, \bar{u}, \bar{v}]$ $\bar{y}, y, 0 [v, \bar{v}, \bar{u}]$	$0, y, \bar{y} [\bar{u}, v, v]$ $\bar{y}, 0, y [v, \bar{u}, v]$ $y, \bar{y}, 0 [v, v, \bar{u}]$	$0, \bar{y}, \bar{y} [u, \bar{v}, v]$ $\bar{y}, 0, \bar{y} [v, u, \bar{v}]$ $\bar{y}, \bar{y}, 0 [v, \bar{v}, u]$
24	g	2..	$x, 1/2, 0 [u, 0, 0]$ $1/2, 0, x [0, 0, u]$ $x, 0, 1/2 [\bar{u}, 0, 0]$	$\bar{x}, 1/2, 0 [\bar{u}, 0, 0]$ $1/2, 0, \bar{x} [0, 0, \bar{u}]$ $\bar{x}, 0, 1/2 [u, 0, 0]$	$0, x, 1/2 [0, u, 0]$ $1/2, x, 0 [0, \bar{u}, 0]$ $0, 1/2, \bar{x} [0, 0, u]$	$0, \bar{x}, 1/2 [0, \bar{u}, 0]$ $1/2, \bar{x}, 0 [0, u, 0]$ $0, 1/2, x [0, 0, \bar{u}]$
16	f	.3.	$x, x, x [u, u, u]$ $x, x, \bar{x} [\bar{u}, \bar{u}, u]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$ $\bar{x}, \bar{x}, \bar{x} [u, u, u]$	$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$ $x, \bar{x}, x [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$ $\bar{x}, x, x [u, \bar{u}, \bar{u}]$
12	e	4..	$x, 0, 0 [u, 0, 0]$ $0, \bar{x}, 0 [0, \bar{u}, 0]$	$\bar{x}, 0, 0 [\bar{u}, 0, 0]$ $0, 0, x [0, 0, u]$	$0, x, 0 [0, u, 0]$ $0, 0, \bar{x} [0, 0, \bar{u}]$	
12	d	2.2'2'	$1/4, 1/2, 0 [u, 0, 0]$ $0, 3/4, 1/2 [0, \bar{u}, 0]$	$3/4, 1/2, 0 [\bar{u}, 0, 0]$ $1/2, 0, 1/4 [0, 0, u]$	$0, 1/4, 1/2 [0, u, 0]$ $1/2, 0, 3/4 [0, 0, \bar{u}]$	
8	c	.32'	$1/4, 1/4, 1/4 [u, u, u]$	$3/4, 3/4, 1/4 [\bar{u}, \bar{u}, u]$	$3/4, 1/4, 3/4 [\bar{u}, u, \bar{u}]$	$1/4, 3/4, 3/4 [u, \bar{u}, \bar{u}]$
6	b	4'2.2'	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$	
2	a	4'32'	$0, 0, 0 [0, 0, 0]$			

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p4'mm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0, 0, z$

Along  $[1, 1, 1]$   $p3m1$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

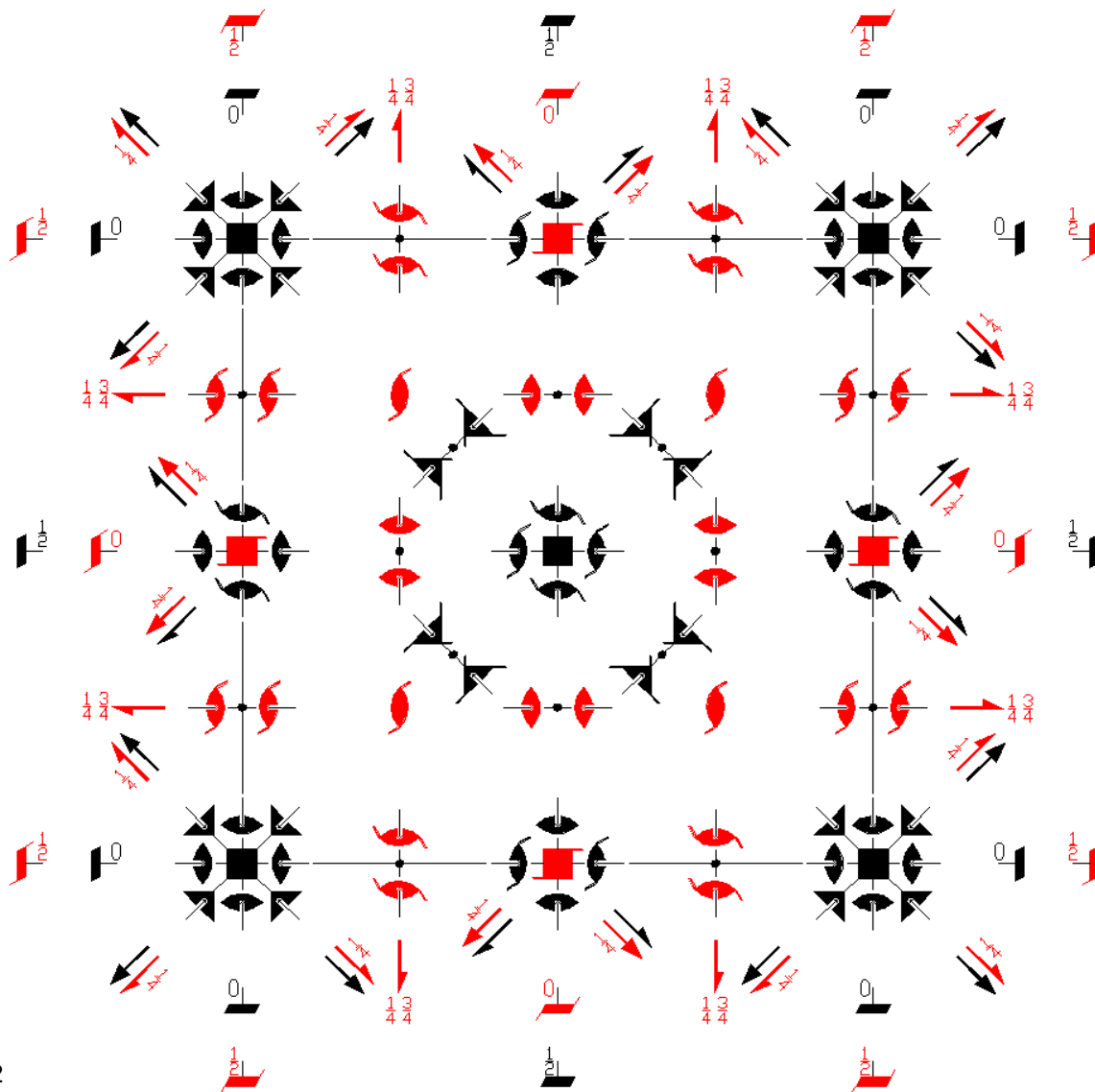
Along  $[1, 1, 0]$   $p2'mm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x, x, 0$



$I_p 432$   
211.4.1559

$4321'$   
 $I_p 432$

Cubic



Origin at 432

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $z \leq \min(x, 1/2-x, y, 1/2-y)$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $0,1/2,0$   $1/4,1/4,1/4$

### Symmetry Operations

For  $(0,0,0)$  + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                  | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                                  | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                  |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) |

(13) $2^- \ x, x, 0$ ( $2_{xy}^-   0, 0, 0$ )	(14) $2^- \ x, \bar{x}, 0$ ( $2_{\bar{xy}}^-   0, 0, 0$ )	(15) $4^- \ 0, 0, z$ ( $4_z^-   0, 0, 0$ )	(16) $4^+ \ 0, 0, z$ ( $4_z^+   0, 0, 0$ )
(17) $4^- \ x, 0, 0$ ( $4_x^-   0, 0, 0$ )	(18) $2^- \ 0, y, y$ ( $2_{yz}^-   0, 0, 0$ )	(19) $2^- \ 0, y, \bar{y}$ ( $2_{\bar{yz}}^-   0, 0, 0$ )	(20) $4^+ \ x, 0, 0$ ( $4_x^+   0, 0, 0$ )
(21) $4^+ \ 0, y, 0$ ( $4_y^+   0, 0, 0$ )	(22) $2^- \ x, 0, x$ ( $2_{xz}^-   0, 0, 0$ )	(23) $4^- \ 0, y, 0$ ( $4_y^-   0, 0, 0$ )	(24) $2^- \ \bar{x}, 0, x$ ( $2_{\bar{xz}}^-   0, 0, 0$ )

For (1/2, 1/2, 1/2)' + set

(1) $t' \ (1/2, 1/2, 1/2)$ ( $1   1/2, 1/2, 1/2$ )'	(2) $2' \ (0, 0, 1/2) \ 1/4, 1/4, z$ ( $2_z   1/2, 1/2, 1/2$ )'	(3) $2' \ (0, 1/2, 0) \ 1/4, y, 1/4$ ( $2_y   1/2, 1/2, 1/2$ )'	(4) $2' \ (1/2, 0, 0) \ x, 1/4, 1/4$ ( $2_x   1/2, 1/2, 1/2$ )'
(5) $3^{+'} \ (1/2, 1/2, 1/2) \ x, x, x$ ( $3_{xyz}   1/2, 1/2, 1/2$ )'	(6) $3^{+'} \ (1/6, -1/6, 1/6) \ \bar{x} + 1/3, \bar{x} + 1/3, \bar{x}$ ( $3_{\bar{xyz}}^-   1/2, 1/2, 1/2$ )'	(7) $3^{+'} \ (-1/6, 1/6, 1/6) \ \bar{x} + 2/3, \bar{x} - 1/3, \bar{x}$ ( $3_{\bar{xyz}}^-   1/2, 1/2, 1/2$ )'	(8) $3^{+'} \ (1/6, 1/6, -1/6) \ \bar{x} + 1/3, \bar{x} + 2/3, \bar{x}$ ( $3_{\bar{xyz}}^-   1/2, 1/2, 1/2$ )'
(9) $3^{-'} \ (1/2, 1/2, 1/2) \ x, x, x$ ( $3_{xyz}^-   1/2, 1/2, 1/2$ )'	(10) $3^{-'} \ (-1/6, 1/6, 1/6) \ \bar{x} + 1/3, \bar{x} + 1/3, \bar{x}$ ( $3_{\bar{xyz}}   1/2, 1/2, 1/2$ )'	(11) $3^{-'} \ (1/6, 1/6, -1/6) \ \bar{x} + 2/3, \bar{x} + 1/3, \bar{x}$ ( $3_{\bar{xyz}}   1/2, 1/2, 1/2$ )'	(12) $3^{-'} \ (1/6, -1/6, 1/6) \ \bar{x} - 1/3, \bar{x} + 2/3, \bar{x}$ ( $3_{\bar{xyz}}   1/2, 1/2, 1/2$ )'
(13) $2' \ (1/2, 1/2, 0) \ x, x, 1/4$ ( $2_{xy}   1/2, 1/2, 1/2$ )'	(14) $2' \ x, \bar{x} + 1/2, 1/4$ ( $2_{\bar{xy}}   1/2, 1/2, 1/2$ )'	(15) $4^{-'} \ (0, 0, 1/2) \ 1/2, 0, z$ ( $4_z^-   1/2, 1/2, 1/2$ )'	(16) $4^{+'} \ (0, 0, 1/2) \ 0, 1/2, z$ ( $4_z^+   1/2, 1/2, 1/2$ )'
(17) $4^{-'} \ (1/2, 0, 0) \ x, 1/2, 0$ ( $4_x^-   1/2, 1/2, 1/2$ )'	(18) $2' \ (0, 1/2, 1/2) \ 1/4, y, y$ ( $2_{yz}   1/2, 1/2, 1/2$ )'	(19) $2' \ 1/4, y + 1/2, \bar{y}$ ( $2_{\bar{yz}}   1/2, 1/2, 1/2$ )'	(20) $4^{+'} \ (1/2, 0, 0) \ x, 0, 1/2$ ( $4_x^+   1/2, 1/2, 1/2$ )'
(21) $4^{+'} \ (0, 1/2, 0) \ 1/2, y, 0$ ( $4_y^+   1/2, 1/2, 1/2$ )'	(22) $2' \ (1/2, 0, 1/2) \ x, 1/4, x$ ( $2_{xz}   1/2, 1/2, 1/2$ )'	(23) $4^{-'} \ (0, 1/2, 0) \ 0, y, 1/2$ ( $4_y^-   1/2, 1/2, 1/2$ )'	(24) $2' \ \bar{x} + 1/2, 1/4, x$ ( $2_{\bar{xz}}   1/2, 1/2, 1/2$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2, 1/2, 1/2); (2); (3); (5); (13).**Positions**Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (1/2, 1/2, 1/2)' +

48	j	1				
(1) $x, y, z$ [u, v, w]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x, \bar{y}, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]			
(5) $z, x, y$ [w, u, v]	(6) $z, \bar{x}, \bar{y}$ [ $w, \bar{u}, \bar{v}$ ]	(7) $\bar{z}, \bar{x}, y$ [ $\bar{w}, \bar{u}, v$ ]	(8) $\bar{z}, x, \bar{y}$ [ $\bar{w}, u, \bar{v}$ ]			
(9) $y, z, x$ [v, w, u]	(10) $\bar{y}, z, \bar{x}$ [ $\bar{v}, w, \bar{u}$ ]	(11) $y, \bar{z}, \bar{x}$ [ $v, \bar{w}, \bar{u}$ ]	(12) $\bar{y}, \bar{z}, x$ [ $\bar{v}, \bar{w}, u$ ]			
(13) $y, x, \bar{z}$ [v, u, $\bar{w}$ ]	(14) $\bar{y}, \bar{x}, \bar{z}$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(15) $y, \bar{x}, z$ [ $v, \bar{u}, w$ ]	(16) $\bar{y}, x, z$ [ $\bar{v}, u, w$ ]			
(17) $x, z, \bar{y}$ [u, w, $\bar{v}$ ]	(18) $\bar{x}, z, y$ [ $\bar{u}, w, v$ ]	(19) $\bar{x}, \bar{z}, \bar{y}$ [ $\bar{u}, \bar{w}, \bar{v}$ ]	(20) $x, \bar{z}, y$ [ $u, \bar{w}, v$ ]			
(21) $z, y, \bar{x}$ [w, v, $\bar{u}$ ]	(22) $z, \bar{y}, x$ [ $w, \bar{v}, u$ ]	(23) $\bar{z}, y, x$ [ $\bar{w}, v, u$ ]	(24) $\bar{z}, \bar{y}, \bar{x}$ [ $\bar{w}, \bar{v}, \bar{u}$ ]			

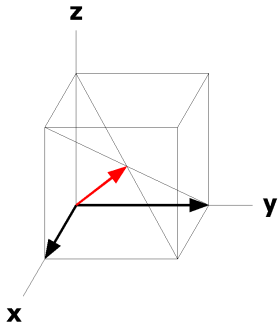
24	i	..2'	$1/4, y, \bar{y} + 1/2 [u, v, v]$ $\bar{y} + 1/2, 1/4, y [v, u, v]$ $y, \bar{y} + 1/2, 1/4 [v, v, u]$	$3/4, \bar{y}, \bar{y} + 1/2 [\bar{u}, \bar{v}, v]$ $\bar{y} + 1/2, 3/4, \bar{y} [v, \bar{u}, \bar{v}]$ $\bar{y}, \bar{y} + 1/2, 3/4 [\bar{v}, v, \bar{u}]$	$3/4, y, y + 1/2 [\bar{u}, v, \bar{v}]$ $y + 1/2, 3/4, y [\bar{v}, \bar{u}, v]$ $y, y + 1/2, 3/4 [v, \bar{v}, \bar{u}]$	$1/4, \bar{y}, y + 1/2 [u, \bar{v}, \bar{v}]$ $y + 1/2, 1/4, \bar{y} [\bar{v}, u, \bar{v}]$ $\bar{y}, y + 1/2, 1/4 [\bar{v}, \bar{v}, u]$
24	h	..2	$0, y, y [0, v, v]$ $y, 0, y [v, 0, v]$ $y, y, 0 [v, v, 0]$	$0, \bar{y}, y [0, \bar{v}, v]$ $y, 0, \bar{y} [v, 0, \bar{v}]$ $\bar{y}, y, 0 [\bar{v}, v, 0]$	$0, y, \bar{y} [0, v, \bar{v}]$ $\bar{y}, 0, y [\bar{v}, 0, v]$ $y, \bar{y}, 0 [v, \bar{v}, 0]$	$0, \bar{y}, \bar{y} [0, \bar{v}, \bar{v}]$ $\bar{y}, 0, \bar{y} [\bar{v}, 0, \bar{v}]$ $\bar{y}, \bar{y}, 0 [\bar{v}, \bar{v}, 0]$
24	g	2..	$x, 1/2, 0 [u, 0, 0]$ $1/2, 0, x [0, 0, u]$ $x, 0, 1/2 [u, 0, 0]$	$\bar{x}, 1/2, 0 [\bar{u}, 0, 0]$ $1/2, 0, \bar{x} [0, 0, \bar{u}]$ $\bar{x}, 0, 1/2 [\bar{u}, 0, 0]$	$0, x, 1/2 [0, u, 0]$ $1/2, x, 0 [0, u, 0]$ $0, 1/2, \bar{x} [0, 0, \bar{u}]$	$0, \bar{x}, 1/2 [0, \bar{u}, 0]$ $1/2, \bar{x}, 0 [0, \bar{u}, 0]$ $0, 1/2, x [0, 0, u]$
16	f	.3.	$x, x, x [u, u, u]$ $x, x, \bar{x} [u, u, \bar{u}]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$ $\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$	$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$ $x, \bar{x}, x [u, \bar{u}, u]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$ $\bar{x}, x, x [\bar{u}, u, u]$
12	e	4..	$x, 0, 0 [u, 0, 0]$ $0, \bar{x}, 0 [0, \bar{u}, 0]$	$\bar{x}, 0, 0 [\bar{u}, 0, 0]$ $0, 0, x [0, 0, u]$	$0, x, 0 [0, u, 0]$ $0, 0, \bar{x} [0, 0, \bar{u}]$	
12	d	2.2'2'	$1/4, 1/2, 0 [u, 0, 0]$ $0, 3/4, 1/2 [0, \bar{u}, 0]$	$3/4, 1/2, 0 [\bar{u}, 0, 0]$ $1/2, 0, 1/4 [0, 0, u]$	$0, 1/4, 1/2 [0, u, 0]$ $1/2, 0, 3/4 [0, 0, \bar{u}]$	
8	c	.32'	$1/4, 1/4, 1/4 [u, u, u]$	$3/4, 3/4, 1/4 [\bar{u}, \bar{u}, u]$	$3/4, 1/4, 3/4 [\bar{u}, u, \bar{u}]$	$1/4, 3/4, 3/4 [u, \bar{u}, \bar{u}]$
6	b	42.2	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$	
2	a	432	$0, 0, 0 [0, 0, 0]$			

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p_4-4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0, 0, z$

Along  $[1, 1, 1]$   $p_3m11'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

Along  $[1, 1, 0]$   $p_{2a}-2m'm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x, x, 0$



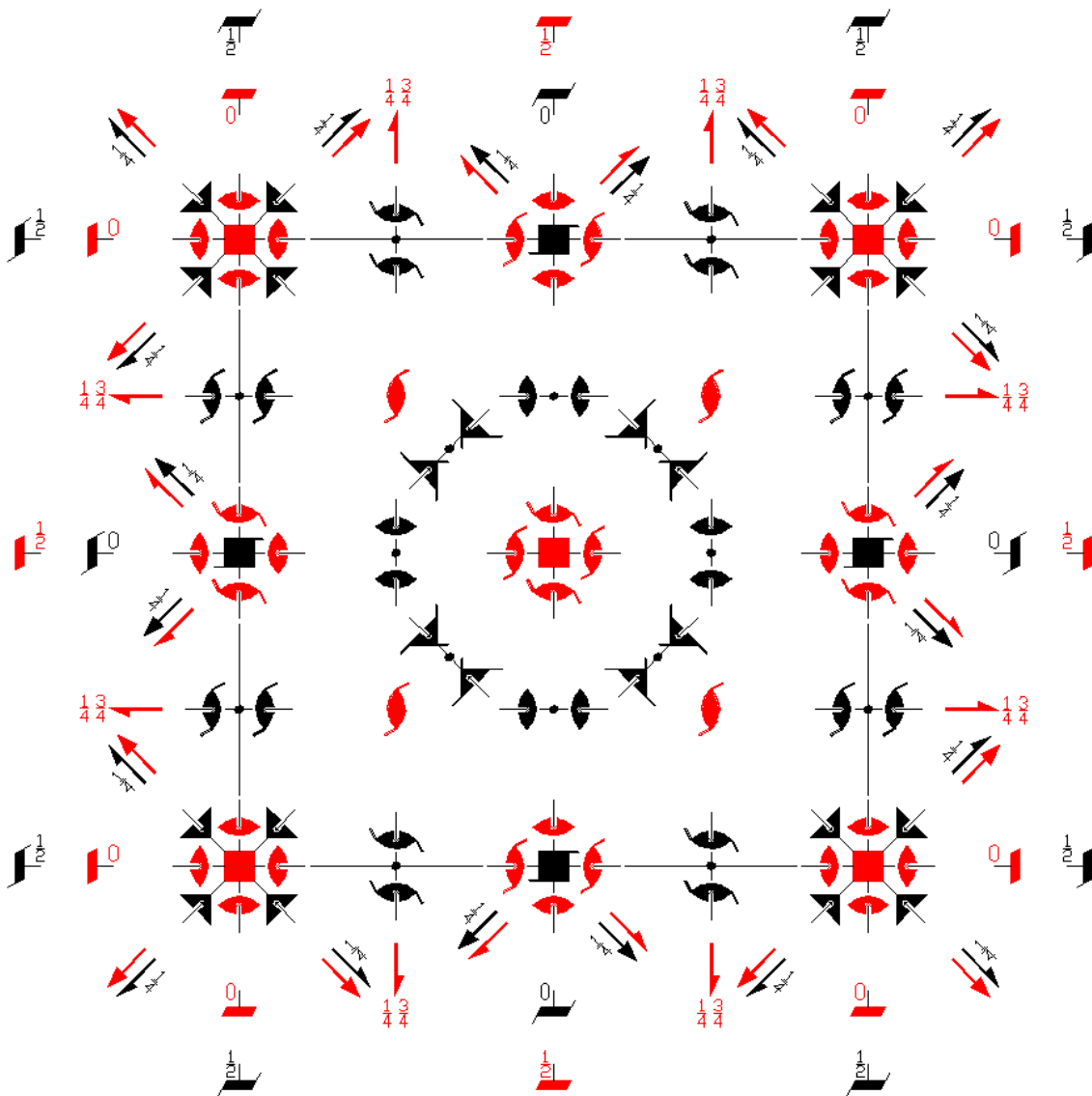
$I_p 4'32'$

$4321'$

Cubic

211.5.1560

$I_p 4'32'$



Origin at  $4'32'$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/4;$   $z \leq \min(x, 1/2-x, y, 1/2-y)$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $0,1/2,0$   $1/4,1/4,1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                          | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                          | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                          |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{xyz^{-1}}$  0,0,0) | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{xyz^{-1}}$  0,0,0) | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{xyz^{-1}}$  0,0,0) |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz^{-1}}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{xyz}$  0,0,0)     | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{xyz}$  0,0,0)     | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{xyz}$  0,0,0)     |

(13) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(14) 2' x,x̄,0 (2 <sub>xy</sub>  0,0,0)'	(15) 4' 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'	(16) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)'
(17) 4' x,0,0 (4 <sub>x</sub> <sup>-1</sup>  0,0,0)'	(18) 2' 0,y,y (2 <sub>yz</sub>  0,0,0)'	(19) 2' 0,y,ȳ (2 <sub>yz</sub>  0,0,0)'	(20) 4 <sup>+</sup> x,0,0 (4 <sub>x</sub>  0,0,0)'
(21) 4 <sup>+</sup> 0,y,0 (4 <sub>y</sub>  0,0,0)'	(22) 2' x,0,x (2 <sub>xz</sub>  0,0,0)'	(23) 4' 0,y,0 (4 <sub>y</sub> <sup>-1</sup>  0,0,0)'	(24) 2' x̄,0,x (2 <sub>xz</sub>  0,0,0)'

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (1 1/2,1/2,1/2)'	(2) 2' (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>  1/2,1/2,1/2)'	(3) 2' (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>  1/2,1/2,1/2)'	(4) 2' (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>  1/2,1/2,1/2)'
(5) 3 <sup>+</sup> (1/2,1/2,1/2) x,x,x (3 <sub>xyz</sub>  1/2,1/2,1/2)'	(6) 3 <sup>+</sup> (1/6,-1/6,1/6) x+1/3,x+1/3,x̄ (3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(7) 3 <sup>+</sup> (-1/6,1/6,1/6) x+2/3,x-1/3,x̄ (3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(8) 3 <sup>+</sup> (1/6,1/6,-1/6) x+1/3,x+2/3,x̄ (3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2)'
(9) 3 <sup>-</sup> (1/2,1/2,1/2) x,x,x (3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(10) 3 <sup>-</sup> (-1/6,1/6,1/6) x+1/3,x+1/3,x̄ (3 <sub>xyz</sub>  1/2,1/2,1/2)'	(11) 3 <sup>-</sup> (1/6,1/6,-1/6) x+2/3,x+1/3,x̄ (3 <sub>xyz</sub>  1/2,1/2,1/2)'	(12) 3 <sup>-</sup> (1/6,-1/6,1/6) x-1/3,x+2/3,x̄ (3 <sub>xyz</sub>  1/2,1/2,1/2)'
(13) 2 (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)	(14) 2 x,x̄+1/2,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)	(15) 4 (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)	(16) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)
(17) 4 <sup>-</sup> (1/2,0,0) x,1/2,0 (4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,1/2)	(18) 2 (0,1/2,1/2) 1/4,y,y (2 <sub>yz</sub>  1/2,1/2,1/2)	(19) 2 1/4,y+1/2,ȳ (2 <sub>yz</sub>  1/2,1/2,1/2)	(20) 4 <sup>+</sup> (1/2,0,0) x,0,1/2 (4 <sub>x</sub>  1/2,1/2,1/2)
(21) 4 <sup>+</sup> (0,1/2,0) 1/2,y,0 (4 <sub>y</sub>  1/2,1/2,1/2)	(22) 2 (1/2,0,1/2) x,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)	(23) 4 <sup>-</sup> (0,1/2,0) 0,y,1/2 (4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,1/2)	(24) 2 x̄+1/2,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (1/2,1/2,1/2)' +

48	j	1									
(1)	x,y,z	[u,v,w]	(2)	x̄,ȳ,z	[ū,v̄,w]	(3)	x̄,y,z	[ū,v,w]	(4)	x,y,z̄	[u,v,w̄]
(5)	z,x,y	[w,u,v]	(6)	z,x̄,ȳ	[w,ū,v̄]	(7)	z̄,x,y	[w̄,ū,v]	(8)	z̄,x,ȳ	[w̄,ū,v̄]
(9)	y,z,x	[v,w,u]	(10)	ȳ,z,x̄	[v̄,w̄,ū]	(11)	y,z̄,x̄	[v,w̄,ū]	(12)	ȳ,z̄,x	[v̄,w̄,ū]
(13)	y,x,z̄	[v̄,ū,w]	(14)	ȳ,x̄,z̄	[v̄,ū,w]	(15)	y,x̄,z	[v̄,ū,w̄]	(16)	ȳ,x,z	[v̄,ū,w̄]
(17)	x,z,ȳ	[ū,w̄,v]	(18)	x̄,z,y	[ū,w̄,v̄]	(19)	x̄,z̄,y	[ū,w,v]	(20)	x,z̄,y	[ū,w̄,v̄]
(21)	z,y,x̄	[w̄,v̄,ū]	(22)	z,ȳ,x	[w̄,v̄,ū]	(23)	z̄,y,x	[w̄,v̄,ū]	(24)	z̄,ȳ,x̄	[w̄,v̄,ū]

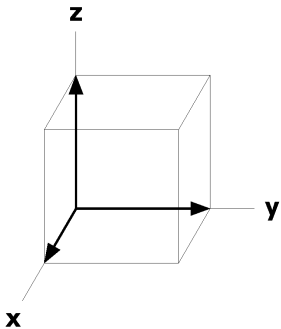
24	i	..2	1/4,y, $\bar{y}$ +1/2 [0, $\bar{v}$ ,v] $\bar{y}$ +1/2,1/4,y [v,0, $\bar{v}$ ] y, $\bar{y}$ +1/2,1/4 [ $\bar{v}$ ,v,0]	3/4, $\bar{y}$ , $\bar{y}$ +1/2 [0,v,v] $\bar{y}$ +1/2,3/4, $\bar{y}$ [v,0,v] $\bar{y}$ , $\bar{y}$ +1/2,3/4 [v,v,0]	3/4,y,y+1/2 [0, $\bar{v}$ , $\bar{v}$ ] y+1/2,3/4,y [ $\bar{v}$ ,0, $\bar{v}$ ] y,y+1/2,3/4 [ $\bar{v}$ , $\bar{v}$ ,0]	1/4, $\bar{y}$ ,y+1/2 [0,v, $\bar{v}$ ] y+1/2,1/4, $\bar{y}$ [ $\bar{v}$ ,0,v] $\bar{y}$ ,y+1/2,1/4 [v, $\bar{v}$ ,0]
24	h	..2'	0,y,y [u,v, $\bar{v}$ ] y,0,y [ $\bar{v}$ ,u,v] y,y,0 [v, $\bar{v}$ ,u]	0, $\bar{y}$ ,y [ $\bar{u}$ , $\bar{v}$ , $\bar{v}$ ] y,0, $\bar{y}$ [ $\bar{v}$ , $\bar{u}$ , $\bar{v}$ ] $\bar{y}$ ,y,0 [ $\bar{v}$ , $\bar{v}$ , $\bar{u}$ ]	0,y, $\bar{y}$ [ $\bar{u}$ ,v,v] $\bar{y}$ ,0,y [v, $\bar{u}$ ,v] y, $\bar{y}$ ,0 [v,v, $\bar{u}$ ]	0, $\bar{y}$ , $\bar{y}$ [u, $\bar{v}$ ,v] $\bar{y}$ ,0, $\bar{y}$ [v,u, $\bar{v}$ ] $\bar{y}$ ,y,0 [ $\bar{v}$ ,v,u]
24	g	2..	x,1/2,0 [u,0,0] 1/2,0,x [0,0,u] x,0,1/2 [ $\bar{u}$ ,0,0]	$\bar{x}$ ,1/2,0 [ $\bar{u}$ ,0,0] 1/2,0, $\bar{x}$ [0,0, $\bar{u}$ ] $\bar{x}$ ,0,1/2 [u,0,0]	0,x,1/2 [0,u,0] 1/2,x,0 [0, $\bar{u}$ ,0] 0,1/2, $\bar{x}$ [0,0,u]	0, $\bar{x}$ ,1/2 [0, $\bar{u}$ ,0] 1/2, $\bar{x}$ ,0 [0,u,0] 0,1/2,x [0,0, $\bar{u}$ ]
16	f	.3.	x,x,x [u,u,u] x,x, $\bar{x}$ [ $\bar{u}$ , $\bar{u}$ ,u]	$\bar{x}$ , $\bar{x}$ ,x [ $\bar{u}$ , $\bar{u}$ ,u] $\bar{x}$ , $\bar{x}$ , $\bar{x}$ [u,u,u]	$\bar{x}$ ,x, $\bar{x}$ [ $\bar{u}$ ,u, $\bar{u}$ ] x, $\bar{x}$ ,x [ $\bar{u}$ ,u, $\bar{u}$ ]	x, $\bar{x}$ , $\bar{x}$ [u, $\bar{u}$ , $\bar{u}$ ] $\bar{x}$ ,x,x [u, $\bar{u}$ , $\bar{u}$ ]
12	e	4..	x,0,0 [u,0,0] 0, $\bar{x}$ ,0 [0, $\bar{u}$ ,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0] 0,0,x [0,0,u]	0,x,0 [0,u,0] 0,0, $\bar{x}$ [0,0, $\bar{u}$ ]	
12	d	2.22	1/4,1/2,0 [0,0,0] 0,3/4,1/2 [0,0,0]	3/4,1/2,0 [0,0,0] 1/2,0,1/4 [0,0,0]	0,1/4,1/2 [0,0,0] 1/2,0,3/4 [0,0,0]	
8	c	.32	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]
6	b	4'2.2'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	
2	a	4'32'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p<sub>p</sub>-4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/2,0,z

Along [1,1,1] p3m11'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

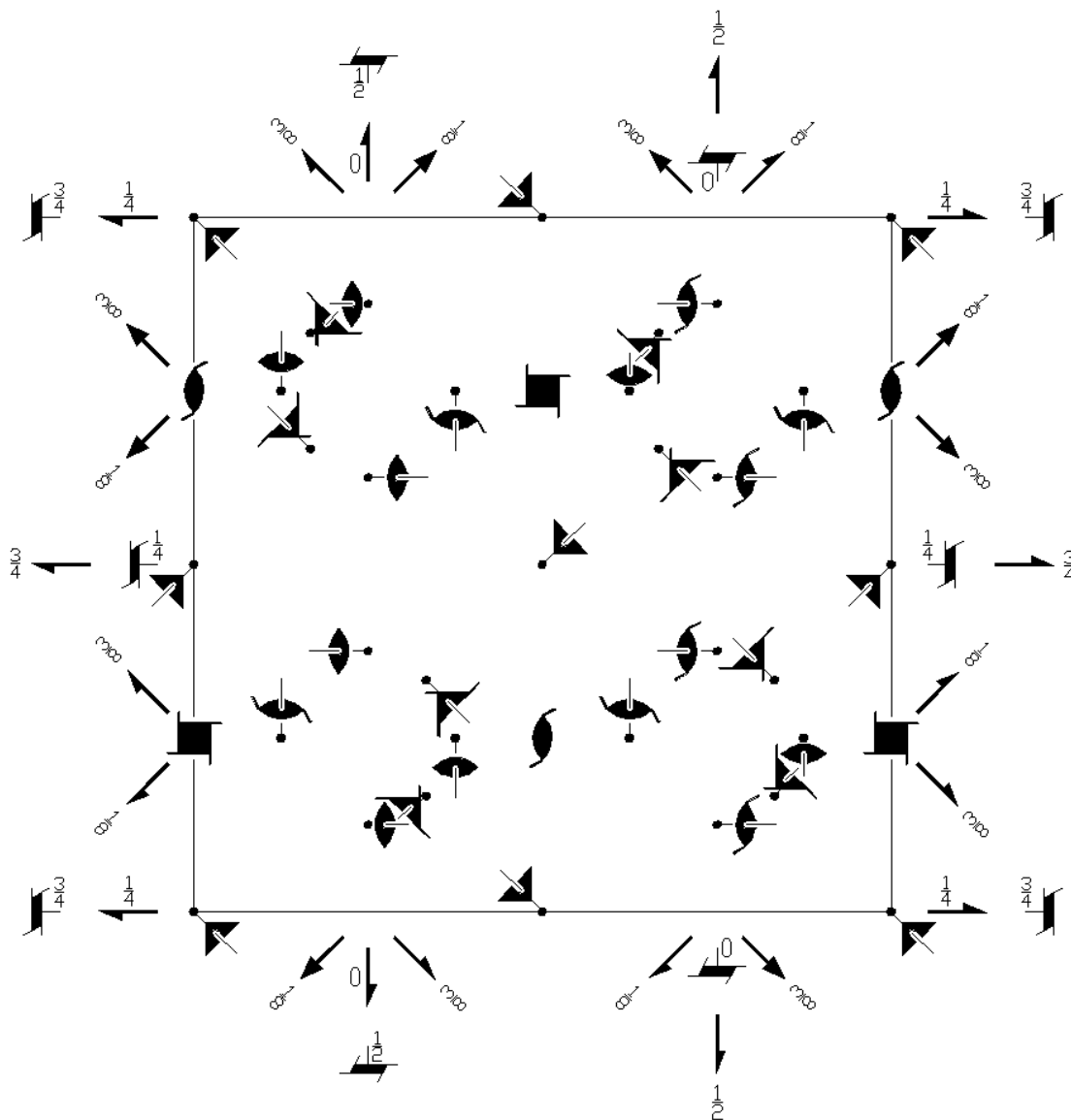
Along [1,1,0] p<sub>2a</sub>-2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



P4<sub>3</sub> 32  
212.1.1561

432  
P4<sub>3</sub> 32

Cubic



**Origin** on 3 [111] at midpoint of three non-intersecting pairs of parallel screw axes 4<sub>3</sub> and 2<sub>1</sub>

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 3/4$ ;  $-1/2 \leq z \leq 1/4$ ;  $\max(-y, x-1/2) \leq y \leq \min(-y+1/2, 2x-y, 2y-x, y-2x+1/2)$

**Vertices** 0,0,0      3/8,1/8,-1/8      1/2,1/2,0      1/4,3/4,-1/4      0,1/2,-1/2      1/4,1/4,1/4

**Symmetry Operations**

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)  | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)  | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}+1/2, \bar{x}, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,1/2,0)      | (7) 3 <sup>+</sup> $x+1/2, \bar{x}-1/2, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,0,1/2)        | (8) 3 <sup>+</sup> $\bar{x}, \bar{x}+1/2, x$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,1/2,1/2)            |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> (-1/3, 1/3, 1/3)<br>x+1/6, $\bar{x}+1/6, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,1/2,1/2) | (11) 3 <sup>-</sup> (1/3, 1/3, -1/3)<br>$\bar{x}+1/3, \bar{x}+1/6, x$<br>(3 <sub><math>\bar{xyz}</math></sub>  1/2,1/2,0) | (12) 3 <sup>-</sup> (1/3, -1/3, 1/3)<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  1/2,0,1/2) |



(13) 2 (1/2,1/2,0) $x, x+1/4, 3/8$ (2 <sub>xy</sub>   1/4, 3/4, 3/4)	(14) 2 $x, \bar{x}+1/4, 1/8$ (2 <sub>xy</sub>   1/4, 1/4, 1/4)	(15) 4 <sup>-</sup> (0,0,1/4) 3/4,0,z (4 <sub>z</sub> <sup>-1</sup>   3/4, 3/4, 1/4)	(16) 4 <sup>+</sup> (0,0,3/4) 1/4,1/2,z (4 <sub>z</sub>   3/4, 1/4, 3/4)
(17) 4 <sup>-</sup> (1/4,0,0) $x, 3/4, 0$ (4 <sub>x</sub> <sup>-1</sup>   1/4, 3/4, 3/4)	(18) 2 (0,1/2,1/2) 3/8,y-1/4,y (2 <sub>yz</sub>   3/4, 1/4, 3/4)	(19) 2 1/8,y+1/4, $\bar{y}$ (2 <sub>yz</sub>   1/4, 1/4, 1/4)	(20) 4 <sup>+</sup> (3/4,0,0) $x, 1/4, 1/2$ (4 <sub>x</sub>   3/4, 3/4, 1/4)
(21) 4 <sup>+</sup> (0,3/4,0) 1/2,y,1/4 (4 <sub>y</sub>   1/4, 3/4, 3/4)	(22) 2 (1/2,0,1/2) $x+1/4, 3/8, x$ (2 <sub>xz</sub>   3/4, 3/4, 1/4)	(23) 4 <sup>-</sup> (0,1/4,0) 0,y,3/4 (4 <sub>y</sub> <sup>-1</sup>   3/4, 1/4, 3/4)	(24) 2 $\bar{x}+1/4, 1/8, x$ (2 <sub>xz</sub>   1/4, 1/4, 1/4)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

24 e 1

(1) x,y,z [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]
(5) z,x,y [w,u,v]	(6) $z+1/2, \bar{x}+1/2, \bar{y}$ [ $w, \bar{u}, \bar{v}$ ]	(7) $\bar{z}+1/2, \bar{x}, y+1/2$ [ $\bar{w}, \bar{u}, v$ ]	(8) $\bar{z}, x+1/2, \bar{y}+1/2$ [ $\bar{w}, u, \bar{v}$ ]
(9) y,z,x [v,w,u]	(10) $\bar{y}, z+1/2, \bar{x}+1/2$ [ $\bar{v}, w, \bar{u}$ ]	(11) $y+1/2, \bar{z}+1/2, \bar{x}$ [ $v, \bar{w}, \bar{u}$ ]	(12) $\bar{y}+1/2, \bar{z}, x+1/2$ [ $\bar{v}, \bar{w}, u$ ]
(13) $y+1/4, x+3/4, \bar{z}+3/4$ [ $v, u, \bar{w}$ ]	(14) $\bar{y}+1/4, \bar{x}+1/4, \bar{z}+1/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(15) $y+3/4, \bar{x}+3/4, z+1/4$ [ $v, \bar{u}, w$ ]	(16) $\bar{y}+3/4, x+1/4, \bar{z}+3/4$ [ $\bar{v}, u, w$ ]
(17) $x+1/4, z+3/4, \bar{y}+3/4$ [ $u, w, \bar{v}$ ]	(18) $\bar{x}+3/4, z+1/4, y+3/4$ [ $\bar{u}, w, v$ ]	(19) $\bar{x}+1/4, \bar{z}+1/4, \bar{y}+1/4$ [ $\bar{u}, \bar{w}, \bar{v}$ ]	(20) $x+3/4, \bar{z}+3/4, y+1/4$ [ $u, \bar{w}, v$ ]
(21) $z+1/4, y+3/4, \bar{x}+3/4$ [ $w, v, \bar{u}$ ]	(22) $z+3/4, \bar{y}+3/4, x+1/4$ [ $w, \bar{v}, u$ ]	(23) $\bar{z}+3/4, y+1/4, x+3/4$ [ $\bar{w}, v, u$ ]	(24) $\bar{z}+1/4, \bar{y}+1/4, \bar{x}+1/4$ [ $\bar{w}, \bar{v}, \bar{u}$ ]

12 d ..2	1/8,y, $\bar{y}+1/4$ [0, $\bar{v},v$ ]	3/8, $\bar{y}, \bar{y}+3/4$ [0,v,v]	7/8,y+1/2,y+1/4 [0, $\bar{v}, \bar{v}$ ]	5/8, $\bar{y}+1/2, y+3/4$ [0,v, $\bar{v}$ ]
	$\bar{y}+1/4, 1/8, y$ [ $v, 0, \bar{v}$ ]	$\bar{y}+3/4, 3/8, \bar{y}$ [ $v, 0, v$ ]	$y+1/4, 7/8, y+1/2$ [ $\bar{v}, 0, \bar{v}$ ]	$y+3/4, 5/8, \bar{y}+1/2$ [ $\bar{v}, 0, v$ ]
	$y, \bar{y}+1/4, 1/8$ [ $\bar{v}, v, 0$ ]	$\bar{y}, \bar{y}+3/4, 3/8$ [ $v, v, 0$ ]	$y+1/2, y+1/4, 7/8$ [ $\bar{v}, \bar{v}, 0$ ]	$\bar{y}+1/2, y+3/4, 5/8$ [ $v, \bar{v}, 0$ ]

8 c .3.	x,x,x [u,u,u]	$\bar{x}+1/2, \bar{x}, x+1/2$ [ $\bar{u}, \bar{u}, u$ ]
	$\bar{x}, x+1/2, \bar{x}+1/2$ [ $\bar{u}, u, \bar{u}$ ]	$x+1/2, \bar{x}+1/2, \bar{x}$ [ $u, \bar{u}, \bar{u}$ ]
	$x+1/4, x+3/4, \bar{x}+3/4$ [ $u, u, \bar{u}$ ]	$\bar{x}+1/4, \bar{x}+1/4, \bar{x}+1/4$ [ $\bar{u}, \bar{u}, \bar{u}$ ]
	$x+3/4, \bar{x}+3/4, x+1/4$ [ $u, \bar{u}, u$ ]	$\bar{x}+3/4, x+1/4, x+3/4$ [ $\bar{u}, u, u$ ]

4 b .32	5/8,5/8,5/8 [0,0,0]	7/8,3/8,1/8 [0,0,0]	3/8,1/8,7/8 [0,0,0]	1/8,7/8,3/8 [0,0,0]
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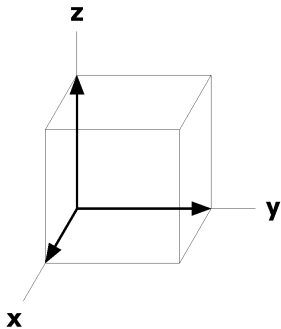
4 a .32	1/8,1/8,1/8 [0,0,0]	3/8,7/8,5/8 [0,0,0]	7/8,5/8,3/8 [0,0,0]	5/8,3/8,7/8 [0,0,0]
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### Symmetry of Special Projections

Along [0,0,1] p4g'm'  
a\* = a b\* = b  
Origin at 1/4,1/2,z

Along [1,1,1] p3m'1  
a\* = (2a - b - c)/3 b\* = (-a + 2b - c)/3  
Origin at x,x,x

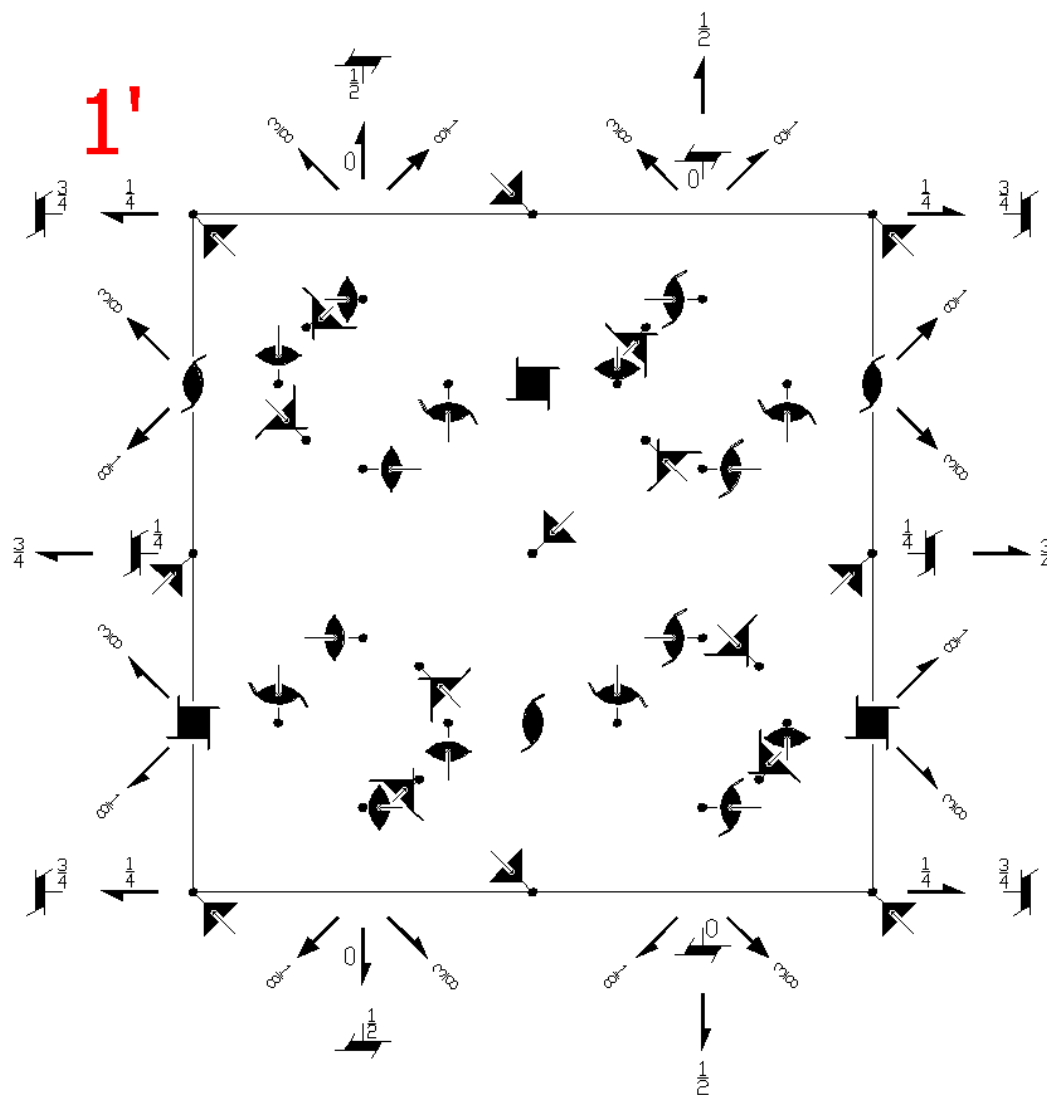
Along [1,1,0] p2m'g'  
a\* = c b\* = -(-a + b)/2  
Origin at x,x+1/4,3/8



$P4_3 321'$   
212.2.1562

$4321'$   
 $P4_3 321'$

Cubic



**Origin** on  $31'$   $[111]$  at midpoint of three non-intersecting pairs of parallel screw axes  $4_3 1'$  and  $2_1 1'$

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 3/4$ ;  $-1/2 \leq z \leq 1/4$ ;  $\max(-y, x-1/2) \leq y \leq \min(-y+1/2, 2x-y, 2y-x, y-2x+1/2)$

Vertices  $0,0,0$   $3/8, 1/8, -1/8$   $1/2, 1/2, 0$   $1/4, 3/4, -1/4$   $0, 1/2, -1/2$   $1/4, 1/4, 1/4$

**Symmetry Operations**

For 1 + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                                  | (2) 2 (0,0,1/2) $1/4, 0, z$<br>( $2_z$   $1/2, 0, 1/2$ )  | (3) 2 (0,1/2,0) $0, y, 1/4$<br>( $2_y$   $0, 1/2, 1/2$ )  | (4) 2 (1/2,0,0) $x, 1/4, 0$<br>( $2_x$   $1/2, 1/2, 0$ )  |
| (5) $3^+$ $x, x, x$<br>( $3_{xyz}$   $0,0,0$ )      | (6) $3^+$ $\bar{x}+1/2, x, \bar{x}$<br>( $3_{x\bar{y}z}^{-1}$   $1/2, 1/2, 0$ )                       | (7) $3^+$ $x+1/2, \bar{x}-1/2, \bar{x}$<br>( $3_{x\bar{y}z}^{-1}$   $1/2, 0, 1/2$ )                   | (8) $3^+$ $\bar{x}, \bar{x}+1/2, x$<br>( $3_{x\bar{y}z}^{-1}$   $0, 1/2, 1/2$ )                       |
| (9) $3^-$ $x, x, x$<br>( $3_{xyz}^{-1}$   $0,0,0$ ) | (10) $3^-$ $(-1/3, 1/3, 1/3)$<br>$x+1/6, \bar{x}+1/6, \bar{x}$<br>( $3_{x\bar{y}z}$   $0, 1/2, 1/2$ ) | (11) $3^-$ $(1/3, 1/3, -1/3)$<br>$\bar{x}+1/3, \bar{x}+1/6, x$<br>( $3_{x\bar{y}z}$   $1/2, 1/2, 0$ ) | (12) $3^-$ $(1/3, -1/3, 1/3)$<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>( $3_{x\bar{y}z}$   $1/2, 0, 1/2$ ) |

(13) 2 (1/2,1/2,0) $\bar{x},x+1/4,3/8$ (2 <sub>xy</sub>  1/4,3/4,3/4)	(14) 2 $\bar{x},\bar{x}+1/4,1/8$ (2 <sub>xy</sub>  1/4,1/4,1/4)	(15) 4 <sup>-</sup> (0,0,1/4) 3/4,0,z (4 <sub>z</sub> <sup>-1</sup>  3/4,3/4,1/4)	(16) 4 <sup>+</sup> (0,0,3/4) 1/4,1/2,z (4 <sub>z</sub>  3/4,1/4,3/4)
(17) 4 <sup>-</sup> (1/4,0,0) $\bar{x},3/4,0$ (4 <sub>x</sub> <sup>-1</sup>  1/4,3/4,3/4)	(18) 2 (0,1/2,1/2) 3/8,y-1/4,y (2 <sub>yz</sub>  3/4,1/4,3/4)	(19) 2 1/8,y+1/4, $\bar{y}$ (2 <sub>yz</sub>  1/4,1/4,1/4)	(20) 4 <sup>+</sup> (3/4,0,0) $\bar{x},1/4,1/2$ (4 <sub>x</sub>  3/4,3/4,1/4)
(21) 4 <sup>+</sup> (0,3/4,0) 1/2,y,1/4 (4 <sub>y</sub>  1/4,3/4,3/4)	(22) 2 (1/2,0,1/2) $\bar{x}+1/4,3/8,x$ (2 <sub>xz</sub>  3/4,3/4,1/4)	(23) 4 <sup>-</sup> (0,1/4,0) 0,y,3/4 (4 <sub>y</sub> <sup>-1</sup>  3/4,1/4,3/4)	(24) 2 $\bar{x}+1/4,1/8,x$ (2 <sub>xz</sub>  1/4,1/4,1/4)

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' (0,0,1/2) 1/4,0,z (2 <sub>z</sub>  1/2,0,1/2)'	(3) 2' (0,1/2,0) 0,y,1/4 (2 <sub>y</sub>  0,1/2,1/2)'	(4) 2' (1/2,0,0) $\bar{x},1/4,0$ (2 <sub>x</sub>  1/2,1/2,0)'
(5) 3 <sup>+</sup> $\bar{x},x,x$ (3 <sub>xyz</sub>  0,0,0)'	(6) 3 <sup>+</sup> $\bar{x}+1/2,x,\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0)'	(7) 3 <sup>+</sup> $\bar{x}+1/2,\bar{x}-1/2,\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2)'	(8) 3 <sup>+</sup> $\bar{x},\bar{x}+1/2,x$ (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)'
(9) 3 <sup>-</sup> $\bar{x},x,x$ (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)'	(10) 3 <sup>-</sup> (-1/3,1/3,1/3) $\bar{x}+1/6,\bar{x}+1/6,\bar{x}$ (3 <sub>xyz</sub>  0,1/2,1/2)'	(11) 3 <sup>-</sup> (1/3,1/3,-1/3) $\bar{x}+1/3,\bar{x}+1/6,x$ (3 <sub>xyz</sub>  1/2,1/2,0)'	(12) 3 <sup>-</sup> (1/3,-1/3,1/3) $\bar{x}-1/6,\bar{x}+1/3,\bar{x}$ (3 <sub>xyz</sub>  1/2,0,1/2)'
(13) 2' (1/2,1/2,0) $\bar{x},x+1/4,3/8$ (2 <sub>xy</sub>  1/4,3/4,3/4)'	(14) 2' $\bar{x},\bar{x}+1/4,1/8$ (2 <sub>xy</sub>  1/4,1/4,1/4)'	(15) 4 <sup>-</sup> (0,0,1/4) 3/4,0,z (4 <sub>z</sub> <sup>-1</sup>  3/4,3/4,1/4)'	(16) 4 <sup>+</sup> (0,0,3/4) 1/4,1/2,z (4 <sub>z</sub>  3/4,1/4,3/4)'
(17) 4 <sup>-</sup> (1/4,0,0) $\bar{x},3/4,0$ (4 <sub>x</sub> <sup>-1</sup>  1/4,3/4,3/4)'	(18) 2' (0,1/2,1/2) 3/8,y-1/4,y (2 <sub>yz</sub>  3/4,1/4,3/4)'	(19) 2' 1/8,y+1/4, $\bar{y}$ (2 <sub>yz</sub>  1/4,1/4,1/4)'	(20) 4 <sup>+</sup> (3/4,0,0) $\bar{x},1/4,1/2$ (4 <sub>x</sub>  3/4,3/4,1/4)'
(21) 4 <sup>+</sup> (0,3/4,0) 1/2,y,1/4 (4 <sub>y</sub>  1/4,3/4,3/4)'	(22) 2' (1/2,0,1/2) $\bar{x}+1/4,3/8,x$ (2 <sub>xz</sub>  3/4,3/4,1/4)'	(23) 4 <sup>-</sup> (0,1/4,0) 0,y,3/4 (4 <sub>y</sub> <sup>-1</sup>  3/4,1/4,3/4)'	(24) 2' $\bar{x}+1/4,1/8,x$ (2 <sub>xz</sub>  1/4,1/4,1/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); 1'.

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +		1' +	
24 e 11'				
(1) x,y,z [0,0,0]	(2) $\bar{x}+1/2,\bar{y},z+1/2$ [0,0,0]	(3) $\bar{x},y+1/2,\bar{z}+1/2$ [0,0,0]	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ [0,0,0]	
(5) z,x,y [0,0,0]	(6) $z+1/2,\bar{x}+1/2,\bar{y}$ [0,0,0]	(7) $\bar{z}+1/2,\bar{x},y+1/2$ [0,0,0]	(8) $\bar{z},x+1/2,\bar{y}+1/2$ [0,0,0]	
(9) y,z,x [0,0,0]	(10) $\bar{y},z+1/2,\bar{x}+1/2$ [0,0,0]	(11) $y+1/2,\bar{z}+1/2,\bar{x}$ [0,0,0]	(12) $\bar{y}+1/2,\bar{z},x+1/2$ [0,0,0]	
(13) $y+1/4,x+3/4,\bar{z}+3/4$ [0,0,0]	(14) $\bar{y}+1/4,\bar{x}+1/4,\bar{z}+1/4$ [0,0,0]	(15) $y+3/4,\bar{x}+3/4,z+1/4$ [0,0,0]	(16) $\bar{y}+3/4,x+1/4,z+3/4$ [0,0,0]	
(17) $x+1/4,z+3/4,\bar{y}+3/4$ [0,0,0]	(18) $\bar{x}+3/4,z+1/4,y+3/4$ [0,0,0]	(19) $\bar{x}+1/4,\bar{z}+1/4,\bar{y}+1/4$ [0,0,0]	(20) $x+3/4,\bar{z}+3/4,y+1/4$ [0,0,0]	
(21) $z+1/4,y+3/4,\bar{x}+3/4$ [0,0,0]	(22) $z+3/4,\bar{y}+3/4,x+1/4$ [0,0,0]	(23) $\bar{z}+3/4,y+1/4,x+3/4$ [0,0,0]	(24) $\bar{z}+1/4,\bar{y}+1/4,\bar{x}+1/4$ [0,0,0]	

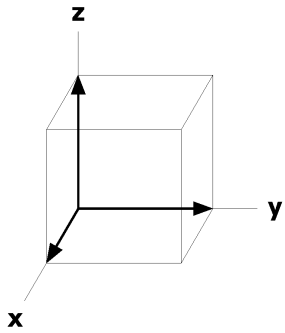
12	d	..21'	$1/8, y, \bar{y}+1/4$ [0,0,0]	$3/8, \bar{y}, \bar{y}+3/4$ [0,0,0]	$7/8, y+1/2, y+1/4$ [0,0,0]	$5/8, \bar{y}+1/2, y+3/4$ [0,0,0]
			$\bar{y}+1/4, 1/8, y$ [0,0,0]	$\bar{y}+3/4, 3/8, \bar{y}$ [0,0,0]	$y+1/4, 7/8, y+1/2$ [0,0,0]	$y+3/4, 5/8, \bar{y}+1/2$ [0,0,0]
			$y, \bar{y}+1/4, 1/8$ [0,0,0]	$\bar{y}, \bar{y}+3/4, 3/8$ [0,0,0]	$y+1/2, y+1/4, 7/8$ [0,0,0]	$\bar{y}+1/2, y+3/4, 5/8$ [0,0,0]
8	c	.3.1'	$x, x, x$ [0,0,0]		$\bar{x}+1/2, \bar{x}, x+1/2$ [0,0,0]	
			$\bar{x}, x+1/2, \bar{x}+1/2$ [0,0,0]		$x+1/2, \bar{x}+1/2, \bar{x}$ [0,0,0]	
			$x+1/4, x+3/4, \bar{x}+3/4$ [0,0,0]		$\bar{x}+1/4, \bar{x}+1/4, \bar{x}+1/4$ [0,0,0]	
			$x+3/4, \bar{x}+3/4, x+1/4$ [0,0,0]		$\bar{x}+3/4, x+1/4, x+3/4$ [0,0,0]	
4	b	.321'	$5/8, 5/8, 5/8$ [0,0,0]	$7/8, 3/8, 1/8$ [0,0,0]	$3/8, 1/8, 7/8$ [0,0,0]	$1/8, 7/8, 3/8$ [0,0,0]
4	a	.321'	$1/8, 1/8, 1/8$ [0,0,0]	$3/8, 7/8, 5/8$ [0,0,0]	$7/8, 5/8, 3/8$ [0,0,0]	$5/8, 3/8, 7/8$ [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $1/4, 1/2, z$

Along [1,1,1] p3m11'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

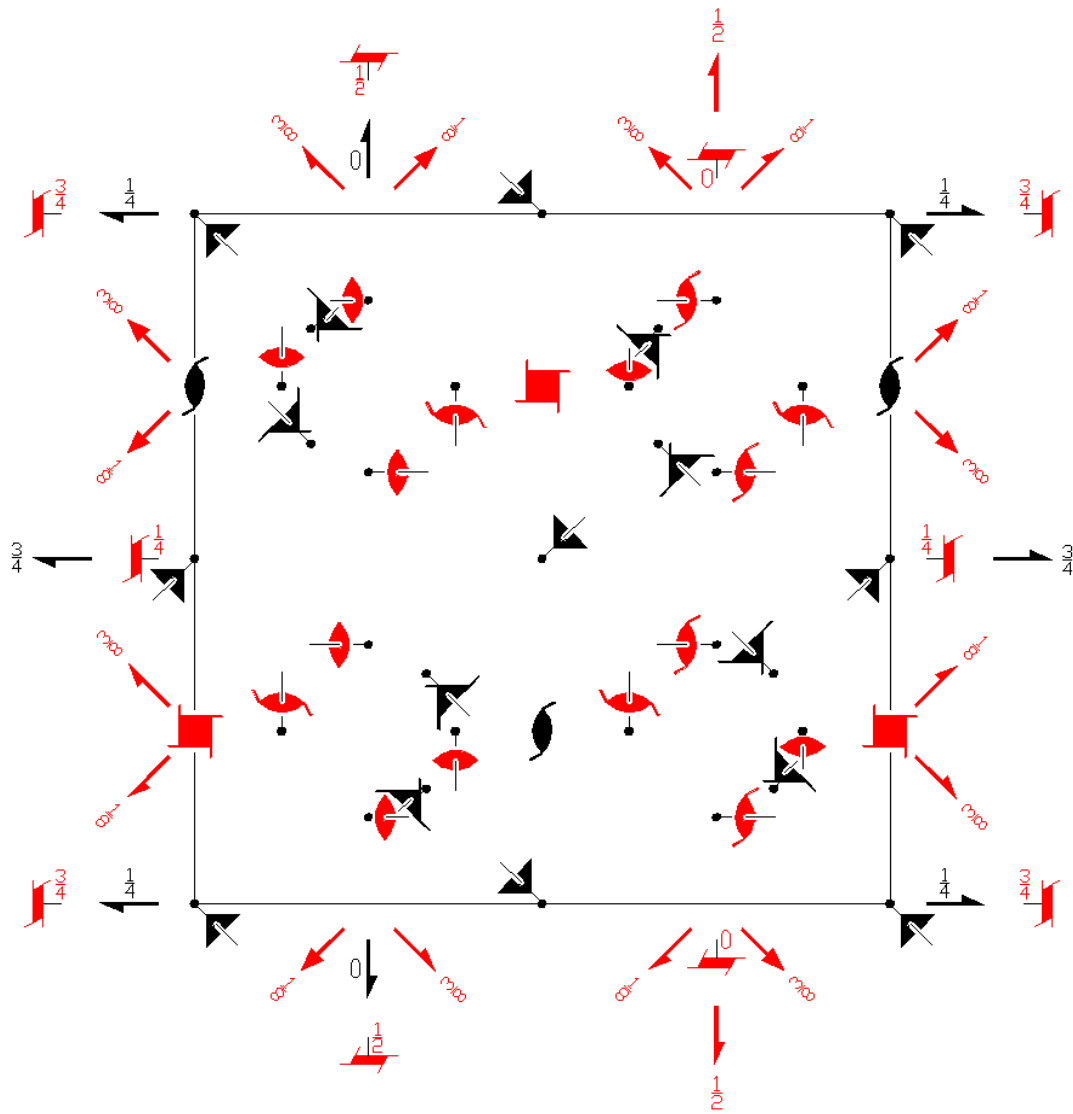
Along [1,1,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = -(-\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x, x+1/4, 3/8$



P4<sub>3</sub>' 32'  
212.3.1563

4'32'  
P4<sub>3</sub>' 32'

Cubic



**Origin** on 3 [111] at midpoint of three non-intersecting pairs of parallel screw axes 4<sub>3</sub>' and 2<sub>1</sub>

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 3/4$ ;  $-1/2 \leq z \leq 1/4$ ;  $\max(-y, x-1/2) \leq y \leq \min(-y+1/2, 2x-y, 2y-x, y-2x+1/2)$

**Vertices** 0,0,0      3/8,1/8,-1/8      1/2,1/2,0      1/4,3/4,-1/4      0,1/2,-1/2      1/4,1/4,1/4

**Symmetry Operations**

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)  | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}+1/2, \bar{x}, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,1/2,0)    | (7) 3 <sup>+</sup> $x+1/2, \bar{x}-1/2, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,0,1/2) | (8) 3 <sup>+</sup> $\bar{x}, \bar{x}+1/2, x$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,1/2,1/2)          |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> (-1/3,1/3,1/3)<br>$x+1/6, \bar{x}+1/6, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,1/2,1/2) | (11) 3 <sup>-</sup> (1/3,1/3,-1/3)<br>$\bar{x}+1/3, x+1/6, x$<br>(3 <sub><math>\bar{xyz}</math></sub>  1/2,1/2,0)  | (12) 3 <sup>-</sup> (1/3,-1/3,1/3)<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  1/2,0,1/2) |

(13) 2' (1/2,1/2,0) x,x+1/4,3/8 (2 <sub>xy</sub>  1/4,3/4,3/4)'	(14) 2' x, $\bar{x}$ +1/4,1/8 (2 <sub>xy</sub>  1/4,1/4,1/4)'	(15) 4' (0,0,1/4) 3/4,0,z (4 <sub>z</sub> <sup>-1</sup>  3/4,3/4,1/4)'	(16) 4 <sup>+</sup> (0,0,3/4) 1/4,1/2,z (4 <sub>z</sub>  3/4,1/4,3/4)'
(17) 4' (1/4,0,0) x,3/4,0 (4 <sub>x</sub> <sup>-1</sup>  1/4,3/4,3/4)'	(18) 2' (0,1/2,1/2) 3/8,y-1/4,y (2 <sub>yz</sub>  3/4,1/4,3/4)'	(19) 2' 1/8,y+1/4, $\bar{y}$ (2 <sub>yz</sub>  1/4,1/4,1/4)'	(20) 4 <sup>+</sup> (3/4,0,0) x,1/4,1/2 (4 <sub>x</sub>  3/4,3/4,1/4)'
(21) 4 <sup>+</sup> (0,3/4,0) 1/2,y,1/4 (4 <sub>y</sub>  1/4,3/4,3/4)'	(22) 2' (1/2,0,1/2) x+1/4,3/8,x (2 <sub>xz</sub>  3/4,3/4,1/4)'	(23) 4' (0,1/4,0) 0,y,3/4 (4 <sub>y</sub> <sup>-1</sup>  3/4,1/4,3/4)'	(24) 2' $\bar{x}$ +1/4,1/8,x (2 <sub>xz</sub>  1/4,1/4,1/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

24 e 1

(1) x,y,z [u,v,w]	(2) $\bar{x}$ +1/2, $\bar{y}$ ,z+1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(3) $\bar{x}$ ,y+1/2, $\bar{z}$ +1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x+1/2, $\bar{y}$ +1/2, $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]
(5) z,x,y [w,u,v]	(6) z+1/2, $\bar{x}$ +1/2, $\bar{y}$ [w, $\bar{u}$ , $\bar{v}$ ]	(7) $\bar{z}$ +1/2, $\bar{x}$ ,y+1/2 [ $\bar{w}$ , $\bar{u}$ ,v]	(8) $\bar{z}$ ,x+1/2, $\bar{y}$ +1/2 [ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ]
(9) y,z,x [v,w,u]	(10) $\bar{y}$ ,z+1/2, $\bar{x}$ +1/2 [ $\bar{v}$ ,w, $\bar{u}$ ]	(11) y+1/2, $\bar{z}$ +1/2, $\bar{x}$ [v, $\bar{w}$ , $\bar{u}$ ]	(12) $\bar{y}$ +1/2, $\bar{z}$ ,x+1/2 [ $\bar{v}$ , $\bar{w}$ ,u]
(13) y+1/4,x+3/4, $\bar{z}$ +3/4 [ $\bar{v}$ , $\bar{u}$ ,w]	(14) $\bar{y}$ +1/4, $\bar{x}$ +1/4, $\bar{z}$ +1/4 [v,u,w]	(15) y+3/4, $\bar{x}$ +3/4,z+1/4 [ $\bar{v}$ ,u, $\bar{w}$ ]	(16) $\bar{y}$ +3/4,x+1/4,z+3/4 [v, $\bar{u}$ , $\bar{w}$ ]
(17) x+1/4,z+3/4, $\bar{y}$ +3/4 [ $\bar{u}$ , $\bar{w}$ ,v]	(18) $\bar{x}$ +3/4,z+1/4,y+3/4 [u, $\bar{w}$ , $\bar{v}$ ]	(19) $\bar{x}$ +1/4, $\bar{z}$ +1/4, $\bar{y}$ +1/4 [u,w,v]	(20) x+3/4, $\bar{z}$ +3/4,y+1/4 [ $\bar{u}$ ,w, $\bar{v}$ ]
(21) z+1/4,y+3/4, $\bar{x}$ +3/4 [ $\bar{w}$ , $\bar{v}$ ,u]	(22) z+3/4, $\bar{y}$ +3/4,x+1/4 [ $\bar{w}$ ,v, $\bar{u}$ ]	(23) $\bar{z}$ +3/4,y+1/4,x+3/4 [w, $\bar{v}$ , $\bar{u}$ ]	(24) $\bar{z}$ +1/4, $\bar{y}$ +1/4, $\bar{x}$ +1/4 [w,v,u]

12 d ..2'	1/8,y, $\bar{y}$ +1/4 [u,v,v]	3/8, $\bar{y}$ , $\bar{y}$ +3/4 [ $\bar{u}$ , $\bar{v}$ ,v]	7/8,y+1/2,y+1/4 [ $\bar{u}$ ,v, $\bar{v}$ ]	5/8, $\bar{y}$ +1/2,y+3/4 [u, $\bar{v}$ , $\bar{v}$ ]
	$\bar{y}$ +1/4,1/8,y [v,u,v]	$\bar{y}$ +3/4,3/8, $\bar{y}$ [v, $\bar{u}$ , $\bar{v}$ ]	y+1/4,7/8,y+1/2 [ $\bar{v}$ , $\bar{u}$ ,v]	y+3/4,5/8, $\bar{y}$ +1/2 [ $\bar{v}$ ,u, $\bar{v}$ ]
	y, $\bar{y}$ +1/4,1/8 [v,v,u]	$\bar{y}$ , $\bar{y}$ +3/4,3/8 [ $\bar{v}$ ,v, $\bar{u}$ ]	y+1/2,y+1/4,7/8 [v, $\bar{v}$ , $\bar{u}$ ]	$\bar{y}$ +1/2,y+3/4,5/8 [ $\bar{v}$ , $\bar{v}$ ,u]

8 c .3.	x,x,x [u,u,u]	$\bar{x}$ +1/2, $\bar{x}$ ,x+1/2 [ $\bar{u}$ , $\bar{u}$ ,u]	$\bar{x}$ +1/2, $\bar{x}$ +1/2,x [u, $\bar{u}$ , $\bar{u}$ ]
	$\bar{x}$ ,x+1/2, $\bar{x}$ +1/2 [ $\bar{u}$ ,u, $\bar{u}$ ]	$\bar{x}$ +1/4, $\bar{x}$ +1/4, $\bar{x}$ +1/4 [u,u,u]	$\bar{x}$ +3/4,x+1/4,x+3/4 [u, $\bar{u}$ , $\bar{u}$ ]
	x+1/4,x+3/4, $\bar{x}$ +3/4 [ $\bar{u}$ , $\bar{u}$ ,u]		
	x+3/4, $\bar{x}$ +3/4,x+1/4 [ $\bar{u}$ ,u, $\bar{u}$ ]		

4 b .32'	5/8,5/8,5/8 [u,u,u]	7/8,3/8,1/8 [ $\bar{u}$ , $\bar{u}$ ,u]	3/8,1/8,7/8 [ $\bar{u}$ ,u, $\bar{u}$ ]	1/8,7/8,3/8 [u, $\bar{u}$ , $\bar{u}$ ]
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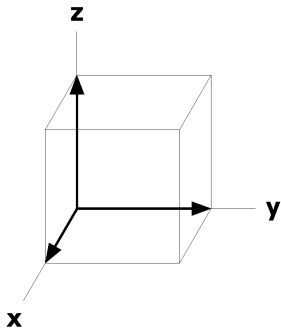
4 a .32'	1/8,1/8,1/8 [u,u,u]	3/8,7/8,5/8 [ $\bar{u}$ , $\bar{u}$ ,u]	7/8,5/8,3/8 [ $\bar{u}$ ,u, $\bar{u}$ ]	5/8,3/8,7/8 [u, $\bar{u}$ , $\bar{u}$ ]
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### Symmetry of Special Projections

Along [0,0,1] p4'g'm  
a\* = a b\* = b  
Origin at 1/4,1/2,z

Along [1,1,1] p3m1  
a\* = (2a - b - c)/3 b\* = (-a + 2b - c)/3  
Origin at x,x,x

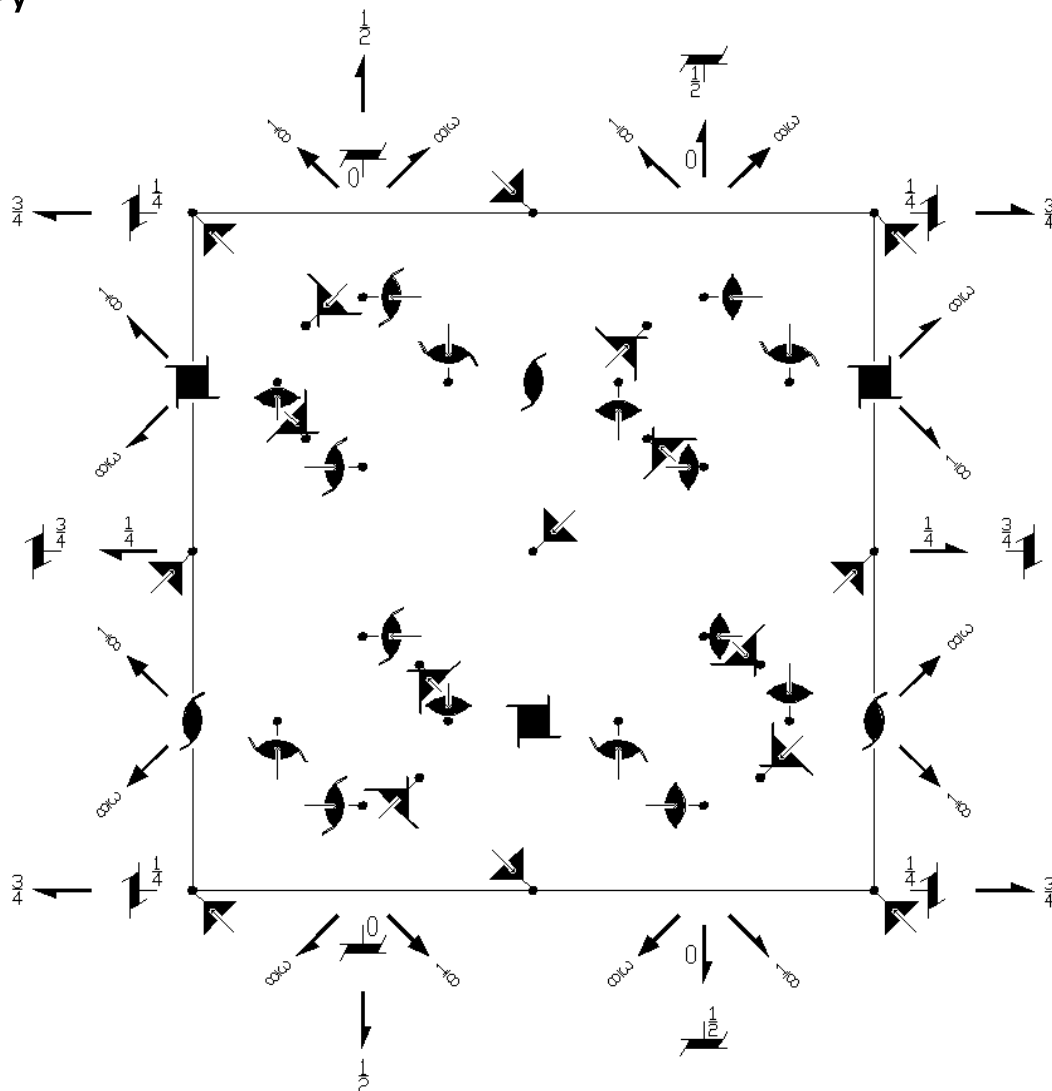
Along [1,1,0] p2'm'g  
a\* = c b\* = -(-a + b)/2  
Origin at x,x+1/4,3/8



P4<sub>1</sub> 32  
213.1.1564

432  
P4<sub>1</sub> 32

Cubic



**Origin** on 3 [111] at midpoint of three non-intersecting pairs of parallel screw axes 4<sub>1</sub> and 2<sub>1</sub>

**Asymmetric unit**  $-1/4 \leq x \leq 1/2$ ;  $0 \leq y \leq 3/4$ ;  $0 \leq z \leq 1/2$ ;  $x \leq y \leq x+1/2$ ;

$(y-x)/2 \leq z \leq \min(y, (-4x-2y+3)/2, (3-2x-2y)/4)$

Vertices 0,0,0      1/2,1/2,0      1/4,3/4,1/4      -1/4,1/4,1/4      0,1/2,1/2      3/8,3/8,3/8

**Symmetry Operations**

- |   |  |   |   |
|---|--|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)  | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}+1/2, \bar{x}, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,1/2,0) | (7) 3 <sup>+</sup> $\bar{x}+1/2, \bar{x}-1/2, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,0,1/2)      | (8) 3 <sup>+</sup> $\bar{x}, \bar{x}+1/2, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,1/2,1/2)          |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> (-1/3,1/3,1/3)<br>x+1/6, $\bar{x}+1/6, \bar{x}$<br>(3 <sub>xyz</sub>  0,1/2,1/2)                 | (11) 3 <sup>-</sup> (1/3,1/3,-1/3)<br>$\bar{x}+1/3, \bar{x}+1/6, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  1/2,1/2,0) | (12) 3 <sup>-</sup> (1/3,-1/3,1/3)<br>$\bar{x}-1/6, \bar{x}+1/3, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  1/2,0,1/2) |

(13) 2 (1/2,1/2,0) $x, x-1/4, 1/8$ ( $2_{xy}   3/4, 1/4, 1/4$ )	(14) 2 $x, \bar{x}+3/4, 3/8$ ( $2_{\bar{xy}}   3/4, 3/4, 3/4$ )	(15) 4 <sup>-</sup> (0,0,3/4) $1/4, 0, z$ ( $4_z^{-1}   1/4, 1/4, 3/4$ )	(16) 4 <sup>+</sup> (0,0,1/4) $-1/4, 1/2, z$ ( $4_z   1/4, 3/4, 1/4$ )
(17) 4 <sup>-</sup> (3/4,0,0) $x, 1/4, 0$ ( $4_x^{-1}   3/4, 1/4, 1/4$ )	(18) 2 (0,1/2,1/2) $1/8, y+1/4, y$ ( $2_{yz}   1/4, 3/4, 1/4$ )	(19) 2 $3/8, y+3/4, \bar{y}$ ( $2_{\bar{yz}}   3/4, 3/4, 3/4$ )	(20) 4 <sup>+</sup> (1/4,0,0) $x, -1/4, 1/2$ ( $4_x   1/4, 1/4, 3/4$ )
(21) 4 <sup>+</sup> (0,1/4,0) $1/2, y, -1/4$ ( $4_y   3/4, 1/4, 1/4$ )	(22) 2 (1/2,0,1/2) $x-1/4, 1/8, x$ ( $2_{xz}   1/4, 1/4, 3/4$ )	(23) 4 <sup>-</sup> (0,3/4,0) $0, y, 1/4$ ( $4_y^{-1}   1/4, 3/4, 1/4$ )	(24) 2 $\bar{x}+3/4, 3/8, x$ ( $2_{\bar{xz}}   3/4, 3/4, 3/4$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

24 e 1

(1) $x, y, z$ [u,v,w]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]
(5) $z, x, y$ [w,u,v]	(6) $z+1/2, \bar{x}+1/2, \bar{y}$ [ $w, \bar{u}, \bar{v}$ ]	(7) $\bar{z}+1/2, \bar{x}, y+1/2$ [ $\bar{w}, \bar{u}, v$ ]	(8) $\bar{z}, x+1/2, \bar{y}+1/2$ [ $\bar{w}, u, \bar{v}$ ]
(9) $y, z, x$ [v,w,u]	(10) $\bar{y}, z+1/2, \bar{x}+1/2$ [ $\bar{v}, w, \bar{u}$ ]	(11) $y+1/2, \bar{z}+1/2, \bar{x}$ [ $v, \bar{w}, \bar{u}$ ]	(12) $\bar{y}+1/2, \bar{z}, x+1/2$ [ $\bar{v}, \bar{w}, u$ ]
(13) $y+3/4, x+1/4, \bar{z}+1/4$ [ $v, u, \bar{w}$ ]	(14) $\bar{y}+3/4, \bar{x}+3/4, \bar{z}+3/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(15) $y+1/4, \bar{x}+1/4, z+3/4$ [ $v, \bar{u}, w$ ]	(16) $\bar{y}+1/4, x+3/4, z+1/4$ [ $\bar{v}, u, w$ ]
(17) $x+3/4, z+1/4, \bar{y}+1/4$ [ $u, w, \bar{v}$ ]	(18) $\bar{x}+1/4, z+3/4, y+1/4$ [ $\bar{u}, w, v$ ]	(19) $\bar{x}+3/4, \bar{z}+3/4, \bar{y}+3/4$ [ $\bar{u}, \bar{w}, \bar{v}$ ]	(20) $x+1/4, \bar{z}+1/4, y+3/4$ [ $u, \bar{w}, v$ ]
(21) $z+3/4, y+1/4, \bar{x}+1/4$ [ $w, v, \bar{u}$ ]	(22) $z+1/4, \bar{y}+1/4, x+3/4$ [ $w, \bar{v}, u$ ]	(23) $\bar{z}+1/4, y+3/4, x+1/4$ [ $\bar{w}, v, u$ ]	(24) $\bar{z}+3/4, \bar{y}+3/4, \bar{x}+3/4$ [ $\bar{w}, \bar{v}, \bar{u}$ ]

12 d ..2	$1/8, y, y+1/4$ [0,v,v]	$3/8, \bar{y}, y+3/4$ [0, $\bar{v}$ ,v]	$7/8, y+1/2, \bar{y}+1/4$ [0,v, $\bar{v}$ ]	$5/8, \bar{y}+1/2, \bar{y}+3/4$ [0, $\bar{v}$ , $\bar{v}$ ]
	$y+1/4, 1/8, y$ [v,0,v]	$y+3/4, 3/8, \bar{y}$ [v,0, $\bar{v}$ ]	$\bar{y}+1/4, 7/8, y+1/2$ [ $\bar{v}$ ,0,v]	$\bar{y}+3/4, 5/8, \bar{y}+1/2$ [ $\bar{v}$ ,0, $\bar{v}$ ]
	$y, y+1/4, 1/8$ [v,v,0]	$\bar{y}, y+3/4, 3/8$ [ $\bar{v}$ ,v,0]	$y+1/2, \bar{y}+1/4, 7/8$ [v, $\bar{v}$ ,0]	$\bar{y}+1/2, \bar{y}+3/4, 5/8$ [ $\bar{v}$ , $\bar{v}$ ,0]

8 c .3.	$x, x, x$ [u,u,u]	$\bar{x}+1/2, \bar{x}, x+1/2$ [ $\bar{u}, \bar{u}, u$ ]
	$\bar{x}, x+1/2, \bar{x}+1/2$ [ $\bar{u}, u, \bar{u}$ ]	$x+1/2, \bar{x}+1/2, \bar{x}$ [u, $\bar{u}, \bar{u}$ ]
	$x+3/4, x+1/4, \bar{x}+1/4$ [u,u, $\bar{u}$ ]	$\bar{x}+3/4, \bar{x}+3/4, \bar{x}+3/4$ [ $\bar{u}, \bar{u}, \bar{u}$ ]
	$x+1/4, \bar{x}+1/4, x+3/4$ [u, $\bar{u}, u$ ]	$\bar{x}+1/4, x+3/4, x+1/4$ [ $\bar{u}, u, u$ ]

4 b .32	$7/8, 7/8, 7/8$ [0,0,0]	$5/8, 1/8, 3/8$ [0,0,0]	$1/8, 3/8, 5/8$ [0,0,0]	$3/8, 5/8, 1/8$ [0,0,0]
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4 a .32	$3/8, 3/8, 3/8$ [0,0,0]	$1/8, 5/8, 7/8$ [0,0,0]	$5/8, 7/8, 1/8$ [0,0,0]	$7/8, 1/8, 5/8$ [0,0,0]
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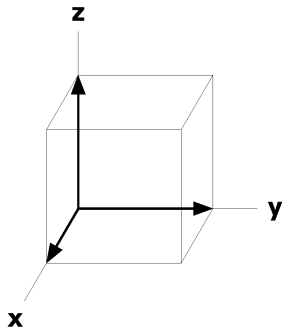
### Symmetry of Special Projections

Along [0,0,1] p4g'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,1,1] p3m'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

Along [1,1,0] p2m'g'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = -(-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x+1/4,1/8

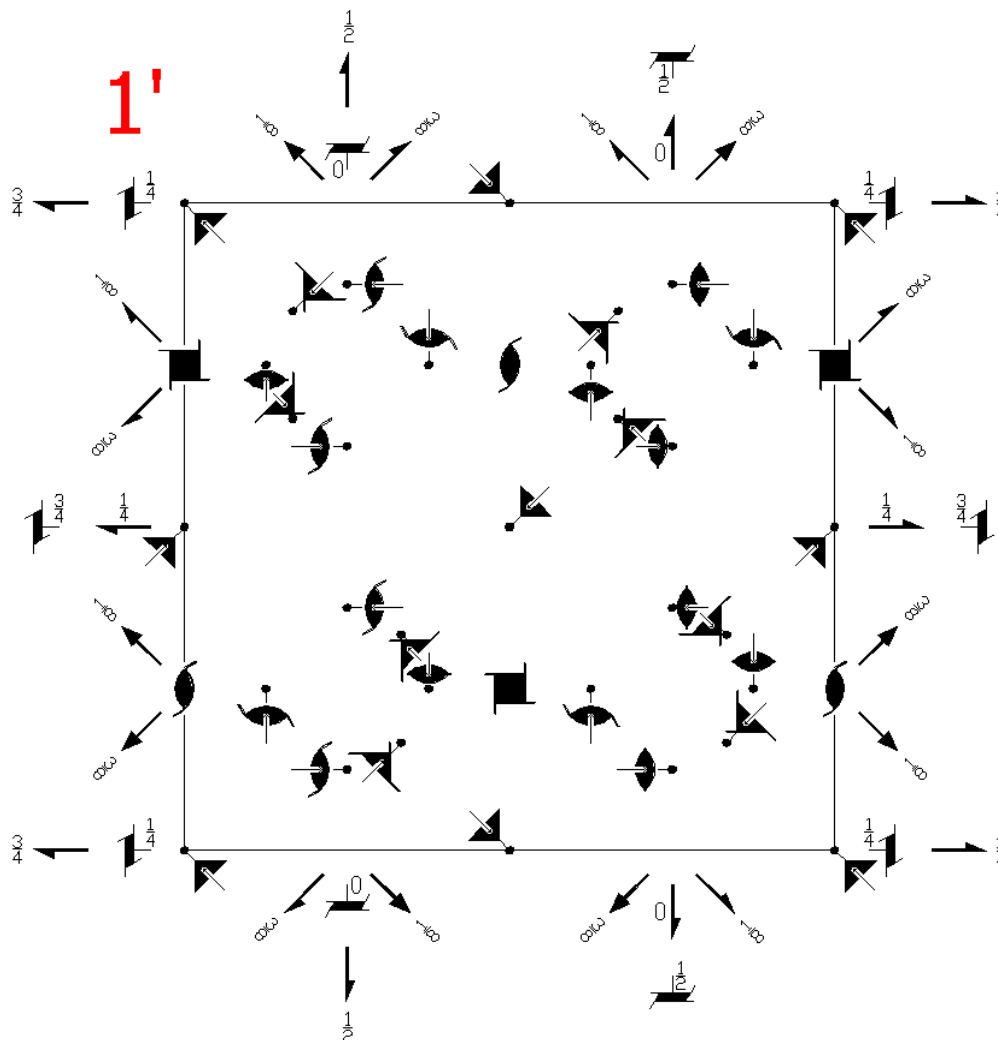




P4<sub>1</sub> 321'  
213.2.1565

4321'  
P4<sub>1</sub> 321'

Cubic



**Origin** on 31' [111] at midpoint of three non-intersecting pairs of parallel screw axes 4<sub>1</sub>1' and 2<sub>1</sub>1'

**Asymmetric unit**  $-1/4 \leq x \leq 1/2$ ;  $0 \leq y \leq 3/4$ ;  $0 \leq z \leq 1/2$ ;  $x \leq y \leq x+1/2$ ;

$(y-x)/2 \leq z \leq \min(y, (-4x-2y+3)/2, (3-2x-2y)/4)$

Vertices 0,0,0      1/2,1/2,0      1/4,3/4,1/4      -1/4,1/4,1/4      0,1/2,1/2      3/8,3/8,3/8

**Symmetry Operations**

For 1 + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)  | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)  | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}+1/2, x, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,1/2,0)            | (7) 3 <sup>+</sup> $x+1/2, \bar{x}-1/2, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,0,1/2)        | (8) 3 <sup>+</sup> $\bar{x}, \bar{x}+1/2, x$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,1/2,1/2)            |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> (-1/3, 1/3, 1/3)<br>x+1/6, $\bar{x}+1/6, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,1/2,1/2) | (11) 3 <sup>-</sup> (1/3, 1/3, -1/3)<br>$\bar{x}+1/3, \bar{x}+1/6, x$<br>(3 <sub><math>\bar{xyz}</math></sub>  1/2,1/2,0) | (12) 3 <sup>-</sup> (1/3, -1/3, 1/3)<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  1/2,0,1/2) |

- |   |   |   |   |
|---|---|---|---|
| (13) $2 (1/2, 1/2, 0) \quad x, x-1/4, 1/8$<br>( $2_{xy}   3/4, 1/4, 1/4$ )' | (14) $2 \quad x, \bar{x}+3/4, 3/8$<br>( $2_{\bar{xy}}   3/4, 3/4, 3/4$ )'   | (15) $4^- (0, 0, 3/4) \quad 1/4, 0, z$<br>( $4_z^{-1}   1/4, 1/4, 3/4$ )' | (16) $4^+ (0, 0, 1/4) \quad -1/4, 1/2, z$<br>( $4_z   1/4, 3/4, 1/4$ )'   |
| (17) $4^- (3/4, 0, 0) \quad x, 1/4, 0$<br>( $4_x^{-1}   3/4, 1/4, 1/4$ )'   | (18) $2 (0, 1/2, 1/2) \quad 1/8, y+1/4, y$<br>( $2_{yz}   1/4, 3/4, 1/4$ )' | (19) $2 \quad 3/8, y+3/4, \bar{y}$<br>( $2_{\bar{yz}}   3/4, 3/4, 3/4$ )' | (20) $4^+ (1/4, 0, 0) \quad x, -1/4, 1/2$<br>( $4_x   1/4, 1/4, 3/4$ )'   |
| (21) $4^+ (0, 1/4, 0) \quad 1/2, y, -1/4$<br>( $4_y   3/4, 1/4, 1/4$ )'     | (22) $2 (1/2, 0, 1/2) \quad x-1/4, 1/8, x$<br>( $2_{xz}   1/4, 1/4, 3/4$ )' | (23) $4^- (0, 3/4, 0) \quad 0, y, 1/4$<br>( $4_y^{-1}   1/4, 3/4, 1/4$ )' | (24) $2 \quad \bar{x}+3/4, 3/8, x$<br>( $2_{\bar{xz}}   3/4, 3/4, 3/4$ )' |

For 1' + set

- |  |   |   |   |
|--|---|---|---|
| (1) $1'$<br>( $1   0, 0, 0$ )'   | (2) $2' (0, 0, 1/2) \quad 1/4, 0, z$<br>( $2_z   1/2, 0, 1/2$ )'  | (3) $2' (0, 1/2, 0) \quad 0, y, 1/4$<br>( $2_y   0, 1/2, 1/2$ )'  | (4) $2' (1/2, 0, 0) \quad x, 1/4, 0$<br>( $2_x   1/2, 1/2, 0$ )'  |
| (5) $3^{+1} \quad x, x, x$<br>( $3_{xyz}   0, 0, 0$ )'                       | (6) $3^{+1} \quad \bar{x}+1/2, x, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   1/2, 1/2, 0$ )'                                     | (7) $3^{+1} \quad x+1/2, \bar{x}-1/2, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ )'                           | (8) $3^{+1} \quad \bar{x}, \bar{x}+1/2, x$<br>( $3_{\bar{xyz}}^{-1}   0, 1/2, 1/2$ )'                               |
| (9) $3^{-1} \quad x, x, x$<br>( $3_{xyz}^{-1}   0, 0, 0$ )'                  | (10) $3^{-1} \quad (-1/3, 1/3, 1/3) \quad \bar{x}$<br>$x+1/6, \bar{x}+1/6, \bar{x}$<br>( $3_{\bar{xyz}}   0, 1/2, 1/2$ )' | (11) $3^{-1} \quad (1/3, 1/3, -1/3) \quad \bar{x}$<br>$x+1/3, \bar{x}+1/6, x$<br>( $3_{\bar{xyz}}   1/2, 1/2, 0$ )' | (12) $3^{-1} \quad (1/3, -1/3, 1/3) \quad \bar{x}$<br>$x-1/6, x+1/3, \bar{x}$<br>( $3_{\bar{xyz}}   1/2, 0, 1/2$ )' |
| (13) $2' (1/2, 1/2, 0) \quad x, x-1/4, 1/8$<br>( $2_{xy}   3/4, 1/4, 1/4$ )' | (14) $2' \quad x, \bar{x}+3/4, 3/8$<br>( $2_{\bar{xy}}   3/4, 3/4, 3/4$ )'  | (15) $4^{-1} (0, 0, 3/4) \quad 1/4, 0, z$<br>( $4_z^{-1}   1/4, 1/4, 3/4$ )'  | (16) $4^{+1} (0, 0, 1/4) \quad -1/4, 1/2, z$<br>( $4_z   1/4, 3/4, 1/4$ )'  |
| (17) $4^{-1} (3/4, 0, 0) \quad x, 1/4, 0$<br>( $4_x^{-1}   3/4, 1/4, 1/4$ )' | (18) $2' (0, 1/2, 1/2) \quad 1/8, y+1/4, y$<br>( $2_{yz}   1/4, 3/4, 1/4$ )'  | (19) $2' \quad 3/8, y+3/4, \bar{y}$<br>( $2_{\bar{yz}}   3/4, 3/4, 3/4$ )'  | (20) $4^{+1} (1/4, 0, 0) \quad x, -1/4, 1/2$<br>( $4_x   1/4, 1/4, 3/4$ )'  |
| (21) $4^{+1} (0, 1/4, 0) \quad 1/2, y, -1/4$<br>( $4_y   3/4, 1/4, 1/4$ )'   | (22) $2' (1/2, 0, 1/2) \quad x-1/4, 1/8, x$<br>( $2_{xz}   1/4, 1/4, 3/4$ )'  | (23) $4^{-1} (0, 3/4, 0) \quad 0, y, 1/4$<br>( $4_y^{-1}   1/4, 3/4, 1/4$ )'  | (24) $2' \quad \bar{x}+3/4, 3/8, x$<br>( $2_{\bar{xz}}   3/4, 3/4, 3/4$ )'  |

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); 1'.

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

1 +                      1' +

- |  |  |  |  |  |  |  |
|--|--|--|--|--|--|--|
| 24                                       | e  | 11'  |  |  |  |  |
| (1) x,y,z [0,0,0]                        | (2) $\bar{x}+1/2, \bar{y}, z+1/2$ [0,0,0]            | (3) $\bar{x}, y+1/2, \bar{z}+1/2$ [0,0,0]            | (4) $x+1/2, \bar{y}+1/2, \bar{z}$ [0,0,0]            |  |  |  |
| (5) z,x,y [0,0,0]                        | (6) $z+1/2, \bar{x}+1/2, \bar{y}$ [0,0,0]            | (7) $\bar{z}+1/2, \bar{x}, y+1/2$ [0,0,0]            | (8) $\bar{z}, x+1/2, \bar{y}+1/2$ [0,0,0]            |  |  |  |
| (9) y,z,x [0,0,0]                        | (10) $\bar{y}, z+1/2, \bar{x}+1/2$ [0,0,0]           | (11) $y+1/2, \bar{z}+1/2, \bar{x}$ [0,0,0]           | (12) $\bar{y}+1/2, \bar{z}, x+1/2$ [0,0,0]           |  |  |  |
| (13) $y+3/4, x+1/4, \bar{z}+1/4$ [0,0,0] | (14) $\bar{y}+3/4, \bar{x}+3/4, \bar{z}+3/4$ [0,0,0] | (15) $y+1/4, \bar{x}+1/4, z+3/4$ [0,0,0]             | (16) $\bar{y}+1/4, x+3/4, z+1/4$ [0,0,0]             |  |  |  |
| (17) $x+3/4, z+1/4, \bar{y}+1/4$ [0,0,0] | (18) $\bar{x}+1/4, z+3/4, y+1/4$ [0,0,0]             | (19) $\bar{x}+3/4, \bar{z}+3/4, \bar{y}+3/4$ [0,0,0] | (20) $x+1/4, \bar{z}+1/4, y+3/4$ [0,0,0]             |  |  |  |
| (21) $z+3/4, y+1/4, \bar{x}+1/4$ [0,0,0] | (22) $z+1/4, \bar{y}+1/4, x+3/4$ [0,0,0]             | (23) $\bar{z}+1/4, y+3/4, x+1/4$ [0,0,0]             | (24) $\bar{z}+3/4, \bar{y}+3/4, \bar{x}+3/4$ [0,0,0] |  |  |  |

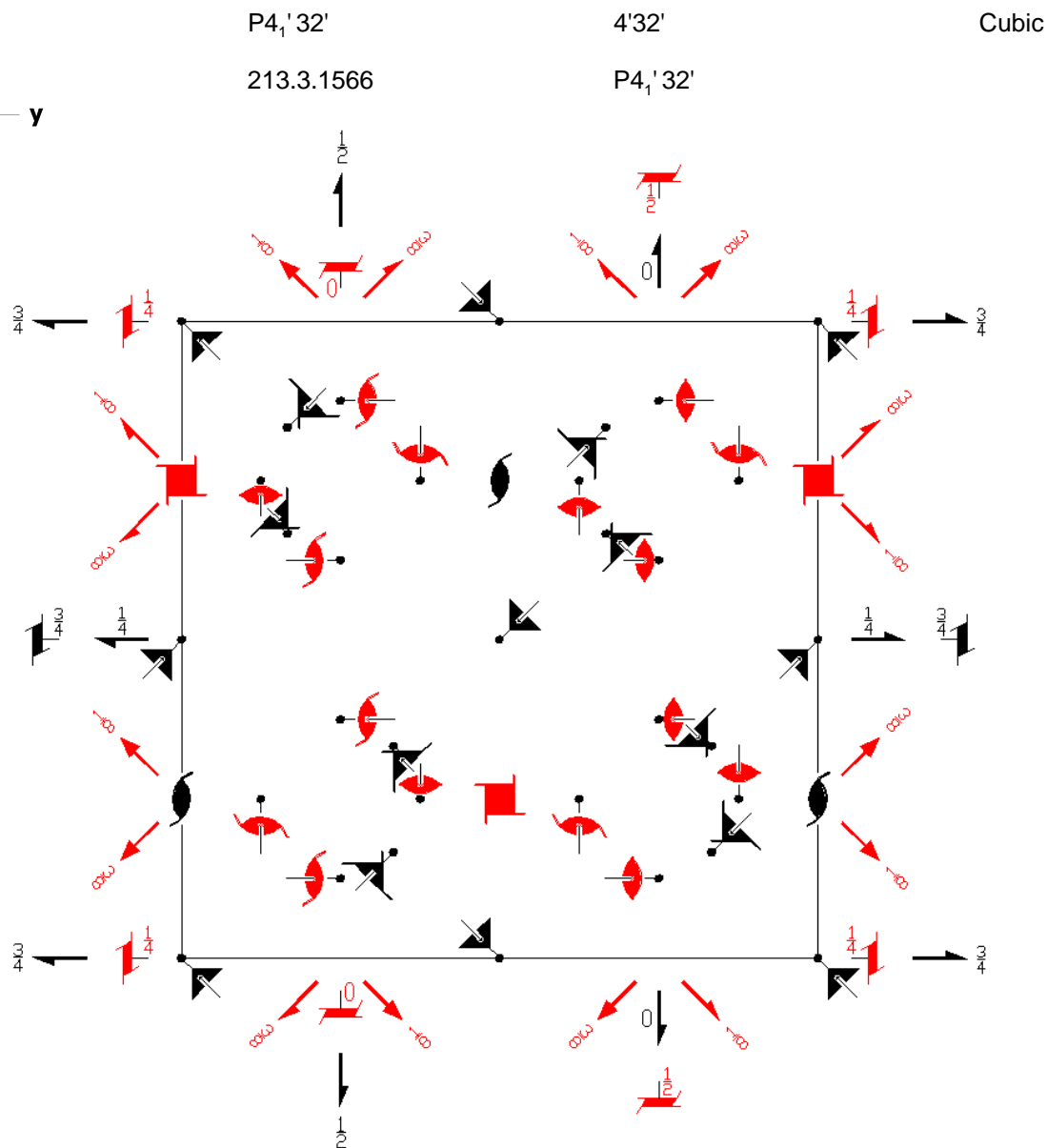
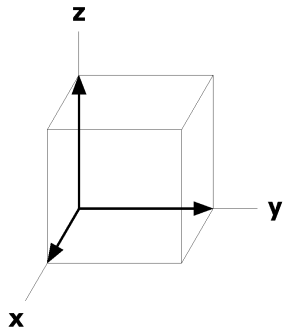
12	d	..21'	1/8,y,y+1/4 [0,0,0]	3/8, $\bar{y}$ ,y+3/4 [0,0,0]	7/8,y+1/2, $\bar{y}$ +1/4 [0,0,0]	5/8, $\bar{y}$ +1/2, $\bar{y}$ +3/4 [0,0,0]
			y+1/4,1/8,y [0,0,0]	y+3/4,3/8, $\bar{y}$ [0,0,0]	$\bar{y}$ +1/4,7/8,y+1/2 [0,0,0]	$\bar{y}$ +3/4,5/8, $\bar{y}$ +1/2 [0,0,0]
			y,y+1/4,1/8 [0,0,0]	$\bar{y}$ ,y+3/4,3/8 [0,0,0]	y+1/2, $\bar{y}$ +1/4,7/8 [0,0,0]	$\bar{y}$ +1/2, $\bar{y}$ +3/4,5/8 [0,0,0]
8	c	.3.1'	x,x,x [0,0,0]		$\bar{x}$ +1/2, $\bar{x}$ ,x+1/2 [0,0,0]	
			$\bar{x}$ ,x+1/2, $\bar{x}$ +1/2 [0,0,0]		x+1/2, $\bar{x}$ +1/2, $\bar{x}$ [0,0,0]	
			x+3/4,x+1/4, $\bar{x}$ +1/4 [0,0,0]		$\bar{x}$ +3/4, $\bar{x}$ +3/4, $\bar{x}$ +3/4 [0,0,0]	
			x+1/4, $\bar{x}$ +1/4,x+3/4 [0,0,0]		$\bar{x}$ +1/4,x+3/4,x+1/4 [0,0,0]	
4	b	.321'	7/8,7/8,7/8 [0,0,0]	5/8,1/8,3/8 [0,0,0]	1/8,3/8,5/8 [0,0,0]	3/8,5/8,1/8 [0,0,0]
4	a	.321'	3/8,3/8,3/8 [0,0,0]	1/8,5/8,7/8 [0,0,0]	5/8,7/8,1/8 [0,0,0]	7/8,1/8,5/8 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4gm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/4,0,z

Along [1,1,1] p3m11'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

Along [1,1,0] p2mg1'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = -(-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x+1/4,1/8



**Origin** on  $3 [111]$  at midpoint of three non-intersecting pairs of parallel screw axes  $4_1'$  and  $2_1$

**Asymmetric unit**  $-1/4 \leq x \leq 1/2; 0 \leq y \leq 3/4; 0 \leq z \leq 1/2; x \leq y \leq x+1/2;$

$(y-x)/2 \leq z \leq \min(y, (-4x-2y+3)/2, (3-2x-2y)/4)$

Vertices       $0,0,0$                $1/2,1/2,0$                $1/4,3/4,1/4$                $-1/4,1/4,1/4$                $0,1/2,1/2$                $3/8,3/8,3/8$

**Symmetry Operations**

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)  | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)  | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}+1/2, \bar{x}, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,1/2,0)              | (7) 3 <sup>+</sup> $x+1/2, \bar{x}-1/2, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,0,1/2)          | (8) 3 <sup>+</sup> $\bar{x}, \bar{x}+1/2, x$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,1/2,1/2)              |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> (-1/3,1/3,1/3) $\bar{x}$<br>$x+1/6, \bar{x}+1/6, \bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,1/2,1/2) | (11) 3 <sup>-</sup> (1/3,1/3,-1/3) $\bar{x}$<br>$x+1/3, \bar{x}+1/6, x$<br>(3 <sub><math>\bar{xyz}</math></sub>  1/2,1/2,0) | (12) 3 <sup>-</sup> (1/3,-1/3,1/3) $\bar{x}$<br>$\bar{x}-1/6, x+1/3, x$<br>(3 <sub><math>\bar{xyz}</math></sub>  1/2,0,1/2) |

(13) 2' (1/2,1/2,0) x,x-1/4,1/8 (2 <sub>xy</sub>  3/4,1/4,1/4)'	(14) 2' x, $\bar{x}$ +3/4,3/8 (2 <sub>xy</sub>  3/4,3/4,3/4)'	(15) 4' (0,0,3/4) 1/4,0,z (4 <sub>z</sub> <sup>-1</sup>  1/4,1/4,3/4)'	(16) 4 <sup>+</sup> (0,0,1/4) -1/4,1/2,z (4 <sub>z</sub>  1/4,3/4,1/4)'
(17) 4' (3/4,0,0) x,1/4,0 (4 <sub>x</sub> <sup>-1</sup>  3/4,1/4,1/4)'	(18) 2' (0,1/2,1/2) 1/8,y+1/4,y (2 <sub>yz</sub>  1/4,3/4,1/4)'	(19) 2' 3/8,y+3/4, $\bar{y}$ (2 <sub>yz</sub>  3/4,3/4,3/4)'	(20) 4 <sup>+</sup> (1/4,0,0) x,-1/4,1/2 (4 <sub>x</sub>  1/4,1/4,3/4)'
(21) 4 <sup>+</sup> (0,1/4,0) 1/2,y,-1/4 (4 <sub>y</sub>  3/4,1/4,1/4)'	(22) 2' (1/2,0,1/2) x-1/4,1/8,x (2 <sub>xz</sub>  1/4,1/4,3/4)'	(23) 4' (0,3/4,0) 0,y,1/4 (4 <sub>y</sub> <sup>-1</sup>  1/4,3/4,1/4)'	(24) 2' $\bar{x}$ +3/4,3/8,x (2 <sub>xz</sub>  3/4,3/4,3/4)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

24 e 1

(1) x,y,z [u,v,w]	(2) $\bar{x}$ +1/2, $\bar{y}$ ,z+1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(3) $\bar{x}$ ,y+1/2, $\bar{z}$ +1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x+1/2, $\bar{y}$ +1/2, $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]
(5) z,x,y [w,u,v]	(6) z+1/2, $\bar{x}$ +1/2, $\bar{y}$ [w, $\bar{u}$ , $\bar{v}$ ]	(7) $\bar{z}$ +1/2, $\bar{x}$ ,y+1/2 [ $\bar{w}$ , $\bar{u}$ ,v]	(8) $\bar{z}$ ,x+1/2, $\bar{y}$ +1/2 [ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ]
(9) y,z,x [v,w,u]	(10) $\bar{y}$ ,z+1/2, $\bar{x}$ +1/2 [ $\bar{v}$ ,w, $\bar{u}$ ]	(11) y+1/2, $\bar{z}$ +1/2, $\bar{x}$ [v, $\bar{w}$ , $\bar{u}$ ]	(12) $\bar{y}$ +1/2, $\bar{z}$ ,x+1/2 [ $\bar{v}$ , $\bar{w}$ ,u]
(13) y+3/4,x+1/4, $\bar{z}$ +1/4 [ $\bar{v}$ , $\bar{u}$ ,w]	(14) $\bar{y}$ +3/4, $\bar{x}$ +3/4, $\bar{z}$ +3/4 [v,u,w]	(15) y+1/4, $\bar{x}$ +1/4,z+3/4 [ $\bar{v}$ ,u, $\bar{w}$ ]	(16) $\bar{y}$ +1/4,x+3/4,z+1/4 [v, $\bar{u}$ , $\bar{w}$ ]
(17) x+3/4,z+1/4, $\bar{y}$ +1/4 [ $\bar{u}$ , $\bar{w}$ ,v]	(18) $\bar{x}$ +1/4,z+3/4,y+1/4 [u, $\bar{w}$ , $\bar{v}$ ]	(19) $\bar{x}$ +3/4, $\bar{z}$ +3/4, $\bar{y}$ +3/4 [u,w,v]	(20) x+1/4, $\bar{z}$ +1/4,y+3/4 [ $\bar{u}$ ,w, $\bar{v}$ ]
(21) z+3/4,y+1/4, $\bar{x}$ +1/4 [ $\bar{w}$ , $\bar{v}$ ,u]	(22) z+1/4, $\bar{y}$ +1/4,x+3/4 [ $\bar{w}$ ,v, $\bar{u}$ ]	(23) $\bar{z}$ +1/4,y+3/4,x+1/4 [w, $\bar{v}$ , $\bar{u}$ ]	(24) $\bar{z}$ +3/4, $\bar{y}$ +3/4, $\bar{x}$ +3/4 [w,v,u]

12 d ..2'	1/8,y,y+1/4 [u,v, $\bar{v}$ ]	3/8, $\bar{y}$ ,y+3/4 [ $\bar{u}$ , $\bar{v}$ , $\bar{v}$ ]	7/8,y+1/2, $\bar{y}$ +1/4 [ $\bar{u}$ ,v,v]	5/8, $\bar{y}$ +1/2, $\bar{y}$ +3/4 [u, $\bar{v}$ ,v]
	y+1/4,1/8,y [ $\bar{v}$ ,u,v]	y+3/4,3/8, $\bar{y}$ [ $\bar{v}$ , $\bar{u}$ , $\bar{v}$ ]	$\bar{y}$ +1/4,7/8,y+1/2 [v, $\bar{u}$ ,v]	$\bar{y}$ +3/4,5/8, $\bar{y}$ +1/2 [v,u, $\bar{v}$ ]
	y,y+1/4,1/8 [v, $\bar{v}$ ,u]	$\bar{y}$ ,y+3/4,3/8 [ $\bar{v}$ , $\bar{v}$ , $\bar{u}$ ]	y+1/2, $\bar{y}$ +1/4,7/8 [v,v, $\bar{u}$ ]	$\bar{y}$ +1/2, $\bar{y}$ +3/4,5/8 [ $\bar{v}$ ,v,u]

8 c .3.	x,x,x [u,u,u]	$\bar{x}$ +1/2, $\bar{x}$ ,x+1/2 [ $\bar{u}$ , $\bar{u}$ ,u]	$\bar{x}$ +1/2, $\bar{x}$ ,x+1/2 [u, $\bar{u}$ , $\bar{u}$ ]
	$\bar{x}$ ,x+1/2, $\bar{x}$ +1/2 [ $\bar{u}$ ,u, $\bar{u}$ ]	x+1/2, $\bar{x}$ +1/2, $\bar{x}$ [u, $\bar{u}$ , $\bar{u}$ ]	
	x+3/4,x+1/4, $\bar{x}$ +1/4 [ $\bar{u}$ , $\bar{u}$ ,u]	$\bar{x}$ +3/4, $\bar{x}$ +3/4, $\bar{x}$ +3/4 [u,u,u]	
	x+1/4, $\bar{x}$ +1/4,x+3/4 [ $\bar{u}$ ,u, $\bar{u}$ ]	$\bar{x}$ +1/4,x+3/4,x+1/4 [u, $\bar{u}$ , $\bar{u}$ ]	

4 b .32'	7/8,7/8,7/8 [u,u,u]	5/8,1/8,3/8 [ $\bar{u}$ , $\bar{u}$ ,u]	1/8,3/8,5/8 [ $\bar{u}$ ,u, $\bar{u}$ ]	3/8,5/8,1/8 [u, $\bar{u}$ , $\bar{u}$ ]
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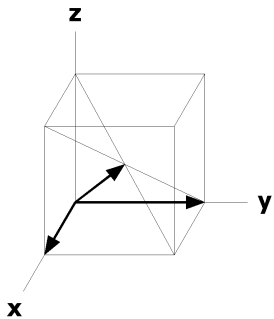
4 a .32'	3/8,3/8,3/8 [u,u,u]	1/8,5/8,7/8 [ $\bar{u}$ , $\bar{u}$ ,u]	5/8,7/8,1/8 [ $\bar{u}$ ,u, $\bar{u}$ ]	7/8,1/8,5/8 [u, $\bar{u}$ , $\bar{u}$ ]
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### Symmetry of Special Projections

Along [0,0,1] p4'g'm  
a\* = a b\* = b  
Origin at 1/4,0,z

Along [1,1,1] p3m1  
a\* = (2a - b - c)/3 b\* = (-a + 2b - c)/3  
Origin at x,x,x

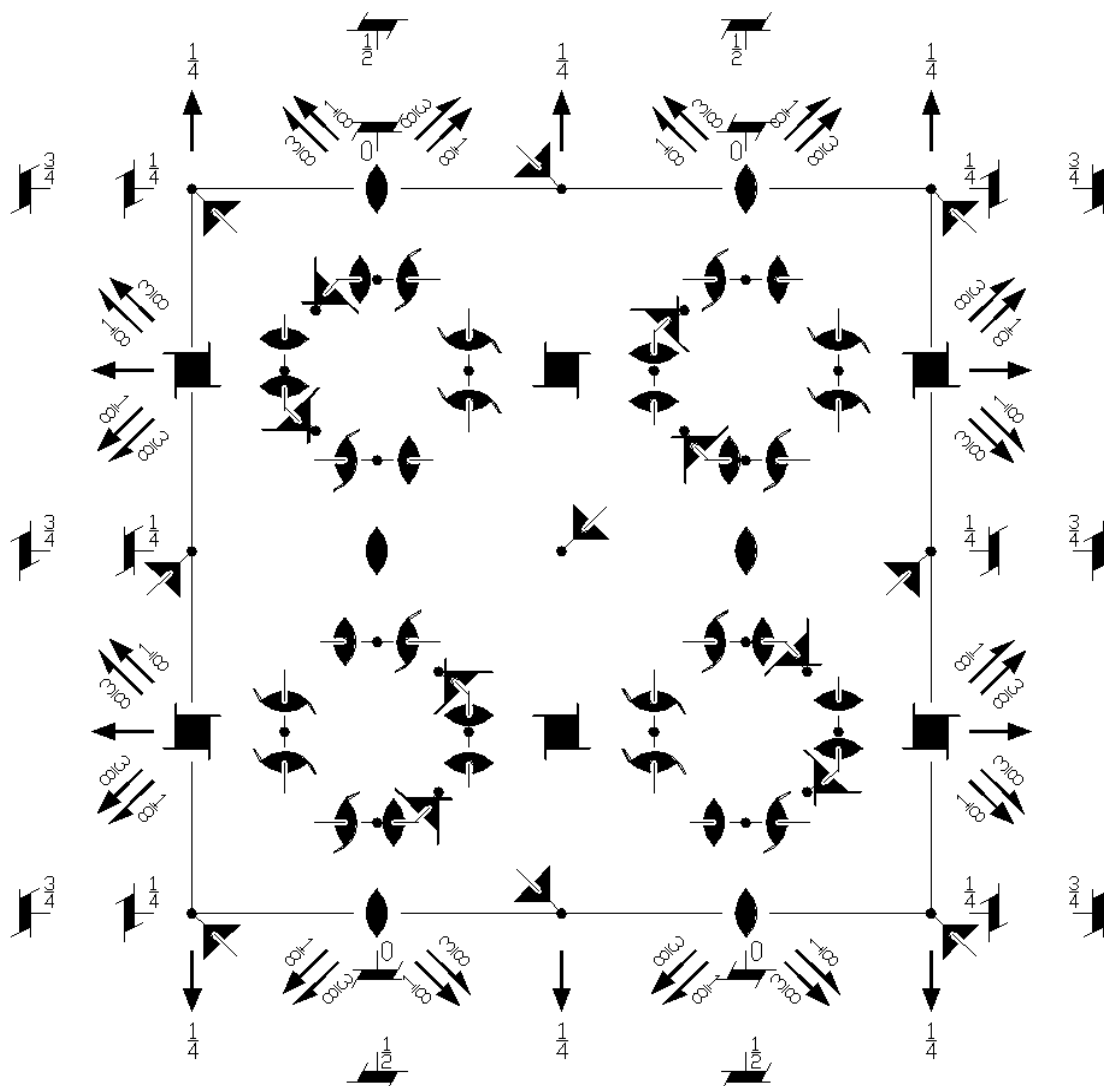
Along [1,1,0] p2'mg'  
a\* = c b\* = -(-a + b)/2  
Origin at x,x+1/4,1/8



$I4_1 32$   
214.1.1567

432  
 $I4_1 32$

Cubic



**Origin** on 3  $[111]$  at midpoint of three non-intersecting pairs of parallel screw axes  $4_1$  and  $4_3$  and of three non-intersection pairs of parallel 2 axes.

**Asymmetric unit**  $-3/8 \leq x \leq 1/8$ ;  $-1/8 \leq y \leq 1/8$ ;  $1/8 \leq z \leq 3/8$ ;  $\max(x, y, y - x - 1/8) \leq z \leq y + 1/4$

Vertices  $1/8, 1/8, 1/8$   $1/8, 1/8, 3/8$   $1/8, -1/8, 1/8$   $-1/8, 1/8, 1/8$   $-1/8, -1/8, -1/8$   $-3/8, 1/8, 3/8$   $-3/8, -1/8, 1/8$

### Symmetry Operations

For  $(0,0,0) +$  set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                                    | (2) 2 (0,0,1/2) $1/4, 0, z$<br>( $2_z$   $1/2, 0, 1/2$ )  | (3) 2 (0,1/2,0) $0, y, 1/4$<br>( $2_y$   $0, 1/2, 1/2$ )  | (4) 2 (1/2,0,0) $x, 1/4, 0$<br>( $2_x$   $1/2, 1/2, 0$ )  |
| (5) $3^+$ $x, x, x$<br>( $3_{xyz}$   $0, 0, 0$ )      | (6) $3^+$ $\bar{x} + 1/2, x, \bar{x}$<br>( $3_{\bar{xyz}^{-1}}$   $1/2, 1/2, 0$ )                         | (7) $3^+$ $x + 1/2, \bar{x} - 1/2, \bar{x}$<br>( $3_{\bar{xyz}^{-1}}$   $1/2, 0, 1/2$ )                   | (8) $3^+$ $\bar{x}, \bar{x} + 1/2, x$<br>( $3_{\bar{xyz}^{-1}}$   $0, 1/2, 1/2$ )                         |
| (9) $3^-$ $x, x, x$<br>( $3_{xyz^{-1}}$   $0, 0, 0$ ) | (10) $3^-$ $(-1/3, 1/3, 1/3)$<br>$x + 1/6, \bar{x} + 1/6, \bar{x}$<br>( $3_{\bar{xyz}}$   $0, 1/2, 1/2$ ) | (11) $3^-$ $(1/3, 1/3, -1/3)$<br>$\bar{x} + 1/3, \bar{x} + 1/6, x$<br>( $3_{\bar{xyz}}$   $1/2, 1/2, 0$ ) | (12) $3^-$ $(1/3, -1/3, 1/3)$<br>$\bar{x} - 1/6, x + 1/3, \bar{x}$<br>( $3_{\bar{xyz}}$   $1/2, 0, 1/2$ ) |

- |  |  |  |  |
|--|--|--|--|
| (13) $2 (1/2, 1/2, 0) \quad x, x-1/4, 1/8$<br>( $2_{xy}   3/4, 1/4, 1/4$ ) | (14) $2 \quad x, \bar{x}+3/4, 3/8$<br>( $2_{\bar{xy}}   3/4, 3/4, 3/4$ )   | (15) $4^- (0, 0, 3/4) \quad 1/4, 0, z$<br>( $4_z^-   1/4, 1/4, 3/4$ )    | (16) $4^+ (0, 0, 1/4) \quad -1/4, 1/2, z$<br>( $4_z   1/4, 3/4, 1/4$ )   |
| (17) $4^- (3/4, 0, 0) \quad x, 1/4, 0$<br>( $4_x^-   3/4, 1/4, 1/4$ )      | (18) $2 (0, 1/2, 1/2) \quad 1/8, y+1/4, y$<br>( $2_{yz}   1/4, 3/4, 1/4$ ) | (19) $2 \quad 3/8, y+3/4, \bar{y}$<br>( $2_{\bar{yz}}   3/4, 3/4, 3/4$ ) | (20) $4^+ (1/4, 0, 0) \quad x, -1/4, 1/2$<br>( $4_x   1/4, 1/4, 3/4$ )   |
| (21) $4^+ (0, 1/4, 0) \quad 1/2, y, -1/4$<br>( $4_y   3/4, 1/4, 1/4$ )     | (22) $2 (1/2, 0, 1/2) \quad x-1/4, 1/8, x$<br>( $2_{xz}   1/4, 1/4, 3/4$ ) | (23) $4^- (0, 3/4, 0) \quad 0, y, 1/4$<br>( $4_y^-   1/4, 3/4, 1/4$ )    | (24) $2 \quad \bar{x}+3/4, 3/8, x$<br>( $2_{\bar{xz}}   3/4, 3/4, 3/4$ ) |

For (1/2, 1/2, 1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) $t (1/2, 1/2, 1/2)$<br>( $1   1/2, 1/2, 1/2$ )                         | (2) $2 \quad 0, 1/4, z$<br>( $2_z   0, 1/2, 0$ )   | (3) $2 \quad 1/4, y, 0$<br>( $2_y   1/2, 0, 0$ )   | (4) $2 \quad x, 0, 1/4$<br>( $2_x   0, 0, 1/2$ )   |
| (5) $3^+ (1/2, 1/2, 1/2) \quad x, x, x$<br>( $3_{xyz}   1/2, 1/2, 1/2$ )   | (6) $3^+ (1/6, -1/6, 1/6)$<br>$\quad \bar{x}-1/6, x+1/3, \bar{x}$<br>( $3_{\bar{xyz}}^-   0, 0, 1/2$ ) | (7) $3^+ (-1/6, 1/6, 1/6)$<br>$\quad x+1/6, \bar{x}+1/6, \bar{x}$<br>( $3_{xyz}^-   0, 1/2, 0$ ) | (8) $3^+ (1/6, 1/6, -1/6)$<br>$\quad \bar{x}+1/3, \bar{x}+1/6, x$<br>( $3_{\bar{xyz}}^-   1/2, 0, 0$ ) |
| (9) $3^- (1/2, 1/2, 1/2) \quad x, x, x$<br>( $3_{xyz}^-   1/2, 1/2, 1/2$ ) | (10) $3^- (1/6, -1/6, -1/6)$<br>$\quad x+1/6, \bar{x}+1/6, \bar{x}$<br>( $3_{\bar{xyz}}   1/2, 0, 0$ ) | (11) $3^- (-1/6, -1/6, 1/6)$<br>$\quad \bar{x}+1/3, \bar{x}+1/6, x$<br>( $3_{xyz}   0, 0, 1/2$ ) | (12) $3^- (-1/6, 1/6, -1/6)$<br>$\quad \bar{x}-1/6, x+1/3, \bar{x}$<br>( $3_{\bar{xyz}}   0, 1/2, 0$ ) |
| (13) $2 (1/2, 1/2, 0) \quad x, x+1/4, 3/8$<br>( $2_{xy}   1/4, 3/4, 3/4$ ) | (14) $2 \quad x, \bar{x}+1/4, 1/8$<br>( $2_{\bar{xy}}   1/4, 1/4, 1/4$ )                               | (15) $4^- (0, 0, 1/4) \quad 3/4, 0, z$<br>( $4_z^-   3/4, 3/4, 1/4$ )                            | (16) $4^+ (0, 0, 3/4) \quad 1/4, 1/2, z$<br>( $4_z   3/4, 1/4, 3/4$ )                                  |
| (17) $4^- (1/4, 0, 0) \quad x, 3/4, 0$<br>( $4_x^-   1/4, 3/4, 3/4$ )      | (18) $2 (0, 1/2, 1/2) \quad 3/8, y-1/4, y$<br>( $2_{yz}   3/4, 1/4, 3/4$ )                             | (19) $2 \quad 1/8, y+1/4, \bar{y}$<br>( $2_{\bar{yz}}   1/4, 1/4, 1/4$ )                         | (20) $4^+ (3/4, 0, 0) \quad x, 1/4, 1/2$<br>( $4_x   3/4, 3/4, 1/4$ )                                  |
| (21) $4^+ (0, 3/4, 0) \quad 1/2, y, 1/4$<br>( $4_y   1/4, 3/4, 3/4$ )      | (22) $2 (1/2, 0, 1/2) \quad x+1/4, 3/8, x$<br>( $2_{xz}   3/4, 3/4, 1/4$ )                             | (23) $4^- (0, 1/4, 0) \quad 0, y, 3/4$<br>( $4_y^-   3/4, 1/4, 3/4$ )                            | (24) $2 \quad \bar{x}+1/4, 1/8, x$<br>( $2_{\bar{xz}}   1/4, 1/4, 1/4$ )                               |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).**Positions**Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (1/2,1/2,1/2) +

48 i 1

- |  |  |  |  |
|--|--|--|--|
| (1) $x, y, z [u, v, w]$                          | (2) $\bar{x}+1/2, \bar{y}, z+1/2 [\bar{u}, \bar{v}, w]$                  | (3) $\bar{x}, y+1/2, \bar{z}+1/2 [\bar{u}, v, \bar{w}]$                  | (4) $x+1/2, \bar{y}+1/2, \bar{z} [u, \bar{v}, \bar{w}]$                  |
| (5) $z, x, y [w, u, v]$                          | (6) $z+1/2, \bar{x}+1/2, \bar{y} [w, \bar{u}, \bar{v}]$                  | (7) $\bar{z}+1/2, \bar{x}, y+1/2 [\bar{w}, \bar{u}, v]$                  | (8) $\bar{z}, x+1/2, \bar{y}+1/2 [\bar{w}, u, \bar{v}]$                  |
| (9) $y, z, x [v, w, u]$                          | (10) $\bar{y}, z+1/2, \bar{x}+1/2 [\bar{v}, w, \bar{u}]$                 | (11) $y+1/2, \bar{z}+1/2, \bar{x} [v, \bar{w}, \bar{u}]$                 | (12) $\bar{y}+1/2, \bar{z}, x+1/2 [\bar{v}, \bar{w}, u]$                 |
| (13) $y+3/4, x+1/4, \bar{z}+1/4 [v, u, \bar{w}]$ | (14) $\bar{y}+3/4, \bar{x}+3/4, \bar{z}+3/4 [\bar{v}, \bar{u}, \bar{w}]$ | (15) $y+1/4, \bar{x}+1/4, z+3/4 [v, \bar{u}, w]$                         | (16) $\bar{y}+1/4, x+3/4, z+1/4 [\bar{v}, u, w]$                         |
| (17) $x+3/4, z+1/4, \bar{y}+1/4 [u, w, \bar{v}]$ | (18) $\bar{x}+1/4, z+3/4, y+1/4 [\bar{u}, w, v]$                         | (19) $\bar{x}+3/4, \bar{z}+3/4, \bar{y}+3/4 [\bar{u}, \bar{w}, \bar{v}]$ | (20) $x+1/4, \bar{z}+1/4, y+3/4 [u, \bar{w}, v]$                         |
| (21) $z+3/4, y+1/4, \bar{x}+1/4 [w, v, \bar{u}]$ | (22) $z+1/4, \bar{y}+1/4, x+3/4 [w, \bar{v}, u]$                         | (23) $\bar{z}+1/4, y+3/4, x+1/4 [\bar{w}, v, u]$                         | (24) $\bar{z}+3/4, \bar{y}+3/4, \bar{x}+3/4 [\bar{w}, \bar{v}, \bar{u}]$ |

24	h	..2	1/8,y, $\bar{y}$ +1/4 [0, $\bar{v}$ ,v] $\bar{y}$ +1/4,1/8,y [v,0, $\bar{v}$ ] y, $\bar{y}$ +1/4,1/8 [ $\bar{v}$ ,v,0]	3/8, $\bar{y}$ , $\bar{y}$ +3/4 [0,v,v] $\bar{y}$ +3/4,3/8, $\bar{y}$ [v,0,v] $\bar{y}$ , $\bar{y}$ +3/4,3/8 [v,v,0]	7/8,y+1/2,y+1/4 [ $\bar{v}$ , $\bar{v}$ ,0] y+1/4,7/8,y+1/2 [ $\bar{v}$ ,0, $\bar{v}$ ] y+1/2,y+1/4,7/8 [ $\bar{v}$ , $\bar{v}$ ,0]	5/8, $\bar{y}$ +1/2,y+3/4 [0,v, $\bar{v}$ ] y+3/4,5/8, $\bar{y}$ +1/2 [ $\bar{v}$ ,0,v] $\bar{y}$ +1/2,y+3/4,5/8 [v, $\bar{v}$ ,0]
24	g	..2	1/8,y,y+1/4 [0,v,v] y+1/4,1/8,y [v,0,v] y,y+1/4,1/8 [v,v,0]	3/8, $\bar{y}$ ,y+3/4 [0, $\bar{v}$ ,v] y+3/4,3/8, $\bar{y}$ [v,0, $\bar{v}$ ] $\bar{y}$ ,y+3/4,3/8 [ $\bar{v}$ ,v,0]	7/8,y+1/2, $\bar{y}$ +1/4 [0,v, $\bar{v}$ ] $\bar{y}$ +1/4,7/8,y+1/2 [ $\bar{v}$ ,0,v] y+1/2, $\bar{y}$ +1/4,7/8 [v, $\bar{v}$ ,0]	5/8, $\bar{y}$ +1/2, $\bar{y}$ +3/4 [0, $\bar{v}$ , $\bar{v}$ ] $\bar{y}$ +3/4,5/8, $\bar{y}$ +1/2 [ $\bar{v}$ ,0, $\bar{v}$ ] $\bar{y}$ +1/2, $\bar{y}$ +3/4,5/8 [ $\bar{v}$ , $\bar{v}$ ,0]
24	f	2..	x,0,1/4 [u,0,0] 0,1/4,x [0,0,u] x+3/4,1/2,1/4 [u,0,0]	$\bar{x}$ +1/2,0,3/4 [ $\bar{u}$ ,0,0] 0,3/4, $\bar{x}$ +1/2 [0,0, $\bar{u}$ ] $\bar{x}$ +1/4,0,1/4 [ $\bar{u}$ ,0,0]	1/4,x,0 [0,u,0] 3/4,x+1/4,0 [0,u,0] 0,1/4, $\bar{x}$ +1/4 [0,0, $\bar{u}$ ]	3/4, $\bar{x}$ +1/2,0 [0, $\bar{u}$ ,0] 3/4, $\bar{x}$ +3/4,1/2 [0, $\bar{u}$ ,0] 1/2,1/4,x+3/4 [0,0,u]
16	e	.3.	x,x,x [u,u,u] $\bar{x}$ ,x+1/2, $\bar{x}$ +1/2 [ $\bar{u}$ ,u, $\bar{u}$ ] x+3/4,x+1/4, $\bar{x}$ +1/4 [u,u, $\bar{u}$ ] x+1/4, $\bar{x}$ +1/4,x+3/4 [u, $\bar{u}$ ,u]	$\bar{x}$ +1/2, $\bar{x}$ ,x+1/2 [ $\bar{u}$ , $\bar{u}$ ,u] x+1/2, $\bar{x}$ +1/2, $\bar{x}$ [u, $\bar{u}$ , $\bar{u}$ ] $\bar{x}$ +3/4, $\bar{x}$ +3/4, $\bar{x}$ +3/4 [ $\bar{u}$ , $\bar{u}$ , $\bar{u}$ ] $\bar{x}$ +1/4,x+3/4,x+1/4 [ $\bar{u}$ ,u,u]		
12	d	2.22	5/8,0,1/4 [0,0,0] 3/4,7/8,0 [0,0,0]	7/8,0,3/4 [0,0,0] 0,1/4,5/8 [0,0,0]	1/4,5/8,0 [0,0,0] 0,3/4,7/8 [0,0,0]	
12	c	2.22	1/8,0,1/4 [0,0,0] 3/4,3/8,0 [0,0,0]	3/8,0,3/4 [0,0,0] 0,1/4,1/8 [0,0,0]	1/4,1/8,0 [0,0,0] 0,3/4,3/8 [0,0,0]	
8	b	.32	7/8,7/8,7/8 [0,0,0]	5/8,1/8,3/8 [0,0,0]	1/8,3/8,5/8 [0,0,0]	3/8,5/8,1/8 [0,0,0]
8	a	.32	1/8,1/8,1/8 [0,0,0]	3/8,7/8,5/8 [0,0,0]	7/8,5/8,3/8 [0,0,0]	5/8,3/8,7/8 [0,0,0]

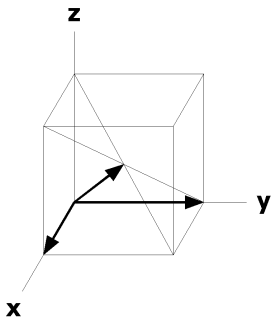
### Symmetry of Special Projections

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,0,z

Along [1,1,1] p3m'1  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x+1/4,1/8





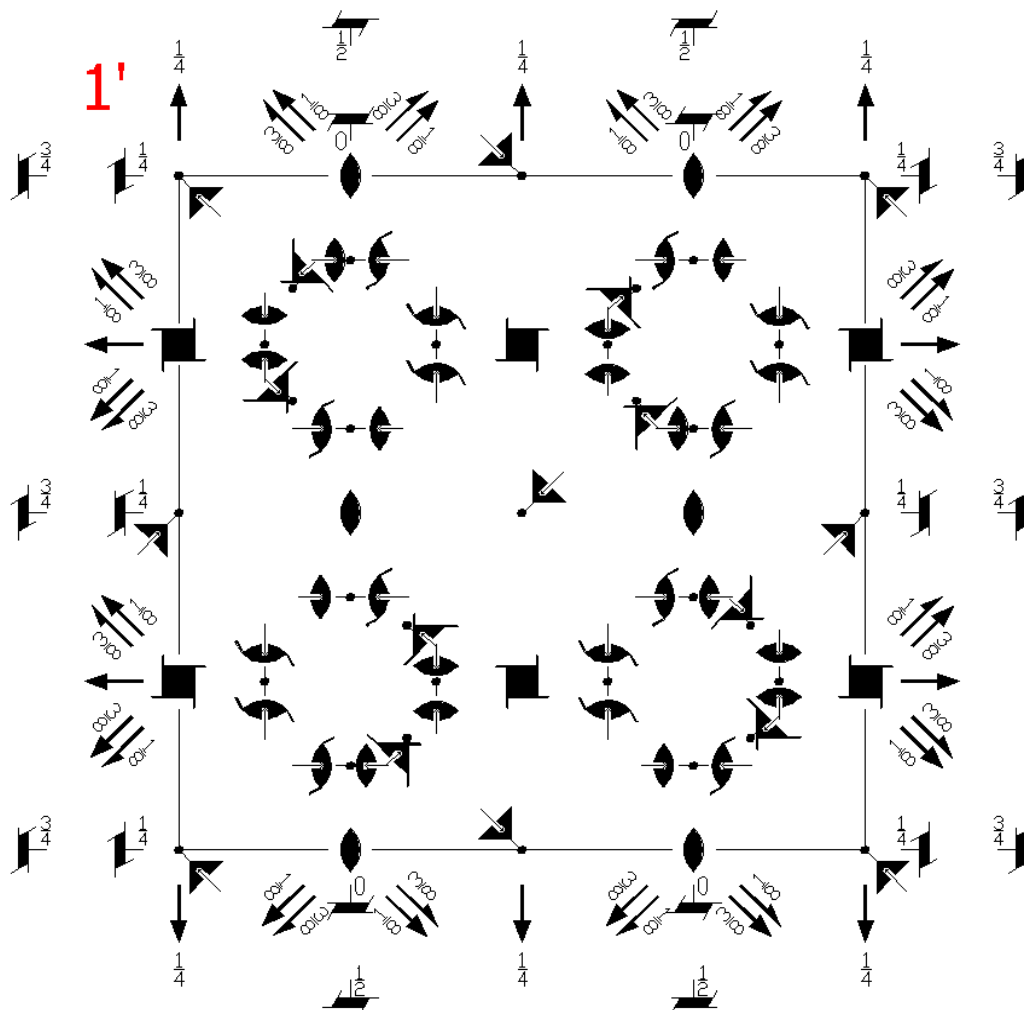
$I4_1 321'$

$4321'$

Cubic

214.2.1568

$I4_1 321'$



**Origin** on  $31'$   $[111]$  at midpoint of three non-intersecting pairs of parallel screw axes  $4_1 1'$  and  $4_3 1'$  and of three non-intersection pairs of parallel 2 axes.

**Asymmetric unit**  $-3/8 \leq x \leq 1/8$ ;  $-1/8 \leq y \leq 1/8$ ;  $1/8 \leq z \leq 3/8$ ;  $\max(x, y, y - x - 1/8) \leq z \leq y + 1/4$

**Vertices**  $1/8, 1/8, 1/8$   $1/8, 1/8, 3/8$   $1/8, -1/8, 1/8$   $-1/8, 1/8, 1/8$   $-1/8, -1/8, -1/8$   $-3/8, 1/8, 3/8$   $-3/8, -1/8, 1/8$

### Symmetry Operations

For  $(0,0,0)$  + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 (0,0,1/2) $1/4, 0, z$<br>( $2_z$  1/2,0,1/2)  | (3) 2 (0,1/2,0) $0, y, 1/4$<br>( $2_y$  0,1/2,1/2)  | (4) 2 (1/2,0,0) $x, 1/4, 0$<br>( $2_x$  1/2,1/2,0)  |
| (5) $3^+$ $x, x, x$<br>( $3_{xyz}$  0,0,0)    | (6) $3^+$ $\bar{x} + 1/2, x, \bar{x}$<br>( $3_{\bar{xyz}}$  -1/2,1/2,0)                             | (7) $3^+$ $x + 1/2, \bar{x} - 1/2, \bar{x}$<br>( $3_{\bar{xyz}}$  -1/2,0,1/2)                 | (8) $3^+$ $\bar{x}, \bar{x} + 1/2, x$<br>( $3_{\bar{xyz}}$  -1/2,1/2,1/2)                           |
| (9) $3^-$ $x, x, x$<br>( $3_{xyz}$  -1/2,0,0) | (10) $3^-$ $(-1/3, 1/3, 1/3)$<br>$x + 1/6, \bar{x} + 1/6, \bar{x}$<br>( $3_{\bar{xyz}}$  0,1/2,1/2) | (11) $3^-$ $(1/3, 1/3, -1/3)$<br>$\bar{x} + 1/3, \bar{x} + 1/6, x$<br>( $3_{xyz}$  1/2,1/2,0) | (12) $3^-$ $(1/3, -1/3, 1/3)$<br>$\bar{x} - 1/6, x + 1/3, \bar{x}$<br>( $3_{\bar{xyz}}$  1/2,0,1/2) |

- |  |  |  |  |
|--|--|--|--|
| (13) $2 (1/2, 1/2, 0) \quad x, x-1/4, 1/8$<br>( $2_{xy}   3/4, 1/4, 1/4$ ) | (14) $2 \quad x, \bar{x}+3/4, 3/8$<br>( $2_{\bar{xy}}   3/4, 3/4, 3/4$ )   | (15) $4^- (0, 0, 3/4) \quad 1/4, 0, z$<br>( $4_{z^-}   1/4, 1/4, 3/4$ )  | (16) $4^+ (0, 0, 1/4) \quad -1/4, 1/2, z$<br>( $4_z   1/4, 3/4, 1/4$ )   |
| (17) $4^- (3/4, 0, 0) \quad x, 1/4, 0$<br>( $4_x^-   3/4, 1/4, 1/4$ )      | (18) $2 (0, 1/2, 1/2) \quad 1/8, y+1/4, y$<br>( $2_{yz}   1/4, 3/4, 1/4$ ) | (19) $2 \quad 3/8, y+3/4, \bar{y}$<br>( $2_{\bar{yz}}   3/4, 3/4, 3/4$ ) | (20) $4^+ (1/4, 0, 0) \quad x, -1/4, 1/2$<br>( $4_x   1/4, 1/4, 3/4$ )   |
| (21) $4^+ (0, 1/4, 0) \quad 1/2, y, -1/4$<br>( $4_y   3/4, 1/4, 1/4$ )     | (22) $2 (1/2, 0, 1/2) \quad x-1/4, 1/8, x$<br>( $2_{xz}   1/4, 1/4, 3/4$ ) | (23) $4^- (0, 3/4, 0) \quad 0, y, 1/4$<br>( $4_y^-   1/4, 3/4, 1/4$ )    | (24) $2 \quad \bar{x}+3/4, 3/8, x$<br>( $2_{\bar{xz}}   3/4, 3/4, 3/4$ ) |

For (1/2, 1/2, 1/2) + set

- |  |  |   |   |
|--|--|---|---|
| (1) $t (1/2, 1/2, 1/2)$<br>( $1   1/2, 1/2, 1/2$ )                         | (2) $2 \quad 0, 1/4, z$<br>( $2_z   0, 1/2, 0$ )   | (3) $2 \quad 1/4, y, 0$<br>( $2_y   1/2, 0, 0$ )  | (4) $2 \quad x, 0, 1/4$<br>( $2_x   0, 0, 1/2$ )  |
| (5) $3^+ (1/2, 1/2, 1/2) \quad x, x, x$<br>( $3_{xyz}   1/2, 1/2, 1/2$ )   | (6) $3^+ (1/6, -1/6, 1/6)$<br>$\quad \bar{x}-1/6, x+1/3, \bar{x}$<br>( $3_{\bar{xyz}}^-   0, 0, 1/2$ ) | (7) $3^+ (-1/6, 1/6, 1/6)$<br>$\quad x+1/6, \bar{x}+1/6, \bar{x}$<br>( $3_{xyz}^-   0, 1/2, 0$ )      | (8) $3^+ (1/6, 1/6, -1/6)$<br>$\quad \bar{x}+1/3, \bar{x}+1/6, x$<br>( $3_{\bar{yz}}^-   1/2, 0, 0$ ) |
| (9) $3^- (1/2, 1/2, 1/2) \quad x, x, x$<br>( $3_{xyz}^-   1/2, 1/2, 1/2$ ) | (10) $3^- (1/6, -1/6, -1/6)$<br>$\quad x+1/6, \bar{x}+1/6, \bar{x}$<br>( $3_{\bar{xyz}}   1/2, 0, 0$ ) | (11) $3^- (-1/6, -1/6, 1/6)$<br>$\quad \bar{x}+1/3, \bar{x}+1/6, x$<br>( $3_{\bar{yz}}   0, 0, 1/2$ ) | (12) $3^- (-1/6, 1/6, -1/6)$<br>$\quad \bar{x}-1/6, x+1/3, \bar{x}$<br>( $3_{\bar{yz}}   0, 1/2, 0$ ) |
| (13) $2 (1/2, 1/2, 0) \quad x, x+1/4, 3/8$<br>( $2_{xy}   1/4, 3/4, 3/4$ ) | (14) $2 \quad x, \bar{x}+1/4, 1/8$<br>( $2_{\bar{xy}}   1/4, 1/4, 1/4$ )                               | (15) $4^- (0, 0, 1/4) \quad 3/4, 0, z$<br>( $4_{z^-}   3/4, 3/4, 1/4$ )                               | (16) $4^+ (0, 0, 3/4) \quad 1/4, 1/2, z$<br>( $4_z   3/4, 1/4, 3/4$ )                                 |
| (17) $4^- (1/4, 0, 0) \quad x, 3/4, 0$<br>( $4_x^-   1/4, 3/4, 3/4$ )      | (18) $2 (0, 1/2, 1/2) \quad 3/8, y-1/4, y$<br>( $2_{yz}   3/4, 1/4, 3/4$ )                             | (19) $2 \quad 1/8, y+1/4, \bar{y}$<br>( $2_{\bar{yz}}   1/4, 1/4, 1/4$ )                              | (20) $4^+ (3/4, 0, 0) \quad x, 1/4, 1/2$<br>( $4_x   3/4, 3/4, 1/4$ )                                 |
| (21) $4^+ (0, 3/4, 0) \quad 1/2, y, 1/4$<br>( $4_y   1/4, 3/4, 3/4$ )      | (22) $2 (1/2, 0, 1/2) \quad x+1/4, 3/8, x$<br>( $2_{xz}   3/4, 3/4, 1/4$ )                             | (23) $4^- (0, 1/4, 0) \quad 0, y, 3/4$<br>( $4_y^-   3/4, 1/4, 3/4$ )                                 | (24) $2 \quad \bar{x}+1/4, 1/8, x$<br>( $2_{\bar{xz}}   1/4, 1/4, 1/4$ )                              |

For (0, 0, 0)' + set

- |  |   |  |  |
|--|---|--|--|
| (1) $1'$<br>( $1   0, 0, 0$ )'   | (2) $2' (0, 0, 1/2) \quad 1/4, 0, z$<br>( $2_z   1/2, 0, 1/2$ )'  | (3) $2' (0, 1/2, 0) \quad 0, y, 1/4$<br>( $2_y   0, 1/2, 1/2$ )'   | (4) $2' (1/2, 0, 0) \quad x, 1/4, 0$<br>( $2_x   1/2, 1/2, 0$ )'   |
| (5) $3^{+'} \quad x, x, x$<br>( $3_{xyz}   0, 0, 0$ )'                       | (6) $3^{+'} \quad \bar{x}+1/2, x, \bar{x}$<br>( $3_{\bar{xyz}}^-   1/2, 1/2, 0$ )'                                | (7) $3^{+'} \quad x+1/2, \bar{x}-1/2, \bar{x}$<br>( $3_{xyz}^-   1/2, 0, 1/2$ )'                                 | (8) $3^{+'} \quad \bar{x}, \bar{x}+1/2, x$<br>( $3_{\bar{yz}}^-   0, 1/2, 1/2$ )'                                |
| (9) $3^{-'} \quad x, x, x$<br>( $3_{xyz}^-   0, 0, 0$ )'                     | (10) $3^{-'} \quad (-1/3, 1/3, 1/3)$<br>$\quad x+1/6, \bar{x}+1/6, \bar{x}$<br>( $3_{\bar{xyz}}   0, 1/2, 1/2$ )' | (11) $3^{-'} \quad (1/3, 1/3, -1/3)$<br>$\quad \bar{x}+1/3, \bar{x}+1/6, x$<br>( $3_{\bar{yz}}   1/2, 1/2, 0$ )' | (12) $3^{-'} \quad (1/3, -1/3, 1/3)$<br>$\quad \bar{x}-1/6, x+1/3, \bar{x}$<br>( $3_{\bar{yz}}   1/2, 0, 1/2$ )' |
| (13) $2' (1/2, 1/2, 0) \quad x, x-1/4, 1/8$<br>( $2_{xy}   3/4, 1/4, 1/4$ )' | (14) $2' \quad x, \bar{x}+3/4, 3/8$<br>( $2_{\bar{xy}}   3/4, 3/4, 3/4$ )'  | (15) $4^{-'} (0, 0, 3/4) \quad 1/4, 0, z$<br>( $4_{z^-}   1/4, 1/4, 3/4$ )'                                      | (16) $4^{+'} (0, 0, 1/4) \quad -1/4, 1/2, z$<br>( $4_z   1/4, 3/4, 1/4$ )'                                       |
| (17) $4^{-'} (3/4, 0, 0) \quad x, 1/4, 0$<br>( $4_x^-   3/4, 1/4, 1/4$ )'    | (18) $2' (0, 1/2, 1/2) \quad 1/8, y+1/4, y$<br>( $2_{yz}   1/4, 3/4, 1/4$ )'                                      | (19) $2' \quad 3/8, y+3/4, \bar{y}$<br>( $2_{\bar{yz}}   3/4, 3/4, 3/4$ )'                                       | (20) $4^{+'} (1/4, 0, 0) \quad x, -1/4, 1/2$<br>( $4_x   1/4, 1/4, 3/4$ )'                                       |
| (21) $4^{+'} (0, 1/4, 0) \quad 1/2, y, -1/4$<br>( $4_y   3/4, 1/4, 1/4$ )'   | (22) $2' (1/2, 0, 1/2) \quad x-1/4, 1/8, x$<br>( $2_{xz}   1/4, 1/4, 3/4$ )'                                      | (23) $4^{-'} (0, 3/4, 0) \quad 0, y, 1/4$<br>( $4_y^-   1/4, 3/4, 1/4$ )'  | (24) $2' \quad \bar{x}+3/4, 3/8, x$<br>( $2_{\bar{xz}}   3/4, 3/4, 3/4$ )'                                       |

For (1/2,1/2,1/2)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) t' (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)'   | (2) 2' 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,0)'   | (3) 2' 1/4,y,0<br>(2 <sub>y</sub>  1/2,0,0)'   | (4) 2' x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)'   |
| (5) 3 <sup>+</sup> ' (1/2,1/2,1/2) x,x,x<br>(3 <sub>xyz</sub>  1/2,1/2,1/2)'               | (6) 3 <sup>+</sup> ' (1/6,-1/6,1/6)<br>x-1/6,x+1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,1/2)' | (7) 3 <sup>+</sup> ' (-1/6,1/6,1/6)<br>x+1/6,x+1/6,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,0)' | (8) 3 <sup>+</sup> ' (1/6,1/6,-1/6)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,0)' |
| (9) 3 <sup>-</sup> ' (1/2,1/2,1/2) x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2)' | (10) 3 <sup>-</sup> ' (1/6,-1/6,-1/6)<br>x+1/6,x+1/6,x<br>(3 <sub>xyz</sub>  1/2,0,0)'             | (11) 3 <sup>-</sup> ' (-1/6,-1/6,1/6)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub>  0,0,1/2)'             | (12) 3 <sup>-</sup> ' (-1/6,1/6,-1/6)<br>x-1/6,x+1/3,x<br>(3 <sub>xyz</sub>  0,1/2,0)'             |
| (13) 2' (1/2,1/2,0) x,x+1/4,3/8<br>(2 <sub>xy</sub>  1/4,3/4,3/4)'                         | (14) 2' x,x+1/4,1/8<br>(2 <sub>xy</sub>  1/4,1/4,1/4)'   | (15) 4 <sup>-</sup> ' (0,0,1/4) 3/4,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  3/4,3/4,1/4)'            | (16) 4 <sup>+</sup> ' (0,0,3/4) 1/4,1/2,z<br>(4 <sub>z</sub>  3/4,1/4,3/4)'                        |
| (17) 4 <sup>-</sup> ' (1/4,0,0) x,3/4,0<br>(4 <sub>x</sub> <sup>-1</sup>  1/4,3/4,3/4)'    | (18) 2' (0,1/2,1/2) 3/8,y-1/4,y<br>(2 <sub>yz</sub>  3/4,1/4,3/4)'                                 | (19) 2' 1/8,y+1/4,y<br>(2 <sub>yz</sub>  1/4,1/4,1/4)'   | (20) 4 <sup>+</sup> ' (3/4,0,0) x,1/4,1/2<br>(4 <sub>x</sub>  3/4,3/4,1/4)'                        |
| (21) 4 <sup>+</sup> ' (0,3/4,0) 1/2,y,1/4<br>(4 <sub>y</sub>  1/4,3/4,3/4)'                | (22) 2' (1/2,0,1/2) x+1/4,3/8,x<br>(2 <sub>xz</sub>  3/4,3/4,1/4)'                                 | (23) 4 <sup>-</sup> ' (0,1/4,0) 0,y,3/4<br>(4 <sub>y</sub> <sup>-1</sup>  3/4,1/4,3/4)'            | (24) 2' x+1/4,1/8,x<br>(2 <sub>xz</sub>  1/4,1/4,1/4)'   |

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); 1'.

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (1/2,1/2,1/2) +  
(0,0,0)' + (1/2,1/2,1/2)' +

48 i 11'

- |                                 |                                   |                                   |                                   |
|---------------------------------|-----------------------------------|-----------------------------------|-----------------------------------|
| (1) x,y,z [0,0,0]               | (2) x̄+1/2,ȳ,z+1/2 [0,0,0]       | (3) x̄,y+1/2,z̄+1/2 [0,0,0]       | (4) x+1/2,ȳ+1/2,z̄ [0,0,0]       |
| (5) z,x,y [0,0,0]               | (6) z+1/2,x̄+1/2,ȳ [0,0,0]       | (7) z̄+1/2,x̄,y+1/2 [0,0,0]       | (8) z̄,x+1/2,ȳ+1/2 [0,0,0]       |
| (9) y,z,x [0,0,0]               | (10) ȳ,z+1/2,x̄+1/2 [0,0,0]      | (11) y+1/2,z̄+1/2,x̄ [0,0,0]      | (12) ȳ+1/2,z̄,x+1/2 [0,0,0]      |
| (13) y+3/4,x+1/4,z̄+1/4 [0,0,0] | (14) ȳ+3/4,x̄+3/4,z̄+3/4 [0,0,0] | (15) y+1/4,x̄+1/4,z+3/4 [0,0,0]   | (16) ȳ+1/4,x+3/4,z+1/4 [0,0,0]   |
| (17) x+3/4,z+1/4,ȳ+1/4 [0,0,0] | (18) x̄+1/4,z+3/4,y+1/4 [0,0,0]   | (19) x̄+3/4,z̄+3/4,ȳ+3/4 [0,0,0] | (20) x+1/4,z̄+1/4,y+3/4 [0,0,0]   |
| (21) z+3/4,y+1/4,x̄+1/4 [0,0,0] | (22) z+1/4,ȳ+1/4,x+3/4 [0,0,0]   | (23) z̄+1/4,y+3/4,x+1/4 [0,0,0]   | (24) z̄+3/4,ȳ+3/4,x̄+3/4 [0,0,0] |

- |            |                       |                       |                         |                          |
|------------|-----------------------|-----------------------|-------------------------|--------------------------|
| 24 h ..21' | 1/8,ȳ,ȳ+1/4 [0,0,0] | 3/8,ȳ,ȳ+3/4 [0,0,0] | 7/8,y+1/2,y+1/4 [0,0,0] | 5/8,ȳ+1/2,y+3/4 [0,0,0] |
|            | ȳ+1/4,1/8,y [0,0,0]  | ȳ+3/4,3/8,ȳ [0,0,0] | y+1/4,7/8,y+1/2 [0,0,0] | y+3/4,5/8,ȳ+1/2 [0,0,0] |
|            | y,ȳ+1/4,1/8 [0,0,0]  | ȳ,ȳ+3/4,3/8 [0,0,0] | y+1/2,y+1/4,7/8 [0,0,0] | ȳ+1/2,y+3/4,5/8 [0,0,0] |

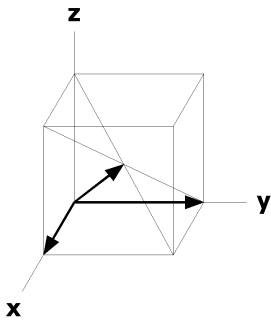
24	g	..21'	1/8,y,y+1/4 [0,0,0] y+1/4,1/8,y [0,0,0] y,y+1/4,1/8 [0,0,0]	3/8, $\bar{y}$ ,y+3/4 [0,0,0] y+3/4,3/8, $\bar{y}$ [0,0,0] $\bar{y}$ ,y+3/4,3/8 [0,0,0]	7/8,y+1/2, $\bar{y}$ +1/4 [0,0,0] $\bar{y}$ +1/4,7/8,y+1/2 [0,0,0] y+1/2, $\bar{y}$ +1/4,7/8 [0,0,0]	5/8, $\bar{y}$ +1/2, $\bar{y}$ +3/4 [0,0,0] $\bar{y}$ +3/4,5/8, $\bar{y}$ +1/2 [0,0,0] $\bar{y}$ +1/2, $\bar{y}$ +3/4,5/8 [0,0,0]
24	f	2..1'	x,0,1/4 [0,0,0] 0,1/4,x [0,0,0] x+3/4,1/2,1/4 [0,0,0]	$\bar{x}$ +1/2,0,3/4 [0,0,0] 0,3/4, $\bar{x}$ +1/2 [0,0,0] $\bar{x}$ +1/4,0,1/4 [0,0,0]	1/4,x,0 [0,0,0] 3/4,x+1/4,0 [0,0,0] 0,1/4, $\bar{x}$ +1/4 [0,0,0]	3/4, $\bar{x}$ +1/2,0 [0,0,0] 3/4, $\bar{x}$ +3/4,1/2 [0,0,0] 1/2,1/4,x+3/4 [0,0,0]
16	e	.3.1'	x,x,x [0,0,0] $\bar{x}$ ,x+1/2, $\bar{x}$ +1/2 [0,0,0] x+3/4,x+1/4, $\bar{x}$ +1/4 [0,0,0] x+1/4, $\bar{x}$ +1/4,x+3/4 [0,0,0]		$\bar{x}$ +1/2, $\bar{x}$ ,x+1/2 [0,0,0] x+1/2, $\bar{x}$ +1/2, $\bar{x}$ [0,0,0] $\bar{x}$ +3/4, $\bar{x}$ +3/4, $\bar{x}$ +3/4 [0,0,0] $\bar{x}$ +1/4,x+3/4,x+1/4 [0,0,0]	
12	d	2.221'	5/8,0,1/4 [0,0,0] 3/4,7/8,0 [0,0,0]	7/8,0,3/4 [0,0,0] 0,1/4,5/8 [0,0,0]	1/4,5/8,0 [0,0,0] 0,3/4,7/8 [0,0,0]	
12	c	2.221'	1/8,0,1/4 [0,0,0] 3/4,3/8,0 [0,0,0]	3/8,0,3/4 [0,0,0] 0,1/4,1/8 [0,0,0]	1/4,1/8,0 [0,0,0] 0,3/4,3/8 [0,0,0]	
8	b	.321'	7/8,7/8,7/8 [0,0,0]	5/8,1/8,3/8 [0,0,0]	1/8,3/8,5/8 [0,0,0]	3/8,5/8,1/8 [0,0,0]
8	a	.321'	1/8,1/8,1/8 [0,0,0]	3/8,7/8,5/8 [0,0,0]	7/8,5/8,3/8 [0,0,0]	5/8,3/8,7/8 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,0,z

Along [1,1,1] p3m11'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

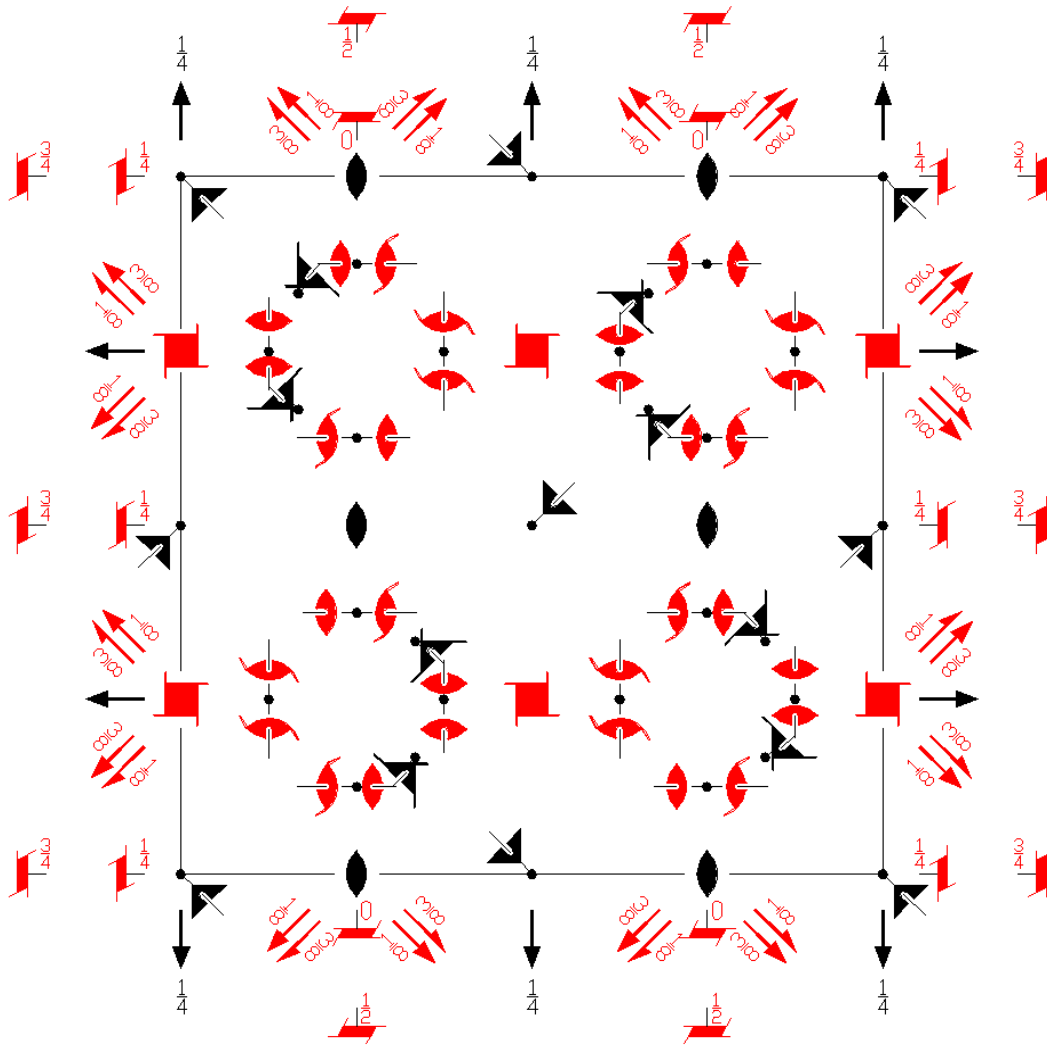
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x+1/4,1/8



$I4_1'32'$   
214.3.1569

$4'32'$   
 $I4_1'32'$

Cubic



**Origin** on  $3 [111]$  at midpoint of three non-intersecting pairs of parallel screw axes  $4_1'$  and  $4_3'$  and of three non-intersection pairs of parallel 2 axes.

**Asymmetric unit**  $-3/8 \leq x \leq 1/8$ ;  $-1/8 \leq y \leq 1/8$ ;  $1/8 \leq z \leq 3/8$ ;  $\max(x,y,y-x-1/8) \leq z \leq y+1/4$

**Vertices**  $1/8, 1/8, 1/8$   $1/8, 1/8, 3/8$   $1/8, -1/8, 1/8$   $-1/8, 1/8, 1/8$   $-1/8, -1/8, -1/8$   $-3/8, 1/8, 3/8$   $-3/8, -1/8, 1/8$

**Symmetry Operations**

For (0,0,0) + set

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                                    | (2) 2 (0,0,1/2) $1/4, 0, z$<br>( $2_z$   $1/2, 0, 1/2$ )  | (3) 2 (0,1/2,0) $0, y, 1/4$<br>( $2_y$   $0, 1/2, 1/2$ )                                  | (4) 2 (1/2,0,0) $x, 1/4, 0$<br>( $2_x$   $1/2, 1/2, 0$ )   |
| (5) $3^+$ $x, x, x$<br>( $3_{xyz}$   $0, 0, 0$ )      | (6) $3^+$ $\bar{x}+1/2, x, \bar{x}$<br>( $3_{\bar{xyz}^{-1}}$   $1/2, 1/2, 0$ )                       | (7) $3^+$ $x+1/2, \bar{x}-1/2, \bar{x}$<br>( $3_{\bar{xyz}^{-1}}$   $1/2, 0, 1/2$ )       | (8) $3^+$ $\bar{x}, \bar{x}+1/2, x$<br>( $3_{\bar{xyz}^{-1}}$   $0, 1/2, 1/2$ )                      |
| (9) $3^-$ $x, x, x$<br>( $3_{xyz^{-1}}$   $0, 0, 0$ ) | (10) $3^-$ $(-1/3, 1/3, 1/3)$<br>$x+1/6, \bar{x}+1/6, \bar{x}$<br>( $3_{\bar{xyz}}$   $0, 1/2, 1/2$ ) | (11) $3^-$ $(1/3, 1/3, -1/3)$<br>$\bar{x}+1/3, x+1/6, x$<br>( $3_{xyz}$   $1/2, 1/2, 0$ ) | (12) $3^-$ $(1/3, -1/3, 1/3)$<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>( $3_{\bar{yz}}$   $1/2, 0, 1/2$ ) |

- |  |  |   |  |
|--|--|---|--|
| (13) 2' (1/2,1/2,0) x,x-1/4,1/8<br>(2 <sub>xy</sub>  3/4,1/4,1/4)'         | (14) 2' x,x+3/4,3/8<br>(2 <sub>xy</sub>  3/4,3/4,3/4)'             | (15) 4' (0,0,3/4) 1/4,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/4,1/4,3/4)' | (16) 4 <sup>+</sup> (0,0,1/4) -1/4,1/2,z<br>(4 <sub>z</sub>  1/4,3/4,1/4)' |
| (17) 4' (3/4,0,0) x,1/4,0<br>(4 <sub>x</sub> <sup>-1</sup>  3/4,1/4,1/4)'  | (18) 2' (0,1/2,1/2) 1/8,y+1/4,y<br>(2 <sub>yz</sub>  1/4,3/4,1/4)' | (19) 2' 3/8,y+3/4,y<br>(2 <sub>yz</sub>  3/4,3/4,3/4)'                    | (20) 4 <sup>+</sup> (1/4,0,0) x,-1/4,1/2<br>(4 <sub>x</sub>  1/4,1/4,3/4)' |
| (21) 4 <sup>+</sup> (0,1/4,0) 1/2,y,-1/4<br>(4 <sub>y</sub>  3/4,1/4,1/4)' | (22) 2' (1/2,0,1/2) x-1/4,1/8,x<br>(2 <sub>xz</sub>  1/4,1/4,3/4)' | (23) 4' (0,3/4,0) 0,y,1/4<br>(4 <sub>y</sub> <sup>-1</sup>  1/4,3/4,1/4)' | (24) 2' x+3/4,3/8,x<br>(2 <sub>xz</sub>  3/4,3/4,3/4)'                     |

For (1/2,1/2,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)  | (2) 2 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,0)  | (3) 2 1/4,y,0<br>(2 <sub>y</sub>  1/2,0,0)  | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)  |
| (5) 3 <sup>+</sup> (1/2,1/2,1/2) x,x,x<br>(3 <sub>xyz</sub>  1/2,1/2,1/2)               | (6) 3 <sup>+</sup> (1/6,-1/6,1/6)<br>x-1/6,x+1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,1/2) | (7) 3 <sup>+</sup> (-1/6,1/6,1/6)<br>x+1/6,x+1/6,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,0) | (8) 3 <sup>+</sup> (1/6,1/6,-1/6)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,0) |
| (9) 3 <sup>-</sup> (1/2,1/2,1/2) x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2) | (10) 3 <sup>-</sup> (1/6,-1/6,-1/6)<br>x+1/6,x+1/6,x<br>(3 <sub>xyz</sub>  1/2,0,0)             | (11) 3 <sup>-</sup> (-1/6,-1/6,1/6)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub>  0,0,1/2)             | (12) 3 <sup>-</sup> (-1/6,1/6,-1/6)<br>x-1/6,x+1/3,x<br>(3 <sub>xyz</sub>  0,1/2,0)             |
| (13) 2' (1/2,1/2,0) x,x+1/4,3/8<br>(2 <sub>xy</sub>  1/4,3/4,3/4)'                      | (14) 2' x,x+1/4,1/8<br>(2 <sub>xy</sub>  1/4,1/4,1/4)'  | (15) 4' (0,0,1/4) 3/4,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  3/4,3/4,1/4)'                       | (16) 4 <sup>+</sup> (0,0,3/4) 1/4,1/2,z<br>(4 <sub>z</sub>  3/4,1/4,3/4)'                       |
| (17) 4' (1/4,0,0) x,3/4,0<br>(4 <sub>x</sub> <sup>-1</sup>  1/4,3/4,3/4)'               | (18) 2' (0,1/2,1/2) 3/8,y-1/4,y<br>(2 <sub>yz</sub>  3/4,1/4,3/4)'                              | (19) 2' 1/8,y+1/4,y<br>(2 <sub>yz</sub>  1/4,1/4,1/4)'  | (20) 4 <sup>+</sup> (3/4,0,0) x,1/4,1/2<br>(4 <sub>x</sub>  3/4,3/4,1/4)'                       |
| (21) 4 <sup>+</sup> (0,3/4,0) 1/2,y,1/4<br>(4 <sub>y</sub>  1/4,3/4,3/4)'               | (22) 2' (1/2,0,1/2) x+1/4,3/8,x<br>(2 <sub>xz</sub>  3/4,3/4,1/4)'                              | (23) 4' (0,1/4,0) 0,y,3/4<br>(4 <sub>y</sub> <sup>-1</sup>  3/4,1/4,3/4)'                       | (24) 2' x+1/4,1/8,x<br>(2 <sub>xz</sub>  1/4,1/4,1/4)'  |

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (1/2,1/2,1/2) +

48 i 1

- |                                |                                |                                |                                |
|--------------------------------|--------------------------------|--------------------------------|--------------------------------|
| (1) x,y,z [u,v,w]              | (2) x+1/2,y,z+1/2 [u,v,w]      | (3) x,y+1/2,z+1/2 [u,v,w]      | (4) x+1/2,y+1/2,z [u,v,w]      |
| (5) z,x,y [w,u,v]              | (6) z+1/2,x+1/2,y [w,u,v]      | (7) z+1/2,x,y+1/2 [w,u,v]      | (8) z,x+1/2,y+1/2 [w,u,v]      |
| (9) y,z,x [v,w,u]              | (10) y,z+1/2,x+1/2 [v,w,u]     | (11) y+1/2,z+1/2,x [v,w,u]     | (12) y+1/2,z,x+1/2 [v,w,u]     |
| (13) y+3/4,x+1/4,z+1/4 [v,u,w] | (14) y+3/4,x+3/4,z+3/4 [v,u,w] | (15) y+1/4,x+1/4,z+3/4 [v,u,w] | (16) y+1/4,x+3/4,z+1/4 [v,u,w] |
| (17) x+3/4,z+1/4,y+1/4 [u,w,v] | (18) x+1/4,z+3/4,y+1/4 [u,w,v] | (19) x+3/4,z+3/4,y+3/4 [u,w,v] | (20) x+1/4,z+1/4,y+3/4 [u,w,v] |
| (21) z+3/4,y+1/4,x+1/4 [w,v,u] | (22) z+1/4,y+1/4,x+3/4 [w,v,u] | (23) z+1/4,y+3/4,x+1/4 [w,v,u] | (24) z+3/4,y+3/4,x+3/4 [w,v,u] |

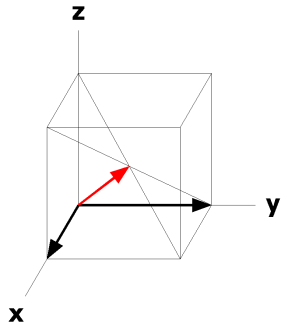
24	h	..2'	1/8,y, $\bar{y}$ +1/4 [u,v,v] $\bar{y}$ +1/4,1/8,y [v,u,v] y, $\bar{y}$ +1/4,1/8 [v,v,u]	3/8, $\bar{y}$ , $\bar{y}$ +3/4 [ $\bar{u}$ , $\bar{v}$ ,v] $\bar{y}$ +3/4,3/8, $\bar{y}$ [v, $\bar{u}$ , $\bar{v}$ ] $\bar{y}$ , $\bar{y}$ +3/4,3/8 [ $\bar{v}$ ,v, $\bar{u}$ ]	7/8,y+1/2,y+1/4 [ $\bar{u}$ ,v, $\bar{v}$ ] y+1/4,7/8,y+1/2 [ $\bar{v}$ , $\bar{u}$ ,v] y+1/2,y+1/4,7/8 [v, $\bar{v}$ , $\bar{u}$ ]	5/8, $\bar{y}$ +1/2,y+3/4 [u, $\bar{v}$ , $\bar{v}$ ] y+3/4,5/8, $\bar{y}$ +1/2 [ $\bar{v}$ ,u, $\bar{v}$ ] $\bar{y}$ +1/2,y+3/4,5/8 [ $\bar{v}$ , $\bar{v}$ ,u]
24	g	..2'	1/8,y,y+1/4 [u,v, $\bar{v}$ ] y+1/4,1/8,y [ $\bar{v}$ ,u,v] y,y+1/4,1/8 [v, $\bar{v}$ ,u]	3/8, $\bar{y}$ ,y+3/4 [ $\bar{u}$ , $\bar{v}$ , $\bar{v}$ ] y+3/4,3/8, $\bar{y}$ [ $\bar{v}$ , $\bar{u}$ , $\bar{v}$ ] $\bar{y}$ ,y+3/4,3/8 [ $\bar{v}$ , $\bar{v}$ , $\bar{u}$ ]	7/8,y+1/2, $\bar{y}$ +1/4 [ $\bar{u}$ ,v,v] $\bar{y}$ +1/4,7/8,y+1/2 [v, $\bar{u}$ ,v] y+1/2, $\bar{y}$ +1/4,7/8 [v,v, $\bar{u}$ ]	5/8, $\bar{y}$ +1/2, $\bar{y}$ +3/4 [u, $\bar{v}$ ,v] $\bar{y}$ +3/4,5/8, $\bar{y}$ +1/2 [v,u, $\bar{v}$ ] $\bar{y}$ +1/2, $\bar{y}$ +3/4,5/8 [ $\bar{v}$ ,v,u]
24	f	2..	x,0,1/4 [u,0,0] 0,1/4,x [0,0,u] x+3/4,1/2,1/4 [ $\bar{u}$ ,0,0]	$\bar{x}$ +1/2,0,3/4 [ $\bar{u}$ ,0,0] 0,3/4, $\bar{x}$ +1/2 [0,0, $\bar{u}$ ] $\bar{x}$ +1/4,0,1/4 [u,0,0]	1/4,x,0 [0,u,0] 3/4,x+1/4,0 [0, $\bar{u}$ ,0] 0,1/4, $\bar{x}$ +1/4 [0,0,u]	3/4, $\bar{x}$ +1/2,0 [0, $\bar{u}$ ,0] 3/4, $\bar{x}$ +3/4,1/2 [0,u,0] 1/2,1/4,x+3/4 [0,0, $\bar{u}$ ]
16	e	.3.	x,x,x [u,u,u] $\bar{x}$ ,x+1/2, $\bar{x}$ +1/2 [ $\bar{u}$ ,u, $\bar{u}$ ] x+3/4,x+1/4, $\bar{x}$ +1/4 [ $\bar{u}$ , $\bar{u}$ ,u] x+1/4, $\bar{x}$ +1/4,x+3/4 [ $\bar{u}$ ,u, $\bar{u}$ ]	$\bar{x}$ +1/2,0,3/4 [ $\bar{u}$ ,0,0] 0,3/4, $\bar{x}$ +1/2 [0,0, $\bar{u}$ ] $\bar{x}$ +1/4,0,1/4 [u,0,0]	$\bar{x}$ +1/2, $\bar{x}$ ,x+1/2 [ $\bar{u}$ , $\bar{u}$ ,u] x+1/2, $\bar{x}$ +1/2, $\bar{x}$ [u, $\bar{u}$ , $\bar{u}$ ] $\bar{x}$ +3/4, $\bar{x}$ +3/4, $\bar{x}$ +3/4 [u,u,u] $\bar{x}$ +1/4,x+3/4,x+1/4 [u, $\bar{u}$ , $\bar{u}$ ]	
12	d	2.2'2'	5/8,0,1/4 [u,0,0] 3/4,7/8,0 [0, $\bar{u}$ ,0]	7/8,0,3/4 [ $\bar{u}$ ,0,0] 0,1/4,5/8 [0,0,u]	1/4,5/8,0 [0,u,0] 0,3/4,7/8 [0,0, $\bar{u}$ ]	
12	c	2.2'2'	1/8,0,1/4 [u,0,0] 3/4,3/8,0 [0, $\bar{u}$ ,0]	3/8,0,3/4 [ $\bar{u}$ ,0,0] 0,1/4,1/8 [0,0,u]	1/4,1/8,0 [0,u,0] 0,3/4,3/8 [0,0, $\bar{u}$ ]	
8	b	.32'	7/8,7/8,7/8 [u,u,u]	5/8,1/8,3/8 [ $\bar{u}$ , $\bar{u}$ ,u]	1/8,3/8,5/8 [ $\bar{u}$ ,u, $\bar{u}$ ]	3/8,5/8,1/8 [u, $\bar{u}$ , $\bar{u}$ ]
8	a	.32'	1/8,1/8,1/8 [u,u,u]	3/8,7/8,5/8 [ $\bar{u}$ , $\bar{u}$ ,u]	7/8,5/8,3/8 [ $\bar{u}$ ,u, $\bar{u}$ ]	5/8,3/8,7/8 [u, $\bar{u}$ , $\bar{u}$ ]

### Symmetry of Special Projections

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,0,z

Along [1,1,1] p3m1  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

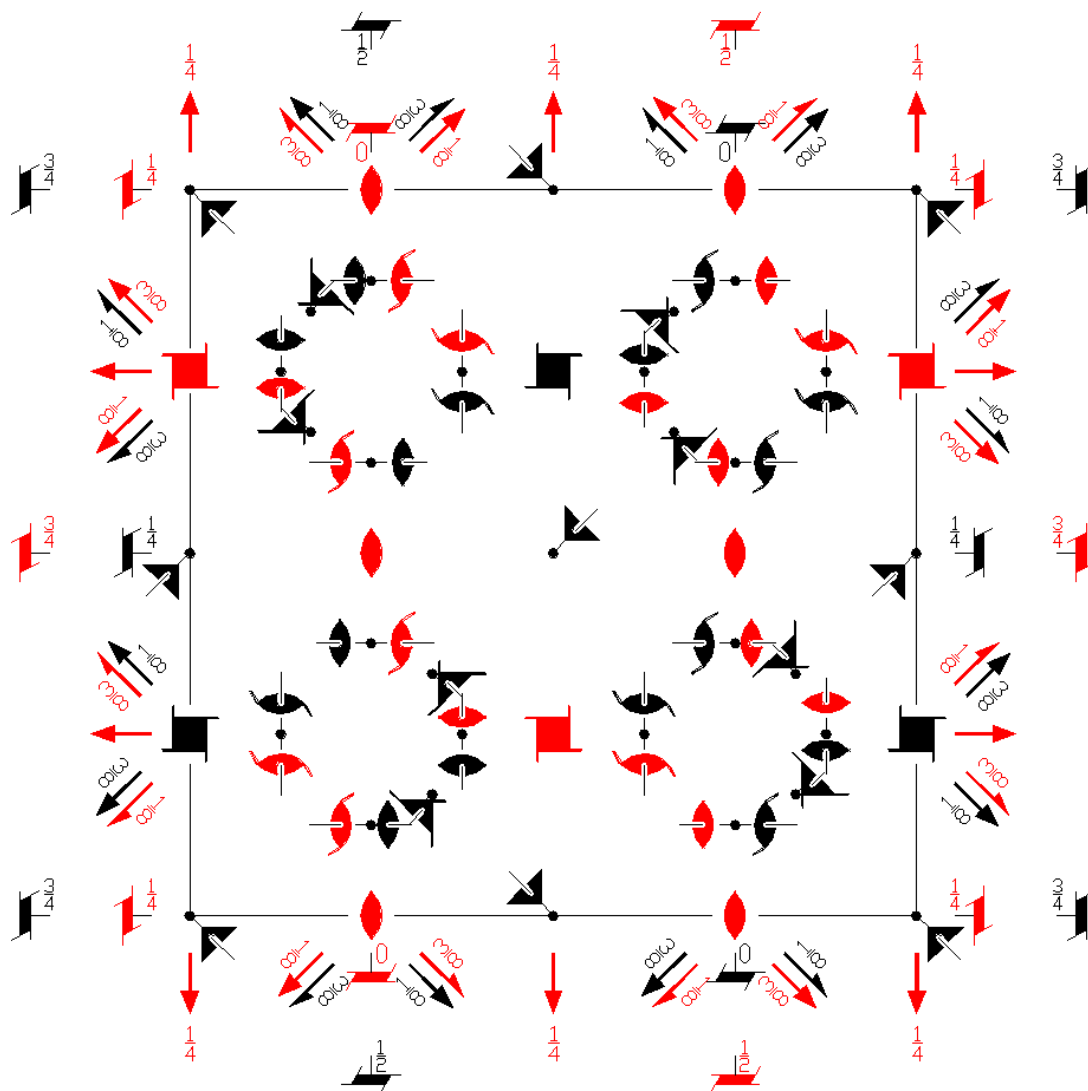
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = -(-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x+1/4,1/8



$I_P 4_1 32$   
214.4.1570

4321'  
 $I_P 4_1 32$

Cubic



**Origin** on 3 [111] at midpoint of three non-intersecting pairs of parallel screw axes  $4_1$  and  $4_3$  and of three non-intersection pairs of parallel 2 axes.

**Asymmetric unit**  $-3/8 \leq x \leq 1/8$ ;  $-1/8 \leq y \leq 1/8$ ;  $1/8 \leq z \leq 3/8$ ;  $\max(x, y, y - x - 1/8) \leq z \leq y + 1/4$

Vertices  $1/8, 1/8, 1/8$   $1/8, 1/8, 3/8$   $1/8, -1/8, 1/8$   $-1/8, 1/8, 1/8$   $-1/8, -1/8, -1/8$   $-3/8, 1/8, 3/8$   $-3/8, -1/8, 1/8$

### Symmetry Operations

For (0,0,0) + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                              | (2) 2 (0,0,1/2) $1/4, 0, z$<br>( $2_z$  1/2,0,1/2)  | (3) 2 (0,1/2,0) $0, y, 1/4$<br>( $2_y$  0,1/2,1/2)  | (4) 2 (1/2,0,0) $x, 1/4, 0$<br>( $2_x$  1/2,1/2,0)  |
| (5) $3^+$ $x, x, x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x} + 1/2, x, \bar{x}$<br>( $3_{\bar{xyz}^{-1}}$  1/2,1/2,0)                         | (7) $3^+$ $x + 1/2, \bar{x} - 1/2, \bar{x}$<br>( $3_{\bar{xyz}^{-1}}$  1/2,0,1/2)                   | (8) $3^+$ $\bar{x}, \bar{x} + 1/2, x$<br>( $3_{\bar{xyz}^{-1}}$  0,1/2,1/2)                         |
| (9) $3^-$ $x, x, x$<br>( $3_{xyz^{-1}}$  0,0,0) | (10) $3^-$ $(-1/3, 1/3, 1/3)$<br>$x + 1/6, \bar{x} + 1/6, \bar{x}$<br>( $3_{\bar{xyz}}$  0,1/2,1/2) | (11) $3^-$ $(1/3, 1/3, -1/3)$<br>$\bar{x} + 1/3, \bar{x} + 1/6, x$<br>( $3_{\bar{xyz}}$  1/2,1/2,0) | (12) $3^-$ $(1/3, -1/3, 1/3)$<br>$\bar{x} - 1/6, x + 1/3, \bar{x}$<br>( $3_{\bar{xyz}}$  1/2,0,1/2) |



- |  |  |   |  |
|--|--|---|--|
| (13) $2 (1/2, 1/2, 0) \quad x, x-1/4, 1/8$<br>( $2_{xy}   3/4, 1/4, 1/4$ ) | (14) $2 \quad x, \bar{x}+3/4, 3/8$<br>( $2_{xy}   3/4, 3/4, 3/4$ )         | (15) $4^- (0, 0, 3/4) \quad 1/4, 0, z$<br>( $4_z^-   1/4, 1/4, 3/4$ ) | (16) $4^+ (0, 0, 1/4) \quad -1/4, 1/2, z$<br>( $4_z   1/4, 3/4, 1/4$ ) |
| (17) $4^- (3/4, 0, 0) \quad x, 1/4, 0$<br>( $4_x^-   3/4, 1/4, 1/4$ )      | (18) $2 (0, 1/2, 1/2) \quad 1/8, y+1/4, y$<br>( $2_{yz}   1/4, 3/4, 1/4$ ) | (19) $2 \quad 3/8, y+3/4, \bar{y}$<br>( $2_{yz}   3/4, 3/4, 3/4$ )    | (20) $4^+ (1/4, 0, 0) \quad x, -1/4, 1/2$<br>( $4_x   1/4, 1/4, 3/4$ ) |
| (21) $4^+ (0, 1/4, 0) \quad 1/2, y, -1/4$<br>( $4_y   3/4, 1/4, 1/4$ )     | (22) $2 (1/2, 0, 1/2) \quad x-1/4, 1/8, x$<br>( $2_{xz}   1/4, 1/4, 3/4$ ) | (23) $4^- (0, 3/4, 0) \quad 0, y, 1/4$<br>( $4_y^-   1/4, 3/4, 1/4$ ) | (24) $2 \quad \bar{x}+3/4, 3/8, x$<br>( $2_{xz}   3/4, 3/4, 3/4$ )     |

For (1/2, 1/2, 1/2)' + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t' (1/2, 1/2, 1/2)$<br>( $1   1/2, 1/2, 1/2$ )'                           | (2) $2' \quad 0, 1/4, z$<br>( $2_z   0, 1/2, 0$ )'  | (3) $2' \quad 1/4, y, 0$<br>( $2_y   1/2, 0, 0$ )'  | (4) $2' \quad x, 0, 1/4$<br>( $2_x   0, 0, 1/2$ )'  |
| (5) $3^{+'} (1/2, 1/2, 1/2) \quad x, x, x$<br>( $3_{xyz}   1/2, 1/2, 1/2$ )'   | (6) $3^{+'} (1/6, -1/6, 1/6) \quad \bar{x}-1/6, x+1/3, \bar{x}$<br>( $3_{xyz}^-   0, 0, 1/2$ )' | (7) $3^{+'} (-1/6, 1/6, 1/6) \quad x+1/6, \bar{x}+1/6, \bar{x}$<br>( $3_{xyz}^-   0, 1/2, 0$ )' | (8) $3^{+'} (1/6, 1/6, -1/6) \quad \bar{x}+1/3, \bar{x}+1/6, x$<br>( $3_{xyz}^-   1/2, 0, 0$ )' |
| (9) $3^{-'} (1/2, 1/2, 1/2) \quad x, x, x$<br>( $3_{xyz}^-   1/2, 1/2, 1/2$ )' | (10) $3^{-'} (1/6, -1/6, -1/6) \quad x+1/6, \bar{x}+1/6, x$<br>( $3_{xyz}   1/2, 0, 0$ )'       | (11) $3^{-'} (-1/6, -1/6, 1/6) \quad \bar{x}+1/3, \bar{x}+1/6, x$<br>( $3_{xyz}   0, 0, 1/2$ )' | (12) $3^{-'} (-1/6, 1/6, -1/6) \quad \bar{x}-1/6, x+1/3, x$<br>( $3_{xyz}   0, 1/2, 0$ )'       |
| (13) $2' (1/2, 1/2, 0) \quad x, x+1/4, 3/8$<br>( $2_{xy}   1/4, 3/4, 3/4$ )'   | (14) $2' \quad x, \bar{x}+1/4, 1/8$<br>( $2_{xy}   1/4, 1/4, 1/4$ )'                            | (15) $4^{-'} (0, 0, 1/4) \quad 3/4, 0, z$<br>( $4_z^-   3/4, 3/4, 1/4$ )'                       | (16) $4^{+'} (0, 0, 3/4) \quad 1/4, 1/2, z$<br>( $4_z   3/4, 1/4, 3/4$ )'                       |
| (17) $4^{-'} (1/4, 0, 0) \quad x, 3/4, 0$<br>( $4_x^-   1/4, 3/4, 3/4$ )'      | (18) $2' (0, 1/2, 1/2) \quad 3/8, y-1/4, y$<br>( $2_{yz}   3/4, 1/4, 3/4$ )'                    | (19) $2' \quad 1/8, y+1/4, \bar{y}$<br>( $2_{yz}   1/4, 1/4, 1/4$ )'                            | (20) $4^{+'} (3/4, 0, 0) \quad x, 1/4, 1/2$<br>( $4_x   3/4, 3/4, 1/4$ )'                       |
| (21) $4^{+'} (0, 3/4, 0) \quad 1/2, y, 1/4$<br>( $4_y   1/4, 3/4, 3/4$ )'      | (22) $2' (1/2, 0, 1/2) \quad x+1/4, 3/8, x$<br>( $2_{xz}   3/4, 3/4, 1/4$ )'                    | (23) $4^{-'} (0, 1/4, 0) \quad 0, y, 3/4$<br>( $4_y^-   3/4, 1/4, 3/4$ )'                       | (24) $2' \quad \bar{x}+1/4, 1/8, x$<br>( $2_{xz}   1/4, 1/4, 1/4$ )'                            |

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2, 1/2, 1/2); (2); (3); (5); (13).

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (1/2, 1/2, 1/2)' +

48 i 1

- |  |  |  |  |
|--|--|--|--|
| (1) $x, y, z [u, v, w]$                          | (2) $\bar{x}+1/2, \bar{y}, z+1/2 [\bar{u}, \bar{v}, w]$                  | (3) $\bar{x}, y+1/2, \bar{z}+1/2 [\bar{u}, v, \bar{w}]$                  | (4) $x+1/2, \bar{y}+1/2, \bar{z} [u, \bar{v}, \bar{w}]$                  |
| (5) $z, x, y [w, u, v]$                          | (6) $z+1/2, \bar{x}+1/2, \bar{y} [w, \bar{u}, \bar{v}]$                  | (7) $\bar{z}+1/2, \bar{x}, y+1/2 [\bar{w}, \bar{u}, v]$                  | (8) $\bar{z}, x+1/2, \bar{y}+1/2 [\bar{w}, u, \bar{v}]$                  |
| (9) $y, z, x [v, w, u]$                          | (10) $\bar{y}, z+1/2, \bar{x}+1/2 [\bar{v}, w, \bar{u}]$                 | (11) $y+1/2, \bar{z}+1/2, \bar{x} [v, \bar{w}, \bar{u}]$                 | (12) $\bar{y}+1/2, \bar{z}, x+1/2 [\bar{v}, \bar{w}, u]$                 |
| (13) $y+3/4, x+1/4, \bar{z}+1/4 [v, u, \bar{w}]$ | (14) $\bar{y}+3/4, \bar{x}+3/4, \bar{z}+3/4 [\bar{v}, \bar{u}, \bar{w}]$ | (15) $y+1/4, \bar{x}+1/4, z+3/4 [v, \bar{u}, w]$                         | (16) $\bar{y}+1/4, x+3/4, z+1/4 [\bar{v}, u, w]$                         |
| (17) $x+3/4, z+1/4, \bar{y}+1/4 [u, w, \bar{v}]$ | (18) $\bar{x}+1/4, z+3/4, y+1/4 [\bar{u}, w, v]$                         | (19) $\bar{x}+3/4, \bar{z}+3/4, \bar{y}+3/4 [\bar{u}, \bar{w}, \bar{v}]$ | (20) $x+1/4, \bar{z}+1/4, y+3/4 [u, \bar{w}, v]$                         |
| (21) $z+3/4, y+1/4, \bar{x}+1/4 [w, v, \bar{u}]$ | (22) $z+1/4, \bar{y}+1/4, x+3/4 [w, \bar{v}, u]$                         | (23) $\bar{z}+1/4, y+3/4, x+1/4 [\bar{w}, v, u]$                         | (24) $\bar{z}+3/4, \bar{y}+3/4, \bar{x}+3/4 [\bar{w}, \bar{v}, \bar{u}]$ |

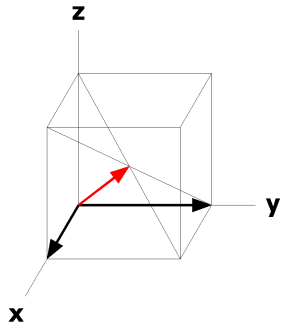
24	h	..2'	1/8,y, $\bar{y}$ +1/4 [u,v,v] $\bar{y}$ +1/4,1/8,y [v,u,v] y, $\bar{y}$ +1/4,1/8 [v,v,u]	3/8, $\bar{y}$ , $\bar{y}$ +3/4 [ $\bar{u}$ , $\bar{v}$ ,v] $\bar{y}$ +3/4,3/8, $\bar{y}$ [v, $\bar{u}$ , $\bar{v}$ ] $\bar{y}$ , $\bar{y}$ +3/4,3/8 [ $\bar{v}$ ,v, $\bar{u}$ ]	7/8,y+1/2,y+1/4 [ $\bar{u}$ ,v, $\bar{v}$ ] y+1/4,7/8,y+1/2 [ $\bar{v}$ , $\bar{u}$ ,v] y+1/2,y+1/4,7/8 [v, $\bar{v}$ , $\bar{u}$ ]	5/8, $\bar{y}$ +1/2,y+3/4 [u, $\bar{v}$ , $\bar{v}$ ] y+3/4,5/8, $\bar{y}$ +1/2 [ $\bar{v}$ ,u, $\bar{v}$ ] $\bar{y}$ +1/2,y+3/4,5/8 [ $\bar{v}$ , $\bar{v}$ ,u]
24	g	..2	1/8,y,y+1/4 [0,v,v] y+1/4,1/8,y [v,0,v] y,y+1/4,1/8 [v,v,0]	3/8, $\bar{y}$ ,y+3/4 [0, $\bar{v}$ ,v] y+3/4,3/8, $\bar{y}$ [v,0, $\bar{v}$ ] $\bar{y}$ ,y+3/4,3/8 [ $\bar{v}$ ,v,0]	7/8,y+1/2, $\bar{y}$ +1/4 [0,v, $\bar{v}$ ] $\bar{y}$ +1/4,7/8,y+1/2 [ $\bar{v}$ ,0,v] y+1/2, $\bar{y}$ +1/4,7/8 [v, $\bar{v}$ ,0]	5/8, $\bar{y}$ +1/2, $\bar{y}$ +3/4 [0, $\bar{v}$ , $\bar{v}$ ] $\bar{y}$ +3/4,5/8, $\bar{y}$ +1/2 [ $\bar{v}$ ,0, $\bar{v}$ ] $\bar{y}$ +1/2, $\bar{y}$ +3/4,5/8 [ $\bar{v}$ , $\bar{v}$ ,0]
24	f	2..	x,0,1/4 [u,0,0] 0,1/4,x [0,0,u] x+3/4,1/2,1/4 [u,0,0]	$\bar{x}$ +1/2,0,3/4 [ $\bar{u}$ ,0,0] 0,3/4, $\bar{x}$ +1/2 [0,0, $\bar{u}$ ] $\bar{x}$ +1/4,0,1/4 [ $\bar{u}$ ,0,0]	1/4,x,0 [0,u,0] 3/4,x+1/4,0 [0,u,0] 0,1/4, $\bar{x}$ +1/4 [0,0, $\bar{u}$ ]	3/4, $\bar{x}$ +1/2,0 [0, $\bar{u}$ ,0] 3/4, $\bar{x}$ +3/4,1/2 [0, $\bar{u}$ ,0] 1/2,1/4,x+3/4 [0,0,u]
16	e	.3.	x,x,x [u,u,u] $\bar{x}$ ,x+1/2, $\bar{x}$ +1/2 [ $\bar{u}$ ,u, $\bar{u}$ ] x+3/4,x+1/4, $\bar{x}$ +1/4 [u,u, $\bar{u}$ ] x+1/4, $\bar{x}$ +1/4,x+3/4 [u, $\bar{u}$ ,u]	$\bar{x}$ +1/2, $\bar{x}$ ,x+1/2 [ $\bar{u}$ , $\bar{u}$ ,u] x+1/2, $\bar{x}$ +1/2, $\bar{x}$ [u, $\bar{u}$ , $\bar{u}$ ] $\bar{x}$ +3/4, $\bar{x}$ +3/4, $\bar{x}$ +3/4 [ $\bar{u}$ , $\bar{u}$ , $\bar{u}$ ] $\bar{x}$ +1/4,x+3/4,x+1/4 [ $\bar{u}$ ,u,u]		
12	d	2'.22'	5/8,0,1/4 [0,v,v] 3/4,7/8,0 [v,0, $\bar{v}$ ]	7/8,0,3/4 [0, $\bar{v}$ ,v] 0,1/4,5/8 [v,v,0]	1/4,5/8,0 [v,0,v] 0,3/4,7/8 [ $\bar{v}$ ,v,0]	
12	c	2'.22'	1/8,0,1/4 [0,v,v] 3/4,3/8,0 [v,0, $\bar{v}$ ]	3/8,0,3/4 [0, $\bar{v}$ ,v] 0,1/4,1/8 [v,v,0]	1/4,1/8,0 [ $\bar{v}$ ,v,0] 0,3/4,3/8 [ $\bar{v}$ ,v,0]	
8	b	.32	7/8,7/8,7/8 [0,0,0]	5/8,1/8,3/8 [0,0,0]	1/8,3/8,5/8 [0,0,0]	3/8,5/8,1/8 [0,0,0]
8	a	.32'	1/8,1/8,1/8 [u,u,u]	3/8,7/8,5/8 [ $\bar{u}$ , $\bar{u}$ ,u]	7/8,5/8,3/8 [ $\bar{u}$ ,u, $\bar{u}$ ]	5/8,3/8,7/8 [u, $\bar{u}$ , $\bar{u}$ ]

### Symmetry of Special Projections

Along [0,0,1]  $p_p$ -4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/4,0,z

Along [1,1,1]  $p_{3m11}'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

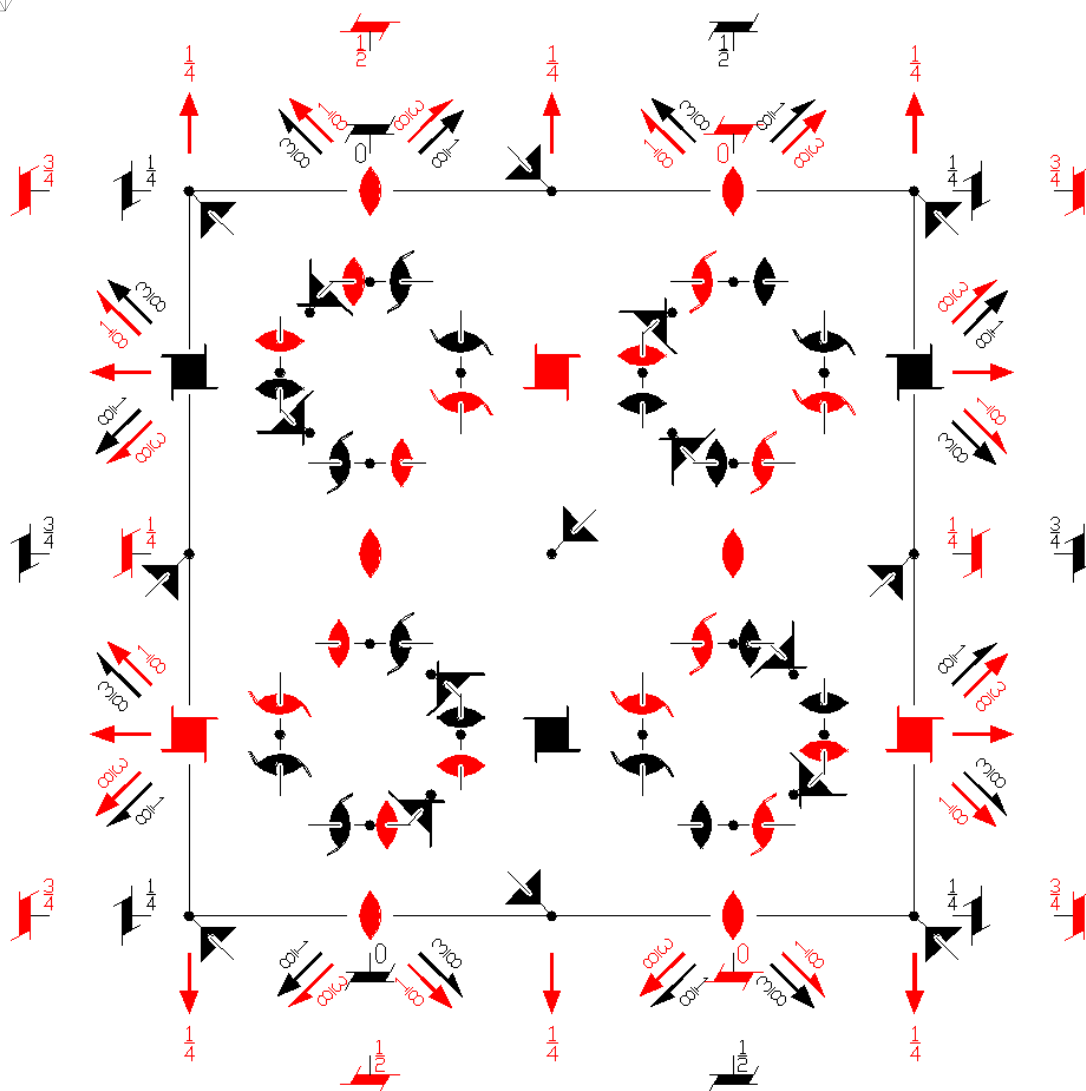
Along [1,1,0]  $p_{2a}$ -2m'm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x+1/4,1/8



$I_p 4_1' 32'$   
214.5.1571

4321'  
 $I_p 4_1' 32'$

Cubic



**Origin** on 3 [111] at midpoint of three non-intersecting pairs of parallel screw axes  $4_1'$  and  $4_3'$  and of three non-intersection pairs of parallel 2 axes.

**Asymmetric unit**  $-3/8 \leq x \leq 1/8$ ;  $-1/8 \leq y \leq 1/8$ ;  $1/8 \leq z \leq 3/8$ ;  $\max(x, y, y - x - 1/8) \leq z \leq y + 1/4$

**Vertices**  $1/8, 1/8, 1/8$   $1/8, 1/8, 3/8$   $1/8, -1/8, 1/8$   $-1/8, 1/8, 1/8$   $-1/8, -1/8, -1/8$   $-3/8, 1/8, 3/8$   $-3/8, -1/8, 1/8$

### Symmetry Operations

For (0,0,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                         | (2) 2 (0,0,1/2) $1/4, 0, z$<br>( $2_z$   $1/2, 0, 1/2$ )  | (3) 2 (0,1/2,0) $0, y, 1/4$<br>( $2_y$   $0, 1/2, 1/2$ )  | (4) 2 (1/2,0,0) $x, 1/4, 0$<br>( $2_x$   $1/2, 1/2, 0$ )  |
| (5) $3^+$ $x, x, x$<br>( $3_{xyz}$  0,0,0) | (6) $3^+$ $\bar{x} + 1/2, x, \bar{x}$<br>( $3_{\bar{xyz}}$   $1/2, 1/2, 0$ )                              | (7) $3^+$ $x + 1/2, \bar{x} - 1/2, \bar{x}$<br>( $3_{\bar{xyz}}$   $1/2, 0, 1/2$ )                        | (8) $3^+$ $\bar{x}, \bar{x} + 1/2, x$<br>( $3_{\bar{xyz}}$   $0, 1/2, 1/2$ )                              |
| (9) $3^-$ $x, x, x$<br>( $3_{xyz}$  0,0,0) | (10) $3^-$ $(-1/3, 1/3, 1/3)$<br>$x + 1/6, \bar{x} + 1/6, \bar{x}$<br>( $3_{\bar{xyz}}$   $0, 1/2, 1/2$ ) | (11) $3^-$ $(1/3, 1/3, -1/3)$<br>$\bar{x} + 1/3, \bar{x} + 1/6, x$<br>( $3_{\bar{xyz}}$   $1/2, 1/2, 0$ ) | (12) $3^-$ $(1/3, -1/3, 1/3)$<br>$\bar{x} - 1/6, x + 1/3, \bar{x}$<br>( $3_{\bar{xyz}}$   $1/2, 0, 1/2$ ) |

(13) 2' (1/2,1/2,0) x,x-1/4,1/8 (2 <sub>xy</sub>  3/4,1/4,1/4)'	(14) 2' x,x+3/4,3/8 (2 <sub>xy</sub>  3/4,3/4,3/4)'	(15) 4' (0,0,3/4) 1/4,0,z (4 <sub>z</sub> <sup>-1</sup>  1/4,1/4,3/4)'	(16) 4 <sup>+</sup> (0,0,1/4) -1/4,1/2,z (4 <sub>z</sub>  1/4,3/4,1/4)'
(17) 4' (3/4,0,0) x,1/4,0 (4 <sub>x</sub> <sup>-1</sup>  3/4,1/4,1/4)'	(18) 2' (0,1/2,1/2) 1/8,y+1/4,y (2 <sub>yz</sub>  1/4,3/4,1/4)'	(19) 2' 3/8,y+3/4,y (2 <sub>yz</sub>  3/4,3/4,3/4)'	(20) 4 <sup>+</sup> (1/4,0,0) x,-1/4,1/2 (4 <sub>x</sub>  1/4,1/4,3/4)'
(21) 4 <sup>+</sup> (0,1/4,0) 1/2,y,-1/4 (4 <sub>y</sub>  3/4,1/4,1/4)'	(22) 2' (1/2,0,1/2) x-1/4,1/8,x (2 <sub>xz</sub>  1/4,1/4,3/4)'	(23) 4' (0,3/4,0) 0,y,1/4 (4 <sub>y</sub> <sup>-1</sup>  1/4,3/4,1/4)'	(24) 2' x+3/4,3/8,x (2 <sub>xz</sub>  3/4,3/4,3/4)'

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (1 1/2,1/2,1/2)'	(2) 2' 0,1/4,z (2 <sub>z</sub>  0,1/2,0)'	(3) 2' 1/4,y,0 (2 <sub>y</sub>  1/2,0,0)'	(4) 2' x,0,1/4 (2 <sub>x</sub>  0,0,1/2)'
(5) 3 <sup>+</sup> (1/2,1/2,1/2) x,x,x (3 <sub>xyz</sub>  1/2,1/2,1/2)'	(6) 3 <sup>+</sup> (1/6,-1/6,1/6) x-1/6,x+1/3,x (3 <sub>xyz</sub> <sup>-1</sup>  0,0,1/2)'	(7) 3 <sup>+</sup> (-1/6,1/6,1/6) x+1/6,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,0)'	(8) 3 <sup>+</sup> (1/6,1/6,-1/6) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,0)'
(9) 3 <sup>-</sup> (1/2,1/2,1/2) x,x,x (3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(10) 3 <sup>-</sup> (1/6,-1/6,-1/6) x+1/6,x+1/6,x (3 <sub>xyz</sub>  1/2,0,0)'	(11) 3 <sup>-</sup> (-1/6,-1/6,1/6) x+1/3,x+1/6,x (3 <sub>xyz</sub>  0,0,1/2)'	(12) 3 <sup>-</sup> (-1/6,1/6,-1/6) x-1/6,x+1/3,x (3 <sub>xyz</sub>  0,1/2,0)'
(13) 2 (1/2,1/2,0) x,x+1/4,3/8 (2 <sub>xy</sub>  1/4,3/4,3/4)	(14) 2 x,x+1/4,1/8 (2 <sub>xy</sub>  1/4,1/4,1/4)	(15) 4 (0,0,1/4) 3/4,0,z (4 <sub>z</sub> <sup>-1</sup>  3/4,3/4,1/4)	(16) 4 <sup>+</sup> (0,0,3/4) 1/4,1/2,z (4 <sub>z</sub>  3/4,1/4,3/4)
(17) 4 (1/4,0,0) x,3/4,0 (4 <sub>x</sub> <sup>-1</sup>  1/4,3/4,3/4)	(18) 2 (0,1/2,1/2) 3/8,y-1/4,y (2 <sub>yz</sub>  3/4,1/4,3/4)	(19) 2 1/8,y+1/4,y (2 <sub>yz</sub>  1/4,1/4,1/4)	(20) 4 <sup>+</sup> (3/4,0,0) x,1/4,1/2 (4 <sub>x</sub>  3/4,3/4,1/4)
(21) 4 <sup>+</sup> (0,3/4,0) 1/2,y,1/4 (4 <sub>y</sub>  1/4,3/4,3/4)	(22) 2 (1/2,0,1/2) x+1/4,3/8,x (2 <sub>xz</sub>  3/4,3/4,1/4)	(23) 4 (0,1/4,0) 0,y,3/4 (4 <sub>y</sub> <sup>-1</sup>  3/4,1/4,3/4)	(24) 2 x+1/4,1/8,x (2 <sub>xz</sub>  1/4,1/4,1/4)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13).**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) +	(1/2,1/2,1/2)' +		
48 i 1				
(1) x,y,z [u,v,w]	(2) x+1/2,y,z+1/2 [u,v,w]	(3) x,y+1/2,z+1/2 [u,v,w]	(4) x+1/2,y+1/2,z [u,v,w]	
(5) z,x,y [w,u,v]	(6) z+1/2,x+1/2,y [w,u,v]	(7) z+1/2,x,y+1/2 [w,u,v]	(8) z,x+1/2,y+1/2 [w,u,v]	
(9) y,z,x [v,w,u]	(10) y,z+1/2,x+1/2 [v,w,u]	(11) y+1/2,z+1/2,x [v,w,u]	(12) y+1/2,z,x+1/2 [v,w,u]	
(13) y+3/4,x+1/4,z+1/4 [v,u,w]	(14) y+3/4,x+3/4,z+3/4 [v,u,w]	(15) y+1/4,x+1/4,z+3/4 [v,u,w]	(16) y+1/4,x+3/4,z+1/4 [v,u,w]	
(17) x+3/4,z+1/4,y+1/4 [u,w,v]	(18) x+1/4,z+3/4,y+1/4 [u,w,v]	(19) x+3/4,z+3/4,y+3/4 [u,w,v]	(20) x+1/4,z+1/4,y+3/4 [u,w,v]	
(21) z+3/4,y+1/4,x+1/4 [w,v,u]	(22) z+1/4,y+1/4,x+3/4 [w,v,u]	(23) z+1/4,y+3/4,x+1/4 [w,v,u]	(24) z+3/4,y+3/4,x+3/4 [w,v,u]	

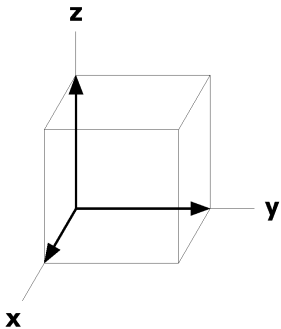
24	h	..2	$1/8, y, \bar{y}+1/4 [0, \bar{v}, v]$ $\bar{y}+1/4, 1/8, y [v, 0, \bar{v}]$ $y, \bar{y}+1/4, 1/8 [\bar{v}, v, 0]$	$3/8, \bar{y}, \bar{y}+3/4 [0, v, v]$ $\bar{y}+3/4, 3/8, \bar{y} [v, 0, v]$ $\bar{y}, \bar{y}+3/4, 3/8 [v, v, 0]$	$7/8, y+1/2, y+1/4 [\bar{v}, \bar{v}, 0]$ $y+1/4, 7/8, y+1/2 [\bar{v}, 0, \bar{v}]$ $y+1/2, y+1/4, 7/8 [\bar{v}, \bar{v}, 0]$	$5/8, \bar{y}+1/2, y+3/4 [0, v, \bar{v}]$ $y+3/4, 5/8, \bar{y}+1/2 [\bar{v}, 0, v]$ $\bar{y}+1/2, y+3/4, 5/8 [v, \bar{v}, 0]$
24	g	..2	$1/8, y, y+1/4 [u, v, \bar{v}]$ $y+1/4, 1/8, y [\bar{v}, u, v]$ $y, y+1/4, 1/8 [v, \bar{v}, u]$	$3/8, \bar{y}, y+3/4 [\bar{u}, \bar{v}, \bar{v}]$ $y+3/4, 3/8, \bar{y} [\bar{v}, \bar{u}, \bar{v}]$ $\bar{y}, y+3/4, 3/8 [\bar{v}, \bar{v}, \bar{u}]$	$7/8, y+1/2, \bar{y}+1/4 [\bar{u}, v, v]$ $\bar{y}+1/4, 7/8, y+1/2 [v, \bar{u}, v]$ $y+1/2, \bar{y}+1/4, 7/8 [v, v, \bar{u}]$	$5/8, \bar{y}+1/2, \bar{y}+3/4 [u, \bar{v}, v]$ $\bar{y}+3/4, 5/8, \bar{y}+1/2 [v, u, \bar{v}]$ $\bar{y}+1/2, \bar{y}+3/4, 5/8 [\bar{v}, v, u]$
24	f	2..	$x, 0, 1/4 [u, 0, 0]$ $0, 1/4, x [0, 0, u]$ $x+3/4, 1/2, 1/4 [\bar{u}, 0, 0]$	$\bar{x}+1/2, 0, 3/4 [\bar{u}, 0, 0]$ $0, 3/4, \bar{x}+1/2 [0, 0, \bar{u}]$ $\bar{x}+1/4, 0, 1/4 [u, 0, 0]$	$1/4, x, 0 [0, u, 0]$ $3/4, x+1/4, 0 [0, \bar{u}, 0]$ $0, 1/4, \bar{x}+1/4 [0, 0, u]$	$3/4, \bar{x}+1/2, 0 [0, \bar{u}, 0]$ $3/4, \bar{x}+3/4, 1/2 [0, u, 0]$ $1/2, 1/4, x+3/4 [0, 0, \bar{u}]$
16	e	.3.	$x, x, x [u, u, u]$ $\bar{x}, x+1/2, \bar{x}+1/2 [\bar{u}, u, \bar{u}]$ $x+3/4, x+1/4, \bar{x}+1/4 [\bar{u}, \bar{u}, u]$ $x+1/4, \bar{x}+1/4, x+3/4 [\bar{u}, u, \bar{u}]$	$\bar{x}+1/2, \bar{x}, x+1/2 [\bar{u}, \bar{u}, u]$ $x+1/2, \bar{x}+1/2, \bar{x} [u, \bar{u}, \bar{u}]$ $\bar{x}+3/4, \bar{x}+3/4, \bar{x}+3/4 [u, u, u]$ $\bar{x}+1/4, x+3/4, x+1/4 [u, \bar{u}, \bar{u}]$		
12	d	2'.2'2	$5/8, 0, 1/4 [0, \bar{v}, v]$ $3/4, 7/8, 0 [v, 0, v]$	$7/8, 0, 3/4 [0, v, v]$ $0, 1/4, 5/8 [\bar{v}, v, 0]$	$1/4, 5/8, 0 [v, 0, \bar{v}]$ $0, 3/4, 7/8 [v, v, 0]$	
12	c	2'.2'2	$1/8, 0, 1/4 [0, \bar{v}, v]$ $3/4, 3/8, 0 [v, 0, v]$	$3/8, 0, 3/4 [0, v, v]$ $0, 1/4, 1/8 [\bar{v}, v, 0]$	$1/4, 1/8, 0 [v, v, 0]$ $0, 3/4, 3/8 [0, 0, \bar{u}]$	
8	b	.32'	$7/8, 7/8, 7/8 [u, u, u]$	$5/8, 1/8, 3/8 [\bar{u}, \bar{u}, u]$	$1/8, 3/8, 5/8 [\bar{u}, u, \bar{u}]$	$3/8, 5/8, 1/8 [u, \bar{u}, \bar{u}]$
8	a	.32	$1/8, 1/8, 1/8 [0, 0, 0]$	$3/8, 7/8, 5/8 [0, 0, 0]$	$7/8, 5/8, 3/8 [0, 0, 0]$	$5/8, 3/8, 7/8 [0, 0, 0]$

**Symmetry of Special Projections**

Along  $[0, 0, 1]$   $p_p \cdot 4'mm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $1/4, 0, z$

Along  $[1, 1, 1]$   $p_{3m}11'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

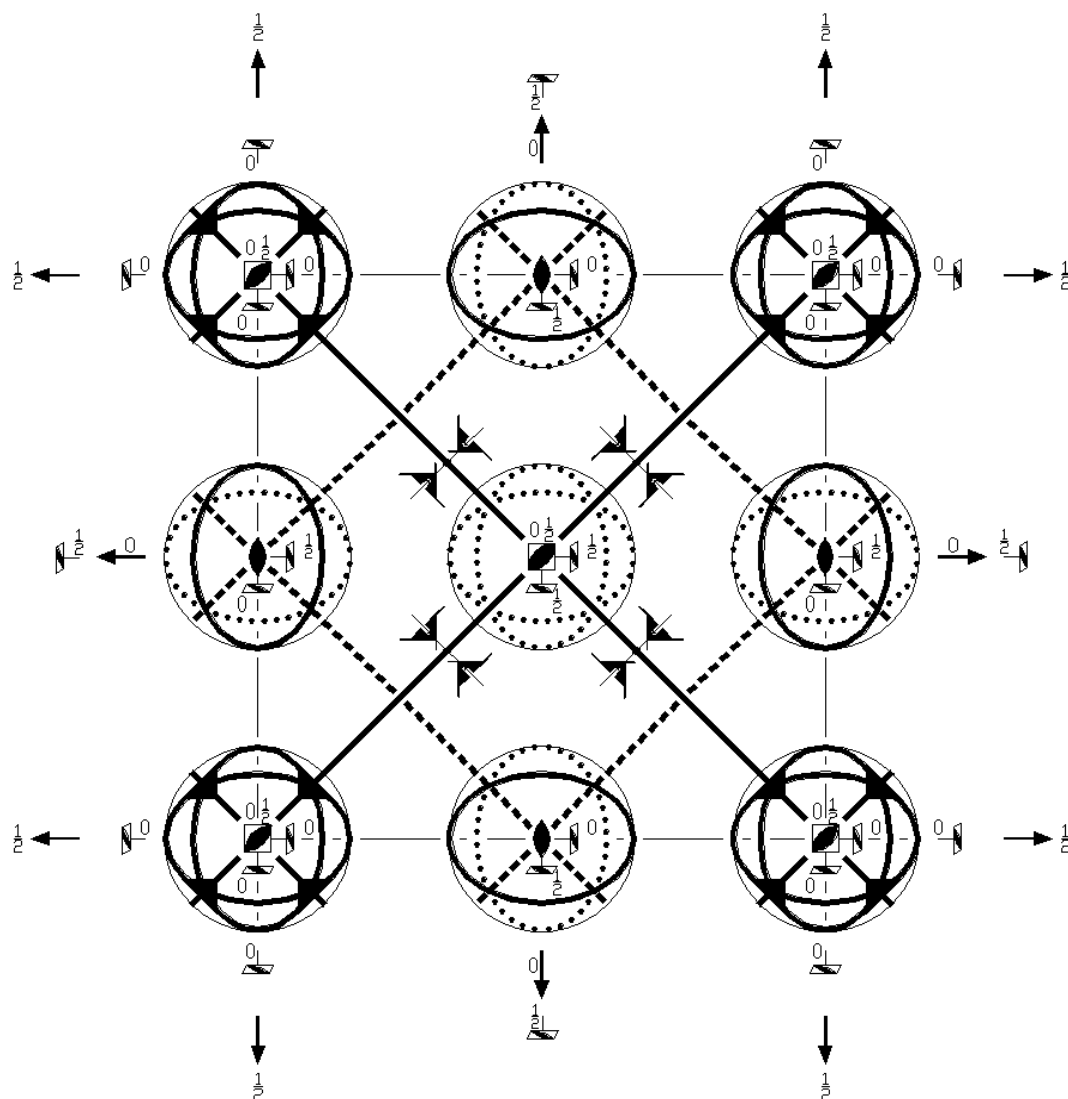
Along  $[1, 1, 0]$   $p_{2a} \cdot 2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, x+1/4, 5/8$



$P\bar{4}3m$   
215.1.1572

$\bar{4}3m$   
 $P\bar{4}3m$

Cubic



Origin at  $\bar{4}3m$

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq \min(x, 1-x);$   $z \leq y$

**Vertices**  $0,0,0$   $1,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                  | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)              |

(13) m $x,x,z$ ( $m_{\bar{xy}} 0,0,0$ )	(14) m $x,\bar{x},z$ ( $m_{xy} 0,0,0$ )	(15) $\bar{4}^+$ $0,0,z; 0,0,0$ ( $\bar{4}_z 0,0,0$ )	(16) $\bar{4}^-$ $0,0,z; 0,0,0$ ( $\bar{4}_z^{-1} 0,0,0$ )
(17) m $x,y,y$ ( $m_{\bar{yz}} 0,0,0$ )	(18) $\bar{4}^+$ $x,0,0; 0,0,0$ ( $\bar{4}_x 0,0,0$ )	(19) $\bar{4}^-$ $x,0,0; 0,0,0$ ( $\bar{4}_x^{-1} 0,0,0$ )	(20) m $x,y,\bar{y}$ ( $m_{yz} 0,0,0$ )
(21) m $x,y,x$ ( $m_{\bar{zx}} 0,0,0$ )	(22) $\bar{4}^-$ $0,y,0; 0,0,0$ ( $\bar{4}_y^{-1} 0,0,0$ )	(23) m $\bar{x},y,x$ ( $m_{xz} 0,0,0$ )	(24) $\bar{4}^+$ $0,y,0; 0,0,0$ ( $\bar{4}_y 0,0,0$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

24	j	1									
(1)	$x,y,z$	[u,v,w]	(2)	$\bar{x},\bar{y},z$	[ $\bar{u},\bar{v},w$ ]	(3)	$\bar{x},y,\bar{z}$	[ $\bar{u},v,\bar{w}$ ]	(4)	$x,\bar{y},\bar{z}$	[ $u,\bar{v},\bar{w}$ ]
(5)	$z,x,y$	[w,u,v]	(6)	$z,\bar{x},\bar{y}$	[ $w,\bar{u},\bar{v}$ ]	(7)	$\bar{z},\bar{x},y$	[ $\bar{w},\bar{u},v$ ]	(8)	$\bar{z},x,\bar{y}$	[ $\bar{w},u,\bar{v}$ ]
(9)	$y,z,x$	[v,w,u]	(10)	$\bar{y},z,\bar{x}$	[ $\bar{v},w,\bar{u}$ ]	(11)	$y,\bar{z},\bar{x}$	[ $v,\bar{w},\bar{u}$ ]	(12)	$\bar{y},\bar{z},x$	[ $\bar{v},\bar{w},u$ ]
(13)	$y,x,z$	[ $\bar{v},\bar{u},\bar{w}$ ]	(14)	$\bar{y},\bar{x},z$	[ $\bar{v},\bar{u},\bar{w}$ ]	(15)	$y,\bar{x},\bar{z}$	[ $\bar{v},\bar{u},\bar{w}$ ]	(16)	$\bar{y},x,\bar{z}$	[ $\bar{v},\bar{u},\bar{w}$ ]
(17)	$x,z,y$	[ $\bar{u},\bar{w},\bar{v}$ ]	(18)	$\bar{x},z,\bar{y}$	[ $\bar{u},\bar{w},\bar{v}$ ]	(19)	$\bar{x},\bar{z},y$	[ $\bar{u},\bar{w},\bar{v}$ ]	(20)	$x,\bar{z},\bar{y}$	[ $\bar{u},\bar{w},\bar{v}$ ]
(21)	$z,y,x$	[ $\bar{w},\bar{v},\bar{u}$ ]	(22)	$z,\bar{y},\bar{x}$	[ $\bar{w},\bar{v},\bar{u}$ ]	(23)	$\bar{z},y,\bar{x}$	[ $\bar{w},\bar{v},\bar{u}$ ]	(24)	$\bar{z},\bar{y},x$	[ $\bar{w},\bar{v},\bar{u}$ ]
12	i	..m	$x,x,z$	[ $u,\bar{u},0$ ]	$\bar{x},\bar{x},z$	[ $\bar{u},u,0$ ]	$\bar{x},x,\bar{z}$	[ $\bar{u},\bar{u},0$ ]	$x,\bar{x},\bar{z}$	[ $u,u,0$ ]	
			$z,x,x$	[ $0,u,\bar{u}$ ]	$z,\bar{x},\bar{x}$	[ $0,\bar{u},u$ ]	$\bar{z},\bar{x},x$	[ $0,\bar{u},\bar{u}$ ]	$\bar{z},x,\bar{x}$	[ $0,u,u$ ]	
			$x,z,x$	[ $\bar{u},0,u$ ]	$\bar{x},z,\bar{x}$	[ $\bar{u},0,\bar{u}$ ]	$x,\bar{z},\bar{x}$	[ $\bar{u},0,\bar{u}$ ]	$\bar{x},z,x$	[ $u,0,u$ ]	
12	h	2..	$x,1/2,0$	[ $u,0,0$ ]	$\bar{x},1/2,0$	[ $\bar{u},0,0$ ]	$0,x,1/2$	[ $0,u,0$ ]	$0,\bar{x},1/2$	[ $0,\bar{u},0$ ]	
			$1/2,0,x$	[ $0,0,u$ ]	$1/2,0,\bar{x}$	[ $0,0,\bar{u}$ ]	$1/2,x,0$	[ $0,\bar{u},0$ ]	$1/2,\bar{x},0$	[ $0,u,0$ ]	
			$x,0,1/2$	[ $\bar{u},0,0$ ]	$\bar{x},0,1/2$	[ $u,0,0$ ]	$0,1/2,x$	[ $0,0,\bar{u}$ ]	$0,1/2,\bar{x}$	[ $0,0,u$ ]	
6	g	2.mm	$x,1/2,1/2$	[ $0,0,0$ ]	$\bar{x},1/2,1/2$	[ $0,0,0$ ]	$1/2,x,1/2$	[ $0,0,0$ ]	$1/2,1/2,\bar{x}$	[ $0,0,0$ ]	
			$1/2,\bar{x},1/2$	[ $0,0,0$ ]	$1/2,1/2,x$	[ $0,0,0$ ]	$1/2,1/2,\bar{x}$	[ $0,0,0$ ]	$1/2,1/2,x$	[ $0,0,0$ ]	
6	f	2.mm	$x,0,0$	[ $0,0,0$ ]	$\bar{x},0,0$	[ $0,0,0$ ]	$0,x,0$	[ $0,0,0$ ]	$0,0,\bar{x}$	[ $0,0,0$ ]	
			$0,\bar{x},0$	[ $0,0,0$ ]	$0,0,x$	[ $0,0,0$ ]	$0,0,\bar{x}$	[ $0,0,0$ ]	$0,0,x$	[ $0,0,0$ ]	
4	e	.3m	$x,x,x$	[ $0,0,0$ ]	$\bar{x},\bar{x},x$	[ $0,0,0$ ]	$\bar{x},x,\bar{x}$	[ $0,0,0$ ]	$x,\bar{x},\bar{x}$	[ $0,0,0$ ]	
3	d	$\bar{4}2.m$	$1/2,0,0$	[ $0,0,0$ ]	$0,1/2,0$	[ $0,0,0$ ]	$0,0,1/2$	[ $0,0,0$ ]	$0,0,1/2$	[ $0,0,0$ ]	

3	c	$\overline{4}2.m$	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
1	b	$\overline{4}3m$	1/2,1/2,1/2 [0,0,0]		
1	a	$\overline{4}3m$	0,0,0 [0,0,0]		

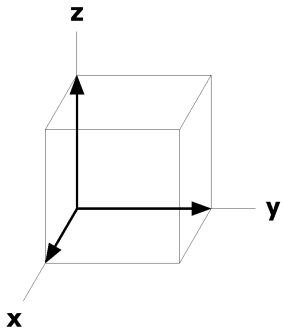
**Symmetry of Special Projections**

Along [0,0,1]  $p4'm'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,1,1]  $p31m$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0

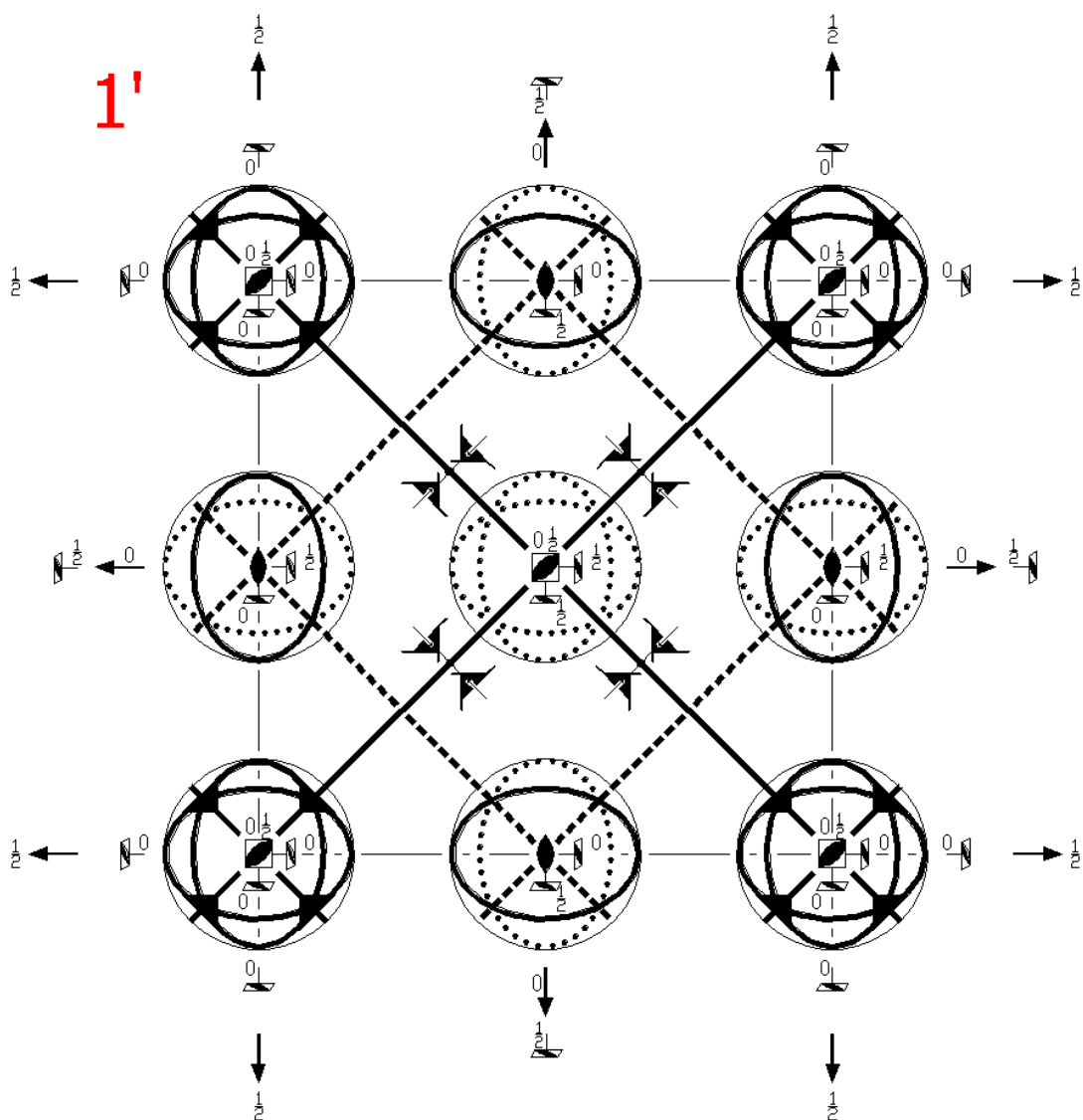




$P\bar{4}3m1'$   
215.2.1573

$\bar{4}3m1'$   
 $P\bar{4}3m1'$

Cubic



Origin at  $\bar{4}3m1'$

**Asymmetric unit**  $0 \leq x \leq 1;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq \min(x, 1-x);$   $z \leq y$

**Vertices**  $0,0,0$   $1,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

For 1 + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                         | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xyz}^{-1}</math></sub>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}^{-1}</math></sub>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xyz}^{-1}</math></sub>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{xyz}^{-1}</math></sub>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)    | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)      | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)     |

(13) m $\bar{x},x,z$ ( $m_{\bar{xy}} 0,0,0$ )	(14) m $x,\bar{x},z$ ( $m_{xy} 0,0,0$ )	(15) $\bar{4}^+$ $0,0,z; 0,0,0$ ( $\bar{4}_z 0,0,0$ )	(16) $\bar{4}^-$ $0,0,z; 0,0,0$ ( $\bar{4}_z^{-1} 0,0,0$ )
(17) m $x,y,y$ ( $m_{\bar{yz}} 0,0,0$ )	(18) $\bar{4}^+$ $x,0,0; 0,0,0$ ( $\bar{4}_x 0,0,0$ )	(19) $\bar{4}^-$ $x,0,0; 0,0,0$ ( $\bar{4}_x^{-1} 0,0,0$ )	(20) m $x,y,\bar{y}$ ( $m_{yz} 0,0,0$ )
(21) m $x,y,x$ ( $m_{\bar{zx}} 0,0,0$ )	(22) $\bar{4}^-$ $0,y,0; 0,0,0$ ( $\bar{4}_y^{-1} 0,0,0$ )	(23) m $\bar{x},y,x$ ( $m_{xz} 0,0,0$ )	(24) $\bar{4}^+$ $0,y,0; 0,0,0$ ( $\bar{4}_y 0,0,0$ )

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' $0,0,z$ ( $2_z 0,0,0$ )'	(3) 2' $0,y,0$ ( $2_y 0,0,0$ )'	(4) 2' $x,0,0$ ( $2_x 0,0,0$ )'
(5) $3^{+ '}$ $x,x,x$ ( $3_{xyz} 0,0,0$ )'	(6) $3^{+ '}$ $\bar{x},x,\bar{x}$ ( $3_{\bar{xyz}}^{-1} 0,0,0$ )'	(7) $3^{+ '}$ $x,\bar{x},\bar{x}$ ( $3_{\bar{xyz}}^{-1} 0,0,0$ )'	(8) $3^{+ '}$ $\bar{x},\bar{x},x$ ( $3_{xyz}^{-1} 0,0,0$ )'
(9) $3^{- '}$ $x,x,x$ ( $3_{xyz}^{-1} 0,0,0$ )'	(10) $3^{- '}$ $x,\bar{x},\bar{x}$ ( $3_{\bar{xyz}} 0,0,0$ )'	(11) $3^{- '}$ $\bar{x},\bar{x},x$ ( $3_{\bar{xyz}} 0,0,0$ )'	(12) $3^{- '}$ $\bar{x},x,\bar{x}$ ( $3_{xyz} 0,0,0$ )'
(13) m' $\bar{x},x,z$ ( $m_{\bar{xy}} 0,0,0$ )'	(14) m' $x,\bar{x},z$ ( $m_{xy} 0,0,0$ )'	(15) $\bar{4}^{+ '}$ $0,0,z; 0,0,0$ ( $\bar{4}_z 0,0,0$ )'	(16) $\bar{4}^{- '}$ $0,0,z; 0,0,0$ ( $\bar{4}_z^{-1} 0,0,0$ )'
(17) m' $x,y,y$ ( $m_{\bar{yz}} 0,0,0$ )'	(18) $\bar{4}^{+ '}$ $x,0,0; 0,0,0$ ( $\bar{4}_x 0,0,0$ )'	(19) $\bar{4}^{- '}$ $x,0,0; 0,0,0$ ( $\bar{4}_x^{-1} 0,0,0$ )'	(20) m' $x,y,\bar{y}$ ( $m_{yz} 0,0,0$ )'
(21) m' $x,y,x$ ( $m_{\bar{zx}} 0,0,0$ )'	(22) $\bar{4}^{- '}$ $0,y,0; 0,0,0$ ( $\bar{4}_y^{-1} 0,0,0$ )'	(23) m' $\bar{x},y,x$ ( $m_{xz} 0,0,0$ )'	(24) $\bar{4}^{+ '}$ $0,y,0; 0,0,0$ ( $\bar{4}_y 0,0,0$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); 1'.

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

24 j 11'

(1) $x,y,z$ [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{x},y,\bar{z}$ [0,0,0]	(4) $x,\bar{y},\bar{z}$ [0,0,0]
(5) $z,x,y$ [0,0,0]	(6) $z,\bar{x},\bar{y}$ [0,0,0]	(7) $\bar{z},\bar{x},y$ [0,0,0]	(8) $\bar{z},x,\bar{y}$ [0,0,0]
(9) $y,z,x$ [0,0,0]	(10) $\bar{y},z,\bar{x}$ [0,0,0]	(11) $y,\bar{z},\bar{x}$ [0,0,0]	(12) $\bar{y},\bar{z},x$ [0,0,0]
(13) $y,x,z$ [0,0,0]	(14) $\bar{y},\bar{x},z$ [0,0,0]	(15) $y,\bar{x},\bar{z}$ [0,0,0]	(16) $\bar{y},x,\bar{z}$ [0,0,0]
(17) $x,z,y$ [0,0,0]	(18) $\bar{x},z,\bar{y}$ [0,0,0]	(19) $\bar{x},\bar{z},y$ [0,0,0]	(20) $x,\bar{z},\bar{y}$ [0,0,0]
(21) $z,y,x$ [0,0,0]	(22) $z,\bar{y},\bar{x}$ [0,0,0]	(23) $\bar{z},y,\bar{x}$ [0,0,0]	(24) $\bar{z},\bar{y},x$ [0,0,0]

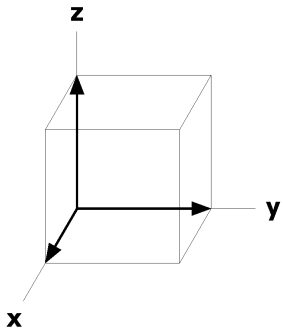
12	i	$\bar{1}m1'$	$x,x,z [0,0,0]$	$\bar{x},\bar{x},z [0,0,0]$	$\bar{x},x,\bar{z} [0,0,0]$	$x,\bar{x},\bar{z} [0,0,0]$
			$z,x,x [0,0,0]$	$z,\bar{x},\bar{x} [0,0,0]$	$\bar{z},\bar{x},x [0,0,0]$	$\bar{z},x,\bar{x} [0,0,0]$
			$x,z,x [0,0,0]$	$\bar{x},z,\bar{x} [0,0,0]$	$x,\bar{z},\bar{x} [0,0,0]$	$\bar{x},\bar{z},x [0,0,0]$
12	h	$2..1'$	$x,1/2,0 [0,0,0]$	$\bar{x},1/2,0 [0,0,0]$	$0,x,1/2 [0,0,0]$	$0,\bar{x},1/2 [0,0,0]$
			$1/2,0,x [0,0,0]$	$1/2,0,\bar{x} [0,0,0]$	$1/2,x,0 [0,0,0]$	$1/2,\bar{x},0 [0,0,0]$
			$x,0,1/2 [0,0,0]$	$\bar{x},0,1/2 [0,0,0]$	$0,1/2,x [0,0,0]$	$0,1/2,\bar{x} [0,0,0]$
6	g	$2.mm1'$	$x,1/2,1/2 [0,0,0]$	$\bar{x},1/2,1/2 [0,0,0]$		$1/2,x,1/2 [0,0,0]$
			$1/2,\bar{x},1/2 [0,0,0]$	$1/2,1/2,x [0,0,0]$		$1/2,1/2,\bar{x} [0,0,0]$
6	f	$2.mm1'$	$x,0,0 [0,0,0]$	$\bar{x},0,0 [0,0,0]$		$0,x,0 [0,0,0]$
			$0,\bar{x},0 [0,0,0]$	$0,0,x [0,0,0]$		$0,0,\bar{x} [0,0,0]$
4	e	$.3m1'$	$x,x,x [0,0,0]$	$\bar{x},\bar{x},x [0,0,0]$	$\bar{x},x,\bar{x} [0,0,0]$	$x,\bar{x},\bar{x} [0,0,0]$
3	d	$\bar{4}2.m1'$	$1/2,0,0 [0,0,0]$		$0,1/2,0 [0,0,0]$	$0,0,1/2 [0,0,0]$
3	c	$\bar{4}2.m1'$	$0,1/2,1/2 [0,0,0]$		$1/2,0,1/2 [0,0,0]$	$1/2,1/2,0 [0,0,0]$
1	b	$\bar{4}3m1'$	$1/2,1/2,1/2 [0,0,0]$			
1	a	$\bar{4}3m1'$	$0,0,0 [0,0,0]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $a^* = a$   $b^* = b$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p31m1'$   
 $a^* = (2a - b - c)/3$   $b^* = (-a + 2b - c)/3$   
 Origin at  $x,x,x$

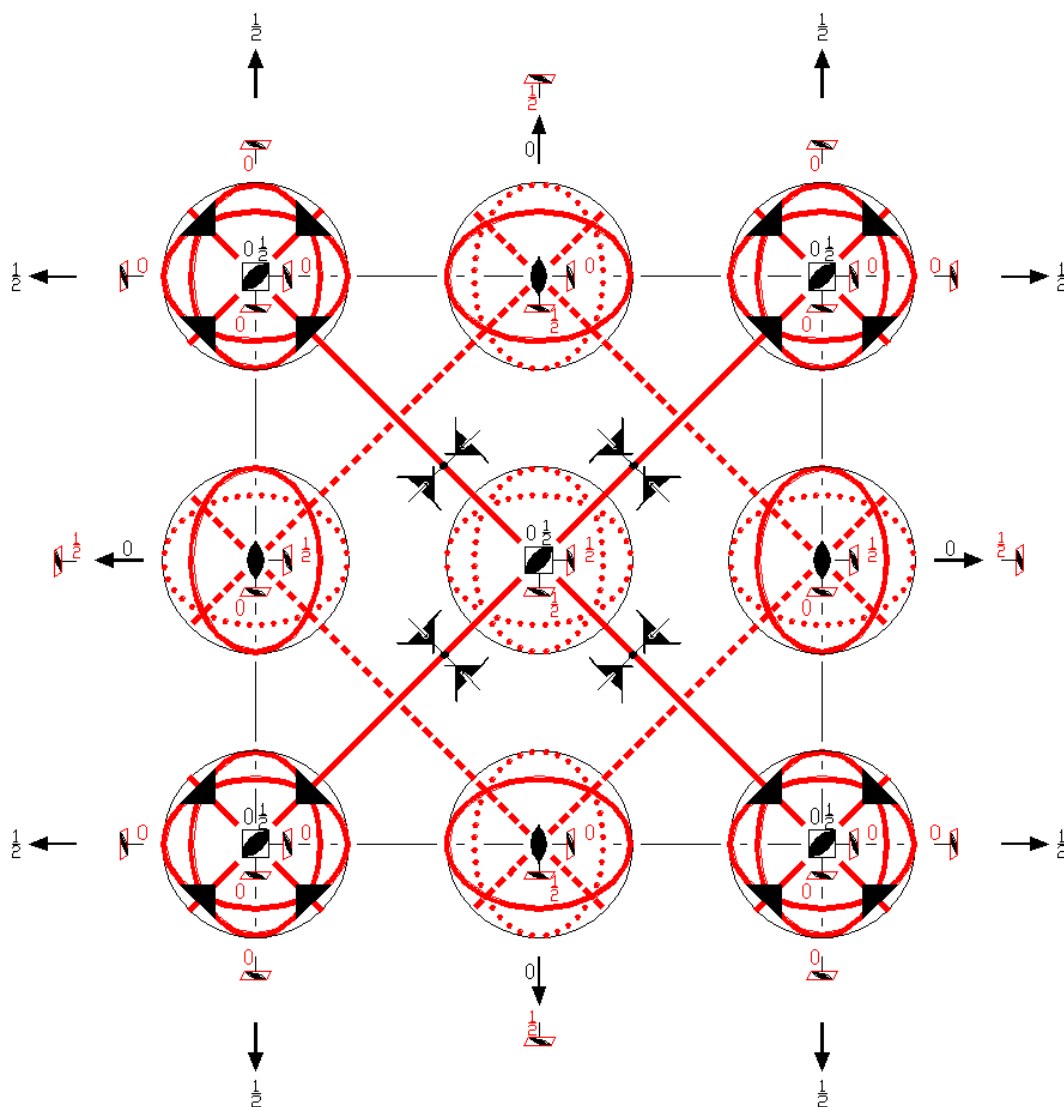
Along  $[1,1,0]$   $p1m11'$   
 $a^* = (-a + b)/2$   $b^* = c$   
 Origin at  $x,x,0$



$P\bar{4}'3m'$   
215.3.1574

$\bar{4}'3m'$   
 $P\bar{4}'3m'$

Cubic



Origin at  $\bar{4}'3m'$

**Asymmetric unit**     $0 \leq x \leq 1;$      $0 \leq y \leq 1/2;$      $0 \leq z \leq 1/2;$      $y \leq \min(x, 1-x);$      $z \leq y$

**Vertices**     $0,0,0$      $1,0,0$      $1/2,1/2,0$      $1/2,1/2,1/2$

**Symmetry Operations**

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                  | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)              |

(13) m' x,x,z (m <sub>xy</sub> ̄ 0,0,0)'	(14) m' x,x̄,z (m <sub>xy</sub>  0,0,0)'	(15) 4 <sup>+</sup> ' 0,0,z; 0,0,0 (4 <sub>z</sub> ̄ 0,0,0)'	(16) 4 <sup>-</sup> ' 0,0,z; 0,0,0 (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'
(17) m' x,y,y (m <sub>yz</sub> ̄ 0,0,0)'	(18) 4 <sup>+</sup> ' x,0,0; 0,0,0 (4 <sub>x</sub> ̄ 0,0,0)'	(19) 4 <sup>-</sup> ' x,0,0; 0,0,0 (4 <sub>x</sub> <sup>-1</sup>  0,0,0)'	(20) m' x,y,ȳ (m <sub>yz</sub>  0,0,0)'
(21) m' x,y,x (m <sub>xz</sub> ̄ 0,0,0)'	(22) 4 <sup>-</sup> ' 0,y,0; 0,0,0 (4 <sub>y</sub> <sup>-1</sup>  0,0,0)'	(23) m' x̄,y,x (m <sub>xz</sub>  0,0,0)'	(24) 4 <sup>+</sup> ' 0,y,0; 0,0,0 (4 <sub>y</sub>  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

24	j	1									
(1)	x,y,z	[u,v,w]	(2)	x̄,ȳ,z	[ū,v̄,w]	(3)	x̄,y,z̄	[ū,v,w̄]	(4)	x,ȳ,z̄	[u,v̄,w̄]
(5)	z,x,y	[w,u,v]	(6)	z,x̄,ȳ	[w,ū,v̄]	(7)	z̄,x̄,y	[w̄,ū,v]	(8)	z̄,x,ȳ	[w̄,ū,v̄]
(9)	y,z,x	[v,w,u]	(10)	ȳ,z,x̄	[v̄,w,ū]	(11)	y,z̄,x̄	[v,w̄,ū]	(12)	ȳ,z̄,x	[v̄,w̄,ū]
(13)	y,x,z	[v,u,w]	(14)	ȳ,x̄,z	[v̄,ū,w]	(15)	y,x̄,z̄	[v,ū,w̄]	(16)	ȳ,x,z̄	[v̄,ū,w̄]
(17)	x,z,y	[u,w,v]	(18)	x̄,z,ȳ	[ū,w̄,v̄]	(19)	x̄,z̄,y	[ū,w̄,v]	(20)	x,z̄,ȳ	[ū,w̄,v̄]
(21)	z,y,x	[w,v,u]	(22)	z,ȳ,x̄	[w̄,v̄,ū]	(23)	z̄,y,x̄	[w̄,v,ū]	(24)	z̄,ȳ,x	[w̄,v̄,ū]
12	i	..m'	x,x,z	[u,u,w]	x̄,x̄,z	[ū,ū,w]	x̄,x,z̄	[ū,u,w̄]	x,x̄,z̄	[u,ū,w̄]	
			z,x,x	[w,u,u]	z,x̄,x̄	[w,ū,ū]	z̄,x̄,x	[w̄,ū,u]	z̄,x,x̄	[w̄,ū,ū]	
			x,z,x	[u,w,u]	x̄,z,x̄	[ū,w,ū]	x̄,z̄,x̄	[ū,w̄,ū]	x̄,z,x̄	[ū,w̄,ū]	
12	h	2..	x,1/2,0	[u,0,0]	x̄,1/2,0	[ū,0,0]	0,x,1/2	[0,u,0]	0,x̄,1/2	[0,ū,0]	
			1/2,0,x	[0,0,u]	1/2,0,x̄	[0,0,ū]	1/2,x,0	[0,u,0]	1/2,x̄,0	[0,ū,0]	
			x,0,1/2	[u,0,0]	x̄,0,1/2	[ū,0,0]	0,1/2,x	[0,0,u]	0,1/2,x̄	[0,0,ū]	
6	g	2.m'm'	x,1/2,1/2	[u,0,0]	x̄,1/2,1/2	[ū,0,0]	1/2,x,1/2	[0,u,0]	1/2,x̄,1/2	[0,ū,0]	
			1/2,x̄,1/2	[0,ū,0]	1/2,1/2,x	[0,0,ū]	1/2,1/2,x̄	[0,0,ū]	1/2,1/2,x̄	[0,0,ū]	
6	f	2.m'm'	x,0,0	[u,0,0]	x̄,0,0	[ū,0,0]	0,x,0	[0,u,0]	0,x̄,0	[0,ū,0]	
			0,x̄,0	[0,ū,0]	0,0,x	[0,0,ū]	0,0,x̄	[0,0,ū]	0,0,x̄	[0,0,ū]	
4	e	.3m'	x,x,x	[u,u,u]	x̄,x̄,x̄	[ū,ū,ū]	x̄,x,x̄	[ū,ū,ū]	x,x̄,x̄	[u,ū,ū]	
3	d	4̄'2.m'	1/2,0,0	[0,0,0]	0,1/2,0	[0,0,0]	0,0,1/2	[0,0,0]	0,0,1/2	[0,0,0]	

Continued

215.3.1574

$\overline{P4}3m'$

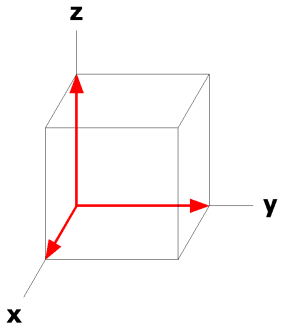
3	c	$\overline{4}2.m'$	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
1	b	$\overline{4}3m'$	1/2,1/2,1/2 [0,0,0]		
1	a	$\overline{4}3m'$	0,0,0 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1]  $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
Origin at 0,0,z

Along [1,1,1]  $p31m'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
Origin at x,x,x

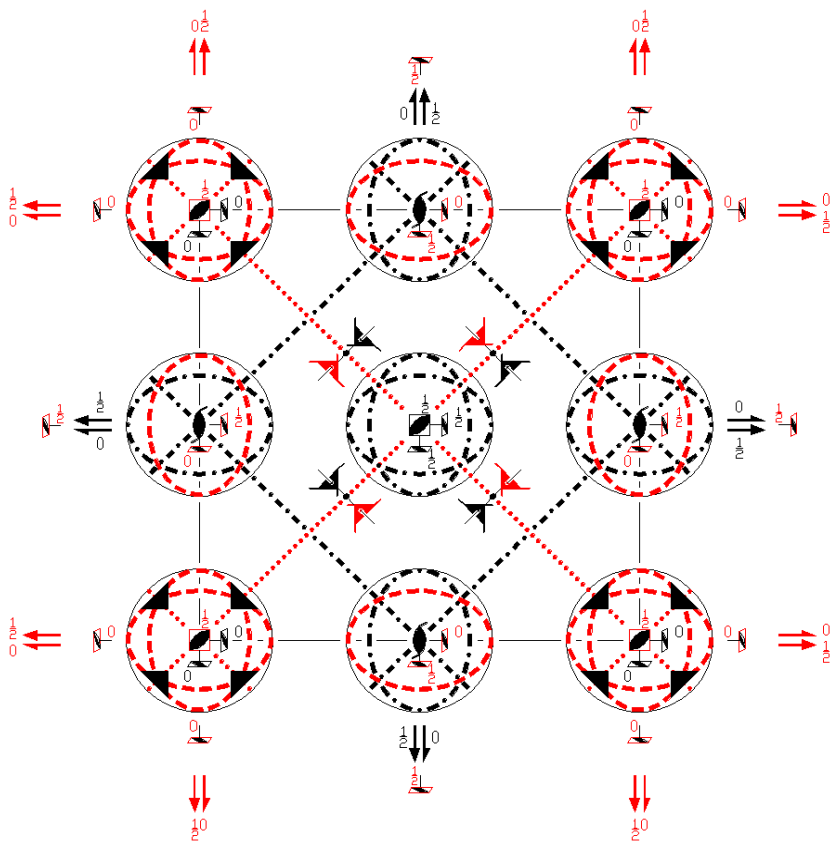
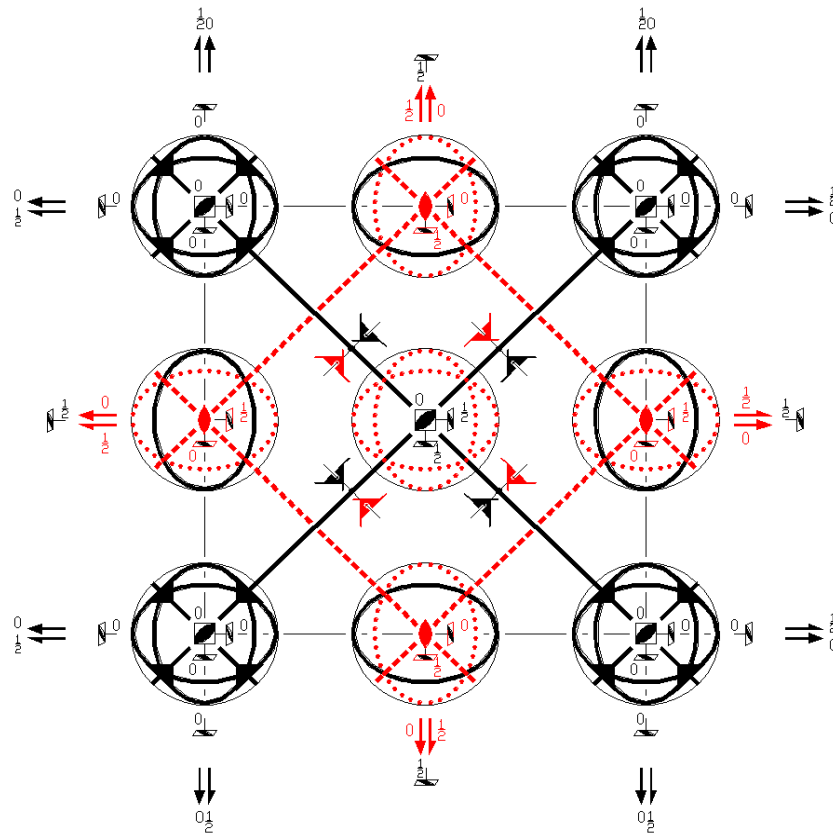
Along [1,1,0]  $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
Origin at x,x,0



$P_F \bar{4}3m$   
215.4.1575

$\bar{4}3m1'$   
 $P_F \bar{4}3m$

Cubic



Origin at  $\bar{4}3m$ 

<b>Asymmetric unit</b>	$0 \leq x \leq 1;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$y \leq \min(x, 1-x);$	$z \leq y$
Vertices	0,0,0	1,0,0	1/2,1/2,0	1/2,1/2,1/2	

## Symmetry Operations

## For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 2 0,y,0 (2 <sub>y</sub>  0,0,0)	(4) 2 x,0,0 (2 <sub>x</sub>  0,0,0)
(5) 3 <sup>+</sup> x,x,x (3 <sub>xyz</sub>  0,0,0)	(6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$ (3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0)	(7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$ (3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0)	(8) 3 <sup>+</sup> $\bar{x},\bar{x},x$ (3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0)
(9) 3 <sup>-</sup> x,x,x (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)	(10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$ (3 <sub><math>\bar{x}yz</math></sub>  0,0,0)	(11) 3 <sup>-</sup> $\bar{x},\bar{x},x$ (3 <sub><math>\bar{x}yz</math></sub>  0,0,0)	(12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$ (3 <sub><math>\bar{x}yz</math></sub>  0,0,0)
(13) m x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,0)	(14) m x, $\bar{x}$ ,z (m <sub><math>\bar{xy}</math></sub>  0,0,0)	(15) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)	(16) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z$ <sup>-1</sup>  0,0,0)
(17) m x,y,y (m <sub><math>\bar{yz}</math></sub>  0,0,0)	(18) $\bar{4}^+$ x,0,0; 0,0,0 ( $\bar{4}_x$  0,0,0)	(19) $\bar{4}^-$ x,0,0; 0,0,0 ( $\bar{4}_x$ <sup>-1</sup>  0,0,0)	(20) m x,y, $\bar{y}$ (m <sub><math>\bar{yz}</math></sub>  0,0,0)
(21) m x,y,x (m <sub><math>\bar{xz}</math></sub>  0,0,0)	(22) $\bar{4}^-$ 0,y,0; 0,0,0 ( $\bar{4}_y$ <sup>-1</sup>  0,0,0)	(23) m $\bar{x}$ ,y,x (m <sub><math>\bar{xz}</math></sub>  0,0,0)	(24) $\bar{4}^+$ 0,y,0; 0,0,0 ( $\bar{4}_y$  0,0,0)

## For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 2' 1/2,y,0 (2 <sub>y</sub>  1,0,0)'	(4) 2' (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)'
(5) 3 <sup>+</sup> ' (1/3,1/3,1/3) x+2/3,x+1/3,x (3 <sub>xyz</sub>  1,0,0)'	(6) 3 <sup>+</sup> ' (1/3,-1/3,1/3) x+2/3,x-1/3,x (3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  1,0,0)'	(7) 3 <sup>+</sup> ' (1/3,-1/3,-1/3) x+2/3,x-1/3,x (3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  1,0,0)'	(8) 3 <sup>+</sup> ' (1/3,1/3,-1/3) x+2/3,x-1/3,x (3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  1,0,0)'
(9) 3 <sup>-</sup> ' (1/3,1/3,1/3) x+1/3,x-1/3,x (3 <sub>xyz</sub> <sup>-1</sup>  1,0,0)'	(10) 3 <sup>-</sup> ' (1/3,-1/3,-1/3) x+1/3,x+1/3,x (3 <sub><math>\bar{x}yz</math></sub>  1,0,0)'	(11) 3 <sup>-</sup> ' (1/3,1/3,-1/3) x+1/3,x-1/3,x (3 <sub><math>\bar{x}yz</math></sub>  1,0,0)'	(12) 3 <sup>-</sup> ' (1/3,-1/3,1/3) x+1/3,x+1/3,x (3 <sub><math>\bar{x}yz</math></sub>  1,0,0)'
(13) g' (1/2,1/2,0) x+1/2,x,z (m <sub><math>\bar{xy}</math></sub>  1,0,0)'	(14) g' (1/2,-1/2,0) x+1/2, $\bar{x}$ ,z (m <sub><math>\bar{xy}</math></sub>  1,0,0)'	(15) $\bar{4}^+$ ' 1/2,-1/2,z; 1/2,-1/2,0 ( $\bar{4}_z$  1,0,0)'	(16) $\bar{4}^-$ ' 1/2,1/2,z; 1/2,1/2,0 ( $\bar{4}_z$ <sup>-1</sup>  1,0,0)'
(17) a' (1,0,0) x,y,y (m <sub><math>\bar{yz}</math></sub>  1,0,0)'	(18) $\bar{4}^+$ ' x+1/2,0,0; 1/2,0,0 ( $\bar{4}_x$  1,0,0)'	(19) $\bar{4}^-$ ' x+1/2,0,0; 1/2,0,0 ( $\bar{4}_x$ <sup>-1</sup>  1,0,0)'	(20) a' (1,0,0) x,y, $\bar{y}$ (m <sub><math>\bar{yz}</math></sub>  1,0,0)'
(21) g' (1/2,0,1/2) x+1/2,y,x (m <sub><math>\bar{xz}</math></sub>  1,0,0)'	(22) $\bar{4}^-$ ' 1/2,y,-1/2; 1/2,0,-1/2 ( $\bar{4}_y$ <sup>-1</sup>  1,0,0)'	(23) g' (1/2,0,-1/2) $\bar{x}$ +1/2,y,x (m <sub><math>\bar{xz}</math></sub>  1,0,0)'	(24) $\bar{4}^+$ ' 1/2,y,1/2; 1/2,0,1/2 ( $\bar{4}_y$  1,0,0)'

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5); (13).



**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (1,0,0)' +

48 j 1

(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
(5) z,x,y [w,u,v]	(6) z, $\bar{x},\bar{y}$ [w, $\bar{u},\bar{v}$ ]	(7) $\bar{z},\bar{x},y$ [ $\bar{w},\bar{u},v$ ]	(8) $\bar{z},x,\bar{y}$ [ $\bar{w},u,\bar{v}$ ]
(9) y,z,x [v,w,u]	(10) $\bar{y},z,\bar{x}$ [ $\bar{v},w,\bar{u}$ ]	(11) y, $\bar{z},\bar{x}$ [v, $\bar{w},\bar{u}$ ]	(12) $\bar{y},\bar{z},x$ [ $\bar{v},\bar{w},u$ ]
(13) y,x,z [ $\bar{v},\bar{u},\bar{w}$ ]	(14) $\bar{y},\bar{x},z$ [v,u, $\bar{w}$ ]	(15) y, $\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(16) $\bar{y},x,\bar{z}$ [v, $\bar{u},\bar{w}$ ]
(17) x,z,y [ $\bar{u},\bar{w},\bar{v}$ ]	(18) $\bar{x},z,\bar{y}$ [u, $\bar{w},\bar{v}$ ]	(19) $\bar{x},\bar{z},y$ [u,w, $\bar{v}$ ]	(20) x, $\bar{z},\bar{y}$ [ $\bar{u},w,\bar{v}$ ]
(21) z,y,x [ $\bar{w},\bar{v},\bar{u}$ ]	(22) z, $\bar{y},\bar{x}$ [ $\bar{w},v,\bar{u}$ ]	(23) $\bar{z},y,\bar{x}$ [w, $\bar{v},\bar{u}$ ]	(24) $\bar{z},\bar{y},x$ [w,v, $\bar{u}$ ]

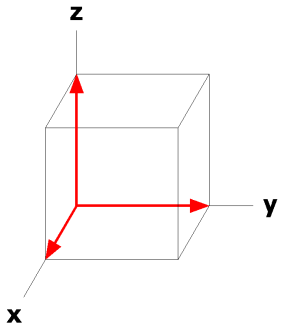
24	i	..m	x,x,z [u, $\bar{u}$ ,0]	$\bar{x},\bar{x},z$ [ $\bar{u},u,0$ ]	$\bar{x},x,\bar{z}$ [ $\bar{u},\bar{u},0$ ]	x, $\bar{x},\bar{z}$ [u,u,0]
			z,x,x [0,u, $\bar{u}$ ]	z, $\bar{x},\bar{x}$ [0, $\bar{u},u$ ]	$\bar{z},\bar{x},x$ [0, $\bar{u},\bar{u}$ ]	$\bar{z},x,\bar{x}$ [0,u,u]
			x,z,x [ $\bar{u}$ ,0,u]	$\bar{x},z,\bar{x}$ [u,0, $\bar{u}$ ]	x, $\bar{z},\bar{x}$ [ $\bar{u}$ ,0, $\bar{u}$ ]	$\bar{x},\bar{z},x$ [u,0,u]
24	h	2'..	x,1/2,0 [0,v,w]	$\bar{x},1/2,0$ [0,v, $\bar{w}$ ]	0,x,1/2 [w,0,v]	0, $\bar{x},1/2$ [ $\bar{w},0,v$ ]
			1/2,0,x [v,w,0]	1/2,0, $\bar{x}$ [v, $\bar{w},0$ ]	1/2,x,0 [ $\bar{v},0,\bar{w}$ ]	1/2, $\bar{x},0$ [ $\bar{v},0,w$ ]
			x,0,1/2 [0, $\bar{w},\bar{v}$ ]	$\bar{x},0,1/2$ [0,w, $\bar{v}$ ]	0,1/2,x [ $\bar{w},\bar{v},0$ ]	0,1/2, $\bar{x}$ [w, $\bar{v},0$ ]
12	g	2.mm	x,1/2,1/2 [0,0,0]	$\bar{x},1/2,1/2$ [0,0,0]	1/2,x,1/2 [0,0,0]	
			1/2, $\bar{x},1/2$ [0,0,0]	1/2,1/2,x [0,0,0]	1/2,1/2, $\bar{x}$ [0,0,0]	
12	f	2.mm	x,0,0 [0,0,0]	$\bar{x},0,0$ [0,0,0]	0,x,0 [0,0,0]	
			0, $\bar{x},0$ [0,0,0]	0,0,x [0,0,0]	0,0, $\bar{x}$ [0,0,0]	
8	e	.3m	x,x,x [0,0,0]	$\bar{x},\bar{x},x$ [0,0,0]	$\bar{x},x,\bar{x}$ [0,0,0]	x, $\bar{x},\bar{x}$ [0,0,0]
6	d	$\bar{4}'2'.m$	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	0,0,1/2 [0,0,0]	
6	c	$\bar{4}'2'.m$	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	
2	b	$\bar{4}3m$	1/2,1/2,1/2 [0,0,0]			
2	a	$\bar{4}3m$	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
a\* = a b\* = b  
Origin at 0,0,z

Along [1,1,1] p31m1'  
a\* = (2a - b - c)/3 b\* = (-a + 2b - c)/3  
Origin at x,x,x

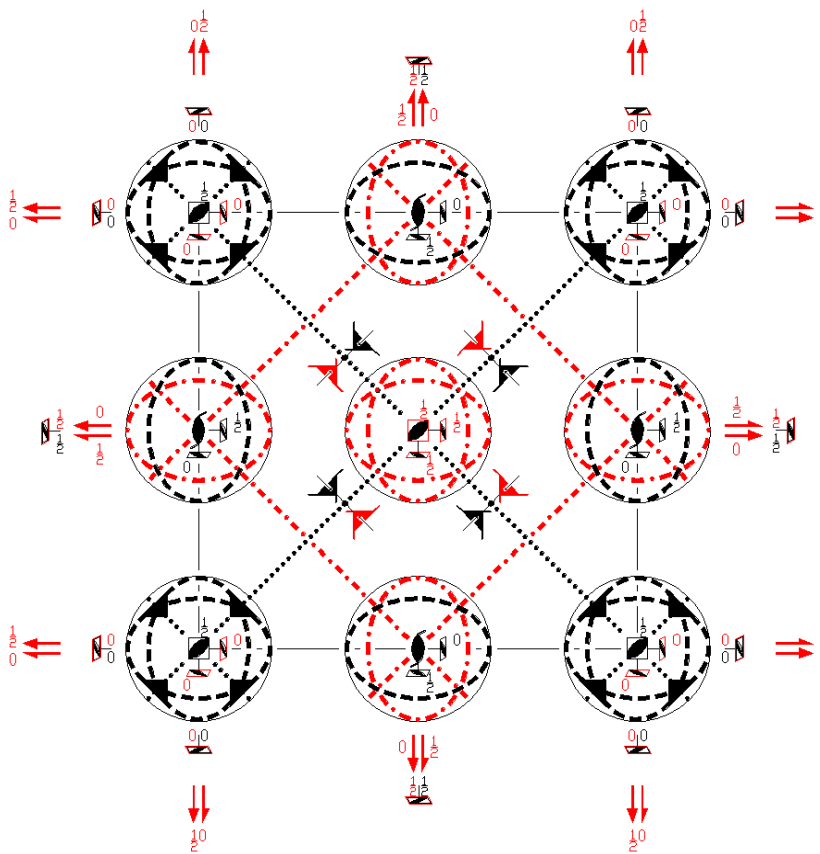
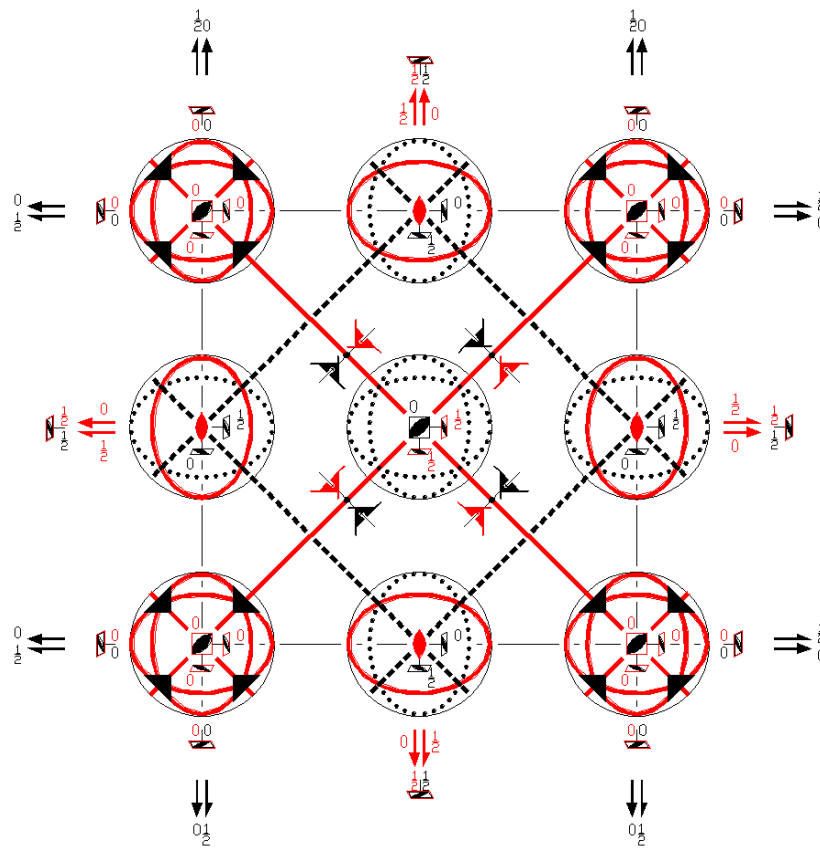
Along [1,1,0] p1m11'  
a\* = (-a + b)/2 b\* = c  
Origin at x,x,0



$P_F\bar{4}3m'$   
215.5.1576

$\bar{4}3m1'$   
 $P_F\bar{4}3m'$

Cubic



Origin at  $\bar{4}3m$ 

<b>Asymmetric unit</b>	$0 \leq x \leq 1;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$y \leq \min(x, 1-x);$	$z \leq y$
Vertices	0,0,0	1,0,0	1/2,1/2,0	1/2,1/2,1/2	

## Symmetry Operations

## For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 2 0,y,0 (2 <sub>y</sub>  0,0,0)	(4) 2 x,0,0 (2 <sub>x</sub>  0,0,0)
(5) 3 <sup>+</sup> x,x,x (3 <sub>xyz</sub>  0,0,0)	(6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$ (3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0)	(7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$ (3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0)	(8) 3 <sup>+</sup> $\bar{x},\bar{x},x$ (3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0)
(9) 3 <sup>-</sup> x,x,x (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)	(10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$ (3 <sub><math>\bar{x}yz</math></sub>  0,0,0)	(11) 3 <sup>-</sup> $\bar{x},\bar{x},x$ (3 <sub><math>\bar{x}yz</math></sub>  0,0,0)	(12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$ (3 <sub><math>\bar{x}yz</math></sub>  0,0,0)
(13) m' x,x,z (m <sub><math>\bar{x}y</math></sub>  0,0,0)'	(14) m' x, $\bar{x}$ ,z (m <sub><math>\bar{x}y</math></sub>  0,0,0)'	(15) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'	(16) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z^{-1}$  0,0,0)'
(17) m' x,y,y (m <sub><math>\bar{y}z</math></sub>  0,0,0)'	(18) $\bar{4}^+$ x,0,0; 0,0,0 ( $\bar{4}_x$  0,0,0)'	(19) $\bar{4}^-$ x,0,0; 0,0,0 ( $\bar{4}_x^{-1}$  0,0,0)'	(20) m' x,y, $\bar{y}$ (m <sub><math>\bar{y}z</math></sub>  0,0,0)'
(21) m' x,y,x (m <sub><math>\bar{z}x</math></sub>  0,0,0)'	(22) $\bar{4}^-$ 0,y,0; 0,0,0 ( $\bar{4}_y^{-1}$  0,0,0)'	(23) m' $\bar{x},y,x$ (m <sub><math>\bar{z}x</math></sub>  0,0,0)'	(24) $\bar{4}^+$ 0,y,0; 0,0,0 ( $\bar{4}_y$  0,0,0)'

## For (1,0,0) + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 2' 1/2,y,0 (2 <sub>y</sub>  1,0,0)'	(4) 2' (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)'
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x+2/3,x+1/3,x (3 <sub>xyz</sub>  1,0,0)'	(6) 3 <sup>+</sup> (1/3,-1/3,1/3) x+2/3,x-1/3,x (3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  1,0,0)'	(7) 3 <sup>+</sup> (1/3,-1/3,-1/3) x+2/3,x-1/3,x (3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  1,0,0)'	(8) 3 <sup>+</sup> (1/3,1/3,-1/3) x+2/3,x-1/3,x (3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  1,0,0)'
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x+1/3,x-1/3,x (3 <sub>xyz</sub> <sup>-1</sup>  1,0,0)'	(10) 3 <sup>-</sup> (1/3,-1/3,-1/3) x+1/3,x+1/3,x (3 <sub><math>\bar{x}yz</math></sub>  1,0,0)'	(11) 3 <sup>-</sup> (1/3,1/3,-1/3) x+1/3,x-1/3,x (3 <sub><math>\bar{x}yz</math></sub>  1,0,0)'	(12) 3 <sup>-</sup> (1/3,-1/3,1/3) x+1/3,x+1/3,x (3 <sub><math>\bar{x}yz</math></sub>  1,0,0)'
(13)g (1/2,1/2,0) x+1/2,x,z (m <sub><math>\bar{x}y</math></sub>  1,0,0)	(14) g (1/2,-1/2,0) x+1/2, $\bar{x}$ ,z (m <sub><math>\bar{x}y</math></sub>  1,0,0)	(15) $\bar{4}^+$ 1/2,-1/2,z; 1/2,-1/2,0 ( $\bar{4}_z$  1,0,0)	(16) $\bar{4}^-$ 1/2,1/2,z; 1/2,1/2,0 ( $\bar{4}_z^{-1}$  1,0,0)
(17) a (1,0,0) x,y,y (m <sub><math>\bar{y}z</math></sub>  1,0,0)	(18) $\bar{4}^+$ x+1/2,0,0; 1/2,0,0 ( $\bar{4}_x$  1,0,0)	(19) $\bar{4}^-$ x+1/2,0,0; 1/2,0,0 ( $\bar{4}_x^{-1}$  1,0,0)	(20) a (1,0,0) x,y, $\bar{y}$ (m <sub><math>\bar{y}z</math></sub>  1,0,0)
(21) g (1/2,0,1/2) x+1/2,y,x (m <sub><math>\bar{z}x</math></sub>  1,0,0)	(22) $\bar{4}^-$ 1/2,y,-1/2; 1/2,0,-1/2 ( $\bar{4}_y^{-1}$  1,0,0)	(23) g (1/2,0,-1/2) $\bar{x}$ +1/2,y,x (m <sub><math>\bar{z}x</math></sub>  1,0,0)	(24) $\bar{4}^+$ 1/2,y,1/2; 1/2,0,1/2 ( $\bar{4}_y$  1,0,0)

**Generators selected** (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5); (13).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (1,0,0)' +

48 j 1

(1) x,y,z [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [u, $\bar{v},\bar{w}$ ]
(5) z,x,y [w,u,v]	(6) z, $\bar{x},\bar{y}$ [ $\bar{w},\bar{u},\bar{v}$ ]	(7) $\bar{z},\bar{x},y$ [ $\bar{w},\bar{u},v$ ]	(8) $\bar{z},x,\bar{y}$ [ $\bar{w},u,\bar{v}$ ]
(9) y,z,x [v,w,u]	(10) $\bar{y},z,\bar{x}$ [ $\bar{v},\bar{w},\bar{u}$ ]	(11) y, $\bar{z},\bar{x}$ [v, $\bar{w},\bar{u}$ ]	(12) $\bar{y},\bar{z},x$ [ $\bar{v},\bar{w},u$ ]
(13) y,x,z [v,u,w]	(14) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(15) y, $\bar{x},\bar{z}$ [v, $\bar{u},\bar{w}$ ]	(16) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]
(17) x,z,y [u,w,v]	(18) $\bar{x},z,\bar{y}$ [ $\bar{u},\bar{w},\bar{v}$ ]	(19) $\bar{x},\bar{z},y$ [ $\bar{u},\bar{w},v$ ]	(20) x, $\bar{z},\bar{y}$ [u, $\bar{w},\bar{v}$ ]
(21) z,y,x [w,v,u]	(22) z, $\bar{y},\bar{x}$ [ $\bar{w},\bar{v},\bar{u}$ ]	(23) $\bar{z},y,\bar{x}$ [ $\bar{w},v,\bar{u}$ ]	(24) $\bar{z},\bar{y},x$ [ $\bar{w},\bar{v},u$ ]

24 i ..m' x,x,z [u,u,w]  $\bar{x},\bar{x},z$  [ $\bar{u},\bar{u},w$ ]  $\bar{x},x,\bar{z}$  [ $\bar{u},u,\bar{w}$ ] x, $\bar{x},\bar{z}$  [u, $\bar{u},\bar{w}$ ]

z,x,x [w,u,u] z, $\bar{x},\bar{x}$  [ $\bar{w},\bar{u},\bar{u}$ ]  $\bar{z},\bar{x},x$  [ $\bar{w},u,u$ ]  $\bar{z},x,\bar{x}$  [ $\bar{w},u,\bar{u}$ ]

x,z,x [u,w,u]  $\bar{x},z,\bar{x}$  [ $\bar{u},w,\bar{u}$ ] x, $\bar{z},\bar{x}$  [u, $\bar{w},\bar{u}$ ]  $\bar{x},\bar{z},x$  [u, $\bar{w},u$ ]

24 h 2'.. x,1/2,0 [0,v,w]  $\bar{x},1/2,0$  [0,v, $\bar{w}$ ] 0,x,1/2 [w,0,v] 0, $\bar{x},1/2$  [ $\bar{w},0,v$ ]

1/2,0,x [v,w,0] 1/2,0, $\bar{x}$  [v, $\bar{w},0$ ] 1/2,x,0 [v,0,w] 1/2, $\bar{x},0$  [v,0, $\bar{w}$ ]

x,0,1/2 [0,w,v]  $\bar{x},0,1/2$  [0, $\bar{w},v$ ] 0,1/2,x [w,v,0] 0,1/2, $\bar{x}$  [ $\bar{w},v,0$ ]

12 g 2.m'm' x,1/2,1/2 [u,0,0]  $\bar{x},1/2,1/2$  [u,0,0] 1/2,x,1/2 [0,u,0]

1/2, $\bar{x},1/2$  [0,u,0] 1/2,1/2,x [0,0,u] 1/2,1/2, $\bar{x}$  [0,0,u]

12 f 2.mm x,0,0 [u,0,0]  $\bar{x},0,0$  [ $\bar{u},0,0$ ] 0,x,0 [0,u,0]

0, $\bar{x},0$  [0, $\bar{u},0$ ] 0,0,x [0,0,u] 0,0, $\bar{x}$  [0,0, $\bar{u}$ ]

8 e .3m x,x,x [u,u,u]  $\bar{x},\bar{x},x$  [ $\bar{u},\bar{u},u$ ]  $\bar{x},x,\bar{x}$  [ $\bar{u},u,\bar{u}$ ] x, $\bar{x},\bar{x}$  [u, $\bar{u},\bar{u}$ ]

6 d  $\bar{4}2'$ .m' 1/2,0,0 [u,0,0] 0,1/2,0 [0,u,0] 0,0,1/2 [0,0,u]

6 c  $\bar{4}2'$ .m' 0,1/2,1/2 [u,0,0] 1/2,0,1/2 [0,u,0] 1/2,1/2,0 [0,0,u]

2 b  $\bar{4}$ '3m' 1/2,1/2,1/2 [0,0,0]

2 a  $\bar{4}$ '3m' 0,0,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'

$\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$

Origin at 0,0,z

Along [1,1,1] p31m1'

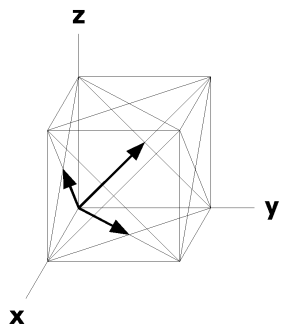
$\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$

Origin at x,x,x

Along [1,1,0] p<sub>c</sub>-1m1

$\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$

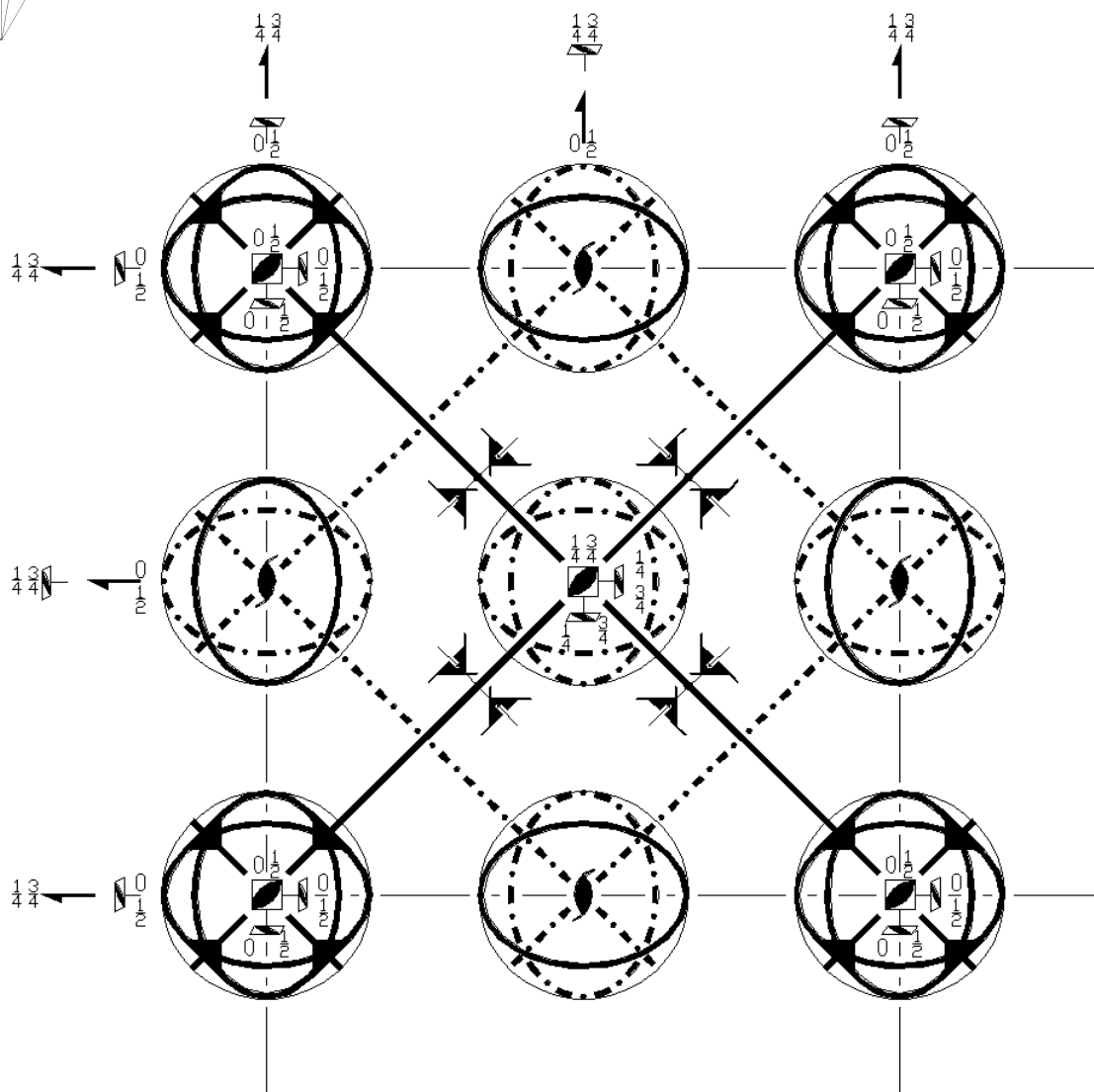
Origin at x-1/4,x+1/4,0



$F\bar{4}3m$   
216.1.1577

$\bar{4}3m$   
 $F\bar{4}3m$

Cubic



Origin at  $\bar{4}3m$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $-1/4 \leq z \leq 1/4$ ;  $y \leq \min(x, 1/2-x)$ ;  $-y \leq z \leq y$

Vertices  $0,0,0$   $1/2,0,0$   $1/4,1/4,1/4$   $1/4,1/4,-1/4$

**Symmetry Operations**

For  $(0,0,0) +$  set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                  | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                                  | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                  |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) |

(13) m $\bar{x},x,z$ ( $m_{\bar{xy}} 0,0,0$ )	(14) m $\bar{x},\bar{x},z$ ( $m_{xy} 0,0,0$ )	(15) $\bar{4}^+$ $0,0,z; 0,0,0$ ( $\bar{4}_z 0,0,0$ )	(16) $\bar{4}^-$ $0,0,z; 0,0,0$ ( $\bar{4}_z^{-1} 0,0,0$ )
(17) m $x,y,y$ ( $m_{\bar{yz}} 0,0,0$ )	(18) $\bar{4}^+$ $x,0,0; 0,0,0$ ( $\bar{4}_x 0,0,0$ )	(19) $\bar{4}^-$ $x,0,0; 0,0,0$ ( $\bar{4}_x^{-1} 0,0,0$ )	(20) m $x,y,\bar{y}$ ( $m_{yz} 0,0,0$ )
(21) m $x,y,x$ ( $m_{\bar{zx}} 0,0,0$ )	(22) $\bar{4}^-$ $0,y,0; 0,0,0$ ( $\bar{4}_y^{-1} 0,0,0$ )	(23) m $\bar{x},y,x$ ( $m_{xz} 0,0,0$ )	(24) $\bar{4}^+$ $0,y,0; 0,0,0$ ( $\bar{4}_y 0,0,0$ )

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2) (1 0,1/2,1/2)	(2) 2 (0,0,1/2) $0,1/4,z$ ( $2_z 0,1/2,1/2$ )	(3) 2 (0,1/2,0) $0,y,1/4$ ( $2_y 0,1/2,1/2$ )	(4) 2 $x,1/4,1/4$ ( $2_x 0,1/2,1/2$ )
(5) $3^+$ (1/3,1/3,1/3) $x-1/3,x-1/6,x$ ( $3_{xyz} 0,1/2,1/2$ )	(6) $3^+$ $\bar{x},x+1/2,\bar{x}$ ( $3_{\bar{xyz}}^{-1} 0,1/2,1/2$ )	(7) $3^+$ (-1/3,1/3,1/3) $x+1/3,\bar{x}-1/6,\bar{x}$ ( $3_{\bar{xyz}}^{-1} 0,1/2,1/2$ )	(8) $3^+$ $\bar{x},\bar{x}+1/2,x$ ( $3_{\bar{xyz}}^{-1} 0,1/2,1/2$ )
(9) $3^-$ (1/3,1/3,1/3) $x-1/6,x+1/6,x$ ( $3_{xyz}^{-1} 0,1/2,1/2$ )	(10) $3^-$ (-1/3,1/3,1/3) $x+1/6,x+1/6,\bar{x}$ ( $3_{\bar{xyz}} 0,1/2,1/2$ )	(11) $3^-$ $\bar{x}+1/2,\bar{x}+1/2,x$ ( $3_{\bar{yz}} 0,1/2,1/2$ )	(12) $3^-$ $\bar{x}-1/2,x+1/2,\bar{x}$ ( $3_{\bar{yz}} 0,1/2,1/2$ )
(13) g (1/4,1/4,1/2) $x-1/4,x,z$ ( $m_{\bar{xy}} 0,1/2,1/2$ )	(14) g (-1/4,1/4,1/2) $x+1/4,\bar{x},z$ ( $m_{xy} 0,1/2,1/2$ )	(15) $\bar{4}^+$ $1/4,1/4,z; 1/4,1/4,1/4$ ( $\bar{4}_z 0,1/2,1/2$ )	(16) $\bar{4}^-$ $-1/4,1/4,z; -1/4,1/4,1/4$ ( $\bar{4}_z^{-1} 0,1/2,1/2$ )
(17) g (0,1/2,1/2) $x,y,y$ ( $m_{\bar{yz}} 0,1/2,1/2$ )	(18) $\bar{4}^+$ $x,1/2,0; 0,1/2,0$ ( $\bar{4}_x 0,1/2,1/2$ )	(19) $\bar{4}^-$ $x,0,1/2; 0,0,1/2$ ( $\bar{4}_x^{-1} 0,1/2,1/2$ )	(20) m $x,y+1/2,\bar{y}$ ( $m_{yz} 0,1/2,1/2$ )
(21) g (1/4,1/2,1/4) $x-1/4,y,x$ ( $m_{\bar{zx}} 0,1/2,1/2$ )	(22) $\bar{4}^-$ $1/4,y,1/4; 1/4,1/4,1/4$ ( $\bar{4}_y^{-1} 0,1/2,1/2$ )	(23) g (-1/4,1/2,1/4) $\bar{x}+1/4,y,x$ ( $m_{xz} 0,1/2,1/2$ )	(24) $\bar{4}^+$ $-1/4,y,1/4; -1/4,1/4,1/4$ ( $\bar{4}_y 0,1/2,1/2$ )

For (1/2,0,1/2) + set

(1) t (1/2,0,1/2) (1 1/2,0,1/2)	(2) 2 (0,0,1/2) $1/4,0,z$ ( $2_z 1/2,0,1/2$ )	(3) 2 $1/4,y,1/4$ ( $2_y 1/2,0,1/2$ )	(4) 2 (1/2,0,0) $x,0,1/2$ ( $2_x 1/2,0,1/2$ )
(5) $3^+$ (1/3,1/3,1/3) $x+1/6,x-1/6,x$ ( $3_{xyz} 1/2,0,1/2$ )	(6) $3^+$ (1/3,-1/3,1/3) $\bar{x}+1/6,x+1/6,\bar{x}$ ( $3_{\bar{xyz}}^{-1} 1/2,0,1/2$ )	(7) $3^+$ $x+1/2,\bar{x}-1/2,\bar{x}$ ( $3_{\bar{yz}}^{-1} 1/2,0,1/2$ )	(8) $3^+$ $\bar{x}+1/2,\bar{x}+1/2,x$ ( $3_{\bar{yz}}^{-1} 1/2,0,1/2$ )
(9) $3^-$ (1/3,1/3,1/3) $x-1/6,x-1/3,x$ ( $3_{xyz}^{-1} 1/2,0,1/2$ )	(10) $3^-$ $x+1/2,\bar{x},\bar{x}$ ( $3_{\bar{yz}} 1/2,0,1/2$ )	(11) $3^-$ $\bar{x}+1/2,\bar{x},x$ ( $3_{\bar{yz}} 1/2,0,1/2$ )	(12) $3^-$ (1/3,-1/3,1/3) $\bar{x}-1/6,x+1/3,\bar{x}$ ( $3_{\bar{yz}} 1/2,0,1/2$ )
(13) g (1/4,1/4,1/2) $x+1/4,x,z$ ( $m_{\bar{xy}} 1/2,0,1/2$ )	(14) g (1/4,-1/4,1/2) $x+1/4,\bar{x},z$ ( $m_{xy} 1/2,0,1/2$ )	(15) $\bar{4}^+$ $1/4,-1/4,z; 1/4,-1/4,1/4$ ( $\bar{4}_z 1/2,0,1/2$ )	(16) $\bar{4}^-$ $1/4,1/4,z; 1/4,1/4,1/4$ ( $\bar{4}_z^{-1} 1/2,0,1/2$ )
(17) g (1/2,1/4,1/4) $x,y-1/4,y$ ( $m_{\bar{yz}} 1/2,0,1/2$ )	(18) $\bar{4}^+$ $x,1/4,1/4; 1/4,1/4,1/4$ ( $\bar{4}_x 1/2,0,1/2$ )	(19) $\bar{4}^-$ $x,-1/4,1/4; 1/4,-1/4,1/4$ ( $\bar{4}_x^{-1} 1/2,0,1/2$ )	(20) g (1/2,-1/4,1/4) $x,y+1/4,\bar{y}$ ( $m_{yz} 1/2,0,1/2$ )
(21) g (1/2,0,1/2) $x,y,x$ ( $m_{\bar{zx}} 1/2,0,1/2$ )	(22) $\bar{4}^-$ $1/2,y,0; 1/2,0,0$ ( $\bar{4}_y^{-1} 1/2,0,1/2$ )	(23) m $\bar{x}+1/2,y,x$ ( $m_{xz} 1/2,0,1/2$ )	(24) $\bar{4}^+$ $0,y,1/2; 0,0,1/2$ ( $\bar{4}_y 1/2,0,1/2$ )

For (1/2,1/2,0) + set

(1) $t$ (1/2,1/2,0) (1   1/2,1/2,0)	(2) $2$ 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,0)	(3) $2$ (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)	(4) $2$ (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)
(5) $3^+$ (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) $3^+$ $\bar{x}$ +1/2,x, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(7) $3^+$ x+1/2, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(8) $3^+$ (1/3,1/3,-1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)
(9) $3^-$ (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) $3^-$ x, $\bar{x}$ +1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)	(11) $3^-$ (1/3,1/3,-1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub>   1/2,1/2,0)	(12) $3^-$ $\bar{x}$ ,x+1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)
(13) $g$ (1/2,1/2,0) x,x,z (m <sub>xy</sub>   1/2,1/2,0)	(14) $m$ x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,0)	(15) $4^+$ 1/2,0,z; 1/2,0,0 (4 <sub>z</sub>   1/2,1/2,0)	(16) $4^-$ 0,1/2,z; 0,1/2,0 (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,0)
(17) $g$ (1/2,1/4,1/4) x,y+1/4,y (m <sub>yz</sub>   1/2,1/2,0)	(18) $4^+$ x,1/4,-1/4; 1/4,1/4,-1/4 (4 <sub>x</sub>   1/2,1/2,0)	(19) $4^-$ x,1/4,1/4; 1/4,1/4,1/4 (4 <sub>x</sub> <sup>-1</sup>   1/2,1/2,0)	(20) $g$ (1/2,1/4,-1/4) x,y+1/4, $\bar{y}$ (m <sub>yz</sub>   1/2,1/2,0)
(21) $g$ (1/4,1/2,1/4) x+1/4,y,x (m <sub>xz</sub>   1/2,1/2,0)	(22) $4^-$ 1/4,y,-1/4; 1/4,1/4,-1/4 (4 <sub>y</sub> <sup>-1</sup>   1/2,1/2,0)	(23) $g$ (1/4,1/2,-1/4) $\bar{x}$ +1/4,y,x (m <sub>xz</sub>   1/2,1/2,0)	(24) $4^+$ 1/4,y,1/4; 1/4,1/4,1/4 (4 <sub>y</sub>   1/2,1/2,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

		(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +		
96	i 1						
(1)	x,y,z [u,v,w]	(2)	$\bar{x}$ , $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w]	(3)	$\bar{x}$ ,y,z [ $\bar{u}$ ,v,w]	(4)	x, $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w]
(5)	z,x,y [w,u,v]	(6)	z,x, $\bar{y}$ [w, $\bar{u}$ , $\bar{v}$ ]	(7)	$\bar{z}$ , $\bar{x}$ ,y [ $\bar{w}$ , $\bar{u}$ ,v]	(8)	$\bar{z}$ ,x,y [ $\bar{w}$ ,u, $\bar{v}$ ]
(9)	y,z,x [v,w,u]	(10)	$\bar{y}$ ,z,x [v,w, $\bar{u}$ ]	(11)	y,z, $\bar{x}$ [v,w, $\bar{u}$ ]	(12)	$\bar{y}$ ,z,x [v,w, $\bar{u}$ ]
(13)	y,x,z [v, $\bar{u}$ ,w]	(14)	$\bar{y}$ , $\bar{x}$ ,z [v,u,w]	(15)	y, $\bar{x}$ ,z [v,u,w]	(16)	$\bar{y}$ ,x,z [v, $\bar{u}$ ,w]
(17)	x,z,y [ $\bar{u}$ , $\bar{w}$ ,v]	(18)	$\bar{x}$ ,z,y [u,w,v]	(19)	$\bar{x}$ ,z,y [u,w,v]	(20)	x,z,y [ $\bar{u}$ ,w,v]
(21)	z,y,x [ $\bar{w}$ , $\bar{v}$ , $\bar{u}$ ]	(22)	z,y, $\bar{x}$ [ $\bar{w}$ ,v,u]	(23)	$\bar{z}$ ,y,x [w,v,u]	(24)	$\bar{z}$ ,y,x [w,v, $\bar{u}$ ]
48	h ..m	x,x,z [u, $\bar{u}$ ,0]	$\bar{x}$ , $\bar{x}$ ,z [ $\bar{u}$ ,u,0]	$\bar{x}$ ,x,z [ $\bar{u}$ , $\bar{u}$ ,0]	x, $\bar{x}$ ,z [u,u,0]		
		z,x,x [0,u, $\bar{u}$ ]	z, $\bar{x}$ , $\bar{x}$ [0, $\bar{u}$ ,u]	$\bar{z}$ , $\bar{x}$ ,x [0, $\bar{u}$ , $\bar{u}$ ]	$\bar{z}$ ,x,x [0,u,u]		
		x,z,x [ $\bar{u}$ ,0,u]	$\bar{x}$ ,z, $\bar{x}$ [u,0, $\bar{u}$ ]	x,z, $\bar{x}$ [ $\bar{u}$ ,0, $\bar{u}$ ]	$\bar{x}$ ,z,x [u,0,u]		
24	g 2.mm	x,1/4,1/4 [0,0,0]	$\bar{x}$ ,3/4,1/4 [0,0,0]	1/4,x,1/4 [0,0,0]			
		1/4, $\bar{x}$ ,3/4 [0,0,0]	1/4,1/4,x [0,0,0]	3/4,1/4, $\bar{x}$ [0,0,0]			

Continued

216.1.1577

 $F\bar{4}3m$ 

24	f	2.mm	$x,0,0 [0,0,0]$	$\bar{x},0,0 [0,0,0]$	$0,x,0 [0,0,0]$
			$0,\bar{x},0 [0,0,0]$	$0,0,x [0,0,0]$	$0,0,\bar{x} [0,0,0]$
16	e	.3m	$x,x,x [0,0,0]$	$\bar{x},\bar{x},x [0,0,0]$	$\bar{x},x,\bar{x} [0,0,0]$
4	d	$\bar{4}3m$	$3/4,3/4,3/4 [0,0,0]$		
4	c	$\bar{4}3m$	$1/4,1/4,1/4 [0,0,0]$		
4	b	$\bar{4}3m$	$1/2,1/2,1/2 [0,0,0]$		
4	a	$\bar{4}3m$	$0,0,0 [0,0,0]$		

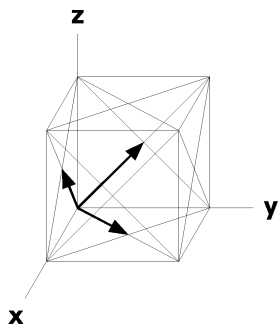
**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4'm'm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p31m$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at  $x,x,x$

Along  $[1,1,0]$   $c1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$

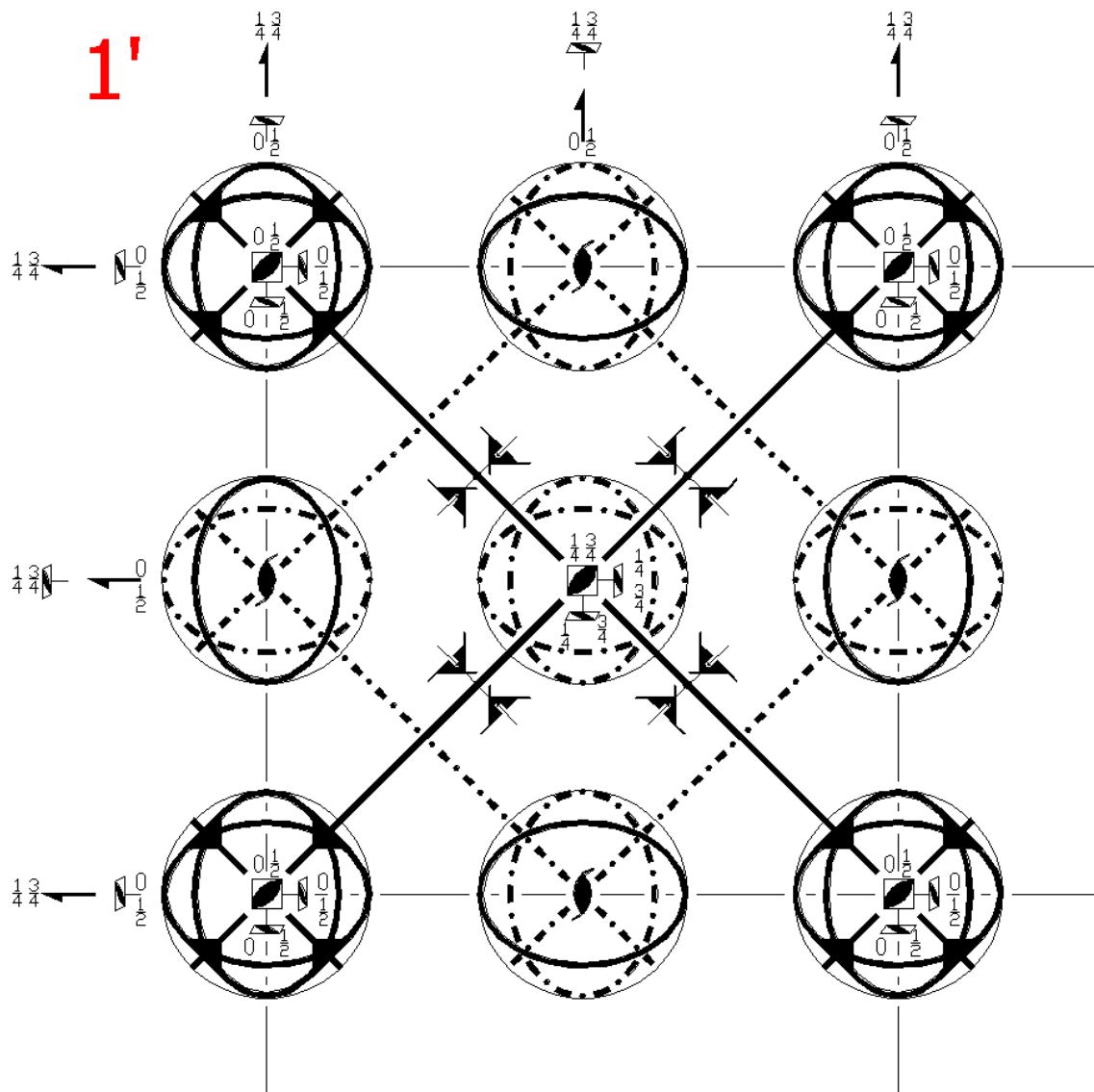




$F\bar{4}3m1'$   
216.2.1578

$\bar{4}3m1'$   
 $F\bar{4}3m1'$

Cubic



Origin at  $\bar{4}3m1'$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/4;$   $-1/4 \leq z \leq 1/4;$   $y \leq \min(x, 1/2-x);$   $-y \leq z \leq y$   
**Vertices**  $0,0,0$   $1/2,0,0$   $1/4,1/4,1/4$   $1/4,1/4,-1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                  | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)              |

(13) $m \bar{x}, x, z$ ( $m_{\bar{xy}}   0, 0, 0$ )	(14) $m \bar{x}, \bar{x}, z$ ( $m_{xy}   0, 0, 0$ )	(15) $\bar{4}^+ 0, 0, z; 0, 0, 0$ ( $\bar{4}_z   0, 0, 0$ )	(16) $\bar{4}^- 0, 0, z; 0, 0, 0$ ( $\bar{4}_z^{-1}   0, 0, 0$ )
(17) $m \bar{x}, y, y$ ( $m_{\bar{yz}}   0, 0, 0$ )	(18) $\bar{4}^+ x, 0, 0; 0, 0, 0$ ( $\bar{4}_x   0, 0, 0$ )	(19) $\bar{4}^- x, 0, 0; 0, 0, 0$ ( $\bar{4}_x^{-1}   0, 0, 0$ )	(20) $m \bar{x}, y, \bar{y}$ ( $m_{yz}   0, 0, 0$ )
(21) $m \bar{x}, y, x$ ( $m_{\bar{zx}}   0, 0, 0$ )	(22) $\bar{4}^- 0, y, 0; 0, 0, 0$ ( $\bar{4}_y^{-1}   0, 0, 0$ )	(23) $m \bar{x}, y, x$ ( $m_{xz}   0, 0, 0$ )	(24) $\bar{4}^+ 0, y, 0; 0, 0, 0$ ( $\bar{4}_y   0, 0, 0$ )
For (0, 1/2, 1/2) + set			
(1) $t (0, 1/2, 1/2)$ ( $1   0, 1/2, 1/2$ )	(2) $2 (0, 0, 1/2) 0, 1/4, z$ ( $2_z   0, 1/2, 1/2$ )	(3) $2 (0, 1/2, 0) 0, y, 1/4$ ( $2_y   0, 1/2, 1/2$ )	(4) $2 \bar{x}, 1/4, 1/4$ ( $2_x   0, 1/2, 1/2$ )
(5) $3^+ (1/3, 1/3, 1/3)$ $x-1/3, x-1/6, x$ ( $3_{xyz}   0, 1/2, 1/2$ )	(6) $3^+ \bar{x}, x+1/2, \bar{x}$ ( $3_{xyz}^{-1}   0, 1/2, 1/2$ )	(7) $3^+ (-1/3, 1/3, 1/3)$ $x+1/3, \bar{x}-1/6, \bar{x}$ ( $3_{xyz}^{-1}   0, 1/2, 1/2$ )	(8) $3^+ \bar{x}, \bar{x}+1/2, x$ ( $3_{xyz}^{-1}   0, 1/2, 1/2$ )
(9) $3^- (1/3, 1/3, 1/3)$ $x-1/6, x+1/6, x$ ( $3_{xyz}^{-1}   0, 1/2, 1/2$ )	(10) $3^- (-1/3, 1/3, 1/3)$ $x+1/6, x+1/6, \bar{x}$ ( $3_{xyz}   0, 1/2, 1/2$ )	(11) $3^- \bar{x}+1/2, \bar{x}+1/2, x$ ( $3_{xyz}   0, 1/2, 1/2$ )	(12) $3^- \bar{x}-1/2, x+1/2, \bar{x}$ ( $3_{xyz}   0, 1/2, 1/2$ )
(13) $g (1/4, 1/4, 1/2) x-1/4, x, z$ ( $m_{\bar{xy}}   0, 1/2, 1/2$ )	(14) $g (-1/4, 1/4, 1/2) x+1/4, \bar{x}, z$ ( $m_{xy}   0, 1/2, 1/2$ )	(15) $\bar{4}^+ 1/4, 1/4, z; 1/4, 1/4, 1/4$ ( $\bar{4}_z   0, 1/2, 1/2$ )	(16) $\bar{4}^- -1/4, 1/4, z; -1/4, 1/4, 1/4$ ( $\bar{4}_z^{-1}   0, 1/2, 1/2$ )
(17) $g (0, 1/2, 1/2) x, y, y$ ( $m_{\bar{yz}}   0, 1/2, 1/2$ )	(18) $\bar{4}^+ x, 1/2, 0; 0, 1/2, 0$ ( $\bar{4}_x   0, 1/2, 1/2$ )	(19) $\bar{4}^- x, 0, 1/2; 0, 0, 1/2$ ( $\bar{4}_x^{-1}   0, 1/2, 1/2$ )	(20) $m \bar{x}, y+1/2, \bar{y}$ ( $m_{yz}   0, 1/2, 1/2$ )
(21) $g (1/4, 1/2, 1/4) x-1/4, y, x$ ( $m_{\bar{zx}}   0, 1/2, 1/2$ )	(22) $\bar{4}^- 1/4, y, 1/4; 1/4, 1/4, 1/4$ ( $\bar{4}_y^{-1}   0, 1/2, 1/2$ )	(23) $g (-1/4, 1/2, 1/4) \bar{x}+1/4, y, x$ ( $m_{xz}   0, 1/2, 1/2$ )	(24) $\bar{4}^+ -1/4, y, 1/4; -1/4, 1/4, 1/4$ ( $\bar{4}_y   0, 1/2, 1/2$ )
For (1/2, 0, 1/2) + set			
(1) $t (1/2, 0, 1/2)$ ( $1   1/2, 0, 1/2$ )	(2) $2 (0, 0, 1/2) 1/4, 0, z$ ( $2_z   1/2, 0, 1/2$ )	(3) $2 1/4, y, 1/4$ ( $2_y   1/2, 0, 1/2$ )	(4) $2 (1/2, 0, 0) x, 0, 1/2$ ( $2_x   1/2, 0, 1/2$ )
(5) $3^+ (1/3, 1/3, 1/3)$ $x+1/6, x-1/6, x$ ( $3_{xyz}   1/2, 0, 1/2$ )	(6) $3^+ (1/3, -1/3, 1/3)$ $\bar{x}+1/6, x+1/6, \bar{x}$ ( $3_{xyz}^{-1}   1/2, 0, 1/2$ )	(7) $3^+ x+1/2, \bar{x}-1/2, \bar{x}$ ( $3_{xyz}^{-1}   1/2, 0, 1/2$ )	(8) $3^+ \bar{x}+1/2, \bar{x}+1/2, x$ ( $3_{xyz}^{-1}   1/2, 0, 1/2$ )
(9) $3^- (1/3, 1/3, 1/3)$ $x-1/6, x-1/3, x$ ( $3_{xyz}^{-1}   1/2, 0, 1/2$ )	(10) $3^- x+1/2, \bar{x}, \bar{x}$ ( $3_{xyz}   1/2, 0, 1/2$ )	(11) $3^- \bar{x}+1/2, \bar{x}, x$ ( $3_{xyz}   1/2, 0, 1/2$ )	(12) $3^- (1/3, -1/3, 1/3)$ $\bar{x}-1/6, x+1/3, \bar{x}$ ( $3_{xyz}   1/2, 0, 1/2$ )
(13) $g (1/4, 1/4, 1/2) x+1/4, x, z$ ( $m_{\bar{xy}}   1/2, 0, 1/2$ )	(14) $g (1/4, -1/4, 1/2) x+1/4, \bar{x}, z$ ( $m_{xy}   1/2, 0, 1/2$ )	(15) $\bar{4}^+ 1/4, -1/4, z; 1/4, -1/4, 1/4$ ( $\bar{4}_z   1/2, 0, 1/2$ )	(16) $\bar{4}^- 1/4, 1/4, z; 1/4, 1/4, 1/4$ ( $\bar{4}_z^{-1}   1/2, 0, 1/2$ )
(17) $g (1/2, 1/4, 1/4) x, y-1/4, y$ ( $m_{\bar{yz}}   1/2, 0, 1/2$ )	(18) $\bar{4}^+ x, 1/4, 1/4; 1/4, 1/4, 1/4$ ( $\bar{4}_x   1/2, 0, 1/2$ )	(19) $\bar{4}^- x, -1/4, 1/4; 1/4, -1/4, 1/4$ ( $\bar{4}_x^{-1}   1/2, 0, 1/2$ )	(20) $g (1/2, -1/4, 1/4) x, y+1/4, \bar{y}$ ( $m_{yz}   1/2, 0, 1/2$ )
(21) $g (1/2, 0, 1/2) x, y, x$ ( $m_{\bar{zx}}   1/2, 0, 1/2$ )	(22) $\bar{4}^- 1/2, y, 0; 1/2, 0, 0$ ( $\bar{4}_y^{-1}   1/2, 0, 1/2$ )	(23) $m \bar{x}+1/2, y, x$ ( $m_{xz}   1/2, 0, 1/2$ )	(24) $\bar{4}^+ 0, y, 1/2; 0, 0, 1/2$ ( $\bar{4}_y   1/2, 0, 1/2$ )

## For (1/2,1/2,0) + set

- |   |  |   |  |
|---|--|---|--|
| (1) $t$ (1/2,1/2,0)<br>(1 1/2,1/2,0)  | (2) $2$ 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)                                       | (3) $2$ (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)                              | (4) $2$ (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)                                 |
| (5) $3^+$ (1/3,1/3,1/3)<br>x+1/6,x+1/3,x<br>(3 <sub>xyz</sub>  1/2,1/2,0)               | (6) $3^+$ $\bar{x}$ +1/2,x, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0)   | (7) $3^+$ x+1/2, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0) | (8) $3^+$ (1/3,1/3,-1/3)<br>x+1/6,x+1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0) |
| (9) $3^-$ (1/3,1/3,1/3)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0) | (10) $3^-$ x, $\bar{x}$ +1/2, $\bar{x}$<br>(3 <sub>xyz</sub>  1/2,1/2,0)               | (11) $3^-$ (1/3,1/3,-1/3)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub>  1/2,1/2,0)           | (12) $3^-$ $\bar{x}$ ,x+1/2, $\bar{x}$<br>(3 <sub>xyz</sub>  1/2,1/2,0)                  |
| (13) $g$ (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)                              | (14) $m$ x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  1/2,1/2,0)                           | (15) $\bar{4}^+$ 1/2,0,z; 1/2,0,0<br>(4 <sub>z</sub>  1/2,1/2,0)                      | (16) $\bar{4}^-$ 0,1/2,z; 0,1/2,0<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,0)           |
| (17) $g$ (1/2,1/4,1/4) x,y+1/4,y<br>(m <sub>yz</sub>  1/2,1/2,0)                        | (18) $\bar{4}^+$ x,1/4,-1/4; 1/4,1/4,-1/4<br>(4 <sub>x</sub>  1/2,1/2,0)               | (19) $\bar{4}^-$ x,1/4,1/4; 1/4,1/4,1/4<br>(4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,0)  | (20) $g$ (1/2,1/4,-1/4) x,y+1/4, $\bar{y}$<br>(m <sub>yz</sub>  1/2,1/2,0)               |
| (21) $g$ (1/4,1/2,1/4) x+1/4,y,x<br>(m <sub>xz</sub>  1/2,1/2,0)                        | (22) $\bar{4}^-$ 1/4,y,-1/4; 1/4,1/4,-1/4<br>(4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,0) | (23) $g$ (1/4,1/2,-1/4) $\bar{x}$ +1/4,y,x<br>(m <sub>xz</sub>  1/2,1/2,0)            | (24) $\bar{4}^+$ 1/4,y,1/4; 1/4,1/4,1/4<br>(4 <sub>y</sub>  1/2,1/2,0)                   |

## For (0,0,0)' + set

- |   |   |  |  |
|---|---|--|--|
| (1) $1'$<br>(1 0,0,0)'  | (2) $2'$ 0,0,z<br>(2 <sub>z</sub>  0,0,0)'                                      | (3) $2'$ 0,y,0<br>(2 <sub>y</sub>  0,0,0)'                                       | (4) $2'$ x,0,0<br>(2 <sub>x</sub>  0,0,0)'                                       |
| (5) $3^+$ ' x,x,x<br>(3 <sub>xyz</sub>  0,0,0)'               | (6) $3^+$ ' $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)' | (7) $3^+$ ' x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)' | (8) $3^+$ ' $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)' |
| (9) $3^-$ ' x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)' | (10) $3^-$ ' x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)'             | (11) $3^-$ ' $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>xyz</sub>  0,0,0)'              | (12) $3^-$ ' $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)'               |
| (13) $m'$ x,x,z<br>(m <sub>xy</sub>  0,0,0)'                  | (14) $m'$ x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0,0)'                          | (15) $\bar{4}^+$ ' 0,0,z; 0,0,0<br>(4 <sub>z</sub>  0,0,0)'                      | (16) $\bar{4}^-$ ' 0,0,z; 0,0,0<br>(4 <sub>z</sub> <sup>-1</sup>  0,0,0)'        |
| (17) $m'$ x,y,y<br>(m <sub>yz</sub>  0,0,0)'                  | (18) $\bar{4}^+$ ' x,0,0; 0,0,0<br>(4 <sub>x</sub>  0,0,0)'                     | (19) $\bar{4}^-$ ' x,0,0; 0,0,0<br>(4 <sub>x</sub> <sup>-1</sup>  0,0,0)'        | (20) $m'$ x,y, $\bar{y}$<br>(m <sub>yz</sub>  0,0,0)'                            |
| (21) $m'$ x,y,x<br>(m <sub>xz</sub>  0,0,0)'                  | (22) $\bar{4}^-$ ' 0,y,0; 0,0,0<br>(4 <sub>y</sub> <sup>-1</sup>  0,0,0)'       | (23) $m'$ $\bar{x}$ ,y,x<br>(m <sub>xz</sub>  0,0,0)'                            | (24) $\bar{4}^+$ ' 0,y,0; 0,0,0<br>(4 <sub>y</sub>  0,0,0)'                      |

## For (0,1/2,1/2)' + set

- |  |   |   |  |
|--|---|---|--|
| (1) $t'$ (0,1/2,1/2)<br>(1 0,1/2,1/2)'   | (2) $2'$ (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)'                              | (3) $2'$ (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)'                                  | (4) $2'$ x,1/4,1/4<br>(2 <sub>x</sub>  0,1/2,1/2)'                                       |
| (5) $3^+$ ' (1/3,1/3,1/3)<br>x-1/3,x-1/6,x<br>(3 <sub>xyz</sub>  0,1/2,1/2)'               | (6) $3^+$ ' $\bar{x}$ ,x+1/2, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)' | (7) $3^+$ ' (-1/3,1/3,1/3)<br>x+1/3,x-1/6,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)' | (8) $3^+$ ' $\bar{x}$ , $\bar{x}$ +1/2,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)' |
| (9) $3^-$ ' (1/3,1/3,1/3)<br>x-1/6,x+1/6,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)' | (10) $3^-$ ' (-1/3,1/3,1/3)<br>x+1/6,x+1/6,x<br>(3 <sub>xyz</sub>  0,1/2,1/2)'          | (11) $3^-$ ' $\bar{x}$ +1/2, $\bar{x}$ +1/2,x<br>(3 <sub>xyz</sub>  0,1/2,1/2)'             | (12) $3^-$ ' $\bar{x}$ -1/2,x+1/2, $\bar{x}$<br>(3 <sub>xyz</sub>  0,1/2,1/2)'           |

- (13)  $g' (1/4, 1/4, 1/2) \quad x^{-1/4}, x, z$   
 $(m_{\bar{xy}} | 0, 1/2, 1/2)'$
- (14)  $g' (-1/4, 1/4, 1/2) \quad x+1/4, \bar{x}, z$   
 $(m_{xy} | 0, 1/2, 1/2)'$
- (15)  $\bar{4}^+ ' 1/4, 1/4, z; 1/4, 1/4, 1/4$   
 $(\bar{4}_z | 0, 1/2, 1/2)'$
- (16)  $\bar{4}^- ' -1/4, 1/4, z; -1/4, 1/4, 1/4$   
 $(\bar{4}_z^{-1} | 0, 1/2, 1/2)'$
- (17)  $g' (0, 1/2, 1/2) \quad x, y, y$   
 $(m_{\bar{yz}} | 0, 1/2, 1/2)'$
- (18)  $\bar{4}^+ ' x, 1/2, 0; 0, 1/2, 0$   
 $(\bar{4}_x | 0, 1/2, 1/2)'$
- (19)  $\bar{4}^- ' x, 0, 1/2; 0, 0, 1/2$   
 $(\bar{4}_x^{-1} | 0, 1/2, 1/2)'$
- (20)  $m' x, y+1/2, \bar{y}$   
 $(m_{yz} | 0, 1/2, 1/2)'$
- (21)  $g' (1/4, 1/2, 1/4) \quad x^{-1/4}, y, x$   
 $(m_{\bar{zx}} | 0, 1/2, 1/2)'$
- (22)  $\bar{4}^- ' 1/4, y, 1/4; 1/4, 1/4, 1/4$   
 $(\bar{4}_y^{-1} | 0, 1/2, 1/2)'$
- (23)  $g' (-1/4, 1/2, 1/4) \quad \bar{x}+1/4, y, x$   
 $(m_{xz} | 0, 1/2, 1/2)'$
- (24)  $\bar{4}^+ ' -1/4, y, 1/4; -1/4, 1/4, 1/4$   
 $(\bar{4}_y | 0, 1/2, 1/2)'$

For (1/2, 0, 1/2)' + set

- (1)  $t' (1/2, 0, 1/2)$   
 $(1 | 1/2, 0, 1/2)'$
- (2)  $2' (0, 0, 1/2) \quad 1/4, 0, z$   
 $(2_z | 1/2, 0, 1/2)'$
- (3)  $2' \quad 1/4, y, 1/4$   
 $(2_y | 1/2, 0, 1/2)'$
- (4)  $2' (1/2, 0, 0) \quad x, 0, 1/2$   
 $(2_x | 1/2, 0, 1/2)'$
- (5)  $3^+ ' (1/3, 1/3, 1/3)$   
 $x+1/6, x-1/6, x$   
 $(3_{xyz} | 1/2, 0, 1/2)'$
- (6)  $3^+ ' (1/3, -1/3, 1/3)$   
 $\bar{x}+1/6, x+1/6, \bar{x}$   
 $(3_{xyz}^{-1} | 1/2, 0, 1/2)'$
- (7)  $3^+ ' x+1/2, \bar{x}-1/2, \bar{x}$   
 $(3_{xyz}^{-1} | 1/2, 0, 1/2)'$
- (8)  $3^+ ' \bar{x}+1/2, \bar{x}+1/2, x$   
 $(3_{xyz}^{-1} | 1/2, 0, 1/2)'$
- (9)  $3^- ' (1/3, 1/3, 1/3)$   
 $x-1/6, x-1/3, x$   
 $(3_{xyz}^{-1} | 1/2, 0, 1/2)'$
- (10)  $3^- ' x+1/2, \bar{x}, \bar{x}$   
 $(3_{xyz} | 1/2, 0, 1/2)'$
- (11)  $3^- ' \bar{x}+1/2, \bar{x}, x$   
 $(3_{xyz} | 1/2, 0, 1/2)'$
- (12)  $3^- ' (1/3, -1/3, 1/3)$   
 $\bar{x}-1/6, x+1/3, \bar{x}$   
 $(3_{xyz} | 1/2, 0, 1/2)'$
- (13)  $g' (1/4, 1/4, 1/2) \quad x+1/4, x, z$   
 $(m_{\bar{xy}} | 1/2, 0, 1/2)'$
- (14)  $g' (1/4, -1/4, 1/2) \quad x+1/4, \bar{x}, z$   
 $(m_{xy} | 1/2, 0, 1/2)'$
- (15)  $\bar{4}^+ ' 1/4, -1/4, z; 1/4, -1/4, 1/4$   
 $(\bar{4}_z | 1/2, 0, 1/2)'$
- (16)  $\bar{4}^- ' 1/4, 1/4, z; 1/4, 1/4, 1/4$   
 $(\bar{4}_z^{-1} | 1/2, 0, 1/2)'$
- (17)  $g' (1/2, 1/4, 1/4) \quad x, y-1/4, y$   
 $(m_{\bar{yz}} | 1/2, 0, 1/2)'$
- (18)  $\bar{4}^+ ' x, 1/4, 1/4; 1/4, 1/4, 1/4$   
 $(\bar{4}_x | 1/2, 0, 1/2)'$
- (19)  $\bar{4}^- ' x, -1/4, 1/4; 1/4, -1/4, 1/4$   
 $(\bar{4}_x^{-1} | 1/2, 0, 1/2)'$
- (20)  $g' (1/2, -1/4, 1/4) \quad x, y+1/4, \bar{y}$   
 $(m_{yz} | 1/2, 0, 1/2)'$
- (21)  $g' (1/2, 0, 1/2) \quad x, y, x$   
 $(m_{\bar{zx}} | 1/2, 0, 1/2)'$
- (22)  $\bar{4}^- ' 1/2, y, 0; 1/2, 0, 0$   
 $(\bar{4}_y^{-1} | 1/2, 0, 1/2)'$
- (23)  $m' \bar{x}+1/2, y, x$   
 $(m_{xz} | 1/2, 0, 1/2)'$
- (24)  $\bar{4}^+ ' 0, y, 1/2; 0, 0, 1/2$   
 $(\bar{4}_y | 1/2, 0, 1/2)'$

For (1/2, 1/2, 0)' + set

- (1)  $t' (1/2, 1/2, 0)$   
 $(1 | 1/2, 1/2, 0)'$
- (2)  $2' \quad 1/4, 1/4, z$   
 $(2_z | 1/2, 1/2, 0)'$
- (3)  $2' (0, 1/2, 0) \quad 1/4, y, 0$   
 $(2_y | 1/2, 1/2, 0)'$
- (4)  $2' (1/2, 0, 0) \quad x, 1/4, 0$   
 $(2_x | 1/2, 1/2, 0)'$
- (5)  $3^+ ' (1/3, 1/3, 1/3)$   
 $x+1/6, x+1/3, x$   
 $(3_{xyz} | 1/2, 1/2, 0)'$
- (6)  $3^+ ' \bar{x}+1/2, x, \bar{x}$   
 $(3_{xyz}^{-1} | 1/2, 1/2, 0)'$
- (7)  $3^+ ' x+1/2, \bar{x}, \bar{x}$   
 $(3_{xyz}^{-1} | 1/2, 1/2, 0)'$
- (8)  $3^+ ' (1/3, 1/3, -1/3)$   
 $\bar{x}+1/6, \bar{x}+1/3, x$   
 $(3_{xyz}^{-1} | 1/2, 1/2, 0)'$
- (9)  $3^- ' (1/3, 1/3, 1/3)$   
 $x+1/3, x+1/6, x$   
 $(3_{xyz}^{-1} | 1/2, 1/2, 0)'$
- (10)  $3^- ' x, \bar{x}+1/2, \bar{x}$   
 $(3_{xyz} | 1/2, 1/2, 0)'$
- (11)  $3^- ' (1/3, 1/3, -1/3)$   
 $\bar{x}+1/3, \bar{x}+1/6, x$   
 $(3_{xyz} | 1/2, 1/2, 0)'$
- (12)  $3^- ' \bar{x}, x+1/2, \bar{x}$   
 $(3_{xyz} | 1/2, 1/2, 0)'$
- (13)  $g' (1/2, 1/2, 0) \quad x, x, z$   
 $(m_{\bar{xy}} | 1/2, 1/2, 0)'$
- (14)  $m' x+1/2, \bar{x}, z$   
 $(m_{xy} | 1/2, 1/2, 0)'$
- (15)  $\bar{4}^+ ' 1/2, 0, z; 1/2, 0, 0$   
 $(\bar{4}_z | 1/2, 1/2, 0)'$
- (16)  $\bar{4}^- ' 0, 1/2, z; 0, 1/2, 0$   
 $(\bar{4}_z^{-1} | 1/2, 1/2, 0)'$
- (17)  $g' (1/2, 1/4, 1/4) \quad x, y+1/4, y$   
 $(m_{\bar{yz}} | 1/2, 1/2, 0)'$
- (18)  $\bar{4}^+ ' x, 1/4, -1/4; 1/4, 1/4, -1/4$   
 $(\bar{4}_x | 1/2, 1/2, 0)'$
- (19)  $\bar{4}^- ' x, 1/4, 1/4; 1/4, 1/4, 1/4$   
 $(\bar{4}_x^{-1} | 1/2, 1/2, 0)'$
- (20)  $g' (1/2, 1/4, -1/4) \quad x, y+1/4, \bar{y}$   
 $(m_{yz} | 1/2, 1/2, 0)'$
- (21)  $g' (1/4, 1/2, 1/4) \quad x+1/4, y, x$   
 $(m_{\bar{zx}} | 1/2, 1/2, 0)'$
- (22)  $\bar{4}^- ' 1/4, y, -1/4; 1/4, 1/4, -1/4$   
 $(\bar{4}_y^{-1} | 1/2, 1/2, 0)'$
- (23)  $g' (1/4, 1/2, -1/4) \quad \bar{x}+1/4, y, x$   
 $(m_{xz} | 1/2, 1/2, 0)'$
- (24)  $\bar{4}^+ ' 1/4, y, 1/4; 1/4, 1/4, 1/4$   
 $(\bar{4}_y | 1/2, 1/2, 0)'$

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); 1'.

## Positions

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

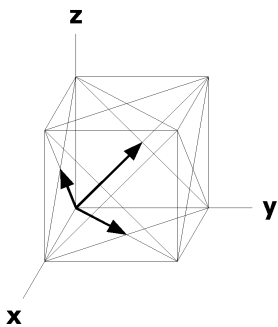
			(0,0,0) + (0,0,0)' +	(0,1/2,1/2) + (0,1/2,1/2)' +	(1/2,0,1/2) + (1/2,0,1/2)' +	(1/2,1/2,0) + (1/2,1/2,0)' +					
96	i	11'									
(1)	x,y,z	[0,0,0]	(2)	$\overline{x},\overline{y},z$	[0,0,0]	(3)	$\overline{x},y,\overline{z}$	[0,0,0]	(4)	$x,\overline{y},\overline{z}$	[0,0,0]
(5)	z,x,y	[0,0,0]	(6)	$z,\overline{x},\overline{y}$	[0,0,0]	(7)	$\overline{z},\overline{x},y$	[0,0,0]	(8)	$\overline{z},x,\overline{y}$	[0,0,0]
(9)	y,z,x	[0,0,0]	(10)	$\overline{y},z,\overline{x}$	[0,0,0]	(11)	$y,\overline{z},\overline{x}$	[0,0,0]	(12)	$\overline{y},\overline{z},x$	[0,0,0]
(13)	y,x,z	[0,0,0]	(14)	$\overline{y},\overline{x},z$	[0,0,0]	(15)	$y,\overline{x},\overline{z}$	[0,0,0]	(16)	$\overline{y},x,\overline{z}$	[0,0,0]
(17)	x,z,y	[0,0,0]	(18)	$\overline{x},z,\overline{y}$	[0,0,0]	(19)	$\overline{x},\overline{z},y$	[0,0,0]	(20)	$x,\overline{z},\overline{y}$	[0,0,0]
(21)	z,y,x	[0,0,0]	(22)	$z,\overline{y},\overline{x}$	[0,0,0]	(23)	$\overline{z},y,\overline{x}$	[0,0,0]	(24)	$\overline{z},\overline{y},x$	[0,0,0]
48	h	$\overline{..}m1'$	x,x,z [0,0,0]	$\overline{x},\overline{x},z$ [0,0,0]	$\overline{x},x,\overline{z}$ [0,0,0]	$x,\overline{x},\overline{z}$ [0,0,0]					
			z,x,x [0,0,0]	$z,\overline{x},\overline{x}$ [0,0,0]	$\overline{z},\overline{x},x$ [0,0,0]	$\overline{z},x,\overline{x}$ [0,0,0]					
			x,z,x [0,0,0]	$\overline{x},z,\overline{x}$ [0,0,0]	$x,\overline{z},\overline{x}$ [0,0,0]	$\overline{x},\overline{z},x$ [0,0,0]					
24	g	2.mm1'	x,1/4,1/4 [0,0,0]	$\overline{x},3/4,1/4$ [0,0,0]	$1/4,x,1/4$ [0,0,0]						
			$1/4,\overline{x},3/4$ [0,0,0]	$1/4,1/4,\overline{x}$ [0,0,0]	$3/4,1/4,\overline{x}$ [0,0,0]						
24	f	2.mm1'	x,0,0 [0,0,0]	$\overline{x},0,0$ [0,0,0]	0,x,0 [0,0,0]						
			0, $\overline{x}$ ,0 [0,0,0]	0,0,x [0,0,0]	0,0, $\overline{x}$ [0,0,0]						
16	e	.3m1'	x,x,x [0,0,0]	$\overline{x},\overline{x},x$ [0,0,0]	$\overline{x},x,\overline{x}$ [0,0,0]	$x,\overline{x},\overline{x}$ [0,0,0]					
4	d	$\overline{4}3m1'$	3/4,3/4,3/4 [0,0,0]								
4	c	$\overline{4}3m1'$	1/4,1/4,1/4 [0,0,0]								
4	b	$\overline{4}3m1'$	1/2,1/2,1/2 [0,0,0]								
4	a	$\overline{4}3m1'$	0,0,0 [0,0,0]								

## Symmetry of Special Projections

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,1,1]  $p31m1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

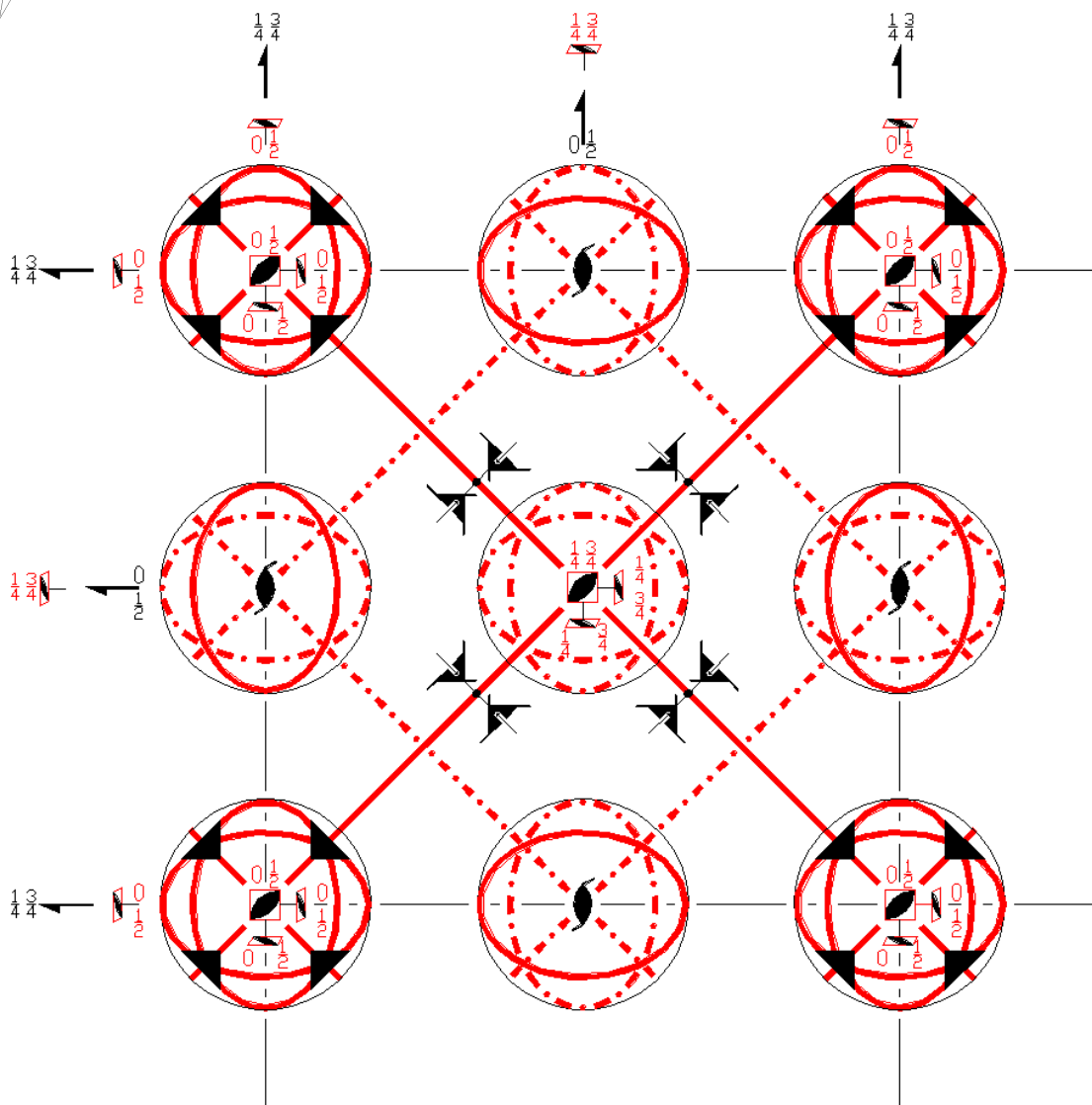
Along [1,1,0]  $c1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$F\bar{4}3m'$   
216.3.1579

$\bar{4}3m'$   
 $F\bar{4}3m'$

Cubic



Origin at  $\bar{4}3m'$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/4;$   $-1/4 \leq z \leq 1/4;$   $y \leq \min(x, 1/2-x);$   $-y \leq z \leq y$   
**Vertices**  $0,0,0$   $1/2,0,0$   $1/4,1/4,1/4$   $1/4,1/4,-1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |  |   |   |
|---|--|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                 | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                            | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                  |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)  | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}yz}$  0,0,0)        |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)      | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}yz}$  0,0,0) | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{\bar{x}y\bar{z}}$  0,0,0) |

(13) $m' \ x,x,z$ ( $m_{\bar{xy}} 0,0,0$ )'	(14) $m' \ x,\bar{x},z$ ( $m_{xy} 0,0,0$ )'	(15) $\bar{4}^+ \ ' \ 0,0,z; 0,0,0$ ( $\bar{4}_z 0,0,0$ )'	(16) $\bar{4}^- \ ' \ 0,0,z; 0,0,0$ ( $\bar{4}_z^{-1} 0,0,0$ )'
(17) $m' \ x,y,y$ ( $m_{\bar{yz}} 0,0,0$ )'	(18) $\bar{4}^+ \ ' \ x,0,0; 0,0,0$ ( $\bar{4}_x 0,0,0$ )'	(19) $\bar{4}^- \ ' \ x,0,0; 0,0,0$ ( $\bar{4}_x^{-1} 0,0,0$ )'	(20) $m' \ x,y,\bar{y}$ ( $m_{yz} 0,0,0$ )'
(21) $m' \ x,y,x$ ( $m_{\bar{zx}} 0,0,0$ )'	(22) $\bar{4}^- \ ' \ 0,y,0; 0,0,0$ ( $\bar{4}_y^{-1} 0,0,0$ )'	(23) $m' \ \bar{x},y,x$ ( $m_{xz} 0,0,0$ )'	(24) $\bar{4}^+ \ ' \ 0,y,0; 0,0,0$ ( $\bar{4}_y 0,0,0$ )'

For (0,1/2,1/2) + set

(1) $t \ (0,1/2,1/2)$ ( $1 0,1/2,1/2$ )	(2) $2 \ (0,0,1/2) \ 0,1/4,z$ ( $2_z 0,1/2,1/2$ )	(3) $2 \ (0,1/2,0) \ 0,y,1/4$ ( $2_y 0,1/2,1/2$ )	(4) $2 \ x,1/4,1/4$ ( $2_x 0,1/2,1/2$ )
(5) $3^+ \ (1/3,1/3,1/3)$ $x-1/3,x-1/6,x$ ( $3_{xyz} 0,1/2,1/2$ )	(6) $3^+ \ \bar{x},x+1/2,\bar{x}$ ( $3_{\bar{xyz}}^{-1} 0,1/2,1/2$ )	(7) $3^+ \ (-1/3,1/3,1/3)$ $x+1/3,\bar{x}-1/6,\bar{x}$ ( $3_{xyz}^{-1} 0,1/2,1/2$ )	(8) $3^+ \ \bar{x},\bar{x}+1/2,x$ ( $3_{\bar{xyz}}^{-1} 0,1/2,1/2$ )
(9) $3^- \ (1/3,1/3,1/3)$ $x-1/6,x+1/6,x$ ( $3_{xyz}^{-1} 0,1/2,1/2$ )	(10) $3^- \ (-1/3,1/3,1/3)$ $x+1/6,x+1/6,\bar{x}$ ( $3_{\bar{xyz}} 0,1/2,1/2$ )	(11) $3^- \ \bar{x}+1/2,\bar{x}+1/2,x$ ( $3_{\bar{yz}} 0,1/2,1/2$ )	(12) $3^- \ \bar{x}-1/2,x+1/2,\bar{x}$ ( $3_{\bar{yz}} 0,1/2,1/2$ )
(13) $g' \ (1/4,1/4,1/2) \ x-1/4,x,z$ ( $m_{\bar{xy}} 0,1/2,1/2$ )'	(14) $g' \ (-1/4,1/4,1/2) \ x+1/4,\bar{x},z$ ( $m_{xy} 0,1/2,1/2$ )'	(15) $\bar{4}^+ \ ' \ 1/4,1/4,z; 1/4,1/4,1/4$ ( $\bar{4}_z 0,1/2,1/2$ )'	(16) $\bar{4}^- \ ' \ -1/4,1/4,z; -1/4,1/4,1/4$ ( $\bar{4}_z^{-1} 0,1/2,1/2$ )'
(17) $g' \ (0,1/2,1/2) \ x,y,y$ ( $m_{\bar{yz}} 0,1/2,1/2$ )'	(18) $\bar{4}^+ \ ' \ x,1/2,0; 0,1/2,0$ ( $\bar{4}_x 0,1/2,1/2$ )'	(19) $\bar{4}^- \ ' \ x,0,1/2; 0,0,1/2$ ( $\bar{4}_x^{-1} 0,1/2,1/2$ )'	(20) $m' \ x,y+1/2,\bar{y}$ ( $m_{yz} 0,1/2,1/2$ )'
(21) $g' \ (1/4,1/2,1/4) \ x-1/4,y,x$ ( $m_{\bar{zx}} 0,1/2,1/2$ )'	(22) $\bar{4}^- \ ' \ 1/4,y,1/4; 1/4,1/4,1/4$ ( $\bar{4}_y^{-1} 0,1/2,1/2$ )'	(23) $g' \ (-1/4,1/2,1/4) \ \bar{x}+1/4,y,x$ ( $m_{xz} 0,1/2,1/2$ )'	(24) $\bar{4}^+ \ ' \ -1/4,y,1/4; -1/4,1/4,1/4$ ( $\bar{4}_y 0,1/2,1/2$ )'

For (1/2,0,1/2) + set

(1) $t \ (1/2,0,1/2)$ ( $1 1/2,0,1/2$ )	(2) $2 \ (0,0,1/2) \ 1/4,0,z$ ( $2_z 1/2,0,1/2$ )	(3) $2 \ 1/4,y,1/4$ ( $2_y 1/2,0,1/2$ )	(4) $2 \ (1/2,0,0) \ x,0,1/2$ ( $2_x 1/2,0,1/2$ )
(5) $3^+ \ (1/3,1/3,1/3)$ $x+1/6,x-1/6,x$ ( $3_{xyz} 1/2,0,1/2$ )	(6) $3^+ \ (1/3,-1/3,1/3)$ $\bar{x}+1/6,x+1/6,\bar{x}$ ( $3_{\bar{xyz}}^{-1} 1/2,0,1/2$ )	(7) $3^+ \ x+1/2,\bar{x}-1/2,\bar{x}$ ( $3_{\bar{yz}}^{-1} 1/2,0,1/2$ )	(8) $3^+ \ \bar{x}+1/2,\bar{x}+1/2,x$ ( $3_{\bar{yz}}^{-1} 1/2,0,1/2$ )
(9) $3^- \ (1/3,1/3,1/3)$ $x-1/6,x-1/3,x$ ( $3_{xyz}^{-1} 1/2,0,1/2$ )	(10) $3^- \ x+1/2,\bar{x},\bar{x}$ ( $3_{\bar{yz}} 1/2,0,1/2$ )	(11) $3^- \ \bar{x}+1/2,\bar{x},x$ ( $3_{\bar{yz}} 1/2,0,1/2$ )	(12) $3^- \ (1/3,-1/3,1/3)$ $\bar{x}-1/6,x+1/3,\bar{x}$ ( $3_{\bar{yz}} 1/2,0,1/2$ )
(13) $g' \ (1/4,1/4,1/2) \ x+1/4,x,z$ ( $m_{\bar{xy}} 1/2,0,1/2$ )'	(14) $g' \ (1/4,-1/4,1/2) \ x+1/4,\bar{x},z$ ( $m_{xy} 1/2,0,1/2$ )'	(15) $\bar{4}^+ \ ' \ 1/4,-1/4,z; 1/4,-1/4,1/4$ ( $\bar{4}_z 1/2,0,1/2$ )'	(16) $\bar{4}^- \ ' \ 1/4,1/4,z; 1/4,1/4,1/4$ ( $\bar{4}_z^{-1} 1/2,0,1/2$ )'
(17) $g' \ (1/2,1/4,1/4) \ x,y-1/4,y$ ( $m_{\bar{yz}} 1/2,0,1/2$ )'	(18) $\bar{4}^+ \ ' \ x,1/4,1/4; 1/4,1/4,1/4$ ( $\bar{4}_x 1/2,0,1/2$ )'	(19) $\bar{4}^- \ ' \ x,-1/4,1/4; 1/4,-1/4,1/4$ ( $\bar{4}_x^{-1} 1/2,0,1/2$ )'	(20) $g' \ (1/2,-1/4,1/4) \ x,y+1/4,\bar{y}$ ( $m_{yz} 1/2,0,1/2$ )'
(21) $g' \ (1/2,0,1/2) \ x,y,x$ ( $m_{\bar{zx}} 1/2,0,1/2$ )'	(22) $\bar{4}^- \ ' \ 1/2,y,0; 1/2,0,0$ ( $\bar{4}_y^{-1} 1/2,0,1/2$ )'	(23) $m' \ \bar{x}+1/2,y,x$ ( $m_{xz} 1/2,0,1/2$ )'	(24) $\bar{4}^+ \ ' \ 0,y,1/2; 0,0,1/2$ ( $\bar{4}_y 1/2,0,1/2$ )'

For (1/2,1/2,0) + set

(1) $t$ (1/2,1/2,0) (1   1/2,1/2,0)	(2) $2$ 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,0)	(3) $2$ (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)	(4) $2$ (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)
(5) $3^+$ (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) $3^+$ $\bar{x}$ +1/2,x, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(7) $3^+$ x+1/2, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(8) $3^+$ (1/3,1/3,-1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)
(9) $3^-$ (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) $3^-$ x, $\bar{x}$ +1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)	(11) $3^-$ (1/3,1/3,-1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub>   1/2,1/2,0)	(12) $3^-$ $\bar{x}$ ,x+1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)
(13) $g'$ (1/2,1/2,0) x,x,z (m <sub>xy</sub>   1/2,1/2,0)'	(14) $m'$ x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,0)'	(15) $\bar{4}^+$ 1/2,0,z; 1/2,0,0 (4 <sub>z</sub>   1/2,1/2,0)'	(16) $\bar{4}^-$ 0,1/2,z; 0,1/2,0 (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,0)'
(17) $g'$ (1/2,1/4,1/4) x,y+1/4,y (m <sub>yz</sub>   1/2,1/2,0)'	(18) $\bar{4}^+$ x,1/4,-1/4; 1/4,1/4,-1/4 (4 <sub>x</sub>   1/2,1/2,0)'	(19) $\bar{4}^-$ x,1/4,1/4; 1/4,1/4,1/4 (4 <sub>x</sub> <sup>-1</sup>   1/2,1/2,0)'	(20) $g'$ (1/2,1/4,-1/4) x,y+1/4, $\bar{y}$ (m <sub>yz</sub>   1/2,1/2,0)'
(21) $g'$ (1/4,1/2,1/4) x+1/4,y,x (m <sub>xz</sub>   1/2,1/2,0)'	(22) $\bar{4}^-$ 1/4,y,-1/4; 1/4,1/4,-1/4 (4 <sub>y</sub> <sup>-1</sup>   1/2,1/2,0)'	(23) $g'$ (1/4,1/2,-1/4) $\bar{x}$ +1/4,y,x (m <sub>xz</sub>   1/2,1/2,0)'	(24) $\bar{4}^+$ 1/4,y,1/4; 1/4,1/4,1/4 (4 <sub>y</sub>   1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

		(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +		
96	i 1						
(1)	x,y,z [u,v,w]	(2)	$\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3)	$\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4)	x, $\bar{y},\bar{z}$ [ $\bar{u},\bar{v},\bar{w}$ ]
(5)	z,x,y [w,u,v]	(6)	z, $\bar{x},\bar{y}$ [ $\bar{w},\bar{u},\bar{v}$ ]	(7)	$\bar{z},\bar{x},y$ [ $\bar{w},\bar{u},v$ ]	(8)	$\bar{z},x,\bar{y}$ [ $\bar{w},\bar{u},\bar{v}$ ]
(9)	y,z,x [v,w,u]	(10)	$\bar{y},z,\bar{x}$ [ $\bar{v},\bar{w},\bar{u}$ ]	(11)	y, $\bar{z},\bar{x}$ [ $\bar{v},\bar{w},\bar{u}$ ]	(12)	$\bar{y},\bar{z},x$ [ $\bar{v},\bar{w},\bar{u}$ ]
(13)	y,x,z [v,u,w]	(14)	$\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(15)	y, $\bar{x},\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]	(16)	$\bar{y},x,\bar{z}$ [ $\bar{v},\bar{u},\bar{w}$ ]
(17)	x,z,y [u,w,v]	(18)	$\bar{x},z,\bar{y}$ [ $\bar{u},\bar{w},\bar{v}$ ]	(19)	$\bar{x},\bar{z},y$ [ $\bar{u},\bar{w},\bar{v}$ ]	(20)	x, $\bar{z},\bar{y}$ [ $\bar{u},\bar{w},\bar{v}$ ]
(21)	z,y,x [w,v,u]	(22)	z, $\bar{y},\bar{x}$ [ $\bar{w},\bar{v},\bar{u}$ ]	(23)	$\bar{z},y,\bar{x}$ [ $\bar{w},\bar{v},\bar{u}$ ]	(24)	$\bar{z},\bar{y},x$ [ $\bar{w},\bar{v},\bar{u}$ ]
48	h ..m'	x,x,z [u,u,w]	$\bar{x},\bar{x},z$ [ $\bar{u},\bar{u},\bar{w}$ ]	$\bar{x},x,\bar{z}$ [ $\bar{u},\bar{u},\bar{w}$ ]	x, $\bar{x},\bar{z}$ [ $\bar{u},\bar{u},\bar{w}$ ]		
		z,x,x [w,u,u]	z, $\bar{x},\bar{x}$ [ $\bar{w},\bar{u},\bar{u}$ ]	$\bar{z},\bar{x},x$ [ $\bar{w},\bar{u},\bar{u}$ ]	$\bar{z},x,\bar{x}$ [ $\bar{w},\bar{u},\bar{u}$ ]		
		x,z,x [u,w,u]	$\bar{x},z,\bar{x}$ [ $\bar{u},\bar{w},\bar{u}$ ]	x, $\bar{z},\bar{x}$ [ $\bar{u},\bar{w},\bar{u}$ ]	$\bar{x},\bar{z},x$ [ $\bar{u},\bar{w},\bar{u}$ ]		
24	g 2.m'm'	x,1/4,1/4 [u,0,0]	$\bar{x},3/4,1/4$ [ $\bar{u},0,0$ ]	1/4,x,1/4 [0,u,0]	1/4,x,1/4 [0,u,0]		
		1/4, $\bar{x},3/4$ [0, $\bar{u},0$ ]	1/4,1/4,x [0,0,u]	3/4,1/4, $\bar{x}$ [0,0, $\bar{u}$ ]	3/4,1/4, $\bar{x}$ [0,0, $\bar{u}$ ]		



Continued

216.3.1579

 $F\bar{4}'3m'$ 

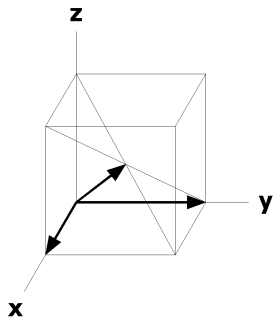
24	f	$2.m'm'$	$x,0,0 [u,0,0]$	$\bar{x},0,0 [\bar{u},0,0]$	$0,x,0 [0,u,0]$
			$0,\bar{x},0 [0,\bar{u},0]$	$0,0,x [0,0,u]$	$0,0,\bar{x} [0,0,\bar{u}]$
16	e	$.3m'$	$x,x,x [u,u,u]$	$\bar{x},\bar{x},\bar{x} [\bar{u},\bar{u},\bar{u}]$	$x,\bar{x},\bar{x} [u,\bar{u},\bar{u}]$
4	d	$\bar{4}'3m'$	$3/4,3/4,3/4 [0,0,0]$		
4	c	$\bar{4}'3m'$	$1/4,1/4,1/4 [0,0,0]$		
4	b	$\bar{4}'3m'$	$1/2,1/2,1/2 [0,0,0]$		
4	a	$\bar{4}'3m'$	$0,0,0 [0,0,0]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p31m'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at  $x,x,x$

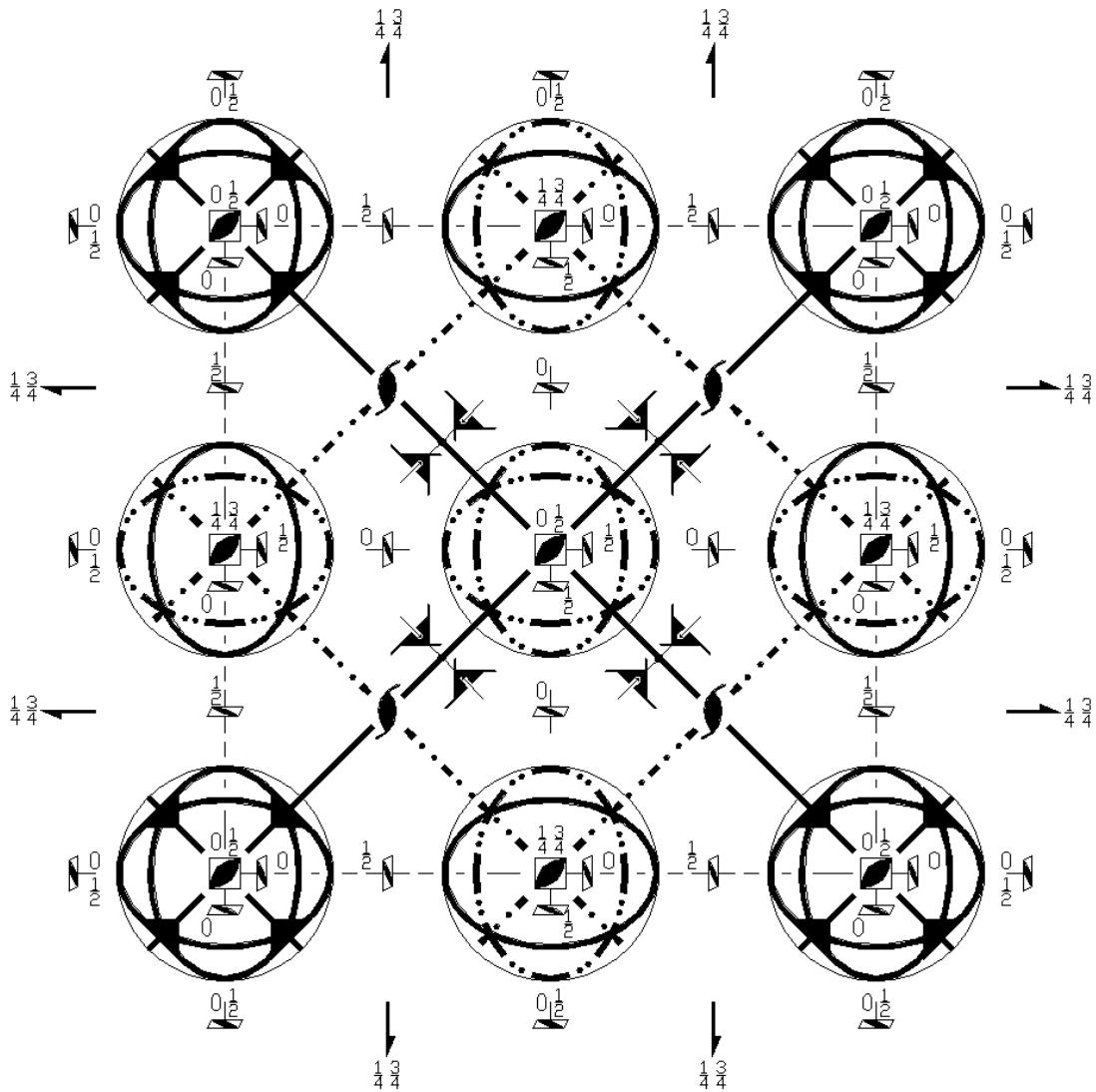
Along  $[1,1,0]$   $c1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$



$\bar{4}3m$   
217.1.1580

$\bar{4}3m$   
 $\bar{4}3m$

Cubic



Origin at  $\bar{4}3m$

Asymmetric unit  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq x;$   $z \leq y$

Vertices  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |  |   |   |
|---|--|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                 | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                            | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                  |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)  | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}yz}$  0,0,0)        |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)      | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}yz}$  0,0,0) | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{\bar{x}y\bar{z}}$  0,0,0) |

(13) m $\bar{x},x,z$ ( $m_{\bar{xy}} 0,0,0$ )	(14) m $\bar{x},\bar{x},z$ ( $m_{xy} 0,0,0$ )	(15) $\bar{4}^+$ $0,0,z; 0,0,0$ ( $\bar{4}_z 0,0,0$ )	(16) $\bar{4}^-$ $0,0,z; 0,0,0$ ( $\bar{4}_z^{-1} 0,0,0$ )
(17) m $x,y,y$ ( $m_{\bar{yz}} 0,0,0$ )	(18) $\bar{4}^+$ $x,0,0; 0,0,0$ ( $\bar{4}_x 0,0,0$ )	(19) $\bar{4}^-$ $x,0,0; 0,0,0$ ( $\bar{4}_x^{-1} 0,0,0$ )	(20) m $x,y,\bar{y}$ ( $m_{yz} 0,0,0$ )
(21) m $x,y,x$ ( $m_{\bar{zx}} 0,0,0$ )	(22) $\bar{4}^-$ $0,y,0; 0,0,0$ ( $\bar{4}_y^{-1} 0,0,0$ )	(23) m $\bar{x},y,x$ ( $m_{xz} 0,0,0$ )	(24) $\bar{4}^+$ $0,y,0; 0,0,0$ ( $\bar{4}_y 0,0,0$ )
For (1/2,1/2,1/2) + set			
(1) t (1/2,1/2,1/2) (1 1/2,1/2,1/2)	(2) 2 (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>  1/2,1/2,1/2)	(3) 2 (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>  1/2,1/2,1/2)	(4) 2 (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>  1/2,1/2,1/2)
(5) 3 <sup>+</sup> (1/2,1/2,1/2) $\bar{x},x,x$ (3 <sub>xyz</sub>  1/2,1/2,1/2)	(6) 3 <sup>+</sup> (1/6,-1/6,1/6) $\bar{x}+1/3,\bar{x}+1/3,\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2)	(7) 3 <sup>+</sup> (-1/6,1/6,1/6) $\bar{x}+2/3,\bar{x}-1/3,\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2)	(8) 3 <sup>+</sup> (1/6,1/6,-1/6) $\bar{x}+1/3,\bar{x}+2/3,\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2)
(9) 3 <sup>-</sup> (1/2,1/2,1/2) $x,x,x$ (3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2)	(10) 3 <sup>-</sup> (-1/6,1/6,1/6) $\bar{x}+1/3,\bar{x}+1/3,\bar{x}$ (3 <sub>xyz</sub>  1/2,1/2,1/2)	(11) 3 <sup>-</sup> (1/6,1/6,-1/6) $\bar{x}+2/3,\bar{x}+1/3,\bar{x}$ (3 <sub>xyz</sub>  1/2,1/2,1/2)	(12) 3 <sup>-</sup> (1/6,-1/6,1/6) $\bar{x}-1/3,\bar{x}+2/3,\bar{x}$ (3 <sub>xyz</sub>  1/2,1/2,1/2)
(13) n (1/2,1/2,1/2) $\bar{x},x,z$ ( $m_{\bar{xy}} 1/2,1/2,1/2$ )	(14) c (0,0,1/2) $\bar{x}+1/2,\bar{x},z$ ( $m_{xy} 1/2,1/2,1/2$ )	(15) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z 1/2,1/2,1/2$ )	(16) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1} 1/2,1/2,1/2$ )
(17) n (1/2,1/2,1/2) $x,y,y$ ( $m_{\bar{yz}} 1/2,1/2,1/2$ )	(18) $\bar{4}^+$ $x,1/2,0; 1/4,1/2,0$ ( $\bar{4}_x 1/2,1/2,1/2$ )	(19) $\bar{4}^-$ $x,0,1/2; 1/4,0,1/2$ ( $\bar{4}_x^{-1} 1/2,1/2,1/2$ )	(20) a (1/2,0,0) $\bar{x},y+1/2,\bar{y}$ ( $m_{yz} 1/2,1/2,1/2$ )
(21) n (1/2,1/2,1/2) $x,y,x$ ( $m_{\bar{zx}} 1/2,1/2,1/2$ )	(22) $\bar{4}^-$ 1/2,y,0; 1/2,1/4,0 ( $\bar{4}_y^{-1} 1/2,1/2,1/2$ )	(23) b (0,1/2,0) $\bar{x}+1/2,y,x$ ( $m_{xz} 1/2,1/2,1/2$ )	(24) $\bar{4}^+$ 0,y,1/2; 0,1/4,1/2 ( $\bar{4}_y 1/2,1/2,1/2$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (1/2,1/2,1/2) +

48	h	1				
(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]			
(5) $z,x,y$ [w,u,v]	(6) $z,\bar{x},\bar{y}$ [ $w,\bar{u},\bar{v}$ ]	(7) $\bar{z},\bar{x},y$ [ $\bar{w},\bar{u},v$ ]	(8) $\bar{z},x,\bar{y}$ [ $\bar{w},u,\bar{v}$ ]			
(9) $y,z,x$ [v,w,u]	(10) $\bar{y},z,\bar{x}$ [ $\bar{v},w,\bar{u}$ ]	(11) $y,\bar{z},\bar{x}$ [ $v,\bar{w},\bar{u}$ ]	(12) $\bar{y},\bar{z},x$ [ $\bar{v},\bar{w},u$ ]			
(13) $y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(14) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(15) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(16) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]			
(17) $x,z,y$ [ $\bar{u},\bar{w},\bar{v}$ ]	(18) $\bar{x},z,\bar{y}$ [ $u,\bar{w},v$ ]	(19) $\bar{x},\bar{z},y$ [ $u,w,\bar{v}$ ]	(20) $x,\bar{z},\bar{y}$ [ $\bar{u},w,v$ ]			
(21) $z,y,x$ [ $\bar{w},\bar{v},\bar{u}$ ]	(22) $z,\bar{y},\bar{x}$ [ $\bar{w},v,u$ ]	(23) $\bar{z},y,\bar{x}$ [ $w,\bar{v},u$ ]	(24) $\bar{z},\bar{y},x$ [ $w,v,\bar{u}$ ]			

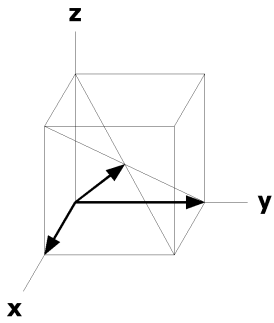
24	g	..m	$x,x,z [u,\bar{u},0]$	$\bar{x},\bar{x},z [\bar{u},u,0]$	$\bar{x},x,\bar{z} [\bar{u},\bar{u},0]$	$x,\bar{x},\bar{z} [u,u,0]$
			$z,x,x [0,u,\bar{u}]$	$z,\bar{x},\bar{x} [0,\bar{u},u]$	$\bar{z},\bar{x},x [0,\bar{u},\bar{u}]$	$\bar{z},x,\bar{x} [0,u,u]$
			$x,z,x [\bar{u},0,u]$	$\bar{x},z,\bar{x} [u,0,\bar{u}]$	$x,\bar{z},\bar{x} [\bar{u},0,\bar{u}]$	$\bar{x},\bar{z},x [u,0,u]$
24	f	2..	$x,1/2,0 [u,0,0]$	$\bar{x},1/2,0 [\bar{u},0,0]$	$0,x,1/2 [0,u,0]$	$0,\bar{x},1/2 [0,\bar{u},0]$
			$1/2,0,x [0,0,u]$	$1/2,0,\bar{x} [0,0,\bar{u}]$	$1/2,x,0 [0,\bar{u},0]$	$1/2,\bar{x},0 [0,u,0]$
			$x,0,1/2 [\bar{u},0,0]$	$\bar{x},0,1/2 [u,0,0]$	$0,1/2,x [0,0,\bar{u}]$	$0,1/2,\bar{x} [0,0,u]$
12	e	2.mm	$x,0,0 [0,0,0]$	$\bar{x},0,0 [0,0,0]$	$0,x,0 [0,0,0]$	$0,x,0 [0,0,0]$
			$0,\bar{x},0 [0,0,0]$	$0,0,x [0,0,0]$	$0,0,\bar{x} [0,0,0]$	$0,0,\bar{x} [0,0,0]$
12	d	$\bar{4}$	$1/4,1/2,0 [u,0,0]$	$3/4,1/2,0 [\bar{u},0,0]$	$0,1/4,1/2 [0,u,0]$	$0,1/4,1/2 [0,u,0]$
			$0,3/4,1/2 [0,\bar{u},0]$	$1/2,0,1/4 [0,0,u]$	$1/2,0,3/4 [0,0,\bar{u}]$	$1/2,0,3/4 [0,0,\bar{u}]$
8	c	.3m	$x,x,x [0,0,0]$	$\bar{x},\bar{x},x [0,0,0]$	$\bar{x},x,\bar{x} [0,0,0]$	$x,\bar{x},\bar{x} [0,0,0]$
6	b	$\bar{4}2.m$	$0,1/2,1/2 [0,0,0]$	$1/2,0,1/2 [0,0,0]$	$1/2,1/2,0 [0,0,0]$	$1/2,1/2,0 [0,0,0]$
2	a	$\bar{4}3m$	$0,0,0 [0,0,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4'mm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p31m$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x,x,x$

Along  $[1,1,0]$   $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



$\bar{I}43m1'$

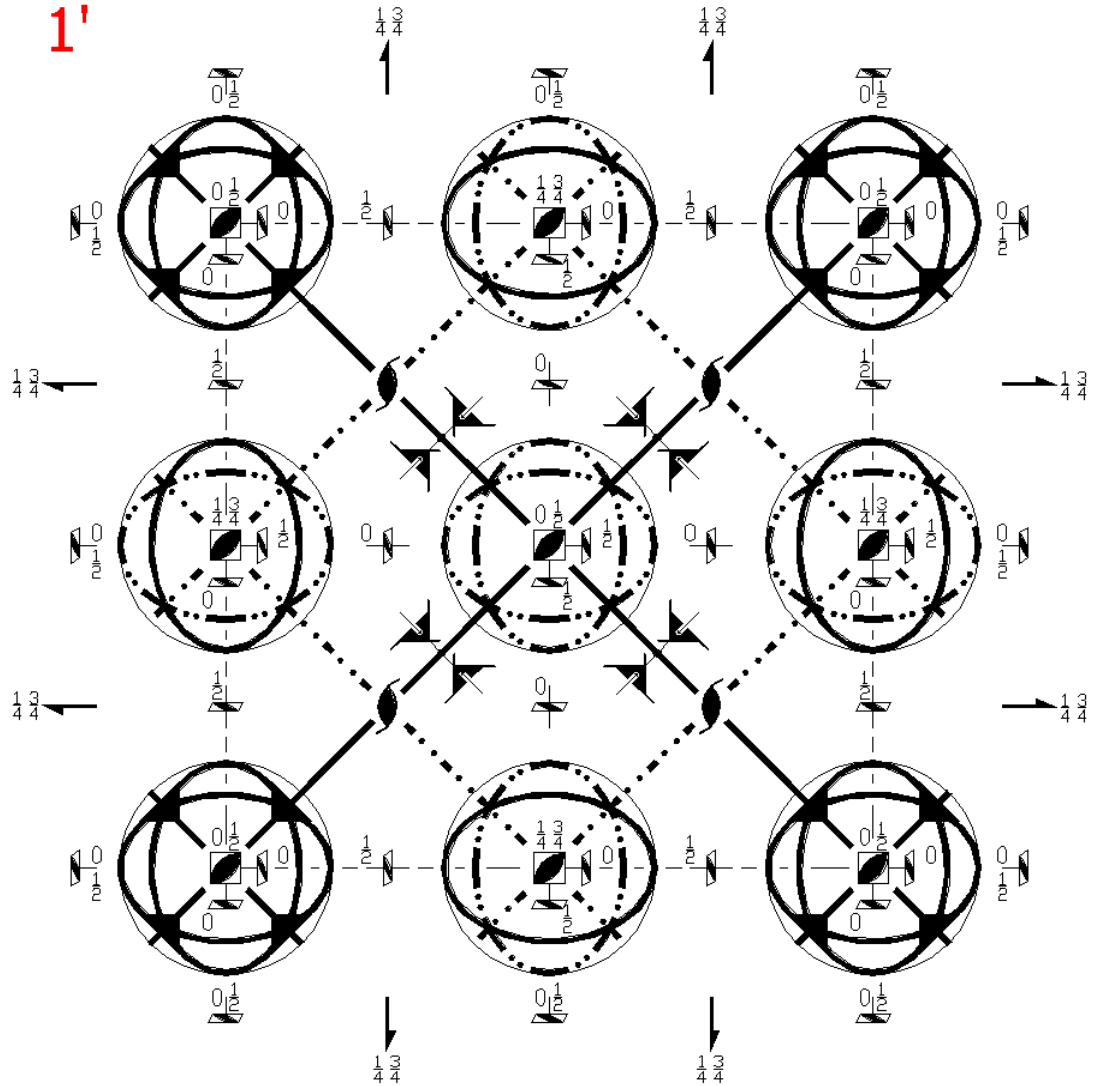
217.2.1581

$\bar{4}3m1'$

$\bar{I}43m1'$

Cubic

1'



Origin at  $\bar{4}3m1'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq x; z \leq y$

Vertices  $0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/2,1/2,1/2$

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                  | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)                   | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)                    |

- |  |   |   |   |
|--|---|---|---|
| (13) m $x,x,z$<br>( $m_{\bar{xy}} 0,0,0$ ) | (14) m $x,\bar{x},z$<br>( $m_{xy} 0,0,0$ )                    | (15) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z 0,0,0$ )      | (16) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^{-1} 0,0,0$ ) |
| (17) m $x,y,y$<br>( $m_{\bar{yz}} 0,0,0$ ) | (18) $\bar{4}^+$ $x,0,0; 0,0,0$<br>( $\bar{4}_x 0,0,0$ )      | (19) $\bar{4}^-$ $x,0,0; 0,0,0$<br>( $\bar{4}_x^{-1} 0,0,0$ ) | (20) m $x,y,\bar{y}$<br>( $m_{yz} 0,0,0$ )                    |
| (21) m $x,y,x$<br>( $m_{\bar{zx}} 0,0,0$ ) | (22) $\bar{4}^-$ $0,y,0; 0,0,0$<br>( $\bar{4}_y^{-1} 0,0,0$ ) | (23) m $\bar{x},y,x$<br>( $m_{xz} 0,0,0$ )                    | (24) $\bar{4}^+$ $0,y,0; 0,0,0$<br>( $\bar{4}_y 0,0,0$ )      |

For (1/2,1/2,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                            | (2) 2 (0,0,1/2) 1/4,1/4,z<br>( $2_z 1/2,1/2,1/2$ )                                    | (3) 2 (0,1/2,0) 1/4,y,1/4<br>( $2_y 1/2,1/2,1/2$ )  | (4) 2 (1/2,0,0) x,1/4,1/4<br>( $2_x 1/2,1/2,1/2$ )                                    |
| (5) $3^+$ (1/2,1/2,1/2) $x,x,x$<br>( $3_{xyz} 1/2,1/2,1/2$ )      | (6) $3^+$ (1/6,-1/6,1/6)<br>$x+1/3,x+1/3,\bar{x}$<br>( $3_{xyz}^{-1} 1/2,1/2,1/2$ )   | (7) $3^+$ (-1/6,1/6,1/6)<br>$x+2/3,\bar{x}-1/3,\bar{x}$<br>( $3_{xyz}^{-1} 1/2,1/2,1/2$ ) | (8) $3^+$ (1/6,1/6,-1/6)<br>$x+1/3,\bar{x}+2/3,x$<br>( $3_{xyz}^{-1} 1/2,1/2,1/2$ )   |
| (9) $3^-$ (1/2,1/2,1/2) $x,x,x$<br>( $3_{xyz}^{-1} 1/2,1/2,1/2$ ) | (10) $3^-$ (-1/6,1/6,1/6)<br>$x+1/3,\bar{x}+1/3,\bar{x}$<br>( $3_{xyz} 1/2,1/2,1/2$ ) | (11) $3^-$ (1/6,1/6,-1/6)<br>$x+2/3,\bar{x}+1/3,x$<br>( $3_{xyz} 1/2,1/2,1/2$ )           | (12) $3^-$ (1/6,-1/6,1/6)<br>$\bar{x}-1/3,x+2/3,\bar{x}$<br>( $3_{xyz} 1/2,1/2,1/2$ ) |
| (13) n (1/2,1/2,1/2) $x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,1/2$ )    | (14) c (0,0,1/2) $x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,1/2$ )                        | (15) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z 1/2,1/2,1/2$ )                        | (16) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1} 1/2,1/2,1/2$ )               |
| (17) n (1/2,1/2,1/2) $x,y,y$<br>( $m_{\bar{yz}} 1/2,1/2,1/2$ )    | (18) $\bar{4}^+$ $x,1/2,0; 1/4,1/2,0$<br>( $\bar{4}_x 1/2,1/2,1/2$ )                  | (19) $\bar{4}^-$ $x,0,1/2; 1/4,0,1/2$<br>( $\bar{4}_x^{-1} 1/2,1/2,1/2$ )                 | (20) a (1/2,0,0) $x,y+1/2,\bar{y}$<br>( $m_{yz} 1/2,1/2,1/2$ )                        |
| (21) n (1/2,1/2,1/2) $x,y,x$<br>( $m_{\bar{zx}} 1/2,1/2,1/2$ )    | (22) $\bar{4}^-$ 1/2,y,0; 1/2,1/4,0<br>( $\bar{4}_y^{-1} 1/2,1/2,1/2$ )               | (23) b (0,1/2,0) $\bar{x}+1/2,y,x$<br>( $m_{xz} 1/2,1/2,1/2$ )                            | (24) $\bar{4}^+$ 0,y,1/2; 0,1/4,1/2<br>( $\bar{4}_y 1/2,1/2,1/2$ )                    |

For (0,0,0)' + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1'<br>(1 0,0,0)'                              | (2) 2' 0,0,z<br>( $2_z 0,0,0$ )'                                | (3) 2' 0,y,0<br>( $2_y 0,0,0$ )'                                  | (4) 2' x,0,0<br>( $2_x 0,0,0$ )'                                |
| (5) $3^{+'}$ $x,x,x$<br>( $3_{xyz} 0,0,0$ )'      | (6) $3^{+'}$ $\bar{x},x,\bar{x}$<br>( $3_{xyz}^{-1} 0,0,0$ )'   | (7) $3^{+'}$ $x,\bar{x},\bar{x}$<br>( $3_{xyz}^{-1} 0,0,0$ )'     | (8) $3^{+'}$ $\bar{x},\bar{x},x$<br>( $3_{xyz}^{-1} 0,0,0$ )'   |
| (9) $3^{-'}$ $x,x,x$<br>( $3_{xyz}^{-1} 0,0,0$ )' | (10) $3^{-'}$ $x,\bar{x},\bar{x}$<br>( $3_{xyz} 0,0,0$ )'       | (11) $3^{-'}$ $\bar{x},\bar{x},x$<br>( $3_{xyz} 0,0,0$ )'         | (12) $3^{-'}$ $\bar{x},x,\bar{x}$<br>( $3_{xyz} 0,0,0$ )'       |
| (13) m' $x,x,z$<br>( $m_{\bar{xy}} 0,0,0$ )'      | (14) m' $x,\bar{x},z$<br>( $m_{xy} 0,0,0$ )'                    | (15) $\bar{4}^{+'}$ 0,0,z; 0,0,0<br>( $\bar{4}_z 0,0,0$ )'        | (16) $\bar{4}^{-'}$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1} 0,0,0$ )' |
| (17) m' $x,y,y$<br>( $m_{\bar{yz}} 0,0,0$ )'      | (18) $\bar{4}^{+'}$ $x,0,0; 0,0,0$<br>( $\bar{4}_x 0,0,0$ )'    | (19) $\bar{4}^{-'}$ $x,0,0; 0,0,0$<br>( $\bar{4}_x^{-1} 0,0,0$ )' | (20) m' $x,y,\bar{y}$<br>( $m_{yz} 0,0,0$ )'                    |
| (21) m' $x,y,x$<br>( $m_{\bar{zx}} 0,0,0$ )'      | (22) $\bar{4}^{-'}$ 0,y,0; 0,0,0<br>( $\bar{4}_y^{-1} 0,0,0$ )' | (23) m' $\bar{x},y,x$<br>( $m_{xz} 0,0,0$ )'                      | (24) $\bar{4}^{+'}$ 0,y,0; 0,0,0<br>( $\bar{4}_y 0,0,0$ )'      |

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (1 1/2,1/2,1/2)'	(2) 2' (0,0,1/2) 1/4,1/4,z (2 <sub>z</sub>  1/2,1/2,1/2)'	(3) 2' (0,1/2,0) 1/4,y,1/4 (2 <sub>y</sub>  1/2,1/2,1/2)'	(4) 2' (1/2,0,0) x,1/4,1/4 (2 <sub>x</sub>  1/2,1/2,1/2)'
(5) 3 <sup>+</sup> ' (1/2,1/2,1/2) x,x,x (3 <sub>xyz</sub>  1/2,1/2,1/2)'	(6) 3 <sup>+</sup> ' (1/6,-1/6,1/6) x+1/3,x+1/3,x (3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(7) 3 <sup>+</sup> ' (-1/6,1/6,1/6) x+2/3,x-1/3,x (3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(8) 3 <sup>+</sup> ' (1/6,1/6,-1/6) x+1/3,x+2/3,x (3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2)'
(9) 3 <sup>-</sup> ' (1/2,1/2,1/2) x,x,x (3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(10) 3 <sup>-</sup> ' (-1/6,1/6,1/6) x+1/3,x+1/3,x (3 <sub>xyz</sub>  1/2,1/2,1/2)'	(11) 3 <sup>-</sup> ' (1/6,1/6,-1/6) x+2/3,x+1/3,x (3 <sub>xyz</sub>  1/2,1/2,1/2)'	(12) 3 <sup>-</sup> ' (1/6,-1/6,1/6) x-1/3,x+2/3,x (3 <sub>xyz</sub>  1/2,1/2,1/2)'
(13) n' (1/2,1/2,1/2) x,x,z (m <sub>xy</sub>  1/2,1/2,1/2)'	(14) c' (0,0,1/2) x+1/2,x,z (m <sub>xy</sub>  1/2,1/2,1/2)'	(15) 4 <sup>+</sup> ' 1/2,0,z; 1/2,0,1/4 (4 <sub>z</sub>  1/2,1/2,1/2)'	(16) 4 <sup>-</sup> ' 0,1/2,z; 0,1/2,1/4 (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'
(17) n' (1/2,1/2,1/2) x,y,y (m <sub>yz</sub>  1/2,1/2,1/2)'	(18) 4 <sup>+</sup> ' x,1/2,0;1/4,1/2,0 (4 <sub>x</sub>  1/2,1/2,1/2)'	(19) 4 <sup>-</sup> ' x,0,1/2; 1/4,0,1/2 (4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(20) a' (1/2,0,0) x,y+1/2,y (m <sub>yz</sub>  1/2,1/2,1/2)'
(21) n' (1/2,1/2,1/2) x,y,x (m <sub>xz</sub>  1/2,1/2,1/2)'	(22) 4 <sup>-</sup> ' 1/2,y,0; 1/2,1/4,0 (4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(23) b' (0,1/2,0) x+1/2,y,x (m <sub>xz</sub>  1/2,1/2,1/2)'	(24) 4 <sup>+</sup> ' 0,y,1/2; 0,1/4,1/2 (4 <sub>y</sub>  1/2,1/2,1/2)'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); 1'.

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

(0,0,0) + (1/2,1/2,1/2) +  
(0,0,0)' + (1/2,1/2,1/2)'

48 h 11'

(1) x,y,z [0,0,0]	(2) x̄,ȳ,z [0,0,0]	(3) x̄,y,z̄ [0,0,0]	(4) x,ȳ,z̄ [0,0,0]
(5) z,x,y [0,0,0]	(6) z,x̄,ȳ [0,0,0]	(7) z̄,x̄,y [0,0,0]	(8) z̄,x,ȳ [0,0,0]
(9) y,z,x [0,0,0]	(10) ȳ,z,x̄ [0,0,0]	(11) y,z̄,x̄ [0,0,0]	(12) ȳ,z̄,x [0,0,0]
(13) y,x,z [0,0,0]	(14) ȳ,x̄,z [0,0,0]	(15) y,x̄,z̄ [0,0,0]	(16) ȳ,x,z̄ [0,0,0]
(17) x,z,y [0,0,0]	(18) x̄,z,ȳ [0,0,0]	(19) x̄,z̄,y [0,0,0]	(20) x,z̄,ȳ [0,0,0]
(21) z,y,x [0,0,0]	(22) z,ȳ,x̄ [0,0,0]	(23) z̄,y,x̄ [0,0,0]	(24) z̄,ȳ,x [0,0,0]

24 g ..m1'	x,x,z [0,0,0]	x̄,x̄,z [0,0,0]	x̄,x,z̄ [0,0,0]	x,x̄,z̄ [0,0,0]
	z,x,x [0,0,0]	z,x̄,x̄ [0,0,0]	z̄,x̄,x [0,0,0]	z̄,x,x̄ [0,0,0]
	x,z,x [0,0,0]	x̄,z,x̄ [0,0,0]	x,z̄,x̄ [0,0,0]	x̄,z̄,x [0,0,0]

Continued

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 $\bar{4}3m1'$ 

24	f	2..1'	$x, 1/2, 0 [0,0,0]$	$\bar{x}, 1/2, 0 [0,0,0]$	$0, x, 1/2 [0,0,0]$	$0, \bar{x}, 1/2 [0,0,0]$
			$1/2, 0, x [0,0,0]$	$1/2, 0, \bar{x} [0,0,0]$	$1/2, x, 0 [0,0,0]$	$1/2, \bar{x}, 0 [0,0,0]$
			$x, 0, 1/2 [0,0,0]$	$\bar{x}, 0, 1/2 [0,0,0]$	$0, 1/2, x [0,0,0]$	$0, 1/2, \bar{x} [0,0,0]$
12	e	2.mm1'	$x, 0, 0 [0,0,0]$	$\bar{x}, 0, 0 [0,0,0]$	$0, x, 0 [0,0,0]$	$0, \bar{x}, 0 [0,0,0]$
			$0, \bar{x}, 0 [0,0,0]$	$0, 0, x [0,0,0]$	$0, 0, \bar{x} [0,0,0]$	
12	d	$\bar{4}1'$	$1/4, 1/2, 0 [0,0,0]$	$3/4, 1/2, 0 [0,0,0]$	$0, 1/4, 1/2 [0,0,0]$	$0, 1/4, 1/2 [0,0,0]$
			$0, 3/4, 1/2 [0,0,0]$	$1/2, 0, 1/4 [0,0,0]$	$1/2, 0, 3/4 [0,0,0]$	
8	c	.3m1'	$x, x, x [0,0,0]$	$\bar{x}, \bar{x}, x [0,0,0]$	$\bar{x}, x, \bar{x} [0,0,0]$	$x, \bar{x}, \bar{x} [0,0,0]$
6	b	$\bar{4}2.m1'$	$0, 1/2, 1/2 [0,0,0]$	$1/2, 0, 1/2 [0,0,0]$	$1/2, 1/2, 0 [0,0,0]$	
2	a	$\bar{4}3m1'$	$0, 0, 0 [0,0,0]$			

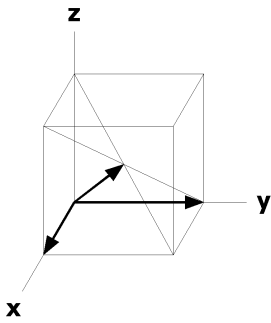
**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p\bar{3}1m1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x,x,x$

Along  $[1,1,0]$   $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$

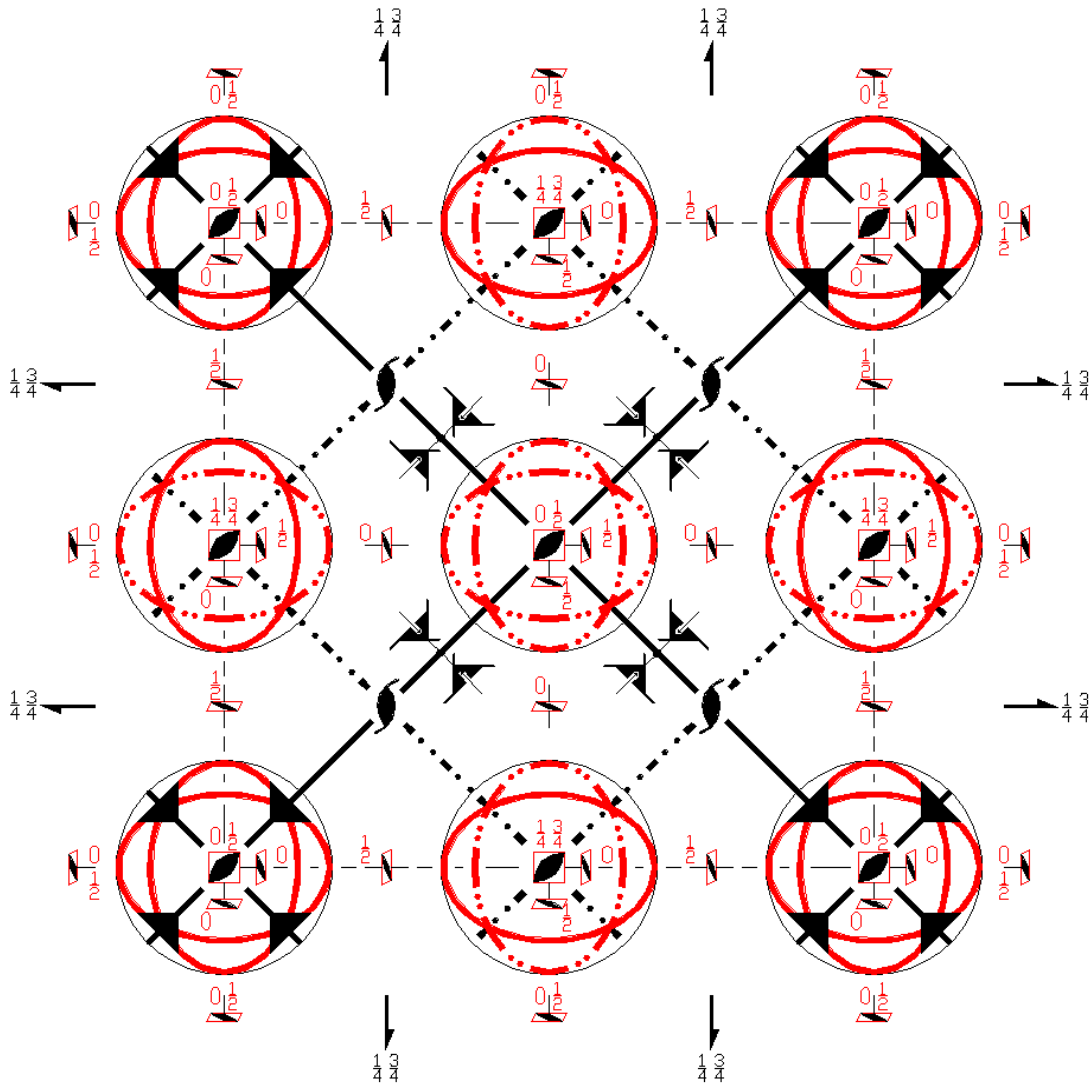




$\bar{1}4'3m'$   
217.3.1582

$\bar{4}'3m'$   
 $\bar{1}4'3m'$

Cubic



Origin at  $\bar{4}'3m'$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq x;$   $z \leq y$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

For  $(0,0,0) + \text{set}$

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                         | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)    | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)      | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)     |

(13) $m' \ x,x,z$ ( $m_{\bar{xy}} 0,0,0$ )'	(14) $m' \ x,\bar{x},z$ ( $m_{xy} 0,0,0$ )'	(15) $\bar{4}^+ \ ' \ 0,0,z; 0,0,0$ ( $\bar{4}_z 0,0,0$ )'	(16) $\bar{4}^- \ ' \ 0,0,z; 0,0,0$ ( $\bar{4}_z^{-1} 0,0,0$ )'
(17) $m' \ x,y,y$ ( $m_{\bar{yz}} 0,0,0$ )'	(18) $\bar{4}^+ \ ' \ x,0,0; 0,0,0$ ( $\bar{4}_x 0,0,0$ )'	(19) $\bar{4}^- \ ' \ x,0,0; 0,0,0$ ( $\bar{4}_x^{-1} 0,0,0$ )'	(20) $m' \ x,y,\bar{y}$ ( $m_{yz} 0,0,0$ )'
(21) $m' \ x,y,x$ ( $m_{\bar{zx}} 0,0,0$ )'	(22) $\bar{4}^- \ ' \ 0,y,0; 0,0,0$ ( $\bar{4}_y^{-1} 0,0,0$ )'	(23) $m' \ \bar{x},y,x$ ( $m_{xz} 0,0,0$ )'	(24) $\bar{4}^+ \ ' \ 0,y,0; 0,0,0$ ( $\bar{4}_y 0,0,0$ )'
For (1/2,1/2,1/2) + set			
(1) $t \ (1/2,1/2,1/2)$ ( $1 1/2,1/2,1/2$ )	(2) $2 \ (0,0,1/2) \ 1/4,1/4,z$ ( $2_z 1/2,1/2,1/2$ )	(3) $2 \ (0,1/2,0) \ 1/4,y,1/4$ ( $2_y 1/2,1/2,1/2$ )	(4) $2 \ (1/2,0,0) \ x,1/4,1/4$ ( $2_x 1/2,1/2,1/2$ )
(5) $3^+ \ (1/2,1/2,1/2) \ x,x,x$ ( $3_{xyz} 1/2,1/2,1/2$ )	(6) $3^+ \ (1/6,-1/6,1/6)$ $\bar{x}+1/3,\bar{x}+1/3,\bar{x}$ ( $3_{xyz}^{-1} 1/2,1/2,1/2$ )	(7) $3^+ \ (-1/6,1/6,1/6)$ $\bar{x}+2/3,\bar{x}-1/3,\bar{x}$ ( $3_{xyz}^{-1} 1/2,1/2,1/2$ )	(8) $3^+ \ (1/6,1/6,-1/6)$ $\bar{x}+1/3,\bar{x}+2/3,\bar{x}$ ( $3_{xyz}^{-1} 1/2,1/2,1/2$ )
(9) $3^- \ (1/2,1/2,1/2) \ x,x,x$ ( $3_{xyz}^{-1} 1/2,1/2,1/2$ )	(10) $3^- \ (-1/6,1/6,1/6)$ $\bar{x}+1/3,\bar{x}+1/3,\bar{x}$ ( $3_{xyz} 1/2,1/2,1/2$ )	(11) $3^- \ (1/6,1/6,-1/6)$ $\bar{x}+2/3,\bar{x}+1/3,\bar{x}$ ( $3_{xyz} 1/2,1/2,1/2$ )	(12) $3^- \ (1/6,-1/6,1/6)$ $\bar{x}-1/3,\bar{x}+2/3,\bar{x}$ ( $3_{xyz} 1/2,1/2,1/2$ )
(13) $n' \ (1/2,1/2,1/2) \ x,x,z$ ( $m_{\bar{xy}} 1/2,1/2,1/2$ )'	(14) $c' \ (0,0,1/2) \ \bar{x}+1/2,\bar{x},z$ ( $m_{xy} 1/2,1/2,1/2$ )'	(15) $\bar{4}^+ \ ' \ 1/2,0,z; 1/2,0,1/4$ ( $\bar{4}_z 1/2,1/2,1/2$ )'	(16) $\bar{4}^- \ ' \ 0,1/2,z; 0,1/2,1/4$ ( $\bar{4}_z^{-1} 1/2,1/2,1/2$ )'
(17) $n' \ (1/2,1/2,1/2) \ x,y,y$ ( $m_{\bar{yz}} 1/2,1/2,1/2$ )'	(18) $\bar{4}^+ \ ' \ x,1/2,0; 1/4,1/2,0$ ( $\bar{4}_x 1/2,1/2,1/2$ )'	(19) $\bar{4}^- \ ' \ x,0,1/2; 1/4,0,1/2$ ( $\bar{4}_x^{-1} 1/2,1/2,1/2$ )'	(20) $a' \ (1/2,0,0) \ x,y+1/2,\bar{y}$ ( $m_{yz} 1/2,1/2,1/2$ )'
(21) $n' \ (1/2,1/2,1/2) \ x,y,x$ ( $m_{\bar{zx}} 1/2,1/2,1/2$ )'	(22) $\bar{4}^- \ ' \ 1/2,y,0; 1/2,1/4,0$ ( $\bar{4}_y^{-1} 1/2,1/2,1/2$ )'	(23) $b' \ (0,1/2,0) \ \bar{x}+1/2,y,x$ ( $m_{xz} 1/2,1/2,1/2$ )'	(24) $\bar{4}^+ \ ' \ 0,y,1/2; 0,1/4,1/2$ ( $\bar{4}_y 1/2,1/2,1/2$ )'

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,1/2)$ ; (2); (3); (5); (13).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (1/2,1/2,1/2) +

48	h	1				
(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]			
(5) $z,x,y$ [w,u,v]	(6) $z,\bar{x},\bar{y}$ [ $w,\bar{u},\bar{v}$ ]	(7) $\bar{z},\bar{x},y$ [ $\bar{w},\bar{u},v$ ]	(8) $\bar{z},x,\bar{y}$ [ $\bar{w},u,\bar{v}$ ]			
(9) $y,z,x$ [v,w,u]	(10) $\bar{y},z,\bar{x}$ [ $\bar{v},w,\bar{u}$ ]	(11) $y,\bar{z},\bar{x}$ [ $v,\bar{w},\bar{u}$ ]	(12) $\bar{y},\bar{z},x$ [ $\bar{v},\bar{w},u$ ]			
(13) $y,x,z$ [v,u,w]	(14) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(15) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(16) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]			
(17) $x,z,y$ [u,w,v]	(18) $\bar{x},z,\bar{y}$ [ $\bar{u},w,\bar{v}$ ]	(19) $\bar{x},\bar{z},y$ [ $\bar{u},\bar{w},v$ ]	(20) $x,\bar{z},\bar{y}$ [ $u,\bar{w},\bar{v}$ ]			
(21) $z,y,x$ [w,v,u]	(22) $z,\bar{y},\bar{x}$ [ $w,\bar{v},\bar{u}$ ]	(23) $\bar{z},y,\bar{x}$ [ $\bar{w},v,\bar{u}$ ]	(24) $\bar{z},\bar{y},x$ [ $\bar{w},\bar{v},u$ ]			

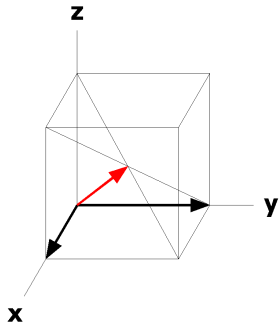
24	g	$\bar{2}m'$	$x,x,z [u,u,w]$	$\bar{x},\bar{x},z [\bar{u},\bar{u},w]$	$\bar{x},x,\bar{z} [\bar{u},u,\bar{w}]$	$x,\bar{x},\bar{z} [u,\bar{u},\bar{w}]$
			$z,x,x [w,u,u]$	$z,\bar{x},\bar{x} [w,\bar{u},\bar{u}]$	$\bar{z},\bar{x},x [\bar{w},\bar{u},u]$	$\bar{z},x,\bar{x} [\bar{w},u,\bar{u}]$
			$x,z,x [u,w,u]$	$\bar{x},z,\bar{x} [\bar{u},w,\bar{u}]$	$x,\bar{z},\bar{x} [u,\bar{w},\bar{u}]$	$\bar{x},\bar{z},x [\bar{u},\bar{w},u]$
24	f	$2..$	$x,1/2,0 [u,0,0]$	$\bar{x},1/2,0 [\bar{u},0,0]$	$0,x,1/2 [0,u,0]$	$0,\bar{x},1/2 [0,\bar{u},0]$
			$1/2,0,x [0,0,u]$	$1/2,0,\bar{x} [0,0,\bar{u}]$	$1/2,x,0 [0,u,0]$	$1/2,\bar{x},0 [0,\bar{u},0]$
			$x,0,1/2 [u,0,0]$	$\bar{x},0,1/2 [\bar{u},0,0]$	$0,1/2,x [0,0,u]$	$0,1/2,\bar{x} [0,0,\bar{u}]$
12	e	$2.m'm'$	$x,0,0 [u,0,0]$	$\bar{x},0,0 [\bar{u},0,0]$		$0,x,0 [0,u,0]$
			$0,\bar{x},0 [0,\bar{u},0]$	$0,0,x [0,0,u]$		$0,0,\bar{x} [0,0,\bar{u}]$
12	d	$\bar{4}'$	$1/4,1/2,0 [0,0,0]$	$3/4,1/2,0 [0,0,0]$		$0,1/4,1/2 [0,0,0]$
			$0,3/4,1/2 [0,0,0]$	$1/2,0,1/4 [0,0,0]$		$1/2,0,3/4 [0,0,0]$
8	c	$.3m'$	$x,x,x [u,u,u]$	$\bar{x},\bar{x},x [\bar{u},\bar{u},u]$	$\bar{x},x,\bar{x} [\bar{u},u,\bar{u}]$	$x,\bar{x},\bar{x} [u,\bar{u},\bar{u}]$
6	b	$\bar{4}'2.m'$	$0,1/2,1/2 [0,0,0]$	$1/2,0,1/2 [0,0,0]$		$1/2,1/2,0 [0,0,0]$
2	a	$\bar{4}'3m'$	$0,0,0 [0,0,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p31m'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x,x,x$

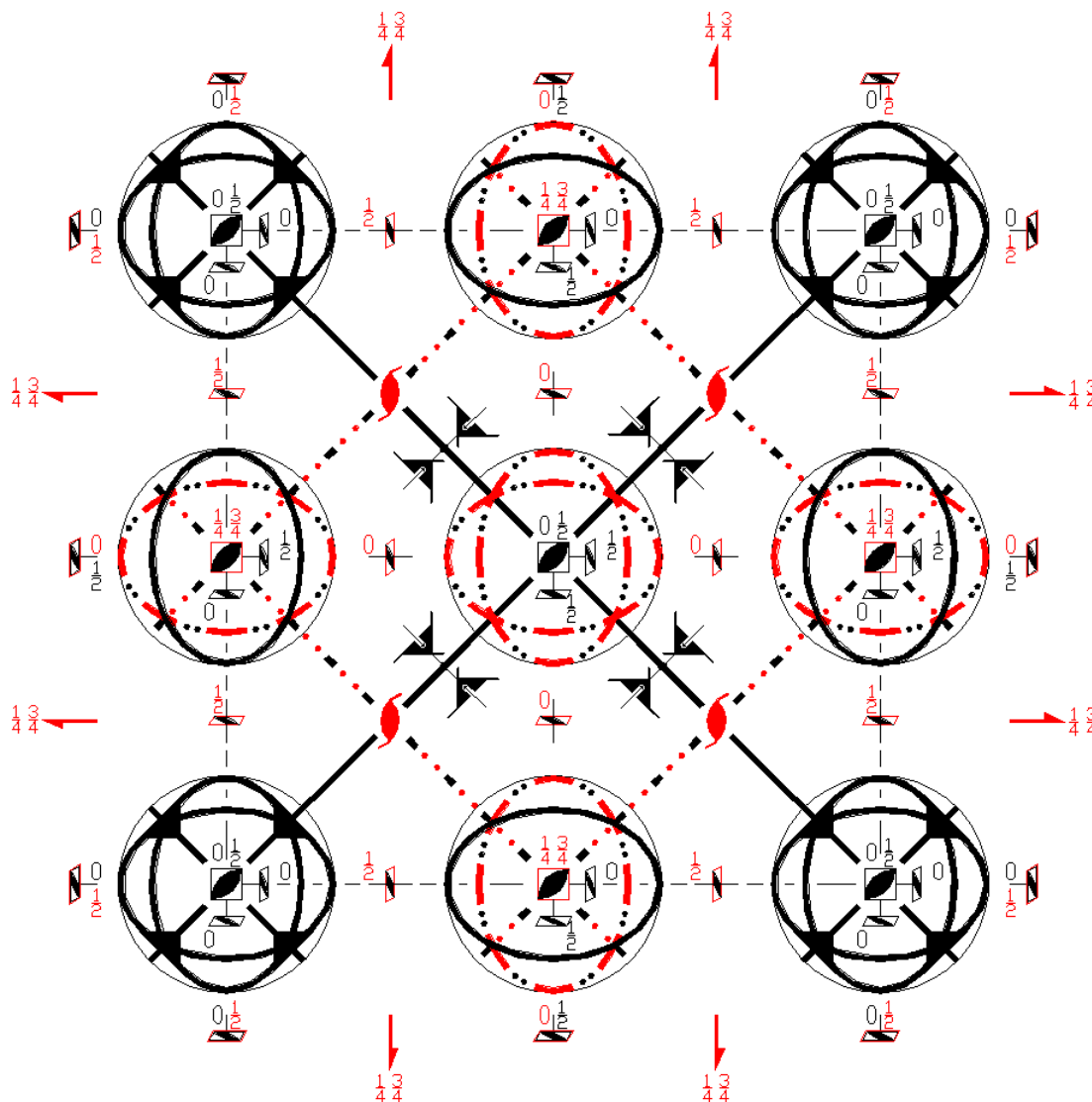
Along  $[1,1,0]$   $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



$I_p \bar{4}3m$   
217.4.1583

$\bar{4}3m1'$   
 $I_p \bar{4}3m$

Cubic



Origin at  $\bar{4}3m$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq x;$   $z \leq y$   
**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

### Symmetry Operations

For  $(0,0,0) + \text{set}$

- |   |  |   |   |
|---|--|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                 | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                            | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                  |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)  | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}yz}$  0,0,0)        |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)      | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}yz}$  0,0,0) | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{\bar{x}y\bar{z}}$  0,0,0) |

(13) m $x,x,z$ ( $m_{\bar{xy}} 0,0,0$ )	(14) m $x,\bar{x},z$ ( $m_{xy} 0,0,0$ )	(15) $\bar{4}^+$ $0,0,z; 0,0,0$ ( $\bar{4}_z 0,0,0$ )	(16) $\bar{4}^-$ $0,0,z; 0,0,0$ ( $\bar{4}_z^{-1} 0,0,0$ )
(17) m $x,y,y$ ( $m_{\bar{yz}} 0,0,0$ )	(18) $\bar{4}^+$ $x,0,0; 0,0,0$ ( $\bar{4}_x 0,0,0$ )	(19) $\bar{4}^-$ $x,0,0; 0,0,0$ ( $\bar{4}_x^{-1} 0,0,0$ )	(20) m $x,y,\bar{y}$ ( $m_{yz} 0,0,0$ )
(21) m $x,y,x$ ( $m_{\bar{zx}} 0,0,0$ )	(22) $\bar{4}^-$ $0,y,0; 0,0,0$ ( $\bar{4}_y^{-1} 0,0,0$ )	(23) m $\bar{x},y,x$ ( $m_{xz} 0,0,0$ )	(24) $\bar{4}^+$ $0,y,0; 0,0,0$ ( $\bar{4}_y 0,0,0$ )

For  $(1/2,1/2,1/2)'$  + set

(1) t' $(1/2,1/2,1/2)$ ( $1 1/2,1/2,1/2$ )'	(2) 2' $(0,0,1/2)$ $1/4,1/4,z$ ( $2_z 1/2,1/2,1/2$ )'	(3) 2' $(0,1/2,0)$ $1/4,y,1/4$ ( $2_y 1/2,1/2,1/2$ )'	(4) 2' $(1/2,0,0)$ $x,1/4,1/4$ ( $2_x 1/2,1/2,1/2$ )'
(5) $3^{+}$ $(1/2,1/2,1/2)$ $x,x,x$ ( $3_{xyz} 1/2,1/2,1/2$ )'	(6) $3^{+}$ $(1/6,-1/6,1/6)$ $\bar{x}+1/3,\bar{x}+1/3,\bar{x}$ ( $3_{xyz}^{-1} 1/2,1/2,1/2$ )'	(7) $3^{+}$ $(-1/6,1/6,1/6)$ $\bar{x}+2/3,\bar{x}-1/3,\bar{x}$ ( $3_{xyz}^{-1} 1/2,1/2,1/2$ )'	(8) $3^{+}$ $(1/6,1/6,-1/6)$ $\bar{x}+1/3,\bar{x}+2/3,\bar{x}$ ( $3_{xyz}^{-1} 1/2,1/2,1/2$ )'
(9) $3^{-}$ $(1/2,1/2,1/2)$ $x,x,x$ ( $3_{xyz}^{-1} 1/2,1/2,1/2$ )'	(10) $3^{-}$ $(-1/6,1/6,1/6)$ $\bar{x}+1/3,\bar{x}+1/3,\bar{x}$ ( $3_{xyz} 1/2,1/2,1/2$ )'	(11) $3^{-}$ $(1/6,1/6,-1/6)$ $\bar{x}+2/3,\bar{x}+1/3,\bar{x}$ ( $3_{xyz} 1/2,1/2,1/2$ )'	(12) $3^{-}$ $(1/6,-1/6,1/6)$ $\bar{x}-1/3,\bar{x}+2/3,\bar{x}$ ( $3_{xyz} 1/2,1/2,1/2$ )'
(13) n' $(1/2,1/2,1/2)$ $x,x,z$ ( $m_{\bar{xy}} 1/2,1/2,1/2$ )'	(14) c' $(0,0,1/2)$ $x+1/2,\bar{x},z$ ( $m_{xy} 1/2,1/2,1/2$ )'	(15) $\bar{4}^+$ $1/2,0,z; 1/2,0,1/4$ ( $\bar{4}_z 1/2,1/2,1/2$ )'	(16) $\bar{4}^-$ $0,1/2,z; 0,1/2,1/4$ ( $\bar{4}_z^{-1} 1/2,1/2,1/2$ )'
(17) n' $(1/2,1/2,1/2)$ $x,y,y$ ( $m_{\bar{yz}} 1/2,1/2,1/2$ )'	(18) $\bar{4}^+$ $x,1/2,0; 1/4,1/2,0$ ( $\bar{4}_x 1/2,1/2,1/2$ )'	(19) $\bar{4}^-$ $x,0,1/2; 1/4,0,1/2$ ( $\bar{4}_x^{-1} 1/2,1/2,1/2$ )'	(20) a' $(1/2,0,0)$ $x,y+1/2,\bar{y}$ ( $m_{yz} 1/2,1/2,1/2$ )'
(21) n' $(1/2,1/2,1/2)$ $x,y,x$ ( $m_{\bar{zx}} 1/2,1/2,1/2$ )'	(22) $\bar{4}^-$ $1/2,y,0; 1/2,1/4,0$ ( $\bar{4}_y^{-1} 1/2,1/2,1/2$ )'	(23) b' $(0,1/2,0)$ $\bar{x}+1/2,y,x$ ( $m_{xz} 1/2,1/2,1/2$ )'	(24) $\bar{4}^+$ $0,y,1/2; 0,1/4,1/2$ ( $\bar{4}_y 1/2,1/2,1/2$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13).**Positions**Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (1/2,1/2,1/2)' +

48	h	1				
(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]			
(5) $z,x,y$ [w,u,v]	(6) $z,\bar{x},\bar{y}$ [ $w,\bar{u},\bar{v}$ ]	(7) $\bar{z},\bar{x},y$ [ $\bar{w},\bar{u},v$ ]	(8) $\bar{z},x,\bar{y}$ [ $\bar{w},u,\bar{v}$ ]			
(9) $y,z,x$ [v,w,u]	(10) $\bar{y},z,\bar{x}$ [ $\bar{v},w,\bar{u}$ ]	(11) $y,\bar{z},\bar{x}$ [ $v,\bar{w},\bar{u}$ ]	(12) $\bar{y},z,x$ [ $\bar{v},w,u$ ]			
(13) $y,x,z$ [ $\bar{v},\bar{u},\bar{w}$ ]	(14) $\bar{y},\bar{x},z$ [ $v,u,\bar{w}$ ]	(15) $y,\bar{x},\bar{z}$ [ $\bar{v},u,w$ ]	(16) $\bar{y},x,\bar{z}$ [ $v,\bar{u},w$ ]			
(17) $x,z,y$ [ $\bar{u},\bar{w},\bar{v}$ ]	(18) $\bar{x},z,\bar{y}$ [ $u,\bar{w},v$ ]	(19) $\bar{x},\bar{z},y$ [ $u,w,\bar{v}$ ]	(20) $x,\bar{z},\bar{y}$ [ $\bar{u},w,v$ ]			
(21) $z,y,x$ [ $\bar{w},\bar{v},\bar{u}$ ]	(22) $z,\bar{y},\bar{x}$ [ $\bar{w},v,u$ ]	(23) $\bar{z},y,\bar{x}$ [ $w,\bar{v},u$ ]	(24) $\bar{z},\bar{y},x$ [ $w,v,\bar{u}$ ]			

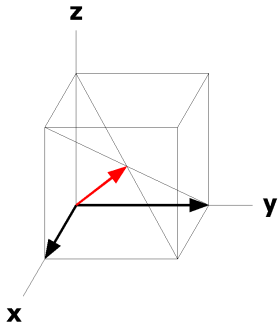
24	g	..m	x,x,z [u, $\bar{u}$ ,0] z,x,x [0,u, $\bar{u}$ ] x,z,x [ $\bar{u}$ ,0,u]	$\bar{x},\bar{x},z$ [ $\bar{u}$ ,u,0] $z,\bar{x},\bar{x}$ [0, $\bar{u}$ ,u] $\bar{x},z,\bar{x}$ [u,0, $\bar{u}$ ]	$\bar{x},x,\bar{z}$ [ $\bar{u}$ , $\bar{u}$ ,0] $\bar{z},\bar{x},x$ [0, $\bar{u}$ , $\bar{u}$ ] x, $\bar{z},\bar{x}$ [ $\bar{u}$ ,0, $\bar{u}$ ]	x, $\bar{x},\bar{z}$ [u,u,0] $\bar{z},x,\bar{x}$ [0,u,u] $\bar{x},\bar{z},x$ [u,0,u]
24	f	2..	x,1/2,0 [u,0,0] 1/2,0,x [0,0,u] x,0,1/2 [ $\bar{u}$ ,0,0]	$\bar{x},1/2,0$ [ $\bar{u}$ ,0,0] 1/2,0, $\bar{x}$ [0,0, $\bar{u}$ ] $\bar{x},0,1/2$ [u,0,0]	0,x,1/2 [0,u,0] 1/2,x,0 [0, $\bar{u}$ ,0] 0,1/2,x [0,0, $\bar{u}$ ]	0, $\bar{x},1/2$ [0, $\bar{u}$ ,0] 1/2, $\bar{x},0$ [0,u,0] 0,1/2, $\bar{x}$ [0,0,u]
12	e	2.mm	x,0,0 [0,0,0] 0, $\bar{x},0$ [0,0,0]	$\bar{x},0,0$ [0,0,0] 0,0,x [0,0,0]	0,x,0 [0,0,0] 0,0, $\bar{x}$ [0,0,0]	
12	d	$\bar{4}'$	1/4,1/2,0 [0,0,0] 0,3/4,1/2 [0,0,0]	3/4,1/2,0 [0,0,0] 1/2,0,1/4 [0,0,0]	0,1/4,1/2 [0,0,0] 1/2,0,3/4 [0,0,0]	
8	c	.3m	x,x,x [0,0,0]	$\bar{x},\bar{x},x$ [0,0,0]	$\bar{x},x,\bar{x}$ [0,0,0]	x, $\bar{x},\bar{x}$ [0,0,0]
6	b	$\bar{4}2.m$	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		1/2,1/2,0 [0,0,0]
2	a	$\bar{4}3m$	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1]  $p_p\bar{4}m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 1/2,0,z

Along [1,1,1]  $p_{31}m1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

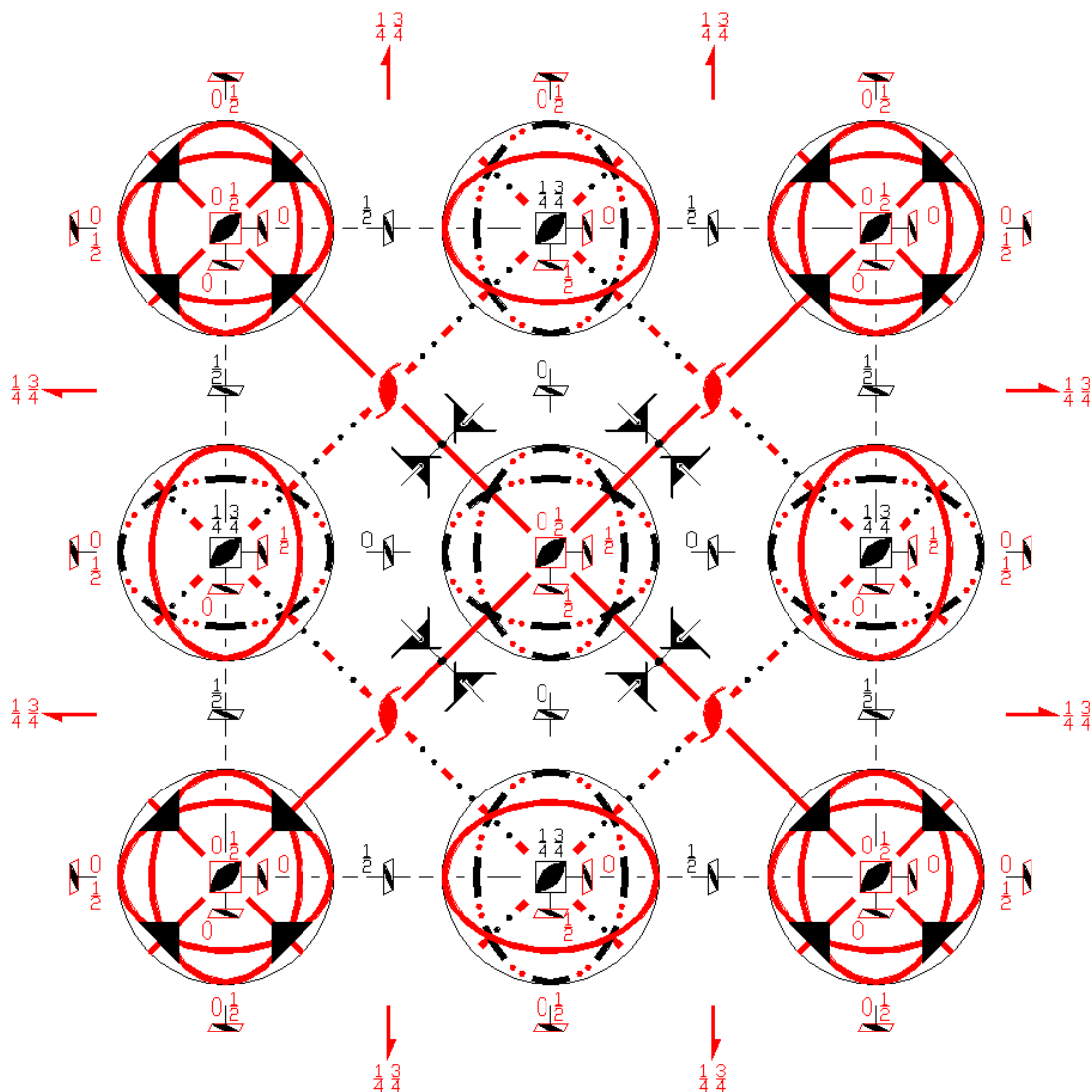
Along [1,1,0]  $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$I_P \bar{4}'3m'$   
217.5.1584

$\bar{4}3m1'$   
 $I_P \bar{4}'3m'$

Cubic



Origin at  $\bar{4}'3m'$

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq x;$   $z \leq y$   
**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                         | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)    | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)      | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)     |

(13) $m' \ x,x,z$ ( $m_{\bar{xy}}   0,0,0$ )'	(14) $m' \ x,\bar{x},z$ ( $m_{xy}   0,0,0$ )'	(15) $\bar{4}^+ \ 0,0,z; 0,0,0$ ( $\bar{4}_z   0,0,0$ )'	(16) $\bar{4}^- \ 0,0,z; 0,0,0$ ( $\bar{4}_z^{-1}   0,0,0$ )'
(17) $m' \ x,y,y$ ( $m_{\bar{yz}}   0,0,0$ )'	(18) $\bar{4}^+ \ x,0,0; 0,0,0$ ( $\bar{4}_x   0,0,0$ )'	(19) $\bar{4}^- \ x,0,0; 0,0,0$ ( $\bar{4}_x^{-1}   0,0,0$ )'	(20) $m' \ x,y,\bar{y}$ ( $m_{yz}   0,0,0$ )'
(21) $m' \ x,y,x$ ( $m_{\bar{zx}}   0,0,0$ )'	(22) $\bar{4}^- \ 0,y,0; 0,0,0$ ( $\bar{4}_y^{-1}   0,0,0$ )'	(23) $m' \ \bar{x},y,x$ ( $m_{xz}   0,0,0$ )'	(24) $\bar{4}^+ \ 0,y,0; 0,0,0$ ( $\bar{4}_y   0,0,0$ )'
For (1/2,1/2,1/2)' + set			
(1) $t' \ (1/2,1/2,1/2)$ ( $1   1/2,1/2,1/2$ )'	(2) $2' \ (0,0,1/2) \ 1/4,1/4,z$ ( $2_z   1/2,1/2,1/2$ )'	(3) $2' \ (0,1/2,0) \ 1/4,y,1/4$ ( $2_y   1/2,1/2,1/2$ )'	(4) $2' \ (1/2,0,0) \ x,1/4,1/4$ ( $2_x   1/2,1/2,1/2$ )'
(5) $3^+ \ (1/2,1/2,1/2) \ x,x,x$ ( $3_{xyz}   1/2,1/2,1/2$ )'	(6) $3^+ \ (1/6,-1/6,1/6)$ $\bar{x}+1/3,\bar{x}+1/3,\bar{x}$ ( $3_{xyz}^{-1}   1/2,1/2,1/2$ )'	(7) $3^+ \ (-1/6,1/6,1/6)$ $x+2/3,x-1/3,x$ ( $3_{xyz}^{-1}   1/2,1/2,1/2$ )'	(8) $3^+ \ (1/6,1/6,-1/6)$ $\bar{x}+1/3,\bar{x}+2/3,\bar{x}$ ( $3_{xyz}^{-1}   1/2,1/2,1/2$ )'
(9) $3^- \ (1/2,1/2,1/2) \ x,x,x$ ( $3_{xyz}^{-1}   1/2,1/2,1/2$ )'	(10) $3^- \ (-1/6,1/6,1/6)$ $x+1/3,\bar{x}+1/3,\bar{x}$ ( $3_{xyz}   1/2,1/2,1/2$ )'	(11) $3^- \ (1/6,1/6,-1/6)$ $x+2/3,\bar{x}+1/3,x$ ( $3_{xyz}   1/2,1/2,1/2$ )'	(12) $3^- \ (1/6,-1/6,1/6)$ $\bar{x}-1/3,\bar{x}+2/3,\bar{x}$ ( $3_{xyz}   1/2,1/2,1/2$ )'
(13) $n \ (1/2,1/2,1/2) \ x,x,z$ ( $m_{\bar{xy}}   1/2,1/2,1/2$ )'	(14) $c \ (0,0,1/2) \ x+1/2,\bar{x},z$ ( $m_{xy}   1/2,1/2,1/2$ )'	(15) $\bar{4}^+ \ 1/2,0,z; 1/2,0,1/4$ ( $\bar{4}_z   1/2,1/2,1/2$ )'	(16) $\bar{4}^- \ 0,1/2,z; 0,1/2,1/4$ ( $\bar{4}_z^{-1}   1/2,1/2,1/2$ )'
(17) $n \ (1/2,1/2,1/2) \ x,y,y$ ( $m_{\bar{yz}}   1/2,1/2,1/2$ )'	(18) $\bar{4}^+ \ x,1/2,0; 1/4,1/2,0$ ( $\bar{4}_x   1/2,1/2,1/2$ )'	(19) $\bar{4}^- \ x,0,1/2; 1/4,0,1/2$ ( $\bar{4}_x^{-1}   1/2,1/2,1/2$ )'	(20) $a \ (1/2,0,0) \ x,y+1/2,\bar{y}$ ( $m_{yz}   1/2,1/2,1/2$ )'
(21) $n \ (1/2,1/2,1/2) \ x,y,x$ ( $m_{\bar{zx}}   1/2,1/2,1/2$ )'	(22) $\bar{4}^- \ 1/2,y,0; 1/2,1/4,0$ ( $\bar{4}_y^{-1}   1/2,1/2,1/2$ )'	(23) $b \ (0,1/2,0) \ \bar{x}+1/2,y,x$ ( $m_{xz}   1/2,1/2,1/2$ )'	(24) $\bar{4}^+ \ 0,y,1/2; 0,1/4,1/2$ ( $\bar{4}_y   1/2,1/2,1/2$ )'

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t'(1/2,1/2,1/2)$ ; (2); (3); (5); (13).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

(0,0,0) + (1/2,1/2,1/2)' +

48	h	1				
(1) $x,y,z$ [u,v,w]	(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]	(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) $x,\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]			
(5) $z,x,y$ [w,u,v]	(6) $z,\bar{x},\bar{y}$ [ $w,\bar{u},\bar{v}$ ]	(7) $\bar{z},\bar{x},y$ [ $\bar{w},\bar{u},v$ ]	(8) $\bar{z},x,\bar{y}$ [ $\bar{w},u,\bar{v}$ ]			
(9) $y,z,x$ [v,w,u]	(10) $\bar{y},z,\bar{x}$ [ $\bar{v},w,\bar{u}$ ]	(11) $y,\bar{z},\bar{x}$ [ $v,\bar{w},\bar{u}$ ]	(12) $\bar{y},\bar{z},x$ [ $\bar{v},\bar{w},u$ ]			
(13) $y,x,z$ [v,u,w]	(14) $\bar{y},\bar{x},z$ [ $\bar{v},\bar{u},w$ ]	(15) $y,\bar{x},\bar{z}$ [ $v,\bar{u},\bar{w}$ ]	(16) $\bar{y},x,\bar{z}$ [ $\bar{v},u,\bar{w}$ ]			
(17) $x,z,y$ [u,w,v]	(18) $\bar{x},z,\bar{y}$ [ $\bar{u},w,\bar{v}$ ]	(19) $\bar{x},\bar{z},y$ [ $\bar{u},\bar{w},v$ ]	(20) $x,\bar{z},\bar{y}$ [ $u,\bar{w},\bar{v}$ ]			
(21) $z,y,x$ [w,v,u]	(22) $z,\bar{y},\bar{x}$ [ $w,\bar{v},\bar{u}$ ]	(23) $\bar{z},y,\bar{x}$ [ $\bar{w},v,\bar{u}$ ]	(24) $\bar{z},\bar{y},x$ [ $\bar{w},\bar{v},u$ ]			



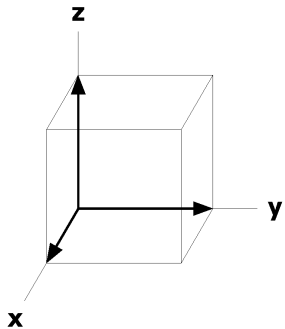
24	g	$\bar{2}m'$	$x,x,z [u,u,w]$	$\bar{x},\bar{x},z [\bar{u},\bar{u},w]$	$\bar{x},x,\bar{z} [\bar{u},u,\bar{w}]$	$x,\bar{x},\bar{z} [u,\bar{u},\bar{w}]$
			$z,x,x [w,u,u]$	$z,\bar{x},\bar{x} [w,\bar{u},\bar{u}]$	$\bar{z},\bar{x},x [\bar{w},\bar{u},u]$	$\bar{z},x,\bar{x} [\bar{w},u,\bar{u}]$
			$x,z,x [u,w,u]$	$\bar{x},z,\bar{x} [\bar{u},w,\bar{u}]$	$x,\bar{z},\bar{x} [u,\bar{w},\bar{u}]$	$\bar{x},\bar{z},x [\bar{u},\bar{w},u]$
24	f	$2..$	$x,1/2,0 [u,0,0]$	$\bar{x},1/2,0 [\bar{u},0,0]$	$0,x,1/2 [0,u,0]$	$0,\bar{x},1/2 [0,\bar{u},0]$
			$1/2,0,x [0,0,u]$	$1/2,0,\bar{x} [0,0,\bar{u}]$	$1/2,x,0 [0,u,0]$	$1/2,\bar{x},0 [0,\bar{u},0]$
			$x,0,1/2 [u,0,0]$	$\bar{x},0,1/2 [\bar{u},0,0]$	$0,1/2,x [0,0,u]$	$0,1/2,\bar{x} [0,0,\bar{u}]$
12	e	$2.m'm'$	$x,0,0 [u,0,0]$	$\bar{x},0,0 [\bar{u},0,0]$		$0,x,0 [0,u,0]$
			$0,\bar{x},0 [0,\bar{u},0]$	$0,0,x [0,0,u]$		$0,0,\bar{x} [0,0,\bar{u}]$
12	d	$\bar{4}$	$1/4,1/2,0 [u,0,0]$	$3/4,1/2,0 [\bar{u},0,0]$		$0,1/4,1/2 [0,u,0]$
			$0,3/4,1/2 [0,\bar{u},0]$	$1/2,0,1/4 [0,0,u]$		$1/2,0,3/4 [0,0,\bar{u}]$
8	c	$.3m'$	$x,x,x [\bar{u},\bar{u},\bar{u}]$	$\bar{x},\bar{x},x [\bar{u},\bar{u},\bar{u}]$	$\bar{x},x,\bar{x} [\bar{u},u,\bar{u}]$	$x,\bar{x},\bar{x} [u,\bar{u},\bar{u}]$
6	b	$\bar{4}'2.m'$	$0,1/2,1/2 [0,0,0]$		$1/2,0,1/2 [0,0,0]$	$1/2,1/2,0 [0,0,0]$
2	a	$\bar{4}'3m'$	$0,0,0 [0,0,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $p_p \bar{4}m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p_{31}m1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x,x,x$

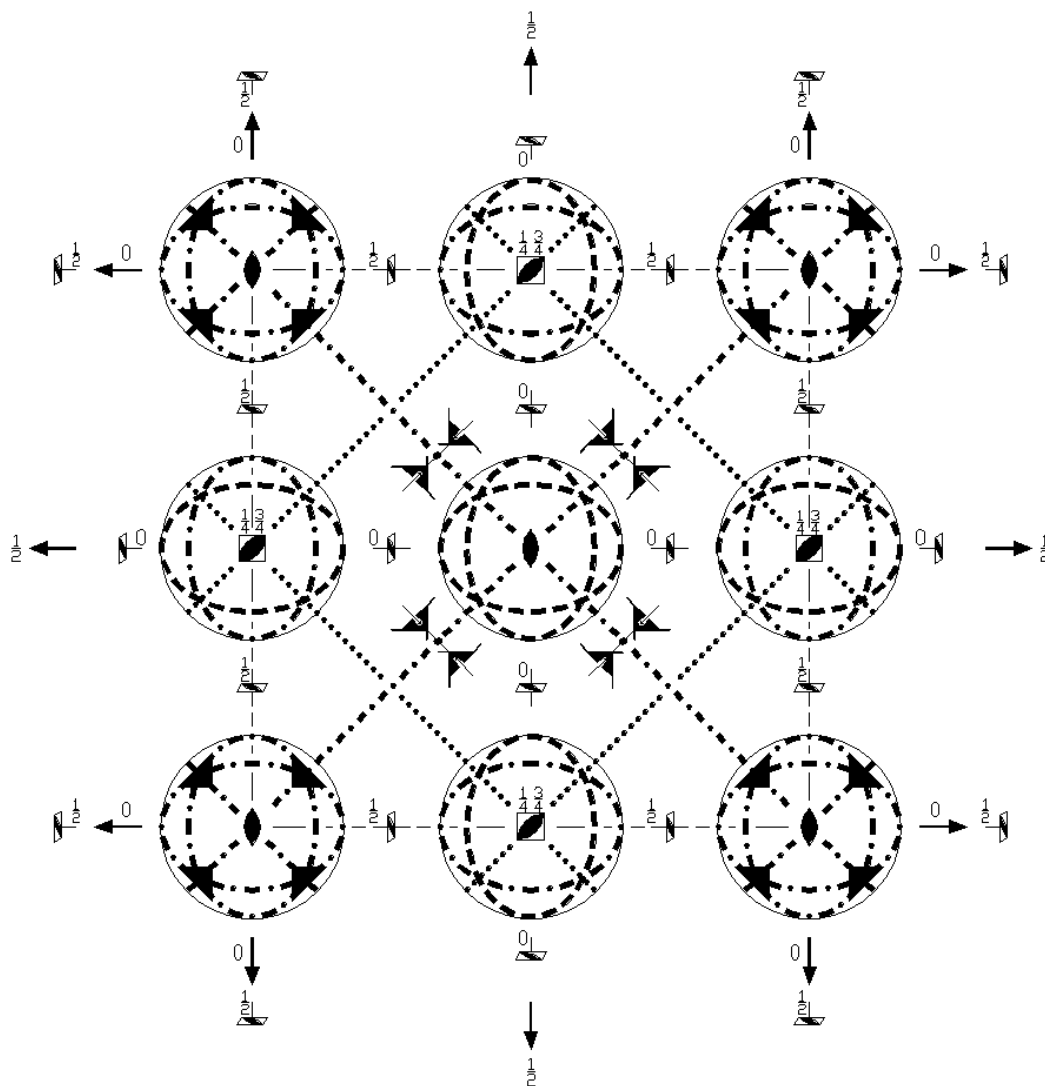
Along  $[1,1,0]$   $p_{2b} \bar{1}m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



$P\bar{4}3n$   
218.1.1585

$\bar{4}3m$   
 $P\bar{4}3n$

Cubic



**Origin at 23**

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $z \leq \min(x,y)$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $0,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

- |   |   |  |  |
|---|---|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                         | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0)   | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0)  |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) |

(13) n (1/2,1/2,1/2) x,x,z (m <sub>xy</sub> <sup>-</sup>  1/2,1/2,1/2)	(14) c (0,0,1/2) x+1/2,x̄,z (m <sub>xy</sub> <sup>-</sup>  1/2,1/2,1/2)	(15) 4 <sup>+</sup> 1/2,0,z;1/2,0,1/4 (4 <sub>z</sub> <sup>-</sup>  1/2,1/2,1/2)	(16) 4 <sup>-</sup> 0,1/2,z; 0,1/2,1/4 (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)
(17) n (1/2,1/2,1/2) x,y,y (m <sub>yz</sub> <sup>-</sup>  1/2,1/2,1/2)	(18) 4 <sup>+</sup> x,1/2,0; 1/4,1/2,0 (4 <sub>x</sub> <sup>-</sup>  1/2,1/2,1/2)	(19) 4 <sup>-</sup> x,0,1/2; 1/4,0,1/2 (4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,1/2)	(20) a (1/2,0,0) x,y+1/2,ȳ (m <sub>yz</sub> <sup>-</sup>  1/2,1/2,1/2)
(21) n (1/2,1/2,1/2) x,y,x (m <sub>xz</sub> <sup>-</sup>  1/2,1/2,1/2)	(22) 4 <sup>-</sup> 1/2,y,0; 1/2,1/4,0 (4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,1/2)	(23) b (0,1/2,0) x̄+1/2,y,x (m <sub>xz</sub> <sup>-</sup>  1/2,1/2,1/2)	(24) 4 <sup>+</sup> 0,y,1/2; 0,1/4,1/2 (4 <sub>y</sub> <sup>-</sup>  1/2,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

24 i 1

(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w̄]	(3) x̄,y,z [ū,v,w̄]	(4) x,y,z̄ [u,v̄,w̄]	
(5) z,x,y [w,u,v]	(6) z,x̄,ȳ [w̄,ū,v̄]	(7) z̄,x̄,y [w̄,ū,v]	(8) z̄,x,ȳ [w̄,u,v̄]	
(9) y,z,x [v,w,u]	(10) ȳ,z,x̄ [v̄,w̄,ū]	(11) y,z̄,x̄ [v,w̄,ū]	(12) ȳ,z̄,x [v̄,w̄,u]	
(13) y+1/2,x+1/2,z+1/2 [v̄,ū,w̄]	(14) ȳ+1/2,x̄+1/2,z+1/2 [v̄,ū,w̄]	(15) y+1/2,x̄+1/2,z̄+1/2 [v̄,ū,w]	(16) ȳ+1/2,x+1/2,z̄+1/2 [v̄,ū,w]	
(17) x+1/2,z+1/2,y+1/2 [ū,w̄,v̄]	(18) x̄+1/2,z+1/2,ȳ+1/2 [ū,w̄,v̄]	(19) x̄+1/2,z̄+1/2,y+1/2 [ū,w̄,v̄]	(20) x+1/2,z̄+1/2,ȳ+1/2 [ū,w̄,v̄]	
(21) z+1/2,y+1/2,x+1/2 [w̄,v̄,ū]	(22) z+1/2,ȳ+1/2,x̄+1/2 [w̄,v̄,ū]	(23) z̄+1/2,y+1/2,x̄+1/2 [w̄,v̄,ū]	(24) z̄+1/2,ȳ+1/2,x+1/2 [w̄,v̄,ū]	
12 h 2..	x,0,1/2 [u,0,0]	x̄,0,1/2 [ū,0,0]	1/2,x,0 [0,u,0]	1/2,x̄,0 [0,ū,0]
	0,1/2,x [0,0,u]	0,1/2,x̄ [0,0,ū]	1/2,x+1/2,0 [0,ū,0]	1/2,x̄+1/2,0 [0,u,0]
	x+1/2,0,1/2 [ū,0,0]	x̄+1/2,0,1/2 [u,0,0]	0,1/2,x+1/2 [0,0,ū]	0,1/2,x̄+1/2 [0,0,u]
12 g 2..	x,1/2,0 [u,0,0]	x̄,1/2,0 [ū,0,0]	0,x,1/2 [0,u,0]	0,x̄,1/2 [0,ū,0]
	1/2,0,x [0,0,u]	1/2,0,x̄ [0,0,ū]	0,x+1/2,1/2 [0,ū,0]	0,x̄+1/2,1/2 [0,u,0]
	x+1/2,1/2,0 [ū,0,0]	x̄+1/2,1/2,0 [u,0,0]	1/2,0,x+1/2 [0,0,ū]	1/2,0,x̄+1/2 [0,0,u]
12 f 2..	x,0,0 [u,0,0]	x̄,0,0 [ū,0,0]	0,x,0 [0,u,0]	0,x̄,0 [0,ū,0]
	0,0,x [0,0,u]	0,0,x̄ [0,0,ū]	1/2,x+1/2,1/2 [0,ū,0]	1/2,x̄+1/2,1/2 [0,u,0]
	x+1/2,1/2,1/2 [ū,0,0]	x̄+1/2,1/2,1/2 [u,0,0]	1/2,1/2,x+1/2 [0,0,ū]	1/2,1/2,x̄+1/2 [0,0,u]

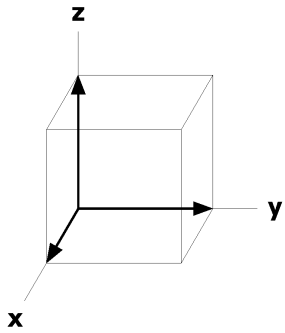
8	e	.3.	$x, x, x [u, u, u]$		$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$
			$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$		$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
			$x+1/2, x+1/2, x+1/2 [\bar{u}, \bar{u}, u]$		$\bar{x}+1/2, \bar{x}+1/2, x+1/2 [u, u, \bar{u}]$
			$x+1/2, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, u, u]$		$\bar{x}+1/2, x+1/2, \bar{x}+1/2 [u, \bar{u}, u]$
6	d	$\bar{4}$	$1/4, 0, 1/2 [u, 0, 0]$	$3/4, 0, 1/2 [\bar{u}, 0, 0]$	$1/2, 1/4, 0 [0, u, 0]$
			$1/2, 3/4, 0 [0, \bar{u}, 0]$	$0, 1/2, 1/4 [0, 0, u]$	$0, 1/2, 3/4 [0, 0, \bar{u}]$
6	c	$\bar{4}$	$1/4, 1/2, 0 [u, 0, 0]$	$3/4, 1/2, 0 [\bar{u}, 0, 0]$	$0, 1/4, 1/2 [0, u, 0]$
			$0, 3/4, 1/2 [0, \bar{u}, 0]$	$1/2, 0, 1/4 [0, 0, u]$	$1/2, 0, 3/4 [0, 0, \bar{u}]$
6	b	222..	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$
			$0, 1/2, 0 [0, 0, 0]$	$1/2, 0, 0 [0, 0, 0]$	$0, 0, 1/2 [0, 0, 0]$
2	a	23.	$0, 0, 0 [0, 0, 0]$	$1/2, 1/2, 1/2 [0, 0, 0]$	

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p4'm'm$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $1/2, 0, z$

Along  $[1, 1, 1]$   $p31m$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

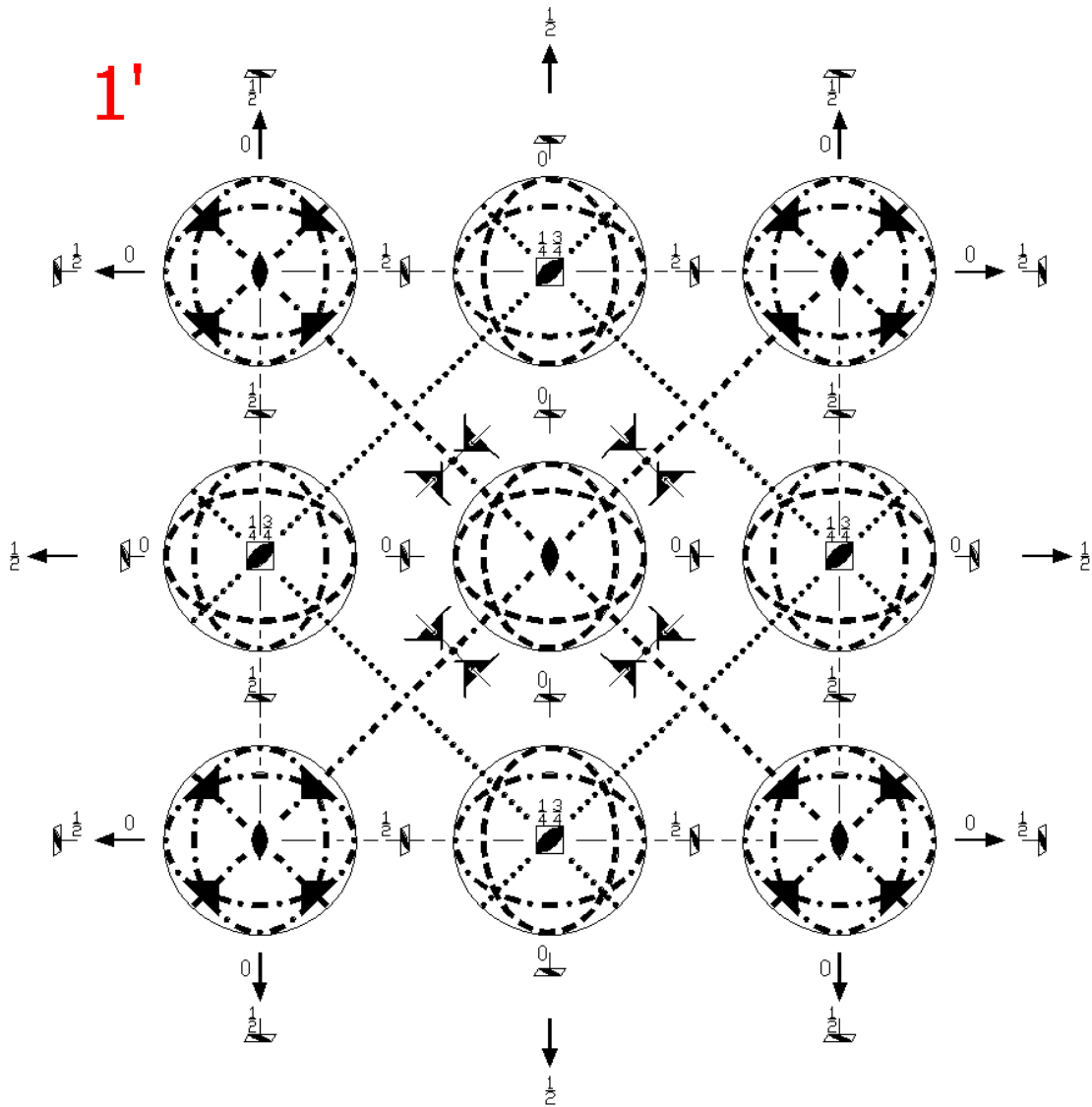
Along  $[1, 1, 0]$   $p_{2b}1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, x, 0$



$P\bar{4}3n1'$   
218.2.1586

$\bar{4}3m1'$   
 $P\bar{4}3n1'$

Cubic



Origin at  $231'$

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; z \leq \min(x,y)$

Vertices  $0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 0,1/2,0 \quad 1/2,1/2,1/2$

**Symmetry Operations**

For 1 + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                      | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                                      | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                      |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}^{-1}}$  0,0,0) | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}^{-1}}$  0,0,0) | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}\bar{z}^{-1}}$  0,0,0) |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz^{-1}}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)     | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)     | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)     |

(13) n (1/2,1/2,1/2) x,x,z ( $m_{\bar{xy}} 1/2,1/2,1/2$ )	(14) c (0,0,1/2) x+1/2, $\bar{x}$ ,z ( $m_{xy} 1/2,1/2,1/2$ )	(15) $\bar{4}^+$ 1/2,0,z;1/2,0,1/4 ( $\bar{4}_z 1/2,1/2,1/2$ )	(16) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1} 1/2,1/2,1/2$ )
(17) n (1/2,1/2,1/2) x,y,y ( $m_{\bar{yz}} 1/2,1/2,1/2$ )	(18) $\bar{4}^+$ x,1/2,0; 1/4,1/2,0 ( $\bar{4}_x 1/2,1/2,1/2$ )	(19) $\bar{4}^-$ x,0,1/2; 1/4,0,1/2 ( $\bar{4}_x^{-1} 1/2,1/2,1/2$ )	(20) a (1/2,0,0) x,y+1/2, $\bar{y}$ ( $m_{yz} 1/2,1/2,1/2$ )
(21) n (1/2,1/2,1/2) x,y,x ( $m_{\bar{zx}} 1/2,1/2,1/2$ )	(22) $\bar{4}^-$ 1/2,y,0; 1/2,1/4,0 ( $\bar{4}_y^{-1} 1/2,1/2,1/2$ )	(23) b (0,1/2,0) $\bar{x}$ +1/2,y,x ( $m_{xz} 1/2,1/2,1/2$ )	(24) $\bar{4}^+$ 0,y,1/2; 0,1/4,1/2 ( $\bar{4}_y 1/2,1/2,1/2$ )

For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 $_z$  0,0,0)'	(3) 2' 0,y,0 (2 $_y$  0,0,0)'	(4) 2' x,0,0 (2 $_x$  0,0,0)'
(5) 3 $^{+1}$ x,x,x (3 $_{xyz}$  0,0,0)'	(6) 3 $^{+1}$ $\bar{x}$ ,x, $\bar{x}$ (3 $_{\bar{xyz}}^{-1}$  0,0,0)'	(7) 3 $^{+1}$ x, $\bar{x}$ , $\bar{x}$ (3 $_{xyz}^{-1}$  0,0,0)'	(8) 3 $^{+1}$ $\bar{x}$ , $\bar{x}$ ,x (3 $_{\bar{yz}}^{-1}$  0,0,0)'
(9) 3 $^{-1}$ x,x,x (3 $_{xyz}^{-1}$  0,0,0)'	(10) 3 $^{-1}$ x, $\bar{x}$ , $\bar{x}$ (3 $_{\bar{xyz}}$  0,0,0)'	(11) 3 $^{-1}$ $\bar{x}$ , $\bar{x}$ ,x (3 $_{\bar{yz}}$  0,0,0)'	(12) 3 $^{-1}$ $\bar{x}$ ,x, $\bar{x}$ (3 $_{xyz}$  0,0,0)'
(13) n' (1/2,1/2,1/2) x,x,z ( $m_{\bar{xy}} 1/2,1/2,1/2$ )'	(14) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z ( $m_{xy} 1/2,1/2,1/2$ )'	(15) $\bar{4}^+$ 1/2,0,z;1/2,0,1/4 ( $\bar{4}_z 1/2,1/2,1/2$ )'	(16) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1} 1/2,1/2,1/2$ )'
(17) n' (1/2,1/2,1/2) x,y,y ( $m_{\bar{yz}} 1/2,1/2,1/2$ )'	(18) $\bar{4}^+$ x,1/2,0; 1/4,1/2,0 ( $\bar{4}_x 1/2,1/2,1/2$ )'	(19) $\bar{4}^-$ x,0,1/2; 1/4,0,1/2 ( $\bar{4}_x^{-1} 1/2,1/2,1/2$ )'	(20) a' (1/2,0,0) x,y+1/2, $\bar{y}$ ( $m_{yz} 1/2,1/2,1/2$ )'
(21) n' (1/2,1/2,1/2) x,y,x ( $m_{\bar{zx}} 1/2,1/2,1/2$ )'	(22) $\bar{4}^-$ 1/2,y,0; 1/2,1/4,0 ( $\bar{4}_y^{-1} 1/2,1/2,1/2$ )'	(23) b' (0,1/2,0) $\bar{x}$ +1/2,y,x ( $m_{xz} 1/2,1/2,1/2$ )'	(24) $\bar{4}^+$ 0,y,1/2; 0,1/4,1/2 ( $\bar{4}_y 1/2,1/2,1/2$ )'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); 1'.

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

1 + 1' +

24 i 11'			
(1) x,y,z [0,0,0]	(2) $\bar{x}$ , $\bar{y}$ ,z [0,0,0]	(3) $\bar{x}$ ,y, $\bar{z}$ [0,0,0]	(4) x, $\bar{y}$ , $\bar{z}$ [0,0,0]
(5) z,x,y [0,0,0]	(6) z, $\bar{x}$ , $\bar{y}$ [0,0,0]	(7) $\bar{z}$ , $\bar{x}$ ,y [0,0,0]	(8) $\bar{z}$ ,x,y [0,0,0]
(9) y,z,x [0,0,0]	(10) $\bar{y}$ ,z, $\bar{x}$ [0,0,0]	(11) y, $\bar{z}$ , $\bar{x}$ [0,0,0]	(12) $\bar{y}$ , $\bar{z}$ ,x [0,0,0]
(13) y+1/2,x+1/2,z+1/2 [0,0,0]	(14) $\bar{y}$ +1/2, $\bar{x}$ +1/2,z+1/2 [0,0,0]	(15) y+1/2, $\bar{x}$ +1/2, $\bar{z}$ +1/2 [0,0,0]	(16) $\bar{y}$ +1/2,x+1/2, $\bar{z}$ +1/2 [0,0,0]
(17) x+1/2,z+1/2,y+1/2 [0,0,0]	(18) $\bar{x}$ +1/2,z+1/2, $\bar{y}$ +1/2 [0,0,0]	(19) $\bar{x}$ +1/2, $\bar{z}$ +1/2,y+1/2 [0,0,0]	(20) x+1/2, $\bar{z}$ +1/2, $\bar{y}$ +1/2 [0,0,0]
(21) z+1/2,y+1/2,x+1/2 [0,0,0]	(22) z+1/2, $\bar{y}$ +1/2, $\bar{x}$ +1/2 [0,0,0]	(23) $\bar{z}$ +1/2,y+1/2, $\bar{x}$ +1/2 [0,0,0]	(24) $\bar{z}$ +1/2, $\bar{y}$ +1/2,x+1/2 [0,0,0]

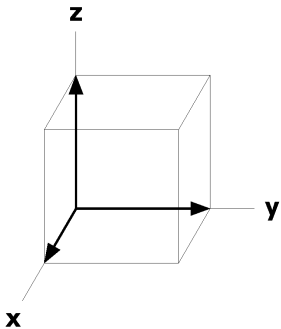
12	h	2..1'	x,0,1/2 [0,0,0]	$\bar{x}$ ,0,1/2 [0,0,0]	1/2,x,0 [0,0,0]	1/2, $\bar{x}$ ,0 [0,0,0]
			0,1/2,x [0,0,0]	0,1/2, $\bar{x}$ [0,0,0]	1/2,x+1/2,0 [0,0,0]	1/2, $\bar{x}$ +1/2,0 [0,0,0]
			x+1/2,0,1/2 [0,0,0]	$\bar{x}$ +1/2,0,1/2 [0,0,0]	0,1/2,x+1/2 [0,0,0]	0,1/2, $\bar{x}$ +1/2 [0,0,0]
12	g	2..1'	x,1/2,0 [0,0,0]	$\bar{x}$ ,1/2,0 [0,0,0]	0,x,1/2 [0,0,0]	0, $\bar{x}$ ,1/2 [0,0,0]
			1/2,0,x [0,0,0]	1/2,0, $\bar{x}$ [0,0,0]	0,x+1/2,1/2 [0,0,0]	0, $\bar{x}$ +1/2,1/2 [0,0,0]
			x+1/2,1/2,0 [0,0,0]	$\bar{x}$ +1/2,1/2,0 [0,0,0]	1/2,0,x+1/2 [0,0,0]	1/2,0, $\bar{x}$ +1/2 [0,0,0]
12	f	2..1'	x,0,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x}$ ,0 [0,0,0]
			0,0,x [0,0,0]	0,0, $\bar{x}$ [0,0,0]	1/2,x+1/2,1/2 [0,0,0]	1/2, $\bar{x}$ +1/2,1/2 [0,0,0]
			x+1/2,1/2,1/2 [0,0,0]	$\bar{x}$ +1/2,1/2,1/2 [0,0,0]	1/2,1/2,x+1/2 [0,0,0]	1/2,1/2, $\bar{x}$ +1/2 [0,0,0]
4	e	.3.1'	x,x,x [0,0,0]		$\bar{x}$ , $\bar{x}$ ,x [0,0,0]	
			$\bar{x}$ ,x, $\bar{x}$ [0,0,0]		x, $\bar{x}$ , $\bar{x}$ [0,0,0]	
			x+1/2,x+1/2,x+1/2 [0,0,0]		$\bar{x}$ +1/2, $\bar{x}$ +1/2,x+1/2 [0,0,0]	
			x+1/2, $\bar{x}$ +1/2, $\bar{x}$ +1/2 [0,0,0]		$\bar{x}$ +1/2,x+1/2, $\bar{x}$ +1/2 [0,0,0]	
6	d	$\bar{4}$ 1'	1/4,0,1/2 [0,0,0]	3/4,0,1/2 [0,0,0]		1/2,1/4,0 [0,0,0]
			1/2,3/4,0 [0,0,0]	0,1/2,1/4 [0,0,0]		0,1/2,3/4 [0,0,0]
6	c	$\bar{4}$ 1'	1/4,1/2,0 [0,0,0]	3/4,1/2,0 [0,0,0]		01/4,1/2 [0,0,0]
			0,3/4,1/2 [0,0,0]	1/2,0,1/4 [0,0,0]		1/2,0,3/4 [0,0,0]
6	b	222..1'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		1/2,1/2,0 [0,0,0]
			0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		0,0,1/2 [0,0,0]
2	a	23.1'	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/2,0,z

Along [1,1,1] p31m1'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

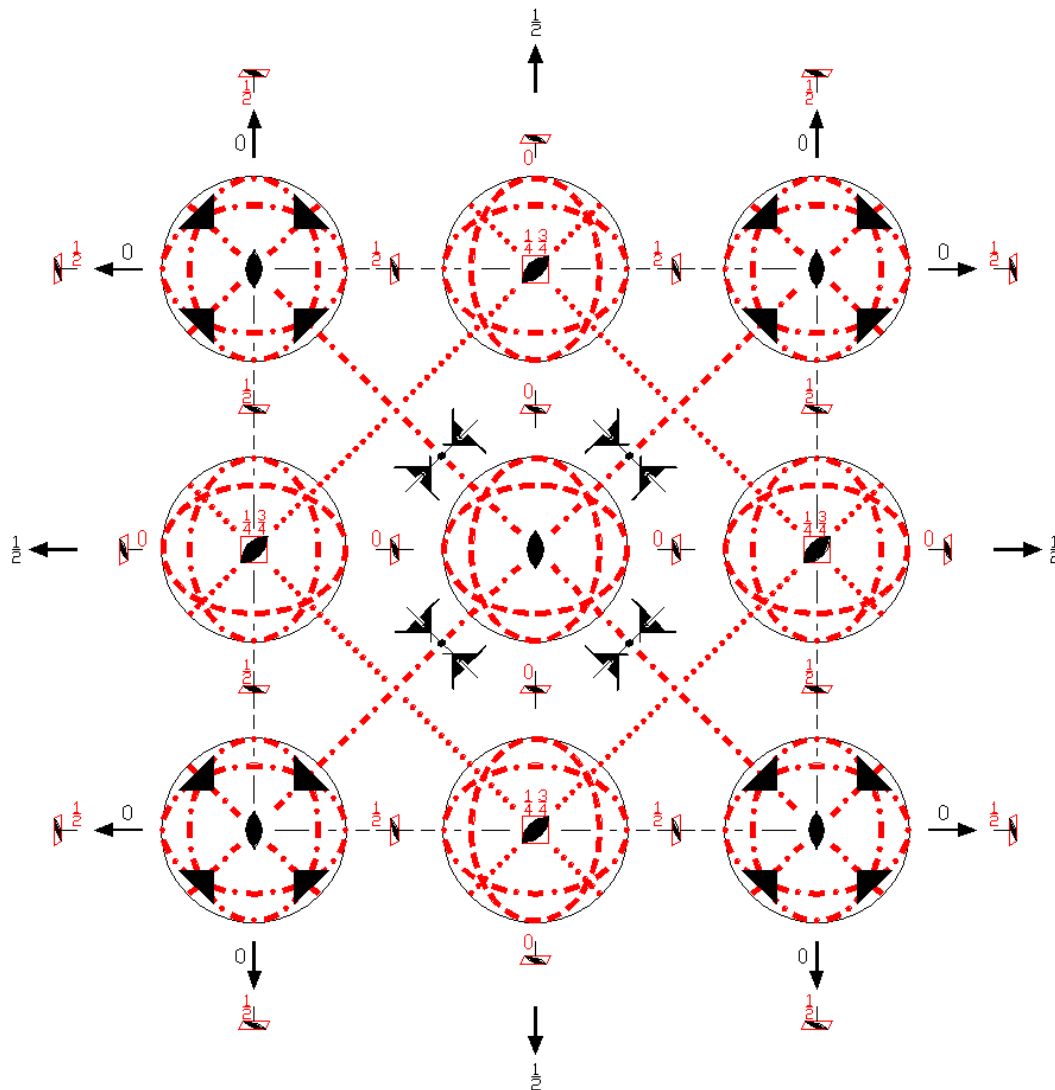
Along [1,1,0] p1m11'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$P\bar{4}'3n'$   
218.3.1587

$\bar{4}'3m'$   
 $P\bar{4}'3n'$

Cubic



Origin at 23

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; z \leq \min(x,y)$

Vertices  $0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 0,1/2,0 \quad 1/2,1/2,1/2$

### Symmetry Operations

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                  | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)        |



(13) n' (1/2,1/2,1/2) x,x,z (m <sub>xy</sub>  1/2,1/2,1/2)'	(14) c' (0,0,1/2) x+1/2,x̄,z (m <sub>xy</sub>  1/2,1/2,1/2)'	(15) 4 <sup>+</sup> ' 1/2,0,z;1/2,0,1/4 (4 <sub>z</sub>  1/2,1/2,1/2)'	(16) 4 <sup>-</sup> ' 0,1/2,z; 0,1/2,1/4 (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'
(17) n' (1/2,1/2,1/2) x,y,y (m <sub>yz</sub>  1/2,1/2,1/2)'	(18) 4 <sup>+</sup> ' x,1/2,0; 1/4,1/2,0 (4 <sub>x</sub>  1/2,1/2,1/2)'	(19) 4 <sup>-</sup> ' x,0,1/2; 1/4,0,1/2 (4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(20) a' (1/2,0,0) x,y+1/2,ȳ (m <sub>yz</sub>  1/2,1/2,1/2)'
(21) n' (1/2,1/2,1/2) x,y,x (m <sub>xz</sub>  1/2,1/2,1/2)'	(22) 4 <sup>-</sup> ' 1/2,y,0; 1/2,1/4,0 (4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(23) b' (0,1/2,0) x̄+1/2,y,x (m <sub>xz</sub>  1/2,1/2,1/2)'	(24) 4 <sup>+</sup> ' 0,y,1/2; 0,1/4,1/2 (4 <sub>y</sub>  1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

24 i 1

(1) x,y,z [u,v,w]	(2) x̄,ȳ,z [ū,v̄,w̄]	(3) x̄,y,z [ū,v,w̄]	(4) x,y,z̄ [u,v̄,w̄]
(5) z,x,y [w,u,v]	(6) z,x̄,ȳ [w̄,ū,v̄]	(7) z̄,x̄,y [w̄,ū,v]	(8) z̄,x,ȳ [w̄,ū,v̄]
(9) y,z,x [v,w,u]	(10) ȳ,z,x̄ [v̄,w̄,ū]	(11) y,z̄,x̄ [v,w̄,ū]	(12) ȳ,z̄,x [v̄,w̄,ū]
(13) y+1/2,x+1/2,z+1/2 [v,u,w]	(14) ȳ+1/2,x̄+1/2,z+1/2 [v̄,ū,w̄]	(15) y+1/2,x̄+1/2,z̄+1/2 [v,ū,w̄]	(16) ȳ+1/2,x+1/2,z̄+1/2 [v̄,ū,w̄]
(17) x+1/2,z+1/2,y+1/2 [u,w,v]	(18) x̄+1/2,z+1/2,ȳ+1/2 [ū,w̄,v̄]	(19) x̄+1/2,z̄+1/2,y+1/2 [ū,w̄,v]	(20) x+1/2,z̄+1/2,ȳ+1/2 [u,w̄,v̄]
(21) z+1/2,y+1/2,x+1/2 [w,v,u]	(22) z+1/2,ȳ+1/2,x̄+1/2 [w̄,v̄,ū]	(23) z̄+1/2,y+1/2,x̄+1/2 [w̄,v,ū]	(24) z̄+1/2,ȳ+1/2,x+1/2 [w̄,v̄,ū]

12	h	2..	x,0,1/2 [u,0,0]	x̄,0,1/2 [ū,0,0]	1/2,x,0 [0,u,0]	1/2,x̄,0 [0,ū,0]
			0,1/2,x [0,0,u]	0,1/2,x̄ [0,0,ū]	1/2,x+1/2,0 [0,u,0]	1/2,x̄+1/2,0 [0,ū,0]
			x+1/2,0,1/2 [u,0,0]	x̄+1/2,0,1/2 [ū,0,0]	0,1/2,x+1/2 [0,0,u]	0,1/2,x̄+1/2 [0,0,ū]
12	g	2..	x,1/2,0 [u,0,0]	x̄,1/2,0 [ū,0,0]	0,x,1/2 [0,u,0]	0,x̄,1/2 [0,ū,0]
			1/2,0,x [0,0,u]	1/2,0,x̄ [0,0,ū]	0,x+1/2,1/2 [0,u,0]	0,x̄+1/2,1/2 [0,ū,0]
			x+1/2,1/2,0 [u,0,0]	x̄+1/2,1/2,0 [ū,0,0]	1/2,0,x+1/2 [0,0,u]	1/2,0,x̄+1/2 [0,0,ū]
12	f	2..	x,0,0 [u,0,0]	x̄,0,0 [ū,0,0]	0,x,0 [0,u,0]	0,x̄,0 [0,ū,0]
			0,0,x [0,0,u]	0,0,x̄ [0,0,ū]	1/2,x+1/2,1/2 [0,u,0]	1/2,x̄+1/2,1/2 [0,ū,0]
			x+1/2,1/2,1/2 [u,0,0]	x̄+1/2,1/2,1/2 [ū,0,0]	1/2,1/2,x+1/2 [0,0,u]	1/2,1/2,x̄+1/2 [0,0,ū]
4	e	.3.	x,x,x [u,u,u]	x̄,x̄,x̄ [ū,ū,ū]	x̄,x̄,x [ū,ū,ū]	x,x̄,x̄ [u,ū,ū]
			x+1/2,x+1/2,x+1/2 [u,u,u]	x̄+1/2,x̄+1/2,x̄+1/2 [ū,ū,ū]	x̄+1/2,x̄+1/2,x+1/2 [ū,ū,ū]	x̄+1/2,x+1/2,x̄+1/2 [u,ū,ū]

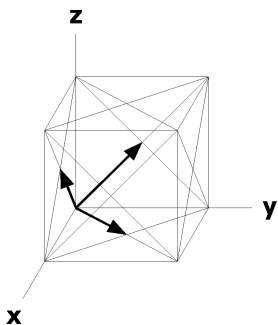
6	d	$\bar{4}'$	1/4,0,1/2 [0,0,0]	3/4,0,1/2 [0,0,0]	1/2,1/4,0 [0,0,0]
			1/2,3/4,0 [0,0,0]	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]
6	c	$\bar{4}'$	1/4,1/2,0 [0,0,0]	3/4,1/2,0 [0,0,0]	01/4,1/2 [0,0,0]
			0,3/4,1/2 [0,0,0]	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]
6	b	222..	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
			0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]	0,0,1/2 [0,0,0]
2	a	23.	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1]  $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 1/2,0,z

Along [1,1,1]  $p31m'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

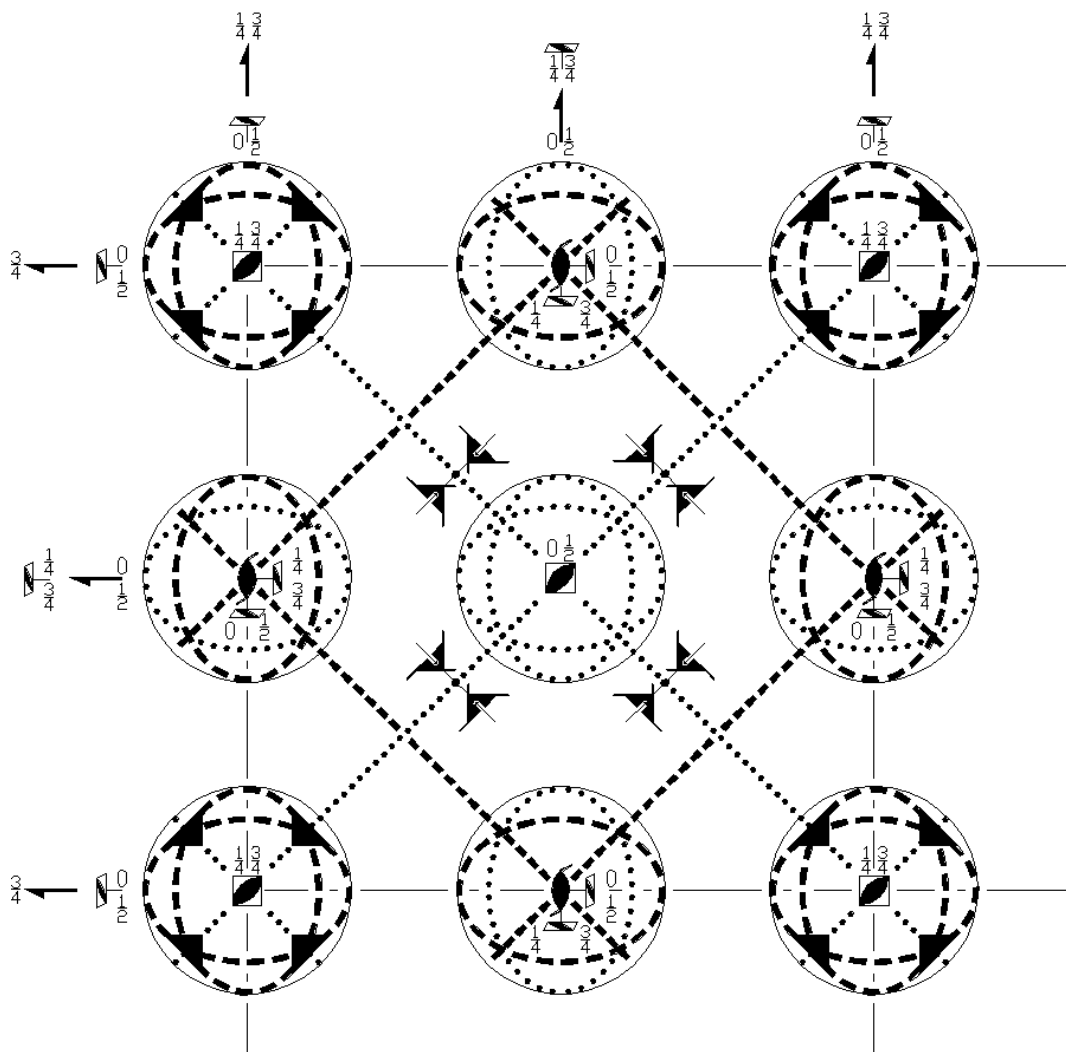
Along [1,1,0]  $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$F\bar{4}3c$   
219.1.1588

$\bar{4}3m$   
 $F\bar{4}3c$

Cubic



Origin at 23

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $-1/4 \leq z \leq 1/4$ ;  $y \leq \min(x, 1/2-x)$ ;  $-y \leq z \leq y$

Vertices  $0,0,0$   $1/2,0,0$   $1/4,1/4,1/4$   $1/4,1/4,-1/4$

### Symmetry Operations

For  $(0,0,0)$  + set

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                          | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                          | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                          |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{xyz^{-1}}$  0,0,0) | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{xyz^{-1}}$  0,0,0) | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{xyz^{-1}}$  0,0,0) |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz^{-1}}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{xyz}$  0,0,0)     | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{xyz}$  0,0,0)     | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{xyz}$  0,0,0)     |

- |  |   |   |   |
|--|---|---|---|
| (13) $n (1/2, 1/2, 1/2) \quad x, x, z$<br>( $m_{\bar{xy}}   1/2, 1/2, 1/2$ ) | (14) $c (0, 0, 1/2) \quad x+1/2, \bar{x}, z$<br>( $m_{xy}   1/2, 1/2, 1/2$ )    | (15) $\bar{4}^+ 1/2, 0, z; 1/2, 0, 1/4$<br>( $\bar{4}_z   1/2, 1/2, 1/2$ )      | (16) $\bar{4}^- 0, 1/2, z; 0, 1/2, 1/4$<br>( $\bar{4}_z^{-1}   1/2, 1/2, 1/2$ ) |
| (17) $n (1/2, 1/2, 1/2) \quad x, y, y$<br>( $m_{\bar{yz}}   1/2, 1/2, 1/2$ ) | (18) $\bar{4}^+ x, 1/2, 0; 1/4, 1/2, 0$<br>( $\bar{4}_x   1/2, 1/2, 1/2$ )      | (19) $\bar{4}^- x, 0, 1/2; 1/4, 0, 1/2$<br>( $\bar{4}_x^{-1}   1/2, 1/2, 1/2$ ) | (20) $a (1/2, 0, 0) \quad x, y+1/2, \bar{y}$<br>( $m_{yz}   1/2, 1/2, 1/2$ )    |
| (21) $n (1/2, 1/2, 1/2) \quad x, y, x$<br>( $m_{\bar{zx}}   1/2, 1/2, 1/2$ ) | (22) $\bar{4}^- 1/2, y, 0; 1/2, 1/4, 0$<br>( $\bar{4}_y^{-1}   1/2, 1/2, 1/2$ ) | (23) $b (0, 1/2, 0) \quad \bar{x}+1/2, y, x$<br>( $m_{xz}   1/2, 1/2, 1/2$ )    | (24) $\bar{4}^+ 0, y, 1/2; 0, 1/4, 1/2$<br>( $\bar{4}_y   1/2, 1/2, 1/2$ )      |

For (0, 1/2, 1/2) + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t (0, 1/2, 1/2)$<br>( $1   0, 1/2, 1/2$ )                                     | (2) $2 (0, 0, 1/2) \quad 0, 1/4, z$<br>( $2_z   0, 1/2, 1/2$ )                              | (3) $2 (0, 1/2, 0) \quad 0, y, 1/4$<br>( $2_y   0, 1/2, 1/2$ )  | (4) $2 \quad x, 1/4, 1/4$<br>( $2_x   0, 1/2, 1/2$ )                          |
| (5) $3^+ (1/3, 1/3, 1/3)$<br>$x-1/3, x-1/6, x$<br>( $3_{xyz}   0, 1/2, 1/2$ )      | (6) $3^+ \bar{x}, x+1/2, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   0, 1/2, 1/2$ )                 | (7) $3^+ (-1/3, 1/3, 1/3)$<br>$x+1/3, \bar{x}-1/6, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   0, 1/2, 1/2$ ) | (8) $3^+ \bar{x}, \bar{x}+1/2, x$<br>( $3_{\bar{xyz}}^{-1}   0, 1/2, 1/2$ )   |
| (9) $3^- (1/3, 1/3, 1/3)$<br>$x-1/6, x+1/6, x$<br>( $3_{xyz}^{-1}   0, 1/2, 1/2$ ) | (10) $3^- (-1/3, 1/3, 1/3)$<br>$x+1/6, x+1/6, \bar{x}$<br>( $3_{\bar{xyz}}   0, 1/2, 1/2$ ) | (11) $3^- \bar{x}+1/2, \bar{x}+1/2, x$<br>( $3_{\bar{yz}}   0, 1/2, 1/2$ )                            | (12) $3^- \bar{x}-1/2, x+1/2, \bar{x}$<br>( $3_{\bar{xyz}}   0, 1/2, 1/2$ )   |
| (13) $g (1/4, 1/4, 0) \quad x+1/4, x, z$<br>( $m_{\bar{xy}}   1/2, 0, 0$ )         | (14) $g (1/4, -1/4, 0) \quad x+1/4, \bar{x}, z$<br>( $m_{xy}   1/2, 0, 0$ )                 | (15) $\bar{4}^+ 1/4, -1/4, z; 1/4, -1/4, 0$<br>( $\bar{4}_z   1/2, 0, 0$ )                            | (16) $\bar{4}^- 1/4, 1/4, z; 1/4, 1/4, 0$<br>( $\bar{4}_z^{-1}   1/2, 0, 0$ ) |
| (17) $a (1/2, 0, 0) \quad x, y, y$<br>( $m_{\bar{yz}}   1/2, 0, 0$ )               | (18) $\bar{4}^+ x, 0, 0; 1/4, 0, 0$<br>( $\bar{4}_x   1/2, 0, 0$ )                          | (19) $\bar{4}^- x, 0, 0; 1/4, 0, 0$<br>( $\bar{4}_x^{-1}   1/2, 0, 0$ )                               | (20) $a (1/2, 0, 0) \quad x, y, \bar{y}$<br>( $m_{yz}   1/2, 0, 0$ )          |
| (21) $g (1/4, 0, 1/4) \quad x+1/4, y, x$<br>( $m_{\bar{zx}}   1/2, 0, 0$ )         | (22) $\bar{4}^- 1/4, y, -1/4; 1/4, 0, -1/4$<br>( $\bar{4}_y^{-1}   1/2, 0, 0$ )             | (23) $g (1/4, 0, -1/4) \quad \bar{x}+1/4, y, x$<br>( $m_{xz}   1/2, 0, 0$ )                           | (24) $\bar{4}^+ 1/4, y, 1/4; 1/4, 0, 1/4$<br>( $\bar{4}_y   1/2, 0, 0$ )      |

For (1/2, 0, 1/2) + set

- |  |   |  |   |
|--|---|--|---|
| (1) $t (1/2, 0, 1/2)$<br>( $1   1/2, 0, 1/2$ )                                     | (2) $2 (0, 0, 1/2) \quad 1/4, 0, z$<br>( $2_z   1/2, 0, 1/2$ )  | (3) $2 \quad 1/4, y, 1/4$<br>( $2_y   1/2, 0, 1/2$ )                           | (4) $2 (1/2, 0, 0) \quad x, 0, 1/4$<br>( $2_x   1/2, 0, 1/2$ )                                    |
| (5) $3^+ (1/3, 1/3, 1/3)$<br>$x+1/6, x-1/6, x$<br>( $3_{xyz}   1/2, 0, 1/2$ )      | (6) $3^+ (1/3, -1/3, 1/3)$<br>$\bar{x}+1/6, x+1/6, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ ) | (7) $3^+ x+1/2, \bar{x}-1/2, \bar{x}$<br>( $3_{\bar{yz}}^{-1}   1/2, 0, 1/2$ ) | (8) $3^+ \bar{x}+1/2, \bar{x}+1/2, x$<br>( $3_{\bar{yz}}^{-1}   1/2, 0, 1/2$ )                    |
| (9) $3^- (1/3, 1/3, 1/3)$<br>$x-1/6, x-1/3, x$<br>( $3_{xyz}^{-1}   1/2, 0, 1/2$ ) | (10) $3^- x+1/2, \bar{x}, \bar{x}$<br>( $3_{\bar{yz}}   1/2, 0, 1/2$ )                                | (11) $3^- \bar{x}+1/2, \bar{x}, x$<br>( $3_{\bar{yz}}   1/2, 0, 1/2$ )         | (12) $3^- (1/3, -1/3, 1/3)$<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>( $3_{\bar{xyz}}   1/2, 0, 1/2$ ) |
| (13) $g (1/4, 1/4, 0) \quad x-1/4, x, z$<br>( $m_{\bar{xy}}   0, 1/2, 0$ )         | (14) $g (-1/4, 1/4, 0) \quad x+1/4, \bar{x}, z$<br>( $m_{xy}   0, 1/2, 0$ )                           | (15) $\bar{4}^+ 1/4, 1/4, z; 1/4, 1/4, 0$<br>( $\bar{4}_z   0, 1/2, 0$ )       | (16) $\bar{4}^- -1/4, 1/4, z; -1/4, 1/4, 0$<br>( $\bar{4}_z^{-1}   0, 1/2, 0$ )                   |
| (17) $g (0, 1/4, 1/4) \quad x, y+1/4, y$<br>( $m_{\bar{yz}}   0, 1/2, 0$ )         | (18) $\bar{4}^+ x, 1/4, -1/4; 0, 1/4, -1/4$<br>( $\bar{4}_x   0, 1/2, 0$ )                            | (19) $\bar{4}^- x, 1/4, 1/4; 0, 1/4, 1/4$<br>( $\bar{4}_x^{-1}   0, 1/2, 0$ )  | (20) $g (0, 1/4, -1/4) \quad x, y+1/4, \bar{y}$<br>( $m_{yz}   0, 1/2, 0$ )                       |
| (21) $b (0, 1/2, 0) \quad x, y, x$<br>( $m_{\bar{zx}}   0, 1/2, 0$ )               | (22) $\bar{4}^- 0, y, 0; 0, 1/4, 0$<br>( $\bar{4}_y^{-1}   0, 1/2, 0$ )                               | (23) $b (0, 1/2, 0) \quad \bar{x}, y, x$<br>( $m_{xz}   0, 1/2, 0$ )           | (24) $\bar{4}^+ 0, y, 0; 0, 1/4, 0$<br>( $\bar{4}_y   0, 1/2, 0$ )                                |

For (1/2,1/2,0) + set

(1) $t$ (1/2,1/2,0) (1   1/2,1/2,0)	(2) $2$ 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,0)	(3) $2$ (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)	(4) $2$ (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)
(5) $3^+$ (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) $3^+$ $\bar{x}$ +1/2,x, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(7) $3^+$ x+1/2, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(8) $3^+$ (1/3,1/3,-1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)
(9) $3^-$ (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) $3^-$ x, $\bar{x}$ +1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)	(11) $3^-$ (1/3,1/3,-1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub>   1/2,1/2,0)	(12) $3^-$ $\bar{x}$ ,x+1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)
(13) $c$ (0,0,1/2) x,x,z (m <sub>xy</sub>   0,0,1/2)	(14) $c$ (0,0,1/2) x, $\bar{x}$ ,z (m <sub>xy</sub>   0,0,1/2)	(15) $4^+$ 0,0,z; 0,0,1/4 (4 <sub>z</sub>   0,0,1/2)	(16) $4^-$ 0,0,z; 0,0,1/4 (4 <sub>z</sub> <sup>-1</sup>   0,0,1/2)
(17) $g$ (0,1/4,1/4) x,y-1/4,y (m <sub>yz</sub>   0,0,1/2)	(18) $4^+$ x,1/4,1/4; 0,1/4,-1/4 (4 <sub>x</sub>   0,0,1/2)	(19) $4^-$ x,-1/4,1/4; 0,-1/4,1/4 (4 <sub>x</sub> <sup>-1</sup>   0,0,1/2)	(20) $g$ (0,-1/4,+1/4) x,y+1/4, $\bar{y}$ (m <sub>yz</sub>   0,0,1/2)
(21) $g$ (1/4,0,1/4) x-1/4,y,x (m <sub>xz</sub>   0,0,1/2)	(22) $4^-$ 1/4,y,1/4; 1/4,0,1/4 (4 <sub>y</sub> <sup>-1</sup>   0,0,1/2)	(23) $g$ (-1/4,0,1/4) $\bar{x}$ +1/4,y,x (m <sub>xz</sub>   0,0,1/2)	(24) $4^+$ -1/4,y,1/4; -1/4,0,1/4 (4 <sub>y</sub>   0,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

		(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +					
96	h	1								
(1)	x,y,z	[u,v,w]	(2) $\bar{x}$ , $\bar{y}$ ,z	[ $\bar{u}$ , $\bar{v}$ ,w]	(3) $\bar{x}$ ,y,z	[ $\bar{u}$ ,v,w]	(4) x, $\bar{y}$ ,z	[u, $\bar{v}$ ,w]		
(5)	z,x,y	[w,u,v]	(6) z, $\bar{x}$ , $\bar{y}$	[w, $\bar{u}$ , $\bar{v}$ ]	(7) $\bar{z}$ , $\bar{x}$ ,y	[ $\bar{w}$ , $\bar{u}$ ,v]	(8) $\bar{z}$ ,x,y	[ $\bar{w}$ ,u,v]		
(9)	y,z,x	[v,w,u]	(10) $\bar{y}$ ,z, $\bar{x}$	[ $\bar{v}$ ,w, $\bar{u}$ ]	(11) y, $\bar{z}$ , $\bar{x}$	[v, $\bar{w}$ , $\bar{u}$ ]	(12) $\bar{y}$ , $\bar{z}$ ,x	[ $\bar{v}$ , $\bar{w}$ ,u]		
(13)	y+1/2,x+1/2,z+1/2	[ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(14) $\bar{y}$ +1/2, $\bar{x}$ +1/2,z+1/2	[v,u, $\bar{w}$ ]	(15) y+1/2, $\bar{x}$ +1/2, $\bar{z}$ +1/2	[ $\bar{v}$ ,u,w]	(16) $\bar{y}$ +1/2,x+1/2, $\bar{z}$ +1/2	[v, $\bar{u}$ ,w]		
(17)	x+1/2,z+1/2,y+1/2	[ $\bar{u}$ , $\bar{w}$ , $\bar{v}$ ]	(18) $\bar{x}$ +1/2,z+1/2, $\bar{y}$ +1/2	[u, $\bar{w}$ ,v]	(19) $\bar{x}$ +1/2, $\bar{z}$ +1/2,y+1/2	[u,w, $\bar{v}$ ]	(20) x+1/2, $\bar{z}$ +1/2, $\bar{y}$ +1/2	[ $\bar{u}$ ,w,v]		
(21)	z+1/2,y+1/2,x+1/2	[ $\bar{w}$ , $\bar{v}$ , $\bar{u}$ ]	(22) z+1/2, $\bar{y}$ +1/2, $\bar{x}$ +1/2	[ $\bar{w}$ ,v,u]	(23) $\bar{z}$ +1/2,y+1/2, $\bar{x}$ +1/2	[w, $\bar{v}$ ,u]	(24) $\bar{z}$ +1/2, $\bar{y}$ +1/2,x+1/2	[w,v, $\bar{u}$ ]		
48	g	2..	x,1/4,1/4	[u,0,0]	$\bar{x}$ ,3/4,1/4	[ $\bar{u}$ ,0,0]	1/4,x,1/4	[0,u,0]	1/4, $\bar{x}$ ,3/4	[0, $\bar{u}$ ,0]
			1/4,1/4,x	[0,0,u]	3/4,1/4, $\bar{x}$	[0,0, $\bar{u}$ ]	3/4,x+1/2,3/4	[0, $\bar{u}$ ,0]	1/4, $\bar{x}$ +1/2,3/4	[0,u,0]
			x+1/2,3/4,3/4	[ $\bar{u}$ ,0,0]	$\bar{x}$ +1/2,3/4,1/4	[u,0,0]	3/4,3/4,x+1/2	[0,0, $\bar{u}$ ]	3/4,1/4, $\bar{x}$ +1/2	[0,0,u]
48	f	2..	x,0,0	[u,0,0]	$\bar{x}$ ,0,0	[ $\bar{u}$ ,0,0]	0,x,0	[0,u,0]	0, $\bar{x}$ ,0	[0, $\bar{u}$ ,0]
			0,0,x	[0,0,u]	0,0, $\bar{x}$	[0,0, $\bar{u}$ ]	1/2,x+1/2,1/2	[0, $\bar{u}$ ,0]	1/2, $\bar{x}$ +1/2,1/2	[0,u,0]
			x+1/2,1/2,1/2	[ $\bar{u}$ ,0,0]	$\bar{x}$ +1/2,1/2,1/2	[u,0,0]	1/2,1/2,x+1/2	[0,0, $\bar{u}$ ]	1/2,1/2, $\bar{x}$ +1/2	[0,0,u]

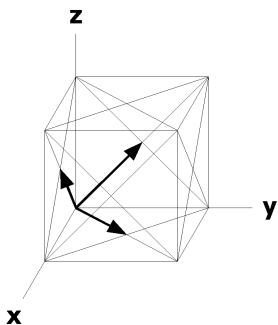
32	e	.3.	$x, x, x [u, u, u]$		$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$
			$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$		$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
			$x+1/2, x+1/2, x+1/2 [\bar{u}, \bar{u}, \bar{u}]$		$\bar{x}+1/2, \bar{x}+1/2, x+1/2 [u, u, \bar{u}]$
			$x+1/2, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, u, u]$		$\bar{x}+1/2, x+1/2, \bar{x}+1/2 [u, \bar{u}, u]$
24	d	$\bar{4}$	$1/4, 0, 0 [u, 0, 0]$	$3/4, 0, 0 [\bar{u}, 0, 0]$	$0, 1/4, 0 [0, u, 0]$
			$0, 3/4, 0 [0, \bar{u}, 0]$	$0, 0, 1/4 [0, 0, u]$	$0, 0, 3/4 [0, 0, \bar{u}]$
24	c	$\bar{4}$	$0, 1/4, 1/4 [u, 0, 0]$	$0, 3/4, 1/4 [\bar{u}, 0, 0]$	$1/4, 0, 1/4 [0, u, 0]$
			$1/4, 0, 3/4 [0, \bar{u}, 0]$	$1/4, 1/4 [0, 0, u]$	$3/4, 1/4 [0, 0, \bar{u}]$
8	b	23.	$1/4, 1/4, 1/4 [0, 0, 0]$	$3/4, 3/4, 3/4 [0, 0, 0]$	
8	a	23.	$0, 0, 0 [0, 0, 0]$	$1/2, 1/2, 1/2 [0, 0, 0]$	

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p4'm'm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $0, 0, z$

Along  $[1, 1, 1]$   $p31m$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at  $x, x, x$

Along  $[1, 1, 0]$   $p_c-1m1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x-1/4, x+1/4, 0$



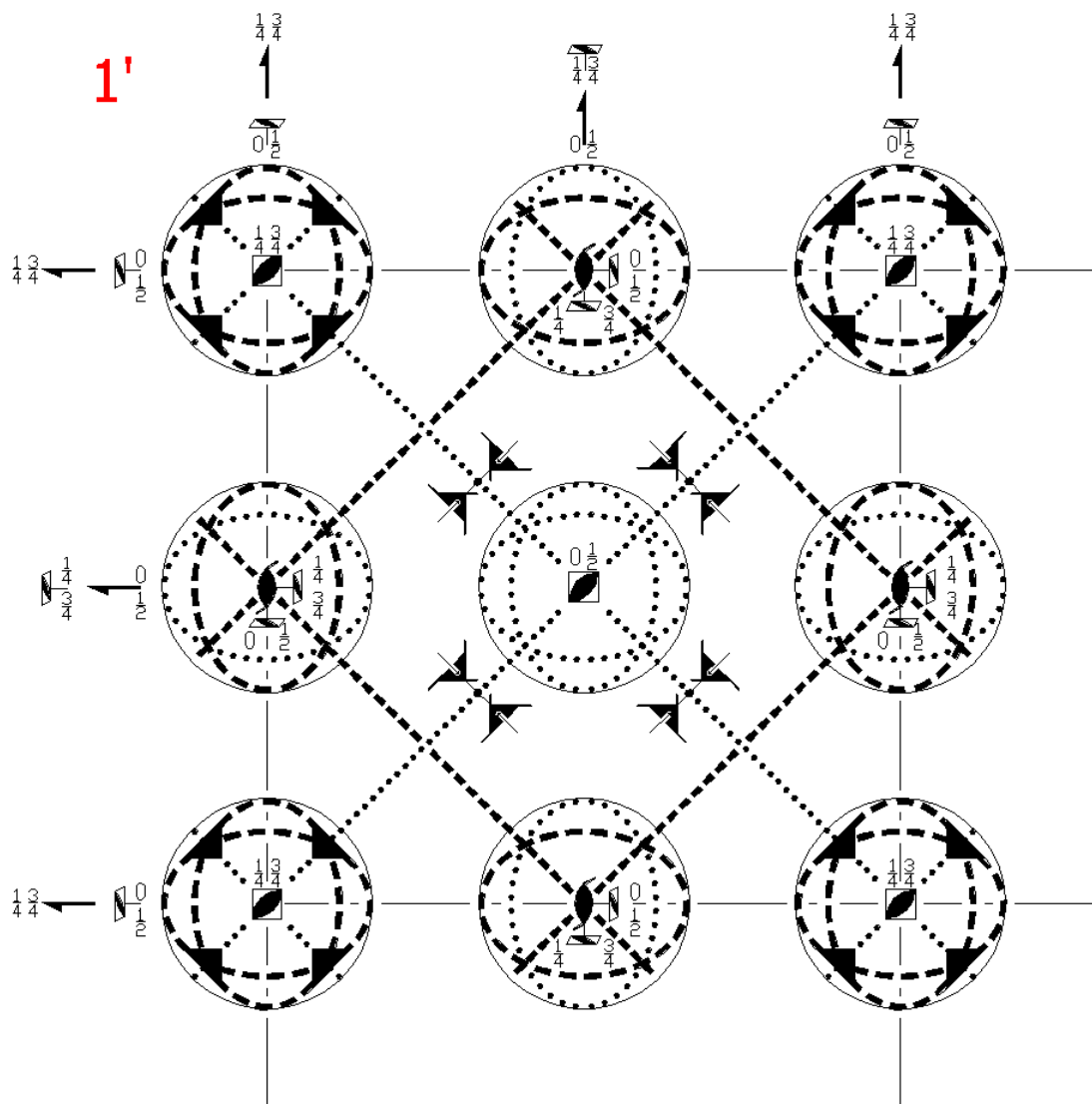
$F\bar{4}3c1'$

219.2.1589

$\bar{4}3m1'$

$F\bar{4}3c1'$

Cubic



Origin at  $231'$

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $-1/4 \leq z \leq 1/4$ ;  $y \leq \min(x, 1/2-x)$ ;  $-y \leq z \leq y$

Vertices  $0,0,0$   $1/2,0,0$   $1/4,1/4,1/4$   $1/4,1/4,-1/4$

**Symmetry Operations**

For  $(0,0,0) + \text{set}$

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                            | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                            | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                            |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{\bar{xyz}}$  0,0,0)  | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{yz}}$  0,0,0)  | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}yz}$  0,0,0)  |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{yz}}$  0,0,0) | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}yz}$  0,0,0) | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{\bar{xyz}}$  0,0,0) |

- |  |   |   |   |
|--|---|---|---|
| (13) $n (1/2, 1/2, 1/2) \quad x, x, z$<br>( $m_{\bar{xy}}   1/2, 1/2, 1/2$ ) | (14) $c (0, 0, 1/2) \quad x+1/2, \bar{x}, z$<br>( $m_{xy}   1/2, 1/2, 1/2$ )    | (15) $\bar{4}^+ 1/2, 0, z; 1/2, 0, 1/4$<br>( $\bar{4}_z   1/2, 1/2, 1/2$ )      | (16) $\bar{4}^- 0, 1/2, z; 0, 1/2, 1/4$<br>( $\bar{4}_z^{-1}   1/2, 1/2, 1/2$ ) |
| (17) $n (1/2, 1/2, 1/2) \quad x, y, y$<br>( $m_{\bar{yz}}   1/2, 1/2, 1/2$ ) | (18) $\bar{4}^+ x, 1/2, 0; 1/4, 1/2, 0$<br>( $\bar{4}_x   1/2, 1/2, 1/2$ )      | (19) $\bar{4}^- x, 0, 1/2; 1/4, 0, 1/2$<br>( $\bar{4}_x^{-1}   1/2, 1/2, 1/2$ ) | (20) $a (1/2, 0, 0) \quad x, y+1/2, \bar{y}$<br>( $m_{yz}   1/2, 1/2, 1/2$ )    |
| (21) $n (1/2, 1/2, 1/2) \quad x, y, x$<br>( $m_{\bar{zx}}   1/2, 1/2, 1/2$ ) | (22) $\bar{4}^- 1/2, y, 0; 1/2, 1/4, 0$<br>( $\bar{4}_y^{-1}   1/2, 1/2, 1/2$ ) | (23) $b (0, 1/2, 0) \quad \bar{x}+1/2, y, x$<br>( $m_{xz}   1/2, 1/2, 1/2$ )    | (24) $\bar{4}^+ 0, y, 1/2; 0, 1/4, 1/2$<br>( $\bar{4}_y   1/2, 1/2, 1/2$ )      |

For (0, 1/2, 1/2) + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t (0, 1/2, 1/2)$<br>( $1   0, 1/2, 1/2$ )                                     | (2) $2 (0, 0, 1/2) \quad 0, 1/4, z$<br>( $2_z   0, 1/2, 1/2$ )                              | (3) $2 (0, 1/2, 0) \quad 0, y, 1/4$<br>( $2_y   0, 1/2, 1/2$ )  | (4) $2 \quad x, 1/4, 1/4$<br>( $2_x   0, 1/2, 1/2$ )                          |
| (5) $3^+ (1/3, 1/3, 1/3)$<br>$x-1/3, x-1/6, x$<br>( $3_{xyz}   0, 1/2, 1/2$ )      | (6) $3^+ \bar{x}, x+1/2, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   0, 1/2, 1/2$ )                 | (7) $3^+ (-1/3, 1/3, 1/3)$<br>$x+1/3, \bar{x}-1/6, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   0, 1/2, 1/2$ ) | (8) $3^+ \bar{x}, \bar{x}+1/2, x$<br>( $3_{\bar{xyz}}^{-1}   0, 1/2, 1/2$ )   |
| (9) $3^- (1/3, 1/3, 1/3)$<br>$x-1/6, x+1/6, x$<br>( $3_{xyz}^{-1}   0, 1/2, 1/2$ ) | (10) $3^- (-1/3, 1/3, 1/3)$<br>$x+1/6, x+1/6, \bar{x}$<br>( $3_{\bar{xyz}}   0, 1/2, 1/2$ ) | (11) $3^- \bar{x}+1/2, \bar{x}+1/2, x$<br>( $3_{\bar{yz}}   0, 1/2, 1/2$ )                            | (12) $3^- \bar{x}-1/2, x+1/2, \bar{x}$<br>( $3_{\bar{xyz}}   0, 1/2, 1/2$ )   |
| (13) $g (1/4, 1/4, 0) \quad x+1/4, x, z$<br>( $m_{\bar{xy}}   1/2, 0, 0$ )         | (14) $g (1/4, -1/4, 0) \quad x+1/4, \bar{x}, z$<br>( $m_{xy}   1/2, 0, 0$ )                 | (15) $\bar{4}^+ 1/4, -1/4, z; 1/4, -1/4, 0$<br>( $\bar{4}_z   1/2, 0, 0$ )                            | (16) $\bar{4}^- 1/4, 1/4, z; 1/4, 1/4, 0$<br>( $\bar{4}_z^{-1}   1/2, 0, 0$ ) |
| (17) $a (1/2, 0, 0) \quad x, y, y$<br>( $m_{\bar{yz}}   1/2, 0, 0$ )               | (18) $\bar{4}^+ x, 0, 0; 1/4, 0, 0$<br>( $\bar{4}_x   1/2, 0, 0$ )                          | (19) $\bar{4}^- x, 0, 0; 1/4, 0, 0$<br>( $\bar{4}_x^{-1}   1/2, 0, 0$ )                               | (20) $a (1/2, 0, 0) \quad x, y, \bar{y}$<br>( $m_{yz}   1/2, 0, 0$ )          |
| (21) $g (1/4, 0, 1/4) \quad x+1/4, y, x$<br>( $m_{\bar{zx}}   1/2, 0, 0$ )         | (22) $\bar{4}^- 1/4, y, -1/4; 1/4, 0, -1/4$<br>( $\bar{4}_y^{-1}   1/2, 0, 0$ )             | (23) $g (1/4, 0, -1/4) \quad \bar{x}+1/4, y, x$<br>( $m_{xz}   1/2, 0, 0$ )                           | (24) $\bar{4}^+ 1/4, y, 1/4; 1/4, 0, 1/4$<br>( $\bar{4}_y   1/2, 0, 0$ )      |

For (1/2, 0, 1/2) + set

- |  |   |  |   |
|--|---|--|---|
| (1) $t (1/2, 0, 1/2)$<br>( $1   1/2, 0, 1/2$ )                                     | (2) $2 (0, 0, 1/2) \quad 1/4, 0, z$<br>( $2_z   1/2, 0, 1/2$ )  | (3) $2 \quad 1/4, y, 1/4$<br>( $2_y   1/2, 0, 1/2$ )                           | (4) $2 (1/2, 0, 0) \quad x, 0, 1/4$<br>( $2_x   1/2, 0, 1/2$ )                                    |
| (5) $3^+ (1/3, 1/3, 1/3)$<br>$x+1/6, x-1/6, x$<br>( $3_{xyz}   1/2, 0, 1/2$ )      | (6) $3^+ (1/3, -1/3, 1/3)$<br>$\bar{x}+1/6, x+1/6, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ ) | (7) $3^+ x+1/2, \bar{x}-1/2, \bar{x}$<br>( $3_{\bar{yz}}^{-1}   1/2, 0, 1/2$ ) | (8) $3^+ \bar{x}+1/2, \bar{x}+1/2, x$<br>( $3_{\bar{yz}}^{-1}   1/2, 0, 1/2$ )                    |
| (9) $3^- (1/3, 1/3, 1/3)$<br>$x-1/6, x-1/3, x$<br>( $3_{xyz}^{-1}   1/2, 0, 1/2$ ) | (10) $3^- x+1/2, \bar{x}, \bar{x}$<br>( $3_{\bar{yz}}   1/2, 0, 1/2$ )                                | (11) $3^- \bar{x}+1/2, \bar{x}, x$<br>( $3_{\bar{yz}}   1/2, 0, 1/2$ )         | (12) $3^- (1/3, -1/3, 1/3)$<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>( $3_{\bar{xyz}}   1/2, 0, 1/2$ ) |
| (13) $g (1/4, 1/4, 0) \quad x-1/4, x, z$<br>( $m_{\bar{xy}}   0, 1/2, 0$ )         | (14) $g (-1/4, 1/4, 0) \quad x+1/4, \bar{x}, z$<br>( $m_{xy}   0, 1/2, 0$ )                           | (15) $\bar{4}^+ 1/4, 1/4, z; 1/4, 1/4, 0$<br>( $\bar{4}_z   0, 1/2, 0$ )       | (16) $\bar{4}^- -1/4, 1/4, z; -1/4, 1/4, 0$<br>( $\bar{4}_z^{-1}   0, 1/2, 0$ )                   |
| (17) $g (0, 1/4, 1/4) \quad x, y+1/4, y$<br>( $m_{\bar{yz}}   0, 1/2, 0$ )         | (18) $\bar{4}^+ x, 1/4, -1/4; 0, 1/4, -1/4$<br>( $\bar{4}_x   0, 1/2, 0$ )                            | (19) $\bar{4}^- x, 1/4, 1/4; 0, 1/4, 1/4$<br>( $\bar{4}_x^{-1}   0, 1/2, 0$ )  | (20) $g (0, 1/4, -1/4) \quad x, y+1/4, \bar{y}$<br>( $m_{yz}   0, 1/2, 0$ )                       |
| (21) $b (0, 1/2, 0) \quad x, y, x$<br>( $m_{\bar{zx}}   0, 1/2, 0$ )               | (22) $\bar{4}^- 0, y, 0; 0, 1/4, 0$<br>( $\bar{4}_y^{-1}   0, 1/2, 0$ )                               | (23) $b (0, 1/2, 0) \quad \bar{x}, y, x$<br>( $m_{xz}   0, 1/2, 0$ )           | (24) $\bar{4}^+ 0, y, 0; 0, 1/4, 0$<br>( $\bar{4}_y   0, 1/2, 0$ )                                |



## For (1/2,1/2,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t \left( \frac{1}{2}, \frac{1}{2}, 0 \right)$<br>$(1   \frac{1}{2}, \frac{1}{2}, 0)$                                | (2) $2 \frac{1}{4}, \frac{1}{4}, z$<br>$(2_z   \frac{1}{2}, \frac{1}{2}, 0)$  | (3) $2 (0, \frac{1}{2}, 0) \frac{1}{4}, y, 0$<br>$(2_y   \frac{1}{2}, \frac{1}{2}, 0)$  | (4) $2 (\frac{1}{2}, 0, 0) x, \frac{1}{4}, 0$<br>$(2_x   \frac{1}{2}, \frac{1}{2}, 0)$  |
| (5) $3^+ (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$<br>$x+1/6, x+1/3, x$<br>$(3_{xyz}   \frac{1}{2}, \frac{1}{2}, 0)$      | (6) $3^+ \bar{x} + \frac{1}{2}, x, \bar{x}$<br>$(3_{xyz}^{-1}   \frac{1}{2}, \frac{1}{2}, 0)$                       | (7) $3^+ x + \frac{1}{2}, \bar{x}, \bar{x}$<br>$(3_{xyz}^{-1}   \frac{1}{2}, \frac{1}{2}, 0)$   | (8) $3^+ (\frac{1}{3}, \frac{1}{3}, -\frac{1}{3})$<br>$\bar{x} + \frac{1}{6}, \bar{x} + \frac{1}{3}, x$<br>$(3_{xyz}^{-1}   \frac{1}{2}, \frac{1}{2}, 0)$ |
| (9) $3^- (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$<br>$x+1/3, x+1/6, x$<br>$(3_{xyz}^{-1}   \frac{1}{2}, \frac{1}{2}, 0)$ | (10) $3^- x, \bar{x} + \frac{1}{2}, \bar{x}$<br>$(3_{xyz}   \frac{1}{2}, \frac{1}{2}, 0)$                           | (11) $3^- (\frac{1}{3}, \frac{1}{3}, -\frac{1}{3})$<br>$\bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$<br>$(3_{xyz}   \frac{1}{2}, \frac{1}{2}, 0)$ | (12) $3^- \bar{x}, x + \frac{1}{2}, \bar{x}$<br>$(3_{xyz}   \frac{1}{2}, \frac{1}{2}, 0)$   |
| (13) $c (0, 0, \frac{1}{2}) x, x, z$<br>$(m_{xy}   0, 0, \frac{1}{2})$   | (14) $c (0, 0, \frac{1}{2}) x, \bar{x}, z$<br>$(m_{xy}   0, 0, \frac{1}{2})$  | (15) $\bar{4}^+ 0, 0, z; 0, 0, \frac{1}{4}$<br>$(\bar{4}_z   0, 0, \frac{1}{2})$  | (16) $\bar{4}^- 0, 0, z; 0, 0, \frac{1}{4}$<br>$(\bar{4}_z^{-1}   0, 0, \frac{1}{2})$   |
| (17) $g (0, \frac{1}{4}, \frac{1}{4}) x, y, -\frac{1}{4}, y$<br>$(m_{yz}   0, 0, \frac{1}{2})$                           | (18) $\bar{4}^+ x, \frac{1}{4}, \frac{1}{4}; 0, \frac{1}{4}, -\frac{1}{4}$<br>$(\bar{4}_x   0, 0, \frac{1}{2})$     | (19) $\bar{4}^- x, -\frac{1}{4}, \frac{1}{4}; 0, -\frac{1}{4}, \frac{1}{4}$<br>$(\bar{4}_x^{-1}   0, 0, \frac{1}{2})$                                 | (20) $g (0, -\frac{1}{4}, \frac{1}{4}) x, y + \frac{1}{4}, \bar{y}$<br>$(m_{yz}   0, 0, \frac{1}{2})$   |
| (21) $g (\frac{1}{4}, 0, \frac{1}{4}) x - \frac{1}{4}, y, x$<br>$(m_{xz}   0, 0, \frac{1}{2})$                           | (22) $\bar{4}^- \frac{1}{4}, y, \frac{1}{4}; \frac{1}{4}, 0, \frac{1}{4}$<br>$(\bar{4}_y^{-1}   0, 0, \frac{1}{2})$ | (23) $g (-\frac{1}{4}, 0, \frac{1}{4}) \bar{x} + \frac{1}{4}, y, x$<br>$(m_{xz}   0, 0, \frac{1}{2})$   | (24) $\bar{4}^+ -\frac{1}{4}, y, \frac{1}{4}; -\frac{1}{4}, 0, \frac{1}{4}$<br>$(\bar{4}_y   0, 0, \frac{1}{2})$  |

## For (0,0,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $1'$<br>$(1   0, 0, 0)'$   | (2) $2' 0, 0, z$<br>$(2_z   0, 0, 0)'$   | (3) $2' 0, y, 0$<br>$(2_y   0, 0, 0)'$   | (4) $2' x, 0, 0$<br>$(2_x   0, 0, 0)'$   |
| (5) $3^{+'} x, x, x$<br>$(3_{xyz}   0, 0, 0)'$   | (6) $3^{+'} \bar{x}, x, \bar{x}$<br>$(3_{xyz}^{-1}   0, 0, 0)'$  | (7) $3^{+'} x, \bar{x}, \bar{x}$<br>$(3_{xyz}^{-1}   0, 0, 0)'$  | (8) $3^{+'} \bar{x}, \bar{x}, x$<br>$(3_{xyz}^{-1}   0, 0, 0)'$  |
| (9) $3^{-'} x, x, x$<br>$(3_{xyz}^{-1}   0, 0, 0)'$  | (10) $3^{-'} x, \bar{x}, \bar{x}$<br>$(3_{xyz}   0, 0, 0)'$  | (11) $3^{-'} \bar{x}, \bar{x}, x$<br>$(3_{xyz}   0, 0, 0)'$  | (12) $3^{-'} \bar{x}, x, \bar{x}$<br>$(3_{xyz}   0, 0, 0)'$  |
| (13) $n' (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, x, z$<br>$(m_{xy}   \frac{1}{2}, \frac{1}{2}, \frac{1}{2})'$ | (14) $c' (0, 0, \frac{1}{2}) x + \frac{1}{2}, \bar{x}, z$<br>$(m_{xy}   \frac{1}{2}, \frac{1}{2}, \frac{1}{2})'$               | (15) $\bar{4}^+ \frac{1}{2}, 0, z; \frac{1}{2}, 0, \frac{1}{4}$<br>$(\bar{4}_z   \frac{1}{2}, \frac{1}{2}, \frac{1}{2})'$      | (16) $\bar{4}^- \frac{1}{2}, 0, z; 0, \frac{1}{2}, \frac{1}{4}$<br>$(\bar{4}_z^{-1}   \frac{1}{2}, \frac{1}{2}, \frac{1}{2})'$ |
| (17) $n' (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, y, y$<br>$(m_{yz}   \frac{1}{2}, \frac{1}{2}, \frac{1}{2})'$ | (18) $\bar{4}^+ x, \frac{1}{2}, 0; \frac{1}{4}, \frac{1}{2}, 0$<br>$(\bar{4}_x   \frac{1}{2}, \frac{1}{2}, \frac{1}{2})'$      | (19) $\bar{4}^- x, 0, \frac{1}{2}; \frac{1}{4}, 0, \frac{1}{2}$<br>$(\bar{4}_x^{-1}   \frac{1}{2}, \frac{1}{2}, \frac{1}{2})'$ | (20) $a' (\frac{1}{2}, 0, 0) x, y + \frac{1}{2}, \bar{y}$<br>$(m_{yz}   \frac{1}{2}, \frac{1}{2}, \frac{1}{2})'$               |
| (21) $n' (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, y, x$<br>$(m_{xz}   \frac{1}{2}, \frac{1}{2}, \frac{1}{2})'$ | (22) $\bar{4}^- \frac{1}{2}, y, 0; \frac{1}{2}, \frac{1}{4}, 0$<br>$(\bar{4}_y^{-1}   \frac{1}{2}, \frac{1}{2}, \frac{1}{2})'$ | (23) $b' (0, \frac{1}{2}, 0) \bar{x} + \frac{1}{2}, y, x$<br>$(m_{xz}   \frac{1}{2}, \frac{1}{2}, \frac{1}{2})'$               | (24) $\bar{4}^+ 0, y, \frac{1}{2}; 0, \frac{1}{4}, \frac{1}{2}$<br>$(\bar{4}_y   \frac{1}{2}, \frac{1}{2}, \frac{1}{2})'$      |

## For (0,1/2,1/2)' + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t' (0, \frac{1}{2}, \frac{1}{2})$<br>$(1   0, \frac{1}{2}, \frac{1}{2})'$   | (2) $2' (0, 0, \frac{1}{2}) 0, \frac{1}{4}, z$<br>$(2_z   0, \frac{1}{2}, \frac{1}{2})'$  | (3) $2' (0, \frac{1}{2}, 0) 0, y, \frac{1}{4}$<br>$(2_y   0, \frac{1}{2}, \frac{1}{2})'$  | (4) $2' x, \frac{1}{4}, \frac{1}{4}$<br>$(2_x   0, \frac{1}{2}, \frac{1}{2})'$                              |
| (5) $3^{+'} (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$<br>$x - \frac{1}{3}, x - \frac{1}{6}, x$<br>$(3_{xyz}   0, \frac{1}{2}, \frac{1}{2})'$      | (6) $3^{+'} \bar{x}, x + \frac{1}{2}, \bar{x}$<br>$(3_{xyz}^{-1}   0, \frac{1}{2}, \frac{1}{2})'$   | (7) $3^{+'} (-\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$<br>$x + \frac{1}{3}, x - \frac{1}{6}, x$<br>$(3_{xyz}^{-1}   0, \frac{1}{2}, \frac{1}{2})'$ | (8) $3^{+'} \bar{x}, \bar{x} + \frac{1}{2}, x$<br>$(3_{xyz}^{-1}   0, \frac{1}{2}, \frac{1}{2})'$           |
| (9) $3^{-'} (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$<br>$x - \frac{1}{6}, x + \frac{1}{6}, x$<br>$(3_{xyz}^{-1}   0, \frac{1}{2}, \frac{1}{2})'$ | (10) $3^{-'} (-\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$<br>$x + \frac{1}{6}, \bar{x} + \frac{1}{6}, x$<br>$(3_{xyz}   0, \frac{1}{2}, \frac{1}{2})'$ | (11) $3^{-'} \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$<br>$(3_{xyz}   0, \frac{1}{2}, \frac{1}{2})'$                                       | (12) $3^{-'} \bar{x} - \frac{1}{2}, x + \frac{1}{2}, \bar{x}$<br>$(3_{xyz}   0, \frac{1}{2}, \frac{1}{2})'$ |

- |  |  |  |   |
|--|--|--|---|
| (13) $g' (1/4, 1/4, 0) \quad x+1/4, x, z$<br>( $m_{\bar{xy}}   1/2, 0, 0$ )' | (14) $g' (1/4, -1/4, 0) \quad x+1/4, \bar{x}, z$<br>( $m_{xy}   1/2, 0, 0$ )'            | (15) $\bar{4}^+ ' 1/4, -1/4, z; 1/4, -1/4, 0$<br>( $\bar{4}_z   1/2, 0, 0$ )'    | (16) $\bar{4}^- ' 1/4, 1/4, z; 1/4, 1/4, 0$<br>( $\bar{4}_z^{-1}   1/2, 0, 0$ )'  |
| (17) $a' (1/2, 0, 0) \quad x, y, y$<br>( $m_{\bar{yz}}   1/2, 0, 0$ )'       | (18) $\bar{4}^+ ' \quad x, 0, 0; 1/4, 0, 0$<br>( $\bar{4}_x   1/2, 0, 0$ )'              | (19) $\bar{4}^- ' \quad x, 0, 0; 1/4, 0, 0$<br>( $\bar{4}_x^{-1}   1/2, 0, 0$ )' | (20) $a' (1/2, 0, 0) \quad x, y, \bar{y}$<br>( $m_{yz}   1/2, 0, 0$ )'            |
| (21) $g' (1/4, 0, 1/4) \quad x+1/4, y, x$<br>( $m_{\bar{xz}}   1/2, 0, 0$ )' | (22) $\bar{4}^- ' \quad 1/4, y, -1/4; 1/4, 0, -1/4$<br>( $\bar{4}_y^{-1}   1/2, 0, 0$ )' | (23) $g' (1/4, 0, -1/4) \quad \bar{x}+1/4, y, x$<br>( $m_{xz}   1/2, 0, 0$ )'    | (24) $\bar{4}^+ ' \quad 1/4, y, 1/4; 1/4, 0, 1/4$<br>( $\bar{4}_y   1/2, 0, 0$ )' |

For (1/2, 0, 1/2)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t' (1/2, 0, 1/2)$<br>( $1   1/2, 0, 1/2$ )'                                      | (2) $2' (0, 0, 1/2) \quad 1/4, 0, z$<br>( $2_z   1/2, 0, 1/2$ )'   | (3) $2' \quad 1/4, y, 1/4$<br>( $2_y   1/2, 0, 1/2$ )'                                   | (4) $2' (1/2, 0, 0) \quad x, 0, 1/4$<br>( $2_x   1/2, 0, 1/2$ )'                                     |
| (5) $3^+ ' (1/3, 1/3, 1/3)$<br>$x+1/6, x-1/6, x$<br>( $3_{xyz}   1/2, 0, 1/2$ )'      | (6) $3^+ ' (1/3, -1/3, 1/3)$<br>$\bar{x}+1/6, x+1/6, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ )' | (7) $3^+ ' \quad x+1/2, \bar{x}-1/2, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ )' | (8) $3^+ ' \quad \bar{x}+1/2, \bar{x}+1/2, x$<br>( $3_{\bar{yz}}^{-1}   1/2, 0, 1/2$ )'              |
| (9) $3^- ' (1/3, 1/3, 1/3)$<br>$x-1/6, x-1/3, x$<br>( $3_{xyz}^{-1}   1/2, 0, 1/2$ )' | (10) $3^- ' \quad x+1/2, \bar{x}, \bar{x}$<br>( $3_{\bar{xyz}}   1/2, 0, 1/2$ )'                         | (11) $3^- ' \quad \bar{x}+1/2, \bar{x}, x$<br>( $3_{\bar{yz}}   1/2, 0, 1/2$ )'          | (12) $3^- ' (1/3, -1/3, 1/3)$<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>( $3_{\bar{xyz}}   1/2, 0, 1/2$ )' |
| (13) $g' (1/4, 1/4, 0) \quad x-1/4, x, z$<br>( $m_{\bar{xy}}   0, 1/2, 0$ )'          | (14) $g' (-1/4, 1/4, 0) \quad x+1/4, \bar{x}, z$<br>( $m_{xy}   0, 1/2, 0$ )'                            | (15) $\bar{4}^+ ' 1/4, 1/4, z; 1/4, 1/4, 0$<br>( $\bar{4}_z   0, 1/2, 0$ )'              | (16) $\bar{4}^- ' -1/4, 1/4, z; -1/4, 1/4, 0$<br>( $\bar{4}_z^{-1}   0, 1/2, 0$ )'                   |
| (17) $g' (0, 1/4, 1/4) \quad x, y+1/4, y$<br>( $m_{\bar{yz}}   0, 1/2, 0$ )'          | (18) $\bar{4}^+ ' \quad x, 1/4, -1/4; 0, 1/4, -1/4$<br>( $\bar{4}_x   0, 1/2, 0$ )'                      | (19) $\bar{4}^- ' \quad x, 1/4, 1/4; 0, 1/4, 1/4$<br>( $\bar{4}_x^{-1}   0, 1/2, 0$ )'   | (20) $g' (0, 1/4, -1/4) \quad x, y+1/4, \bar{y}$<br>( $m_{yz}   0, 1/2, 0$ )'                        |
| (21) $b' (0, 1/2, 0) \quad x, y, x$<br>( $m_{\bar{xz}}   0, 1/2, 0$ )'                | (22) $\bar{4}^- ' \quad 0, y, 0; 0, 1/4, 0$<br>( $\bar{4}_y^{-1}   0, 1/2, 0$ )'                         | (23) $b' (0, 1/2, 0) \quad \bar{x}, y, x$<br>( $m_{xz}   0, 1/2, 0$ )'                   | (24) $\bar{4}^+ ' \quad 0, y, 0; 0, 1/4, 0$<br>( $\bar{4}_y   0, 1/2, 0$ )'                          |

For (1/2, 1/2, 0)' + set

- |   |  |   |   |
|---|--|---|---|
| (1) $t' (1/2, 1/2, 0)$<br>( $1   1/2, 1/2, 0$ )'                                      | (2) $2' \quad 1/4, 1/4, z$<br>( $2_z   1/2, 1/2, 0$ )'                                 | (3) $2' (0, 1/2, 0) \quad 1/4, y, 0$<br>( $2_y   1/2, 1/2, 0$ )'  | (4) $2' (1/2, 0, 0) \quad x, 1/4, 0$<br>( $2_x   1/2, 1/2, 0$ )'  |
| (5) $3^+ ' (1/3, 1/3, 1/3)$<br>$x+1/6, x+1/3, x$<br>( $3_{xyz}   1/2, 1/2, 0$ )'      | (6) $3^+ ' \quad \bar{x}+1/2, x, \bar{x}$<br>( $3_{\bar{yz}}^{-1}   1/2, 1/2, 0$ )'    | (7) $3^+ ' \quad x+1/2, \bar{x}, \bar{x}$<br>( $3_{\bar{yz}}^{-1}   1/2, 1/2, 0$ )'                       | (8) $3^+ ' (1/3, 1/3, -1/3)$<br>$\bar{x}+1/6, \bar{x}+1/3, \bar{x}$<br>( $3_{\bar{yz}}^{-1}   1/2, 1/2, 0$ )' |
| (9) $3^- ' (1/3, 1/3, 1/3)$<br>$x+1/3, x+1/6, x$<br>( $3_{xyz}^{-1}   1/2, 1/2, 0$ )' | (10) $3^- ' \quad x, \bar{x}+1/2, \bar{x}$<br>( $3_{\bar{yz}}   1/2, 1/2, 0$ )'        | (11) $3^- ' (1/3, 1/3, -1/3)$<br>$\bar{x}+1/3, \bar{x}+1/6, \bar{x}$<br>( $3_{\bar{yz}}   1/2, 1/2, 0$ )' | (12) $3^- ' \quad \bar{x}, x+1/2, \bar{x}$<br>( $3_{\bar{yz}}   1/2, 1/2, 0$ )'                               |
| (13) $c' (0, 0, 1/2) \quad x, x, z$<br>( $m_{\bar{xy}}   0, 0, 1/2$ )'                | (14) $c' (0, 0, 1/2) \quad x, \bar{x}, z$<br>( $m_{xy}   0, 0, 1/2$ )'                 | (15) $\bar{4}^+ ' 0, 0, z; 0, 0, 1/4$<br>( $\bar{4}_z   0, 0, 1/2$ )'                                     | (16) $\bar{4}^- ' 0, 0, z; 0, 0, 1/4$<br>( $\bar{4}_z^{-1}   0, 0, 1/2$ )'                                    |
| (17) $g' (0, 1/4, 1/4) \quad x, y-1/4, y$<br>( $m_{\bar{yz}}   0, 0, 1/2$ )'          | (18) $\bar{4}^+ ' \quad x, 1/4, 1/4; 0, 1/4, -1/4$<br>( $\bar{4}_x   0, 0, 1/2$ )'     | (19) $\bar{4}^- ' \quad x, -1/4, 1/4; 0, -1/4, 1/4$<br>( $\bar{4}_x^{-1}   0, 0, 1/2$ )'                  | (20) $g' (0, -1/4, +1/4) \quad x, y+1/4, \bar{y}$<br>( $m_{yz}   0, 0, 1/2$ )'                                |
| (21) $g' (1/4, 0, 1/4) \quad x-1/4, y, x$<br>( $m_{\bar{xz}}   0, 0, 1/2$ )'          | (22) $\bar{4}^- ' \quad 1/4, y, 1/4; 1/4, 0, 1/4$<br>( $\bar{4}_y^{-1}   0, 0, 1/2$ )' | (23) $g' (-1/4, 0, 1/4) \quad \bar{x}+1/4, y, x$<br>( $m_{xz}   0, 0, 1/2$ )'                             | (24) $\bar{4}^+ ' -1/4, y, 1/4; -1/4, 0, 1/4$<br>( $\bar{4}_y   0, 0, 1/2$ )'                                 |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); 1'.

## Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

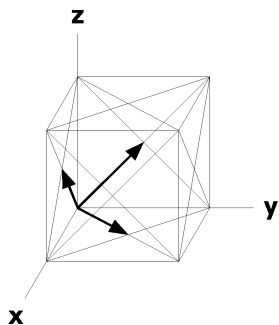
			(0,0,0) + (0,0,0)' +	(0,1/2,1/2) + (0,1/2,1/2)' +	(1/2,0,1/2) + (1/2,0,1/2)' +	(1/2,1/2,0) + (1/2,1/2,0)' +				
96	h	11'								
(1)	x,y,z	[0,0,0]	(2) $\bar{x},\bar{y},z$	[0,0,0]	(3) $\bar{x},y,\bar{z}$	[0,0,0]	(4) $x,\bar{y},\bar{z}$	[0,0,0]		
(5)	z,x,y	[0,0,0]	(6) $z,\bar{x},\bar{y}$	[0,0,0]	(7) $\bar{z},\bar{x},y$	[0,0,0]	(8) $\bar{z},x,\bar{y}$	[0,0,0]		
(9)	y,z,x	[0,0,0]	(10) $\bar{y},z,\bar{x}$	[0,0,0]	(11) $y,\bar{z},\bar{x}$	[0,0,0]	(12) $\bar{y},\bar{z},x$	[0,0,0]		
(13)	$y+1/2,x+1/2,z+1/2$	[0,0,0]	(14) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$	[0,0,0]	(15) $y+1/2,\bar{x}+1/2,\bar{z}+1/2$	[0,0,0]	(16) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$	[0,0,0]		
(17)	$x+1/2,z+1/2,y+1/2$	[0,0,0]	(18) $\bar{x}+1/2,z+1/2,\bar{y}+1/2$	[0,0,0]	(19) $\bar{x}+1/2,\bar{z}+1/2,y+1/2$	[0,0,0]	(20) $x+1/2,\bar{z}+1/2,\bar{y}+1/2$	[0,0,0]		
(21)	$z+1/2,y+1/2,x+1/2$	[0,0,0]	(22) $z+1/2,\bar{y}+1/2,\bar{x}+1/2$	[0,0,0]	(23) $\bar{z}+1/2,y+1/2,\bar{x}+1/2$	[0,0,0]	(24) $\bar{z}+1/2,\bar{y}+1/2,x+1/2$	[0,0,0]		
48	g	2..1'	$x,1/4,1/4$	[0,0,0]	$\bar{x},3/4,1/4$	[0,0,0]	$1/4,x,1/4$	[0,0,0]	$1/4,\bar{x},3/4$	[0,0,0]
			$1/4,1/4,x$	[0,0,0]	$3/4,1/4,\bar{x}$	[0,0,0]	$3/4,x+1/2,3/4$	[0,0,0]	$1/4,\bar{x}+1/2,3/4$	[0,0,0]
			$x+1/2,3/4,3/4$	[0,0,0]	$\bar{x}+1/2,3/4,1/4$	[0,0,0]	$3/4,3/4,x+1/2$	[0,0,0]	$3/4,1/4,\bar{x}+1/2$	[0,0,0]
48	f	2..1'	$x,0,0$	[0,0,0]	$\bar{x},0,0$	[0,0,0]	$0,x,0$	[0,0,0]	$0,\bar{x},0$	[0,0,0]
			$0,0,x$	[0,0,0]	$0,0,\bar{x}$	[0,0,0]	$1/2,x+1/2,1/2$	[0,0,0]	$1/2,\bar{x}+1/2,1/2$	[0,0,0]
			$x+1/2,1/2,1/2$	[0,0,0]	$\bar{x}+1/2,1/2,1/2$	[0,0,0]	$1/2,1/2,x+1/2$	[0,0,0]	$1/2,1/2,\bar{x}+1/2$	[0,0,0]
32	e	.3.1'	$x,x,x$	[0,0,0]			$\bar{x},\bar{x},x$	[0,0,0]		
			$\bar{x},x,\bar{x}$	[0,0,0]			$x,\bar{x},\bar{x}$	[0,0,0]		
			$x+1/2,x+1/2,x+1/2$	[0,0,0]			$\bar{x}+1/2,\bar{x}+1/2,x+1/2$	[0,0,0]		
			$x+1/2,\bar{x}+1/2,\bar{x}+1/2$	[0,0,0]			$\bar{x}+1/2,x+1/2,\bar{x}+1/2$	[0,0,0]		
24	d	$\bar{4}1'$	$1/4,0,0$	[0,0,0]	$3/4,0,0$	[0,0,0]	$0,1/4,0$	[0,0,0]		
			$0,3/4,0$	[0,0,0]	$0,0,1/4$	[0,0,0]	$0,0,3/4$	[0,0,0]		
24	c	$\bar{4}1'$	$0,1/4,1/4$	[0,0,0]	$0,3/4,1/4$	[0,0,0]	$1/4,0,1/4$	[0,0,0]		
			$1/4,0,3/4$	[0,0,0]	$1/4,1/4$	[0,0,0]	$3/4,1/4$	[0,0,0]		
8	b	23.1'	$1/4,1/4,1/4$	[0,0,0]	$3/4,3/4,3/4$	[0,0,0]				
8	a	23.1'	$0,0,0$	[0,0,0]	$1/2,1/2,1/2$	[0,0,0]				

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
Origin at  $0,0,z$

Along  $[1,1,1]$   $p31m1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
Origin at  $x,x,x$

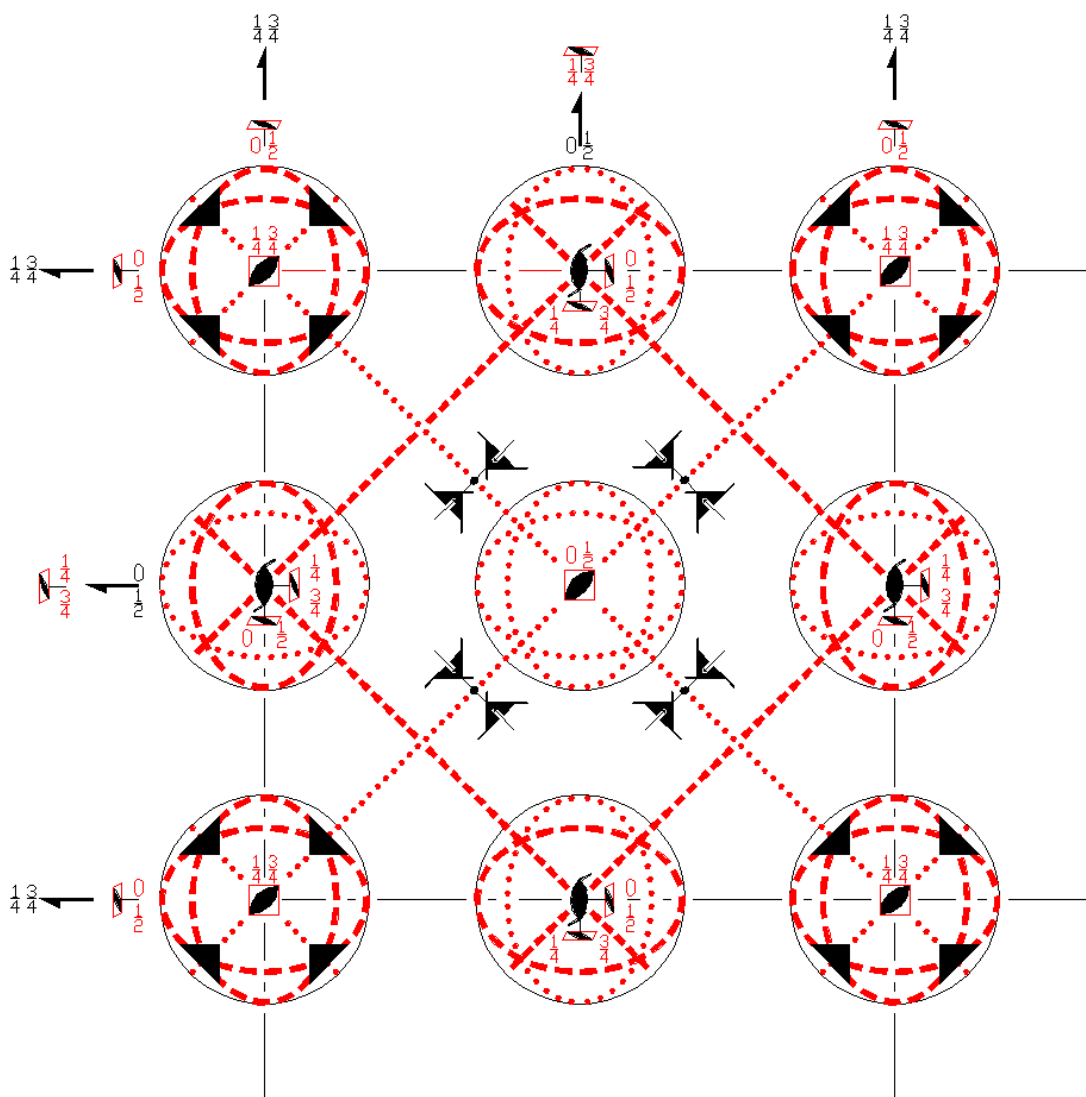
Along  $[1,1,0]$   $p1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at  $x,x,0$



$F\bar{4}'3c'$   
219.3.1590

$\bar{4}'3m'$   
 $F\bar{4}'3c'$

Cubic



Origin at 23

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/4;$   $-1/4 \leq z \leq 1/4;$   $y \leq \min(x, 1/2-x);$   $-y \leq z \leq y$   
**Vertices**  $0,0,0$   $1/2,0,0$   $1/4,1/4,1/4$   $1/4,1/4,-1/4$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)              |

(13) $n' (1/2, 1/2, 1/2) \quad x, x, z$ ( $m_{\bar{xy}}   1/2, 1/2, 1/2$ )'	(14) $c' (0, 0, 1/2) \quad x+1/2, \bar{x}, z$ ( $m_{xy}   1/2, 1/2, 1/2$ )'	(15) $\bar{4}^+ ' 1/2, 0, z; 1/2, 0, 1/4$ ( $\bar{4}_z   1/2, 1/2, 1/2$ )'	(16) $\bar{4}^- ' 0, 1/2, z; 0, 1/2, 1/4$ ( $\bar{4}_z^{-1}   1/2, 1/2, 1/2$ )'
(17) $n' (1/2, 1/2, 1/2) \quad x, y, y$ ( $m_{\bar{yz}}   1/2, 1/2, 1/2$ )'	(18) $\bar{4}^+ ' x, 1/2, 0; 1/4, 1/2, 0$ ( $\bar{4}_x   1/2, 1/2, 1/2$ )'	(19) $\bar{4}^- ' x, 0, 1/2; 1/4, 0, 1/2$ ( $\bar{4}_x^{-1}   1/2, 1/2, 1/2$ )'	(20) $a' (1/2, 0, 0) \quad x, y+1/2, \bar{y}$ ( $m_{yz}   1/2, 1/2, 1/2$ )'
(21) $n' (1/2, 1/2, 1/2) \quad x, y, x$ ( $m_{\bar{zx}}   1/2, 1/2, 1/2$ )'	(22) $\bar{4}^- ' 1/2, y, 0; 1/2, 1/4, 0$ ( $\bar{4}_y^{-1}   1/2, 1/2, 1/2$ )'	(23) $b' (0, 1/2, 0) \quad \bar{x}+1/2, y, x$ ( $m_{xz}   1/2, 1/2, 1/2$ )'	(24) $\bar{4}^+ ' 0, y, 1/2; 0, 1/4, 1/2$ ( $\bar{4}_y   1/2, 1/2, 1/2$ )'

For (0, 1/2, 1/2) + set

(1) $t (0, 1/2, 1/2)$ ( $1   0, 1/2, 1/2$ )	(2) $2 (0, 0, 1/2) \quad 0, 1/4, z$ ( $2_z   0, 1/2, 1/2$ )	(3) $2 (0, 1/2, 0) \quad 0, y, 1/4$ ( $2_y   0, 1/2, 1/2$ )	(4) $2 \quad x, 1/4, 1/4$ ( $2_x   0, 1/2, 1/2$ )
(5) $3^+ (1/3, 1/3, 1/3)$ $x-1/3, x-1/6, x$ ( $3_{xyz}   0, 1/2, 1/2$ )	(6) $3^+ \quad \bar{x}, x+1/2, \bar{x}$ ( $3_{\bar{xyz}}^{-1}   0, 1/2, 1/2$ )	(7) $3^+ (-1/3, 1/3, 1/3)$ $x+1/3, \bar{x}-1/6, \bar{x}$ ( $3_{\bar{xyz}}^{-1}   0, 1/2, 1/2$ )	(8) $3^+ \quad \bar{x}, \bar{x}+1/2, x$ ( $3_{\bar{xyz}}^{-1}   0, 1/2, 1/2$ )
(9) $3^- (1/3, 1/3, 1/3)$ $x-1/6, x+1/6, x$ ( $3_{xyz}^{-1}   0, 1/2, 1/2$ )	(10) $3^- (-1/3, 1/3, 1/3)$ $x+1/6, x+1/6, \bar{x}$ ( $3_{\bar{xyz}}   0, 1/2, 1/2$ )	(11) $3^- \quad \bar{x}+1/2, \bar{x}+1/2, x$ ( $3_{\bar{yz}}   0, 1/2, 1/2$ )	(12) $3^- \quad \bar{x}-1/2, x+1/2, \bar{x}$ ( $3_{\bar{yz}}   0, 1/2, 1/2$ )
(13) $g' (1/4, 1/4, 0) \quad x+1/4, x, z$ ( $m_{\bar{xy}}   1/2, 0, 0$ )'	(14) $g' (1/4, -1/4, 0) \quad x+1/4, \bar{x}, z$ ( $m_{xy}   1/2, 0, 0$ )'	(15) $\bar{4}^+ ' 1/4, -1/4, z; 1/4, -1/4, 0$ ( $\bar{4}_z   1/2, 0, 0$ )'	(16) $\bar{4}^- ' 1/4, 1/4, z; 1/4, 1/4, 0$ ( $\bar{4}_z^{-1}   1/2, 0, 0$ )'
(17) $a' (1/2, 0, 0) \quad x, y, y$ ( $m_{\bar{yz}}   1/2, 0, 0$ )'	(18) $\bar{4}^+ ' x, 0, 0; 1/4, 0, 0$ ( $\bar{4}_x   1/2, 0, 0$ )'	(19) $\bar{4}^- ' x, 0, 0; 1/4, 0, 0$ ( $\bar{4}_x^{-1}   1/2, 0, 0$ )'	(20) $a' (1/2, 0, 0) \quad x, y, \bar{y}$ ( $m_{yz}   1/2, 0, 0$ )'
(21) $g' (1/4, 0, 1/4) \quad x+1/4, y, x$ ( $m_{\bar{zx}}   1/2, 0, 0$ )'	(22) $\bar{4}^- ' 1/4, y, -1/4; 1/4, 0, -1/4$ ( $\bar{4}_y^{-1}   1/2, 0, 0$ )'	(23) $g' (1/4, 0, -1/4) \quad \bar{x}+1/4, y, x$ ( $m_{xz}   1/2, 0, 0$ )'	(24) $\bar{4}^+ ' 1/4, y, 1/4; 1/4, 0, 1/4$ ( $\bar{4}_y   1/2, 0, 0$ )'

For (1/2, 0, 1/2) + set

(1) $t (1/2, 0, 1/2)$ ( $1   1/2, 0, 1/2$ )	(2) $2 (0, 0, 1/2) \quad 1/4, 0, z$ ( $2_z   1/2, 0, 1/2$ )	(3) $2 \quad 1/4, y, 1/4$ ( $2_y   1/2, 0, 1/2$ )	(4) $2 (1/2, 0, 0) \quad x, 0, 1/4$ ( $2_x   1/2, 0, 1/2$ )
(5) $3^+ (1/3, 1/3, 1/3)$ $x+1/6, x-1/6, x$ ( $3_{xyz}   1/2, 0, 1/2$ )	(6) $3^+ (1/3, -1/3, 1/3)$ $\bar{x}+1/6, x+1/6, \bar{x}$ ( $3_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ )	(7) $3^+ \quad x+1/2, \bar{x}-1/2, \bar{x}$ ( $3_{\bar{yz}}^{-1}   1/2, 0, 1/2$ )	(8) $3^+ \quad \bar{x}+1/2, \bar{x}+1/2, x$ ( $3_{\bar{yz}}^{-1}   1/2, 0, 1/2$ )
(9) $3^- (1/3, 1/3, 1/3)$ $x-1/6, x-1/3, x$ ( $3_{xyz}^{-1}   1/2, 0, 1/2$ )	(10) $3^- \quad x+1/2, \bar{x}, \bar{x}$ ( $3_{\bar{yz}}   1/2, 0, 1/2$ )	(11) $3^- \quad \bar{x}+1/2, \bar{x}, x$ ( $3_{\bar{yz}}   1/2, 0, 1/2$ )	(12) $3^- (1/3, -1/3, 1/3)$ $\bar{x}-1/6, x+1/3, \bar{x}$ ( $3_{\bar{yz}}   1/2, 0, 1/2$ )
(13) $g' (1/4, 1/4, 0) \quad x-1/4, x, z$ ( $m_{\bar{xy}}   0, 1/2, 0$ )'	(14) $g' (-1/4, 1/4, 0) \quad x+1/4, \bar{x}, z$ ( $m_{xy}   0, 1/2, 0$ )'	(15) $\bar{4}^+ ' 1/4, 1/4, z; 1/4, 1/4, 0$ ( $\bar{4}_z   0, 1/2, 0$ )'	(16) $\bar{4}^- ' -1/4, 1/4, z; -1/4, 1/4, 0$ ( $\bar{4}_z^{-1}   0, 1/2, 0$ )'
(17) $g' (0, 1/4, 1/4) \quad x, y+1/4, y$ ( $m_{\bar{yz}}   0, 1/2, 0$ )'	(18) $\bar{4}^+ ' x, 1/4, -1/4; 0, 1/4, -1/4$ ( $\bar{4}_x   0, 1/2, 0$ )'	(19) $\bar{4}^- ' x, 1/4, 1/4; 0, 1/4, 1/4$ ( $\bar{4}_x^{-1}   0, 1/2, 0$ )'	(20) $g' (0, 1/4, -1/4) \quad x, y+1/4, \bar{y}$ ( $m_{yz}   0, 1/2, 0$ )'
(21) $b' (0, 1/2, 0) \quad x, y, x$ ( $m_{\bar{zx}}   0, 1/2, 0$ )'	(22) $\bar{4}^- ' 0, y, 0; 0, 1/4, 0$ ( $\bar{4}_y^{-1}   0, 1/2, 0$ )'	(23) $b' (0, 1/2, 0) \quad \bar{x}, y, x$ ( $m_{xz}   0, 1/2, 0$ )'	(24) $\bar{4}^+ ' 0, y, 0; 0, 1/4, 0$ ( $\bar{4}_y   0, 1/2, 0$ )'

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (1   1/2,1/2,0)	(2) 2 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,0)	(3) 2 (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)	(4) 2 (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) 3 <sup>+</sup> $\bar{x}+1/2,x,\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(7) 3 <sup>+</sup> x+1/2, $\bar{x},\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(8) 3 <sup>+</sup> (1/3,1/3,-1/3) $\bar{x}+1/6,\bar{x}+1/3,x$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) 3 <sup>-</sup> x, $\bar{x}+1/2,\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)	(11) 3 <sup>-</sup> (1/3,1/3,-1/3) $\bar{x}+1/3,\bar{x}+1/6,x$ (3 <sub>xyz</sub>   1/2,1/2,0)	(12) 3 <sup>-</sup> $\bar{x},x+1/2,\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)
(13) c' (0,0,1/2) x,x,z (m <sub>xy</sub>   0,0,1/2)'	(14) c' (0,0,1/2) x, $\bar{x},z$ (m <sub>xy</sub>   0,0,1/2)'	(15) $\bar{4}^+$ ' 0,0,z; 0,0,1/4 (4 <sub>z</sub>   0,0,1/2)'	(16) $\bar{4}^-$ ' 0,0,z; 0,0,1/4 (4 <sub>z</sub> <sup>-1</sup>   0,0,1/2)'
(17) g' (0,1/4,1/4) x,y-1/4,y (m <sub>yz</sub>   0,0,1/2)'	(18) $\bar{4}^+$ ' x,1/4,1/4; 0,1/4,-1/4 (4 <sub>x</sub>   0,0,1/2)'	(19) $\bar{4}^-$ ' x,-1/4,1/4; 0,-1/4,1/4 (4 <sub>x</sub> <sup>-1</sup>   0,0,1/2)'	(20) g' (0,-1/4,+1/4) x,y+1/4, $\bar{y}$ (m <sub>yz</sub>   0,0,1/2)'
(21) g' (1/4,0,1/4) x-1/4,y,x (m <sub>xz</sub>   0,0,1/2)'	(22) $\bar{4}^-$ ' 1/4,y,1/4; 1/4,0,1/4 (4 <sub>y</sub> <sup>-1</sup>   0,0,1/2)'	(23) g' (-1/4,0,1/4) $\bar{x}+1/4,y,x$ (m <sub>xz</sub>   0,0,1/2)'	(24) $\bar{4}^+$ ' -1/4,y,1/4; -1/4,0,1/4 (4 <sub>y</sub>   0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

			(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +
96	h	1				
(1)	x,y,z [u,v,w]		(2) $\bar{x},\bar{y},z$ [ $\bar{u},\bar{v},w$ ]		(3) $\bar{x},y,\bar{z}$ [ $\bar{u},v,\bar{w}$ ]	(4) x, $\bar{y},\bar{z}$ [ $u,\bar{v},\bar{w}$ ]
(5)	z,x,y [w,u,v]		(6) z, $\bar{x},\bar{y}$ [ $w,\bar{u},\bar{v}$ ]		(7) $\bar{z},\bar{x},y$ [ $\bar{w},\bar{u},v$ ]	(8) $\bar{z},x,\bar{y}$ [ $\bar{w},u,\bar{v}$ ]
(9)	y,z,x [v,w,u]		(10) $\bar{y},z,\bar{x}$ [ $\bar{v},w,\bar{u}$ ]		(11) y, $\bar{z},\bar{x}$ [ $v,\bar{w},\bar{u}$ ]	(12) $\bar{y},\bar{z},x$ [ $\bar{v},\bar{w},u$ ]
(13)	y+1/2,x+1/2,z+1/2 [v,u,w]		(14) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [ $\bar{v},\bar{u},w$ ]		(15) y+1/2, $\bar{x}+1/2,\bar{z}+1/2$ [ $v,\bar{u},\bar{w}$ ]	(16) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [ $\bar{v},u,\bar{w}$ ]
(17)	x+1/2,z+1/2,y+1/2 [u,w,v]		(18) $\bar{x}+1/2,z+1/2,\bar{y}+1/2$ [ $\bar{u},w,\bar{v}$ ]		(19) $\bar{x}+1/2,\bar{z}+1/2,y+1/2$ [ $\bar{u},\bar{w},v$ ]	(20) x+1/2, $\bar{z}+1/2,\bar{y}+1/2$ [ $u,\bar{w},\bar{v}$ ]
(21)	z+1/2,y+1/2,x+1/2 [w,v,u]		(22) z+1/2, $\bar{y}+1/2,\bar{x}+1/2$ [ $w,\bar{v},\bar{u}$ ]		(23) $\bar{z}+1/2,y+1/2,\bar{x}+1/2$ [ $\bar{w},v,\bar{u}$ ]	(24) $\bar{z}+1/2,\bar{y}+1/2,x+1/2$ [ $\bar{w},\bar{v},u$ ]
48	g	2..	x,1/4,1/4 [u,0,0]	$\bar{x},3/4,1/4$ [ $\bar{u},0,0$ ]	1/4,x,1/4 [0,u,0]	1/4, $\bar{x},3/4$ [0, $\bar{u},0$ ]
			1/4,1/4,x [0,0,u]	3/4,1/4, $\bar{x}$ [0,0, $\bar{u}$ ]	3/4,x+1/2,3/4 [0,u,0]	1/4, $\bar{x}+1/2,3/4$ [0, $\bar{u},0$ ]
			x+1/2,3/4,3/4 [u,0,0]	$\bar{x}+1/2,3/4,1/4$ [ $\bar{u},0,0$ ]	3/4,3/4,x+1/2 [0,0,u]	3/4,1/4, $\bar{x}+1/2$ [0,0, $\bar{u}$ ]
48	f	2..	x,0,0 [u,0,0]	$\bar{x},0,0$ [ $\bar{u},0,0$ ]	0,x,0 [0,u,0]	0, $\bar{x},0$ [0, $\bar{u},0$ ]
			0,0,x [0,0,u]	0,0, $\bar{x}$ [0,0, $\bar{u}$ ]	1/2,x+1/2,1/2 [0,u,0]	1/2, $\bar{x}+1/2,1/2$ [0, $\bar{u},0$ ]
			x+1/2,1/2,1/2 [u,0,0]	$\bar{x}+1/2,1/2,1/2$ [ $\bar{u},0,0$ ]	1/2,1/2,x+1/2 [0,0,u]	1/2,1/2, $\bar{x}+1/2$ [0,0, $\bar{u}$ ]

32	e	.3.	$x,x,x [u,u,u]$		$\bar{x},\bar{x},x [\bar{u},\bar{u},u]$
			$\bar{x},x,\bar{x} [\bar{u},u,\bar{u}]$		$x,\bar{x},\bar{x} [u,\bar{u},\bar{u}]$
			$x+1/2,x+1/2,x+1/2 [u,u,u]$		$\bar{x}+1/2,\bar{x}+1/2,x+1/2 [\bar{u},\bar{u},u]$
			$x+1/2,\bar{x}+1/2,\bar{x}+1/2 [u,\bar{u},\bar{u}]$		$\bar{x}+1/2,x+1/2,\bar{x}+1/2 [\bar{u},u,\bar{u}]$
24	d	$\bar{4}'$	$1/4,0,0 [0,0,0]$	$3/4,0,0 [0,0,0]$	$0,1/4,0 [0,0,0]$
			$0,3/4,0 [0,0,0]$	$0,0,1/4 [0,0,0]$	$0,0,3/4 [0,0,0]$
24	c	$\bar{4}'$	$0,1/4,1/4 [0,0,0]$	$0,3/4,1/4 [0,0,0]$	$1/4,0,1/4 [0,0,0]$
			$1/4,0,3/4 [0,0,0]$	$1/4,1/4 [0,0,0]$	$3/4,1/4 [0,0,0]$
8	b	23.	$1/4,1/4,1/4 [0,0,0]$	$3/4,3/4,3/4 [0,0,0]$	
8	a	23.	$0,0,0 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$	

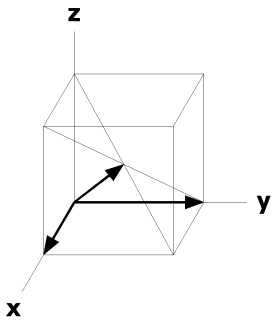
### Symmetry of Special Projections

Along  $[0,0,1]$   $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p31m'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at  $x,x,x$

Along  $[1,1,0]$   $p1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$

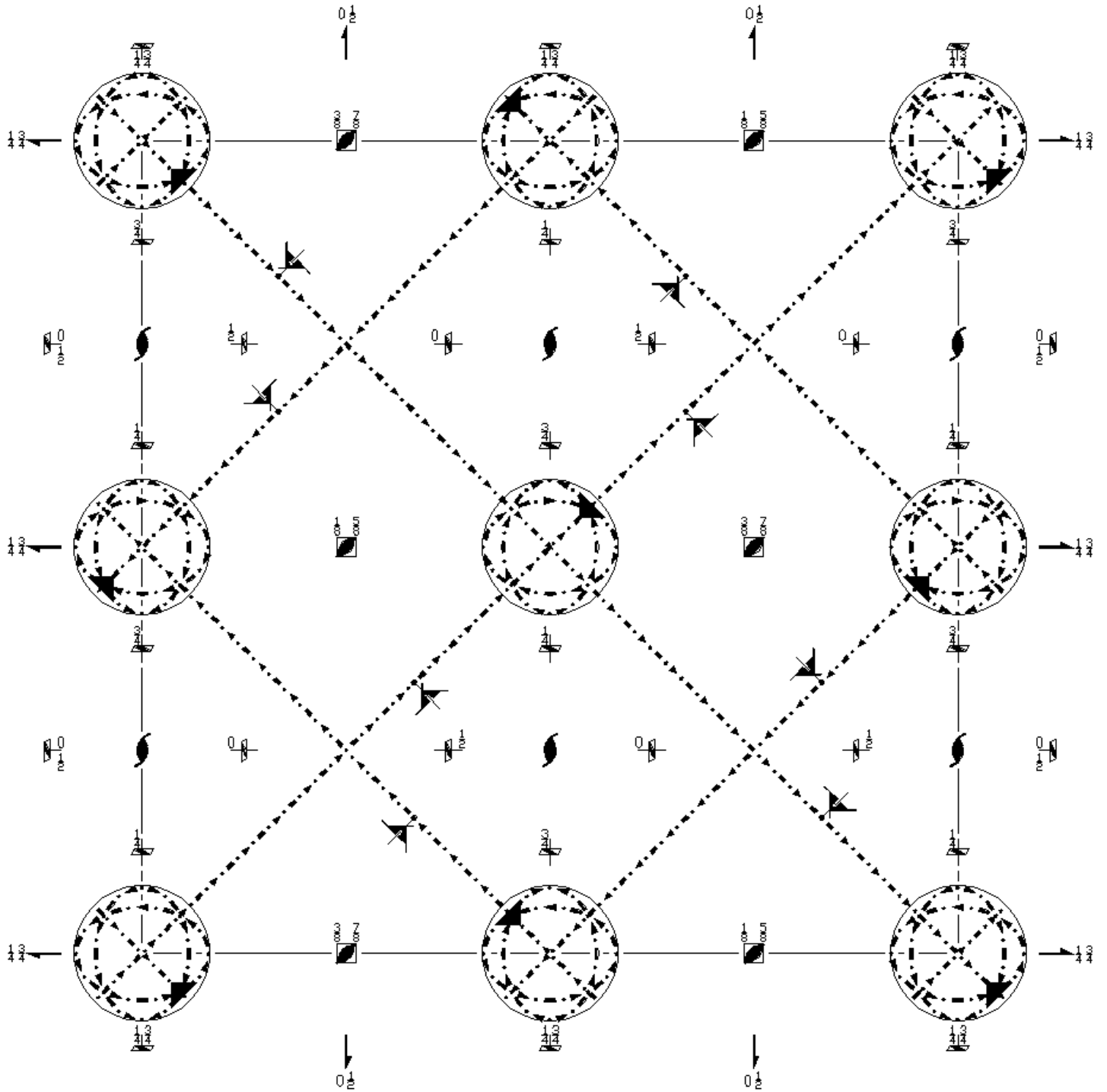




$\bar{4}3d$   
220.1.1591

$\bar{4}3m$   
 $\bar{4}3d$

Cubic



**Origin** on 3 [1,1,1] at midpoint of three non-intersecting pairs of parallel 2 axes and of three non-intersecting pairs of parallel 2<sub>1</sub> axes

**Asymmetric unit**  $1/4 \leq x \leq 1/2$ ;  $1/4 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$ ;  $z \leq \min(x,y)$

Vertices  $1/4, 1/4, 0$   $1/2, 1/4, 0$   $1/2, 1/2, 0$   $1/4, 1/2, 0$   
 $1/4, 1/4, 1/4$   $1/2, 1/4, 1/2$   $1/2, 1/2, 1/2$   $1/4, 1/2, 1/4$

### Symmetry Operations

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) $1/4, 0, z$<br>(2 <sub>z</sub>  1/2,0,1/2)                                       | (3) 2 (0,1/2,0) $0, y, 1/4$<br>(2 <sub>y</sub>  0,1/2,1/2)                                       | (4) 2 (1/2,0,0) $x, 1/4, 0$<br>(2 <sub>x</sub>  1/2,1/2,0)                                       |
| (5) 3 <sup>+</sup> $\bar{x}, x, x$<br>(3 <sub>xyz</sub>  0,0,0)         | (6) 3 <sup>+</sup> $\bar{x}+1/2, x, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0)      | (7) 3 <sup>+</sup> $x+1/2, \bar{x}-1/2, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2)  | (8) 3 <sup>+</sup> $\bar{x}, \bar{x}+1/2, x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)      |
| (9) 3 <sup>-</sup> $x, x, x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> (-1/3, 1/3, 1/3)<br>$x+1/6, x+1/6, \bar{x}$<br>(3 <sub>xyz</sub>  0,1/2,1/2) | (11) 3 <sup>-</sup> (1/3, 1/3, -1/3)<br>$x+1/3, \bar{x}+1/6, x$<br>(3 <sub>xyz</sub>  1/2,1/2,0) | (12) 3 <sup>-</sup> (1/3, -1/3, 1/3)<br>$x-1/6, x+1/3, \bar{x}$<br>(3 <sub>xyz</sub>  1/2,0,1/2) |
| (13) d (1/4, 1/4, 1/4) $x, x, z$<br>(m <sub>xy</sub>  1/4,1/4,1/4)      | (14) d (-1/4, 1/4, 3/4) $x+1/2, \bar{x}, z$<br>(m <sub>xy</sub>  1/4,3/4,3/4)                    | (15) $\bar{4}^+$ 1/2, -1/4, z; 1/2, -1/4, 3/8<br>( $\bar{4}_z$  3/4,1/4,3/4)                     | (16) $\bar{4}^-$ 0, 3/4, z; 0, 3/4, 1/8<br>( $\bar{4}_z$ <sup>-1</sup>  3/4,3/4,1/4)             |
| (17) d (1/4, 1/4, 1/4) $x, y, y$<br>(m <sub>yz</sub>  1/4,1/4,1/4)      | (18) $\bar{4}^+$ $x, 1/2, -1/4$ ; 3/8, 1/2, -1/4<br>( $\bar{4}_x$  3/4,3/4,1/4)                  | (19) $\bar{4}^-$ $x, 0, 3/4$ ; 1/8, 0, 3/4<br>( $\bar{4}_x$ <sup>-1</sup>  1/4,3/4,3/4)          | (20) d (3/4, -1/4, 1/4) $x, y+1/2, \bar{y}$<br>(m <sub>yz</sub>  3/4,1/4,3/4)                    |
| (21) d (1/4, 1/4, 1/4) $x, y, x$<br>(m <sub>xz</sub>  1/4,1/4,1/4)      | (22) $\bar{4}^-$ 3/4, y, 0; 3/4, 1/8, 0<br>( $\bar{4}_y$ <sup>-1</sup>  3/4,1/4,3/4)             | (23) d (1/4, 3/4, -1/4) $\bar{x}+1/2, y, x$<br>(m <sub>xz</sub>  3/4,3/4,1/4)                    | (24) $\bar{4}^+$ -1/4, y, 1/2; -1/4, 3/8, 1/2<br>( $\bar{4}_y$  1/4,3/4,3/4)                     |

For (1/2,1/2,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2, 1/2, 1/2)<br>(1 1/2,1/2,1/2)  | (2) 2 0, 1/4, z<br>(2 <sub>z</sub>  0,1/2,0)  | (3) 2 1/4, y, 0<br>(2 <sub>y</sub>  1/2,0,0)  | (4) 2 x, 0, 1/4<br>(2 <sub>x</sub>  0,0,1/2)  |
| (5) 3 <sup>+</sup> (1/2, 1/2, 1/2) $x, x, x$<br>(3 <sub>xyz</sub>  1/2,1/2,1/2)               | (6) 3 <sup>+</sup> (1/6, -1/6, 1/6)<br>$x-1/6, x+1/3, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,1/2) | (7) 3 <sup>+</sup> (-1/6, 1/6, 1/6)<br>$x+1/6, \bar{x}+1/6, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,0) | (8) 3 <sup>+</sup> (1/6, 1/6, -1/6)<br>$x+1/3, \bar{x}+1/6, x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,0) |
| (9) 3 <sup>-</sup> (1/2, 1/2, 1/2) $x, x, x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2) | (10) 3 <sup>-</sup> (1/6, -1/6, -1/6)<br>$x+1/6, \bar{x}+1/6, \bar{x}$<br>(3 <sub>xyz</sub>  1/2,0,0)       | (11) 3 <sup>-</sup> (-1/6, -1/6, 1/6)<br>$x+1/3, \bar{x}+1/6, x$<br>(3 <sub>xyz</sub>  0,0,1/2)                   | (12) 3 <sup>-</sup> (-1/6, 1/6, -1/6)<br>$x-1/6, x+1/3, \bar{x}$<br>(3 <sub>xyz</sub>  0,1/2,0)             |
| (13) d (3/4, 3/4, 3/4) $x, x, z$<br>(m <sub>xy</sub>  3/4,3/4,3/4)                            | (14) d (1/4, -1/4, 1/4) $x+1/2, \bar{x}, z$<br>(m <sub>xy</sub>  3/4,1/4,1/4)                               | (15) $\bar{4}^+$ 1/2, 1/4, z; 1/2, 1/4, 1/8<br>( $\bar{4}_z$  1/4,3/4,1/4)  | (16) $\bar{4}^-$ 0, 1/4, z; 0, 1/4, 3/8<br>( $\bar{4}_z$ <sup>-1</sup>  1/4,1/4,3/4)                        |
| (17) d (3/4, 3/4, 3/4) $x, y, y$<br>(m <sub>yz</sub>  3/4,3/4,3/4)                            | (18) $\bar{4}^+$ $x, 1/2, 1/4$ ; 1/8, 1/2, 1/4<br>( $\bar{4}_x$  1/4,1/4,3/4)                               | (19) $\bar{4}^-$ $x, 0, 1/4$ ; 3/8, 0, 1/4<br>( $\bar{4}_x$ <sup>-1</sup>  3/4,1/4,1/4)                           | (20) d (1/4, 1/4, -1/4) $x, y+1/2, \bar{y}$<br>(m <sub>yz</sub>  1/4,3/4,1/4)                               |
| (21) d (3/4, 3/4, 3/4) $x, y, x$<br>(m <sub>xz</sub>  3/4,3/4,3/4)                            | (22) $\bar{4}^-$ 1/4, y, 0; 1/4, 0, 3/8<br>( $\bar{4}_y$ <sup>-1</sup>  1/4,3/4,1/4)                        | (23) d (-1/4, 1/4, 1/4) $\bar{x}+1/2, y, x$<br>(m <sub>xz</sub>  1/4,1/4,3/4)                                     | (24) $\bar{4}^+$ 1/4, y, 1/2; 1/4, 1/8, 1/2<br>( $\bar{4}_y$  3/4,1/4,1/4)                                  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).

**Positions**

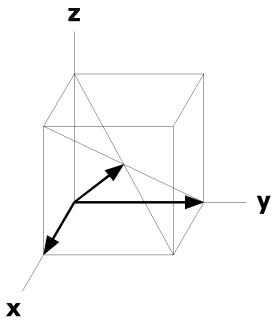
Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates		
48	e	1	(0,0,0) +	(1/2,1/2,1/2) +	
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}+1/2, \bar{y}, z+1/2$	$[\bar{u}, \bar{v}, w]$
(3)	$\bar{x}, y+1/2, \bar{z}+1/2$	$[\bar{u}, v, \bar{w}]$	(4)	$x+1/2, \bar{y}+1/2, \bar{z}$	$[u, \bar{v}, \bar{w}]$
(5)	z,x,y	[w,u,v]	(6)	$z+1/2, \bar{x}+1/2, \bar{y}$	$[w, \bar{u}, \bar{v}]$
(7)	$\bar{z}+1/2, \bar{x}, y+1/2$	$[\bar{w}, \bar{u}, v]$	(8)	$\bar{z}, x+1/2, \bar{y}+1/2$	$[\bar{w}, u, \bar{v}]$
(9)	y,z,x	[v,w,u]	(10)	$\bar{y}, z+1/2, \bar{x}+1/2$	$[\bar{v}, w, \bar{u}]$
(11)	$y+1/2, \bar{z}+1/2, \bar{x}$	$[v, \bar{w}, \bar{u}]$	(12)	$\bar{y}+1/2, \bar{z}, x+1/2$	$[\bar{v}, \bar{w}, u]$
(13)	$y+1/4, x+1/4, z+1/4$	$[\bar{v}, \bar{u}, \bar{w}]$	(14)	$\bar{y}+1/4, \bar{x}+3/4, z+3/4$	$[v, u, \bar{w}]$
(15)	$y+3/4, \bar{x}+1/4, \bar{z}+3/4$	$[\bar{v}, u, w]$	(16)	$\bar{y}+3/4, x+3/4, \bar{z}+1/4$	$[v, \bar{u}, \bar{w}]$
(17)	$x+1/4, z+1/4, y+1/4$	$[\bar{u}, \bar{w}, \bar{v}]$	(18)	$\bar{x}+3/4, z+3/4, \bar{y}+1/4$	$[u, \bar{w}, v]$
(19)	$\bar{x}+1/4, \bar{z}+3/4, y+3/4$	$[u, w, \bar{v}]$	(20)	$x+3/4, \bar{z}+1/4, \bar{y}+3/4$	$[\bar{u}, w, v]$
(21)	$z+1/4, y+1/4, x+1/4$	$[\bar{w}, \bar{v}, \bar{u}]$	(22)	$z+3/4, \bar{y}+1/4, \bar{x}+3/4$	$[\bar{w}, v, u]$
(23)	$\bar{z}+3/4, y+3/4, \bar{x}+1/4$	$[w, \bar{v}, u]$	(24)	$\bar{z}+1/4, \bar{y}+3/4, x+3/4$	$[w, v, \bar{u}]$
24	d	2..	x,0,1/4 [u,0,0]	$\bar{x}+1/2, 0, 3/4$ $[\bar{u}, 0, 0]$	1/4,x,0 [0,u,0]
			3/4, $\bar{x}+1/2, 0$ $[0, \bar{u}, 0]$	0,1/4,x [0,0,u]	0,3/4, $\bar{x}+1/2$ $[0, 0, \bar{u}]$
			1/4,x+1/4,1/2 $[0, \bar{u}, 0]$	1/4, $\bar{x}+3/4, 0$ $[0, u, 0]$	x+1/4,1/2,1/4 $[\bar{u}, 0, 0]$
			$\bar{x}+3/4, 0, 1/4$ $[u, 0, 0]$	1/2,1/4,x+1/4 $[0, 0, \bar{u}]$	0,1/4, $\bar{x}+3/4$ $[0, 0, u]$
16	c	.3.	x,x,x [u,u,u]	$\bar{x}+1/2, \bar{x}, x+1/2$ $[\bar{u}, \bar{u}, u]$	
			$\bar{x}, x+1/2, \bar{x}+1/2$ $[\bar{u}, u, \bar{u}]$	$x+1/2, \bar{x}+1/2, \bar{x}$ $[u, \bar{u}, \bar{u}]$	
			$x+1/4, x+1/4, x+1/4$ $[\bar{u}, \bar{u}, \bar{u}]$	$\bar{x}+1/4, \bar{x}+3/4, x+3/4$ $[u, u, \bar{u}]$	
			$x+3/4, \bar{x}+1/4, \bar{x}+3/4$ $[\bar{u}, u, u]$	$\bar{x}+3/4, x+3/4, \bar{x}+1/4$ $[u, \bar{u}, u]$	
12	b	$\bar{4}$	7/8,0,1/4 [u,0,0]	5/8,0,3/4 $[\bar{u}, 0, 0]$	1/4,7/8,0 [0,u,0]
			3/4,5/8,0 $[0, \bar{u}, 0]$	0,1/4,7/8 $[0, 0, u]$	0,3/4,5/8 $[0, 0, \bar{u}]$
12	a	$\bar{4}$	3/8,0,1/4 [u,0,0]	1/8,0,3/4 $[\bar{u}, 0, 0]$	1/4,3/8,0 [0,u,0]
			3/4,1/8,0 $[0, \bar{u}, 0]$	0,1/4,3/8 $[0, 0, u]$	0,3/4,1/8 $[0, 0, \bar{u}]$

**Symmetry of Special Projections**

Along [0,0,1]  $p4'gm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,1/4,z

Along [1,1,1]  $p31m$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

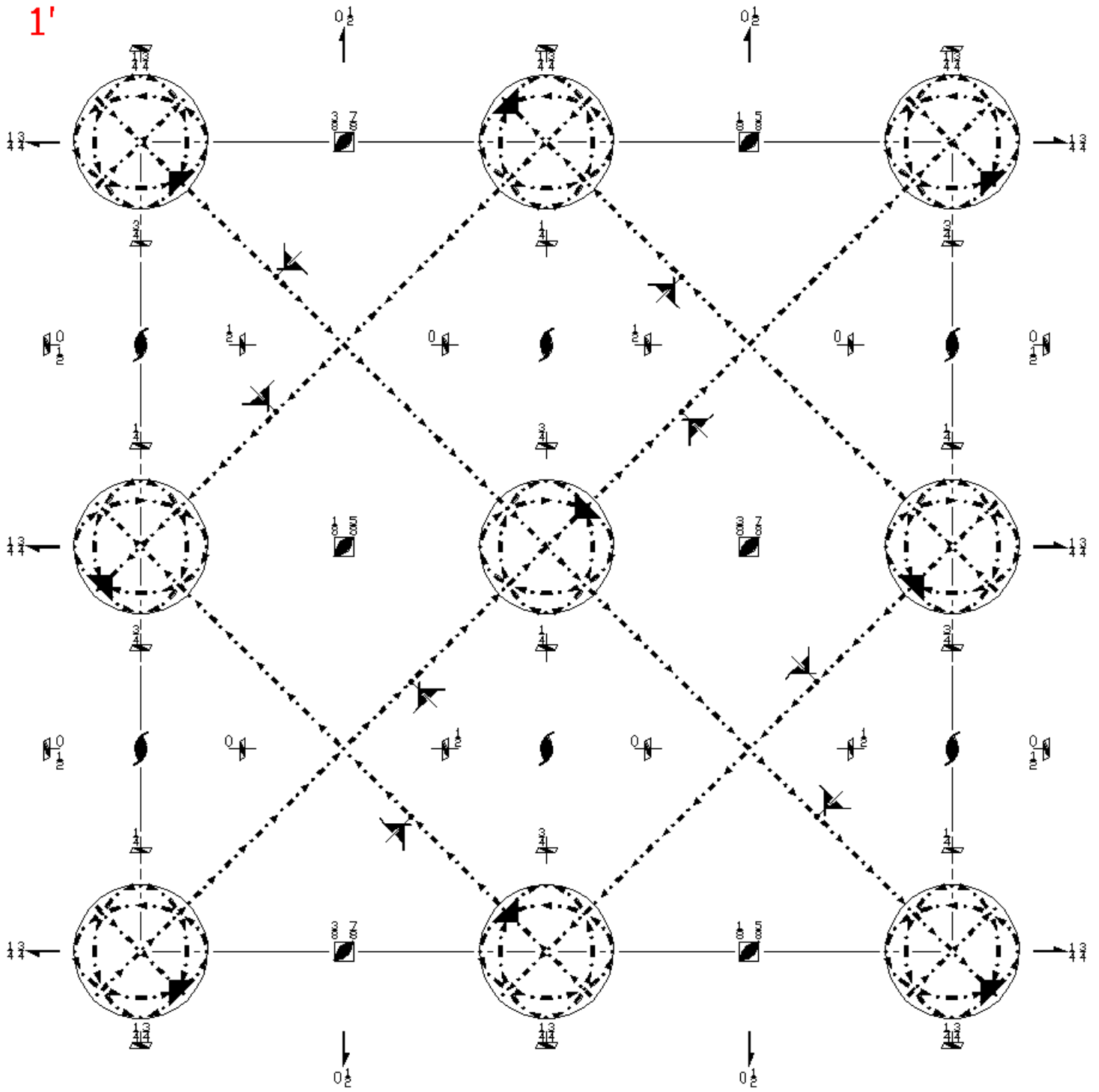
Along [1,1,0]  $c_2'1m1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x+1/4,0



$\bar{4}3d1'$   
220.2.1592

$\bar{4}3m1'$   
 $\bar{4}3d1'$

Cubic



**Origin** on 31' [1,1,1] at midpoint of three non-intersecting pairs of parallel 21' axes and of three non-intersecting pairs of parallel 2,1' axes

**Asymmetric unit**  $1/4 \leq x \leq 1/2$ ;  $1/4 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$ ;  $z \leq \min(x,y)$

Vertices  $1/4, 1/4, 0$   $1/2, 1/4, 0$   $1/2, 1/2, 0$   $1/4, 1/2, 0$   
 $1/4, 1/4, 1/4$   $1/2, 1/4, 1/2$   $1/2, 1/2, 1/2$   $1/4, 1/2, 1/4$

### Symmetry Operations

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) $1/4, 0, z$<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 (0,1/2,0) $0, y, 1/4$<br>(2 <sub>y</sub>  0,1/2,1/2)                                       | (4) 2 (1/2,0,0) $x, 1/4, 0$<br>(2 <sub>x</sub>  1/2,1/2,0)                                       |
| (5) 3 <sup>+</sup> $\bar{x}, x, x$<br>(3 <sub>xyz</sub>  0,0,0)         | (6) 3 <sup>+</sup> $\bar{x}+1/2, x, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0)            | (7) 3 <sup>+</sup> $x+1/2, \bar{x}-1/2, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2)  | (8) 3 <sup>+</sup> $\bar{x}, \bar{x}+1/2, x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)      |
| (9) 3 <sup>-</sup> $x, x, x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> (-1/3, 1/3, 1/3)<br>$x+1/6, \bar{x}+1/6, \bar{x}$<br>(3 <sub>xyz</sub>  0,1/2,1/2) | (11) 3 <sup>-</sup> (1/3, 1/3, -1/3)<br>$x+1/3, \bar{x}+1/6, x$<br>(3 <sub>xyz</sub>  1/2,1/2,0) | (12) 3 <sup>-</sup> (1/3, -1/3, 1/3)<br>$x-1/6, x+1/3, \bar{x}$<br>(3 <sub>xyz</sub>  1/2,0,1/2) |
| (13) d (1/4, 1/4, 1/4) $x, x, z$<br>(m <sub>xy</sub>  1/4,1/4,1/4)      | (14) d (-1/4, 1/4, 3/4) $x+1/2, \bar{x}, z$<br>(m <sub>xy</sub>  1/4,3/4,3/4)                          | (15) $\bar{4}^+$ 1/2, -1/4, z; 1/2, -1/4, 3/8<br>( $\bar{4}_z$  3/4,1/4,3/4)                     | (16) $\bar{4}^-$ 0, 3/4, z; 0, 3/4, 1/8<br>( $\bar{4}_z$ <sup>-1</sup>  3/4,3/4,1/4)             |
| (17) d (1/4, 1/4, 1/4) $x, y, y$<br>(m <sub>yz</sub>  1/4,1/4,1/4)      | (18) $\bar{4}^+$ $x, 1/2, -1/4$ ; 3/8, 1/2, -1/4<br>( $\bar{4}_x$  3/4,3/4,1/4)                        | (19) $\bar{4}^-$ $x, 0, 3/4$ ; 1/8, 0, 3/4<br>( $\bar{4}_x$ <sup>-1</sup>  1/4,3/4,3/4)          | (20) d (3/4, -1/4, 1/4) $x, y+1/2, \bar{y}$<br>(m <sub>yz</sub>  3/4,1/4,3/4)                    |
| (21) d (1/4, 1/4, 1/4) $x, y, x$<br>(m <sub>xz</sub>  1/4,1/4,1/4)      | (22) $\bar{4}^-$ 3/4, y, 0; 3/4, 1/8, 0<br>( $\bar{4}_y$ <sup>-1</sup>  3/4,1/4,3/4)                   | (23) d (1/4, 3/4, -1/4) $\bar{x}+1/2, y, x$<br>(m <sub>xz</sub>  3/4,3/4,1/4)                    | (24) $\bar{4}^+$ -1/4, y, 1/2; -1/4, 3/8, 1/2<br>( $\bar{4}_y$  1/4,3/4,3/4)                     |

For (1/2,1/2,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2, 1/2, 1/2)<br>(1 1/2,1/2,1/2)  | (2) 2 0, 1/4, z<br>(2 <sub>z</sub>  0,1/2,0)  | (3) 2 1/4, y, 0<br>(2 <sub>y</sub>  1/2,0,0)  | (4) 2 x, 0, 1/4<br>(2 <sub>x</sub>  0,0,1/2)  |
| (5) 3 <sup>+</sup> (1/2, 1/2, 1/2) $x, x, x$<br>(3 <sub>xyz</sub>  1/2,1/2,1/2)               | (6) 3 <sup>+</sup> (1/6, -1/6, 1/6)<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,1/2) | (7) 3 <sup>+</sup> (-1/6, 1/6, 1/6)<br>$x+1/6, \bar{x}+1/6, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,0) | (8) 3 <sup>+</sup> (1/6, 1/6, -1/6)<br>$\bar{x}+1/3, \bar{x}+1/6, x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,0) |
| (9) 3 <sup>-</sup> (1/2, 1/2, 1/2) $x, x, x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,1/2) | (10) 3 <sup>-</sup> (1/6, -1/6, -1/6)<br>$x+1/6, \bar{x}+1/6, \bar{x}$<br>(3 <sub>xyz</sub>  1/2,0,0)             | (11) 3 <sup>-</sup> (-1/6, -1/6, 1/6)<br>$x+1/3, \bar{x}+1/6, x$<br>(3 <sub>xyz</sub>  0,0,1/2)                   | (12) 3 <sup>-</sup> (-1/6, 1/6, -1/6)<br>$x-1/6, x+1/3, \bar{x}$<br>(3 <sub>xyz</sub>  0,1/2,0)                   |
| (13) d (3/4, 3/4, 3/4) $x, x, z$<br>(m <sub>xy</sub>  3/4,3/4,3/4)                            | (14) d (1/4, -1/4, 1/4) $x+1/2, \bar{x}, z$<br>(m <sub>xy</sub>  3/4,1/4,1/4)                                     | (15) $\bar{4}^+$ 1/2, 1/4, z; 1/2, 1/4, 1/8<br>( $\bar{4}_z$  1/4,3/4,1/4)  | (16) $\bar{4}^-$ 0, 1/4, z; 0, 1/4, 3/8<br>( $\bar{4}_z$ <sup>-1</sup>  1/4,1/4,3/4)                              |
| (17) d (3/4, 3/4, 3/4) $x, y, y$<br>(m <sub>yz</sub>  3/4,3/4,3/4)                            | (18) $\bar{4}^+$ $x, 1/2, 1/4$ ; 1/8, 1/2, 1/4<br>( $\bar{4}_x$  1/4,1/4,3/4)                                     | (19) $\bar{4}^-$ $x, 0, 1/4$ ; 3/8, 0, 1/4<br>( $\bar{4}_x$ <sup>-1</sup>  3/4,1/4,1/4)                           | (20) d (1/4, 1/4, -1/4) $x, y+1/2, \bar{y}$<br>(m <sub>yz</sub>  1/4,3/4,1/4)                                     |
| (21) d (3/4, 3/4, 3/4) $x, y, x$<br>(m <sub>xz</sub>  3/4,3/4,3/4)                            | (22) $\bar{4}^-$ 1/4, y, 0; 1/4, 0, 3/8<br>( $\bar{4}_y$ <sup>-1</sup>  1/4,3/4,1/4)                              | (23) d (-1/4, 1/4, 1/4) $\bar{x}+1/2, y, x$<br>(m <sub>xz</sub>  1/4,1/4,3/4)                                     | (24) $\bar{4}^+$ 1/4, y, 1/2; 1/4, 1/8, 1/2<br>( $\bar{4}_y$  3/4,1/4,1/4)  |

## For (0,0,0)' + set

- |  |  |  |  |
|--|--|--|--|
| (1) $1'$<br>( $1 0,0,0$ )'   | (2) $2'$ (0,0,1/2) $1/4,0,z$<br>( $2_z 1/2,0,1/2$ )'                                   | (3) $2'$ (0,1/2,0) $0,y,1/4$<br>( $2_y 0,1/2,1/2$ )'                             | (4) $2'$ (1/2,0,0) $x,1/4,0$<br>( $2_x 1/2,1/2,0$ )'                             |
| (5) $3^{+}$ $x,x,x$<br>( $3_{xyz} 0,0,0$ )'                        | (6) $3^{+}$ $\bar{x}+1/2,x,\bar{x}$<br>( $3_{xyz}^{-1} 1/2,1/2,0$ )'                   | (7) $3^{+}$ $x+1/2,\bar{x}-1/2,\bar{x}$<br>( $3_{xyz}^{-1} 1/2,0,1/2$ )'         | (8) $3^{+}$ $\bar{x},\bar{x}+1/2,x$<br>( $3_{xyz}^{-1} 0,1/2,1/2$ )'             |
| (9) $3^{-}$ $x,x,x$<br>( $3_{xyz}^{-1} 0,0,0$ )'                   | (10) $3^{-}$ (-1/3,1/3,1/3)<br>$x+1/6,\bar{x}+1/6,\bar{x}$<br>( $3_{xyz} 0,1/2,1/2$ )' | (11) $3^{-}$ (1/3,1/3,-1/3)<br>$x+1/3,\bar{x}+1/6,x$<br>( $3_{xyz} 1/2,1/2,0$ )' | (12) $3^{-}$ (1/3,-1/3,1/3)<br>$x-1/6,x+1/3,\bar{x}$<br>( $3_{xyz} 1/2,0,1/2$ )' |
| (13) $d'$ (1/4,1/4,1/4) $x,x,z$<br>( $m_{\bar{xy}} 1/4,1/4,1/4$ )' | (14) $d'$ (-1/4,1/4,3/4) $x+1/2,\bar{x},z$<br>( $m_{xy} 1/4,3/4,3/4$ )'                | (15) $\bar{4}^{+}$ $1/2,-1/4,z; 1/2,-1/4,3/8$<br>( $\bar{4}_z 3/4,1/4,3/4$ )'    | (16) $\bar{4}^{-}$ $0,3/4,z; 0,3/4,1/8$<br>( $\bar{4}_z^{-1} 3/4,3/4,1/4$ )'     |
| (17) $d'$ (1/4,1/4,1/4) $x,y,y$<br>( $m_{\bar{yz}} 1/4,1/4,1/4$ )' | (18) $\bar{4}^{+}$ $x,1/2,-1/4; 3/8,1/2,-1/4$<br>( $\bar{4}_x 3/4,3/4,1/4$ )'          | (19) $\bar{4}^{-}$ $x,0,3/4; 1/8,0,3/4$<br>( $\bar{4}_x^{-1} 1/4,3/4,3/4$ )'     | (20) $d'$ (3/4,-1/4,1/4) $x,y+1/2,\bar{y}$<br>( $m_{yz} 3/4,1/4,3/4$ )'          |
| (21) $d'$ (1/4,1/4,1/4) $x,y,x$<br>( $m_{\bar{zx}} 1/4,1/4,1/4$ )' | (22) $\bar{4}^{-}$ $3/4,y,0; 3/4,1/8,0$<br>( $\bar{4}_y^{-1} 3/4,1/4,3/4$ )'           | (23) $d'$ (1/4,3/4,-1/4) $\bar{x}+1/2,y,x$<br>( $m_{xz} 3/4,3/4,1/4$ )'          | (24) $\bar{4}^{+}$ $-1/4,y,1/2; -1/4,3/8,1/2$<br>( $\bar{4}_y 1/4,3/4,3/4$ )'    |

## For (1/2,1/2,1/2)' + set

- |  |   |  |  |
|--|---|--|--|
| (1) $t'$ (1/2,1/2,1/2)<br>( $1 1/2,1/2,1/2$ )'                       | (2) $2'$ $0,1/4,z$<br>( $2_z 0,1/2,0$ )'  | (3) $2'$ $1/4,y,0$<br>( $2_y 1/2,0,0$ )'   | (4) $2'$ $x,0,1/4$<br>( $2_x 0,0,1/2$ )'   |
| (5) $3^{+}$ (1/2,1/2,1/2) $x,x,x$<br>( $3_{xyz} 1/2,1/2,1/2$ )'      | (6) $3^{+}$ (1/6,-1/6,1/6)<br>$x-1/6,x+1/3,\bar{x}$<br>( $3_{xyz}^{-1} 0,0,1/2$ )'    | (7) $3^{+}$ (-1/6,1/6,1/6)<br>$x+1/6,\bar{x}+1/6,\bar{x}$<br>( $3_{xyz}^{-1} 0,1/2,0$ )' | (8) $3^{+}$ (1/6,1/6,-1/6)<br>$x+1/3,\bar{x}+1/6,x$<br>( $3_{xyz}^{-1} 1/2,0,0$ )' |
| (9) $3^{-}$ (1/2,1/2,1/2) $x,x,x$<br>( $3_{xyz}^{-1} 1/2,1/2,1/2$ )' | (10) $3^{-}$ (1/6,-1/6,-1/6)<br>$x+1/6,\bar{x}+1/6,\bar{x}$<br>( $3_{xyz} 1/2,0,0$ )' | (11) $3^{-}$ (-1/6,-1/6,1/6)<br>$x+1/3,\bar{x}+1/6,x$<br>( $3_{xyz} 0,0,1/2$ )'          | (12) $3^{-}$ (-1/6,1/6,-1/6)<br>$x-1/6,x+1/3,\bar{x}$<br>( $3_{xyz} 0,1/2,0$ )'    |
| (13) $d'$ (3/4,3/4,3/4) $x,x,z$<br>( $m_{\bar{xy}} 3/4,3/4,3/4$ )'   | (14) $d'$ (1/4,-1/4,1/4) $x+1/2,\bar{x},z$<br>( $m_{xy} 3/4,1/4,1/4$ )'               | (15) $\bar{4}^{+}$ $1/2,1/4,z; 1/2,1/4,1/8$<br>( $\bar{4}_z 1/4,3/4,1/4$ )'              | (16) $\bar{4}^{-}$ $0,1/4,z; 0,1/4,3/8$<br>( $\bar{4}_z^{-1} 1/4,1/4,3/4$ )'       |
| (17) $d'$ (3/4,3/4,3/4) $x,y,y$<br>( $m_{\bar{yz}} 3/4,3/4,3/4$ )'   | (18) $\bar{4}^{+}$ $x,1/2,1/4; 1/8,1/2,1/4$<br>( $\bar{4}_x 1/4,1/4,3/4$ )'           | (19) $\bar{4}^{-}$ $x,0,1/4; 3/8,0,1/4$<br>( $\bar{4}_x^{-1} 3/4,1/4,1/4$ )'             | (20) $d'$ (1/4,1/4,-1/4) $x,y+1/2,\bar{y}$<br>( $m_{yz} 1/4,3/4,1/4$ )'            |
| (21) $d'$ (3/4,3/4,3/4) $x,y,x$<br>( $m_{\bar{zx}} 3/4,3/4,3/4$ )'   | (22) $\bar{4}^{-}$ $1/4,y,0; 1/4,0,3/8$<br>( $\bar{4}_y^{-1} 1/4,3/4,1/4$ )'          | (23) $d'$ (-1/4,1/4,1/4) $\bar{x}+1/2,y,x$<br>( $m_{xz} 1/4,1/4,3/4$ )'                  | (24) $\bar{4}^{+}$ $1/4,y,1/2; 1/4,1/8,1/2$<br>( $\bar{4}_y 3/4,1/4,1/4$ )'        |

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,1/2)$ ; (2); (3); (5); (13);  $1'$ .

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

48 e 11'

(0,0,0) + (1/2,1/2,1/2) +  
(0,0,0)' + (1/2,1/2,1/2)' +

- |                     |   |   |   |
|---------------------|---|---|---|
| (1) $x,y,z$ [0,0,0] | (2) $\bar{x}+1/2,\bar{y},z+1/2$ [0,0,0] | (3) $\bar{x},y+1/2,\bar{z}+1/2$ [0,0,0] | (4) $x+1/2,\bar{y}+1/2,\bar{z}$ [0,0,0] |
| (5) $z,x,y$ [0,0,0] | (6) $z+1/2,\bar{x}+1/2,\bar{y}$ [0,0,0] | (7) $\bar{z}+1/2,\bar{x},y+1/2$ [0,0,0] | (8) $\bar{z},x+1/2,\bar{y}+1/2$ [0,0,0] |

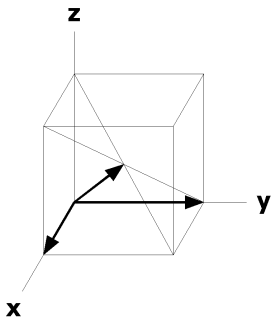
(9) $y, z, x [0,0,0]$	(10) $\bar{y}, z+1/2, \bar{x}+1/2 [0,0,0]$	(11) $y+1/2, \bar{z}+1/2, \bar{x} [0,0,0]$	(12) $\bar{y}+1/2, \bar{z}, x+1/2 [0,0,0]$		
(13) $y+1/4, x+1/4, z+1/4 [0,0,0]$	(14) $\bar{y}+1/4, \bar{x}+3/4, z+3/4 [0,0,0]$	(15) $y+3/4, \bar{x}+1/4, \bar{z}+3/4 [0,0,0]$	(16) $\bar{y}+3/4, x+3/4, \bar{z}+1/4 [0,0,0]$		
(17) $x+1/4, z+1/4, y+1/4 [0,0,0]$	(18) $\bar{x}+3/4, z+3/4, \bar{y}+1/4 [0,0,0]$	(19) $\bar{x}+1/4, \bar{z}+3/4, y+3/4 [0,0,0]$	(20) $x+3/4, \bar{z}+1/4, \bar{y}+3/4 [0,0,0]$		
(21) $z+1/4, y+1/4, x+1/4 [0,0,0]$	(22) $z+3/4, \bar{y}+1/4, \bar{x}+3/4 [0,0,0]$	(23) $\bar{z}+3/4, y+3/4, \bar{x}+1/4 [0,0,0]$	(24) $\bar{z}+1/4, \bar{y}+3/4, x+3/4 [0,0,0]$		
24	d	2..1'	$x, 0, 1/4 [0,0,0]$ $3/4, \bar{x}+1/2, 0 [0,0,0]$ $1/4, x+1/4, 1/2 [0,0,0]$ $\bar{x}+3/4, 0, 1/4 [0,0,0]$	$\bar{x}+1/2, 0, 3/4 [0,0,0]$ $0, 1/4, x [0,0,0]$ $1/4, \bar{x}+3/4, 0 [0,0,0]$ $1/2, 1/4, x+1/4 [0,0,0]$	$1/4, x, 0 [0,0,0]$ $0, 3/4, \bar{x}+1/2 [0,0,0]$ $x+1/4, 1/2, 1/4 [0,0,0]$ $0, 1/4, \bar{x}+3/4 [0,0,0]$
16	c	.3.1'	$x, x, x [0,0,0]$ $\bar{x}, x+1/2, \bar{x}+1/2 [0,0,0]$ $x+1/4, x+1/4, x+1/4 [0,0,0]$ $x+3/4, \bar{x}+1/4, \bar{x}+3/4 [0,0,0]$	$\bar{x}+1/2, \bar{x}, x+1/2 [0,0,0]$ $x+1/2, \bar{x}+1/2, \bar{x} [0,0,0]$ $\bar{x}+1/4, \bar{x}+3/4, x+3/4 [0,0,0]$ $\bar{x}+3/4, x+3/4, \bar{x}+1/4 [0,0,0]$	
12	b	$\bar{4}1'$	$7/8, 0, 1/4 [0,0,0]$ $3/4, 5/8, 0 [0,0,0]$	$5/8, 0, 3/4 [0,0,0]$ $0, 1/4, 7/8 [0,0,0]$	$1/4, 7/8, 0 [0,0,0]$ $0, 3/4, 5/8 [0,0,0]$
12	a	$\bar{4}1'$	$3/8, 0, 1/4 [0,0,0]$ $3/4, 1/8, 0 [0,0,0]$	$1/8, 0, 3/4 [0,0,0]$ $0, 1/4, 3/8 [0,0,0]$	$1/4, 3/8, 0 [0,0,0]$ $0, 3/4, 1/8 [0,0,0]$

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4gm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0, 1/4, z$

Along  $[1,1,1]$   $p31m1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

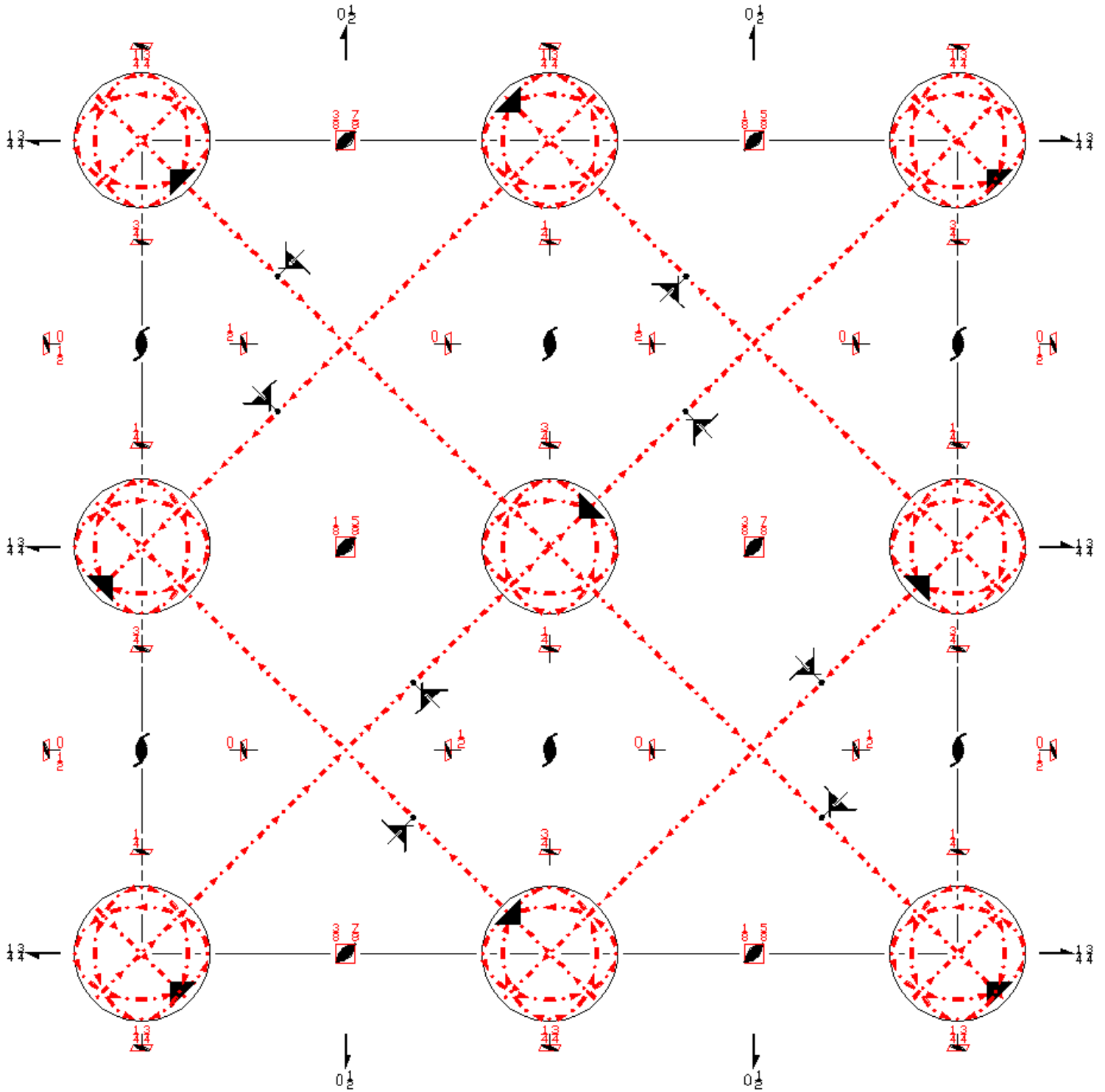
Along  $[1,1,0]$   $c1m11'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, x+1/4, 0$



$\bar{4}3d'$   
220.3.1593

$\bar{4}3m'$   
 $\bar{4}3d'$

Cubic





**Origin** on 3 [1,1,1] at midpoint of three non-intersecting pairs of parallel 2 axes and of three non-intersecting pairs of parallel 2<sub>1</sub> axes

**Asymmetric unit**  $1/4 \leq x \leq 1/2$ ;  $1/4 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$ ;  $z \leq \min(x,y)$

Vertices  $1/4, 1/4, 0$   $1/2, 1/4, 0$   $1/2, 1/2, 0$   $1/4, 1/2, 0$   
 $1/4, 1/4, 1/4$   $1/2, 1/4, 1/2$   $1/2, 1/2, 1/2$   $1/4, 1/2, 1/4$

### Symmetry Operations

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) $1/4, 0, z$<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 (0,1/2,0) $0, y, 1/4$<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2 (1/2,0,0) $x, 1/4, 0$<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) 3 <sup>+</sup> $\bar{x}, x, x$<br>(3 <sub>xyz</sub>  0,0,0)         | (6) 3 <sup>+</sup> $\bar{x}+1/2, x, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0)            | (7) 3 <sup>+</sup> $x+1/2, \bar{x}-1/2, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2)        | (8) 3 <sup>+</sup> $\bar{x}, \bar{x}+1/2, x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)            |
| (9) 3 <sup>-</sup> $x, x, x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> (-1/3, 1/3, 1/3)<br>$x+1/6, \bar{x}+1/6, \bar{x}$<br>(3 <sub>xyz</sub>  0,1/2,1/2) | (11) 3 <sup>-</sup> (1/3, 1/3, -1/3)<br>$\bar{x}+1/3, \bar{x}+1/6, x$<br>(3 <sub>xyz</sub>  1/2,1/2,0) | (12) 3 <sup>-</sup> (1/3, -1/3, 1/3)<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>(3 <sub>xyz</sub>  1/2,0,1/2) |
| (13) d' (1/4, 1/4, 1/4) $x, x, z$<br>(m <sub>xy</sub>  1/4, 1/4, 1/4)'  | (14) d' (-1/4, 1/4, 3/4) $x+1/2, \bar{x}, z$<br>(m <sub>xy</sub>  1/4, 3/4, 3/4)'                      | (15) $\bar{4}^+$ ' 1/2, -1/4, z; 1/2, -1/4, 3/8<br>( $\bar{4}_z$  3/4, 1/4, 3/4)'                      | (16) $\bar{4}^-$ ' 0, 3/4, z; 0, 3/4, 1/8<br>( $\bar{4}_z$ <sup>-1</sup>  3/4, 3/4, 1/4)'              |
| (17) d' (1/4, 1/4, 1/4) $x, y, y$<br>(m <sub>yz</sub>  1/4, 1/4, 1/4)'  | (18) $\bar{4}^+$ ' $x, 1/2, -1/4$ ; 3/8, 1/2, -1/4<br>( $\bar{4}_x$  3/4, 3/4, 1/4)'                   | (19) $\bar{4}^-$ ' $x, 0, 3/4$ ; 1/8, 0, 3/4<br>( $\bar{4}_x$ <sup>-1</sup>  1/4, 3/4, 3/4)'           | (20) d' (3/4, -1/4, 1/4) $x, y+1/2, \bar{y}$<br>(m <sub>yz</sub>  3/4, 1/4, 3/4)'                      |
| (21) d' (1/4, 1/4, 1/4) $x, y, x$<br>(m <sub>xz</sub>  1/4, 1/4, 1/4)'  | (22) $\bar{4}^-$ ' 3/4, y, 0; 3/4, 1/8, 0<br>( $\bar{4}_y$ <sup>-1</sup>  3/4, 1/4, 3/4)'              | (23) d' (1/4, 3/4, -1/4) $\bar{x}+1/2, y, x$<br>(m <sub>xz</sub>  3/4, 3/4, 1/4)'                      | (24) $\bar{4}^+$ ' -1/4, y, 1/2; -1/4, 3/8, 1/2<br>( $\bar{4}_y$  1/4, 3/4, 3/4)'                      |

For (1/2,1/2,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2, 1/2, 1/2)<br>(1 1/2, 1/2, 1/2)  | (2) 2 0, 1/4, z<br>(2 <sub>z</sub>  0, 1/2, 0)  | (3) 2 1/4, y, 0<br>(2 <sub>y</sub>  1/2, 0, 0)  | (4) 2 x, 0, 1/4<br>(2 <sub>x</sub>  0, 0, 1/2)  |
| (5) 3 <sup>+</sup> (1/2, 1/2, 1/2) $x, x, x$<br>(3 <sub>xyz</sub>  1/2, 1/2, 1/2)               | (6) 3 <sup>+</sup> (1/6, -1/6, 1/6)<br>$\bar{x}-1/6, \bar{x}+1/3, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0, 0, 1/2) | (7) 3 <sup>+</sup> (-1/6, 1/6, 1/6)<br>$\bar{x}+1/6, \bar{x}+1/6, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0, 1/2, 0) | (8) 3 <sup>+</sup> (1/6, 1/6, -1/6)<br>$\bar{x}+1/3, \bar{x}+1/6, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2, 0, 0) |
| (9) 3 <sup>-</sup> (1/2, 1/2, 1/2) $x, x, x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2, 1/2, 1/2) | (10) 3 <sup>-</sup> (1/6, -1/6, -1/6)<br>$\bar{x}+1/6, \bar{x}+1/6, \bar{x}$<br>(3 <sub>xyz</sub>  1/2, 0, 0)             | (11) 3 <sup>-</sup> (-1/6, -1/6, 1/6)<br>$\bar{x}+1/3, \bar{x}+1/6, \bar{x}$<br>(3 <sub>xyz</sub>  0, 0, 1/2)             | (12) 3 <sup>-</sup> (-1/6, 1/6, -1/6)<br>$\bar{x}-1/6, \bar{x}+1/3, \bar{x}$<br>(3 <sub>xyz</sub>  0, 1/2, 0)             |
| (13) d' (3/4, 3/4, 3/4) $x, x, z$<br>(m <sub>xy</sub>  3/4, 3/4, 3/4)'                          | (14) d' (1/4, -1/4, 1/4) $x+1/2, \bar{x}, z$<br>(m <sub>xy</sub>  3/4, 1/4, 1/4)'   | (15) $\bar{4}^+$ ' 1/2, 1/4, z; 1/2, 1/4, 1/8<br>( $\bar{4}_z$  1/4, 3/4, 1/4)'   | (16) $\bar{4}^-$ ' 0, 1/4, z; 0, 1/4, 3/8<br>( $\bar{4}_z$ <sup>-1</sup>  1/4, 1/4, 3/4)'                                 |
| (17) d' (3/4, 3/4, 3/4) $x, y, y$<br>(m <sub>yz</sub>  3/4, 3/4, 3/4)'                          | (18) $\bar{4}^+$ ' $x, 1/2, 1/4$ ; 1/8, 1/2, 1/4<br>( $\bar{4}_x$  1/4, 1/4, 3/4)'  | (19) $\bar{4}^-$ ' $x, 0, 1/4$ ; 3/8, 0, 1/4<br>( $\bar{4}_x$ <sup>-1</sup>  3/4, 1/4, 1/4)'                              | (20) d' (1/4, 1/4, -1/4) $x, y+1/2, \bar{y}$<br>(m <sub>yz</sub>  1/4, 3/4, 1/4)'   |
| (21) d' (3/4, 3/4, 3/4) $x, y, x$<br>(m <sub>xz</sub>  3/4, 3/4, 3/4)'                          | (22) $\bar{4}^-$ ' 1/4, y, 0; 1/4, 0, 3/8<br>( $\bar{4}_y$ <sup>-1</sup>  1/4, 3/4, 1/4)'                                 | (23) d' (-1/4, 1/4, 1/4) $\bar{x}+1/2, y, x$<br>(m <sub>xz</sub>  1/4, 1/4, 3/4)'   | (24) $\bar{4}^+$ ' 1/4, y, 1/2; 1/4, 1/8, 1/2<br>( $\bar{4}_y$  3/4, 1/4, 1/4)'   |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

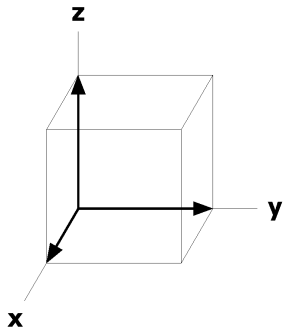
				(0,0,0) +	(1/2,1/2,1/2) +						
48	e	1									
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}+1/2, \bar{y}, z+1/2$	$[\bar{u}, \bar{v}, w]$	(3)	$\bar{x}, y+1/2, \bar{z}+1/2$	$[\bar{u}, v, \bar{w}]$	(4)	$x+1/2, \bar{y}+1/2, \bar{z}$	$[u, \bar{v}, \bar{w}]$
(5)	z,x,y	[w,u,v]	(6)	$z+1/2, \bar{x}+1/2, \bar{y}$	$[w, \bar{u}, \bar{v}]$	(7)	$\bar{z}+1/2, \bar{x}, y+1/2$	$[\bar{w}, \bar{u}, v]$	(8)	$\bar{z}, x+1/2, \bar{y}+1/2$	$[\bar{w}, u, \bar{v}]$
(9)	y,z,x	[v,w,u]	(10)	$\bar{y}, z+1/2, \bar{x}+1/2$	$[\bar{v}, w, \bar{u}]$	(11)	$y+1/2, \bar{z}+1/2, \bar{x}$	$[v, \bar{w}, \bar{u}]$	(12)	$\bar{y}+1/2, \bar{z}, x+1/2$	$[\bar{v}, \bar{w}, u]$
(13)	$y+1/4, x+1/4, z+1/4$	$[v, u, w]$	(14)	$\bar{y}+1/4, \bar{x}+3/4, z+3/4$	$[\bar{v}, \bar{u}, w]$	(15)	$y+3/4, \bar{x}+1/4, \bar{z}+3/4$	$[v, \bar{u}, \bar{w}]$	(16)	$\bar{y}+3/4, x+3/4, \bar{z}+1/4$	$[\bar{v}, u, \bar{w}]$
(17)	$x+1/4, z+1/4, y+1/4$	$[u, w, v]$	(18)	$\bar{x}+3/4, z+3/4, \bar{y}+1/4$	$[\bar{u}, w, \bar{v}]$	(19)	$\bar{x}+1/4, \bar{z}+3/4, y+3/4$	$[\bar{u}, \bar{w}, v]$	(20)	$x+3/4, \bar{z}+1/4, \bar{y}+3/4$	$[u, \bar{w}, \bar{v}]$
(21)	$z+1/4, y+1/4, x+1/4$	$[w, v, u]$	(22)	$z+3/4, \bar{y}+1/4, \bar{x}+3/4$	$[w, \bar{v}, \bar{u}]$	(23)	$\bar{z}+3/4, y+3/4, \bar{x}+1/4$	$[\bar{w}, v, \bar{u}]$	(24)	$\bar{z}+1/4, \bar{y}+3/4, x+3/4$	$[\bar{w}, \bar{v}, u]$
24	d	2..	$x, 0, 1/4$	$[u, 0, 0]$	$\bar{x}+1/2, 0, 3/4$	$[\bar{u}, 0, 0]$	$1/4, x, 0$	$[0, u, 0]$			
			$3/4, \bar{x}+1/2, 0$	$[0, \bar{u}, 0]$	$0, 1/4, x$	$[0, 0, u]$	$0, 3/4, \bar{x}+1/2$	$[0, 0, \bar{u}]$			
			$1/4, x+1/4, 1/2$	$[0, u, 0]$	$1/4, \bar{x}+3/4, 0$	$[0, \bar{u}, 0]$	$x+1/4, 1/2, 1/4$	$[u, 0, 0]$			
			$\bar{x}+3/4, 0, 1/4$	$[\bar{u}, 0, 0]$	$1/2, 1/4, x+1/4$	$[0, 0, u]$	$0, 1/4, \bar{x}+3/4$	$[0, 0, \bar{u}]$			
16	c	.3.	$x, x, x$	$[u, u, u]$	$\bar{x}+1/2, \bar{x}, x+1/2$	$[\bar{u}, \bar{u}, u]$					
			$\bar{x}, x+1/2, \bar{x}+1/2$	$[\bar{u}, u, \bar{u}]$	$x+1/2, \bar{x}+1/2, \bar{x}$	$[u, \bar{u}, \bar{u}]$					
			$x+1/4, x+1/4, x+1/4$	$[u, u, u]$	$\bar{x}+1/4, \bar{x}+3/4, x+3/4$	$[\bar{u}, \bar{u}, u]$					
			$x+3/4, \bar{x}+1/4, \bar{x}+3/4$	$[u, \bar{u}, \bar{u}]$	$\bar{x}+3/4, x+3/4, \bar{x}+1/4$	$[\bar{u}, u, \bar{u}]$					
12	b	$\bar{4}'$	$7/8, 0, 1/4$	$[0, 0, 0]$	$5/8, 0, 3/4$	$[0, 0, 0]$	$1/4, 7/8, 0$	$[0, 0, 0]$			
			$3/4, 5/8, 0$	$[0, 0, 0]$	$0, 1/4, 7/8$	$[0, 0, 0]$	$0, 3/4, 5/8$	$[0, 0, 0]$			
12	a	$\bar{4}'$	$3/8, 0, 1/4$	$[0, 0, 0]$	$1/8, 0, 3/4$	$[0, 0, 0]$	$1/4, 3/8, 0$	$[0, 0, 0]$			
			$3/4, 1/8, 0$	$[0, 0, 0]$	$0, 1/4, 3/8$	$[0, 0, 0]$	$0, 3/4, 1/8$	$[0, 0, 0]$			

**Symmetry of Special Projections**

Along  $[0, 0, 1]$   $p4g'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0, 1/4, z$

Along  $[1, 1, 1]$   $p31m'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

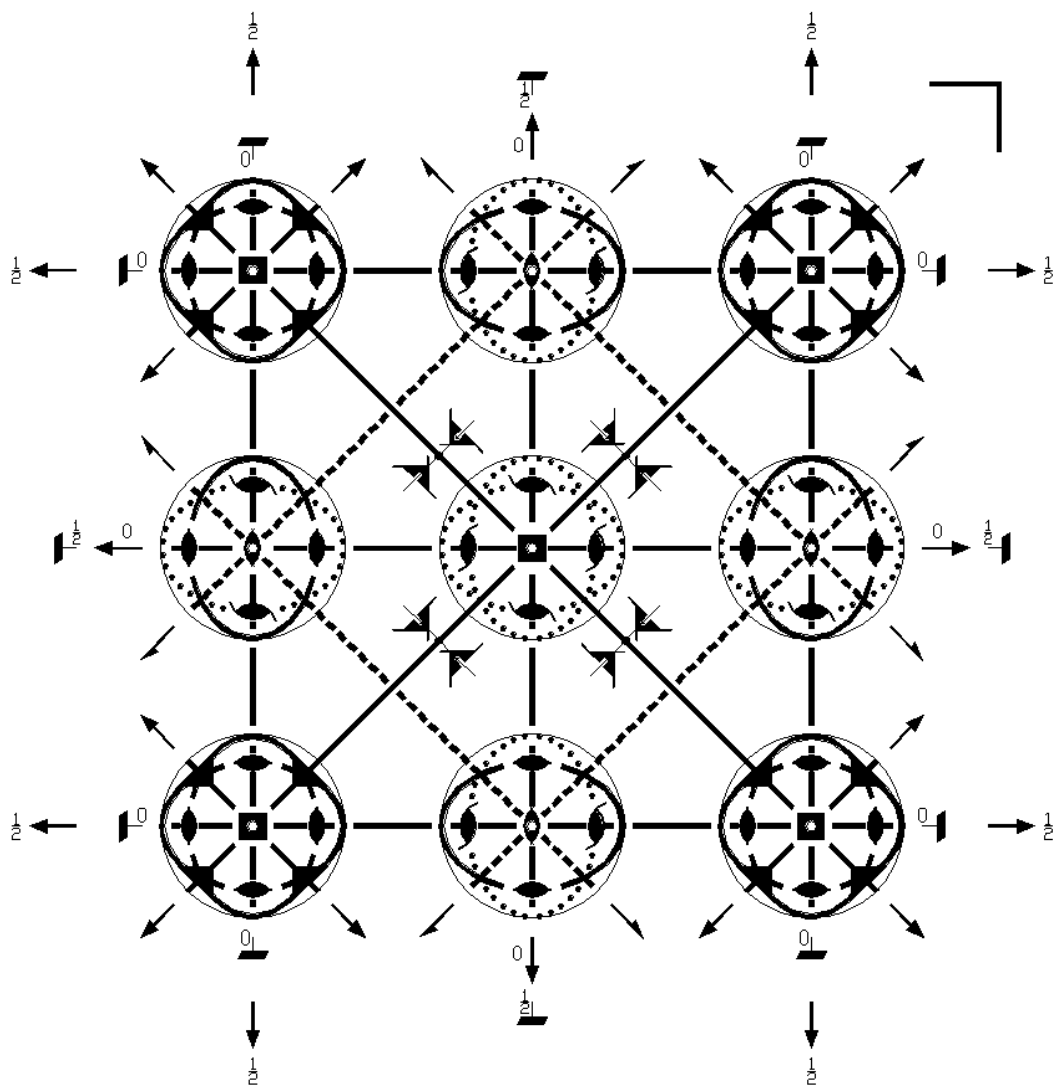
Along  $[1, 1, 0]$   $c1m'1$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, x+1/4, 0$



$Pm\bar{3}m$   
221.1.1594

$m\bar{3}m$   
 $P4/m\bar{3}2/m$

Cubic



**Origin** at center ( $m\bar{3}m$ )

<b>Asymmetric unit</b>	$0 \leq x \leq 1/2;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$y \leq x;$	$z \leq y$
<b>Vertices</b>	0,0,0	1/2,0,0	1/2,1/2,0	1/2,1/2,1/2	

**Symmetry Operations**

- |   |  |  |   |
|---|--|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>xyz</sub>  0,0,0)              | (12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)               |

(13) $2 \ x,x,0$ ( $2_{xy} 0,0,0$ )	(14) $2 \ x,\bar{x},0$ ( $2_{\bar{xy}} 0,0,0$ )	(15) $4^- \ 0,0,z$ ( $4_z^{-1} 0,0,0$ )	(16) $4^+ \ 0,0,z$ ( $4_z 0,0,0$ )
(17) $4^- \ x,0,0$ ( $4_x^{-1} 0,0,0$ )	(18) $2 \ 0,y,y$ ( $2_{yz} 0,0,0$ )	(19) $2 \ 0,y,\bar{y}$ ( $2_{\bar{yz}} 0,0,0$ )	(20) $4^+ \ x,0,0$ ( $4_x 0,0,0$ )
(21) $4^+ \ 0,y,0$ ( $4_y 0,0,0$ )	(22) $2 \ x,0,x$ ( $2_{xz} 0,0,0$ )	(23) $4^- \ 0,y,0$ ( $4_y^{-1} 0,0,0$ )	(24) $2 \ \bar{x},0,x$ ( $2_{\bar{xz}} 0,0,0$ )
(25) $\bar{1} \ 0,0,0$ ( $\bar{1} 0,0,0$ )	(26) $m \ x,y,0$ ( $m_z 0,0,0$ )	(27) $m \ x,0,z$ ( $m_y 0,0,0$ )	(28) $m \ 0,y,z$ ( $m_x 0,0,0$ )
(29) $\bar{3}^+ \ x,x,x; 0,0,0$ ( $\bar{3}_{xyz} 0,0,0$ )	(30) $\bar{3}^+ \ \bar{x},x,\bar{x}; 0,0,0$ ( $\bar{3}_{x\bar{y}\bar{z}^{-1}} 0,0,0$ )	(31) $\bar{3}^+ \ x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{y}\bar{z}^{-1}} 0,0,0$ )	(32) $\bar{3}^+ \ \bar{x},\bar{x},x; 0,0,0$ ( $\bar{3}_{x\bar{y}\bar{z}^{-1}} 0,0,0$ )
(33) $\bar{3}^- \ x,x,x; 0,0,0$ ( $\bar{3}_{xyz^{-1}} 0,0,0$ )	(34) $\bar{3}^- \ x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{y}\bar{z}} 0,0,0$ )	(35) $\bar{3}^- \ \bar{x},\bar{x},x; 0,0,0$ ( $\bar{3}_{\bar{y}\bar{z}} 0,0,0$ )	(36) $\bar{3}^- \ \bar{x},x,\bar{x}; 0,0,0$ ( $\bar{3}_{x\bar{y}\bar{z}} 0,0,0$ )
(37) $m \ x,\bar{x},z$ ( $m_{xy} 0,0,0$ )	(38) $m \ x,x,z$ ( $m_{\bar{xy}} 0,0,0$ )	(39) $\bar{4}^- \ 0,0,z; 0,0,0$ ( $\bar{4}_z^{-1} 0,0,0$ )	(40) $\bar{4}^+ \ 0,0,z; 0,0,0$ ( $\bar{4}_z 0,0,0$ )
(41) $\bar{4}^- \ x,0,0; 0,0,0$ ( $\bar{4}_x^{-1} 0,0,0$ )	(42) $m \ x,y,\bar{y}$ ( $m_{yz} 0,0,0$ )	(43) $m \ x,y,y$ ( $m_{\bar{yz}} 0,0,0$ )	(44) $\bar{4}^+ \ x,0,0; 0,0,0$ ( $\bar{4}_x 0,0,0$ )
(45) $\bar{4}^+ \ 0,y,0; 0,0,0$ ( $\bar{4}_y 0,0,0$ )	(46) $m \ \bar{x},y,x$ ( $m_{xz} 0,0,0$ )	(47) $\bar{4}^- \ 0,y,0; 0,0,0$ ( $\bar{4}_y^{-1} 0,0,0$ )	(48) $m \ x,y,x$ ( $m_{\bar{xz}} 0,0,0$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

48 n 1

### Coordinates

(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $\bar{x},y,\bar{z} [\bar{u},v,\bar{w}]$	(4) $x,\bar{y},\bar{z} [u,\bar{v},\bar{w}]$
(5) $z,x,y [w,u,v]$	(6) $z,\bar{x},\bar{y} [w,\bar{u},\bar{v}]$	(7) $\bar{z},\bar{x},y [\bar{w},\bar{u},v]$	(8) $\bar{z},x,\bar{y} [\bar{w},u,\bar{v}]$
(9) $y,z,x [v,w,u]$	(10) $\bar{y},z,\bar{x} [\bar{v},w,\bar{u}]$	(11) $y,\bar{z},\bar{x} [v,\bar{w},\bar{u}]$	(12) $\bar{y},\bar{z},x [\bar{v},\bar{w},u]$
(13) $y,x,\bar{z} [v,u,\bar{w}]$	(14) $\bar{y},\bar{x},\bar{z} [\bar{v},\bar{u},\bar{w}]$	(15) $y,\bar{x},z [v,\bar{u},w]$	(16) $\bar{y},x,z [\bar{v},u,w]$
(17) $x,z,\bar{y} [u,w,\bar{v}]$	(18) $\bar{x},z,y [\bar{u},w,v]$	(19) $\bar{x},\bar{z},\bar{y} [\bar{u},\bar{w},\bar{v}]$	(20) $x,\bar{z},y [u,\bar{w},v]$
(21) $z,y,\bar{x} [w,v,\bar{u}]$	(22) $z,\bar{y},x [w,\bar{v},u]$	(23) $\bar{z},y,x [\bar{w},v,u]$	(24) $\bar{z},\bar{y},\bar{x} [\bar{w},\bar{v},\bar{u}]$
(25) $\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$	(26) $x,y,\bar{z} [u,v,w]$	(27) $x,\bar{y},z [u,\bar{v},w]$	(28) $\bar{x},y,z [\bar{u},v,\bar{w}]$
(29) $\bar{z},\bar{x},\bar{y} [\bar{w},\bar{u},\bar{v}]$	(30) $\bar{z},x,y [w,\bar{u},v]$	(31) $z,x,\bar{y} [\bar{w},\bar{u},v]$	(32) $z,\bar{x},y [w,\bar{u},\bar{v}]$
(33) $\bar{y},\bar{z},\bar{x} [\bar{v},\bar{w},\bar{u}]$	(34) $y,\bar{z},x [v,\bar{w},u]$	(35) $\bar{y},z,x [\bar{v},w,u]$	(36) $y,z,\bar{x} [v,w,\bar{u}]$

(37)	$\bar{y}, \bar{x}, z$	$[v, u, \bar{w}]$	(38)	$y, x, z$	$[\bar{v}, \bar{u}, \bar{w}]$	(39)	$\bar{y}, x, \bar{z}$	$[v, \bar{u}, w]$	(40)	$y, \bar{x}, \bar{z}$	$[\bar{v}, u, w]$	
(41)	$\bar{x}, \bar{z}, y$	$[u, w, \bar{v}]$	(42)	$x, \bar{z}, y$	$[\bar{u}, w, v]$	(43)	$x, z, y$	$[\bar{u}, \bar{w}, \bar{v}]$	(44)	$\bar{x}, z, y$	$[u, \bar{w}, v]$	
(45)	$\bar{z}, \bar{y}, x$	$[w, v, \bar{u}]$	(46)	$\bar{z}, y, \bar{x}$	$[w, \bar{v}, u]$	(47)	$z, y, \bar{x}$	$[\bar{w}, v, u]$	(48)	$z, y, x$	$[\bar{w}, \bar{v}, \bar{u}]$	
24	m	..m	$x, x, z$	$[u, \bar{u}, 0]$	$\bar{x}, \bar{x}, z$	$[\bar{u}, u, 0]$	$\bar{x}, x, \bar{z}$	$[\bar{u}, \bar{u}, 0]$	$x, \bar{x}, \bar{z}$	$[u, u, 0]$	$x, \bar{x}, \bar{z}$	$[u, u, 0]$
			$z, x, x$	$[0, u, \bar{u}]$	$z, \bar{x}, \bar{x}$	$[0, \bar{u}, u]$	$\bar{z}, \bar{x}, x$	$[0, \bar{u}, \bar{u}]$	$\bar{z}, x, \bar{x}$	$[0, u, u]$	$\bar{z}, x, \bar{x}$	$[0, u, u]$
			$x, z, x$	$[\bar{u}, 0, u]$	$\bar{x}, z, \bar{x}$	$[u, 0, \bar{u}]$	$x, \bar{z}, \bar{x}$	$[\bar{u}, 0, \bar{u}]$	$\bar{x}, \bar{z}, x$	$[u, 0, u]$	$\bar{x}, \bar{z}, x$	$[u, 0, u]$
			$x, x, \bar{z}$	$[\bar{u}, u, 0]$	$\bar{x}, \bar{x}, \bar{z}$	$[u, \bar{u}, 0]$	$x, \bar{x}, z$	$[\bar{u}, \bar{u}, 0]$	$\bar{x}, x, z$	$[u, u, 0]$	$\bar{x}, x, z$	$[u, u, 0]$
			$x, z, \bar{x}$	$[u, 0, u]$	$\bar{x}, z, x$	$[\bar{u}, 0, \bar{u}]$	$\bar{x}, z, \bar{x}$	$[\bar{u}, 0, u]$	$x, \bar{z}, x$	$[u, 0, \bar{u}]$	$\bar{x}, z, x$	$[u, 0, \bar{u}]$
			$z, x, \bar{x}$	$[0, \bar{u}, \bar{u}]$	$z, \bar{x}, x$	$[0, u, u]$	$\bar{z}, x, x$	$[0, \bar{u}, u]$	$\bar{z}, \bar{x}, \bar{x}$	$[0, u, \bar{u}]$	$\bar{z}, \bar{x}, \bar{x}$	$[0, u, \bar{u}]$
24	l	m..	$1/2, y, z$	$[u, 0, 0]$	$1/2, \bar{y}, z$	$[\bar{u}, 0, 0]$	$1/2, y, \bar{z}$	$[\bar{u}, 0, 0]$	$1/2, \bar{y}, \bar{z}$	$[u, 0, 0]$	$1/2, \bar{y}, \bar{z}$	$[u, 0, 0]$
			$z, 1/2, y$	$[0, u, 0]$	$z, 1/2, \bar{y}$	$[0, \bar{u}, 0]$	$\bar{z}, 1/2, y$	$[0, \bar{u}, 0]$	$\bar{z}, 1/2, \bar{y}$	$[0, u, 0]$	$\bar{z}, 1/2, \bar{y}$	$[0, u, 0]$
			$y, z, 1/2$	$[0, 0, u]$	$\bar{y}, z, 1/2$	$[0, 0, \bar{u}]$	$y, \bar{z}, 1/2$	$[0, 0, \bar{u}]$	$\bar{y}, \bar{z}, 1/2$	$[0, 0, u]$	$\bar{y}, \bar{z}, 1/2$	$[0, 0, u]$
			$y, 1/2, \bar{z}$	$[0, u, 0]$	$\bar{y}, 1/2, \bar{z}$	$[0, \bar{u}, 0]$	$y, 1/2, z$	$[0, \bar{u}, 0]$	$\bar{y}, 1/2, z$	$[0, u, 0]$	$\bar{y}, 1/2, z$	$[0, u, 0]$
			$1/2, z, \bar{y}$	$[u, 0, 0]$	$1/2, z, y$	$[\bar{u}, 0, 0]$	$1/2, \bar{z}, \bar{y}$	$[\bar{u}, 0, 0]$	$1/2, \bar{z}, y$	$[u, 0, 0]$	$1/2, \bar{z}, y$	$[u, 0, 0]$
			$z, y, 1/2$	$[0, 0, \bar{u}]$	$z, \bar{y}, 1/2$	$[0, 0, u]$	$\bar{z}, y, 1/2$	$[0, 0, u]$	$\bar{z}, \bar{y}, 1/2$	$[0, 0, \bar{u}]$	$\bar{z}, \bar{y}, 1/2$	$[0, 0, \bar{u}]$
24	k	m..	$0, y, z$	$[u, 0, 0]$	$0, \bar{y}, z$	$[\bar{u}, 0, 0]$	$0, y, \bar{z}$	$[\bar{u}, 0, 0]$	$0, \bar{y}, \bar{z}$	$[u, 0, 0]$	$0, \bar{y}, \bar{z}$	$[u, 0, 0]$
			$z, 0, y$	$[0, u, 0]$	$z, 0, \bar{y}$	$[0, \bar{u}, 0]$	$\bar{z}, 0, y$	$[0, \bar{u}, 0]$	$\bar{z}, 0, \bar{y}$	$[0, u, 0]$	$\bar{z}, 0, \bar{y}$	$[0, u, 0]$
			$y, z, 0$	$[0, 0, u]$	$\bar{y}, z, 0$	$[0, 0, \bar{u}]$	$y, \bar{z}, 0$	$[0, 0, \bar{u}]$	$\bar{y}, \bar{z}, 0$	$[0, 0, u]$	$\bar{y}, \bar{z}, 0$	$[0, 0, u]$
			$y, 0, \bar{z}$	$[0, u, 0]$	$\bar{y}, 0, \bar{z}$	$[0, \bar{u}, 0]$	$y, 0, z$	$[0, \bar{u}, 0]$	$\bar{y}, 0, z$	$[0, u, 0]$	$\bar{y}, 0, z$	$[0, u, 0]$
			$0, z, \bar{y}$	$[u, 0, 0]$	$0, z, y$	$[\bar{u}, 0, 0]$	$0, \bar{z}, \bar{y}$	$[\bar{u}, 0, 0]$	$0, \bar{z}, y$	$[u, 0, 0]$	$0, \bar{z}, y$	$[u, 0, 0]$
			$z, y, 0$	$[0, 0, \bar{u}]$	$z, \bar{y}, 0$	$[0, 0, u]$	$\bar{z}, y, 0$	$[0, 0, u]$	$\bar{z}, \bar{y}, 0$	$[0, 0, \bar{u}]$	$\bar{z}, \bar{y}, 0$	$[0, 0, \bar{u}]$
12	j	m.m2	$1/2, y, y$	$[0, 0, 0]$	$1/2, \bar{y}, y$	$[0, 0, 0]$	$1/2, y, \bar{y}$	$[0, 0, 0]$	$1/2, \bar{y}, \bar{y}$	$[0, 0, 0]$	$1/2, \bar{y}, \bar{y}$	$[0, 0, 0]$
			$y, 1/2, y$	$[0, 0, 0]$	$y, 1/2, \bar{y}$	$[0, 0, 0]$	$\bar{y}, 1/2, y$	$[0, 0, 0]$	$\bar{y}, 1/2, \bar{y}$	$[0, 0, 0]$	$\bar{y}, 1/2, \bar{y}$	$[0, 0, 0]$
			$y, y, 1/2$	$[0, 0, 0]$	$\bar{y}, y, 1/2$	$[0, 0, 0]$	$y, \bar{y}, 1/2$	$[0, 0, 0]$	$\bar{y}, \bar{y}, 1/2$	$[0, 0, 0]$	$\bar{y}, \bar{y}, 1/2$	$[0, 0, 0]$
12	i	m.m2	$0, y, y$	$[0, 0, 0]$	$0, \bar{y}, y$	$[0, 0, 0]$	$0, y, \bar{y}$	$[0, 0, 0]$	$0, \bar{y}, \bar{y}$	$[0, 0, 0]$	$0, \bar{y}, \bar{y}$	$[0, 0, 0]$
			$y, 0, y$	$[0, 0, 0]$	$y, 0, \bar{y}$	$[0, 0, 0]$	$\bar{y}, 0, y$	$[0, 0, 0]$	$\bar{y}, 0, \bar{y}$	$[0, 0, 0]$	$\bar{y}, 0, \bar{y}$	$[0, 0, 0]$
			$y, y, 0$	$[0, 0, 0]$	$\bar{y}, y, 0$	$[0, 0, 0]$	$y, \bar{y}, 0$	$[0, 0, 0]$	$\bar{y}, \bar{y}, 0$	$[0, 0, 0]$	$\bar{y}, \bar{y}, 0$	$[0, 0, 0]$

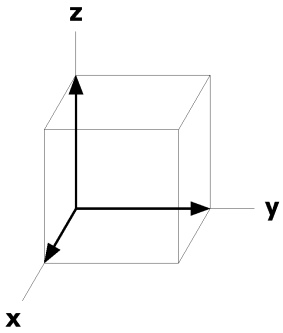
12	h	mm2..	x,1/2,0 [0,0,0]	$\bar{x}$ ,1/2,0 [0,0,0]	0,x,1/2 [0,0,0]	0, $\bar{x}$ ,1/2 [0,0,0]
			1/2,0,x [0,0,0]	1/2,0, $\bar{x}$ [0,0,0]	1/2,x,0 [0,0,0]	1/2, $\bar{x}$ ,0 [0,0,0]
			x,0,1/2 [0,0,0]	$\bar{x}$ ,0,1/2 [0,0,0]	0,1/2, $\bar{x}$ [0,0,0]	0,1/2,x [0,0,0]
8	g	.3m	x,x,x [0,0,0]	$\bar{x}$ , $\bar{x}$ ,x [0,0,0]	$\bar{x}$ ,x, $\bar{x}$ [0,0,0]	x, $\bar{x}$ , $\bar{x}$ [0,0,0]
			x,x, $\bar{x}$ [0,0,0]	$\bar{x}$ , $\bar{x}$ , $\bar{x}$ [0,0,0]	x, $\bar{x}$ ,x [0,0,0]	$\bar{x}$ ,x,x [0,0,0]
6	f	4m.m	x,1/2,1/2 [0,0,0]	$\bar{x}$ ,1/2,1/2 [0,0,0]		1/2,x,1/2 [0,0,0]
			1/2, $\bar{x}$ ,1/2 [0,0,0]	1/2,1/2,x [0,0,0]		1/2,1/2, $\bar{x}$ [0,0,0]
6	e	4m.m	x,0,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0]		0,x,0 [0,0,0]
			0, $\bar{x}$ ,0 [0,0,0]	0,0,x [0,0,0]		0,0, $\bar{x}$ [0,0,0]
3	d	4/mm.m	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]		0,0,1/2 [0,0,0]
3	c	4/mm.m	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		1/2,1/2,0 [0,0,0]
1	b	m $\bar{3}$ m	1/2,1/2,1/2 [0,0,0]			
1	a	m $\bar{3}$ m	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,1,1] p6'm'm  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

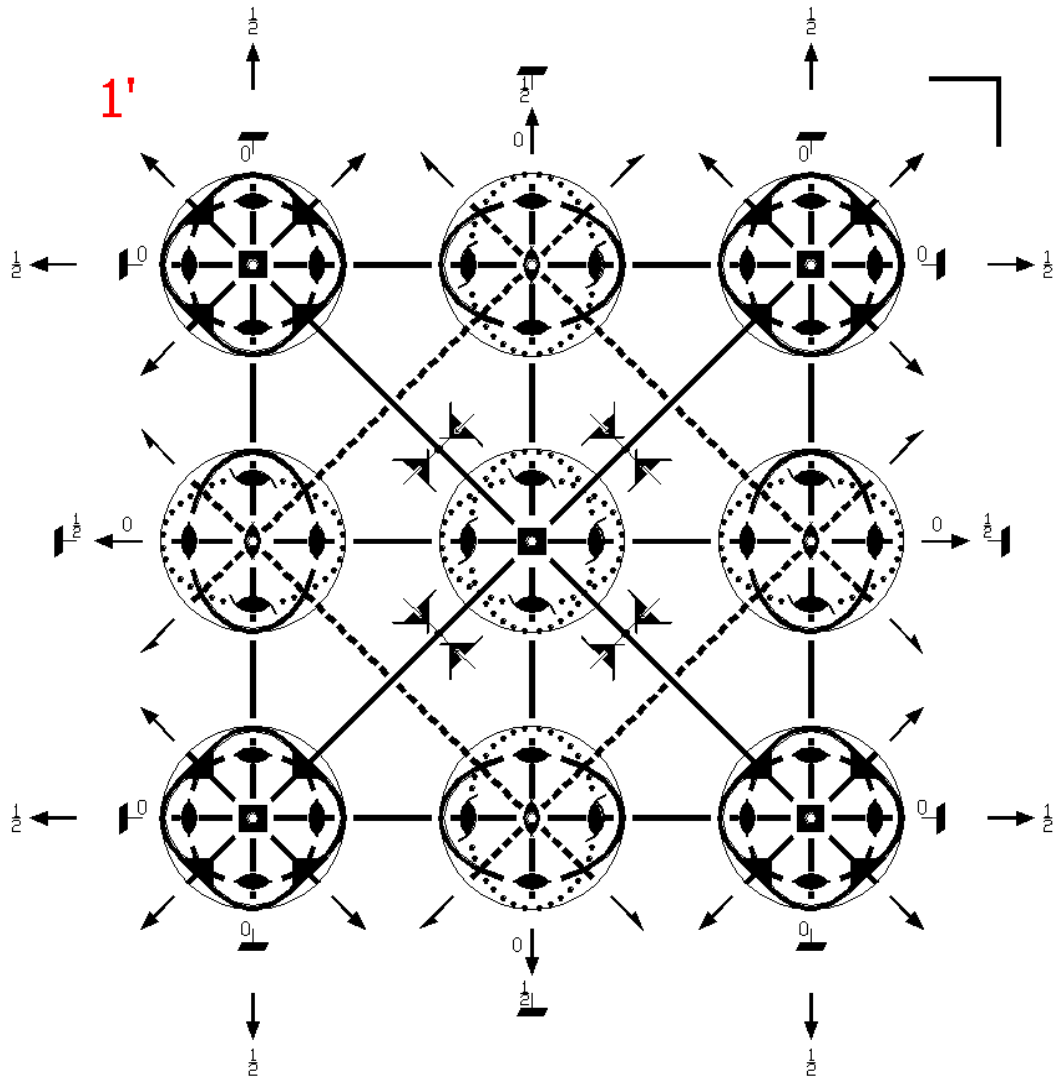
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$Pm\bar{3}m1'$   
221.2.1595

$m\bar{3}m1'$   
 $P4/m\bar{3}2/m1'$

Cubic



**Origin** at center ( $m\bar{3}m1'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq x;$   $z \leq y$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

For 1 + set

- |   |  |   |  |
|---|--|---|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)            | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)                                      | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0) | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)              |

(13) $2^- x,x,0$ ( $2_{xy} 0,0,0$ )	(14) $2^- x,\bar{x},0$ ( $2_{\bar{xy}} 0,0,0$ )	(15) $4^- 0,0,z$ ( $4_z^{-1} 0,0,0$ )	(16) $4^+ 0,0,z$ ( $4_z 0,0,0$ )
(17) $4^- x,0,0$ ( $4_x^{-1} 0,0,0$ )	(18) $2^- 0,y,y$ ( $2_{yz} 0,0,0$ )	(19) $2^- 0,y,\bar{y}$ ( $2_{\bar{yz}} 0,0,0$ )	(20) $4^+ x,0,0$ ( $4_x 0,0,0$ )
(21) $4^+ 0,y,0$ ( $4_y 0,0,0$ )	(22) $2^- x,0,x$ ( $2_{xz} 0,0,0$ )	(23) $4^- 0,y,0$ ( $4_y^{-1} 0,0,0$ )	(24) $2^- \bar{x},0,x$ ( $2_{\bar{xz}} 0,0,0$ )
(25) $\bar{1}^- 0,0,0$ ( $\bar{1} 0,0,0$ )	(26) $m^- x,y,0$ ( $m_z 0,0,0$ )	(27) $m^- x,0,z$ ( $m_y 0,0,0$ )	(28) $m^- 0,y,z$ ( $m_x 0,0,0$ )
(29) $\bar{3}^+ x,x,x; 0,0,0$ ( $\bar{3}_{xyz} 0,0,0$ )	(30) $\bar{3}^+ \bar{x},x,\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{xyz}}^{-1} 0,0,0$ )	(31) $\bar{3}^+ x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{xyz}}^{-1} 0,0,0$ )	(32) $\bar{3}^+ \bar{x},\bar{x},x; 0,0,0$ ( $\bar{3}_{xyz}^{-1} 0,0,0$ )
(33) $\bar{3}^- x,x,x; 0,0,0$ ( $\bar{3}_{xyz}^{-1} 0,0,0$ )	(34) $\bar{3}^- x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{xyz}} 0,0,0$ )	(35) $\bar{3}^- \bar{x},\bar{x},x; 0,0,0$ ( $\bar{3}_{\bar{xyz}} 0,0,0$ )	(36) $\bar{3}^- \bar{x},x,\bar{x}; 0,0,0$ ( $\bar{3}_{xyz}^{-1} 0,0,0$ )
(37) $m^- x,\bar{x},z$ ( $m_{xy} 0,0,0$ )	(38) $m^- x,x,z$ ( $m_{\bar{xy}} 0,0,0$ )	(39) $\bar{4}^- 0,0,z; 0,0,0$ ( $\bar{4}_z^{-1} 0,0,0$ )	(40) $\bar{4}^+ 0,0,z; 0,0,0$ ( $\bar{4}_z 0,0,0$ )
(41) $\bar{4}^- x,0,0; 0,0,0$ ( $\bar{4}_x^{-1} 0,0,0$ )	(42) $m^- x,y,\bar{y}$ ( $m_{yz} 0,0,0$ )	(43) $m^- x,y,y$ ( $m_{\bar{yz}} 0,0,0$ )	(44) $\bar{4}^+ x,0,0; 0,0,0$ ( $\bar{4}_x 0,0,0$ )
(45) $\bar{4}^+ 0,y,0; 0,0,0$ ( $\bar{4}_y 0,0,0$ )	(46) $m^- \bar{x},y,x$ ( $m_{xz} 0,0,0$ )	(47) $\bar{4}^- 0,y,0; 0,0,0$ ( $\bar{4}_y^{-1} 0,0,0$ )	(48) $m^- x,y,x$ ( $m_{\bar{xz}} 0,0,0$ )

For  $1'$  + set

(1) $1'$ ( $1 0,0,0$ )'	(2) $2'$ $0,0,z$ ( $2_z 0,0,0$ )'	(3) $2'$ $0,y,0$ ( $2_y 0,0,0$ )'	(4) $2'$ $x,0,0$ ( $2_x 0,0,0$ )'
(5) $3^{+'}$ $x,x,x$ ( $3_{xyz} 0,0,0$ )'	(6) $3^{+'}$ $\bar{x},x,\bar{x}$ ( $3_{\bar{xyz}}^{-1} 0,0,0$ )'	(7) $3^{+'}$ $x,\bar{x},\bar{x}$ ( $3_{\bar{xyz}}^{-1} 0,0,0$ )'	(8) $3^{+'}$ $\bar{x},\bar{x},x$ ( $3_{xyz}^{-1} 0,0,0$ )'
(9) $3^{-'}$ $x,x,x$ ( $3_{xyz}^{-1} 0,0,0$ )'	(10) $3^{-'}$ $x,\bar{x},\bar{x}$ ( $3_{\bar{xyz}} 0,0,0$ )'	(11) $3^{-'}$ $\bar{x},\bar{x},x$ ( $3_{\bar{xyz}} 0,0,0$ )'	(12) $3^{-'}$ $\bar{x},x,\bar{x}$ ( $3_{xyz}^{-1} 0,0,0$ )'
(13) $2'$ $x,x,0$ ( $2_{xy} 0,0,0$ )'	(14) $2'$ $x,\bar{x},0$ ( $2_{\bar{xy}} 0,0,0$ )'	(15) $4^{-'}$ $0,0,z$ ( $4_z^{-1} 0,0,0$ )'	(16) $4^{+'}$ $0,0,z$ ( $4_z 0,0,0$ )'
(17) $4^{-'}$ $x,0,0$ ( $4_x^{-1} 0,0,0$ )'	(18) $2'$ $0,y,y$ ( $2_{yz} 0,0,0$ )'	(19) $2'$ $0,y,\bar{y}$ ( $2_{\bar{yz}} 0,0,0$ )'	(20) $4^{+'}$ $x,0,0$ ( $4_x 0,0,0$ )'
(21) $4^{+'}$ $0,y,0$ ( $4_y 0,0,0$ )'	(22) $2'$ $x,0,x$ ( $2_{xz} 0,0,0$ )'	(23) $4^{-'}$ $0,y,0$ ( $4_y^{-1} 0,0,0$ )'	(24) $2'$ $\bar{x},0,x$ ( $2_{\bar{xz}} 0,0,0$ )'
(25) $\bar{1}'$ $0,0,0$ ( $\bar{1} 0,0,0$ )'	(26) $m'$ $x,y,0$ ( $m_z 0,0,0$ )'	(27) $m'$ $x,0,z$ ( $m_y 0,0,0$ )'	(28) $m'$ $0,y,z$ ( $m_x 0,0,0$ )'
(29) $\bar{3}^{+'}$ $x,x,x; 0,0,0$ ( $\bar{3}_{xyz} 0,0,0$ )'	(30) $\bar{3}^{+'}$ $\bar{x},x,\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{xyz}}^{-1} 0,0,0$ )'	(31) $\bar{3}^{+'}$ $x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{xyz}}^{-1} 0,0,0$ )'	(32) $\bar{3}^{+'}$ $\bar{x},\bar{x},x; 0,0,0$ ( $\bar{3}_{xyz}^{-1} 0,0,0$ )'
(33) $\bar{3}^{-'}$ $x,x,x; 0,0,0$ ( $\bar{3}_{xyz}^{-1} 0,0,0$ )'	(34) $\bar{3}^{-'}$ $x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{xyz}} 0,0,0$ )'	(35) $\bar{3}^{-'}$ $\bar{x},\bar{x},x; 0,0,0$ ( $\bar{3}_{\bar{xyz}} 0,0,0$ )'	(36) $\bar{3}^{-'}$ $\bar{x},x,\bar{x}; 0,0,0$ ( $\bar{3}_{xyz}^{-1} 0,0,0$ )'



(37) $m' \quad x, \bar{x}, z$ ( $m_{xy}   0, 0, 0$ )'	(38) $m' \quad x, x, z$ ( $m_{\bar{xy}}   0, 0, 0$ )'	(39) $\bar{4}^- ' \quad 0, 0, z; 0, 0, 0$ ( $\bar{4}_z^{-1}   0, 0, 0$ )'	(40) $\bar{4}^+ ' \quad 0, 0, z; 0, 0, 0$ ( $\bar{4}_z   0, 0, 0$ )'
(41) $\bar{4}^- ' \quad x, 0, 0; 0, 0, 0$ ( $\bar{4}_x^{-1}   0, 0, 0$ )'	(42) $m' \quad x, y, \bar{y}$ ( $m_{yz}   0, 0, 0$ )'	(43) $m' \quad x, y, y$ ( $m_{\bar{yz}}   0, 0, 0$ )'	(44) $\bar{4}^+ ' \quad x, 0, 0; 0, 0, 0$ ( $\bar{4}_x   0, 0, 0$ )'
(45) $\bar{4}^+ ' \quad 0, y, 0; 0, 0, 0$ ( $\bar{4}_y   0, 0, 0$ )'	(46) $m' \quad \bar{x}, y, x$ ( $m_{xz}   0, 0, 0$ )'	(47) $\bar{4}^- ' \quad 0, y, 0; 0, 0, 0$ ( $\bar{4}_y^{-1}   0, 0, 0$ )'	(48) $m' \quad x, y, x$ ( $m_{\bar{xz}}   0, 0, 0$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

1 +                      1' +

48	n	11'									
(1)	x, y, z	[0, 0, 0]	(2)	$\bar{x}, \bar{y}, z$	[0, 0, 0]	(3)	$\bar{x}, y, \bar{z}$	[0, 0, 0]	(4)	x, $\bar{y}, \bar{z}$	[0, 0, 0]
(5)	z, x, y	[0, 0, 0]	(6)	z, $\bar{x}, \bar{y}$	[0, 0, 0]	(7)	$\bar{z}, \bar{x}, y$	[0, 0, 0]	(8)	$\bar{z}, x, \bar{y}$	[0, 0, 0]
(9)	y, z, x	[0, 0, 0]	(10)	$\bar{y}, z, \bar{x}$	[0, 0, 0]	(11)	y, $\bar{z}, \bar{x}$	[0, 0, 0]	(12)	$\bar{y}, \bar{z}, x$	[0, 0, 0]
(13)	y, x, $\bar{z}$	[0, 0, 0]	(14)	$\bar{y}, \bar{x}, \bar{z}$	[0, 0, 0]	(15)	y, $\bar{x}, z$	[0, 0, 0]	(16)	$\bar{y}, x, z$	[0, 0, 0]
(17)	x, z, $\bar{y}$	[0, 0, 0]	(18)	$\bar{x}, z, y$	[0, 0, 0]	(19)	$\bar{x}, \bar{z}, \bar{y}$	[0, 0, 0]	(20)	x, $\bar{z}, y$	[0, 0, 0]
(21)	z, y, $\bar{x}$	[0, 0, 0]	(22)	z, $\bar{y}, x$	[0, 0, 0]	(23)	$\bar{z}, y, x$	[0, 0, 0]	(24)	$\bar{z}, \bar{y}, \bar{x}$	[0, 0, 0]
(25)	$\bar{x}, \bar{y}, \bar{z}$	[0, 0, 0]	(26)	x, y, $\bar{z}$	[0, 0, 0]	(27)	x, $\bar{y}, z$	[0, 0, 0]	(28)	$\bar{x}, y, z$	[0, 0, 0]
(29)	$\bar{z}, \bar{x}, \bar{y}$	[0, 0, 0]	(30)	$\bar{z}, x, y$	[0, 0, 0]	(31)	z, x, $\bar{y}$	[0, 0, 0]	(32)	z, $\bar{x}, y$	[0, 0, 0]
(33)	$\bar{y}, \bar{z}, \bar{x}$	[0, 0, 0]	(34)	y, $\bar{z}, x$	[0, 0, 0]	(35)	$\bar{y}, z, x$	[0, 0, 0]	(36)	y, z, $\bar{x}$	[0, 0, 0]
(37)	$\bar{y}, \bar{x}, z$	[0, 0, 0]	(38)	y, x, z	[0, 0, 0]	(39)	$\bar{y}, x, \bar{z}$	[0, 0, 0]	(40)	y, $\bar{x}, \bar{z}$	[0, 0, 0]
(41)	$\bar{x}, \bar{z}, y$	[0, 0, 0]	(42)	x, $\bar{z}, \bar{y}$	[0, 0, 0]	(43)	x, z, y	[0, 0, 0]	(44)	$\bar{x}, z, \bar{y}$	[0, 0, 0]
(45)	$\bar{z}, \bar{y}, x$	[0, 0, 0]	(46)	$\bar{z}, y, \bar{x}$	[0, 0, 0]	(47)	z, $\bar{y}, \bar{x}$	[0, 0, 0]	(48)	z, y, x	[0, 0, 0]
24	m	..m1'	x, x, z	[0, 0, 0]	$\bar{x}, \bar{x}, z$	[0, 0, 0]	$\bar{x}, x, \bar{z}$	[0, 0, 0]	x, $\bar{x}, \bar{z}$	[0, 0, 0]	
			z, x, x	[0, 0, 0]	z, $\bar{x}, \bar{x}$	[0, 0, 0]	$\bar{z}, \bar{x}, x$	[0, 0, 0]	$\bar{z}, x, \bar{x}$	[0, 0, 0]	
			x, z, x	[0, 0, 0]	$\bar{x}, z, \bar{x}$	[0, 0, 0]	x, $\bar{z}, \bar{x}$	[0, 0, 0]	$\bar{x}, \bar{z}, x$	[0, 0, 0]	
			x, x, $\bar{z}$	[0, 0, 0]	$\bar{x}, \bar{x}, \bar{z}$	[0, 0, 0]	x, $\bar{x}, z$	[0, 0, 0]	$\bar{x}, x, z$	[0, 0, 0]	
			x, z, $\bar{x}$	[0, 0, 0]	$\bar{x}, z, x$	[0, 0, 0]	$\bar{x}, \bar{z}, \bar{x}$	[0, 0, 0]	x, $\bar{z}, x$	[0, 0, 0]	
			z, x, $\bar{x}$	[0, 0, 0]	z, $\bar{x}, x$	[0, 0, 0]	$\bar{z}, x, x$	[0, 0, 0]	$\bar{z}, \bar{x}, \bar{x}$	[0, 0, 0]	

24	l	m..1'	1/2,y,z [0,0,0] z,1/2,y [0,0,0] y,z,1/2 [0,0,0] y,1/2, $\bar{z}$ [0,0,0] 1/2,z, $\bar{y}$ [0,0,0] z,y,1/2 [0,0,0]	1/2, $\bar{y}$ ,z [0,0,0] z,1/2, $\bar{y}$ [0,0,0] $\bar{y}$ ,z,1/2 [0,0,0] $\bar{y}$ ,1/2, $\bar{z}$ [0,0,0] 1/2,z,y [0,0,0] z, $\bar{y}$ ,1/2 [0,0,0]	1/2,y, $\bar{z}$ [0,0,0] $\bar{z}$ ,1/2,y [0,0,0] y, $\bar{z}$ ,1/2 [0,0,0] y,1/2,z [0,0,0] 1/2, $\bar{z}$ , $\bar{y}$ [0,0,0] $\bar{z}$ ,y,1/2 [0,0,0]	1/2, $\bar{y}$ , $\bar{z}$ [0,0,0] $\bar{z}$ ,1/2, $\bar{y}$ [0,0,0] $\bar{y}$ , $\bar{z}$ ,1/2 [0,0,0] $\bar{y}$ ,1/2,z [0,0,0] 1/2, $\bar{z}$ ,y [0,0,0] $\bar{z}$ , $\bar{y}$ ,1/2 [0,0,0]
24	k	m..1'	0,y,z [0,0,0] z,0,y [0,0,0] y,z,0 [0,0,0] y,0, $\bar{z}$ [0,0,0] 0,z, $\bar{y}$ [0,0,0] z,y,0 [0,0,0]	0, $\bar{y}$ ,z [0,0,0] z,0, $\bar{y}$ [0,0,0] $\bar{y}$ ,z,0 [0,0,0] $\bar{y}$ ,0, $\bar{z}$ [0,0,0] 0,z,y [0,0,0] z, $\bar{y}$ ,0 [0,0,0]	0,y, $\bar{z}$ [0,0,0] $\bar{z}$ ,0,y [0,0,0] y, $\bar{z}$ ,0 [0,0,0] y,0,z [0,0,0] 0, $\bar{z}$ , $\bar{y}$ [0,0,0] $\bar{z}$ ,y,0 [0,0,0]	0, $\bar{y}$ , $\bar{z}$ [0,0,0] $\bar{z}$ ,0, $\bar{y}$ [0,0,0] $\bar{y}$ , $\bar{z}$ ,0 [0,0,0] $\bar{y}$ ,0,z [0,0,0] 0, $\bar{z}$ ,y [0,0,0] $\bar{z}$ , $\bar{y}$ ,0 [0,0,0]
12	j	m.m21'	1/2,y,y [0,0,0] y,1/2,y [0,0,0] y,y,1/2 [0,0,0]	1/2, $\bar{y}$ ,y [0,0,0] y,1/2, $\bar{y}$ [0,0,0] $\bar{y}$ ,y,1/2 [0,0,0]	1/2,y, $\bar{y}$ [0,0,0] $\bar{y}$ ,1/2,y [0,0,0] y, $\bar{y}$ ,1/2 [0,0,0]	1/2, $\bar{y}$ , $\bar{y}$ [0,0,0] $\bar{y}$ ,1/2, $\bar{y}$ [0,0,0] $\bar{y}$ , $\bar{y}$ ,1/2 [0,0,0]
12	i	m.m21'	0,y,y [0,0,0] y,0,y [0,0,0] y,y,0 [0,0,0]	0, $\bar{y}$ ,y [0,0,0] y,0, $\bar{y}$ [0,0,0] $\bar{y}$ ,y,0 [0,0,0]	0,y, $\bar{y}$ [0,0,0] $\bar{y}$ ,0,y [0,0,0] y, $\bar{y}$ ,0 [0,0,0]	0, $\bar{y}$ , $\bar{y}$ [0,0,0] $\bar{y}$ ,0, $\bar{y}$ [0,0,0] $\bar{y}$ , $\bar{y}$ ,0 [0,0,0]
12	h	mm2..1'	x,1/2,0 [0,0,0] 1/2,0,x [0,0,0] x,0,1/2 [0,0,0]	$\bar{x}$ ,1/2,0 [0,0,0] 1/2,0, $\bar{x}$ [0,0,0] $\bar{x}$ ,0,1/2 [0,0,0]	0,x,1/2 [0,0,0] 1/2,x,0 [0,0,0] 0,1/2, $\bar{x}$ [0,0,0]	0, $\bar{x}$ ,1/2 [0,0,0] 1/2, $\bar{x}$ ,0 [0,0,0] 0,1/2,x [0,0,0]
8	g	.3m1'	x,x,x [0,0,0] x,x, $\bar{x}$ [0,0,0]	$\bar{x}$ , $\bar{x}$ ,x [0,0,0] $\bar{x}$ , $\bar{x}$ , $\bar{x}$ [0,0,0]	$\bar{x}$ ,x, $\bar{x}$ [0,0,0] x, $\bar{x}$ ,x [0,0,0]	x, $\bar{x}$ , $\bar{x}$ [0,0,0] $\bar{x}$ ,x,x [0,0,0]
6	f	4m.m1'	x,1/2,1/2 [0,0,0] 1/2, $\bar{x}$ ,1/2 [0,0,0]	$\bar{x}$ ,1/2,1/2 [0,0,0] 1/2,1/2,x [0,0,0]	1/2,x,1/2 [0,0,0] 1/2,1/2, $\bar{x}$ [0,0,0]	1/2,x,1/2 [0,0,0] 1/2,1/2, $\bar{x}$ [0,0,0]
6	e	4m.m1'	x,0,0 [0,0,0] 0, $\bar{x}$ ,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0] 0,0,x [0,0,0]	0,x,0 [0,0,0] 0,0, $\bar{x}$ [0,0,0]	0,x,0 [0,0,0] 0,0, $\bar{x}$ [0,0,0]
3	d	4/mm.m1'	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	0,0,1/2 [0,0,0]	0,0,1/2 [0,0,0]
3	c	4/mm.m1'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0]

1      b       $m\bar{3}m1'$   $1/2, 1/2, 1/2$  [0,0,0]

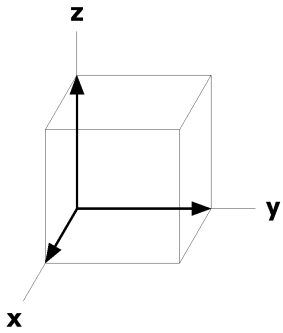
1      a       $m\bar{3}m1'$  0,0,0 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]       $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$     $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,1,1]       $p6mm1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$     $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

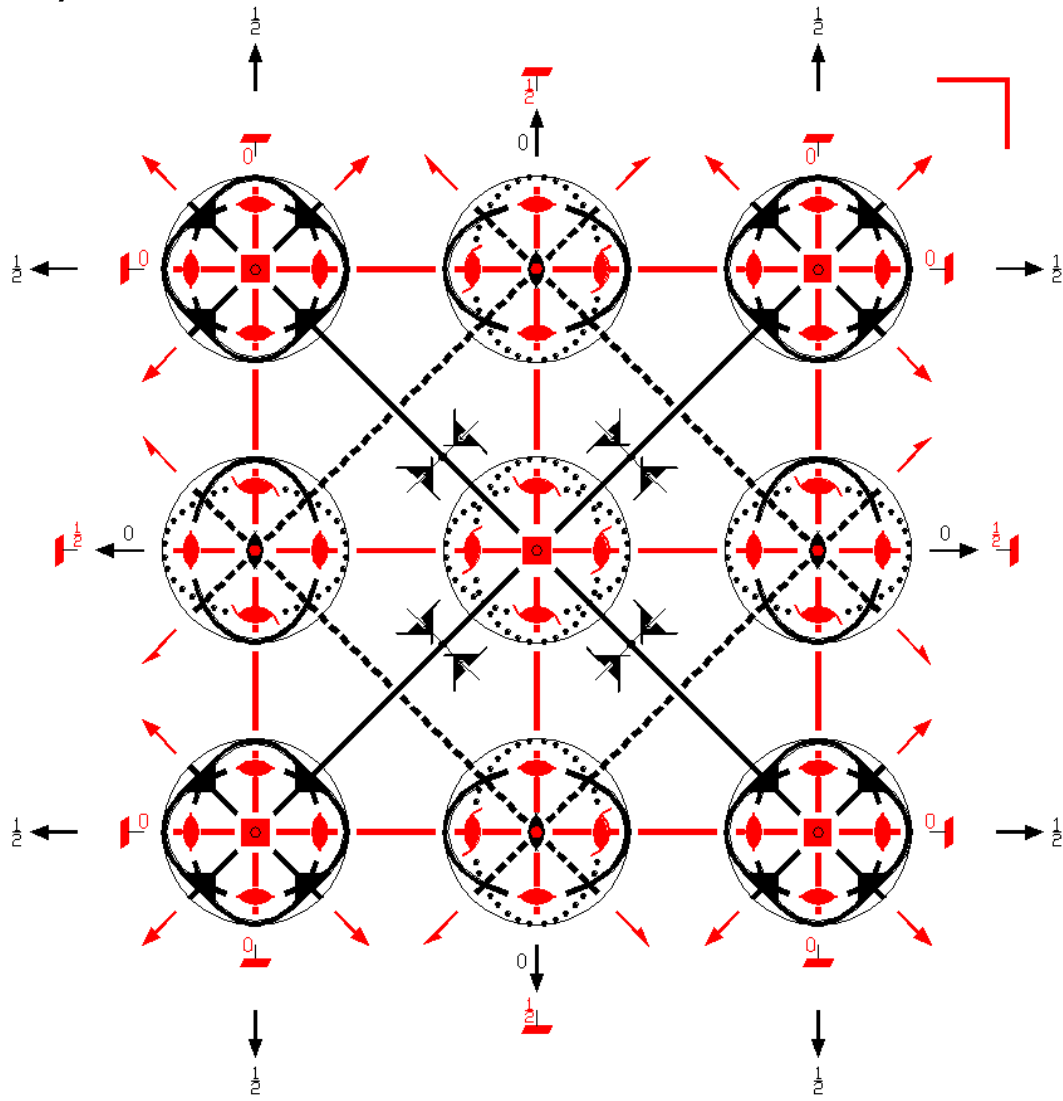
Along [1,1,0]       $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$     $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



Pm $\bar{3}$ 'm  
221.3.1596

m $\bar{3}$ 'm  
P4'/m $\bar{3}$ '2'/m

Cubic



**Origin** at center (m $\bar{3}$ 'm)

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$ ;  $y \leq x$ ;  $z \leq y$   
**Vertices** 0,0,0      1/2,0,0      1/2,1/2,0      1/2,1/2,1/2

**Symmetry Operations**

- |   |  |  |   |
|---|--|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>xyz</sub>  0,0,0)              | (12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)               |

(13) $2' \ x, x, 0$ ( $2_{xy}   0, 0, 0$ )'	(14) $2' \ x, \bar{x}, 0$ ( $2_{\bar{xy}}   0, 0, 0$ )'	(15) $4' \ 0, 0, z$ ( $4_z^{-1}   0, 0, 0$ )'	(16) $4' \ 0, 0, z$ ( $4_z   0, 0, 0$ )'
(17) $4' \ x, 0, 0$ ( $4_x^{-1}   0, 0, 0$ )'	(18) $2' \ 0, y, y$ ( $2_{yz}   0, 0, 0$ )'	(19) $2' \ 0, y, \bar{y}$ ( $2_{\bar{yz}}   0, 0, 0$ )'	(20) $4' \ x, 0, 0$ ( $4_x   0, 0, 0$ )'
(21) $4' \ 0, y, 0$ ( $4_y   0, 0, 0$ )'	(22) $2' \ x, 0, x$ ( $2_{xz}   0, 0, 0$ )'	(23) $4' \ 0, y, 0$ ( $4_y^{-1}   0, 0, 0$ )'	(24) $2' \ \bar{x}, 0, x$ ( $2_{\bar{xz}}   0, 0, 0$ )'
(25) $\bar{1} \ 0, 0, 0$ ( $\bar{1}   0, 0, 0$ )'	(26) $m' \ x, y, 0$ ( $m_z   0, 0, 0$ )'	(27) $m' \ x, 0, z$ ( $m_y   0, 0, 0$ )'	(28) $m' \ 0, y, z$ ( $m_x   0, 0, 0$ )'
(29) $\bar{3}^+ \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}   0, 0, 0$ )'	(30) $\bar{3}^+ \ \bar{x}, x, \bar{x}; 0, 0, 0$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1}   0, 0, 0$ )'	(31) $\bar{3}^+ \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xy}\bar{z}}^{-1}   0, 0, 0$ )'	(32) $\bar{3}^+ \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1}   0, 0, 0$ )'
(33) $\bar{3}^- \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}^{-1}   0, 0, 0$ )'	(34) $\bar{3}^- \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xy}\bar{z}}   0, 0, 0$ )'	(35) $\bar{3}^- \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{x\bar{y}\bar{z}}   0, 0, 0$ )'	(36) $\bar{3}^- \ \bar{x}, x, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xy}\bar{z}}   0, 0, 0$ )'
(37) $m \ x, \bar{x}, z$ ( $m_{xy}   0, 0, 0$ )	(38) $m \ x, x, z$ ( $m_{\bar{xy}}   0, 0, 0$ )	(39) $\bar{4} \ 0, 0, z; 0, 0, 0$ ( $\bar{4}_z^{-1}   0, 0, 0$ )	(40) $\bar{4}^+ \ 0, 0, z; 0, 0, 0$ ( $\bar{4}_z   0, 0, 0$ )
(41) $\bar{4} \ x, 0, 0; 0, 0, 0$ ( $\bar{4}_x^{-1}   0, 0, 0$ )	(42) $m \ x, y, \bar{y}$ ( $m_{yz}   0, 0, 0$ )	(43) $m \ x, y, y$ ( $m_{\bar{yz}}   0, 0, 0$ )	(44) $\bar{4}^+ \ x, 0, 0; 0, 0, 0$ ( $\bar{4}_x   0, 0, 0$ )
(45) $\bar{4}^+ \ 0, y, 0; 0, 0, 0$ ( $\bar{4}_y   0, 0, 0$ )	(46) $m \ \bar{x}, y, x$ ( $m_{xz}   0, 0, 0$ )	(47) $\bar{4} \ 0, y, 0; 0, 0, 0$ ( $\bar{4}_y^{-1}   0, 0, 0$ )	(48) $m \ x, y, x$ ( $m_{\bar{xz}}   0, 0, 0$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

### Coordinates

48 n 1

(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x, \bar{y}, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]
(5) $z, x, y$ [ $w, u, v$ ]	(6) $z, \bar{x}, \bar{y}$ [ $w, \bar{u}, \bar{v}$ ]	(7) $\bar{z}, \bar{x}, y$ [ $\bar{w}, \bar{u}, v$ ]	(8) $\bar{z}, x, \bar{y}$ [ $\bar{w}, u, \bar{v}$ ]
(9) $y, z, x$ [ $v, w, u$ ]	(10) $\bar{y}, z, \bar{x}$ [ $\bar{v}, w, \bar{u}$ ]	(11) $y, \bar{z}, \bar{x}$ [ $v, \bar{w}, \bar{u}$ ]	(12) $\bar{y}, \bar{z}, x$ [ $\bar{v}, \bar{w}, u$ ]
(13) $y, x, \bar{z}$ [ $\bar{v}, \bar{u}, w$ ]	(14) $\bar{y}, \bar{x}, \bar{z}$ [ $\bar{v}, u, w$ ]	(15) $y, \bar{x}, z$ [ $\bar{v}, u, \bar{w}$ ]	(16) $\bar{y}, x, z$ [ $v, u, \bar{w}$ ]
(17) $x, z, \bar{y}$ [ $\bar{u}, \bar{w}, v$ ]	(18) $\bar{x}, z, y$ [ $u, \bar{w}, \bar{v}$ ]	(19) $\bar{x}, \bar{z}, \bar{y}$ [ $u, w, v$ ]	(20) $x, \bar{z}, y$ [ $\bar{u}, w, \bar{v}$ ]
(21) $z, y, \bar{x}$ [ $\bar{w}, \bar{v}, u$ ]	(22) $z, \bar{y}, x$ [ $\bar{w}, v, \bar{u}$ ]	(23) $\bar{z}, y, x$ [ $w, \bar{v}, \bar{u}$ ]	(24) $\bar{z}, \bar{y}, \bar{x}$ [ $w, v, u$ ]
(25) $\bar{x}, \bar{y}, \bar{z}$ [ $\bar{u}, \bar{v}, \bar{w}$ ]	(26) $x, y, \bar{z}$ [ $u, v, \bar{w}$ ]	(27) $x, \bar{y}, z$ [ $u, \bar{v}, w$ ]	(28) $\bar{x}, y, z$ [ $\bar{u}, v, w$ ]
(29) $\bar{z}, \bar{x}, \bar{y}$ [ $\bar{w}, \bar{u}, \bar{v}$ ]	(30) $\bar{z}, x, y$ [ $\bar{w}, u, v$ ]	(31) $z, x, \bar{y}$ [ $w, u, \bar{v}$ ]	(32) $z, \bar{x}, y$ [ $w, \bar{u}, v$ ]
(33) $\bar{y}, \bar{z}, \bar{x}$ [ $\bar{v}, \bar{w}, \bar{u}$ ]	(34) $y, \bar{z}, x$ [ $v, \bar{w}, u$ ]	(35) $\bar{y}, z, x$ [ $\bar{v}, w, u$ ]	(36) $y, z, \bar{x}$ [ $v, w, \bar{u}$ ]

(37)	$\bar{y}, \bar{x}, z$	$[v, u, \bar{w}]$	(38)	$y, x, z$	$[\bar{v}, \bar{u}, \bar{w}]$	(39)	$\bar{y}, x, \bar{z}$	$[v, \bar{u}, w]$	(40)	$y, \bar{x}, \bar{z}$	$[\bar{v}, u, w]$	
(41)	$\bar{x}, \bar{z}, y$	$[u, w, \bar{v}]$	(42)	$x, \bar{z}, y$	$[\bar{u}, w, v]$	(43)	$x, z, y$	$[\bar{u}, \bar{w}, \bar{v}]$	(44)	$\bar{x}, z, y$	$[u, \bar{w}, v]$	
(45)	$\bar{z}, \bar{y}, x$	$[w, v, \bar{u}]$	(46)	$\bar{z}, y, \bar{x}$	$[w, \bar{v}, u]$	(47)	$z, y, \bar{x}$	$[\bar{w}, v, u]$	(48)	$z, y, x$	$[\bar{w}, \bar{v}, \bar{u}]$	
24	m	..m	$x, x, z$	$[u, \bar{u}, 0]$	$\bar{x}, \bar{x}, z$	$[\bar{u}, u, 0]$	$\bar{x}, x, \bar{z}$	$[\bar{u}, \bar{u}, 0]$	$x, x, \bar{z}$	$[u, u, 0]$	$\bar{x}, x, \bar{z}$	$[u, u, 0]$
			$z, x, x$	$[0, u, \bar{u}]$	$z, \bar{x}, \bar{x}$	$[0, \bar{u}, u]$	$\bar{z}, \bar{x}, x$	$[0, \bar{u}, \bar{u}]$	$\bar{z}, x, \bar{x}$	$[0, u, u]$	$\bar{z}, x, \bar{x}$	$[0, u, u]$
			$x, z, x$	$[\bar{u}, 0, u]$	$\bar{x}, z, \bar{x}$	$[u, 0, \bar{u}]$	$x, \bar{z}, \bar{x}$	$[\bar{u}, 0, \bar{u}]$	$\bar{x}, \bar{z}, x$	$[u, 0, u]$	$\bar{x}, \bar{z}, x$	$[u, 0, u]$
			$x, x, \bar{z}$	$[u, \bar{u}, 0]$	$\bar{x}, \bar{x}, \bar{z}$	$[\bar{u}, u, 0]$	$x, \bar{x}, z$	$[u, u, 0]$	$\bar{x}, x, z$	$[\bar{u}, \bar{u}, 0]$	$\bar{x}, x, z$	$[\bar{u}, \bar{u}, 0]$
			$x, z, \bar{x}$	$[\bar{u}, 0, \bar{u}]$	$\bar{x}, z, x$	$[u, 0, u]$	$\bar{x}, \bar{z}, \bar{x}$	$[u, 0, \bar{u}]$	$x, \bar{z}, x$	$[\bar{u}, 0, u]$	$\bar{x}, \bar{z}, x$	$[\bar{u}, 0, u]$
			$z, x, \bar{x}$	$[0, u, u]$	$z, \bar{x}, x$	$[0, \bar{u}, \bar{u}]$	$\bar{z}, x, x$	$[0, u, \bar{u}]$	$\bar{z}, \bar{x}, \bar{x}$	$[0, \bar{u}, u]$	$\bar{z}, \bar{x}, \bar{x}$	$[0, \bar{u}, u]$
24	l	m'..	$1/2, y, z$	$[0, v, w]$	$1/2, \bar{y}, z$	$[0, \bar{v}, w]$	$1/2, y, \bar{z}$	$[0, v, \bar{w}]$	$1/2, \bar{y}, \bar{z}$	$[0, \bar{v}, \bar{w}]$	$1/2, \bar{y}, \bar{z}$	$[0, \bar{v}, \bar{w}]$
			$z, 1/2, y$	$[w, 0, v]$	$z, 1/2, \bar{y}$	$[w, 0, \bar{v}]$	$\bar{z}, 1/2, y$	$[w, 0, v]$	$\bar{z}, 1/2, \bar{y}$	$[w, 0, \bar{v}]$	$\bar{z}, 1/2, \bar{y}$	$[w, 0, \bar{v}]$
			$y, z, 1/2$	$[v, w, 0]$	$\bar{y}, z, 1/2$	$[\bar{v}, w, 0]$	$y, \bar{z}, 1/2$	$[v, w, 0]$	$\bar{y}, \bar{z}, 1/2$	$[\bar{v}, w, 0]$	$\bar{y}, \bar{z}, 1/2$	$[\bar{v}, w, 0]$
			$y, 1/2, \bar{z}$	$[\bar{v}, 0, w]$	$\bar{y}, 1/2, \bar{z}$	$[v, 0, w]$	$y, 1/2, z$	$[\bar{v}, 0, \bar{w}]$	$\bar{y}, 1/2, z$	$[v, 0, w]$	$\bar{y}, 1/2, z$	$[v, 0, w]$
			$1/2, z, \bar{y}$	$[0, \bar{w}, v]$	$1/2, z, y$	$[0, \bar{w}, \bar{v}]$	$1/2, \bar{z}, \bar{y}$	$[0, w, v]$	$1/2, \bar{z}, y$	$[0, w, \bar{v}]$	$1/2, \bar{z}, y$	$[0, w, \bar{v}]$
			$z, y, 1/2$	$[\bar{w}, \bar{v}, 0]$	$z, \bar{y}, 1/2$	$[\bar{w}, v, 0]$	$\bar{z}, y, 1/2$	$[w, \bar{v}, 0]$	$\bar{z}, \bar{y}, 1/2$	$[w, v, 0]$	$\bar{z}, \bar{y}, 1/2$	$[w, v, 0]$
24	k	m'..	$0, y, z$	$[0, v, w]$	$0, \bar{y}, z$	$[0, \bar{v}, w]$	$0, y, \bar{z}$	$[0, v, \bar{w}]$	$0, \bar{y}, \bar{z}$	$[0, \bar{v}, \bar{w}]$	$0, \bar{y}, \bar{z}$	$[0, \bar{v}, \bar{w}]$
			$z, 0, y$	$[w, 0, v]$	$z, 0, \bar{y}$	$[w, 0, \bar{v}]$	$\bar{z}, 0, y$	$[w, 0, v]$	$\bar{z}, 0, \bar{y}$	$[w, 0, \bar{v}]$	$\bar{z}, 0, \bar{y}$	$[w, 0, \bar{v}]$
			$y, z, 0$	$[v, w, 0]$	$\bar{y}, z, 0$	$[\bar{v}, w, 0]$	$y, \bar{z}, 0$	$[v, w, 0]$	$\bar{y}, \bar{z}, 0$	$[\bar{v}, w, 0]$	$\bar{y}, \bar{z}, 0$	$[\bar{v}, w, 0]$
			$y, 0, \bar{z}$	$[\bar{v}, 0, w]$	$\bar{y}, 0, \bar{z}$	$[v, 0, w]$	$y, 0, z$	$[\bar{v}, 0, \bar{w}]$	$\bar{y}, 0, z$	$[v, 0, w]$	$\bar{y}, 0, z$	$[v, 0, w]$
			$0, z, \bar{y}$	$[0, \bar{w}, v]$	$0, z, y$	$[0, \bar{w}, \bar{v}]$	$0, \bar{z}, \bar{y}$	$[0, w, v]$	$0, \bar{z}, y$	$[0, w, \bar{v}]$	$0, \bar{z}, y$	$[0, w, \bar{v}]$
			$z, y, 0$	$[\bar{w}, \bar{v}, 0]$	$z, \bar{y}, 0$	$[\bar{w}, v, 0]$	$\bar{z}, y, 0$	$[w, \bar{v}, 0]$	$\bar{z}, \bar{y}, 0$	$[w, v, 0]$	$\bar{z}, \bar{y}, 0$	$[w, v, 0]$
12	j	m'.m2'	$1/2, y, y$	$[u, v, v]$	$1/2, \bar{y}, y$	$[\bar{u}, \bar{v}, \bar{v}]$	$1/2, y, \bar{y}$	$[\bar{u}, v, \bar{v}]$	$1/2, \bar{y}, y$	$[\bar{u}, \bar{v}, \bar{v}]$	$1/2, \bar{y}, y$	$[\bar{u}, \bar{v}, \bar{v}]$
			$y, 1/2, y$	$[v, u, v]$	$y, 1/2, \bar{y}$	$[v, \bar{u}, \bar{v}]$	$\bar{y}, 1/2, y$	$[v, u, v]$	$\bar{y}, 1/2, \bar{y}$	$[v, \bar{u}, \bar{v}]$	$\bar{y}, 1/2, \bar{y}$	$[v, \bar{u}, \bar{v}]$
			$y, y, 1/2$	$[v, v, u]$	$\bar{y}, y, 1/2$	$[\bar{v}, v, \bar{u}]$	$y, \bar{y}, 1/2$	$[v, v, u]$	$\bar{y}, \bar{y}, 1/2$	$[\bar{v}, \bar{v}, \bar{u}]$	$\bar{y}, \bar{y}, 1/2$	$[\bar{v}, \bar{v}, \bar{u}]$
12	i	m'.m2'	$0, y, y$	$[u, v, v]$	$0, \bar{y}, y$	$[\bar{u}, \bar{v}, \bar{v}]$	$0, y, \bar{y}$	$[\bar{u}, v, \bar{v}]$	$0, \bar{y}, y$	$[\bar{u}, \bar{v}, \bar{v}]$	$0, \bar{y}, y$	$[\bar{u}, \bar{v}, \bar{v}]$
			$y, 0, y$	$[v, u, v]$	$y, 0, \bar{y}$	$[v, \bar{u}, \bar{v}]$	$\bar{y}, 0, y$	$[v, u, v]$	$\bar{y}, 0, \bar{y}$	$[v, \bar{u}, \bar{v}]$	$\bar{y}, 0, \bar{y}$	$[v, \bar{u}, \bar{v}]$
			$y, y, 0$	$[v, v, u]$	$\bar{y}, y, 0$	$[\bar{v}, v, \bar{u}]$	$y, \bar{y}, 0$	$[v, v, u]$	$\bar{y}, \bar{y}, 0$	$[\bar{v}, \bar{v}, \bar{u}]$	$\bar{y}, \bar{y}, 0$	$[\bar{v}, \bar{v}, \bar{u}]$

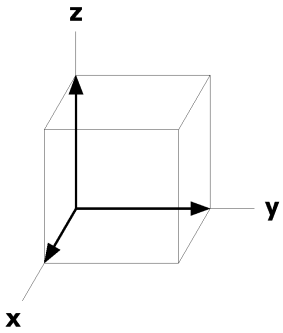
12	h	m'm'2..	x,1/2,0 [u,0,0]	$\bar{x}$ ,1/2,0 [ $\bar{u}$ ,0,0]	0,x,1/2 [0,u,0]	0, $\bar{x}$ ,1/2 [0, $\bar{u}$ ,0]
			1/2,0,x [0,0,u]	1/2,0, $\bar{x}$ [0,0, $\bar{u}$ ]	1/2,x,0 [0, $\bar{u}$ ,0]	1/2, $\bar{x}$ ,0 [0,u,0]
			x,0,1/2 [ $\bar{u}$ ,0,0]	$\bar{x}$ ,0,1/2 [u,0,0]	0,1/2, $\bar{x}$ [0,0,u]	0,1/2,x [0,0, $\bar{u}$ ]
8	g	.3m	x,x,x [0,0,0]	$\bar{x}$ , $\bar{x}$ ,x [0,0,0]	$\bar{x}$ ,x, $\bar{x}$ [0,0,0]	x, $\bar{x}$ , $\bar{x}$ [0,0,0]
			x,x, $\bar{x}$ [0,0,0]	$\bar{x}$ , $\bar{x}$ , $\bar{x}$ [0,0,0]	x, $\bar{x}$ ,x [0,0,0]	$\bar{x}$ ,x,x [0,0,0]
6	f	4'm'.m	x,1/2,1/2 [0,0,0]	$\bar{x}$ ,1/2,1/2 [0,0,0]		1/2,x,1/2 [0,0,0]
			1/2, $\bar{x}$ ,1/2 [0,0,0]	1/2,1/2,x [0,0,0]		1/2,1/2, $\bar{x}$ [0,0,0]
6	e	4'm'.m	x,0,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0]		0,x,0 [0,0,0]
			0, $\bar{x}$ ,0 [0,0,0]	0,0,x [0,0,0]		0,0, $\bar{x}$ [0,0,0]
3	d	4'/m'm'.m	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]		0,0,1/2 [0,0,0]
3	c	4'/m'm'.m	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		1/2,1/2,0 [0,0,0]
1	b	m' $\bar{3}$ 'm	1/2,1/2,1/2 [0,0,0]			
1	a	m' $\bar{3}$ 'm	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p4'm'm  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,1,1] p6mm  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

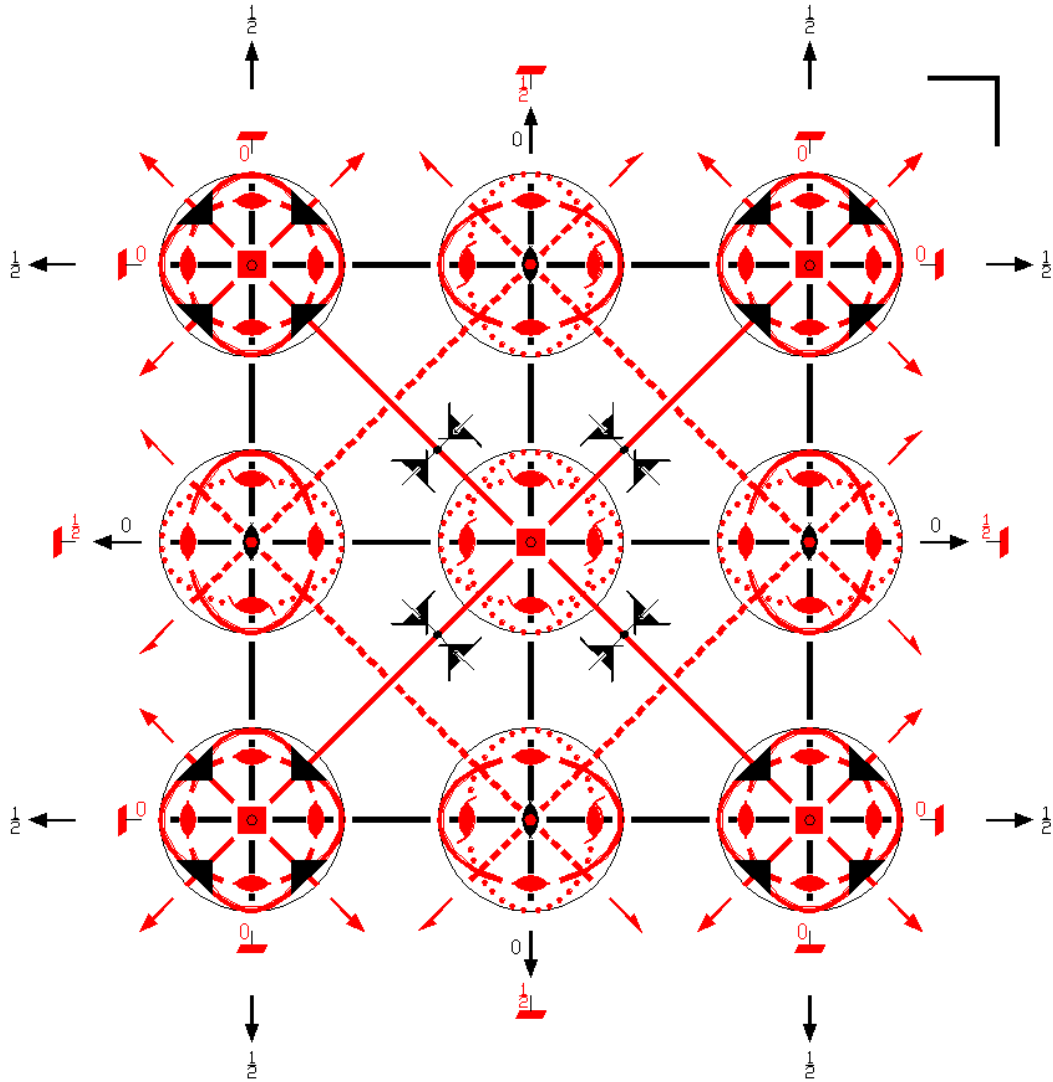
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$Pm\bar{3}m'$   
221.4.1597

$m\bar{3}m'$   
 $P4'/m\bar{3}2'/m'$

Cubic



**Origin** at center ( $m\bar{3}m'$ )

<b>Asymmetric unit</b>	$0 \leq x \leq 1/2;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$y \leq x;$	$z \leq y$
Vertices	0,0,0	1/2,0,0	1/2,1/2,0	1/2,1/2,1/2	

**Symmetry Operations**

- |   |  |   |  |
|---|--|---|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)      | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0) | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)              |



(13) $2' \ x, x, 0$ ( $2_{xy}   0, 0, 0$ )'	(14) $2' \ x, \bar{x}, 0$ ( $2_{\bar{xy}}   0, 0, 0$ )'	(15) $4' \ 0, 0, z$ ( $4_z^{-1}   0, 0, 0$ )'	(16) $4^+ \ 0, 0, z$ ( $4_z   0, 0, 0$ )'
(17) $4' \ x, 0, 0$ ( $4_x^{-1}   0, 0, 0$ )'	(18) $2' \ 0, y, y$ ( $2_{yz}   0, 0, 0$ )'	(19) $2' \ 0, y, \bar{y}$ ( $2_{\bar{yz}}   0, 0, 0$ )'	(20) $4^+ \ x, 0, 0$ ( $4_x   0, 0, 0$ )'
(21) $4^+ \ 0, y, 0$ ( $4_y   0, 0, 0$ )'	(22) $2' \ x, 0, x$ ( $2_{xz}   0, 0, 0$ )'	(23) $4' \ 0, y, 0$ ( $4_y^{-1}   0, 0, 0$ )'	(24) $2' \ \bar{x}, 0, x$ ( $2_{\bar{xz}}   0, 0, 0$ )'
(25) $\bar{1} \ 0, 0, 0$ ( $\bar{1}   0, 0, 0$ )	(26) $m \ x, y, 0$ ( $m_z   0, 0, 0$ )	(27) $m \ x, 0, z$ ( $m_y   0, 0, 0$ )	(28) $m \ 0, y, z$ ( $m_x   0, 0, 0$ )
(29) $\bar{3}^+ \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}   0, 0, 0$ )	(30) $\bar{3}^+ \ \bar{x}, x, \bar{x}; 0, 0, 0$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1}   0, 0, 0$ )	(31) $\bar{3}^+ \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xy}\bar{z}}^{-1}   0, 0, 0$ )	(32) $\bar{3}^+ \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1}   0, 0, 0$ )
(33) $\bar{3}^- \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}^{-1}   0, 0, 0$ )	(34) $\bar{3}^- \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xy}\bar{z}}   0, 0, 0$ )	(35) $\bar{3}^- \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{x\bar{y}\bar{z}}   0, 0, 0$ )	(36) $\bar{3}^- \ \bar{x}, x, \bar{x}; 0, 0, 0$ ( $\bar{3}_{x\bar{y}\bar{z}}   0, 0, 0$ )
(37) $m' \ x, \bar{x}, z$ ( $m_{xy}   0, 0, 0$ )'	(38) $m' \ x, x, z$ ( $m_{\bar{xy}}   0, 0, 0$ )'	(39) $\bar{4}^- \ 0, 0, z; 0, 0, 0$ ( $\bar{4}_z^{-1}   0, 0, 0$ )'	(40) $\bar{4}^+ \ 0, 0, z; 0, 0, 0$ ( $\bar{4}_z   0, 0, 0$ )'
(41) $\bar{4}^- \ x, 0, 0; 0, 0, 0$ ( $\bar{4}_x^{-1}   0, 0, 0$ )'	(42) $m' \ x, y, \bar{y}$ ( $m_{yz}   0, 0, 0$ )'	(43) $m' \ x, y, y$ ( $m_{\bar{yz}}   0, 0, 0$ )'	(44) $\bar{4}^+ \ x, 0, 0; 0, 0, 0$ ( $\bar{4}_x   0, 0, 0$ )'
(45) $\bar{4}^+ \ 0, y, 0; 0, 0, 0$ ( $\bar{4}_y   0, 0, 0$ )'	(46) $m' \ \bar{x}, y, x$ ( $m_{xz}   0, 0, 0$ )'	(47) $\bar{4}^- \ 0, y, 0; 0, 0, 0$ ( $\bar{4}_y^{-1}   0, 0, 0$ )'	(48) $m' \ x, y, x$ ( $m_{\bar{xz}}   0, 0, 0$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

### Coordinates

48 n 1

(1) $x, y, z$ [ $u, v, w$ ]	(2) $\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3) $\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4) $x, \bar{y}, \bar{z}$ [ $u, \bar{v}, \bar{w}$ ]
(5) $z, x, y$ [ $w, u, v$ ]	(6) $z, \bar{x}, \bar{y}$ [ $w, \bar{u}, \bar{v}$ ]	(7) $\bar{z}, \bar{x}, y$ [ $\bar{w}, \bar{u}, v$ ]	(8) $\bar{z}, x, \bar{y}$ [ $\bar{w}, u, \bar{v}$ ]
(9) $y, z, x$ [ $v, w, u$ ]	(10) $\bar{y}, z, \bar{x}$ [ $\bar{v}, w, \bar{u}$ ]	(11) $y, \bar{z}, \bar{x}$ [ $v, \bar{w}, \bar{u}$ ]	(12) $\bar{y}, \bar{z}, x$ [ $\bar{v}, \bar{w}, u$ ]
(13) $y, x, \bar{z}$ [ $\bar{v}, \bar{u}, w$ ]	(14) $\bar{y}, \bar{x}, \bar{z}$ [ $\bar{v}, u, w$ ]	(15) $y, \bar{x}, z$ [ $\bar{v}, u, \bar{w}$ ]	(16) $\bar{y}, x, z$ [ $v, \bar{u}, \bar{w}$ ]
(17) $x, z, \bar{y}$ [ $\bar{u}, \bar{w}, v$ ]	(18) $\bar{x}, z, y$ [ $u, \bar{w}, \bar{v}$ ]	(19) $\bar{x}, \bar{z}, \bar{y}$ [ $u, w, v$ ]	(20) $x, \bar{z}, y$ [ $\bar{u}, w, \bar{v}$ ]
(21) $z, y, \bar{x}$ [ $\bar{w}, \bar{v}, u$ ]	(22) $z, \bar{y}, x$ [ $\bar{w}, v, \bar{u}$ ]	(23) $\bar{z}, y, x$ [ $w, \bar{v}, \bar{u}$ ]	(24) $\bar{z}, \bar{y}, \bar{x}$ [ $w, v, u$ ]
(25) $\bar{x}, \bar{y}, \bar{z}$ [ $u, v, w$ ]	(26) $x, y, \bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(27) $x, \bar{y}, z$ [ $\bar{u}, v, \bar{w}$ ]	(28) $\bar{x}, y, z$ [ $u, \bar{v}, \bar{w}$ ]
(29) $\bar{z}, \bar{x}, \bar{y}$ [ $w, u, v$ ]	(30) $\bar{z}, x, y$ [ $w, \bar{u}, \bar{v}$ ]	(31) $z, x, \bar{y}$ [ $\bar{w}, \bar{u}, v$ ]	(32) $z, \bar{x}, y$ [ $\bar{w}, u, \bar{v}$ ]
(33) $\bar{y}, \bar{z}, \bar{x}$ [ $v, w, u$ ]	(34) $y, \bar{z}, x$ [ $\bar{v}, w, \bar{u}$ ]	(35) $\bar{y}, z, x$ [ $v, \bar{w}, \bar{u}$ ]	(36) $y, z, \bar{x}$ [ $\bar{v}, w, u$ ]

(37)	$\bar{y}, \bar{x}, z$	$[\bar{v}, \bar{u}, w]$	(38)	$y, x, z$	$[v, u, w]$	(39)	$\bar{y}, x, \bar{z}$	$[\bar{v}, u, \bar{w}]$	(40)	$y, \bar{x}, \bar{z}$	$[v, \bar{u}, \bar{w}]$
(41)	$\bar{x}, \bar{z}, y$	$[\bar{u}, \bar{w}, v]$	(42)	$x, \bar{z}, y$	$[u, \bar{w}, v]$	(43)	$x, z, y$	$[u, w, v]$	(44)	$\bar{x}, z, y$	$[\bar{u}, w, \bar{v}]$
(45)	$\bar{z}, \bar{y}, x$	$[\bar{w}, \bar{v}, u]$	(46)	$\bar{z}, y, \bar{x}$	$[\bar{w}, v, \bar{u}]$	(47)	$z, \bar{y}, \bar{x}$	$[w, \bar{v}, \bar{u}]$	(48)	$z, y, x$	$[w, v, u]$
24	m	..m'	$x, x, z$	$[u, u, w]$	$\bar{x}, \bar{x}, \bar{z}$	$[\bar{u}, \bar{u}, \bar{w}]$	$\bar{x}, x, \bar{z}$	$[\bar{u}, u, \bar{w}]$	$x, \bar{x}, \bar{z}$	$[u, \bar{u}, \bar{w}]$	
			$z, x, x$	$[w, u, u]$	$z, \bar{x}, \bar{x}$	$[w, \bar{u}, \bar{u}]$	$\bar{z}, \bar{x}, x$	$[\bar{w}, \bar{u}, u]$	$\bar{z}, x, \bar{x}$	$[\bar{w}, u, \bar{u}]$	
			$x, z, x$	$[u, w, u]$	$\bar{x}, z, \bar{x}$	$[w, \bar{u}, \bar{u}]$	$x, \bar{z}, \bar{x}$	$[u, \bar{w}, \bar{u}]$	$\bar{x}, z, x$	$[\bar{u}, \bar{w}, u]$	
			$x, x, \bar{z}$	$[\bar{u}, \bar{u}, w]$	$\bar{x}, \bar{x}, \bar{z}$	$[u, u, w]$	$x, \bar{x}, z$	$[\bar{u}, u, \bar{w}]$	$\bar{x}, x, z$	$[u, \bar{u}, \bar{w}]$	
			$x, z, \bar{x}$	$[\bar{u}, \bar{w}, u]$	$\bar{x}, z, \bar{x}$	$[u, \bar{w}, \bar{u}]$	$\bar{x}, z, x$	$[u, w, u]$	$x, \bar{z}, x$	$[\bar{u}, w, \bar{u}]$	
			$z, x, \bar{x}$	$[\bar{w}, \bar{u}, u]$	$z, \bar{x}, \bar{x}$	$[w, u, \bar{u}]$	$\bar{z}, x, x$	$[w, \bar{u}, \bar{u}]$	$\bar{z}, \bar{x}, \bar{x}$	$[w, u, u]$	
24	l	m..	$1/2, y, z$	$[u, 0, 0]$	$1/2, \bar{y}, z$	$[\bar{u}, 0, 0]$	$1/2, y, \bar{z}$	$[\bar{u}, 0, 0]$	$1/2, \bar{y}, \bar{z}$	$[u, 0, 0]$	
			$z, 1/2, y$	$[0, u, 0]$	$z, 1/2, \bar{y}$	$[0, \bar{u}, 0]$	$\bar{z}, 1/2, y$	$[0, \bar{u}, 0]$	$\bar{z}, 1/2, \bar{y}$	$[0, u, 0]$	
			$y, z, 1/2$	$[0, 0, u]$	$\bar{y}, z, 1/2$	$[0, 0, \bar{u}]$	$y, \bar{z}, 1/2$	$[0, 0, \bar{u}]$	$\bar{y}, \bar{z}, 1/2$	$[0, 0, u]$	
			$y, 1/2, \bar{z}$	$[0, \bar{u}, 0]$	$\bar{y}, 1/2, \bar{z}$	$[0, u, 0]$	$y, 1/2, z$	$[0, u, 0]$	$\bar{y}, 1/2, z$	$[0, \bar{u}, 0]$	
			$1/2, z, \bar{y}$	$[\bar{u}, 0, 0]$	$1/2, z, y$	$[u, 0, 0]$	$1/2, \bar{z}, \bar{y}$	$[u, 0, 0]$	$1/2, \bar{z}, y$	$[\bar{u}, 0, 0]$	
			$z, y, 1/2$	$[0, 0, u]$	$z, \bar{y}, 1/2$	$[0, 0, \bar{u}]$	$\bar{z}, y, 1/2$	$[0, 0, \bar{u}]$	$\bar{z}, \bar{y}, 1/2$	$[0, 0, u]$	
24	k	m..	$0, y, z$	$[u, 0, 0]$	$0, \bar{y}, z$	$[\bar{u}, 0, 0]$	$0, y, \bar{z}$	$[\bar{u}, 0, 0]$	$0, \bar{y}, \bar{z}$	$[u, 0, 0]$	
			$z, 0, y$	$[0, u, 0]$	$z, 0, \bar{y}$	$[0, \bar{u}, 0]$	$\bar{z}, 0, y$	$[0, \bar{u}, 0]$	$\bar{z}, 0, \bar{y}$	$[0, u, 0]$	
			$y, z, 0$	$[0, 0, u]$	$\bar{y}, z, 0$	$[0, 0, \bar{u}]$	$y, \bar{z}, 0$	$[0, 0, \bar{u}]$	$\bar{y}, \bar{z}, 0$	$[0, 0, u]$	
			$y, 0, \bar{z}$	$[0, \bar{u}, 0]$	$\bar{y}, 0, \bar{z}$	$[0, u, 0]$	$y, 0, z$	$[0, u, 0]$	$\bar{y}, 0, z$	$[0, \bar{u}, 0]$	
			$0, z, \bar{y}$	$[\bar{u}, 0, 0]$	$0, z, y$	$[u, 0, 0]$	$0, \bar{z}, \bar{y}$	$[u, 0, 0]$	$0, \bar{z}, y$	$[\bar{u}, 0, 0]$	
			$z, y, 0$	$[0, 0, u]$	$z, \bar{y}, 0$	$[0, 0, \bar{u}]$	$\bar{z}, y, 0$	$[0, 0, \bar{u}]$	$\bar{z}, \bar{y}, 0$	$[0, 0, u]$	
12	j	m.m'2'	$1/2, y, y$	$[u, 0, 0]$	$1/2, \bar{y}, y$	$[\bar{u}, 0, 0]$	$1/2, y, \bar{y}$	$[\bar{u}, 0, 0]$	$1/2, \bar{y}, \bar{y}$	$[u, 0, 0]$	
			$y, 1/2, y$	$[0, u, 0]$	$y, 1/2, \bar{y}$	$[0, \bar{u}, 0]$	$\bar{y}, 1/2, y$	$[0, \bar{u}, 0]$	$\bar{y}, 1/2, \bar{y}$	$[0, u, 0]$	
			$y, y, 1/2$	$[0, 0, u]$	$\bar{y}, y, 1/2$	$[0, 0, \bar{u}]$	$y, \bar{y}, 1/2$	$[0, 0, \bar{u}]$	$\bar{y}, \bar{y}, 1/2$	$[0, 0, u]$	
12	i	m.m'2'	$0, y, y$	$[u, 0, 0]$	$0, \bar{y}, y$	$[\bar{u}, 0, 0]$	$0, y, \bar{y}$	$[\bar{u}, 0, 0]$	$0, \bar{y}, \bar{y}$	$[u, 0, 0]$	
			$y, 0, y$	$[0, u, 0]$	$y, 0, \bar{y}$	$[0, \bar{u}, 0]$	$\bar{y}, 0, y$	$[0, \bar{u}, 0]$	$\bar{y}, 0, \bar{y}$	$[0, u, 0]$	
			$y, y, 0$	$[0, 0, u]$	$\bar{y}, y, 0$	$[0, 0, \bar{u}]$	$y, \bar{y}, 0$	$[0, 0, \bar{u}]$	$\bar{y}, \bar{y}, 0$	$[0, 0, u]$	

Continued

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 $Pm\bar{3}m'$ 

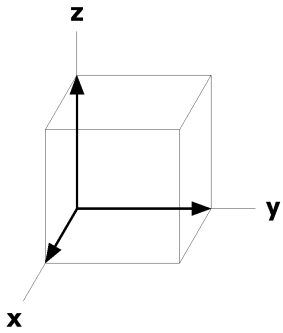
12	h	$mm2..$	$x, 1/2, 0 [0, 0, 0]$	$\bar{x}, 1/2, 0 [0, 0, 0]$	$0, x, 1/2 [0, 0, 0]$	$0, \bar{x}, 1/2 [0, 0, 0]$
			$1/2, 0, x [0, 0, 0]$	$1/2, 0, \bar{x} [0, 0, 0]$	$1/2, x, 0 [0, 0, 0]$	$1/2, \bar{x}, 0 [0, 0, 0]$
			$x, 0, 1/2 [0, 0, 0]$	$\bar{x}, 0, 1/2 [0, 0, 0]$	$0, 1/2, \bar{x} [0, 0, 0]$	$0, 1/2, x [0, 0, 0]$
8	g	$.3m'$	$x, x, x [u, u, u]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$	$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
			$x, x, \bar{x} [\bar{u}, \bar{u}, u]$	$\bar{x}, \bar{x}, \bar{x} [u, u, u]$	$x, \bar{x}, x [\bar{u}, u, \bar{u}]$	$\bar{x}, x, x [u, \bar{u}, \bar{u}]$
6	f	$4'm.m'$	$x, 1/2, 1/2 [0, 0, 0]$	$\bar{x}, 1/2, 1/2 [0, 0, 0]$		$1/2, x, 1/2 [0, 0, 0]$
			$1/2, \bar{x}, 1/2 [0, 0, 0]$	$1/2, 1/2, x [0, 0, 0]$		$1/2, 1/2, \bar{x} [0, 0, 0]$
6	e	$4'm.m'$	$x, 0, 0 [0, 0, 0]$	$\bar{x}, 0, 0 [0, 0, 0]$		$0, x, 0 [0, 0, 0]$
			$0, \bar{x}, 0 [0, 0, 0]$	$0, 0, x [0, 0, 0]$		$0, 0, \bar{x} [0, 0, 0]$
3	d	$4'/mm.m'$	$1/2, 0, 0 [0, 0, 0]$		$0, 1/2, 0 [0, 0, 0]$	$0, 0, 1/2 [0, 0, 0]$
3	c	$4'/mm.m'$	$0, 1/2, 1/2 [0, 0, 0]$		$1/2, 0, 1/2 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$
1	b	$m\bar{3}m'$	$1/2, 1/2, 1/2 [0, 0, 0]$			
1	a	$m\bar{3}m'$	$0, 0, 0 [0, 0, 0]$			

**Symmetry of Special Projections**

Along  $[0, 0, 1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 1, 1]$   $p6'mm'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

Along  $[1, 1, 0]$   $p2'mm'$   
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x, x, 0$



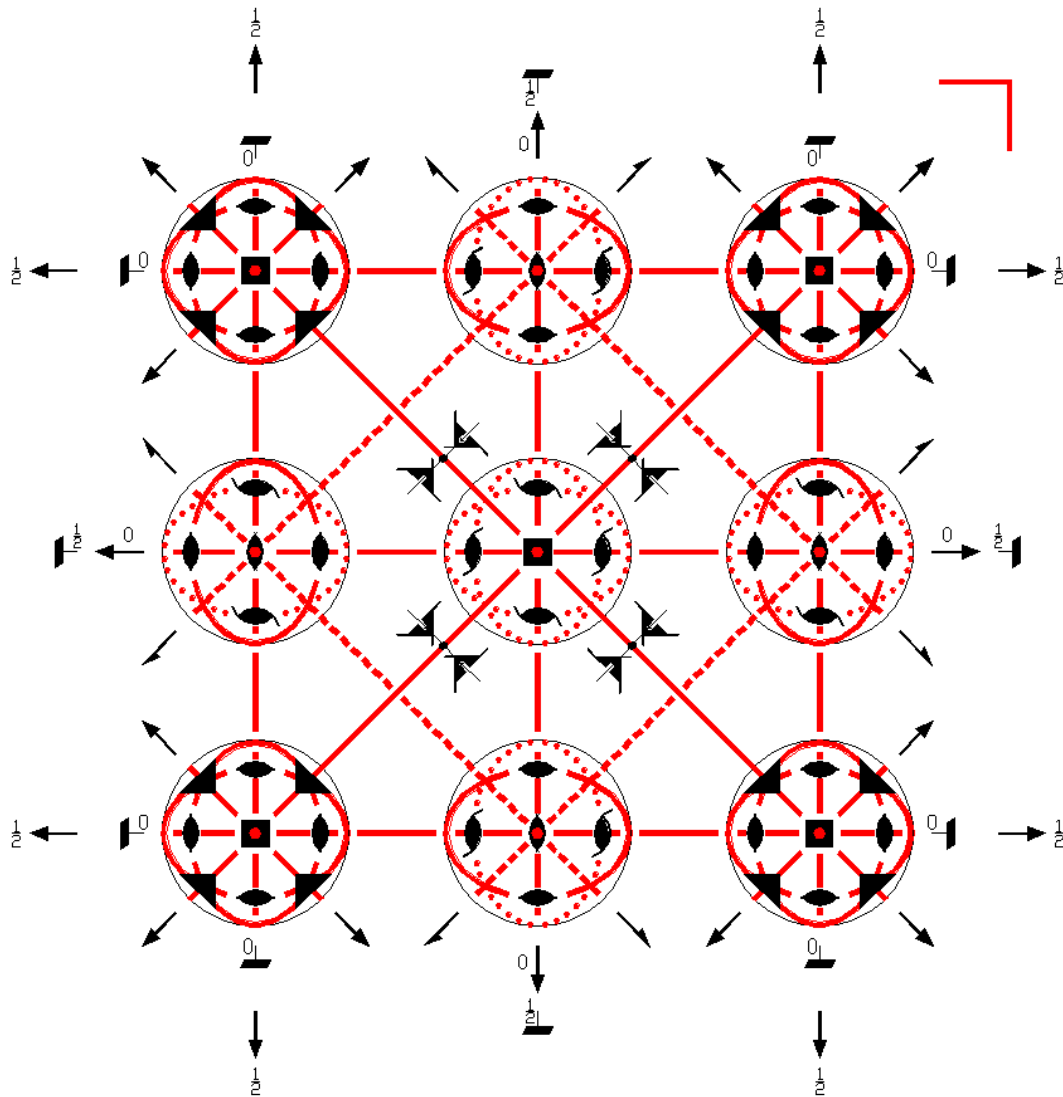
$Pm\bar{3}'m'$

221.5.1598

$m\bar{3}'m'$

$P4/m\bar{3}'2/m'$

Cubic



**Origin** at center ( $m\bar{3}'m'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq x;$   $z \leq y$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                  | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                            | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                            |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)  | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}yz}$  0,0,0)  |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}z}$  0,0,0) | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{\bar{x}yz}$  0,0,0) |

(13) $2 \ x,x,0$ ( $2_{xy} 0,0,0$ )	(14) $2 \ x,\bar{x},0$ ( $2_{\bar{xy}} 0,0,0$ )	(15) $4^- \ 0,0,z$ ( $4_z^{-1} 0,0,0$ )	(16) $4^+ \ 0,0,z$ ( $4_z 0,0,0$ )
(17) $4^- \ x,0,0$ ( $4_x^{-1} 0,0,0$ )	(18) $2 \ 0,y,y$ ( $2_{yz} 0,0,0$ )	(19) $2 \ 0,y,\bar{y}$ ( $2_{\bar{yz}} 0,0,0$ )	(20) $4^+ \ x,0,0$ ( $4_x 0,0,0$ )
(21) $4^+ \ 0,y,0$ ( $4_y 0,0,0$ )	(22) $2 \ x,0,x$ ( $2_{xz} 0,0,0$ )	(23) $4^- \ 0,y,0$ ( $4_y^{-1} 0,0,0$ )	(24) $2 \ \bar{x},0,x$ ( $2_{\bar{xz}} 0,0,0$ )
(25) $\bar{1} \ 0,0,0$ ( $\bar{1} 0,0,0$ )'	(26) $m' \ x,y,0$ ( $m_z 0,0,0$ )'	(27) $m' \ x,0,z$ ( $m_y 0,0,0$ )'	(28) $m' \ 0,y,z$ ( $m_x 0,0,0$ )'
(29) $\bar{3}^+ \ x,x,x; 0,0,0$ ( $\bar{3}_{xyz} 0,0,0$ )'	(30) $\bar{3}^+ \ \bar{x},x,\bar{x}; 0,0,0$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1} 0,0,0$ )'	(31) $\bar{3}^+ \ x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{xy}\bar{z}}^{-1} 0,0,0$ )'	(32) $\bar{3}^+ \ \bar{x},\bar{x},x; 0,0,0$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1} 0,0,0$ )'
(33) $\bar{3}^- \ x,x,x; 0,0,0$ ( $\bar{3}_{xyz}^{-1} 0,0,0$ )'	(34) $\bar{3}^- \ x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{xy}\bar{z}} 0,0,0$ )'	(35) $\bar{3}^- \ \bar{x},\bar{x},x; 0,0,0$ ( $\bar{3}_{\bar{xy}\bar{z}} 0,0,0$ )'	(36) $\bar{3}^- \ \bar{x},x,\bar{x}; 0,0,0$ ( $\bar{3}_{x\bar{y}\bar{z}} 0,0,0$ )'
(37) $m' \ x,\bar{x},z$ ( $m_{xy} 0,0,0$ )'	(38) $m' \ x,x,z$ ( $m_{\bar{xy}} 0,0,0$ )'	(39) $\bar{4}^- \ 0,0,z; 0,0,0$ ( $\bar{4}_z^{-1} 0,0,0$ )'	(40) $\bar{4}^+ \ 0,0,z; 0,0,0$ ( $\bar{4}_z 0,0,0$ )'
(41) $\bar{4}^- \ x,0,0; 0,0,0$ ( $\bar{4}_x^{-1} 0,0,0$ )'	(42) $m' \ x,y,\bar{y}$ ( $m_{yz} 0,0,0$ )'	(43) $m' \ x,y,y$ ( $m_{\bar{yz}} 0,0,0$ )'	(44) $\bar{4}^+ \ x,0,0; 0,0,0$ ( $\bar{4}_x 0,0,0$ )'
(45) $\bar{4}^+ \ 0,y,0; 0,0,0$ ( $\bar{4}_y 0,0,0$ )'	(46) $m' \ \bar{x},y,x$ ( $m_{xz} 0,0,0$ )'	(47) $\bar{4}^- \ 0,y,0; 0,0,0$ ( $\bar{4}_y^{-1} 0,0,0$ )'	(48) $m' \ x,y,x$ ( $m_{\bar{xz}} 0,0,0$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

### Coordinates

48 n 1

(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $\bar{x},y,\bar{z} [\bar{u},v,\bar{w}]$	(4) $x,\bar{y},\bar{z} [u,\bar{v},\bar{w}]$
(5) $z,x,y [w,u,v]$	(6) $z,\bar{x},\bar{y} [w,\bar{u},\bar{v}]$	(7) $\bar{z},\bar{x},y [\bar{w},\bar{u},v]$	(8) $\bar{z},x,\bar{y} [\bar{w},u,\bar{v}]$
(9) $y,z,x [v,w,u]$	(10) $\bar{y},z,\bar{x} [\bar{v},w,\bar{u}]$	(11) $y,\bar{z},\bar{x} [v,\bar{w},\bar{u}]$	(12) $\bar{y},\bar{z},x [\bar{v},\bar{w},u]$
(13) $y,x,\bar{z} [v,u,\bar{w}]$	(14) $\bar{y},\bar{x},\bar{z} [\bar{v},\bar{u},\bar{w}]$	(15) $y,\bar{x},z [v,\bar{u},w]$	(16) $\bar{y},x,z [\bar{v},u,w]$
(17) $x,z,\bar{y} [u,w,\bar{v}]$	(18) $\bar{x},z,y [\bar{u},w,\bar{v}]$	(19) $\bar{x},\bar{z},\bar{y} [\bar{u},\bar{w},\bar{v}]$	(20) $x,\bar{z},y [u,\bar{w},\bar{v}]$
(21) $z,y,\bar{x} [w,v,\bar{u}]$	(22) $z,\bar{y},x [w,\bar{v},u]$	(23) $\bar{z},y,x [\bar{w},v,u]$	(24) $\bar{z},\bar{y},\bar{x} [\bar{w},\bar{v},\bar{u}]$
(25) $\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$	(26) $x,y,\bar{z} [u,v,\bar{w}]$	(27) $x,\bar{y},z [u,\bar{v},w]$	(28) $\bar{x},y,z [\bar{u},v,w]$
(29) $\bar{z},\bar{x},\bar{y} [\bar{w},\bar{u},\bar{v}]$	(30) $\bar{z},x,y [\bar{w},u,\bar{v}]$	(31) $z,x,\bar{y} [w,u,\bar{v}]$	(32) $z,\bar{x},y [w,\bar{u},\bar{v}]$
(33) $\bar{y},\bar{z},\bar{x} [\bar{v},\bar{w},\bar{u}]$	(34) $y,\bar{z},x [v,\bar{w},u]$	(35) $\bar{y},z,x [\bar{v},w,u]$	(36) $y,z,\bar{x} [v,w,\bar{u}]$

(37)	$\bar{y}, \bar{x}, z$	$[\bar{v}, \bar{u}, w]$	(38)	$y, x, z$	$[v, u, w]$	(39)	$\bar{y}, x, \bar{z}$	$[\bar{v}, u, \bar{w}]$	(40)	$y, \bar{x}, \bar{z}$	$[v, \bar{u}, \bar{w}]$	
(41)	$\bar{x}, \bar{z}, y$	$[\bar{u}, \bar{w}, v]$	(42)	$x, \bar{z}, \bar{y}$	$[u, \bar{w}, \bar{v}]$	(43)	$x, z, y$	$[u, w, v]$	(44)	$\bar{x}, z, \bar{y}$	$[\bar{u}, w, \bar{v}]$	
(45)	$\bar{z}, \bar{y}, x$	$[\bar{w}, \bar{v}, u]$	(46)	$\bar{z}, y, \bar{x}$	$[\bar{w}, v, \bar{u}]$	(47)	$z, \bar{y}, \bar{x}$	$[w, \bar{v}, \bar{u}]$	(48)	$z, y, x$	$[w, v, u]$	
24	m	..m'	$x, x, z$	$[u, u, w]$	$\bar{x}, \bar{x}, z$	$[\bar{u}, \bar{u}, \bar{w}]$	$\bar{x}, x, \bar{z}$	$[\bar{u}, u, \bar{w}]$	$x, \bar{x}, \bar{z}$	$[u, \bar{u}, \bar{w}]$	$x, x, z$	$[u, u, w]$
			$z, x, x$	$[w, u, u]$	$z, \bar{x}, \bar{x}$	$[w, \bar{u}, \bar{u}]$	$\bar{z}, \bar{x}, x$	$[w, \bar{u}, u]$	$\bar{z}, x, \bar{x}$	$[w, u, \bar{u}]$	$z, x, x$	$[w, u, u]$
			$x, z, x$	$[u, w, u]$	$\bar{x}, z, \bar{x}$	$[\bar{u}, w, \bar{u}]$	$x, \bar{z}, \bar{x}$	$[u, \bar{w}, \bar{u}]$	$\bar{x}, z, x$	$[\bar{u}, w, \bar{u}]$	$x, z, x$	$[u, w, u]$
			$x, x, \bar{z}$	$[u, u, \bar{w}]$	$\bar{x}, \bar{x}, \bar{z}$	$[\bar{u}, \bar{u}, \bar{w}]$	$x, \bar{x}, z$	$[u, \bar{u}, w]$	$\bar{x}, x, z$	$[\bar{u}, u, w]$	$x, x, z$	$[u, u, w]$
			$x, z, \bar{x}$	$[u, w, \bar{u}]$	$\bar{x}, z, \bar{x}$	$[\bar{u}, w, \bar{u}]$	$\bar{x}, z, x$	$[u, \bar{w}, \bar{u}]$	$x, \bar{z}, x$	$[\bar{u}, w, \bar{u}]$	$x, z, x$	$[u, w, u]$
			$z, x, \bar{x}$	$[w, u, \bar{u}]$	$z, \bar{x}, x$	$[w, \bar{u}, u]$	$\bar{z}, x, x$	$[w, u, u]$	$\bar{z}, x, \bar{x}$	$[w, \bar{u}, \bar{u}]$	$z, x, x$	$[w, u, u]$
24	l	m'..	$1/2, y, z$	$[0, v, w]$	$1/2, \bar{y}, z$	$[0, \bar{v}, w]$	$1/2, y, \bar{z}$	$[0, v, \bar{w}]$	$1/2, \bar{y}, z$	$[0, \bar{v}, \bar{w}]$	$1/2, y, z$	$[0, v, w]$
			$z, 1/2, y$	$[w, 0, v]$	$z, 1/2, \bar{y}$	$[w, 0, \bar{v}]$	$\bar{z}, 1/2, y$	$[w, 0, v]$	$\bar{z}, 1/2, \bar{y}$	$[w, 0, \bar{v}]$	$z, 1/2, y$	$[w, 0, v]$
			$y, z, 1/2$	$[v, w, 0]$	$\bar{y}, z, 1/2$	$[\bar{v}, w, 0]$	$y, \bar{z}, 1/2$	$[v, \bar{w}, 0]$	$\bar{y}, z, 1/2$	$[\bar{v}, w, 0]$	$y, z, 1/2$	$[v, w, 0]$
			$y, 1/2, \bar{z}$	$[v, 0, \bar{w}]$	$\bar{y}, 1/2, \bar{z}$	$[\bar{v}, 0, \bar{w}]$	$y, 1/2, z$	$[v, 0, w]$	$\bar{y}, 1/2, z$	$[\bar{v}, 0, \bar{w}]$	$y, 1/2, z$	$[v, 0, w]$
			$1/2, z, \bar{y}$	$[0, w, \bar{v}]$	$1/2, z, y$	$[0, w, v]$	$1/2, \bar{z}, \bar{y}$	$[0, \bar{w}, \bar{v}]$	$1/2, z, y$	$[0, w, v]$	$1/2, z, \bar{y}$	$[0, w, \bar{v}]$
			$z, y, 1/2$	$[w, v, 0]$	$z, \bar{y}, 1/2$	$[w, \bar{v}, 0]$	$\bar{z}, y, 1/2$	$[w, v, 0]$	$\bar{z}, \bar{y}, 1/2$	$[w, \bar{v}, 0]$	$z, y, 1/2$	$[w, v, 0]$
24	k	m'..	$0, y, z$	$[0, v, w]$	$0, \bar{y}, z$	$[0, \bar{v}, w]$	$0, y, \bar{z}$	$[0, v, \bar{w}]$	$0, \bar{y}, z$	$[0, \bar{v}, \bar{w}]$	$0, y, z$	$[0, v, w]$
			$z, 0, y$	$[w, 0, v]$	$z, 0, \bar{y}$	$[w, 0, \bar{v}]$	$\bar{z}, 0, y$	$[w, 0, v]$	$\bar{z}, 0, \bar{y}$	$[w, 0, \bar{v}]$	$z, 0, y$	$[w, 0, v]$
			$y, z, 0$	$[v, w, 0]$	$\bar{y}, z, 0$	$[\bar{v}, w, 0]$	$y, \bar{z}, 0$	$[v, \bar{w}, 0]$	$\bar{y}, z, 0$	$[\bar{v}, w, 0]$	$y, z, 0$	$[v, w, 0]$
			$y, 0, \bar{z}$	$[v, 0, \bar{w}]$	$\bar{y}, 0, \bar{z}$	$[\bar{v}, 0, \bar{w}]$	$y, 0, z$	$[v, 0, w]$	$\bar{y}, 0, z$	$[\bar{v}, 0, \bar{w}]$	$y, 0, z$	$[v, 0, w]$
			$0, z, \bar{y}$	$[0, w, \bar{v}]$	$0, z, y$	$[0, w, v]$	$0, \bar{z}, \bar{y}$	$[0, \bar{w}, \bar{v}]$	$0, z, y$	$[0, w, v]$	$0, \bar{z}, \bar{y}$	$[0, \bar{w}, \bar{v}]$
			$z, y, 0$	$[w, v, 0]$	$z, \bar{y}, 0$	$[w, \bar{v}, 0]$	$\bar{z}, y, 0$	$[w, v, 0]$	$\bar{z}, \bar{y}, 0$	$[w, \bar{v}, 0]$	$z, y, 0$	$[w, v, 0]$
12	j	m'.m'2	$1/2, y, y$	$[0, v, v]$	$1/2, \bar{y}, y$	$[0, \bar{v}, v]$	$1/2, y, \bar{y}$	$[0, v, \bar{v}]$	$1/2, \bar{y}, y$	$[0, \bar{v}, \bar{v}]$	$1/2, y, y$	$[0, v, v]$
			$y, 1/2, y$	$[v, 0, v]$	$y, 1/2, \bar{y}$	$[v, 0, \bar{v}]$	$\bar{y}, 1/2, y$	$[v, 0, v]$	$\bar{y}, 1/2, \bar{y}$	$[v, 0, \bar{v}]$	$y, 1/2, y$	$[v, 0, v]$
			$y, y, 1/2$	$[v, v, 0]$	$\bar{y}, y, 1/2$	$[\bar{v}, v, 0]$	$y, \bar{y}, 1/2$	$[v, \bar{v}, 0]$	$\bar{y}, y, 1/2$	$[\bar{v}, v, 0]$	$y, y, 1/2$	$[v, v, 0]$
12	i	m'.m'2	$0, y, y$	$[0, v, v]$	$0, \bar{y}, y$	$[0, \bar{v}, v]$	$0, y, \bar{y}$	$[0, v, \bar{v}]$	$0, \bar{y}, y$	$[0, \bar{v}, \bar{v}]$	$0, y, y$	$[0, v, v]$
			$y, 0, y$	$[v, 0, v]$	$y, 0, \bar{y}$	$[v, 0, \bar{v}]$	$\bar{y}, 0, y$	$[v, 0, v]$	$\bar{y}, 0, \bar{y}$	$[v, 0, \bar{v}]$	$y, 0, y$	$[v, 0, v]$
			$y, y, 0$	$[v, v, 0]$	$\bar{y}, y, 0$	$[\bar{v}, v, 0]$	$y, \bar{y}, 0$	$[v, \bar{v}, 0]$	$\bar{y}, y, 0$	$[\bar{v}, v, 0]$	$y, y, 0$	$[v, v, 0]$

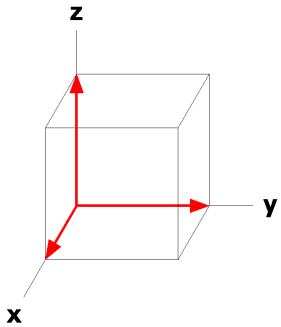
12	h	m'm'2..	x,1/2,0 [u,0,0]	$\bar{x}$ ,1/2,0 [ $\bar{u}$ ,0,0]	0,x,1/2 [0,u,0]	0, $\bar{x}$ ,1/2 [0, $\bar{u}$ ,0]
			1/2,0,x [0,0,u]	1/2,0, $\bar{x}$ [0,0, $\bar{u}$ ]	1/2,x,0 [0,u,0]	1/2, $\bar{x}$ ,0 [0, $\bar{u}$ ,0]
			x,0,1/2 [u,0,0]	$\bar{x}$ ,0,1/2 [ $\bar{u}$ ,0,0]	0,1/2, $\bar{x}$ [0,0, $\bar{u}$ ]	0,1/2,x [0,0,u]
8	g	.3m'	x,x,x [u,u,u]	$\bar{x}$ , $\bar{x}$ ,x [ $\bar{u}$ , $\bar{u}$ ,u]	$\bar{x}$ ,x, $\bar{x}$ [ $\bar{u}$ ,u, $\bar{u}$ ]	x, $\bar{x}$ , $\bar{x}$ [u, $\bar{u}$ , $\bar{u}$ ]
			x,x, $\bar{x}$ [u,u, $\bar{u}$ ]	$\bar{x}$ , $\bar{x}$ , $\bar{x}$ [ $\bar{u}$ , $\bar{u}$ , $\bar{u}$ ]	x, $\bar{x}$ ,x [u, $\bar{u}$ ,u]	$\bar{x}$ ,x,x [ $\bar{u}$ ,u,u]
6	f	4m'.m'	x,1/2,1/2 [u,0,0]	$\bar{x}$ ,1/2,1/2 [ $\bar{u}$ ,0,0]		1/2,x,1/2 [0,u,0]
			1/2, $\bar{x}$ ,1/2 [0, $\bar{u}$ ,0]	1/2,1/2,x [0,0,u]		1/2,1/2, $\bar{x}$ [0,0, $\bar{u}$ ]
6	e	4m'.m'	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0]		0,x,0 [0,u,0]
			0, $\bar{x}$ ,0 [0, $\bar{u}$ ,0]	0,0,x [0,0,u]		0,0, $\bar{x}$ [0,0, $\bar{u}$ ]
3	d	4/m'm'.m'	1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]		0,0,1/2 [0,0,0]
3	c	4/m'm'.m'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		1/2,1/2,0 [0,0,0]
1	b	m' $\bar{3}$ 'm'	1/2,1/2,1/2 [0,0,0]			
1	a	m' $\bar{3}$ 'm'	0,0,0 [0,0,0]			

### Symmetry of Special Projections

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,0,z

Along [1,1,1] p6m'm'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



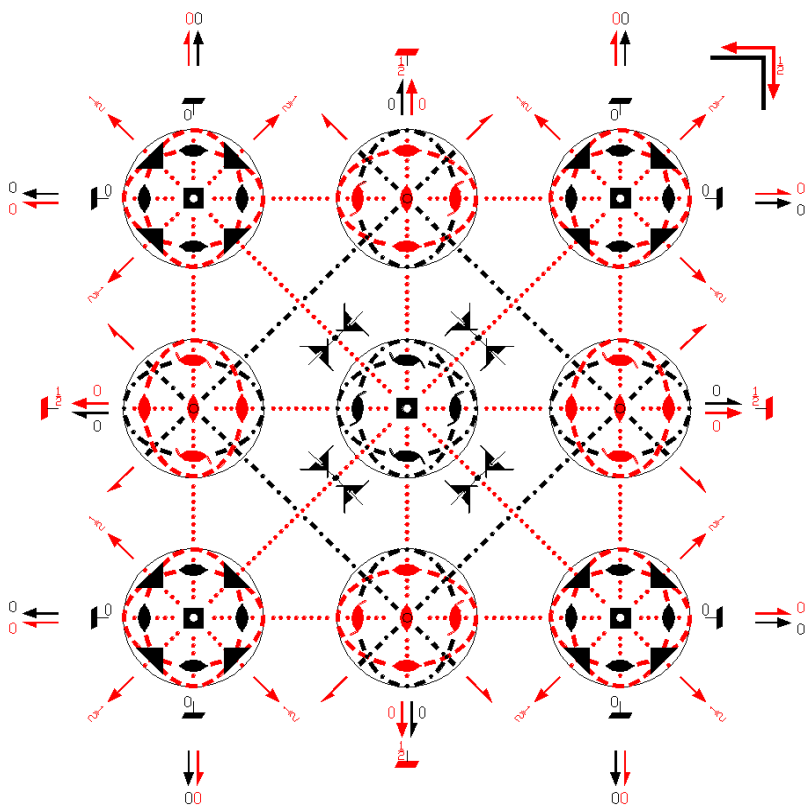
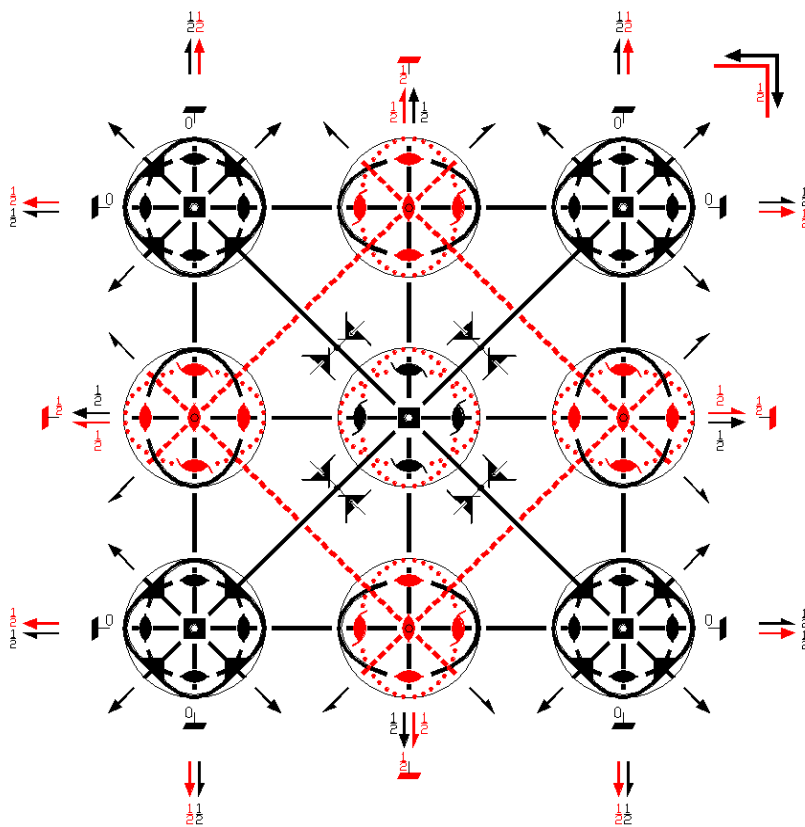
$P_F m\bar{3}m$

221.6.1599

$m\bar{3}m1'$

$P_F 4/m\bar{3}2/m$

Cubic





Origin at center (m $\bar{3}$ m)

<b>Asymmetric unit</b>	$0 \leq x \leq 1/2;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$y \leq x;$	$z \leq y$
Vertices	0,0,0	1/2,0,0	1/2,1/2,0	1/2,1/2,1/2	

## Symmetry Operations

## For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 2 0,y,0 (2 <sub>y</sub>  0,0,0)	(4) 2 x,0,0 (2 <sub>x</sub>  0,0,0)
(5) 3 <sup>+</sup> x,x,x (3 <sub>xyz</sub>  0,0,0)	(6) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)	(7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)
(9) 3 <sup>-</sup> x,x,x (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)	(10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub>  0,0,0)	(11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x (3 <sub>xyz</sub>  0,0,0)	(12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$ (3 <sub>xyz</sub>  0,0,0)
(13) 2 x,x,0 (2 <sub>xy</sub>  0,0,0)	(14) 2 x, $\bar{x}$ ,0 (2 <sub>xy</sub>  0,0,0)	(15) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)	(16) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)
(17) 4 <sup>-</sup> x,0,0 (4 <sub>x</sub> <sup>-1</sup>  0,0,0)	(18) 2 0,y,y (2 <sub>yz</sub>  0,0,0)	(19) 2 0,y, $\bar{y}$ (2 <sub>yz</sub>  0,0,0)	(20) 4 <sup>+</sup> x,0,0 (4 <sub>x</sub>  0,0,0)
(21) 4 <sup>+</sup> 0,y,0 (4 <sub>y</sub>  0,0,0)	(22) 2 x,0,x (2 <sub>xz</sub>  0,0,0)	(23) 4 <sup>-</sup> 0,y,0 (4 <sub>y</sub> <sup>-1</sup>  0,0,0)	(24) 2 $\bar{x}$ ,0,x (2 <sub>xz</sub>  0,0,0)
(25) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(26) m x,y,0 (m <sub>z</sub>  0,0,0)	(27) m x,0,z (m <sub>y</sub>  0,0,0)	(28) m 0,y,z (m <sub>x</sub>  0,0,0)
(29) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)	(30) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)	(31) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)	(32) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)
(33) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)	(34) $\bar{3}^-$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)	(35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)	(36) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)
(37) m x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)	(38) m x,x,z (m <sub>xy</sub>  0,0,0)	(39) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z$ <sup>-1</sup>  0,0,0)	(40) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)
(41) $\bar{4}^-$ x,0,0; 0,0,0 ( $\bar{4}_x$ <sup>-1</sup>  0,0,0)	(42) m x,y, $\bar{y}$ (m <sub>yz</sub>  0,0,0)	(43) m x,y,y (m <sub>yz</sub>  0,0,0)	(44) $\bar{4}^+$ x,0,0; 0,0,0 ( $\bar{4}_x$  0,0,0)
(45) $\bar{4}^+$ 0,y,0; 0,0,0 ( $\bar{4}_y$  0,0,0)	(46) m $\bar{x}$ ,y,x (m <sub>xz</sub>  0,0,0)	(47) $\bar{4}^-$ 0,y,0; 0,0,0 ( $\bar{4}_y$ <sup>-1</sup>  0,0,0)	(48) m x,y,x (m <sub>xz</sub>  0,0,0)

## For (1,0,0)' + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 2' 1/2,y,0 (2 <sub>y</sub>  1,0,0)'	(4) 2' (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)'
(5) 3 <sup>+</sup> ' (1/3,1/3,1/3) x+2/3,x+1/3,x (3 <sub>xyz</sub>  1,0,0)'	(6) 3 <sup>+</sup> ' (1/3,-1/3,1/3) x+2/3,x-1/3,x (3 <sub>xyz</sub> <sup>-1</sup>  1,0,0)'	(7) 3 <sup>+</sup> ' (1/3,-1/3,-1/3) x+2/3,x-1/3,x (3 <sub>xyz</sub> <sup>-1</sup>  1,0,0)'	(8) 3 <sup>+</sup> ' (1/3,1/3,-1/3) x+2/3,x-1/3,x (3 <sub>xyz</sub> <sup>-1</sup>  1,0,0)'
(9) 3 <sup>-</sup> ' (1/3,1/3,1/3) x+1/3,x-1/3,x (3 <sub>xyz</sub> <sup>-1</sup>  1,0,0)'	(10) 3 <sup>-</sup> ' (1/3,-1/3,-1/3) x+1/3,x+1/3,x (3 <sub>xyz</sub>  1,0,0)'	(11) 3 <sup>-</sup> ' (1/3,1/3,-1/3) x+1/3,x-1/3,x (3 <sub>xyz</sub>  1,0,0)'	(12) 3 <sup>-</sup> ' (1/3,-1/3,1/3) x+1/3,x+1/3,x (3 <sub>xyz</sub>  1,0,0)'

(13) $2' (1/2, 1/2, 0) \quad x+1, x+1/2, 0$ $(2_{xy}   1, 0, 0)'$	(14) $2' (-1/2, 1/2, 0) \quad x+1, \bar{x}-1/2, 0$ $(2_{\bar{xy}}   1, 0, 0)'$	(15) $4' 1/2, -1/2, z$ $(4_z^{-1}   1, 0, 0)'$	(16) $4^+ 1/2, 1/2, z$ $(4_z   1, 0, 0)'$
(17) $4' (1, 0, 0) \quad x, 0, 0$ $(4_x^{-1}   1, 0, 0)'$	(18) $2' 1/2, y, y$ $(2_{yz}   1, 0, 0)'$	(19) $2' 1/2, y, \bar{y}$ $(2_{\bar{yz}}   1, 0, 0)'$	(20) $4^+ (1, 0, 0) \quad x, 0, 0$ $(4_x   1, 0, 0)'$
(21) $4^+ 1/2, y, -1/2$ $(4_y   1, 0, 0)'$	(22) $2' (1/2, 0, 1/2) \quad x+1/2, 0, x$ $(2_{xz}   1, 0, 0)'$	(23) $4' 1/2, y, 1/2$ $(4_y^{-1}   1, 0, 0)'$	(24) $2' \bar{x}+1/2, 0, x$ $(2_{\bar{xz}}   1, 0, 0)'$
(25) $\bar{1}' 1/2, 0, 0$ $(\bar{1}   1, 0, 0)'$	(26) $a' (1, 0, 0) \quad x, y, 0$ $(m_z   1, 0, 0)'$	(27) $a' (1, 0, 0) \quad x, 0, z$ $(m_y   1, 0, 0)'$	(28) $m' 1/2, y, z$ $(m_x   1, 0, 0)'$
(29) $\bar{3}^+ x, x-1, x;$ $1/2, -1/2, 1/2$ $(\bar{3}_{xyz}   1, 0, 0)'$	(30) $\bar{3}^+ \bar{x}, x+1/2, \bar{x};$ $1/2, 1/2, 1/2$ $(\bar{3}_{\bar{xyz}}^{-1}   1, 0, 0)'$	(31) $\bar{3}^+ x, \bar{x}+1, \bar{x};$ $1/2, 1/2, -1/2$ $(\bar{3}_{\bar{xyz}}^{-1}   1, 0, 0)'$	(32) $\bar{3}^+ \bar{x}, \bar{x}+1, x;$ $1/2, -1/2, 1/2$ $(\bar{3}_{xyz}^{-1}   1, 0, 0)'$
(33) $\bar{3}^- x+1, x+1, x;$ $1/2, 1/2, -1/2$ $(\bar{3}_{xyz}^{-1}   1, 0, 0)'$	(34) $\bar{3}^- x+1, \bar{x}-1, \bar{x};$ $1/2, -1/2, 1/2$ $(\bar{3}_{\bar{xyz}}   1, 0, 0)'$	(35) $\bar{3}^- \bar{x}+1, \bar{x}+1, x;$ $1/2, 1/2, 1/2$ $(\bar{3}_{\bar{xyz}}   1, 0, 0)'$	(36) $\bar{3}^- \bar{x}+1, x-1, \bar{x};$ $1/2, -1/2, -1/2$ $(\bar{3}_{xyz}   1, 0, 0)'$
(37) $g' (1/2, -1/2, 0) \quad x+1/2, \bar{x}, z$ $(m_{xy}   1, 0, 0)'$	(38) $g' (1/2, 1/2, 0) \quad x+1/2, x, z$ $(m_{\bar{xy}}   1, 0, 0)'$	(39) $\bar{4}^- 1/2, 1/2, z; 1/2, 1/2, 0$ $(\bar{4}_z^{-1}   1, 0, 0)'$	(40) $\bar{4}^+ 1/2, -1/2, z; 1/2, -1/2, 0$ $(\bar{4}_z   1, 0, 0)'$
(41) $\bar{4}^- x+1/2, 0, 0; 1/2, 0, 0$ $(\bar{4}_x^{-1}   1, 0, 0)'$	(42) $a' (1, 0, 0) \quad x, y, \bar{y}$ $(m_{yz}   1, 0, 0)'$	(43) $a' (1, 0, 0) \quad x, y, y$ $(m_{\bar{yz}}   1, 0, 0)'$	(44) $\bar{4}^+ x+1/2, 0, 0; 1/2, 0, 0$ $(\bar{4}_x   1, 0, 0)'$
(45) $\bar{4}^+ 1/2, y, 1/2; 1/2, 0, 1/2$ $(\bar{4}_y   1, 0, 0)'$	(46) $g' (1/2, 0, -1/2) \quad \bar{x}+1/2, y, x$ $(m_{xz}   1, 0, 0)'$	(47) $\bar{4}^- 1/2, y, -1/2; 1/2, 0, -1/2$ $(\bar{4}_y^{-1}   1, 0, 0)'$	(48) $g' (1/2, 0, 1/2) \quad x+1/2, y, x$ $(m_{\bar{xz}}   1, 0, 0)'$

**Generators selected** (1);  $t'(1, 0, 0)$ ;  $t'(0, 1, 0)$ ;  $t'(0, 0, 1)$ ; (2); (3); (5); (13); (25).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

$(0, 0, 0) + (1, 0, 0)'$

96 n 1

(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{x}, y, \bar{z} [\bar{u}, v, \bar{w}]$	(4) $x, \bar{y}, \bar{z} [u, \bar{v}, \bar{w}]$
(5) $z, x, y [w, u, v]$	(6) $z, \bar{x}, \bar{y} [w, \bar{u}, \bar{v}]$	(7) $\bar{z}, \bar{x}, y [\bar{w}, \bar{u}, v]$	(8) $\bar{z}, x, \bar{y} [\bar{w}, u, \bar{v}]$
(9) $y, z, x [v, w, u]$	(10) $\bar{y}, z, \bar{x} [\bar{v}, w, \bar{u}]$	(11) $y, \bar{z}, \bar{x} [v, \bar{w}, \bar{u}]$	(12) $\bar{y}, z, x [\bar{v}, w, u]$
(13) $y, x, \bar{z} [v, u, \bar{w}]$	(14) $\bar{y}, \bar{x}, \bar{z} [\bar{v}, \bar{u}, \bar{w}]$	(15) $y, \bar{x}, z [v, \bar{u}, w]$	(16) $\bar{y}, x, z [\bar{v}, u, w]$
(17) $x, z, \bar{y} [u, w, \bar{v}]$	(18) $\bar{x}, z, y [\bar{u}, w, \bar{v}]$	(19) $\bar{x}, \bar{z}, \bar{y} [\bar{u}, \bar{w}, \bar{v}]$	(20) $x, \bar{z}, y [u, \bar{w}, \bar{v}]$
(21) $z, y, \bar{x} [w, v, \bar{u}]$	(22) $z, \bar{y}, x [w, \bar{v}, u]$	(23) $\bar{z}, y, x [\bar{w}, v, u]$	(24) $\bar{z}, \bar{y}, \bar{x} [\bar{w}, \bar{v}, \bar{u}]$
(25) $\bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$	(26) $x, y, z [u, v, w]$	(27) $x, \bar{y}, z [u, \bar{v}, w]$	(28) $\bar{x}, y, z [\bar{u}, v, \bar{w}]$
(29) $\bar{z}, \bar{x}, \bar{y} [\bar{w}, \bar{u}, \bar{v}]$	(30) $\bar{z}, x, y [\bar{w}, u, \bar{v}]$	(31) $z, x, \bar{y} [w, \bar{u}, \bar{v}]$	(32) $z, \bar{x}, y [w, u, \bar{v}]$
(33) $\bar{y}, \bar{z}, \bar{x} [\bar{v}, \bar{w}, \bar{u}]$	(34) $y, \bar{z}, x [v, w, \bar{u}]$	(35) $\bar{y}, z, x [\bar{v}, w, u]$	(36) $y, z, \bar{x} [v, w, u]$

(37)	$\bar{y}, \bar{x}, z$	$[v, u, \bar{w}]$	(38)	$y, x, z$	$[\bar{v}, \bar{u}, \bar{w}]$	(39)	$\bar{y}, x, \bar{z}$	$[v, \bar{u}, w]$	(40)	$y, \bar{x}, \bar{z}$	$[\bar{v}, u, w]$	
(41)	$\bar{x}, \bar{z}, y$	$[u, w, \bar{v}]$	(42)	$x, \bar{z}, \bar{y}$	$[\bar{u}, w, v]$	(43)	$x, z, y$	$[\bar{u}, \bar{w}, \bar{v}]$	(44)	$\bar{x}, z, \bar{y}$	$[u, \bar{w}, v]$	
(45)	$\bar{z}, \bar{y}, x$	$[w, v, \bar{u}]$	(46)	$\bar{z}, y, \bar{x}$	$[w, \bar{v}, u]$	(47)	$z, \bar{y}, \bar{x}$	$[\bar{w}, v, u]$	(48)	$z, y, x$	$[\bar{w}, \bar{v}, \bar{u}]$	
48	m	..m	$x, x, z$	$[u, \bar{u}, 0]$	$\bar{x}, \bar{x}, z$	$[\bar{u}, u, 0]$	$\bar{x}, x, \bar{z}$	$[\bar{u}, \bar{u}, 0]$	$x, \bar{x}, \bar{z}$	$[u, u, 0]$	$x, \bar{x}, \bar{z}$	$[u, u, 0]$
			$z, x, x$	$[0, u, \bar{u}]$	$z, \bar{x}, \bar{x}$	$[0, \bar{u}, u]$	$\bar{z}, \bar{x}, x$	$[0, \bar{u}, \bar{u}]$	$\bar{z}, x, \bar{x}$	$[0, u, u]$	$\bar{z}, x, \bar{x}$	$[0, u, u]$
			$x, z, x$	$[\bar{u}, 0, u]$	$\bar{x}, z, \bar{x}$	$[u, 0, \bar{u}]$	$x, \bar{z}, \bar{x}$	$[\bar{u}, 0, \bar{u}]$	$\bar{x}, \bar{z}, x$	$[u, 0, u]$	$\bar{x}, \bar{z}, x$	$[u, 0, u]$
			$x, x, \bar{z}$	$[\bar{u}, u, 0]$	$\bar{x}, \bar{x}, \bar{z}$	$[u, \bar{u}, 0]$	$x, \bar{x}, z$	$[\bar{u}, \bar{u}, 0]$	$\bar{x}, x, z$	$[u, u, 0]$	$\bar{x}, x, z$	$[u, u, 0]$
			$x, z, \bar{x}$	$[u, 0, u]$	$\bar{x}, z, x$	$[\bar{u}, 0, \bar{u}]$	$\bar{x}, z, \bar{x}$	$[\bar{u}, 0, u]$	$x, \bar{z}, x$	$[u, 0, \bar{u}]$	$\bar{x}, \bar{z}, x$	$[u, 0, \bar{u}]$
			$z, x, \bar{x}$	$[0, \bar{u}, \bar{u}]$	$z, \bar{x}, x$	$[0, u, u]$	$\bar{z}, x, x$	$[0, \bar{u}, u]$	$\bar{z}, \bar{x}, \bar{x}$	$[0, u, \bar{u}]$	$\bar{z}, \bar{x}, \bar{x}$	$[0, u, \bar{u}]$
48	l	m'..	$1/2, y, z$	$[0, v, w]$	$1/2, \bar{y}, z$	$[0, \bar{v}, \bar{w}]$	$1/2, y, \bar{z}$	$[0, \bar{v}, w]$	$1/2, \bar{y}, z$	$[0, \bar{v}, \bar{w}]$	$1/2, \bar{y}, z$	$[0, \bar{v}, \bar{w}]$
			$z, 1/2, y$	$[w, 0, v]$	$z, 1/2, \bar{y}$	$[\bar{w}, 0, \bar{v}]$	$\bar{z}, 1/2, y$	$[w, 0, \bar{v}]$	$\bar{z}, 1/2, \bar{y}$	$[\bar{w}, 0, \bar{v}]$	$\bar{z}, 1/2, \bar{y}$	$[\bar{w}, 0, \bar{v}]$
			$y, z, 1/2$	$[v, w, 0]$	$\bar{y}, z, 1/2$	$[v, \bar{w}, 0]$	$y, \bar{z}, 1/2$	$[v, w, 0]$	$\bar{y}, z, 1/2$	$[v, \bar{w}, 0]$	$\bar{y}, z, 1/2$	$[v, \bar{w}, 0]$
			$y, 1/2, \bar{z}$	$[v, 0, \bar{w}]$	$\bar{y}, 1/2, z$	$[v, 0, w]$	$y, 1/2, z$	$[v, 0, \bar{w}]$	$\bar{y}, 1/2, z$	$[v, 0, w]$	$\bar{y}, 1/2, z$	$[v, 0, w]$
			$1/2, z, \bar{y}$	$[0, w, \bar{v}]$	$1/2, z, y$	$[0, \bar{w}, \bar{v}]$	$1/2, \bar{z}, \bar{y}$	$[0, w, v]$	$1/2, z, y$	$[0, \bar{w}, \bar{v}]$	$1/2, \bar{z}, \bar{y}$	$[0, w, v]$
			$z, y, 1/2$	$[\bar{w}, \bar{v}, 0]$	$z, \bar{y}, 1/2$	$[w, \bar{v}, 0]$	$\bar{z}, y, 1/2$	$[\bar{w}, v, 0]$	$\bar{z}, \bar{y}, 1/2$	$[w, v, 0]$	$\bar{z}, \bar{y}, 1/2$	$[w, v, 0]$
48	k	m..	$0, y, z$	$[u, 0, 0]$	$0, \bar{y}, z$	$[\bar{u}, 0, 0]$	$0, y, \bar{z}$	$[\bar{u}, 0, 0]$	$0, \bar{y}, z$	$[u, 0, 0]$	$0, \bar{y}, z$	$[u, 0, 0]$
			$z, 0, y$	$[0, u, 0]$	$z, 0, \bar{y}$	$[0, \bar{u}, 0]$	$\bar{z}, 0, y$	$[0, \bar{u}, 0]$	$\bar{z}, 0, \bar{y}$	$[0, u, 0]$	$\bar{z}, 0, \bar{y}$	$[0, u, 0]$
			$y, z, 0$	$[0, 0, u]$	$\bar{y}, z, 0$	$[0, 0, \bar{u}]$	$y, \bar{z}, 0$	$[0, 0, \bar{u}]$	$\bar{y}, z, 0$	$[0, 0, u]$	$\bar{y}, z, 0$	$[0, 0, u]$
			$y, 0, \bar{z}$	$[0, u, 0]$	$\bar{y}, 0, z$	$[0, \bar{u}, 0]$	$y, 0, z$	$[0, \bar{u}, 0]$	$\bar{y}, 0, z$	$[0, u, 0]$	$\bar{y}, 0, z$	$[0, u, 0]$
			$0, z, \bar{y}$	$[u, 0, 0]$	$0, z, y$	$[\bar{u}, 0, 0]$	$0, \bar{z}, \bar{y}$	$[\bar{u}, 0, 0]$	$0, z, y$	$[u, 0, 0]$	$0, \bar{z}, \bar{y}$	$[u, 0, 0]$
			$z, y, 0$	$[0, 0, \bar{u}]$	$z, \bar{y}, 0$	$[0, 0, u]$	$\bar{z}, y, 0$	$[0, 0, u]$	$\bar{z}, \bar{y}, 0$	$[0, 0, \bar{u}]$	$\bar{z}, \bar{y}, 0$	$[0, 0, \bar{u}]$
24	j	m.m'2'	$1/2, y, y$	$[0, \bar{v}, v]$	$1/2, \bar{y}, y$	$[0, \bar{v}, \bar{v}]$	$1/2, y, \bar{y}$	$[0, v, v]$	$1/2, \bar{y}, y$	$[0, v, \bar{v}]$	$1/2, \bar{y}, y$	$[0, v, \bar{v}]$
			$y, 1/2, y$	$[v, 0, \bar{v}]$	$y, 1/2, \bar{y}$	$[\bar{v}, 0, \bar{v}]$	$\bar{y}, 1/2, y$	$[v, 0, v]$	$\bar{y}, 1/2, \bar{y}$	$[\bar{v}, 0, \bar{v}]$	$\bar{y}, 1/2, \bar{y}$	$[\bar{v}, 0, \bar{v}]$
			$y, y, 1/2$	$[\bar{v}, v, 0]$	$\bar{y}, y, 1/2$	$[\bar{v}, \bar{v}, 0]$	$y, \bar{y}, 1/2$	$[v, v, 0]$	$\bar{y}, \bar{y}, 1/2$	$[v, \bar{v}, 0]$	$\bar{y}, \bar{y}, 1/2$	$[v, \bar{v}, 0]$
24	i	m.m2	$0, y, y$	$[0, 0, 0]$	$0, \bar{y}, y$	$[0, 0, 0]$	$0, y, \bar{y}$	$[0, 0, 0]$	$0, \bar{y}, y$	$[0, 0, 0]$	$0, \bar{y}, y$	$[0, 0, 0]$
			$y, 0, y$	$[0, 0, 0]$	$y, 0, \bar{y}$	$[0, 0, 0]$	$\bar{y}, 0, y$	$[0, 0, 0]$	$\bar{y}, 0, \bar{y}$	$[0, 0, 0]$	$\bar{y}, 0, \bar{y}$	$[0, 0, 0]$
			$y, y, 0$	$[0, 0, 0]$	$\bar{y}, y, 0$	$[0, 0, 0]$	$y, \bar{y}, 0$	$[0, 0, 0]$	$\bar{y}, \bar{y}, 0$	$[0, 0, 0]$	$\bar{y}, \bar{y}, 0$	$[0, 0, 0]$

Continued

221.6.1599

 $P_{\bar{c}}m\bar{3}m$ 

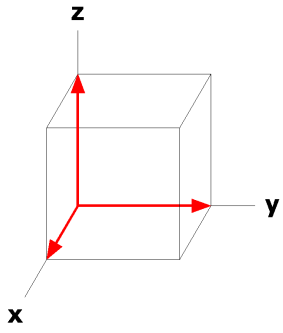
24	h	mm2..	$x, 1/2, 0 [0, 0, w]$	$\bar{x}, 1/2, 0 [0, 0, \bar{w}]$	$0, x, 1/2 [w, 0, 0]$	$0, \bar{x}, 1/2 [\bar{w}, 0, 0]$
			$1/2, 0, x [0, w, 0]$	$1/2, 0, \bar{x} [0, \bar{w}, 0]$	$1/2, x, 0 [0, 0, \bar{w}]$	$1/2, \bar{x}, 0 [0, 0, w]$
			$x, 0, 1/2 [0, \bar{w}, 0]$	$\bar{x}, 0, 1/2 [0, w, 0]$	$0, 1/2, \bar{x} [w, 0, 0]$	$0, 1/2, x [\bar{w}, 0, 0]$
16	g	.3m	$x, x, x [0, 0, 0]$	$\bar{x}, \bar{x}, x [0, 0, 0]$	$\bar{x}, x, \bar{x} [0, 0, 0]$	$x, \bar{x}, \bar{x} [0, 0, 0]$
			$x, x, \bar{x} [0, 0, 0]$	$\bar{x}, \bar{x}, \bar{x} [0, 0, 0]$	$x, \bar{x}, x [0, 0, 0]$	$\bar{x}, x, x [0, 0, 0]$
16	f	4'm'.m	$x, 1/2, 1/2 [0, 0, 0]$	$\bar{x}, 1/2, 1/2 [0, 0, 0]$		$1/2, x, 1/2 [0, 0, 0]$
			$1/2, \bar{x}, 1/2 [0, 0, 0]$	$1/2, 1/2, x [0, 0, 0]$		$1/2, 1/2, \bar{x} [0, 0, 0]$
12	e	4m.m	$x, 0, 0 [0, 0, 0]$	$\bar{x}, 0, 0 [0, 0, 0]$		$0, x, 0 [0, 0, 0]$
			$0, \bar{x}, 0 [0, 0, 0]$	$0, 0, x [0, 0, 0]$		$0, 0, \bar{x} [0, 0, 0]$
6	d	4/m'm.m	$1/2, 0, 0 [0, 0, 0]$		$0, 1/2, 0 [0, 0, 0]$	$0, 0, 1/2 [0, 0, 0]$
6	c	4'/mm'.m	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$		$1/2, 1/2, 0 [0, 0, 0]$
2	b	$m\bar{3}m$	$1/2, 1/2, 1/2 [0, 0, 0]$			
2	a	$m\bar{3}m$	$0, 0, 0 [0, 0, 0]$			

**Symmetry of Special Projections**

Along  $[0, 0, 1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 1, 1]$   $p6mm1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

Along  $[1, 1, 0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 0$



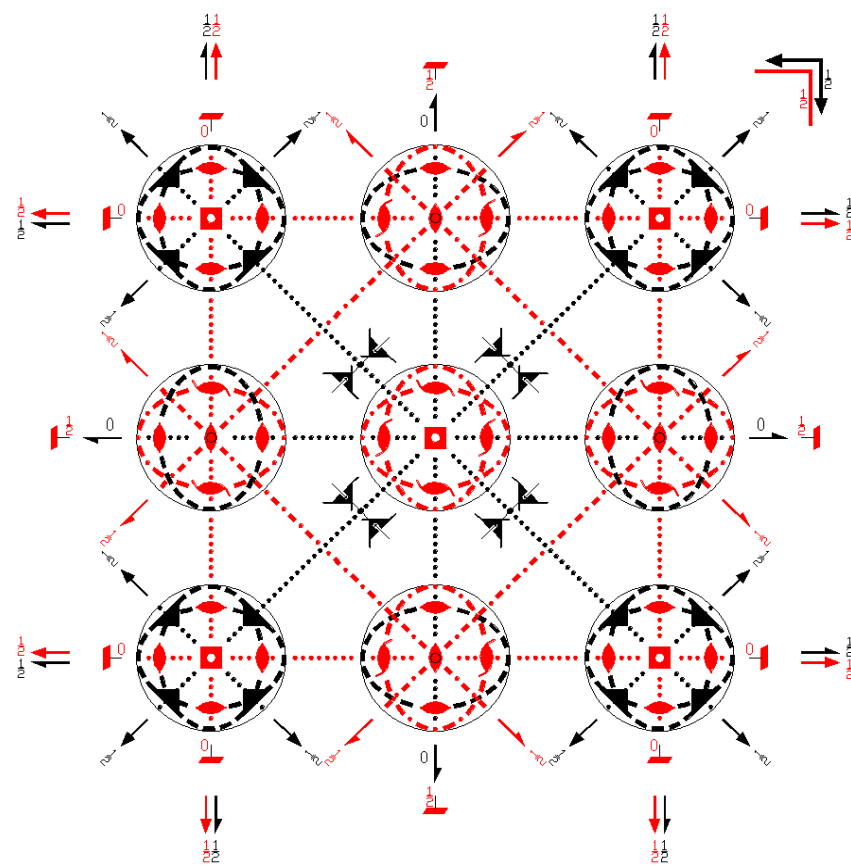
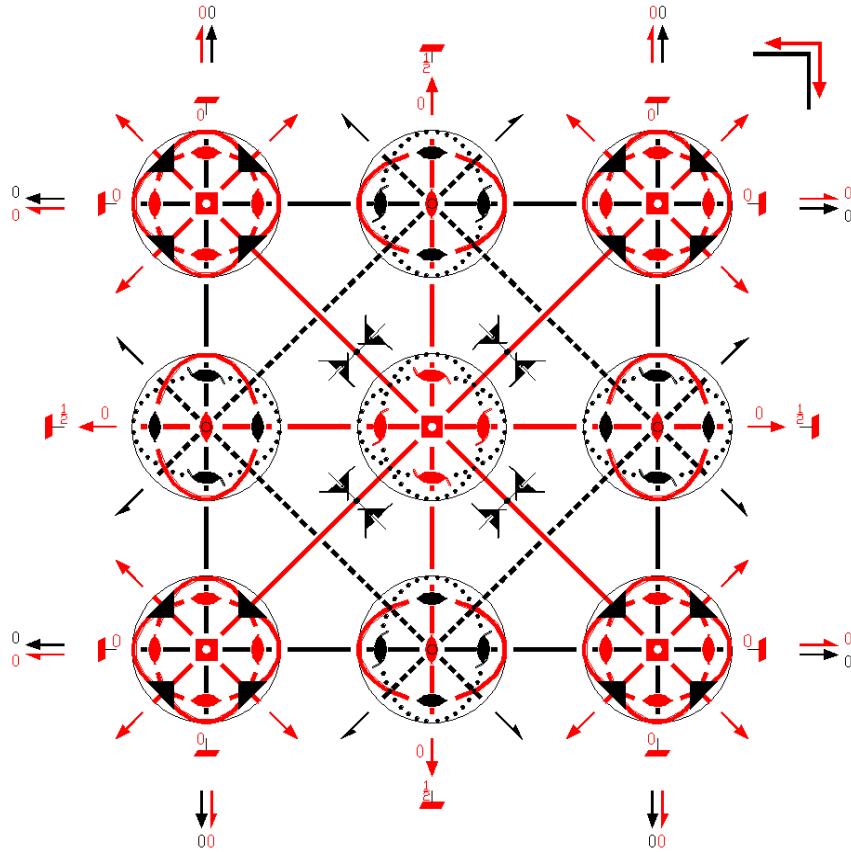
$P_F\bar{m}3m'$

221.7.1600

$m\bar{3}m1'$

$P4'/m\bar{3}2'/m'$

Cubic



Origin at center ( $m\bar{3}m'$ )

<b>Asymmetric unit</b>	$0 \leq x \leq 1/2;$	$0 \leq y \leq 1/2;$	$0 \leq z \leq 1/2;$	$y \leq x;$	$z \leq y$
Vertices	0,0,0	1/2,0,0	1/2,1/2,0	1/2,1/2,1/2	

## Symmetry Operations

For (0,0,0) + set

(1) 1 (1 0,0,0)	(2) 2 0,0,z (2 <sub>z</sub>  0,0,0)	(3) 2 0,y,0 (2 <sub>y</sub>  0,0,0)	(4) 2 x,0,0 (2 <sub>x</sub>  0,0,0)
(5) 3 <sup>+</sup> x,x,x (3 <sub>xyz</sub>  0,0,0)	(6) 3 <sup>+</sup> $\bar{x},\bar{x},\bar{x}$ (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0)	(7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$ (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0)	(8) 3 <sup>+</sup> $\bar{x},\bar{x},x$ (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0)
(9) 3 <sup>-</sup> x,x,x (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)	(10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$ (3 <sub><math>\bar{xyz}</math></sub>  0,0,0)	(11) 3 <sup>-</sup> $\bar{x},\bar{x},x$ (3 <sub>xyz</sub>  0,0,0)	(12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$ (3 <sub>xyz</sub>  0,0,0)
(13) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(14) 2' x, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  0,0,0)'	(15) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'	(16) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)'
(17) 4 <sup>-</sup> x,0,0 (4 <sub>x</sub> <sup>-1</sup>  0,0,0)'	(18) 2' 0,y,y (2 <sub>yz</sub>  0,0,0)'	(19) 2' 0,y, $\bar{y}$ (2 <sub><math>\bar{yz}</math></sub>  0,0,0)'	(20) 4 <sup>+</sup> x,0,0 (4 <sub>x</sub>  0,0,0)'
(21) 4 <sup>+</sup> 0,y,0 (4 <sub>y</sub>  0,0,0)'	(22) 2' x,0,x (2 <sub>zx</sub>  0,0,0)'	(23) 4 <sup>-</sup> 0,y,0 (4 <sub>y</sub> <sup>-1</sup>  0,0,0)'	(24) 2' $\bar{x}$ ,0,x (2 <sub><math>\bar{zx}</math></sub>  0,0,0)'
(25) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(26) m x,y,0 (m <sub>z</sub>  0,0,0)	(27) m x,0,z (m <sub>y</sub>  0,0,0)	(28) m 0,y,z (m <sub>x</sub>  0,0,0)
(29) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)	(30) $\bar{3}^+$ $\bar{x},\bar{x},\bar{x}$ ; 0,0,0 ( $\bar{3}_{\bar{xyz}}$ <sup>-1</sup>  0,0,0)	(31) $\bar{3}^+$ x, $\bar{x},\bar{x}$ ; 0,0,0 ( $\bar{3}_{\bar{xyz}}$ <sup>-1</sup>  0,0,0)	(32) $\bar{3}^+$ $\bar{x},\bar{x},x$ ; 0,0,0 ( $\bar{3}_{\bar{xyz}}$ <sup>-1</sup>  0,0,0)
(33) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)	(34) $\bar{3}^-$ x, $\bar{x},\bar{x}$ ; 0,0,0 ( $\bar{3}_{\bar{xyz}}$  0,0,0)	(35) $\bar{3}^-$ $\bar{x},\bar{x},x$ ; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)	(36) $\bar{3}^-$ $\bar{x},x,\bar{x}$ ; 0,0,0 ( $\bar{3}_{\bar{xyz}}$  0,0,0)
(37) m' x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)'	(38) m' x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,0)'	(39) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z$ <sup>-1</sup>  0,0,0)'	(40) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'
(41) $\bar{4}^-$ x,0,0; 0,0,0 ( $\bar{4}_x$ <sup>-1</sup>  0,0,0)'	(42) m' x,y, $\bar{y}$ (m <sub>yz</sub>  0,0,0)'	(43) m' x,y,y (m <sub><math>\bar{yz}</math></sub>  0,0,0)'	(44) $\bar{4}^+$ x,0,0; 0,0,0 ( $\bar{4}_x$  0,0,0)'
(45) $\bar{4}^+$ 0,y,0; 0,0,0 ( $\bar{4}_y$  0,0,0)'	(46) m' $\bar{x}$ ,y,x (m <sub>zx</sub>  0,0,0)'	(47) $\bar{4}^-$ 0,y,0; 0,0,0 ( $\bar{4}_y$ <sup>-1</sup>  0,0,0)'	(48) m' x,y,x (m <sub><math>\bar{zx}</math></sub>  0,0,0)'

For (1,0,0) + set

(1) t' (1,0,0) (1 1,0,0)'	(2) 2' 1/2,0,z (2 <sub>z</sub>  1,0,0)'	(3) 2' 1/2,y,0 (2 <sub>y</sub>  1,0,0)'	(4) 2' (1,0,0) x,0,0 (2 <sub>x</sub>  1,0,0)'
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x+2/3,x+1/3,x (3 <sub>xyz</sub>  1,0,0)'	(6) 3 <sup>+</sup> (1/3,-1/3,1/3) x+2/3,x-1/3,x (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1,0,0)'	(7) 3 <sup>+</sup> (1/3,-1/3,-1/3) x+2/3,x-1/3,x (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1,0,0)'	(8) 3 <sup>+</sup> (1/3,1/3,-1/3) x+2/3,x-1/3,x (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1,0,0)'
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x+1/3,x-1/3,x (3 <sub>xyz</sub> <sup>-1</sup>  1,0,0)'	(10) 3 <sup>-</sup> (1/3,-1/3,-1/3) x+1/3,x+1/3,x (3 <sub><math>\bar{xyz}</math></sub>  1,0,0)'	(11) 3 <sup>-</sup> (1/3,1/3,-1/3) x+1/3,x-1/3,x (3 <sub>xyz</sub>  1,0,0)'	(12) 3 <sup>-</sup> (1/3,-1/3,1/3) x+1/3,x+1/3,x (3 <sub><math>\bar{xyz}</math></sub>  1,0,0)'

(13) $2 (1/2, 1/2, 0) \quad x+1, x+1/2, 0$ $(2_{xy}   1, 0, 0)$	(14) $2 (-1/2, 1/2, 0) \quad x+1, \bar{x}-1/2, 0$ $(2_{\bar{xy}}   1, 0, 0)$	(15) $4^- 1/2, -1/2, z$ $(4_z^{-1}   1, 0, 0)$	(16) $4^+ 1/2, 1/2, z$ $(4_z   1, 0, 0)$
(17) $4^- (1, 0, 0) \quad x, 0, 0$ $(4_x^{-1}   1, 0, 0)$	(18) $2 1/2, y, y$ $(2_{yz}   1, 0, 0)$	(19) $2 1/2, y, \bar{y}$ $(2_{\bar{yz}}   1, 0, 0)$	(20) $4^+ (1, 0, 0) \quad x, 0, 0$ $(4_x   1, 0, 0)$
(21) $4^+ 1/2, y, -1/2$ $(4_y   1, 0, 0)$	(22) $2 (1/2, 0, 1/2) \quad x+1/2, 0, x$ $(2_{xz}   1, 0, 0)$	(23) $4^- 1/2, y, 1/2$ $(4_y^{-1}   1, 0, 0)$	(24) $2 \bar{x}+1/2, 0, x$ $(2_{\bar{xz}}   1, 0, 0)$
(25) $\bar{1}^+ 1/2, 0, 0$ $(\bar{1}   1, 0, 0)'$	(26) $a' (1, 0, 0) \quad x, y, 0$ $(m_z   1, 0, 0)'$	(27) $a' (1, 0, 0) \quad x, 0, z$ $(m_y   1, 0, 0)'$	(28) $m' 1/2, y, z$ $(m_x   1, 0, 0)'$
(29) $\bar{3}^+ x, x-1, x;$ $1/2, -1/2, 1/2$ $(\bar{3}_{xyz}   1, 0, 0)'$	(30) $\bar{3}^+ \bar{x}, x+1/2, \bar{x};$ $1/2, 1/2, 1/2$ $(\bar{3}_{\bar{xyz}}^{-1}   1, 0, 0)'$	(31) $\bar{3}^+ x, \bar{x}+1, \bar{x};$ $1/2, 1/2, -1/2$ $(\bar{3}_{\bar{xyz}}^{-1}   1, 0, 0)'$	(32) $\bar{3}^+ \bar{x}, \bar{x}+1, x;$ $1/2, -1/2, 1/2$ $(\bar{3}_{\bar{xyz}}^{-1}   1, 0, 0)'$
(33) $\bar{3}^- x+1, x+1, x;$ $1/2, 1/2, -1/2$ $(\bar{3}_{xyz}^{-1}   1, 0, 0)'$	(34) $\bar{3}^- x+1, \bar{x}-1, \bar{x};$ $1/2, -1/2, 1/2$ $(\bar{3}_{\bar{xyz}}   1, 0, 0)'$	(35) $\bar{3}^- \bar{x}+1, \bar{x}+1, x;$ $1/2, 1/2, 1/2$ $(\bar{3}_{\bar{xyz}}   1, 0, 0)'$	(36) $\bar{3}^- \bar{x}+1, x-1, \bar{x};$ $1/2, -1/2, -1/2$ $(\bar{3}_{\bar{xyz}}   1, 0, 0)'$
(37) $g (1/2, -1/2, 0) \quad x+1/2, \bar{x}, z$ $(m_{xy}   1, 0, 0)$	(38) $g (1/2, 1/2, 0) \quad x+1/2, x, z$ $(m_{\bar{xy}}   1, 0, 0)$	(39) $\bar{4}^- 1/2, 1/2, z; 1/2, 1/2, 0$ $(\bar{4}_z^{-1}   1, 0, 0)$	(40) $\bar{4}^+ 1/2, -1/2, z; 1/2, -1/2, 0$ $(\bar{4}_z   1, 0, 0)$
(41) $\bar{4}^- x+1/2, 0, 0; 1/2, 0, 0$ $(\bar{4}_x^{-1}   1, 0, 0)$	(42) $a (1, 0, 0) \quad x, y, \bar{y}$ $(m_{yz}   1, 0, 0)$	(43) $a (1, 0, 0) \quad x, y, y$ $(m_{\bar{yz}}   1, 0, 0)$	(44) $\bar{4}^+ x+1/2, 0, 0; 1/2, 0, 0$ $(\bar{4}_x   1, 0, 0)$
(45) $\bar{4}^+ 1/2, y, 1/2; 1/2, 0, 1/2$ $(\bar{4}_y   1, 0, 0)$	(46) $g (1/2, 0, -1/2) \quad \bar{x}+1/2, y, x$ $(m_{xz}   1, 0, 0)$	(47) $\bar{4}^- 1/2, y, -1/2; 1/2, 0, -1/2$ $(\bar{4}_y^{-1}   1, 0, 0)$	(48) $g (1/2, 0, 1/2) \quad x+1/2, y, x$ $(m_{\bar{xz}}   1, 0, 0)$

**Generators selected** (1);  $t'(1, 0, 0)$ ;  $t'(0, 1, 0)$ ;  $t'(0, 0, 1)$ ; (2); (3); (5); (13); (25).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

			(0,0,0) +	(1,0,0)' +				
96	n	1						
(1)	$x, y, z$	$[u, v, w]$	(2)	$\bar{x}, \bar{y}, z$	$[\bar{u}, \bar{v}, w]$	(3)	$\bar{x}, y, \bar{z}$	$[\bar{u}, v, \bar{w}]$
(5)	$z, x, y$	$[w, u, v]$	(6)	$z, \bar{x}, \bar{y}$	$[w, \bar{u}, \bar{v}]$	(7)	$\bar{z}, \bar{x}, y$	$[\bar{w}, \bar{u}, v]$
(9)	$y, z, x$	$[v, w, u]$	(10)	$\bar{y}, z, \bar{x}$	$[\bar{v}, w, \bar{u}]$	(11)	$y, \bar{z}, \bar{x}$	$[v, \bar{w}, \bar{u}]$
(13)	$y, x, \bar{z}$	$[\bar{v}, \bar{u}, w]$	(14)	$\bar{y}, \bar{x}, \bar{z}$	$[\bar{v}, \bar{u}, w]$	(15)	$y, \bar{x}, z$	$[\bar{v}, \bar{u}, w]$
(17)	$x, z, \bar{y}$	$[\bar{u}, \bar{w}, \bar{v}]$	(18)	$\bar{x}, z, y$	$[\bar{u}, \bar{w}, \bar{v}]$	(19)	$\bar{x}, \bar{z}, \bar{y}$	$[\bar{u}, w, v]$
(21)	$z, y, \bar{x}$	$[\bar{w}, \bar{v}, \bar{u}]$	(22)	$z, \bar{y}, x$	$[\bar{w}, \bar{v}, \bar{u}]$	(23)	$\bar{z}, y, x$	$[w, \bar{v}, \bar{u}]$
(25)	$\bar{x}, \bar{y}, \bar{z}$	$[\bar{u}, \bar{v}, \bar{w}]$	(26)	$x, y, \bar{z}$	$[\bar{u}, \bar{v}, \bar{w}]$	(27)	$x, \bar{y}, z$	$[\bar{u}, \bar{v}, \bar{w}]$
(29)	$\bar{z}, \bar{x}, \bar{y}$	$[\bar{w}, \bar{u}, \bar{v}]$	(30)	$\bar{z}, x, y$	$[\bar{w}, \bar{u}, \bar{v}]$	(31)	$z, x, \bar{y}$	$[\bar{w}, \bar{u}, \bar{v}]$
(33)	$\bar{y}, \bar{z}, \bar{x}$	$[\bar{v}, \bar{w}, \bar{u}]$	(34)	$y, \bar{z}, x$	$[\bar{v}, \bar{w}, \bar{u}]$	(35)	$\bar{y}, z, x$	$[\bar{v}, \bar{w}, \bar{u}]$
(4)	$x, \bar{y}, \bar{z}$	$[\bar{u}, \bar{v}, \bar{w}]$	(8)	$\bar{z}, x, \bar{y}$	$[\bar{w}, \bar{u}, \bar{v}]$	(12)	$\bar{y}, \bar{z}, x$	$[\bar{v}, \bar{w}, \bar{u}]$
(16)	$\bar{y}, x, z$	$[\bar{v}, \bar{u}, \bar{w}]$	(20)	$x, \bar{z}, y$	$[\bar{u}, \bar{w}, \bar{v}]$	(24)	$\bar{z}, \bar{y}, \bar{x}$	$[w, v, u]$
(28)	$\bar{x}, y, z$	$[u, \bar{v}, \bar{w}]$	(32)	$z, \bar{x}, y$	$[\bar{w}, \bar{u}, \bar{v}]$	(36)	$y, z, \bar{x}$	$[\bar{v}, \bar{w}, \bar{u}]$

(37)	$\bar{y}, \bar{x}, z$	$[\bar{v}, \bar{u}, w]$	(38)	$y, x, z$	$[v, u, w]$	(39)	$\bar{y}, x, \bar{z}$	$[\bar{v}, u, \bar{w}]$	(40)	$y, \bar{x}, \bar{z}$	$[v, \bar{u}, \bar{w}]$	
(41)	$\bar{x}, \bar{z}, y$	$[\bar{u}, \bar{w}, v]$	(42)	$x, \bar{z}, y$	$[u, \bar{w}, v]$	(43)	$x, z, y$	$[u, w, v]$	(44)	$\bar{x}, z, y$	$[\bar{u}, w, \bar{v}]$	
(45)	$\bar{z}, \bar{y}, x$	$[\bar{w}, \bar{v}, u]$	(46)	$\bar{z}, y, \bar{x}$	$[\bar{w}, v, \bar{u}]$	(47)	$z, \bar{y}, \bar{x}$	$[w, \bar{v}, \bar{u}]$	(48)	$z, y, x$	$[w, v, u]$	
48	m	..m'	$x, x, z$	$[u, u, w]$	$\bar{x}, \bar{x}, z$	$[\bar{u}, \bar{u}, \bar{w}]$	$\bar{x}, x, \bar{z}$	$[\bar{u}, u, \bar{w}]$	$x, \bar{x}, \bar{z}$	$[u, \bar{u}, \bar{w}]$	$x, x, z$	$[u, u, w]$
			$z, x, x$	$[w, u, u]$	$z, \bar{x}, \bar{x}$	$[w, \bar{u}, \bar{u}]$	$\bar{z}, \bar{x}, x$	$[w, \bar{u}, u]$	$\bar{z}, x, \bar{x}$	$[w, u, \bar{u}]$	$z, x, x$	$[w, u, u]$
			$x, z, x$	$[u, w, u]$	$\bar{x}, z, \bar{x}$	$[w, \bar{u}, \bar{u}]$	$x, \bar{z}, \bar{x}$	$[u, \bar{w}, \bar{u}]$	$\bar{x}, z, x$	$[u, w, u]$	$x, z, x$	$[u, w, u]$
			$x, x, \bar{z}$	$[\bar{u}, \bar{u}, w]$	$\bar{x}, \bar{x}, \bar{z}$	$[u, u, w]$	$x, \bar{x}, z$	$[\bar{u}, u, \bar{w}]$	$\bar{x}, x, z$	$[u, \bar{u}, \bar{w}]$	$x, x, z$	$[u, u, w]$
			$x, z, \bar{x}$	$[\bar{u}, \bar{w}, u]$	$\bar{x}, z, \bar{x}$	$[u, \bar{w}, \bar{u}]$	$\bar{x}, z, x$	$[u, w, u]$	$x, \bar{z}, x$	$[\bar{u}, w, \bar{u}]$	$x, z, x$	$[u, w, u]$
			$z, x, \bar{x}$	$[w, \bar{u}, u]$	$z, \bar{x}, \bar{x}$	$[w, u, \bar{u}]$	$\bar{z}, x, x$	$[w, \bar{u}, \bar{u}]$	$\bar{z}, \bar{x}, \bar{x}$	$[w, u, u]$	$z, x, x$	$[w, u, u]$
48	l	m'..	$1/2, y, z$	$[0, v, w]$	$1/2, \bar{y}, z$	$[0, \bar{v}, \bar{w}]$	$1/2, y, \bar{z}$	$[0, v, \bar{w}]$	$1/2, \bar{y}, z$	$[0, \bar{v}, \bar{w}]$	$1/2, y, z$	$[0, v, w]$
			$z, 1/2, y$	$[w, 0, v]$	$z, 1/2, \bar{y}$	$[w, 0, \bar{v}]$	$\bar{z}, 1/2, y$	$[w, 0, v]$	$\bar{z}, 1/2, \bar{y}$	$[w, 0, \bar{v}]$	$z, 1/2, y$	$[w, 0, v]$
			$y, z, 1/2$	$[v, w, 0]$	$\bar{y}, z, 1/2$	$[v, \bar{w}, 0]$	$y, \bar{z}, 1/2$	$[v, w, 0]$	$\bar{y}, z, 1/2$	$[v, \bar{w}, 0]$	$y, z, 1/2$	$[v, w, 0]$
			$y, 1/2, \bar{z}$	$[\bar{v}, 0, w]$	$\bar{y}, 1/2, z$	$[v, 0, \bar{w}]$	$y, 1/2, z$	$[v, 0, w]$	$\bar{y}, 1/2, z$	$[v, 0, \bar{w}]$	$y, 1/2, z$	$[v, 0, w]$
			$1/2, z, \bar{y}$	$[0, \bar{w}, v]$	$1/2, z, y$	$[0, w, v]$	$1/2, \bar{z}, \bar{y}$	$[0, \bar{w}, \bar{v}]$	$1/2, z, y$	$[0, w, v]$	$1/2, z, \bar{y}$	$[0, \bar{w}, v]$
			$z, y, 1/2$	$[w, v, 0]$	$z, \bar{y}, 1/2$	$[w, \bar{v}, 0]$	$\bar{z}, y, 1/2$	$[w, v, 0]$	$\bar{z}, \bar{y}, 1/2$	$[w, \bar{v}, 0]$	$z, y, 1/2$	$[w, v, 0]$
48	k	m..	$0, y, z$	$[u, 0, 0]$	$0, \bar{y}, z$	$[\bar{u}, 0, 0]$	$0, y, \bar{z}$	$[\bar{u}, 0, 0]$	$0, \bar{y}, z$	$[u, 0, 0]$	$0, y, z$	$[u, 0, 0]$
			$z, 0, y$	$[0, u, 0]$	$z, 0, \bar{y}$	$[0, \bar{u}, 0]$	$\bar{z}, 0, y$	$[0, u, 0]$	$\bar{z}, 0, \bar{y}$	$[0, \bar{u}, 0]$	$z, 0, y$	$[0, u, 0]$
			$y, z, 0$	$[0, 0, u]$	$\bar{y}, z, 0$	$[0, 0, \bar{u}]$	$y, \bar{z}, 0$	$[0, 0, u]$	$\bar{y}, z, 0$	$[0, 0, \bar{u}]$	$y, z, 0$	$[0, 0, u]$
			$y, 0, \bar{z}$	$[0, \bar{u}, 0]$	$\bar{y}, 0, z$	$[0, u, 0]$	$y, 0, z$	$[0, u, 0]$	$\bar{y}, 0, z$	$[0, \bar{u}, 0]$	$y, 0, z$	$[0, u, 0]$
			$0, z, \bar{y}$	$[\bar{u}, 0, 0]$	$0, z, y$	$[u, 0, 0]$	$0, \bar{z}, \bar{y}$	$[u, 0, 0]$	$0, z, y$	$[\bar{u}, 0, 0]$	$0, z, \bar{y}$	$[\bar{u}, 0, 0]$
			$z, y, 0$	$[0, 0, u]$	$z, \bar{y}, 0$	$[0, 0, \bar{u}]$	$\bar{z}, y, 0$	$[0, 0, u]$	$\bar{z}, \bar{y}, 0$	$[0, 0, \bar{u}]$	$z, y, 0$	$[0, 0, u]$
24	j	m'.m'2	$1/2, y, y$	$[0, v, v]$	$1/2, \bar{y}, y$	$[0, \bar{v}, \bar{v}]$	$1/2, y, \bar{y}$	$[0, v, \bar{v}]$	$1/2, \bar{y}, y$	$[0, \bar{v}, \bar{v}]$	$1/2, y, y$	$[0, v, v]$
			$y, 1/2, y$	$[v, 0, v]$	$y, 1/2, \bar{y}$	$[v, 0, \bar{v}]$	$\bar{y}, 1/2, y$	$[v, 0, v]$	$\bar{y}, 1/2, \bar{y}$	$[v, 0, \bar{v}]$	$y, 1/2, y$	$[v, 0, v]$
			$y, y, 1/2$	$[v, v, 0]$	$\bar{y}, y, 1/2$	$[v, \bar{v}, 0]$	$y, \bar{y}, 1/2$	$[v, v, 0]$	$\bar{y}, y, 1/2$	$[v, \bar{v}, 0]$	$y, y, 1/2$	$[v, v, 0]$
24	i	m.m'2'	$0, y, y$	$[u, 0, 0]$	$0, \bar{y}, y$	$[\bar{u}, 0, 0]$	$0, y, \bar{y}$	$[\bar{u}, 0, 0]$	$0, \bar{y}, y$	$[u, 0, 0]$	$0, y, y$	$[u, 0, 0]$
			$y, 0, y$	$[0, u, 0]$	$y, 0, \bar{y}$	$[0, \bar{u}, 0]$	$\bar{y}, 0, y$	$[0, u, 0]$	$\bar{y}, 0, \bar{y}$	$[0, \bar{u}, 0]$	$y, 0, y$	$[0, u, 0]$
			$y, y, 0$	$[0, 0, u]$	$\bar{y}, y, 0$	$[0, 0, \bar{u}]$	$y, \bar{y}, 0$	$[0, 0, u]$	$\bar{y}, y, 0$	$[0, 0, \bar{u}]$	$y, y, 0$	$[0, 0, u]$



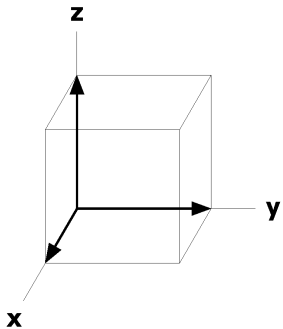
24	h	$mm'2'..$	$x, 1/2, 0 [0, 0, w]$	$\bar{x}, 1/2, 0 [0, 0, \bar{w}]$	$0, x, 1/2 [w, 0, 0]$	$0, \bar{x}, 1/2 [\bar{w}, 0, 0]$
			$1/2, 0, x [0, w, 0]$	$1/2, 0, \bar{x} [0, \bar{w}, 0]$	$1/2, x, 0 [0, 0, \bar{w}]$	$1/2, \bar{x}, 0 [0, 0, w]$
			$x, 0, 1/2 [0, \bar{w}, 0]$	$\bar{x}, 0, 1/2 [0, w, 0]$	$0, 1/2, \bar{x} [w, 0, 0]$	$0, 1/2, x [\bar{w}, 0, 0]$
16	g	$.3m'$	$x, x, x [u, u, u]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$	$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
			$x, x, \bar{x} [\bar{u}, \bar{u}, u]$	$\bar{x}, \bar{x}, \bar{x} [u, u, u]$	$x, \bar{x}, x [\bar{u}, u, \bar{u}]$	$\bar{x}, x, x [u, \bar{u}, \bar{u}]$
12	f	$4m'.m'$	$x, 1/2, 1/2 [u, 0, 0]$	$\bar{x}, 1/2, 1/2 [u, 0, 0]$	$1/2, x, 1/2 [0, u, 0]$	$1/2, \bar{x}, 1/2 [0, u, 0]$
			$1/2, \bar{x}, 1/2 [0, u, 0]$	$1/2, 1/2, x [0, 0, u]$	$1/2, 1/2, \bar{x} [0, 0, u]$	
12	e	$4'm.m'$	$x, 0, 0 [0, 0, 0]$	$\bar{x}, 0, 0 [0, 0, 0]$	$0, x, 0 [0, 0, 0]$	$0, x, 0 [0, 0, 0]$
			$0, \bar{x}, 0 [0, 0, 0]$	$0, 0, x [0, 0, 0]$	$0, 0, \bar{x} [0, 0, 0]$	
6	d	$4'/m'm.m'$	$1/2, 0, 0 [0, 0, 0]$	$0, 1/2, 0 [0, 0, 0]$	$0, 0, 1/2 [0, 0, 0]$	$0, 0, 1/2 [0, 0, 0]$
6	c	$4/mm'.m'$	$0, 1/2, 1/2 [u, 0, 0]$	$1/2, 0, 1/2 [0, u, 0]$	$1/2, 1/2, 0 [0, 0, u]$	$1/2, 1/2, 0 [0, 0, u]$
2	b	$m\bar{3}m'$	$1/2, 1/2, 1/2 [0, 0, 0]$			
2	a	$m\bar{3}m'$	$0, 0, 0 [0, 0, 0]$			

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[1, 1, 1]$   $p6mm1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

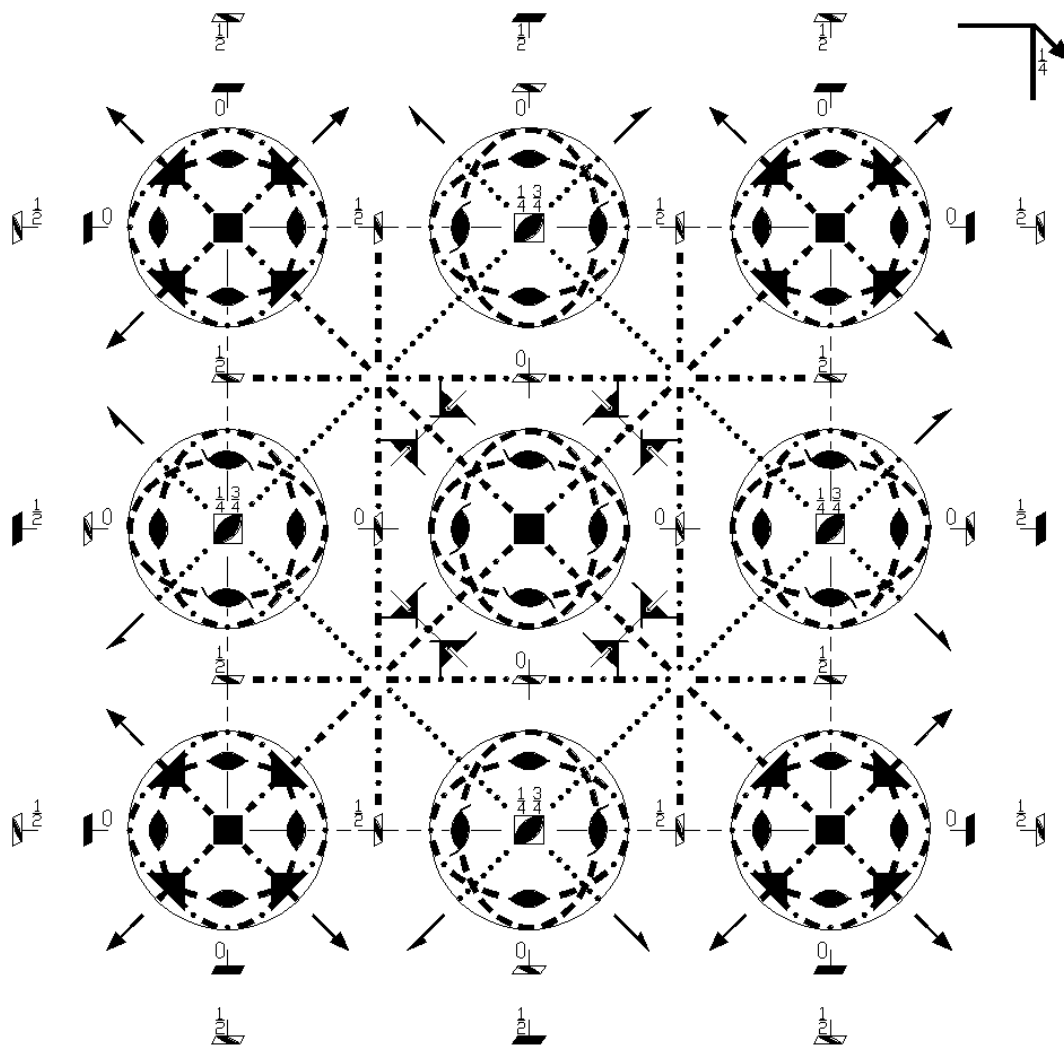
Along  $[1, 1, 0]$   $p_6c-2mm$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 1/2$



$Pn\bar{3}n$   
222.1.1601

$m\bar{3}m$   
 $P4/n\bar{3}2/n$

Cubic



**Origin** at 432, at  $-1/4, -1/4, -1/4$  from center ( $\bar{3}$ )

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq x; z \leq y$

**Vertices**  $0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/2,1/2,1/2$

**Symmetry Operations**

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{y}z</math></sub>  0,0,0)              |

(13) $2^-$ x,x,0 ( $2_{xy}$  0,0,0)	(14) $2^-$ x, $\bar{x}$ ,0 ( $2_{\bar{xy}}$  0,0,0)	(15) $4^-$ 0,0,z ( $4_z^{-1}$  0,0,0)	(16) $4^+$ 0,0,z ( $4_z$  0,0,0)
(17) $4^-$ x,0,0 ( $4_x^{-1}$  0,0,0)	(18) $2^-$ 0,y,y ( $2_{yz}$  0,0,0)	(19) $2^-$ 0,y, $\bar{y}$ ( $2_{\bar{yz}}$  0,0,0)	(20) $4^+$ x,0,0 ( $4_x$  0,0,0)
(21) $4^+$ 0,y,0 ( $4_y$  0,0,0)	(22) $2^-$ x,0,x ( $2_{xz}$  0,0,0)	(23) $4^-$ 0,y,0 ( $4_y^{-1}$  0,0,0)	(24) $2^-$ $\bar{x}$ ,0,x ( $2_{\bar{xz}}$  0,0,0)
(25) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$  1/2,1/2,12)	(26) n (1/2,1/2,0) x,y,1/4 ( $m_z$  1/2,1/2,12)	(27) n (1/2,0,1/2) x,1/4,z ( $m_y$  1/2,1/2,12)	(28) n (0,1/2,1/2) 1/4,y,z ( $m_x$  1/2,1/2,12)
(29) $\bar{3}^+$ x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}$  1/2,1/2,12)	(30) $\bar{3}^+$ $\bar{x}$ -1,x+1, $\bar{x}$ ; -1/4,1/4,3/4 ( $\bar{3}_{x\bar{y}\bar{z}^{-1}}$  1/2,1/2,12)	(31) $\bar{3}^+$ x, $\bar{x}$ +1, $\bar{x}$ ; 1/4,3/4,-1/4 ( $\bar{3}_{\bar{y}\bar{z}^{-1}}$  1/2,1/2,12)	(32) $\bar{3}^+$ $\bar{x}$ +1, $\bar{x}$ ,x; 3/4,-1/4,1/4 ( $\bar{3}_{x\bar{y}\bar{z}^{-1}}$  1/2,1/2,12)
(33) $\bar{3}^-$ x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz^{-1}}$  1/2,1/2,12)	(34) $\bar{3}^-$ x+1, $\bar{x}$ -1, $\bar{x}$ ; 1/4,-1/4,3/4 ( $\bar{3}_{\bar{y}\bar{z}}$  1/2,1/2,12)	(35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1,x; -1/4,3/4,1/4 ( $\bar{3}_{x\bar{y}\bar{z}}$  1/2,1/2,12)	(36) $\bar{3}^-$ $\bar{x}$ +1,x, $\bar{x}$ ; 3/4,1/4,-1/4 ( $\bar{3}_{x\bar{y}\bar{z}}$  1/2,1/2,12)
(37) c (0,0,1/2) x+1/2, $\bar{x}$ ,z ( $m_{xy}$  1/2,1/2,12)	(38) n (1/2,1/2,1/2) x,x,z ( $m_{\bar{xy}}$  1/2,1/2,12)	(39) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$  1/2,1/2,12)	(40) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$  1/2,1/2,12)
(41) $\bar{4}^-$ x,0,1/2; 1/4,0,1/2 ( $\bar{4}_x^{-1}$  1/2,1/2,12)	(42) a (1/2,0,0) x,y+1/2, $\bar{y}$ ( $m_{yz}$  1/2,1/2,12)	(43) n (1/2,1/2,1/2) x,y,y ( $m_{\bar{yz}}$  1/2,1/2,12)	(44) $\bar{4}^+$ x,1/2,0; 1/4,1/2,0 ( $\bar{4}_x$  1/2,1/2,12)
(45) $\bar{4}^+$ 0,y,1/2; 0,1/4,1/2 ( $\bar{4}_y$  1/2,1/2,12)	(46) b (0,1/2,0) $\bar{x}$ +1/2,y,x ( $m_{xz}$  1/2,1/2,12)	(47) $\bar{4}^-$ 1/2,y,0; 1/2,1/4,0 ( $\bar{4}_y^{-1}$  1/2,1/2,12)	(48) n (1/2,1/2,1/2) x,y,x ( $m_{\bar{xz}}$  1/2,1/2,12)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

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(1) x,y,z [u,v,w]	(2) $\bar{x}$ , $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w]	(3) $\bar{x}$ ,y, $\bar{z}$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x, $\bar{y}$ , $\bar{z}$ [u, $\bar{v}$ , $\bar{w}$ ]
(5) z,x,y [w,u,v]	(6) z, $\bar{x}$ , $\bar{y}$ [w, $\bar{u}$ , $\bar{v}$ ]	(7) $\bar{z}$ , $\bar{x}$ ,y [ $\bar{w}$ , $\bar{u}$ ,v]	(8) $\bar{z}$ ,x,y [w,u, $\bar{v}$ ]
(9) y,z,x [v,w,u]	(10) $\bar{y}$ ,z, $\bar{x}$ [ $\bar{v}$ ,w, $\bar{u}$ ]	(11) y, $\bar{z}$ , $\bar{x}$ [v, $\bar{w}$ , $\bar{u}$ ]	(12) $\bar{y}$ , $\bar{z}$ ,x [ $\bar{v}$ , $\bar{w}$ ,u]
(13) y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(14) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(15) y, $\bar{x}$ ,z [v, $\bar{u}$ ,w]	(16) $\bar{y}$ ,x,z [ $\bar{v}$ ,u,w]
(17) x,z, $\bar{y}$ [u,w, $\bar{v}$ ]	(18) $\bar{x}$ ,z,y [ $\bar{u}$ ,w,v]	(19) $\bar{x}$ , $\bar{z}$ ,y [ $\bar{u}$ , $\bar{w}$ , $\bar{v}$ ]	(20) x, $\bar{z}$ ,y [u, $\bar{w}$ ,v]
(21) z,y, $\bar{x}$ [w,v, $\bar{u}$ ]	(22) z, $\bar{y}$ ,x [w, $\bar{v}$ ,u]	(23) $\bar{z}$ ,y,x [ $\bar{w}$ ,v,u]	(24) $\bar{z}$ , $\bar{y}$ , $\bar{x}$ [ $\bar{w}$ , $\bar{v}$ , $\bar{u}$ ]
(25) $\bar{x}$ +1/2, $\bar{y}$ +1/2, $\bar{z}$ +1/2 [u,v,w]	(26) x+1/2,y+1/2, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(27) x+1/2, $\bar{y}$ +1/2,z+1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	(28) $\bar{x}$ +1/2,y+1/2,z+1/2 [u, $\bar{v}$ , $\bar{w}$ ]
(29) $\bar{z}$ +1/2, $\bar{x}$ +1/2, $\bar{y}$ +1/2 [w,u,v]	(30) $\bar{z}$ +1/2,x+1/2,y+1/2 [w, $\bar{u}$ , $\bar{v}$ ]	(31) z+1/2,x+1/2, $\bar{y}$ +1/2 [ $\bar{w}$ , $\bar{u}$ ,v]	(32) z+1/2, $\bar{x}$ +1/2,y+1/2 [ $\bar{w}$ ,u, $\bar{v}$ ]
(33) $\bar{y}$ +1/2, $\bar{z}$ +1/2, $\bar{x}$ +1/2 [v,w,u]	(34) y+1/2, $\bar{z}$ +1/2,x+1/2 [ $\bar{v}$ ,w, $\bar{u}$ ]	(35) $\bar{y}$ +1/2,z+1/2,x+1/2 [v, $\bar{w}$ , $\bar{u}$ ]	(36) y+1/2,z+1/2, $\bar{x}$ +1/2 [ $\bar{v}$ , $\bar{w}$ ,u]

- (37)  $\bar{y}+1/2, \bar{x}+1/2, z+1/2 [v, u, \bar{w}]$  (38)  $y+1/2, x+1/2, z+1/2 [\bar{v}, \bar{u}, \bar{w}]$  (39)  $\bar{y}+1/2, x+1/2, \bar{z}+1/2 [v, \bar{u}, w]$  (40)  $y+1/2, \bar{x}+1/2, \bar{z}+1/2 [\bar{v}, u, w]$   
 (41)  $\bar{x}+1/2, \bar{z}+1/2, y+1/2 [u, w, \bar{v}]$  (42)  $x+1/2, \bar{z}+1/2, \bar{y}+1/2 [\bar{u}, w, v]$  (43)  $x+1/2, z+1/2, y+1/2 [\bar{u}, \bar{w}, \bar{v}]$  (44)  $\bar{x}+1/2, z+1/2, \bar{y}+1/2 [u, \bar{w}, v]$   
 (45)  $\bar{z}+1/2, \bar{y}+1/2, x+1/2 [w, v, \bar{u}]$  (46)  $\bar{z}+1/2, y+1/2, \bar{x}+1/2 [w, \bar{v}, u]$  (47)  $z+1/2, \bar{y}+1/2, \bar{x}+1/2 [\bar{w}, v, u]$  (48)  $z+1/2, y+1/2, x+1/2 [\bar{w}, \bar{v}, \bar{u}]$

24 h ..2

$0, y, y [0, v, v]$	$0, \bar{y}, y [0, \bar{v}, v]$	$0, y, \bar{y} [0, v, \bar{v}]$	$0, \bar{y}, \bar{y} [0, \bar{v}, \bar{v}]$
$y, 0, y [v, 0, v]$	$y, 0, \bar{y} [v, 0, \bar{v}]$	$\bar{y}, 0, y [\bar{v}, 0, v]$	$\bar{y}, 0, \bar{y} [\bar{v}, 0, \bar{v}]$
$y, y, 0 [v, v, 0]$	$\bar{y}, y, 0 [\bar{v}, v, 0]$	$y, \bar{y}, 0 [v, \bar{v}, 0]$	$\bar{y}, \bar{y}, 0 [\bar{v}, \bar{v}, 0]$
$1/2, \bar{y}+1/2, \bar{y}+1/2 [0, v, v]$	$1/2, y+1/2, \bar{y}+1/2 [0, \bar{v}, v]$	$1/2, \bar{y}+1/2, y+1/2 [0, v, \bar{v}]$	$1/2, y+1/2, y+1/2 [0, \bar{v}, \bar{v}]$
$\bar{y}+1/2, 1/2, \bar{y}+1/2 [v, 0, v]$	$\bar{y}+1/2, 1/2, y+1/2 [v, 0, \bar{v}]$	$y+1/2, 1/2, \bar{y}+1/2 [\bar{v}, 0, v]$	$y+1/2, 1/2, y+1/2 [\bar{v}, 0, \bar{v}]$
$\bar{y}+1/2, \bar{y}+1/2, 1/2 [v, v, 0]$	$y+1/2, \bar{y}+1/2, 1/2 [\bar{v}, v, 0]$	$\bar{y}+1/2, y+1/2, 1/2 [v, \bar{v}, 0]$	$y+1/2, y+1/2, 1/2 [\bar{v}, \bar{v}, 0]$

24	g	2..	$x, 0, 1/2 [u, 0, 0]$	$\bar{x}, 0, 1/2 [\bar{u}, 0, 0]$	$1/2, x, 0 [0, u, 0]$	$1/2, \bar{x}, 0 [0, \bar{u}, 0]$
			$0, 1/2, x [0, 0, u]$	$0, 1/2, \bar{x} [0, 0, \bar{u}]$	$0, x, 1/2 [0, u, 0]$	$0, \bar{x}, 1/2 [0, \bar{u}, 0]$
			$x, 1/2, 0 [u, 0, 0]$	$\bar{x}, 1/2, 0 [\bar{u}, 0, 0]$	$1/2, 0, \bar{x} [0, 0, \bar{u}]$	$1/2, 0, x [0, 0, u]$
			$\bar{x}+1/2, 1/2, 0 [u, 0, 0]$	$x+1/2, 1/2, 0 [\bar{u}, 0, 0]$	$0, \bar{x}+1/2, 1/2 [0, u, 0]$	$0, x+1/2, 1/2 [0, \bar{u}, 0]$
			$1/2, 0, \bar{x}+1/2 [0, 0, u]$	$1/2, 0, x+1/2 [0, 0, \bar{u}]$	$1/2, \bar{x}+1/2, 0 [0, u, 0]$	$1/2, x+1/2, 0 [0, \bar{u}, 0]$
			$\bar{x}+1/2, 0, 1/2 [u, 0, 0]$	$x+1/2, 0, 1/2 [\bar{u}, 0, 0]$	$0, 1/2, x+1/2 [0, 0, \bar{u}]$	$0, 1/2, \bar{x}+1/2 [0, 0, u]$

16	f	.3.	$x, x, x [u, u, u]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$
			$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
			$x, x, \bar{x} [u, u, \bar{u}]$	$\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$
			$x, \bar{x}, x [u, \bar{u}, u]$	$\bar{x}, x, x [\bar{u}, u, u]$
			$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [u, u, u]$	$x+1/2, x+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, u]$
			$x+1/2, \bar{x}+1/2, x+1/2 [\bar{u}, u, \bar{u}]$	$\bar{x}+1/2, x+1/2, x+1/2 [u, \bar{u}, \bar{u}]$
			$\bar{x}+1/2, \bar{x}+1/2, x+1/2 [u, u, \bar{u}]$	$x+1/2, x+1/2, x+1/2 [\bar{u}, \bar{u}, \bar{u}]$
			$\bar{x}+1/2, x+1/2, \bar{x}+1/2 [u, \bar{u}, u]$	$x+1/2, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, u, u]$

12	e	4..	$x, 0, 0 [u, 0, 0]$	$\bar{x}, 0, 0 [0, \bar{u}, 0]$	$0, x, 0 [0, u, 0]$
			$0, \bar{x}, 0 [0, \bar{u}, 0]$	$0, 0, x [0, 0, u]$	$0, 0, \bar{x} [0, 0, \bar{u}]$
			$\bar{x}+1/2, 1/2, 1/2 [u, 0, 0]$	$x+1/2, 1/2, 1/2 [0, \bar{u}, 0]$	$1/2, \bar{x}+1/2, 1/2 [0, u, 0]$
			$1/2, x+1/2, 1/2 [0, \bar{u}, 0]$	$1/2, 1/2, \bar{x}+1/2 [0, 0, u]$	$1/2, 1/2, x+1/2 [0, 0, \bar{u}]$

Continued

222.1.1601

 $Pn\bar{3}n$ 

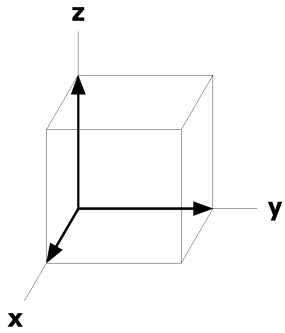
12	d	$\bar{4}..$	1/4,0,1/2 [u,0,0] 0,1/2,1/4 [0,0,u] 1/4,1/2,0 [u,0,0]	3/4,0,1/2 [ $\bar{u}$ ,0,0] 0,1/2,3/4 [0,0, $\bar{u}$ ] 3/4,1/2,0 [ $\bar{u}$ ,0,0]	1/2,1/4 [0,u,0] 0,1/4,1/2 [0,u,0] 1/2,0,3/4 [0,0, $\bar{u}$ ]	1/2,3/4,0 [0, $\bar{u}$ ,0] 0,3/4,1/2 [0, $\bar{u}$ ,0] 1/2,0,1/4 [0,0,u]
8	c	$\bar{3}..$	1/4,1/4,1/4 [u,u,u] 1/4,1/4,3/4 [u,u, $\bar{u}$ ]	3/4,3/4,1/4 [ $\bar{u}$ , $\bar{u}$ ,u] 3/4,3/4,3/4 [ $\bar{u}$ , $\bar{u}$ , $\bar{u}$ ]	3/4,1/4,3/4 [ $\bar{u}$ ,u, $\bar{u}$ ] 1/4,3/4,1/4 [u, $\bar{u}$ ,u]	1/4,3/4,3/4 [u, $\bar{u}$ , $\bar{u}$ ] 3/4,1/4,1/4 [ $\bar{u}$ ,u,u]
6	b	42.2	0,1/2,1/2 [0,0,0] 1/2,0,0 [0,0,0]	1/2,0,1/2 [0,0,0] 0,1/2,0 [0,0,0]	1/2,1/2,0 [0,0,0] 0,0,1/2 [0,0,0]	
2	a	432	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,1,1]  $p6'm'm$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

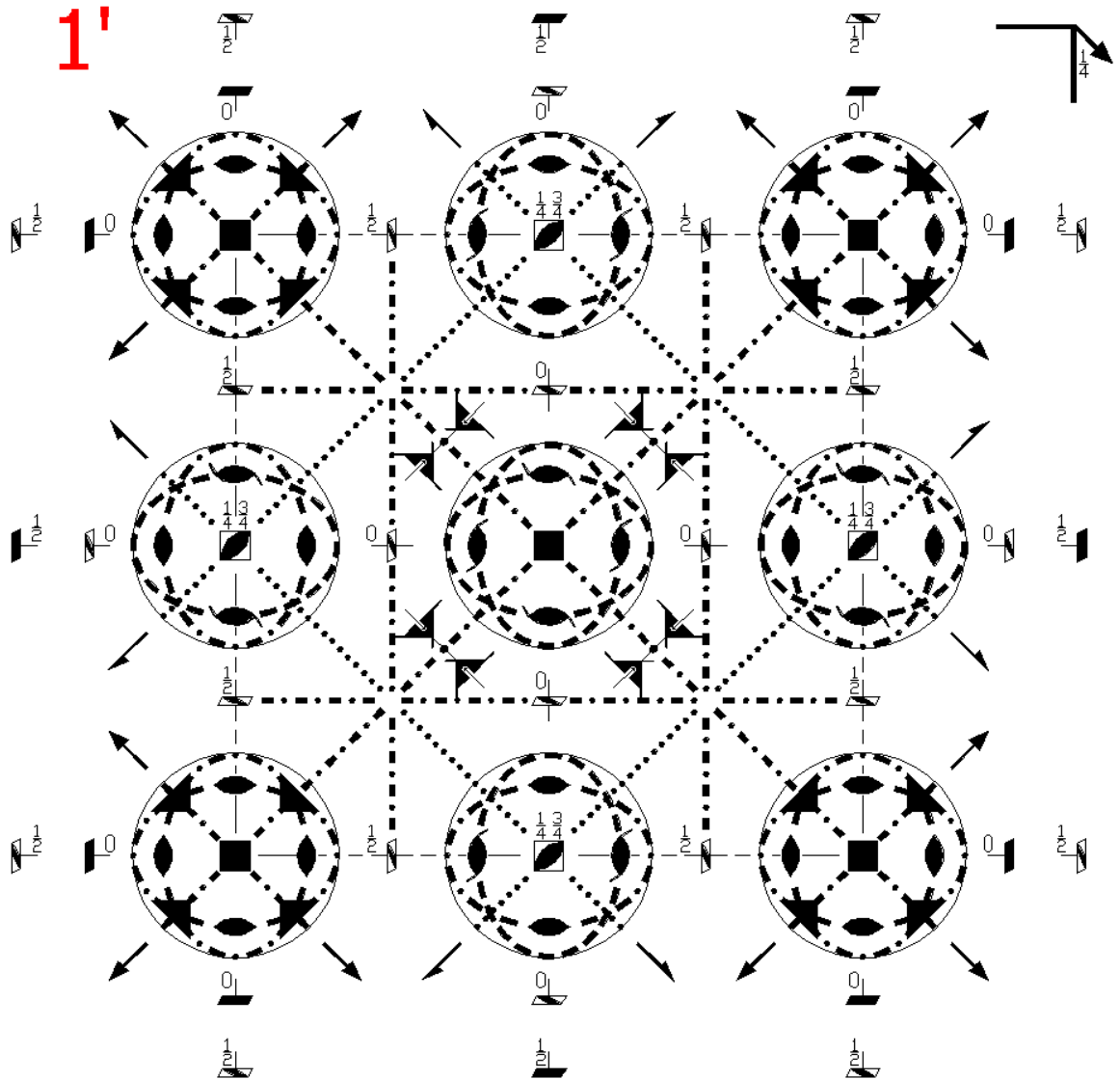
Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$Pn\bar{3}n1'$   
222.2.1602

$m\bar{3}m1'$   
 $P4/n\bar{3}2/n1'$

Cubic



**Origin** at  $4321'$ , at  $-1/4, -1/4, -1/4$  from center ( $\bar{3}1'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/2$ ;  $y \leq x$ ;  $z \leq y$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

For 1 + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                                   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                  | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                                  | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                  |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)             | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  |
| (9) $3^-$ $x,x,x$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) |

- |  |  |   |  |
|--|--|---|--|
| (13) $2^-$ x,x,0<br>( $2_{xy}$  0,0,0)                                     | (14) $2^-$ x, $\bar{x}$ ,0<br>( $2_{\bar{xy}}$  0,0,0)   | (15) $4^-$ 0,0,z<br>( $4_z^{-1}$  0,0,0)  | (16) $4^+$ 0,0,z<br>( $4_z$  0,0,0)  |
| (17) $4^-$ x,0,0<br>( $4_x^{-1}$  0,0,0)                                   | (18) $2^-$ 0,y,y<br>( $2_{yz}$  0,0,0)   | (19) $2^-$ 0,y, $\bar{y}$<br>( $2_{\bar{yz}}$  0,0,0)   | (20) $4^+$ x,0,0<br>( $4_x$  0,0,0)  |
| (21) $4^+$ 0,y,0<br>( $4_y$  0,0,0)  | (22) $2^-$ x,0,x<br>( $2_{xz}$  0,0,0)   | (23) $4^-$ 0,y,0<br>( $4_y^{-1}$  0,0,0)  | (24) $2^-$ $\bar{x}$ ,0,x<br>( $2_{\bar{xz}}$  0,0,0)  |
| (25) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,12)                     | (26) n (1/2,1/2,0) x,y,1/4<br>( $m_z$  1/2,1/2,12)   | (27) n (1/2,0,1/2) x,1/4,z<br>( $m_y$  1/2,1/2,12)  | (28) n (0,1/2,1/2) 1/4,y,z<br>( $m_x$  1/2,1/2,12)   |
| (29) $\bar{3}^+$ x,x,x; 1/4,1/4,1/4<br>( $\bar{3}_{xyz}$  1/2,1/2,12)      | (30) $\bar{3}^+$ $\bar{x}$ -1,x+1, $\bar{x}$ ; -1/4,1/4,3/4<br>( $\bar{3}_{\bar{xyz}^{-1}}$  1/2,1/2,12) | (31) $\bar{3}^+$ x, $\bar{x}$ +1, $\bar{x}$ ; 1/4,3/4,-1/4<br>( $\bar{3}_{\bar{xyz}^{-1}}$  1/2,1/2,12) | (32) $\bar{3}^+$ $\bar{x}$ +1, $\bar{x}$ ,x; 3/4,-1/4,1/4<br>( $\bar{3}_{\bar{xyz}^{-1}}$  1/2,1/2,12) |
| (33) $\bar{3}^-$ x,x,x; 1/4,1/4,1/4<br>( $\bar{3}_{xyz^{-1}}$  1/2,1/2,12) | (34) $\bar{3}^-$ x+1, $\bar{x}$ -1, $\bar{x}$ ; 1/4,-1/4,3/4<br>( $\bar{3}_{\bar{xyz}}$  1/2,1/2,12)     | (35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1,x; -1/4,3/4,1/4<br>( $\bar{3}_{\bar{xyz}}$  1/2,1/2,12)       | (36) $\bar{3}^-$ $\bar{x}$ +1,x, $\bar{x}$ ; 3/4,1/4,-1/4<br>( $\bar{3}_{\bar{xyz}}$  1/2,1/2,12)      |
| (37) c (0,0,1/2) x+1/2, $\bar{x}$ ,z<br>( $m_{xy}$  1/2,1/2,12)            | (38) n (1/2,1/2,1/2) x,x,z<br>( $m_{\bar{xy}}$  1/2,1/2,12)  | (39) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1}$  1/2,1/2,12)                                  | (40) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z$  1/2,1/2,12)                                      |
| (41) $\bar{4}^-$ x,0,1/2; 1/4,0,1/2<br>( $\bar{4}_x^{-1}$  1/2,1/2,12)     | (42) a (1/2,0,0) x,y+1/2, $\bar{y}$<br>( $m_{yz}$  1/2,1/2,12)   | (43) n (1/2,1/2,1/2) x,y,y<br>( $m_{\bar{yz}}$  1/2,1/2,12)   | (44) $\bar{4}^+$ x,1/2,0; 1/4,1/2,0<br>( $\bar{4}_x$  1/2,1/2,12)                                      |
| (45) $\bar{4}^+$ 0,y,1/2; 0,1/4,1/2<br>( $\bar{4}_y$  1/2,1/2,12)          | (46) b (0,1/2,0) $\bar{x}$ +1/2,y,x<br>( $m_{xz}$  1/2,1/2,12)   | (47) $\bar{4}^-$ 1/2,y,0; 1/2,1/4,0<br>( $\bar{4}_y^{-1}$  1/2,1/2,12)                                  | (48) n (1/2,1/2,1/2) x,y,x<br>( $m_{\bar{xz}}$  1/2,1/2,12)  |

For 1' + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1'<br>(1 0,0,0)'   | (2) 2' 0,0,z<br>( $2_z$  0,0,0)'   | (3) 2' 0,y,0<br>( $2_y$  0,0,0)'  | (4) 2' x,0,0<br>( $2_x$  0,0,0)'   |
| (5) $3^{+'}$ x,x,x<br>( $3_{xyz}$  0,0,0)'                                     | (6) $3^{+'}$ $\bar{x}$ ,x, $\bar{x}$<br>( $3_{\bar{xyz}^{-1}}$  0,0,0)'                                      | (7) $3^{+'}$ x, $\bar{x}$ , $\bar{x}$<br>( $3_{\bar{xyz}^{-1}}$  0,0,0)'                                    | (8) $3^{+'}$ $\bar{x}$ , $\bar{x}$ ,x<br>( $3_{\bar{xyz}^{-1}}$  0,0,0)'                                   |
| (9) $3^{-'}$ x,x,x<br>( $3_{xyz^{-1}}$  0,0,0)'                                | (10) $3^{-'}$ x, $\bar{x}$ , $\bar{x}$<br>( $3_{\bar{xyz}}$  0,0,0)'   | (11) $3^{-'}$ $\bar{x}$ , $\bar{x}$ ,x<br>( $3_{\bar{xyz}}$  0,0,0)'  | (12) $3^{-'}$ $\bar{x}$ ,x, $\bar{x}$<br>( $3_{\bar{xyz}}$  0,0,0)'  |
| (13) 2' x,x,0<br>( $2_{xy}$  0,0,0)'   | (14) 2' x, $\bar{x}$ ,0<br>( $2_{\bar{xy}}$  0,0,0)'   | (15) $4^{-'}$ 0,0,z<br>( $4_z^{-1}$  0,0,0)'  | (16) $4^{+'}$ 0,0,z<br>( $4_z$  0,0,0)'  |
| (17) $4^{-'}$ x,0,0<br>( $4_x^{-1}$  0,0,0)'                                   | (18) 2' 0,y,y<br>( $2_{yz}$  0,0,0)'   | (19) 2' 0,y, $\bar{y}$<br>( $2_{\bar{yz}}$  0,0,0)'   | (20) $4^{+'}$ x,0,0<br>( $4_x$  0,0,0)'  |
| (21) $4^{+'}$ 0,y,0<br>( $4_y$  0,0,0)'  | (22) 2' x,0,x<br>( $2_{xz}$  0,0,0)'   | (23) $4^{-'}$ 0,y,0<br>( $4_y^{-1}$  0,0,0)'  | (24) 2' $\bar{x}$ ,0,x<br>( $2_{\bar{xz}}$  0,0,0)'  |
| (25) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,12)'                        | (26) n' (1/2,1/2,0) x,y,1/4<br>( $m_z$  1/2,1/2,12)'   | (27) n' (1/2,0,1/2) x,1/4,z<br>( $m_y$  1/2,1/2,12)'  | (28) n' (0,1/2,1/2) 1/4,y,z<br>( $m_x$  1/2,1/2,12)'   |
| (29) $\bar{3}^{+'}$ x,x,x; 1/4,1/4,1/4<br>( $\bar{3}_{xyz}$  1/2,1/2,12)'      | (30) $\bar{3}^{+'}$ $\bar{x}$ -1,x+1, $\bar{x}$ ; -1/4,1/4,3/4<br>( $\bar{3}_{\bar{xyz}^{-1}}$  1/2,1/2,12)' | (31) $\bar{3}^{+'}$ x, $\bar{x}$ +1, $\bar{x}$ ; 1/4,3/4,-1/4<br>( $\bar{3}_{\bar{xyz}^{-1}}$  1/2,1/2,12)' | (32) $\bar{3}^{+'}$ $\bar{x}$ +1, $\bar{x}$ ,x; 3/4,-1/4,1/4<br>( $\bar{3}_{\bar{xyz}^{-1}}$  1/2,1/2,12)' |
| (33) $\bar{3}^{-'}$ x,x,x; 1/4,1/4,1/4<br>( $\bar{3}_{xyz^{-1}}$  1/2,1/2,12)' | (34) $\bar{3}^{-'}$ x+1, $\bar{x}$ -1, $\bar{x}$ ; 1/4,-1/4,3/4<br>( $\bar{3}_{\bar{xyz}}$  1/2,1/2,12)'     | (35) $\bar{3}^{-'}$ $\bar{x}$ , $\bar{x}$ +1,x; -1/4,3/4,1/4<br>( $\bar{3}_{\bar{xyz}}$  1/2,1/2,12)'       | (36) $\bar{3}^{-'}$ $\bar{x}$ +1,x, $\bar{x}$ ; 3/4,1/4,-1/4<br>( $\bar{3}_{\bar{xyz}}$  1/2,1/2,12)'      |

(37) c' (0,0,1/2) $\bar{x}+1/2,\bar{z}$ ( $m_{xy} 1/2,1/2,12$ )'	(38) n' (1/2,1/2,1/2) x,x,z ( $m_{\bar{xy}} 1/2,1/2,12$ )'	(39) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1} 1/2,1/2,12$ )'	(40) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z 1/2,1/2,12$ )'
(41) $\bar{4}^-$ ' x,0,1/2; 1/4,0,1/2 ( $\bar{4}_x^{-1} 1/2,1/2,12$ )'	(42) a' (1/2,0,0) x,y+1/2, $\bar{y}$ ( $m_{yz} 1/2,1/2,12$ )'	(43) n' (1/2,1/2,1/2) x,y,y ( $m_{\bar{yz}} 1/2,1/2,12$ )'	(44) $\bar{4}^+$ ' x,1/2,0; 1/4,1/2,0 ( $\bar{4}_x 1/2,1/2,12$ )'
(45) $\bar{4}^+$ ' 0,y,1/2; 0,1/4,1/2 ( $\bar{4}_y 1/2,1/2,12$ )'	(46) b' (0,1/2,0) $\bar{x}+1/2,y,x$ ( $m_{xz} 1/2,1/2,12$ )'	(47) $\bar{4}^-$ ' 1/2,y,0; 1/2,1/4,0 ( $\bar{4}_y^{-1} 1/2,1/2,12$ )'	(48) n' (1/2,1/2,1/2) x,y,x ( $m_{\bar{xz}} 1/2,1/2,12$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25); 1'.

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	1 +		1' +	
48 i 11'				
(1) x,y,z [0,0,0]	(2) $\bar{x},\bar{y},z$ [0,0,0]	(3) $\bar{x},y,\bar{z}$ [0,0,0]	(4) x, $\bar{y},\bar{z}$ [0,0,0]	
(5) z,x,y [0,0,0]	(6) z, $\bar{x},\bar{y}$ [0,0,0]	(7) $\bar{z},\bar{x},y$ [0,0,0]	(8) $\bar{z},x,\bar{y}$ [0,0,0]	
(9) y,z,x [0,0,0]	(10) $\bar{y},z,\bar{x}$ [0,0,0]	(11) y, $\bar{z},\bar{x}$ [0,0,0]	(12) $\bar{y},\bar{z},x$ [0,0,0]	
(13) y,x, $\bar{z}$ [0,0,0]	(14) $\bar{y},\bar{x},\bar{z}$ [0,0,0]	(15) y, $\bar{x},z$ [0,0,0]	(16) $\bar{y},x,z$ [0,0,0]	
(17) x,z, $\bar{y}$ [0,0,0]	(18) $\bar{x},z,y$ [0,0,0]	(19) $\bar{x},\bar{z},\bar{y}$ [0,0,0]	(20) x, $\bar{z},y$ [0,0,0]	
(21) z,y, $\bar{x}$ [0,0,0]	(22) z, $\bar{y},x$ [0,0,0]	(23) $\bar{z},y,x$ [0,0,0]	(24) $\bar{z},\bar{y},\bar{x}$ [0,0,0]	
(25) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2$ [0,0,0]	(26) $x+1/2,y+1/2,\bar{z}+1/2$ [0,0,0]	(27) $x+1/2,\bar{y}+1/2,z+1/2$ [0,0,0]	(28) $\bar{x}+1/2,y+1/2,z+1/2$ [0,0,0]	
(29) $\bar{z}+1/2,\bar{x}+1/2,\bar{y}+1/2$ [0,0,0]	(30) $\bar{z}+1/2,x+1/2,y+1/2$ [0,0,0]	(31) $z+1/2,x+1/2,\bar{y}+1/2$ [0,0,0]	(32) $z+1/2,\bar{x}+1/2,y+1/2$ [0,0,0]	
(33) $\bar{y}+1/2,\bar{z}+1/2,\bar{x}+1/2$ [0,0,0]	(34) $y+1/2,\bar{z}+1/2,x+1/2$ [0,0,0]	(35) $\bar{y}+1/2,z+1/2,x+1/2$ [0,0,0]	(36) $y+1/2,z+1/2,\bar{x}+1/2$ [0,0,0]	
(37) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [0,0,0]	(38) $y+1/2,x+1/2,z+1/2$ [0,0,0]	(39) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [0,0,0]	(40) $y+1/2,\bar{x}+1/2,\bar{z}+1/2$ [0,0,0]	
(41) $\bar{x}+1/2,\bar{z}+1/2,y+1/2$ [0,0,0]	(42) $x+1/2,\bar{z}+1/2,\bar{y}+1/2$ [0,0,0]	(43) $x+1/2,z+1/2,y+1/2$ [0,0,0]	(44) $\bar{x}+1/2,z+1/2,\bar{y}+1/2$ [0,0,0]	
(45) $\bar{z}+1/2,\bar{y}+1/2,x+1/2$ [0,0,0]	(46) $\bar{z}+1/2,y+1/2,\bar{x}+1/2$ [0,0,0]	(47) $z+1/2,\bar{y}+1/2,\bar{x}+1/2$ [0,0,0]	(48) $z+1/2,y+1/2,x+1/2$ [0,0,0]	
24 h ..21'				
0,y,y [0,0,0]	0, $\bar{y},y$ [0,0,0]	0,y, $\bar{y}$ [0,0,0]	0, $\bar{y},\bar{y}$ [0,0,0]	
y,0,y [0,0,0]	y,0, $\bar{y}$ [0,0,0]	$\bar{y},0,y$ [0,0,0]	$\bar{y},0,\bar{y}$ [0,0,0]	
y,y,0 [0,0,0]	$\bar{y},y,0$ [0,0,0]	y, $\bar{y},0$ [0,0,0]	$\bar{y},\bar{y},0$ [0,0,0]	



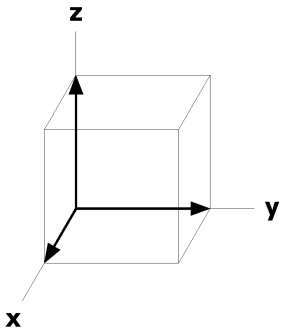
			$1/2, \bar{y}+1/2, \bar{y}+1/2 [0,0,0]$	$1/2, y+1/2, \bar{y}+1/2 [0,0,0]$	$1/2, \bar{y}+1/2, y+1/2 [0,0,0]$	$1/2, y+1/2, y+1/2 [0,0,0]$
			$\bar{y}+1/2, 1/2, \bar{y}+1/2 [0,0,0]$	$\bar{y}+1/2, 1/2, y+1/2 [0,0,0]$	$y+1/2, 1/2, \bar{y}+1/2 [0,0,0]$	$y+1/2, 1/2, y+1/2 [0,0,0]$
			$\bar{y}+1/2, \bar{y}+1/2, 1/2 [0,0,0]$	$y+1/2, \bar{y}+1/2, 1/2 [0,0,0]$	$\bar{y}+1/2, y+1/2, 1/2 [0,0,0]$	$y+1/2, y+1/2, 1/2 [0,0,0]$
24	g	2..1'	$x, 0, 1/2 [0,0,0]$	$\bar{x}, 0, 1/2 [0,0,0]$	$1/2, x, 0 [0,0,0]$	$1/2, \bar{x}, 0 [0,0,0]$
			$0, 1/2, x [0,0,0]$	$0, 1/2, \bar{x} [0,0,0]$	$0, x, 1/2 [0,0,0]$	$0, \bar{x}, 1/2 [0,0,0]$
			$x, 1/2, 0 [0,0,0]$	$\bar{x}, 1/2, 0 [0,0,0]$	$1/2, 0, \bar{x} [0,0,0]$	$1/2, 0, x [0,0,0]$
			$\bar{x}+1/2, 1/2, 0 [0,0,0]$	$x+1/2, 1/2, 0 [0,0,0]$	$0, \bar{x}+1/2, 1/2 [0,0,0]$	$0, x+1/2, 1/2 [0,0,0]$
			$1/2, 0, \bar{x}+1/2 [0,0,0]$	$1/2, 0, x+1/2 [0,0,0]$	$1/2, \bar{x}+1/2, 0 [0,0,0]$	$1/2, x+1/2, 0 [0,0,0]$
			$\bar{x}+1/2, 0, 1/2 [0,0,0]$	$x+1/2, 0, 1/2 [0,0,0]$	$0, 1/2, x+1/2 [0,0,0]$	$0, 1/2, \bar{x}+1/2 [0,0,0]$
16	f	.3.1'	$x, x, x [0,0,0]$		$\bar{x}, \bar{x}, x [0,0,0]$	
			$\bar{x}, x, \bar{x} [0,0,0]$		$x, \bar{x}, \bar{x} [0,0,0]$	
			$x, x, \bar{x} [0,0,0]$		$\bar{x}, \bar{x}, \bar{x} [0,0,0]$	
			$x, \bar{x}, x [0,0,0]$		$\bar{x}, x, x [0,0,0]$	
			$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [0,0,0]$		$x+1/2, x+1/2, \bar{x}+1/2 [0,0,0]$	
			$x+1/2, \bar{x}+1/2, x+1/2 [0,0,0]$		$\bar{x}+1/2, x+1/2, x+1/2 [0,0,0]$	
			$\bar{x}+1/2, \bar{x}+1/2, x+1/2 [0,0,0]$		$x+1/2, x+1/2, x+1/2 [0,0,0]$	
			$\bar{x}+1/2, x+1/2, \bar{x}+1/2 [0,0,0]$		$x+1/2, \bar{x}+1/2, \bar{x}+1/2 [0,0,0]$	
12	e	4..1'	$x, 0, 0 [0,0,0]$	$\bar{x}, 0, 0 [0,0,0]$	$0, x, 0 [0,0,0]$	$0, 0, \bar{x} [0,0,0]$
			$0, \bar{x}, 0 [0,0,0]$	$0, 0, x [0,0,0]$	$0, 0, \bar{x} [0,0,0]$	$0, 0, x [0,0,0]$
			$\bar{x}+1/2, 1/2, 1/2 [0,0,0]$	$x+1/2, 1/2, 1/2 [0,0,0]$	$1/2, \bar{x}+1/2, 1/2 [0,0,0]$	$1/2, \bar{x}+1/2, 1/2 [0,0,0]$
			$1/2, x+1/2, 1/2 [0,0,0]$	$1/2, 1/2, \bar{x}+1/2 [0,0,0]$	$1/2, 1/2, x+1/2 [0,0,0]$	$1/2, 1/2, x+1/2 [0,0,0]$
12	d	$\bar{4}..1'$	$1/4, 0, 1/2 [0,0,0]$	$3/4, 0, 1/2 [0,0,0]$	$1/2, 1/4 [0,0,0]$	$1/2, 3/4, 0 [0,0,0]$
			$0, 1/2, 1/4 [0,0,0]$	$0, 1/2, 3/4 [0,0,0]$	$0, 1/4, 1/2 [0,0,0]$	$0, 3/4, 1/2 [0,0,0]$
			$1/4, 1/2, 0 [0,0,0]$	$3/4, 1/2, 0 [0,0,0]$	$1/2, 0, 3/4 [0,0,0]$	$1/2, 0, 1/4 [0,0,0]$
8	c	$\bar{3}..1'$	$1/4, 1/4, 1/4 [0,0,0]$	$3/4, 3/4, 1/4 [0,0,0]$	$3/4, 1/4, 3/4 [0,0,0]$	$1/4, 3/4, 3/4 [0,0,0]$
			$1/4, 1/4, 3/4 [0,0,0]$	$3/4, 3/4, 3/4 [0,0,0]$	$1/4, 3/4, 1/4 [0,0,0]$	$3/4, 1/4, 1/4 [0,0,0]$
6	b	42.21'	$0, 1/2, 1/2 [0,0,0]$	$1/2, 0, 1/2 [0,0,0]$	$1/2, 1/2, 0 [0,0,0]$	$1/2, 1/2, 0 [0,0,0]$
			$1/2, 0, 0 [0,0,0]$	$0, 1/2, 0 [0,0,0]$	$0, 0, 1/2 [0,0,0]$	$0, 0, 1/2 [0,0,0]$
2	a	4321'	$0, 0, 0 [0,0,0]$	$1/2, 1/2, 1/2 [0,0,0]$		

**Symmetry of Special Projections**

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at 0,0,z

Along [1,1,1]  $p6mm1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
Origin at x,x,x

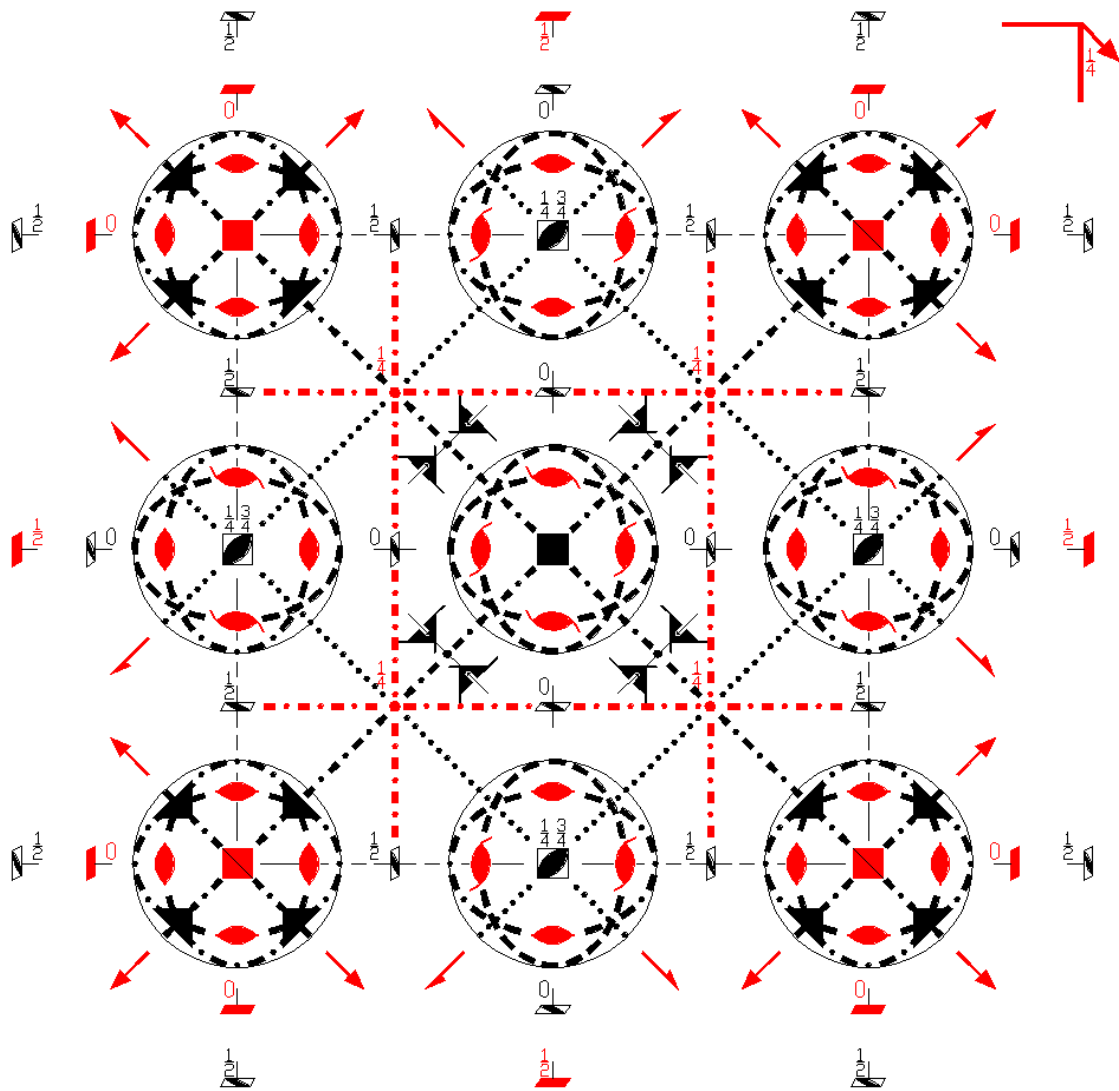
Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at x,x,0



$Pn\bar{3}n$   
222.3.1603

$m\bar{3}m$   
 $P4/n\bar{3}2/n$

Cubic



Origin at  $4'32'$ , at  $-1/4, -1/4, -1/4$  from center ( $\bar{3}'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq x; z \leq y$

Vertices  $0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/2,1/2,1/2$

### Symmetry Operations

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                  | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)              |

(13) $2' \ x, x, 0$ ( $2_{xy}   0, 0, 0$ )'	(14) $2' \ x, \bar{x}, 0$ ( $2_{\bar{xy}}   0, 0, 0$ )'	(15) $4' \ 0, 0, z$ ( $4_z^{-1}   0, 0, 0$ )'	(16) $4^+ \ 0, 0, z$ ( $4_z   0, 0, 0$ )'
(17) $4' \ x, 0, 0$ ( $4_x^{-1}   0, 0, 0$ )'	(18) $2' \ 0, y, y$ ( $2_{yz}   0, 0, 0$ )'	(19) $2' \ 0, y, \bar{y}$ ( $2_{\bar{yz}}   0, 0, 0$ )'	(20) $4^+ \ x, 0, 0$ ( $4_x   0, 0, 0$ )'
(21) $4^+ \ 0, y, 0$ ( $4_y   0, 0, 0$ )'	(22) $2' \ x, 0, x$ ( $2_{xz}   0, 0, 0$ )'	(23) $4' \ 0, y, 0$ ( $4_y^{-1}   0, 0, 0$ )'	(24) $2' \ \bar{x}, 0, x$ ( $2_{\bar{xz}}   0, 0, 0$ )'
(25) $\bar{1} \ 1/4, 1/4, 1/4$ ( $\bar{1}   1/2, 1/2, 12$ )'	(26) $n' \ (1/2, 1/2, 0) \ x, y, 1/4$ ( $m_z   1/2, 1/2, 12$ )'	(27) $n' \ (1/2, 0, 1/2) \ x, 1/4, z$ ( $m_y   1/2, 1/2, 12$ )'	(28) $n' \ (0, 1/2, 1/2) \ 1/4, y, z$ ( $m_x   1/2, 1/2, 12$ )'
(29) $\bar{3}^+ \ x, x, x; 1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 1/2, 12$ )'	(30) $\bar{3}^+ \ \bar{x}-1, x+1, \bar{x}; -1/4, 1/4, 3/4$ ( $\bar{3}_{\bar{xyz}^{-1}}   1/2, 1/2, 12$ )'	(31) $\bar{3}^+ \ x, \bar{x}+1, \bar{x}; 1/4, 3/4, -1/4$ ( $\bar{3}_{\bar{xyz}^{-1}}   1/2, 1/2, 12$ )'	(32) $\bar{3}^+ \ \bar{x}+1, \bar{x}, x; 3/4, -1/4, 1/4$ ( $\bar{3}_{\bar{xyz}^{-1}}   1/2, 1/2, 12$ )'
(33) $\bar{3}^- \ x, x, x; 1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 12$ )'	(34) $\bar{3}^- \ x+1, \bar{x}-1, \bar{x}; 1/4, -1/4, 3/4$ ( $\bar{3}_{\bar{xyz}}   1/2, 1/2, 12$ )'	(35) $\bar{3}^- \ \bar{x}, \bar{x}+1, x; -1/4, 3/4, 1/4$ ( $\bar{3}_{\bar{xyz}}   1/2, 1/2, 12$ )'	(36) $\bar{3}^- \ \bar{x}+1, x, \bar{x}; 3/4, 1/4, -1/4$ ( $\bar{3}_{\bar{xyz}}   1/2, 1/2, 12$ )'
(37) $c \ (0, 0, 1/2) \ x+1/2, \bar{x}, z$ ( $m_{xy}   1/2, 1/2, 12$ )	(38) $n \ (1/2, 1/2, 1/2) \ x, x, z$ ( $m_{\bar{xy}}   1/2, 1/2, 12$ )	(39) $\bar{4}^- \ 0, 1/2, z; 0, 1/2, 1/4$ ( $\bar{4}_z^{-1}   1/2, 1/2, 12$ )	(40) $\bar{4}^+ \ 1/2, 0, z; 1/2, 0, 1/4$ ( $\bar{4}_z   1/2, 1/2, 12$ )
(41) $\bar{4}^- \ x, 0, 1/2; 1/4, 0, 1/2$ ( $\bar{4}_x^{-1}   1/2, 1/2, 12$ )	(42) $a \ (1/2, 0, 0) \ x, y+1/2, \bar{y}$ ( $m_{yz}   1/2, 1/2, 12$ )	(43) $n \ (1/2, 1/2, 1/2) \ x, y, y$ ( $m_{\bar{yz}}   1/2, 1/2, 12$ )	(44) $\bar{4}^+ \ x, 1/2, 0; 1/4, 1/2, 0$ ( $\bar{4}_x   1/2, 1/2, 12$ )
(45) $\bar{4}^+ \ 0, y, 1/2; 0, 1/4, 1/2$ ( $\bar{4}_y   1/2, 1/2, 12$ )	(46) $b \ (0, 1/2, 0) \ \bar{x}+1/2, y, x$ ( $m_{xz}   1/2, 1/2, 12$ )	(47) $\bar{4}^- \ 1/2, y, 0; 1/2, 1/4, 0$ ( $\bar{4}_y^{-1}   1/2, 1/2, 12$ )	(48) $n \ (1/2, 1/2, 1/2) \ x, y, x$ ( $m_{\bar{xz}}   1/2, 1/2, 12$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

### Coordinates

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(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{x}, y, \bar{z} [\bar{u}, v, \bar{w}]$	(4) $x, \bar{y}, \bar{z} [u, \bar{v}, \bar{w}]$
(5) $z, x, y [w, u, v]$	(6) $z, \bar{x}, \bar{y} [w, \bar{u}, \bar{v}]$	(7) $\bar{z}, \bar{x}, y [\bar{w}, \bar{u}, v]$	(8) $\bar{z}, x, \bar{y} [\bar{w}, u, \bar{v}]$
(9) $y, z, x [v, w, u]$	(10) $\bar{y}, z, \bar{x} [\bar{v}, w, \bar{u}]$	(11) $y, \bar{z}, \bar{x} [v, \bar{w}, \bar{u}]$	(12) $\bar{y}, \bar{z}, x [\bar{v}, \bar{w}, u]$
(13) $y, x, \bar{z} [\bar{v}, \bar{u}, w]$	(14) $\bar{y}, \bar{x}, \bar{z} [\bar{v}, u, w]$	(15) $y, \bar{x}, z [v, u, \bar{w}]$	(16) $\bar{y}, x, z [v, u, \bar{w}]$
(17) $x, z, \bar{y} [\bar{u}, \bar{w}, \bar{v}]$	(18) $\bar{x}, z, y [u, \bar{w}, \bar{v}]$	(19) $\bar{x}, \bar{z}, \bar{y} [u, w, v]$	(20) $x, \bar{z}, y [\bar{u}, w, \bar{v}]$
(21) $z, y, \bar{x} [\bar{w}, \bar{v}, u]$	(22) $z, \bar{y}, x [\bar{w}, v, \bar{u}]$	(23) $\bar{z}, y, x [w, \bar{v}, \bar{u}]$	(24) $\bar{z}, \bar{y}, \bar{x} [w, v, u]$
(25) $\bar{x}+1/2, \bar{y}+1/2, \bar{z}+1/2 [\bar{u}, \bar{v}, \bar{w}]$	(26) $x+1/2, y+1/2, \bar{z}+1/2 [u, v, \bar{w}]$	(27) $x+1/2, \bar{y}+1/2, z+1/2 [u, \bar{v}, w]$	(28) $\bar{x}+1/2, y+1/2, z+1/2 [\bar{u}, v, w]$
(29) $\bar{z}+1/2, \bar{x}+1/2, \bar{y}+1/2 [\bar{w}, \bar{u}, \bar{v}]$	(30) $\bar{z}+1/2, x+1/2, y+1/2 [\bar{w}, u, v]$	(31) $z+1/2, x+1/2, \bar{y}+1/2 [w, u, \bar{v}]$	(32) $z+1/2, \bar{x}+1/2, y+1/2 [w, \bar{u}, v]$
(33) $\bar{y}+1/2, \bar{z}+1/2, \bar{x}+1/2 [\bar{v}, \bar{w}, \bar{u}]$	(34) $y+1/2, \bar{z}+1/2, x+1/2 [v, \bar{w}, u]$	(35) $\bar{y}+1/2, z+1/2, x+1/2 [\bar{v}, w, u]$	(36) $y+1/2, z+1/2, \bar{x}+1/2 [v, w, \bar{u}]$

- (37)  $\bar{y}+1/2, \bar{x}+1/2, z+1/2 [v, u, \bar{w}]$  (38)  $y+1/2, x+1/2, z+1/2 [\bar{v}, \bar{u}, \bar{w}]$  (39)  $\bar{y}+1/2, x+1/2, \bar{z}+1/2 [v, \bar{u}, w]$  (40)  $y+1/2, \bar{x}+1/2, \bar{z}+1/2 [\bar{v}, u, w]$   
 (41)  $\bar{x}+1/2, \bar{z}+1/2, y+1/2 [u, w, \bar{v}]$  (42)  $x+1/2, \bar{z}+1/2, \bar{y}+1/2 [\bar{u}, w, v]$  (43)  $x+1/2, z+1/2, y+1/2 [\bar{u}, \bar{w}, \bar{v}]$  (44)  $\bar{x}+1/2, z+1/2, \bar{y}+1/2 [u, \bar{w}, v]$   
 (45)  $\bar{z}+1/2, \bar{y}+1/2, x+1/2 [w, v, \bar{u}]$  (46)  $\bar{z}+1/2, y+1/2, \bar{x}+1/2 [w, \bar{v}, u]$  (47)  $z+1/2, \bar{y}+1/2, \bar{x}+1/2 [\bar{w}, v, u]$  (48)  $z+1/2, y+1/2, x+1/2 [\bar{w}, \bar{v}, \bar{u}]$

24 h ..2'

$0, y, y [u, v, \bar{v}]$	$0, \bar{y}, y [\bar{u}, \bar{v}, \bar{v}]$	$0, y, \bar{y} [\bar{u}, v, v]$	$0, \bar{y}, \bar{y} [u, \bar{v}, v]$
$y, 0, y [\bar{v}, u, v]$	$y, 0, \bar{y} [\bar{v}, \bar{u}, \bar{v}]$	$\bar{y}, 0, y [v, \bar{u}, v]$	$\bar{y}, 0, \bar{y} [v, u, \bar{v}]$
$y, y, 0 [v, \bar{v}, u]$	$\bar{y}, y, 0 [\bar{v}, \bar{v}, \bar{u}]$	$y, \bar{y}, 0 [v, v, \bar{u}]$	$\bar{y}, \bar{y}, 0 [\bar{v}, v, u]$
$1/2, \bar{y}+1/2, \bar{y}+1/2 [\bar{u}, \bar{v}, v]$	$1/2, y+1/2, \bar{y}+1/2 [u, v, v]$	$1/2, \bar{y}+1/2, y+1/2 [u, \bar{v}, \bar{v}]$	$1/2, y+1/2, y+1/2 [\bar{u}, v, \bar{v}]$
$\bar{y}+1/2, 1/2, \bar{y}+1/2 [v, \bar{u}, \bar{v}]$	$\bar{y}+1/2, 1/2, y+1/2 [v, u, v]$	$y+1/2, 1/2, \bar{y}+1/2 [\bar{v}, u, \bar{v}]$	$y+1/2, 1/2, y+1/2 [\bar{v}, \bar{u}, \bar{v}]$
$\bar{y}+1/2, \bar{y}+1/2, 1/2 [\bar{v}, v, \bar{u}]$	$y+1/2, \bar{y}+1/2, 1/2 [v, v, u]$	$\bar{y}+1/2, y+1/2, 1/2 [\bar{v}, \bar{v}, u]$	$y+1/2, y+1/2, 1/2 [v, \bar{v}, \bar{u}]$

24	g	2..	$x, 0, 1/2 [u, 0, 0]$	$\bar{x}, 0, 1/2 [\bar{u}, 0, 0]$	$1/2, x, 0 [0, u, 0]$	$1/2, \bar{x}, 0 [0, \bar{u}, 0]$
			$0, 1/2, x [0, 0, u]$	$0, 1/2, \bar{x} [0, 0, \bar{u}]$	$0, x, 1/2 [0, \bar{u}, 0]$	$0, \bar{x}, 1/2 [0, u, 0]$
			$x, 1/2, 0 [\bar{u}, 0, 0]$	$\bar{x}, 1/2, 0 [u, 0, 0]$	$1/2, 0, \bar{x} [0, 0, u]$	$1/2, 0, x [0, 0, \bar{u}]$
			$\bar{x}+1/2, 1/2, 0 [\bar{u}, 0, 0]$	$x+1/2, 1/2, 0 [u, 0, 0]$	$0, \bar{x}+1/2, 1/2 [0, \bar{u}, 0]$	$0, x+1/2, 1/2 [0, u, 0]$
			$1/2, 0, \bar{x}+1/2 [0, 0, \bar{u}]$	$1/2, 0, x+1/2 [0, 0, u]$	$1/2, \bar{x}+1/2, 0 [0, u, 0]$	$1/2, x+1/2, 0 [0, \bar{u}, 0]$
			$\bar{x}+1/2, 0, 1/2 [u, 0, 0]$	$x+1/2, 0, 1/2 [\bar{u}, 0, 0]$	$0, 1/2, x+1/2 [0, 0, \bar{u}]$	$0, 1/2, \bar{x}+1/2 [0, 0, u]$

16	f	.3.	$x, x, x [u, u, u]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$
			$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
			$x, x, \bar{x} [\bar{u}, \bar{u}, u]$	$\bar{x}, \bar{x}, \bar{x} [u, u, u]$
			$x, \bar{x}, x [\bar{u}, u, \bar{u}]$	$\bar{x}, x, x [u, \bar{u}, \bar{u}]$
			$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, \bar{u}]$	$x+1/2, x+1/2, \bar{x}+1/2 [u, u, \bar{u}]$
			$x+1/2, \bar{x}+1/2, x+1/2 [u, \bar{u}, u]$	$\bar{x}+1/2, x+1/2, x+1/2 [\bar{u}, u, u]$
			$\bar{x}+1/2, \bar{x}+1/2, x+1/2 [u, u, \bar{u}]$	$x+1/2, x+1/2, x+1/2 [\bar{u}, \bar{u}, \bar{u}]$
			$\bar{x}+1/2, x+1/2, \bar{x}+1/2 [u, \bar{u}, u]$	$x+1/2, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, u, u]$

12	e	4'..	$x, 0, 0 [0, 0, 0]$	$\bar{x}, 0, 0 [0, 0, 0]$	$0, x, 0 [0, 0, 0]$
			$0, \bar{x}, 0 [0, 0, 0]$	$0, 0, x [0, 0, 0]$	$0, 0, \bar{x} [0, 0, 0]$
			$\bar{x}+1/2, 1/2, 1/2 [0, 0, 0]$	$x+1/2, 1/2, 1/2 [0, 0, 0]$	$1/2, \bar{x}+1/2, 1/2 [0, 0, 0]$
			$1/2, x+1/2, 1/2 [0, 0, 0]$	$1/2, 1/2, \bar{x}+1/2 [0, 0, 0]$	$1/2, 1/2, x+1/2 [0, 0, 0]$

Continued

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 $Pn\bar{3}'n$ 

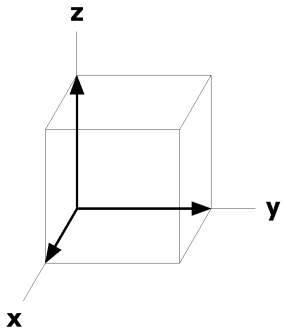
12	d	$\bar{4}..$	$1/4, 0, 1/2 [u, 0, 0]$	$3/4, 0, 1/2 [\bar{u}, 0, 0]$	$1/2, 1/4 [0, u, 0]$	$1/2, 3/4, 0 [0, \bar{u}, 0]$
			$0, 1/2, 1/4 [0, 0, u]$	$0, 1/2, 3/4 [0, 0, \bar{u}]$	$0, 1/4, 1/2 [0, \bar{u}, 0]$	$0, 3/4, 1/2 [0, u, 0]$
			$1/4, 1/2, 0 [\bar{u}, 0, 0]$	$3/4, 1/2, 0 [u, 0, 0]$	$1/2, 0, 3/4 [0, 0, u]$	$1/2, 0, 1/4 [0, 0, \bar{u}]$
8	c	$\bar{3}'..$	$1/4, 1/4, 1/4 [0, 0, 0]$	$3/4, 3/4, 1/4 [0, 0, 0]$	$3/4, 1/4, 3/4 [0, 0, 0]$	$1/4, 3/4, 3/4 [0, 0, 0]$
			$1/4, 1/4, 3/4 [0, 0, 0]$	$3/4, 3/4, 3/4 [0, 0, 0]$	$1/4, 3/4, 1/4 [0, 0, 0]$	$3/4, 1/4, 1/4 [0, 0, 0]$
6	b	$4'2.2'$	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$	
			$1/2, 0, 0 [0, 0, 0]$	$0, 1/2, 0 [0, 0, 0]$	$0, 0, 1/2 [0, 0, 0]$	
2	a	$4'32'$	$0, 0, 0 [0, 0, 0]$	$1/2, 1/2, 1/2 [0, 0, 0]$		

**Symmetry of Special Projections**

Along  $[0, 0, 1]$   $p4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0, 0, z$

Along  $[1, 1, 1]$   $p6mm$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

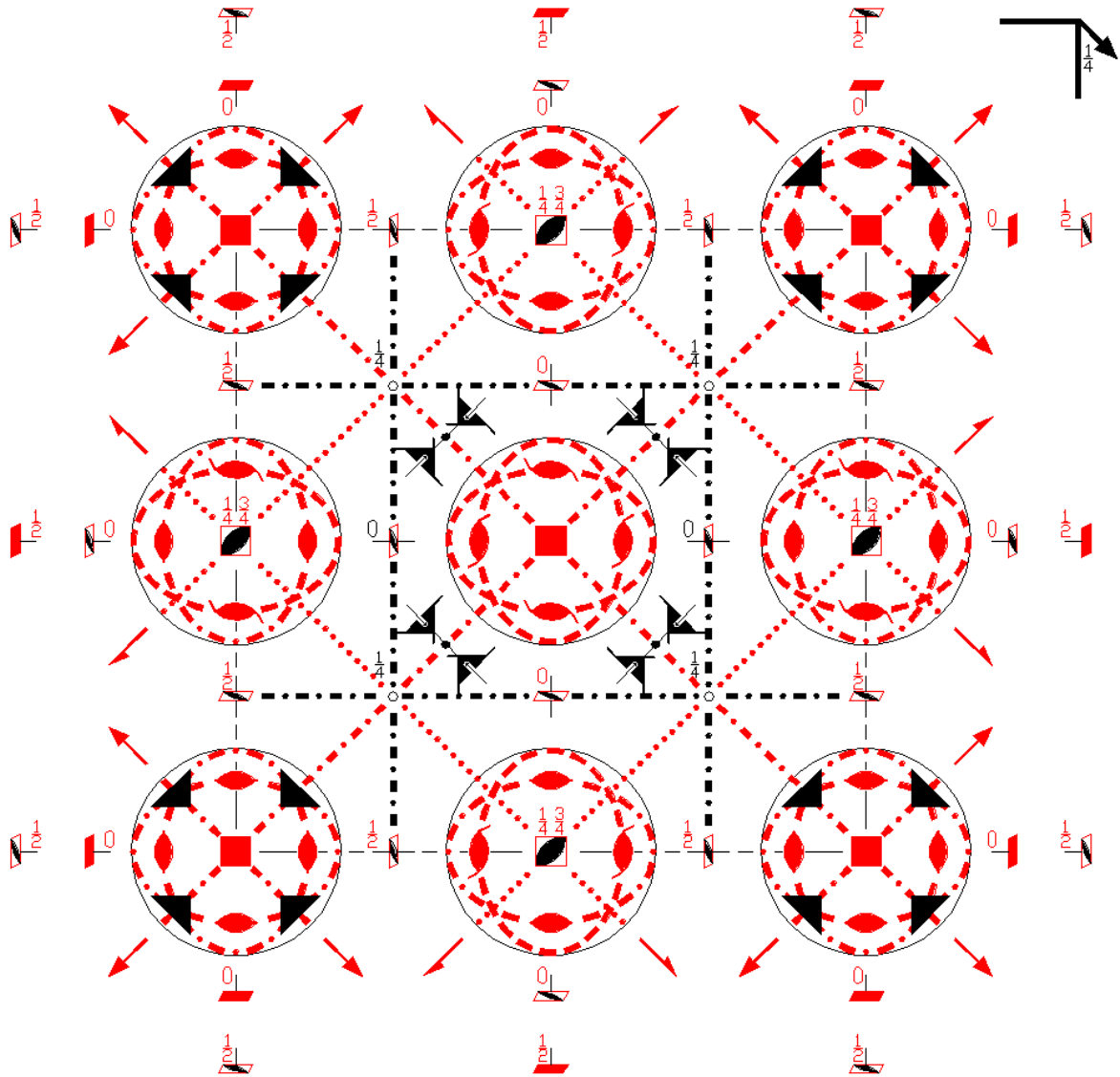
Along  $[1, 1, 0]$   $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, x, 1/4$



$Pn\bar{3}n'$   
222.4.1604

$m\bar{3}m'$   
 $P4'/n\bar{3}2'/n'$

Cubic



**Origin** at  $4'32$ , at  $-1/4, -1/4, -1/4$  from center ( $\bar{3}$ )

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq x; z \leq y$

**Vertices**  $0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/2,1/2,1/2$

**Symmetry Operations**

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                  | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)              |

(13) $2' \ x, x, 0$ ( $2_{xy}   0, 0, 0$ )'	(14) $2' \ x, \bar{x}, 0$ ( $2_{xy}   0, 0, 0$ )'	(15) $4' \ 0, 0, z$ ( $4_z^{-1}   0, 0, 0$ )'	(16) $4^+ \ 0, 0, z$ ( $4_z   0, 0, 0$ )'
(17) $4' \ x, 0, 0$ ( $4_x^{-1}   0, 0, 0$ )'	(18) $2' \ 0, y, y$ ( $2_{yz}   0, 0, 0$ )'	(19) $2' \ 0, y, \bar{y}$ ( $2_{yz}   0, 0, 0$ )'	(20) $4^+ \ x, 0, 0$ ( $4_x   0, 0, 0$ )'
(21) $4^+ \ 0, y, 0$ ( $4_y   0, 0, 0$ )'	(22) $2' \ x, 0, x$ ( $2_{xz}   0, 0, 0$ )'	(23) $4' \ 0, y, 0$ ( $4_y^{-1}   0, 0, 0$ )'	(24) $2' \ \bar{x}, 0, x$ ( $2_{xz}   0, 0, 0$ )'
(25) $\bar{1} \ 1/4, 1/4, 1/4$ ( $\bar{1}   1/2, 1/2, 12$ )	(26) $n \ (1/2, 1/2, 0) \ x, y, 1/4$ ( $m_z   1/2, 1/2, 12$ )	(27) $n \ (1/2, 0, 1/2) \ x, 1/4, z$ ( $m_y   1/2, 1/2, 12$ )	(28) $n \ (0, 1/2, 1/2) \ 1/4, y, z$ ( $m_x   1/2, 1/2, 12$ )
(29) $\bar{3}^+ \ x, x, x; 1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 1/2, 12$ )	(30) $\bar{3}^+ \ \bar{x} - 1, x + 1, \bar{x}; -1/4, 1/4, 3/4$ ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 12$ )	(31) $\bar{3}^+ \ x, \bar{x} + 1, \bar{x}; 1/4, 3/4, -1/4$ ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 12$ )	(32) $\bar{3}^+ \ \bar{x} + 1, \bar{x}, x; 3/4, -1/4, 1/4$ ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 12$ )
(33) $\bar{3}^- \ x, x, x; 1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 12$ )	(34) $\bar{3}^- \ x + 1, \bar{x} - 1, \bar{x}; 1/4, -1/4, 3/4$ ( $\bar{3}_{xyz}   1/2, 1/2, 12$ )	(35) $\bar{3}^- \ \bar{x} + 1, x; -1/4, 3/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 1/2, 12$ )	(36) $\bar{3}^- \ \bar{x} + 1, x, \bar{x}; 3/4, 1/4, -1/4$ ( $\bar{3}_{xyz}   1/2, 1/2, 12$ )
(37) $c' \ (0, 0, 1/2) \ x + 1/2, \bar{x}, z$ ( $m_{xy}   1/2, 1/2, 12$ )'	(38) $n' \ (1/2, 1/2, 1/2) \ x, x, z$ ( $m_{xy}   1/2, 1/2, 12$ )'	(39) $\bar{4}^- \ 0, 1/2, z; 0, 1/2, 1/4$ ( $\bar{4}_z^{-1}   1/2, 1/2, 12$ )'	(40) $\bar{4}^+ \ 1/2, 0, z; 1/2, 0, 1/4$ ( $\bar{4}_z   1/2, 1/2, 12$ )'
(41) $\bar{4}^- \ x, 0, 1/2; 1/4, 0, 1/2$ ( $\bar{4}_x^{-1}   1/2, 1/2, 12$ )'	(42) $a' \ (1/2, 0, 0) \ x, y + 1/2, \bar{y}$ ( $m_{yz}   1/2, 1/2, 12$ )'	(43) $n' \ (1/2, 1/2, 1/2) \ x, y, y$ ( $m_{yz}   1/2, 1/2, 12$ )'	(44) $\bar{4}^+ \ x, 1/2, 0; 1/4, 1/2, 0$ ( $\bar{4}_x   1/2, 1/2, 12$ )'
(45) $\bar{4}^+ \ 0, y, 1/2; 0, 1/4, 1/2$ ( $\bar{4}_y   1/2, 1/2, 12$ )'	(46) $b' \ (0, 1/2, 0) \ \bar{x} + 1/2, y, x$ ( $m_{xz}   1/2, 1/2, 12$ )'	(47) $\bar{4}^- \ 1/2, y, 0; 1/2, 1/4, 0$ ( $\bar{4}_y^{-1}   1/2, 1/2, 12$ )'	(48) $n' \ (1/2, 1/2, 1/2) \ x, y, x$ ( $m_{xz}   1/2, 1/2, 12$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

48 i 1

(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{x}, y, \bar{z} [\bar{u}, v, \bar{w}]$	(4) $x, \bar{y}, \bar{z} [u, \bar{v}, \bar{w}]$
(5) $z, x, y [w, u, v]$	(6) $z, \bar{x}, \bar{y} [w, \bar{u}, \bar{v}]$	(7) $\bar{z}, \bar{x}, y [\bar{w}, \bar{u}, v]$	(8) $\bar{z}, x, \bar{y} [\bar{w}, u, \bar{v}]$
(9) $y, z, x [v, w, u]$	(10) $\bar{y}, z, \bar{x} [\bar{v}, w, \bar{u}]$	(11) $y, \bar{z}, \bar{x} [v, \bar{w}, \bar{u}]$	(12) $\bar{y}, \bar{z}, x [\bar{v}, \bar{w}, u]$
(13) $y, x, \bar{z} [\bar{v}, \bar{u}, w]$	(14) $\bar{y}, \bar{x}, \bar{z} [\bar{v}, u, w]$	(15) $y, \bar{x}, z [v, u, \bar{w}]$	(16) $\bar{y}, x, z [v, \bar{u}, \bar{w}]$
(17) $x, z, \bar{y} [\bar{u}, \bar{w}, v]$	(18) $\bar{x}, z, y [u, \bar{w}, \bar{v}]$	(19) $\bar{x}, \bar{z}, \bar{y} [u, w, v]$	(20) $x, \bar{z}, y [\bar{u}, w, \bar{v}]$
(21) $z, y, \bar{x} [\bar{w}, \bar{v}, u]$	(22) $z, \bar{y}, x [\bar{w}, v, \bar{u}]$	(23) $\bar{z}, y, x [w, \bar{v}, \bar{u}]$	(24) $\bar{z}, \bar{y}, \bar{x} [w, v, u]$
(25) $\bar{x} + 1/2, \bar{y} + 1/2, \bar{z} + 1/2 [u, v, w]$	(26) $x + 1/2, y + 1/2, \bar{z} + 1/2 [\bar{u}, \bar{v}, w]$	(27) $x + 1/2, \bar{y} + 1/2, z + 1/2 [\bar{u}, v, \bar{w}]$	(28) $\bar{x} + 1/2, y + 1/2, z + 1/2 [u, \bar{v}, \bar{w}]$
(29) $\bar{z} + 1/2, \bar{x} + 1/2, \bar{y} + 1/2 [w, u, v]$	(30) $\bar{z} + 1/2, x + 1/2, y + 1/2 [w, \bar{u}, \bar{v}]$	(31) $z + 1/2, x + 1/2, \bar{y} + 1/2 [\bar{w}, \bar{u}, v]$	(32) $z + 1/2, \bar{x} + 1/2, y + 1/2 [\bar{w}, u, \bar{v}]$
(33) $\bar{y} + 1/2, \bar{z} + 1/2, \bar{x} + 1/2 [v, w, u]$	(34) $y + 1/2, \bar{z} + 1/2, x + 1/2 [\bar{v}, w, \bar{u}]$	(35) $\bar{y} + 1/2, z + 1/2, x + 1/2 [v, \bar{w}, \bar{u}]$	(36) $y + 1/2, z + 1/2, \bar{x} + 1/2 [v, w, u]$



- (37)  $\bar{y}+1/2, \bar{x}+1/2, z+1/2 [\bar{v}, \bar{u}, w]$  (38)  $y+1/2, x+1/2, z+1/2 [v, u, w]$  (39)  $\bar{y}+1/2, x+1/2, \bar{z}+1/2 [\bar{v}, \bar{u}, \bar{w}]$  (40)  $y+1/2, \bar{x}+1/2, \bar{z}+1/2 [v, \bar{u}, \bar{w}]$   
 (41)  $\bar{x}+1/2, \bar{z}+1/2, y+1/2 [\bar{u}, \bar{w}, v]$  (42)  $x+1/2, \bar{z}+1/2, \bar{y}+1/2 [u, \bar{w}, \bar{v}]$  (43)  $x+1/2, z+1/2, y+1/2 [u, w, v]$  (44)  $\bar{x}+1/2, z+1/2, \bar{y}+1/2 [\bar{u}, \bar{w}, \bar{v}]$   
 (45)  $\bar{z}+1/2, \bar{y}+1/2, x+1/2 [\bar{w}, \bar{v}, u]$  (46)  $\bar{z}+1/2, y+1/2, \bar{x}+1/2 [\bar{w}, v, \bar{u}]$  (47)  $z+1/2, \bar{y}+1/2, \bar{x}+1/2 [w, \bar{v}, \bar{u}]$  (48)  $z+1/2, y+1/2, x+1/2 [w, v, u]$

24 h ..2'

$0, y, y [u, v, \bar{v}]$	$0, \bar{y}, y [\bar{u}, \bar{v}, \bar{v}]$	$0, y, \bar{y} [\bar{u}, v, v]$	$0, \bar{y}, \bar{y} [u, \bar{v}, v]$
$y, 0, y [\bar{v}, u, v]$	$y, 0, \bar{y} [\bar{v}, \bar{u}, \bar{v}]$	$\bar{y}, 0, y [v, \bar{u}, v]$	$\bar{y}, 0, \bar{y} [v, u, \bar{v}]$
$y, y, 0 [v, \bar{v}, u]$	$\bar{y}, y, 0 [\bar{v}, \bar{v}, \bar{u}]$	$y, \bar{y}, 0 [v, v, \bar{u}]$	$\bar{y}, \bar{y}, 0 [\bar{v}, v, u]$
$1/2, \bar{y}+1/2, \bar{y}+1/2 [u, v, \bar{v}]$	$1/2, y+1/2, \bar{y}+1/2 [\bar{u}, \bar{v}, \bar{v}]$	$1/2, \bar{y}+1/2, y+1/2 [\bar{u}, v, v]$	$1/2, y+1/2, y+1/2 [u, \bar{v}, v]$
$\bar{y}+1/2, 1/2, \bar{y}+1/2 [\bar{v}, u, v]$	$\bar{y}+1/2, 1/2, y+1/2 [\bar{v}, \bar{u}, \bar{v}]$	$y+1/2, 1/2, \bar{y}+1/2 [v, \bar{u}, v]$	$y+1/2, 1/2, y+1/2 [v, u, \bar{v}]$
$\bar{y}+1/2, \bar{y}+1/2, 1/2 [v, \bar{v}, u]$	$y+1/2, \bar{y}+1/2, 1/2 [\bar{v}, \bar{v}, \bar{u}]$	$\bar{y}+1/2, y+1/2, 1/2 [v, v, \bar{u}]$	$y+1/2, y+1/2, 1/2 [\bar{v}, v, u]$

24 g 2..	$x, 0, 1/2 [u, 0, 0]$	$\bar{x}, 0, 1/2 [\bar{u}, 0, 0]$	$1/2, x, 0 [0, u, 0]$	$1/2, \bar{x}, 0 [0, \bar{u}, 0]$
	$0, 1/2, x [0, 0, u]$	$0, 1/2, \bar{x} [0, 0, \bar{u}]$	$0, x, 1/2 [0, u, 0]$	$0, \bar{x}, 1/2 [0, \bar{u}, 0]$
	$x, 1/2, 0 [u, 0, 0]$	$\bar{x}, 1/2, 0 [\bar{u}, 0, 0]$	$1/2, 0, \bar{x} [0, 0, \bar{u}]$	$1/2, 0, x [0, 0, u]$
	$\bar{x}+1/2, 1/2, 0 [u, 0, 0]$	$x+1/2, 1/2, 0 [\bar{u}, 0, 0]$	$0, \bar{x}+1/2, 1/2 [0, u, 0]$	$0, x+1/2, 1/2 [0, \bar{u}, 0]$
	$1/2, 0, \bar{x}+1/2 [0, 0, u]$	$1/2, 0, x+1/2 [0, 0, \bar{u}]$	$1/2, \bar{x}+1/2, 0 [0, u, 0]$	$1/2, x+1/2, 0 [0, \bar{u}, 0]$
	$\bar{x}+1/2, 0, 1/2 [u, 0, 0]$	$x+1/2, 0, 1/2 [\bar{u}, 0, 0]$	$0, 1/2, x+1/2 [0, 0, \bar{u}]$	$0, 1/2, \bar{x}+1/2 [0, 0, u]$

16 f .3.	$x, x, x [u, u, u]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$
	$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
	$x, x, \bar{x} [\bar{u}, \bar{u}, u]$	$\bar{x}, \bar{x}, \bar{x} [u, u, u]$
	$x, \bar{x}, x [\bar{u}, u, \bar{u}]$	$\bar{x}, x, x [u, \bar{u}, \bar{u}]$
	$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [u, u, u]$	$x+1/2, x+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, u]$
	$x+1/2, \bar{x}+1/2, x+1/2 [\bar{u}, u, \bar{u}]$	$\bar{x}+1/2, x+1/2, x+1/2 [u, \bar{u}, \bar{u}]$
	$\bar{x}+1/2, \bar{x}+1/2, x+1/2 [\bar{u}, \bar{u}, u]$	$x+1/2, x+1/2, x+1/2 [u, u, u]$
	$\bar{x}+1/2, x+1/2, \bar{x}+1/2 [\bar{u}, u, \bar{u}]$	$x+1/2, \bar{x}+1/2, \bar{x}+1/2 [u, \bar{u}, \bar{u}]$

12 e 4'.	$x, 0, 0 [0, 0, 0]$	$\bar{x}, 0, 0 [0, 0, 0]$	$0, x, 0 [0, 0, 0]$
	$0, \bar{x}, 0 [0, 0, 0]$	$0, 0, x [0, 0, 0]$	$0, 0, \bar{x} [0, 0, 0]$
	$\bar{x}+1/2, 1/2, 1/2 [0, 0, 0]$	$x+1/2, 1/2, 1/2 [0, 0, 0]$	$1/2, \bar{x}+1/2, 1/2 [0, 0, 0]$
	$1/2, x+1/2, 1/2 [0, 0, 0]$	$1/2, 1/2, \bar{x}+1/2 [0, 0, 0]$	$1/2, 1/2, x+1/2 [0, 0, 0]$

Continued

222.4.1604

 $Pn\bar{3}n'$ 

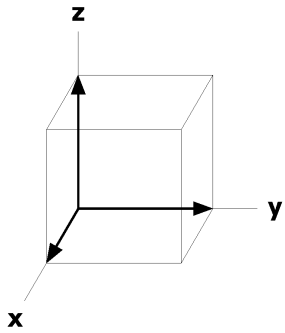
12	d	$\bar{4}'..$	1/4,0,1/2 [0,0,0]	3/4,0,1/2 [0,0,0]	1/2,1/4 [0,0,0]	1/2,3/4,0 [0,0,0]
			0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	0,1/4,1/2 [0,0,0]	0,3/4,1/2 [0,0,0]
			1/4,1/2,0 [0,0,0]	3/4,1/2,0 [0,0,0]	1/2,0,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]
8	c	$\bar{3}..$	1/4,1/4,1/4 [u,u,u]	3/4,3/4,1/4 [ $\bar{u},\bar{u},u$ ]	3/4,1/4,3/4 [ $\bar{u},u,\bar{u}$ ]	1/4,3/4,3/4 [u, $\bar{u},\bar{u}$ ]
			1/4,1/4,3/4 [ $\bar{u},\bar{u},u$ ]	3/4,3/4,3/4 [u,u,u]	1/4,3/4,1/4 [ $\bar{u},u,\bar{u}$ ]	3/4,1/4,1/4 [u, $\bar{u},\bar{u}$ ]
6	b	4'2.2'	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	
			1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	0,0,1/2 [0,0,0]	
2	a	4'32'	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,1,1]  $p6'mm'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

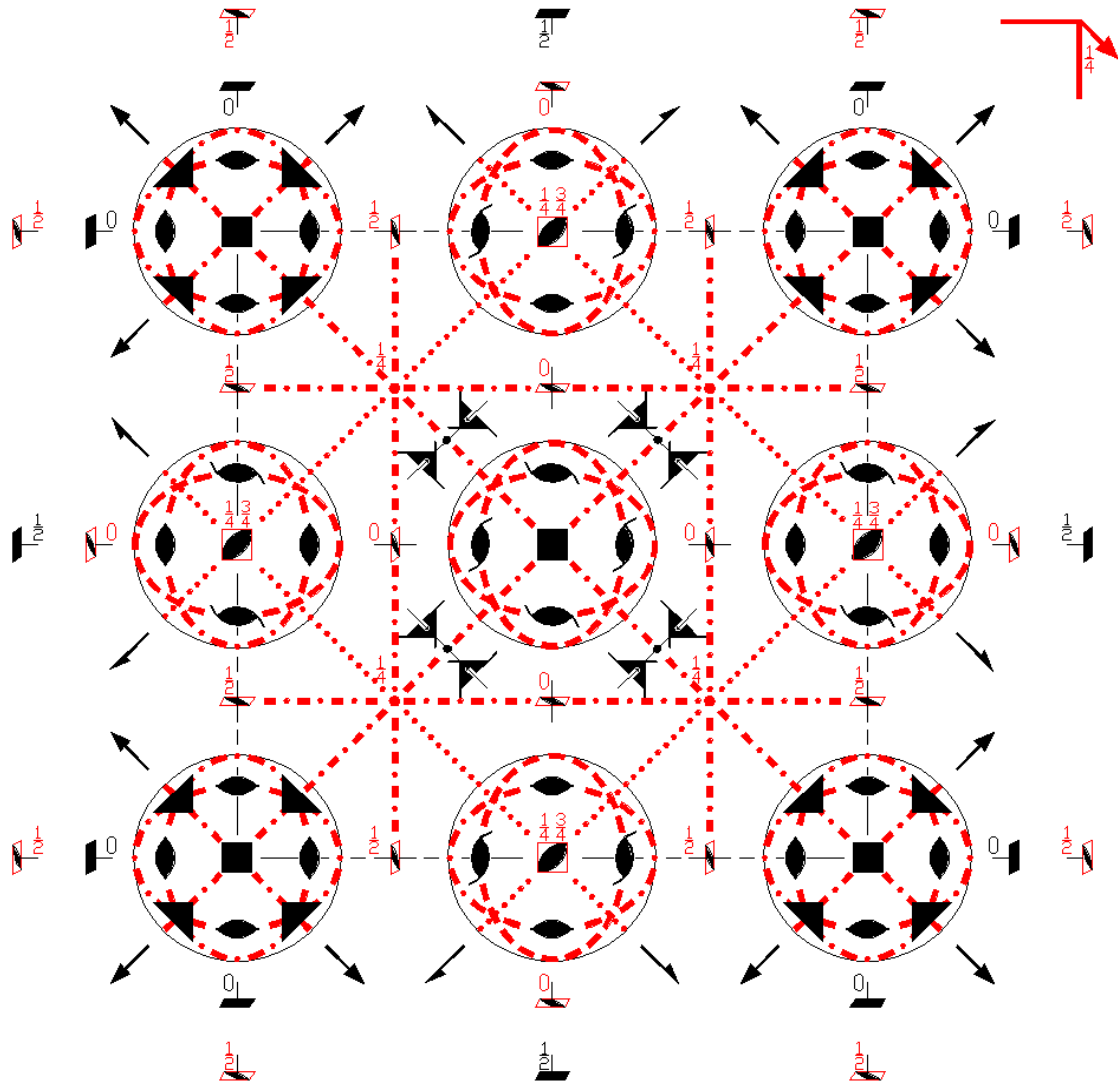
Along [1,1,0]  $p2'mm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



$Pn\bar{3}n'$   
222.5.1605

$m\bar{3}'m'$   
 $P4/n\bar{3}'2/n'$

Cubic



**Origin** at 432, at  $-1/4, -1/4, -1/4$  from center ( $\bar{3}'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/2;$   $y \leq x;$   $z \leq y$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/2,1/2,1/2$

**Symmetry Operations**

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                  | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)              |

(13) $2^- x,x,0$ ( $2_{xy} 0,0,0$ )	(14) $2^- x,\bar{x},0$ ( $2_{\bar{xy}} 0,0,0$ )	(15) $4^- 0,0,z$ ( $4_z^{-1} 0,0,0$ )	(16) $4^+ 0,0,z$ ( $4_z 0,0,0$ )
(17) $4^- x,0,0$ ( $4_x^{-1} 0,0,0$ )	(18) $2^- 0,y,y$ ( $2_{yz} 0,0,0$ )	(19) $2^- 0,y,\bar{y}$ ( $2_{\bar{yz}} 0,0,0$ )	(20) $4^+ x,0,0$ ( $4_x 0,0,0$ )
(21) $4^+ 0,y,0$ ( $4_y 0,0,0$ )	(22) $2^- x,0,x$ ( $2_{xz} 0,0,0$ )	(23) $4^- 0,y,0$ ( $4_y^{-1} 0,0,0$ )	(24) $2^- \bar{x},0,x$ ( $2_{\bar{xz}} 0,0,0$ )
(25) $\bar{1}^- 1/4,1/4,1/4$ ( $\bar{1} 1/2,1/2,12$ )'	(26) $n' (1/2,1/2,0) x,y,1/4$ ( $m_z 1/2,1/2,12$ )'	(27) $n' (1/2,0,1/2) x,1/4,z$ ( $m_y 1/2,1/2,12$ )'	(28) $n' (0,1/2,1/2) 1/4,y,z$ ( $m_x 1/2,1/2,12$ )'
(29) $\bar{3}^+ x,x,x; 1/4,1/4,1/4$ ( $\bar{3}_{xyz} 1/2,1/2,12$ )'	(30) $\bar{3}^+ \bar{x}-1,x+1,\bar{x}; -1/4,1/4,3/4$ ( $\bar{3}_{\bar{xyz}^{-1}} 1/2,1/2,12$ )'	(31) $\bar{3}^+ x,\bar{x}+1,\bar{x}; 1/4,3/4,-1/4$ ( $\bar{3}_{\bar{xyz}^{-1}} 1/2,1/2,12$ )'	(32) $\bar{3}^+ \bar{x}+1,\bar{x},x; 3/4,-1/4,1/4$ ( $\bar{3}_{\bar{xyz}^{-1}} 1/2,1/2,12$ )'
(33) $\bar{3}^- x,x,x; 1/4,1/4,1/4$ ( $\bar{3}_{xyz}^{-1} 1/2,1/2,12$ )'	(34) $\bar{3}^- x+1,\bar{x}-1,\bar{x}; 1/4,-1/4,3/4$ ( $\bar{3}_{\bar{xyz}} 1/2,1/2,12$ )'	(35) $\bar{3}^- \bar{x},\bar{x}+1,x; -1/4,3/4,1/4$ ( $\bar{3}_{\bar{xyz}} 1/2,1/2,12$ )'	(36) $\bar{3}^- \bar{x}+1,x,\bar{x}; 3/4,1/4,-1/4$ ( $\bar{3}_{\bar{xyz}} 1/2,1/2,12$ )'
(37) $c' (0,0,1/2) x+1/2,\bar{x},z$ ( $m_{xy} 1/2,1/2,12$ )'	(38) $n' (1/2,1/2,1/2) x,x,z$ ( $m_{\bar{xy}} 1/2,1/2,12$ )'	(39) $\bar{4}^- 0,1/2,z; 0,1/2,1/4$ ( $\bar{4}_z^{-1} 1/2,1/2,12$ )'	(40) $\bar{4}^+ 1/2,0,z; 1/2,0,1/4$ ( $\bar{4}_z 1/2,1/2,12$ )'
(41) $\bar{4}^- x,0,1/2; 1/4,0,1/2$ ( $\bar{4}_x^{-1} 1/2,1/2,12$ )'	(42) $a' (1/2,0,0) x,y+1/2,\bar{y}$ ( $m_{yz} 1/2,1/2,12$ )'	(43) $n' (1/2,1/2,1/2) x,y,y$ ( $m_{\bar{yz}} 1/2,1/2,12$ )'	(44) $\bar{4}^+ x,1/2,0; 1/4,1/2,0$ ( $\bar{4}_x 1/2,1/2,12$ )'
(45) $\bar{4}^+ 0,y,1/2; 0,1/4,1/2$ ( $\bar{4}_y 1/2,1/2,12$ )'	(46) $b' (0,1/2,0) \bar{x}+1/2,y,x$ ( $m_{xz} 1/2,1/2,12$ )'	(47) $\bar{4}^- 1/2,y,0; 1/2,1/4,0$ ( $\bar{4}_y^{-1} 1/2,1/2,12$ )'	(48) $n' (1/2,1/2,1/2) x,y,x$ ( $m_{\bar{xz}} 1/2,1/2,12$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

### Coordinates

48 i 1

(1) $x,y,z [u,v,w]$	(2) $\bar{x},\bar{y},z [\bar{u},\bar{v},w]$	(3) $\bar{x},y,\bar{z} [\bar{u},v,\bar{w}]$	(4) $x,\bar{y},\bar{z} [u,\bar{v},\bar{w}]$
(5) $z,x,y [w,u,v]$	(6) $z,\bar{x},\bar{y} [w,\bar{u},\bar{v}]$	(7) $\bar{z},\bar{x},y [\bar{w},\bar{u},v]$	(8) $\bar{z},x,\bar{y} [\bar{w},u,\bar{v}]$
(9) $y,z,x [v,w,u]$	(10) $\bar{y},z,\bar{x} [\bar{v},w,\bar{u}]$	(11) $y,\bar{z},\bar{x} [v,\bar{w},\bar{u}]$	(12) $\bar{y},\bar{z},x [\bar{v},\bar{w},u]$
(13) $y,x,\bar{z} [v,u,\bar{w}]$	(14) $\bar{y},\bar{x},\bar{z} [\bar{v},\bar{u},\bar{w}]$	(15) $y,\bar{x},z [v,\bar{u},w]$	(16) $\bar{y},x,z [\bar{v},u,w]$
(17) $x,z,\bar{y} [u,w,\bar{v}]$	(18) $\bar{x},z,y [\bar{u},w,v]$	(19) $\bar{x},\bar{z},\bar{y} [\bar{u},\bar{w},\bar{v}]$	(20) $x,\bar{z},y [u,\bar{w},v]$
(21) $z,y,\bar{x} [w,v,\bar{u}]$	(22) $z,\bar{y},x [w,\bar{v},u]$	(23) $\bar{z},y,x [\bar{w},v,u]$	(24) $\bar{z},\bar{y},\bar{x} [\bar{w},\bar{v},\bar{u}]$
(25) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2 [\bar{u},\bar{v},\bar{w}]$	(26) $x+1/2,y+1/2,\bar{z}+1/2 [u,v,\bar{w}]$	(27) $x+1/2,\bar{y}+1/2,z+1/2 [u,\bar{v},w]$	(28) $\bar{x}+1/2,y+1/2,z+1/2 [\bar{u},v,w]$
(29) $\bar{z}+1/2,\bar{x}+1/2,\bar{y}+1/2 [\bar{w},\bar{u},\bar{v}]$	(30) $\bar{z}+1/2,x+1/2,y+1/2 [\bar{w},u,v]$	(31) $z+1/2,x+1/2,\bar{y}+1/2 [w,u,\bar{v}]$	(32) $z+1/2,\bar{x}+1/2,y+1/2 [w,\bar{u},v]$
(33) $\bar{y}+1/2,\bar{z}+1/2,\bar{x}+1/2 [\bar{v},\bar{w},\bar{u}]$	(34) $y+1/2,\bar{z}+1/2,x+1/2 [v,\bar{w},u]$	(35) $\bar{y}+1/2,z+1/2,x+1/2 [\bar{v},w,u]$	(36) $y+1/2,z+1/2,\bar{x}+1/2 [v,w,\bar{u}]$

(37)  $\bar{y}+1/2, \bar{x}+1/2, z+1/2 [\bar{v}, \bar{u}, w]$  (38)  $y+1/2, x+1/2, z+1/2 [v, u, w]$  (39)  $\bar{y}+1/2, x+1/2, \bar{z}+1/2 [\bar{v}, u, \bar{w}]$  (40)  $y+1/2, \bar{x}+1/2, \bar{z}+1/2 [v, \bar{u}, \bar{w}]$   
 (41)  $\bar{x}+1/2, \bar{z}+1/2, y+1/2 [\bar{u}, \bar{w}, v]$  (42)  $x+1/2, \bar{z}+1/2, \bar{y}+1/2 [u, \bar{w}, \bar{v}]$  (43)  $x+1/2, z+1/2, y+1/2 [u, w, v]$  (44)  $\bar{x}+1/2, z+1/2, \bar{y}+1/2 [\bar{u}, \bar{w}, \bar{v}]$   
 (45)  $\bar{z}+1/2, \bar{y}+1/2, x+1/2 [\bar{w}, \bar{v}, u]$  (46)  $\bar{z}+1/2, y+1/2, \bar{x}+1/2 [\bar{w}, v, \bar{u}]$  (47)  $z+1/2, \bar{y}+1/2, \bar{x}+1/2 [w, \bar{v}, \bar{u}]$  (48)  $z+1/2, y+1/2, x+1/2 [w, v, u]$

24 h ..2

$0, y, y [0, v, v]$	$0, \bar{y}, y [0, \bar{v}, v]$	$0, y, \bar{y} [0, v, \bar{v}]$	$0, \bar{y}, \bar{y} [0, \bar{v}, \bar{v}]$
$y, 0, y [v, 0, v]$	$y, 0, \bar{y} [v, 0, \bar{v}]$	$\bar{y}, 0, y [\bar{v}, 0, v]$	$\bar{y}, 0, \bar{y} [\bar{v}, 0, \bar{v}]$
$y, y, 0 [v, v, 0]$	$\bar{y}, y, 0 [\bar{v}, v, 0]$	$y, \bar{y}, 0 [v, \bar{v}, 0]$	$\bar{y}, \bar{y}, 0 [\bar{v}, \bar{v}, 0]$
$1/2, \bar{y}+1/2, \bar{y}+1/2 [0, \bar{v}, \bar{v}]$	$1/2, y+1/2, \bar{y}+1/2 [0, v, \bar{v}]$	$1/2, \bar{y}+1/2, y+1/2 [0, \bar{v}, v]$	$1/2, y+1/2, y+1/2 [0, v, v]$
$\bar{y}+1/2, 1/2, \bar{y}+1/2 [\bar{v}, 0, \bar{v}]$	$\bar{y}+1/2, 1/2, y+1/2 [\bar{v}, 0, v]$	$y+1/2, 1/2, \bar{y}+1/2 [v, 0, \bar{v}]$	$y+1/2, 1/2, y+1/2 [v, 0, v]$
$\bar{y}+1/2, \bar{y}+1/2, 1/2 [\bar{v}, \bar{v}, 0]$	$y+1/2, \bar{y}+1/2, 1/2 [v, \bar{v}, 0]$	$\bar{y}+1/2, y+1/2, 1/2 [\bar{v}, v, 0]$	$y+1/2, y+1/2, 1/2 [v, v, 0]$

24	g	2..	$x, 0, 1/2 [u, 0, 0]$	$\bar{x}, 0, 1/2 [\bar{u}, 0, 0]$	$1/2, x, 0 [0, u, 0]$	$1/2, \bar{x}, 0 [0, \bar{u}, 0]$
			$0, 1/2, x [0, 0, u]$	$0, 1/2, \bar{x} [0, 0, \bar{u}]$	$0, x, 1/2 [0, u, 0]$	$0, \bar{x}, 1/2 [0, \bar{u}, 0]$
			$x, 1/2, 0 [u, 0, 0]$	$\bar{x}, 1/2, 0 [\bar{u}, 0, 0]$	$1/2, 0, \bar{x} [0, 0, \bar{u}]$	$1/2, 0, x [0, 0, u]$
			$\bar{x}+1/2, 1/2, 0 [\bar{u}, 0, 0]$	$x+1/2, 1/2, 0 [u, 0, 0]$	$0, \bar{x}+1/2, 1/2 [0, \bar{u}, 0]$	$0, x+1/2, 1/2 [0, u, 0]$
			$1/2, 0, \bar{x}+1/2 [0, 0, \bar{u}]$	$1/2, 0, x+1/2 [0, 0, u]$	$1/2, \bar{x}+1/2, 0 [0, \bar{u}, 0]$	$1/2, x+1/2, 0 [0, u, 0]$
			$\bar{x}+1/2, 0, 1/2 [\bar{u}, 0, 0]$	$x+1/2, 0, 1/2 [u, 0, 0]$	$0, 1/2, x+1/2 [0, 0, u]$	$0, 1/2, \bar{x}+1/2 [0, 0, \bar{u}]$

16	f	.3.	$x, x, x [u, u, u]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$
			$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
			$x, x, \bar{x} [u, u, \bar{u}]$	$\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$
			$x, \bar{x}, x [u, \bar{u}, u]$	$\bar{x}, x, x [\bar{u}, u, u]$
			$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, \bar{u}]$	$x+1/2, x+1/2, \bar{x}+1/2 [u, u, \bar{u}]$
			$x+1/2, \bar{x}+1/2, x+1/2 [u, \bar{u}, u]$	$\bar{x}+1/2, x+1/2, x+1/2 [\bar{u}, u, u]$
			$\bar{x}+1/2, \bar{x}+1/2, x+1/2 [\bar{u}, \bar{u}, u]$	$x+1/2, x+1/2, x+1/2 [u, u, u]$
			$\bar{x}+1/2, x+1/2, \bar{x}+1/2 [\bar{u}, u, \bar{u}]$	$x+1/2, \bar{x}+1/2, \bar{x}+1/2 [u, \bar{u}, \bar{u}]$

12	e	4..	$x, 0, 0 [u, 0, 0]$	$\bar{x}, 0, 0 [0, \bar{u}, 0]$	$0, x, 0 [0, u, 0]$
			$0, \bar{x}, 0 [0, \bar{u}, 0]$	$0, 0, x [0, 0, u]$	$0, 0, \bar{x} [0, 0, \bar{u}]$
			$\bar{x}+1/2, 1/2, 1/2 [\bar{u}, 0, 0]$	$x+1/2, 1/2, 1/2 [0, u, 0]$	$1/2, \bar{x}+1/2, 1/2 [0, \bar{u}, 0]$
			$1/2, x+1/2, 1/2 [0, u, 0]$	$1/2, 1/2, \bar{x}+1/2 [0, 0, \bar{u}]$	$1/2, 1/2, x+1/2 [0, 0, u]$

Continued

222.5.1605

 $Pn\bar{3}'n'$ 

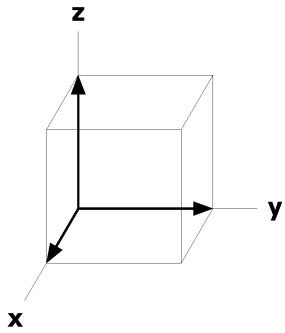
12	d	$\bar{4}'..$	1/4,0,1/2 [0,0,0]	3/4,0,1/2 [0,0,0]	1/2,1/4 [0,0,0]	1/2,3/4,0 [0,0,0]
			0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	0,1/4,1/2 [0,0,0]	0,3/4,1/2 [0,0,0]
			1/4,1/2,0 [0,0,0]	3/4,1/2,0 [0,0,0]	1/2,0,3/4 [0,0,0]	1/2,0,1/4 [0,0,0]
8	c	$\bar{3}'..$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]
			1/4,1/4,3/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
6	b	42.2	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	
			1/2,0,0 [0,0,0]	0,1/2,0 [0,0,0]	0,0,1/2 [0,0,0]	
2	a	432	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1]  $p4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,1,1]  $p6m'm'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

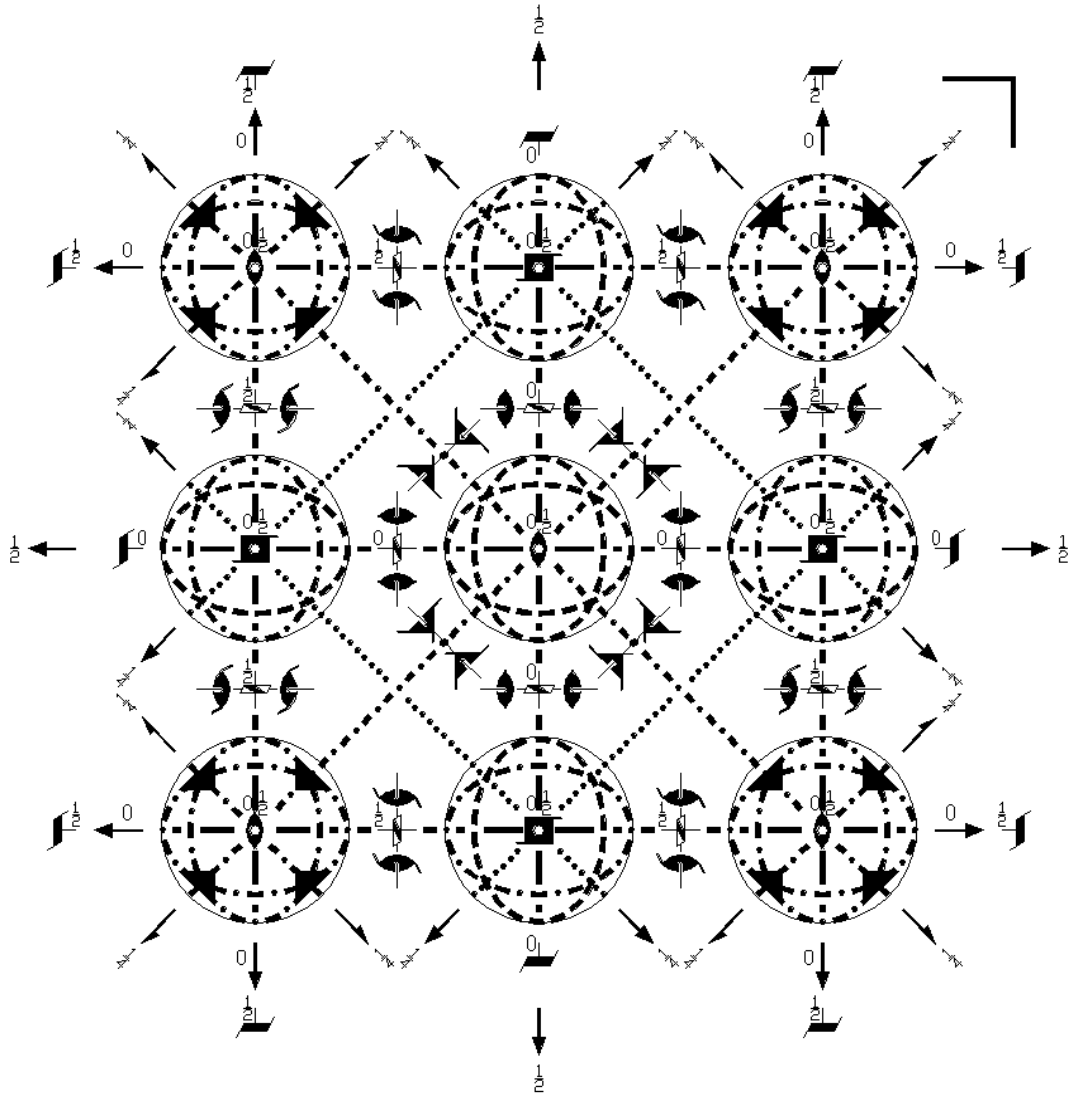
Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$Pm\bar{3}n$   
223.1.1606

$m\bar{3}n$   
 $P4_2/m\bar{3}2/n$

Cubic



**Origin** at center ( $m\bar{3}$ )

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $z \leq \min(x, 1/2-x, y, 1/2-y)$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $0,1/2,0$   $1/4,1/4,1/4$

**Symmetry Operations**

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)   | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)   | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)   |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)               | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0) | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{\bar{x}yz}$ <sup>-1</sup>  0,0,0) | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}y\bar{z}}$ <sup>-1</sup>  0,0,0) |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}$ <sup>-1</sup>  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{\bar{x}yz}$  0,0,0)                    | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)        | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)              |

(13) $2 (1/2, 1/2, 0) \ x, x, 1/4$ ( $2_{xy}   1/2, 1/2, 1/2$ )	(14) $2 \ x, \bar{x} + 1/2, 1/4$ ( $2_{\bar{xy}}   1/2, 1/2, 1/2$ )	(15) $4^- (0, 0, 1/2) \ 1/2, 0, z$ ( $4_z^{-1}   1/2, 1/2, 1/2$ )	(16) $4^+ (0, 0, 1/2) \ 0, 1/2, z$ ( $4_z   1/2, 1/2, 1/2$ )
(17) $4^- (1/2, 0, 0) \ x, 1/2, 0$ ( $4_x^{-1}   1/2, 1/2, 1/2$ )	(18) $2 (0, 1/2, 1/2) \ 1/4, y, y$ ( $2_{yz}   1/2, 1/2, 1/2$ )	(19) $2 \ 1/4, y + 1/2, \bar{y}$ ( $2_{\bar{yz}}   1/2, 1/2, 1/2$ )	(20) $4^+ (1/2, 0, 0) \ x, 0, 1/2$ ( $4_x   1/2, 1/2, 1/2$ )
(21) $4^+ (0, 1/2, 0) \ 1/2, y, 0$ ( $4_y   1/2, 1/2, 1/2$ )	(22) $2 (1/2, 0, 1/2) \ x, 1/4, x$ ( $2_{xz}   1/2, 1/2, 1/2$ )	(23) $4^- (0, 1/2, 0) \ 0, y, 1/2$ ( $4_y^{-1}   1/2, 1/2, 1/2$ )	(24) $2 \ \bar{x} + 1/2, 1/4, x$ ( $2_{\bar{xz}}   1/2, 1/2, 1/2$ )
(25) $\bar{1} \ 0, 0, 0$ ( $\bar{1}   0, 0, 0$ )	(26) $m \ x, y, 0$ ( $m_z   0, 0, 0$ )	(27) $m \ x, 0, z$ ( $m_y   0, 0, 0$ )	(28) $m \ 0, y, z$ ( $m_x   0, 0, 0$ )
(29) $\bar{3}^+ \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}   0, 0, 0$ )	(30) $\bar{3}^+ \ \bar{x}, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}^{-1}   0, 0, 0$ )	(31) $\bar{3}^+ \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xy}z}^{-1}   0, 0, 0$ )	(32) $\bar{3}^+ \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{xy\bar{z}}^{-1}   0, 0, 0$ )
(33) $\bar{3}^- \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}^{-1}   0, 0, 0$ )	(34) $\bar{3}^- \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}   0, 0, 0$ )	(35) $\bar{3}^- \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{\bar{xy}z}   0, 0, 0$ )	(36) $\bar{3}^- \ \bar{x}, x, \bar{x}; 0, 0, 0$ ( $\bar{3}_{xy\bar{z}}   0, 0, 0$ )
(37) $c (0, 0, 1/2) \ x + 1/2, \bar{x}, z$ ( $m_{xy}   1/2, 1/2, 12$ )	(38) $n (1/2, 1/2, 1/2) \ x, x, z$ ( $m_{\bar{xy}}   1/2, 1/2, 12$ )	(39) $\bar{4}^- \ 0, 1/2, z; 0, 1/2, 1/4$ ( $\bar{4}_z^{-1}   1/2, 1/2, 12$ )	(40) $\bar{4}^+ \ 1/2, 0, z; 1/2, 0, 1/4$ ( $\bar{4}_z   1/2, 1/2, 12$ )
(41) $\bar{4}^- \ x, 0, 1/2; 1/4, 0, 1/2$ ( $\bar{4}_x^{-1}   1/2, 1/2, 12$ )	(42) $a (1/2, 0, 0) \ x, y + 1/2, \bar{y}$ ( $m_{yz}   1/2, 1/2, 12$ )	(43) $n (1/2, 1/2, 1/2) \ x, y, y$ ( $m_{\bar{yz}}   1/2, 1/2, 12$ )	(44) $\bar{4}^+ \ x, 1/2, 0; 1/4, 1/2, 0$ ( $\bar{4}_x   1/2, 1/2, 12$ )
(45) $\bar{4}^+ \ 0, y, 1/2; 0, 1/4, 1/2$ ( $\bar{4}_y   1/2, 1/2, 12$ )	(46) $b (0, 1/2, 0) \ \bar{x} + 1/2, y, x$ ( $m_{xz}   1/2, 1/2, 12$ )	(47) $\bar{4}^- \ 1/2, y, 0; 1/2, 1/4, 0$ ( $\bar{4}_y^{-1}   1/2, 1/2, 12$ )	(48) $n (1/2, 1/2, 1/2) \ x, y, x$ ( $m_{\bar{xz}}   1/2, 1/2, 12$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

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(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$	(3) $\bar{x}, y, \bar{z} [\bar{u}, v, \bar{w}]$	(4) $x, \bar{y}, \bar{z} [u, \bar{v}, \bar{w}]$
(5) $z, x, y [w, u, v]$	(6) $z, \bar{x}, \bar{y} [w, \bar{u}, \bar{v}]$	(7) $\bar{z}, \bar{x}, y [\bar{w}, \bar{u}, v]$	(8) $\bar{z}, x, \bar{y} [\bar{w}, u, \bar{v}]$
(9) $y, z, x [v, w, u]$	(10) $\bar{y}, \bar{z}, \bar{x} [\bar{v}, \bar{w}, \bar{u}]$	(11) $y, \bar{z}, \bar{x} [v, \bar{w}, \bar{u}]$	(12) $\bar{y}, \bar{z}, x [\bar{v}, \bar{w}, u]$
(13) $y + 1/2, x + 1/2, \bar{z} + 1/2 [v, u, \bar{w}]$	(14) $\bar{y} + 1/2, \bar{x} + 1/2, \bar{z} + 1/2 [\bar{v}, \bar{u}, \bar{w}]$	(15) $y + 1/2, \bar{x} + 1/2, z + 1/2 [v, \bar{u}, w]$	(16) $\bar{y} + 1/2, x + 1/2, z + 1/2 [\bar{v}, u, w]$
(17) $x + 1/2, z + 1/2, \bar{y} + 1/2 [u, w, \bar{v}]$	(18) $\bar{x} + 1/2, \bar{z} + 1/2, y + 1/2 [\bar{u}, \bar{w}, v]$	(19) $\bar{x} + 1/2, \bar{z} + 1/2, \bar{y} + 1/2 [\bar{u}, \bar{w}, \bar{v}]$	(20) $x + 1/2, \bar{z} + 1/2, y + 1/2 [u, \bar{w}, v]$
(21) $z + 1/2, y + 1/2, \bar{x} + 1/2 [w, v, \bar{u}]$	(22) $z + 1/2, \bar{y} + 1/2, x + 1/2 [w, \bar{v}, u]$	(23) $\bar{z} + 1/2, y + 1/2, x + 1/2 [\bar{w}, v, u]$	(24) $\bar{z} + 1/2, \bar{y} + 1/2, \bar{x} + 1/2 [\bar{w}, \bar{v}, \bar{u}]$
(25) $\bar{x}, \bar{y}, \bar{z} [u, v, w]$	(26) $x, y, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$	(27) $x, \bar{y}, z [u, \bar{v}, w]$	(28) $\bar{x}, y, z [u, v, \bar{w}]$
(29) $\bar{z}, \bar{x}, \bar{y} [w, u, v]$	(30) $\bar{z}, x, y [w, \bar{u}, \bar{v}]$	(31) $z, x, \bar{y} [\bar{w}, \bar{u}, v]$	(32) $z, \bar{x}, y [\bar{w}, u, \bar{v}]$
(33) $\bar{y}, \bar{z}, \bar{x} [v, w, u]$	(34) $y, \bar{z}, x [\bar{v}, \bar{w}, \bar{u}]$	(35) $\bar{y}, z, x [v, \bar{w}, u]$	(36) $y, z, \bar{x} [\bar{v}, \bar{w}, u]$



(37)  $\bar{y}+1/2, \bar{x}+1/2, z+1/2 [v, u, \bar{w}]$  (38)  $y+1/2, x+1/2, z+1/2 [\bar{v}, \bar{u}, \bar{w}]$  (39)  $\bar{y}+1/2, x+1/2, \bar{z}+1/2 [v, \bar{u}, w]$  (40)  $y+1/2, \bar{x}+1/2, \bar{z}+1/2 [\bar{v}, u, w]$

(41)  $\bar{x}+1/2, \bar{z}+1/2, y+1/2 [u, w, \bar{v}]$  (42)  $x+1/2, \bar{z}+1/2, \bar{y}+1/2 [\bar{u}, w, v]$  (43)  $x+1/2, z+1/2, y+1/2 [\bar{u}, \bar{w}, \bar{v}]$  (44)  $\bar{x}+1/2, z+1/2, \bar{y}+1/2 [u, \bar{w}, v]$

(45)  $\bar{z}+1/2, \bar{y}+1/2, x+1/2 [w, v, \bar{u}]$  (46)  $\bar{z}+1/2, y+1/2, \bar{x}+1/2 [w, \bar{v}, u]$  (47)  $z+1/2, \bar{y}+1/2, \bar{x}+1/2 [\bar{w}, v, u]$  (48)  $z+1/2, y+1/2, x+1/2 [\bar{w}, \bar{v}, \bar{u}]$

24	k	m..	0,y,z [u,0,0]	0, $\bar{y}$ ,z [ $\bar{u}$ ,0,0]	0,y, $\bar{z}$ [ $\bar{u}$ ,0,0]	0, $\bar{y}$ , $\bar{z}$ [u,0,0]
			z,0,y [0,u,0]	z,0, $\bar{y}$ [0, $\bar{u}$ ,0]	$\bar{z}$ ,0,y [0, $\bar{u}$ ,0]	$\bar{z}$ ,0, $\bar{y}$ [0,u,0]
			y,z,0 [0,0,u]	$\bar{y}$ ,z,0 [0,0, $\bar{u}$ ]	y, $\bar{z}$ ,0 [0,0, $\bar{u}$ ]	$\bar{y}$ , $\bar{z}$ ,0 [0,0,u]
			$y+1/2, 1/2, \bar{z}+1/2 [0,u,0]$	$\bar{y}+1/2, 1/2, \bar{z}+1/2 [0, \bar{u}, 0]$	$y+1/2, 1/2, z+1/2 [0, \bar{u}, 0]$	$\bar{y}+1/2, 1/2, z+1/2 [0,u,0]$
			$1/2, z+1/2, \bar{y}+1/2 [u,0,0]$	$1/2, z+1/2, y+1/2 [\bar{u},0,0]$	$1/2, \bar{z}+1/2, \bar{y}+1/2 [\bar{u},0,0]$	$1/2, \bar{z}+1/2, y+1/2 [u,0,0]$
			$z+1/2, y+1/2, 1/2 [0,0, \bar{u}]$	$1/2+1/2, \bar{y}+1/2, 0 [0,0,u]$	$\bar{z}+1/2, y+1/2, 1/2 [0,0,u]$	$\bar{z}+1/2, \bar{y}+1/2, 1/2 [0,0, \bar{u}]$

24 j ..2

1/4,y,y+1/2 [0,v,v]	3/4, $\bar{y}$ ,y+1/2 [0, $\bar{v}$ ,v]	3/4,y, $\bar{y}+1/2 [0,v, \bar{v}]$	1/4, $\bar{y}$ , $\bar{y}+1/2 [0, \bar{v}, \bar{v}]$
y+1/2, 1/4,y [v,0,v]	y+1/2, 3/4, $\bar{y}$ [v,0, $\bar{v}]$	$\bar{y}+1/2, 3/4,y [\bar{v},0,v]$	$\bar{y}+1/2, 1/4, \bar{y} [\bar{v},0, \bar{v}]$
y,y+1/2, 1/4 [v,v,0]	$\bar{y}$ ,y+1/2, 3/4 [ $\bar{v}$ ,v,0]	y, $\bar{y}+1/2, 3/4 [v, \bar{v}, 0]$	$\bar{y}$ , $\bar{y}+1/2, 1/4 [\bar{v}, \bar{v}, 0]$
3/4, $\bar{y}$ , $\bar{y}+1/2 [0,v,v]$	1/4,y, $\bar{y}+1/2 [0, \bar{v}, v]$	1/4, $\bar{y}$ ,y+1/2 [0,v, $\bar{v}]$	3/4,y,y+1/2 [0, $\bar{v}, \bar{v}]$
$\bar{y}+1/2, 3/4, \bar{y} [v,0,v]$	$\bar{y}+1/2, 1/4, y [v,0, \bar{v}]$	y+1/2, 1/4, $\bar{y} [\bar{v},0,v]$	y+1/2, 3/4,y [ $\bar{v},0, \bar{v}]$
$\bar{y}$ , $\bar{y}+1/2, 3/4 [v,v,0]$	y, $\bar{y}+1/2, 1/4 [\bar{v},v,0]$	$\bar{y}$ ,y+1/2, 1/4 [v, $\bar{v},0]$	y,y+1/2, 3/4 [ $\bar{v}, \bar{v}, 0]$

16	i	.3.	x,x,x [u,u,u]	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$
			$\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$	x, $\bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
			$x+1/2, x+1/2, \bar{x}+1/2 [u, u, \bar{u}]$	$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, \bar{u}]$
			$x+1/2, \bar{x}+1/2, x+1/2 [u, \bar{u}, u]$	$\bar{x}+1/2, x+1/2, x+1/2 [\bar{u}, u, u]$
			$\bar{x}, \bar{x}, \bar{x} [u, u, u]$	x,x, $\bar{x} [\bar{u}, \bar{u}, u]$
			x, $\bar{x}, x [\bar{u}, u, \bar{u}]$	$\bar{x}, x, x [u, \bar{u}, \bar{u}]$
			$\bar{x}+1/2, \bar{x}+1/2, x+1/2 [u, u, \bar{u}]$	$x+1/2, x+1/2, x+1/2 [\bar{u}, \bar{u}, \bar{u}]$
			$\bar{x}+1/2, x+1/2, \bar{x}+1/2 [u, \bar{u}, u]$	$x+1/2, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, u, u]$

12	h	mm2..	x,1/2,0 [0,0,0]	$\bar{x}$ ,1/2,0 [0,0,0]	0,x,1/2 [0,0,0]	0, $\bar{x}$ ,1/2 [0,0,0]
			1/2,0,x [0,0,0]	1/2,0, $\bar{x}$ [0,0,0]	0,x+1/2,1/2 [0,0,0]	0, $\bar{x}+1/2, 1/2 [0,0,0]$
			x+1/2,1/2,0 [0,0,0]	$\bar{x}+1/2, 1/2, 0 [0,0,0]$	1/2,0, $\bar{x}+1/2 [0,0,0]$	1/2,0,x+1/2 [0,0,0]

Continued

223.1.1606

 $Pm\bar{3}n$ 

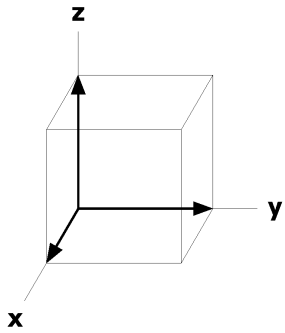
12	g	$mm2..$	$x,0,1/2 [0,0,0]$	$\bar{x},0,1/2 [0,0,0]$	$1/2,x,0 [0,0,0]$	$1/2,\bar{x},0 [0,0,0]$
			$0,1/2,x [0,0,0]$	$0,1/2,\bar{x} [0,0,0]$	$1/2,x+1/2,0 [0,0,0]$	$1/2,\bar{x}+1/2,0 [0,0,0]$
			$x+1/2,0,1/2 [0,0,0]$	$\bar{x}+1/2,0,1/2 [0,0,0]$	$0,1/2,\bar{x}+1/2 [0,0,0]$	$0,1/2,x+1/2 [0,0,0]$
12	f	$mm2..$	$x,0,0 [0,0,0]$	$\bar{x},0,0 [0,0,0]$	$0,x,0 [0,0,0]$	$0,\bar{x},0 [0,0,0]$
			$0,0,x [0,0,0]$	$0,0,\bar{x} [0,0,0]$	$1/2,x+1/2,1/2 [0,0,0]$	$1/2,\bar{x}+1/2,1/2 [0,0,0]$
			$x+1/2,1/2,1/2 [0,0,0]$	$\bar{x}+1/2,1/2,1/2 [0,0,0]$	$1/2,1/2,\bar{x}+1/2 [0,0,0]$	$1/2,1/2,x+1/2 [0,0,0]$
8	e	$.32$	$1/4,1/4,1/4 [0,0,0]$	$3/4,3/4,1/4 [0,0,0]$	$3/4,1/4,3/4 [0,0,0]$	$1/4,3/4,3/4 [0,0,0]$
			$3/4,3/4,3/4 [0,0,0]$	$1/4,1/4,3/4 [0,0,0]$	$1/4,3/4,1/4 [0,0,0]$	$3/4,1/4,1/4 [0,0,0]$
6	d	$\bar{4}m.2$	$1/4,1/2,0 [0,0,0]$	$3/4,1/2,0 [0,0,0]$	$0,1/4,1/2 [0,0,0]$	
			$0,3/4,1/2 [0,0,0]$	$1/2,0,1/4 [0,0,0]$	$1/2,0,3/4 [0,0,0]$	
6	c	$\bar{4}m.2$	$1/4,0,1/2 [0,0,0]$	$3/4,0,1/2 [0,0,0]$	$1/2,1/4,0 [0,0,0]$	
			$1/2,3/4,0 [0,0,0]$	$0,1/2,1/4 [0,0,0]$	$0,1/2,3/4 [0,0,0]$	
6	b	$mmm..$	$0,1/2,1/2 [0,0,0]$	$1/2,0,1/2 [0,0,0]$	$1/2,1/2,0 [0,0,0]$	
			$0,1/2,0 [0,0,0]$	$1/2,0,0 [0,0,0]$	$0,0,1/2 [0,0,0]$	
2	a	$m\bar{3}.$	$0,0,0 [0,0,0]$	$1/2,1/2,1/2 [0,0,0]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at  $0,1/2,z$

Along  $[1,1,1]$   $p6'm'm$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x,x,x$

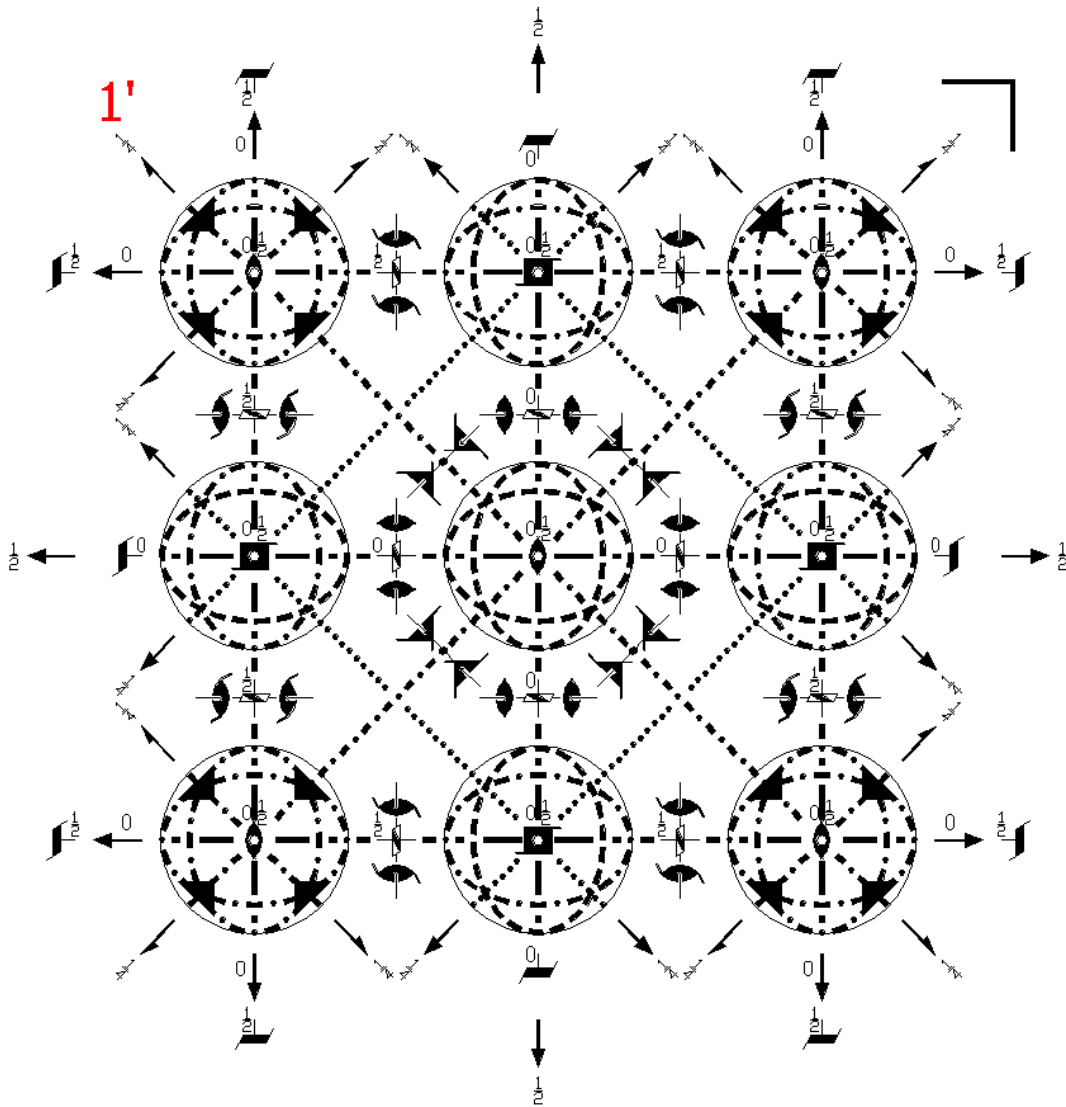
Along  $[1,1,0]$   $p_{2a}2mm$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,1/4$



$Pm\bar{3}n1'$   
223.2.1607

$m\bar{3}n1'$   
 $P4_2/m\bar{3}2/n1'$

Cubic



**Origin** at center ( $m\bar{3}1'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $z \leq \min(x, 1/2-x, y, 1/2-y)$

**Vertices** 0,0,0      1/2,0,0      1/2,1/2,0      0,1/2,0      1/4,1/4,1/4

**Symmetry Operations**

For 1 + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                  | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)              |

(13) 2 (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)	(14) 2 x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)	(15) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)	(16) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)
(17) 4 <sup>-</sup> (1/2,0,0) x,1/2,0 (4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,1/2)	(18) 2 (0,1/2,1/2) 1/4,y,y (2 <sub>yz</sub>  1/2,1/2,1/2)	(19) 2 1/4,y+1/2, $\bar{y}$ (2 <sub>yz</sub>  1/2,1/2,1/2)	(20) 4 <sup>+</sup> (1/2,0,0) x,0,1/2 (4 <sub>x</sub>  1/2,1/2,1/2)
(21) 4 <sup>+</sup> (0,1/2,0) 1/2,y,0 (4 <sub>y</sub>  1/2,1/2,1/2)	(22) 2 (1/2,0,1/2) x,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)	(23) 4 <sup>-</sup> (0,1/2,0) 0,y,1/2 (4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,1/2)	(24) 2 $\bar{x}$ +1/2,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)
(25) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(26) m x,y,0 (m <sub>z</sub>  0,0,0)	(27) m x,0,z (m <sub>y</sub>  0,0,0)	(28) m 0,y,z (m <sub>x</sub>  0,0,0)
(29) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)	(30) $\bar{3}^+$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)	(31) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)	(32) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)
(33) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)	(34) $\bar{3}^-$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)	(35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)	(36) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)
(37) c (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,12)	(38) n (1/2,1/2,1/2) x,x,z (m <sub>xy</sub>  1/2,1/2,12)	(39) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>  1/2,1/2,12)	(40) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$  1/2,1/2,12)
(41) $\bar{4}^-$ x,0,1/2; 1/4,0,1/2 ( $\bar{4}_x$ <sup>-1</sup>  1/2,1/2,12)	(42) a (1/2,0,0) x,y+1/2, $\bar{y}$ (m <sub>yz</sub>  1/2,1/2,12)	(43) n (1/2,1/2,1/2) x,y,y (m <sub>yz</sub>  1/2,1/2,12)	(44) $\bar{4}^+$ x,1/2,0; 1/4,1/2,0 ( $\bar{4}_x$  1/2,1/2,12)
(45) $\bar{4}^+$ 0,y,1/2; 0,1/4,1/2 ( $\bar{4}_y$  1/2,1/2,12)	(46) b (0,1/2,0) $\bar{x}$ +1/2,y,x (m <sub>xz</sub>  1/2,1/2,12)	(47) $\bar{4}^-$ 1/2,y,0; 1/2,1/4,0 ( $\bar{4}_y$ <sup>-1</sup>  1/2,1/2,12)	(48) n (1/2,1/2,1/2) x,y,x (m <sub>xz</sub>  1/2,1/2,12)

## For 1' + set

(1) 1' ( $\bar{1}$  0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(4) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'
(5) 3 <sup>+</sup> x,x,x ( $\bar{3}_{xyz}$  0,0,0)'	(6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$ ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$ ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'
(9) 3 <sup>-</sup> x,x,x ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$ ( $\bar{3}_{xyz}$  0,0,0)'	(11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x ( $\bar{3}_{xyz}$  0,0,0)'	(12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$ ( $\bar{3}_{xyz}$  0,0,0)'
(13) 2' (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(14) 2' x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(15) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(16) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)'
(17) 4 <sup>-</sup> (1/2,0,0) x,1/2,0 (4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(18) 2' (0,1/2,1/2) 1/4,y,y (2 <sub>yz</sub>  1/2,1/2,1/2)'	(19) 2' 1/4,y+1/2, $\bar{y}$ (2 <sub>yz</sub>  1/2,1/2,1/2)'	(20) 4 <sup>+</sup> (1/2,0,0) x,0,1/2 (4 <sub>x</sub>  1/2,1/2,1/2)'
(21) 4 <sup>+</sup> (0,1/2,0) 1/2,y,0 (4 <sub>y</sub>  1/2,1/2,1/2)'	(22) 2' (1/2,0,1/2) x,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)'	(23) 4 <sup>-</sup> (0,1/2,0) 0,y,1/2 (4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(24) 2' $\bar{x}$ +1/2,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)'
(25) $\bar{1}$ ' 0,0,0 ( $\bar{1}$  0,0,0)'	(26) m' x,y,0 (m <sub>z</sub>  0,0,0)'	(27) m' x,0,z (m <sub>y</sub>  0,0,0)'	(28) m' 0,y,z (m <sub>x</sub>  0,0,0)'
(29) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'	(30) $\bar{3}^+$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(31) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(32) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'
(33) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(34) $\bar{3}^-$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'	(35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'	(36) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'

Continued

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Pm $\bar{3}$ n1'

- |   |   |   |  |
|---|---|---|--|
| (37) $c'$ (0,0,1/2) $x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,12$ )'           | (38) $n'$ (1/2,1/2,1/2) $x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,12$ )' | (39) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1} 1/2,1/2,12$ )' | (40) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z 1/2,1/2,12$ )'   |
| (41) $\bar{4}^-$ ' $x,0,1/2; 1/4,0,1/2$<br>( $\bar{4}_x^{-1} 1/2,1/2,12$ )' | (42) $a'$ (1/2,0,0) $x,y+1/2,\bar{y}$<br>( $m_{yz} 1/2,1/2,12$ )' | (43) $n'$ (1/2,1/2,1/2) $x,y,y$<br>( $m_{\bar{yz}} 1/2,1/2,12$ )'         | (44) $\bar{4}^+$ ' $x,1/2,0; 1/4,1/2,0$<br>( $\bar{4}_x 1/2,1/2,12$ )' |
| (45) $\bar{4}^+$ ' 0,y,1/2; 0,1/4,1/2<br>( $\bar{4}_y 1/2,1/2,12$ )'        | (46) $b'$ (0,1/2,0) $\bar{x}+1/2,y,x$<br>( $m_{xz} 1/2,1/2,12$ )' | (47) $\bar{4}^-$ ' 1/2,y,0; 1/2,1/4,0<br>( $\bar{4}_y^{-1} 1/2,1/2,12$ )' | (48) $n'$ (1/2,1/2,1/2) $x,y,x$<br>( $m_{\bar{xz}} 1/2,1/2,12$ )'      |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

1 + 1'

Continued

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Pm $\bar{3}$ n1'

48 l 11'

- |  |  |  |  |
|--|--|--|--|
| (1) $x,y,z$ [0,0,0]                          | (2) $\bar{x},\bar{y},z$ [0,0,0]                    | (3) $\bar{x},y,\bar{z}$ [0,0,0]                    | (4) $x,\bar{y},\bar{z}$ [0,0,0]                    |
| (5) $z,x,y$ [0,0,0]                          | (6) $z,\bar{x},\bar{y}$ [0,0,0]                    | (7) $\bar{z},\bar{x},y$ [0,0,0]                    | (8) $\bar{z},x,\bar{y}$ [0,0,0]                    |
| (9) $y,z,x$ [0,0,0]                          | (10) $\bar{y},z,\bar{x}$ [0,0,0]                   | (11) $y,\bar{z},\bar{x}$ [0,0,0]                   | (12) $\bar{y},\bar{z},x$ [0,0,0]                   |
| (13) $y+1/2,x+1/2,\bar{z}+1/2$ [0,0,0]       | (14) $\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2$ [0,0,0] | (15) $y+1/2,\bar{x}+1/2,z+1/2$ [0,0,0]             | (16) $\bar{y}+1/2,x+1/2,z+1/2$ [0,0,0]             |
| (17) $x+1/2,z+1/2,\bar{y}+1/2$ [0,0,0]       | (18) $\bar{x}+1/2,z+1/2,y+1/2$ [0,0,0]             | (19) $\bar{x}+1/2,\bar{z}+1/2,\bar{y}+1/2$ [0,0,0] | (20) $x+1/2,\bar{z}+1/2,y+1/2$ [0,0,0]             |
| (21) $z+1/2,y+1/2,\bar{x}+1/2$ [0,0,0]       | (22) $z+1/2,\bar{y}+1/2,x+1/2$ [0,0,0]             | (23) $\bar{z}+1/2,y+1/2,x+1/2$ [0,0,0]             | (24) $\bar{z}+1/2,\bar{y}+1/2,\bar{x}+1/2$ [0,0,0] |
| (25) $\bar{x},\bar{y},\bar{z}$ [0,0,0]       | (26) $x,y,\bar{z}$ [0,0,0]                         | (27) $x,\bar{y},z$ [0,0,0]                         | (28) $\bar{x},y,z$ [0,0,0]                         |
| (29) $\bar{z},\bar{x},\bar{y}$ [0,0,0]       | (30) $\bar{z},x,y$ [0,0,0]                         | (31) $z,x,\bar{y}$ [0,0,0]                         | (32) $z,\bar{x},y$ [0,0,0]                         |
| (33) $\bar{y},\bar{z},\bar{x}$ [0,0,0]       | (34) $y,\bar{z},x$ [0,0,0]                         | (35) $\bar{y},z,x$ [0,0,0]                         | (36) $y,z,\bar{x}$ [0,0,0]                         |
| (37) $\bar{y}+1/2,\bar{x}+1/2,z+1/2$ [0,0,0] | (38) $y+1/2,x+1/2,z+1/2$ [0,0,0]                   | (39) $\bar{y}+1/2,x+1/2,\bar{z}+1/2$ [0,0,0]       | (40) $y+1/2,\bar{x}+1/2,\bar{z}+1/2$ [0,0,0]       |
| (41) $\bar{x}+1/2,\bar{z}+1/2,y+1/2$ [0,0,0] | (42) $x+1/2,\bar{z}+1/2,\bar{y}+1/2$ [0,0,0]       | (43) $x+1/2,z+1/2,y+1/2$ [0,0,0]                   | (44) $\bar{x}+1/2,z+1/2,\bar{y}+1/2$ [0,0,0]       |
| (45) $\bar{z}+1/2,\bar{y}+1/2,x+1/2$ [0,0,0] | (46) $\bar{z}+1/2,y+1/2,\bar{x}+1/2$ [0,0,0]       | (47) $z+1/2,\bar{y}+1/2,\bar{x}+1/2$ [0,0,0]       | (48) $z+1/2,y+1/2,x+1/2$ [0,0,0]                   |
| 24 k m..1'                                   | 0,y,z [0,0,0]                                      | 0, $\bar{y}$ ,z [0,0,0]                            | 0, $\bar{y}$ , $\bar{z}$ [0,0,0]                   |
|  | z,0,y [0,0,0]                                      | z,0, $\bar{y}$ [0,0,0]                             | $\bar{z}$ ,0, $\bar{y}$ [0,0,0]                    |
|  | y,z,0 [0,0,0]                                      | $\bar{y}$ ,z,0 [0,0,0]                             | $\bar{y}$ , $\bar{z}$ ,0 [0,0,0]                   |

$y+1/2, 1/2, \bar{z}+1/2 [0,0,0]$   $\bar{y}+1/2, 1/2, \bar{z}+1/2 [0,0,0]$   $y+1/2, 1/2, z+1/2 [0,0,0]$   $\bar{y}+1/2, 1/2, z+1/2 [0,0,0]$   
 $1/2, z+1/2, \bar{y}+1/2 [0,0,0]$   $1/2, z+1/2, y+1/2 [0,0,0]$   $1/2, \bar{z}+1/2, \bar{y}+1/2 [0,0,0]$   $1/2, \bar{z}+1/2, y+1/2 [0,0,0]$   
 $z+1/2, y+1/2, 1/2 [0,0,0]$   $1/2+1/2, \bar{y}+1/2, 0 [0,0,0]$   $\bar{z}+1/2, y+1/2, 1/2 [0,0,0]$   $\bar{z}+1/2, \bar{y}+1/2, 1/2 [0,0,0]$

24 j ..21'

$1/4, y, y+1/2 [0,0,0]$	$3/4, \bar{y}, y+1/2 [0,0,0]$	$3/4, y, \bar{y}+1/2 [0,0,0]$	$1/4, \bar{y}, \bar{y}+1/2 [0,0,0]$
$y+1/2, 1/4, y [0,0,0]$	$y+1/2, 3/4, \bar{y} [0,0,0]$	$\bar{y}+1/2, 3/4, y [0,0,0]$	$\bar{y}+1/2, 1/4, \bar{y} [0,0,0]$
$y, y+1/2, 1/4 [0,0,0]$	$\bar{y}, y+1/2, 3/4 [0,0,0]$	$y, \bar{y}+1/2, 3/4 [0,0,0]$	$\bar{y}, \bar{y}+1/2, 1/4 [0,0,0]$
$3/4, \bar{y}, \bar{y}+1/2 [0,0,0]$	$1/4, y, \bar{y}+1/2 [0,0,0]$	$1/4, \bar{y}, y+1/2 [0,0,0]$	$3/4, y, y+1/2 [0,0,0]$
$\bar{y}+1/2, 3/4, \bar{y} [0,0,0]$	$\bar{y}+1/2, 1/4, y [0,0,0]$	$y+1/2, 1/4, \bar{y} [0,0,0]$	$y+1/2, 3/4, y [0,0,0]$
$\bar{y}, \bar{y}+1/2, 3/4 [0,0,0]$	$y, \bar{y}+1/2, 1/4 [0,0,0]$	$\bar{y}, y+1/2, 1/4 [0,0,0]$	$y, y+1/2, 3/4 [0,0,0]$

16 i .3.1'

$x, x, x [0,0,0]$	$\bar{x}, \bar{x}, x [0,0,0]$
$\bar{x}, x, \bar{x} [0,0,0]$	$x, \bar{x}, \bar{x} [0,0,0]$
$x+1/2, x+1/2, \bar{x}+1/2 [0,0,0]$	$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [0,0,0]$
$x+1/2, \bar{x}+1/2, x+1/2 [0,0,0]$	$\bar{x}+1/2, x+1/2, x+1/2 [0,0,0]$
$\bar{x}, \bar{x}, \bar{x} [0,0,0]$	$x, x, \bar{x} [0,0,0]$
$x, \bar{x}, x [0,0,0]$	$\bar{x}, x, x [0,0,0]$
$\bar{x}+1/2, \bar{x}+1/2, x+1/2 [0,0,0]$	$x+1/2, x+1/2, x+1/2 [0,0,0]$
$\bar{x}+1/2, x+1/2, \bar{x}+1/2 [0,0,0]$	$x+1/2, \bar{x}+1/2, \bar{x}+1/2 [0,0,0]$

12 h mm2..1'	$x, 1/2, 0 [0,0,0]$	$\bar{x}, 1/2, 0 [0,0,0]$	$0, x, 1/2 [0,0,0]$	$0, \bar{x}, 1/2 [0,0,0]$
	$1/2, 0, x [0,0,0]$	$1/2, 0, \bar{x} [0,0,0]$	$0, x+1/2, 1/2 [0,0,0]$	$0, \bar{x}+1/2, 1/2 [0,0,0]$
	$x+1/2, 1/2, 0 [0,0,0]$	$\bar{x}+1/2, 1/2, 0 [0,0,0]$	$1/2, 0, \bar{x}+1/2 [0,0,0]$	$1/2, 0, x+1/2 [0,0,0]$

12 g mm2..1'	$x, 0, 1/2 [0,0,0]$	$\bar{x}, 0, 1/2 [0,0,0]$	$1/2, x, 0 [0,0,0]$	$1/2, \bar{x}, 0 [0,0,0]$
	$0, 1/2, x [0,0,0]$	$0, 1/2, \bar{x} [0,0,0]$	$1/2, x+1/2, 0 [0,0,0]$	$1/2, \bar{x}+1/2, 0 [0,0,0]$
	$x+1/2, 0, 1/2 [0,0,0]$	$\bar{x}+1/2, 0, 1/2 [0,0,0]$	$0, 1/2, \bar{x}+1/2 [0,0,0]$	$0, 1/2, x+1/2 [0,0,0]$

12 f mm2..1'	$x, 0, 0 [0,0,0]$	$\bar{x}, 0, 0 [0,0,0]$	$0, x, 0 [0,0,0]$	$0, \bar{x}, 0 [0,0,0]$
	$0, 0, x [0,0,0]$	$0, 0, \bar{x} [0,0,0]$	$1/2, x+1/2, 1/2 [0,0,0]$	$1/2, \bar{x}+1/2, 1/2 [0,0,0]$
	$x+1/2, 1/2, 1/2 [0,0,0]$	$\bar{x}+1/2, 1/2, 1/2 [0,0,0]$	$1/2, 1/2, \bar{x}+1/2 [0,0,0]$	$1/2, 1/2, x+1/2 [0,0,0]$

8 e .321'	$1/4, 1/4, 1/4 [0,0,0]$	$3/4, 3/4, 1/4 [0,0,0]$	$3/4, 1/4, 3/4 [0,0,0]$	$1/4, 3/4, 3/4 [0,0,0]$
	$3/4, 3/4, 3/4 [0,0,0]$	$1/4, 1/4, 3/4 [0,0,0]$	$1/4, 3/4, 1/4 [0,0,0]$	$3/4, 1/4, 1/4 [0,0,0]$

Continued

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 $Pm\bar{3}n1'$ 

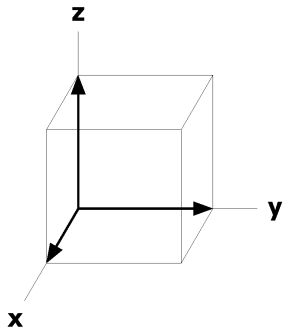
6	d	$\bar{4}m.21'$ 1/4,1/2,0 [0,0,0]	3/4,1/2,0 [0,0,0]	0,1/4,1/2 [0,0,0]
		0,3/4,1/2 [0,0,0]	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]
6	c	$\bar{4}m.21'$ 1/4,0,1/2 [0,0,0]	3/4,0,1/2 [0,0,0]	1/2,1/4,0 [0,0,0]
		1/2,3/4,0 [0,0,0]	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]
6	b	mmm..1' 0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
		0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]	0,0,1/2 [0,0,0]
2	a	$m\bar{3}.1'$ 0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	

**Symmetry of Special Projections**

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,1,1]  $p6mm1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

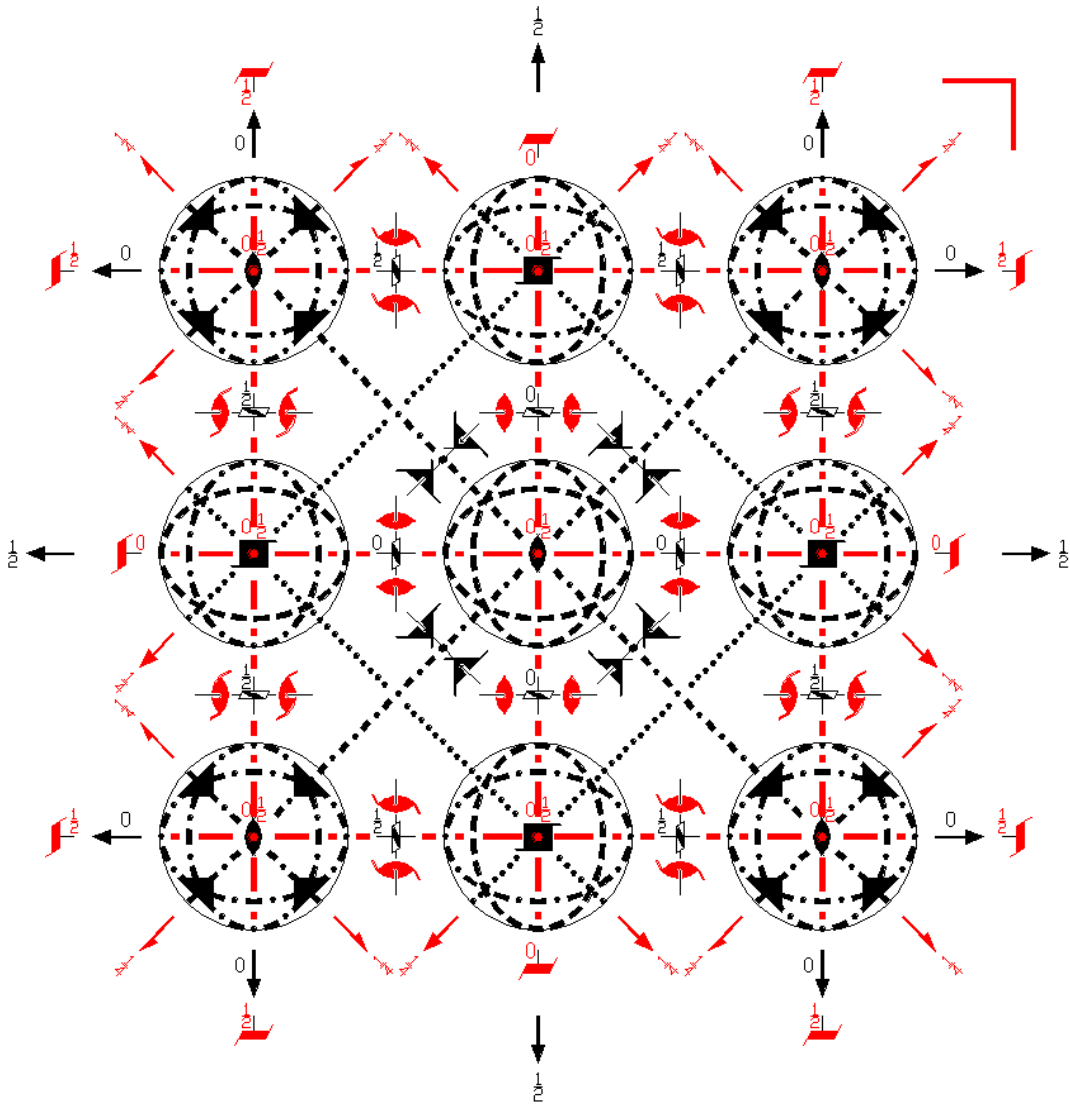
Along [1,1,0]  $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



Pm $\bar{3}$ 'n  
223.3.1608

m $\bar{3}$ 'n  
P4 $_2$ 'm $\bar{3}$ '2'/n

Cubic



**Origin** at center (m $\bar{3}$ 'n)

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $z \leq \min(x, 1/2-x, y, 1/2-y)$

**Vertices** 0,0,0    1/2,0,0    1/2,1/2,0    0,1/2,0    1/4,1/4,1/4

**Symmetry Operations**

- |   |  |  |   |
|---|--|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)       | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>x<math>\bar{y}z</math></sub>  0,0,0) | (12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub>  0,0,0)               |



13) 2' (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(14) 2' x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(15) 4' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(16) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)'
(17) 4' (1/2,0,0) x,1/2,0 (4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(18) 2' (0,1/2,1/2) 1/4,y,y (2 <sub>yz</sub>  1/2,1/2,1/2)'	(19) 2' 1/4,y+1/2, $\bar{y}$ (2 <sub>yz</sub>  1/2,1/2,1/2)'	(20) 4 <sup>+</sup> (1/2,0,0) x,0,1/2 (4 <sub>x</sub>  1/2,1/2,1/2)'
(21) 4 <sup>+</sup> (0,1/2,0) 1/2,y,0 (4 <sub>y</sub>  1/2,1/2,1/2)'	(22) 2' (1/2,0,1/2) x,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)'	(23) 4' (0,1/2,0) 0,y,1/2 (4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(24) 2' $\bar{x}$ +1/2,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)'
(25) $\bar{1}$ ' 0,0,0 ( $\bar{1}$  0,0,0)'	(26) m' x,y,0 (m <sub>z</sub>  0,0,0)'	(27) m' x,0,z (m <sub>y</sub>  0,0,0)'	(28) m' 0,y,z (m <sub>x</sub>  0,0,0)'
(29) $\bar{3}^+$ ' x,x,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'	(30) $\bar{3}^+$ ' $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(31) $\bar{3}^+$ ' x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(32) $\bar{3}^+$ ' $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'
(33) $\bar{3}^-$ ' x,x,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(34) $\bar{3}^-$ ' x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'	(35) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'	(36) $\bar{3}^-$ ' $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'
(37) c (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,12)	(38) n (1/2,1/2,1/2) x,x,z (m <sub>xy</sub>  1/2,1/2,12)	(39) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>  1/2,1/2,12)	(40) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$  1/2,1/2,12)
(41) $\bar{4}^-$ x,0,1/2; 1/4,0,1/2 ( $\bar{4}_x$ <sup>-1</sup>  1/2,1/2,12)	(42) a (1/2,0,0) x,y+1/2, $\bar{y}$ (m <sub>yz</sub>  1/2,1/2,12)	(43) n (1/2,1/2,1/2) x,y,y (m <sub>yz</sub>  1/2,1/2,12)	(44) $\bar{4}^+$ x,1/2,0; 1/4,1/2,0 ( $\bar{4}_x$  1/2,1/2,12)
(45) $\bar{4}^+$ 0,y,1/2; 0,1/4,1/2 ( $\bar{4}_y$  1/2,1/2,12)	(46) b (0,1/2,0) $\bar{x}$ +1/2,y,x (m <sub>xz</sub>  1/2,1/2,12)	(47) $\bar{4}^-$ 1/2,y,0; 1/2,1/4,0 ( $\bar{4}_y$ <sup>-1</sup>  1/2,1/2,12)	(48) n (1/2,1/2,1/2) x,y,x (m <sub>xz</sub>  1/2,1/2,12)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

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(1) x,y,z [u,v,w]	(2) $\bar{x}$ , $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w]	(3) $\bar{x}$ ,y, $\bar{z}$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x, $\bar{y}$ , $\bar{z}$ [u, $\bar{v}$ , $\bar{w}$ ]
(5) z,x,y [w,u,v]	(6) z, $\bar{x}$ , $\bar{y}$ [w, $\bar{u}$ , $\bar{v}$ ]	(7) $\bar{z}$ , $\bar{x}$ ,y [ $\bar{w}$ , $\bar{u}$ ,v]	(8) $\bar{z}$ ,x,y [w,u, $\bar{v}$ ]
(9) y,z,x [v,w,u]	(10) $\bar{y}$ ,z, $\bar{x}$ [ $\bar{v}$ ,w, $\bar{u}$ ]	(11) y, $\bar{z}$ , $\bar{x}$ [v, $\bar{w}$ , $\bar{u}$ ]	(12) $\bar{y}$ , $\bar{z}$ ,x [ $\bar{v}$ , $\bar{w}$ ,u]
(13) y+1/2,x+1/2, $\bar{z}$ +1/2 [ $\bar{v}$ , $\bar{u}$ ,w]	(14) $\bar{y}$ +1/2, $\bar{x}$ +1/2, $\bar{z}$ +1/2 [v,u,w]	(15) y+1/2, $\bar{x}$ +1/2,z+1/2 [ $\bar{v}$ ,u, $\bar{w}$ ]	(16) $\bar{y}$ +1/2,x+1/2,z+1/2 [v, $\bar{u}$ , $\bar{w}$ ]
(17) x+1/2,z+1/2, $\bar{y}$ +1/2 [ $\bar{u}$ , $\bar{w}$ ,v]	(18) $\bar{x}$ +1/2,z+1/2,y+1/2 [u, $\bar{w}$ , $\bar{v}$ ]	(19) $\bar{x}$ +1/2, $\bar{z}$ +1/2, $\bar{y}$ +1/2 [u,w,v]	(20) x+1/2, $\bar{z}$ +1/2,y+1/2 [ $\bar{u}$ ,w, $\bar{v}$ ]
(21) z+1/2,y+1/2, $\bar{x}$ +1/2 [ $\bar{w}$ , $\bar{v}$ ,u]	(22) z+1/2, $\bar{y}$ +1/2,x+1/2 [ $\bar{w}$ ,v, $\bar{u}$ ]	(23) $\bar{z}$ +1/2,y+1/2,x+1/2 [w, $\bar{v}$ , $\bar{u}$ ]	(24) $\bar{z}$ +1/2, $\bar{y}$ +1/2, $\bar{x}$ +1/2 [w,v,u]
(25) $\bar{x}$ , $\bar{y}$ , $\bar{z}$ [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(26) x,y, $\bar{z}$ [u,v, $\bar{w}$ ]	(27) x, $\bar{y}$ ,z [u, $\bar{v}$ ,w]	(28) $\bar{x}$ ,y,z [ $\bar{u}$ ,v,w]
(29) $\bar{z}$ , $\bar{x}$ , $\bar{y}$ [ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ]	(30) $\bar{z}$ ,x,y [ $\bar{w}$ ,u,v]	(31) z,x, $\bar{y}$ [w,u, $\bar{v}$ ]	(32) z, $\bar{x}$ ,y [w, $\bar{u}$ ,v]
(33) $\bar{y}$ , $\bar{z}$ , $\bar{x}$ [ $\bar{v}$ , $\bar{w}$ , $\bar{u}$ ]	(34) y, $\bar{z}$ ,x [v, $\bar{w}$ ,u]	(35) $\bar{y}$ ,z,x [ $\bar{v}$ ,w,u]	(36) y,z, $\bar{x}$ [v,w, $\bar{u}$ ]

$$(37) \bar{y}+1/2, \bar{x}+1/2, z+1/2 [v, u, \bar{w}] \quad (38) y+1/2, x+1/2, z+1/2 [\bar{v}, \bar{u}, \bar{w}] \quad (39) \bar{y}+1/2, x+1/2, \bar{z}+1/2 [v, \bar{u}, w] \quad (40) y+1/2, \bar{x}+1/2, \bar{z}+1/2 [\bar{v}, u, w]$$

$$(41) \bar{x}+1/2, \bar{z}+1/2, y+1/2 [u, w, \bar{v}] \quad (42) x+1/2, \bar{z}+1/2, \bar{y}+1/2 [\bar{u}, w, v] \quad (43) x+1/2, z+1/2, y+1/2 [\bar{u}, \bar{w}, \bar{v}] \quad (44) \bar{x}+1/2, z+1/2, \bar{y}+1/2 [u, \bar{w}, v]$$

$$(45) \bar{z}+1/2, \bar{y}+1/2, x+1/2 [w, v, \bar{u}] \quad (46) \bar{z}+1/2, y+1/2, \bar{x}+1/2 [w, \bar{v}, u] \quad (47) z+1/2, \bar{y}+1/2, \bar{x}+1/2 [\bar{w}, v, u] \quad (48) z+1/2, y+1/2, x+1/2 [\bar{w}, \bar{v}, \bar{u}]$$

24	k	m'..	0,y,z [0,v,w]	0, $\bar{y}$ ,z [0, $\bar{v}$ ,w]	0,y, $\bar{z}$ [0,v, $\bar{w}$ ]	0, $\bar{y}$ , $\bar{z}$ [0, $\bar{v}$ , $\bar{w}$ ]
			z,0,y [w,0,v]	z,0, $\bar{y}$ [w,0, $\bar{v}$ ]	$\bar{z}$ ,0,y [w,0,v]	$\bar{z}$ ,0, $\bar{y}$ [w,0, $\bar{v}$ ]
			y,z,0 [v,w,0]	$\bar{y}$ ,z,0 [v,w,0]	y, $\bar{z}$ ,0 [v,w,0]	$\bar{y}$ , $\bar{z}$ ,0 [v,w,0]
			$y+1/2, 1/2, \bar{z}+1/2 [\bar{v}, 0, w]$	$\bar{y}+1/2, 1/2, \bar{z}+1/2 [v, 0, w]$	$y+1/2, 1/2, z+1/2 [\bar{v}, 0, \bar{w}]$	$\bar{y}+1/2, 1/2, z+1/2 [v, 0, \bar{w}]$
			$1/2, z+1/2, \bar{y}+1/2 [0, \bar{w}, v]$	$1/2, z+1/2, y+1/2 [0, \bar{w}, \bar{v}]$	$1/2, \bar{z}+1/2, \bar{y}+1/2 [0, w, v]$	$1/2, \bar{z}+1/2, y+1/2 [0, w, \bar{v}]$
			$z+1/2, y+1/2, 1/2 [\bar{w}, \bar{v}, 0]$	$1/2+1/2, \bar{y}+1/2, 0 [\bar{w}, v, 0]$	$\bar{z}+1/2, y+1/2, 1/2 [w, \bar{v}, 0]$	$\bar{z}+1/2, \bar{y}+1/2, 1/2 [w, v, 0]$

$$24 \quad j \quad ..2'$$

1/4,y,y+1/2 [u,v, $\bar{v}$ ]	3/4, $\bar{y}$ ,y+1/2 [ $\bar{u}$ , $\bar{v}$ , $\bar{v}$ ]	3/4,y, $\bar{y}+1/2 [\bar{u}$ ,v,v]	1/4, $\bar{y}$ , $\bar{y}+1/2 [u,\bar{v},v]$
y+1/2,1/4,y [ $\bar{v}$ ,u,v]	y+1/2,3/4, $\bar{y}$ [ $\bar{v}$ , $\bar{u}$ , $\bar{v}$ ]	$\bar{y}+1/2, 3/4, y [v, \bar{u}, v]$	$\bar{y}+1/2, 1/4, \bar{y} [v, u, \bar{v}]$
y,y+1/2,1/4 [v, $\bar{v}$ ,u]	$\bar{y}$ ,y+1/2,3/4 [ $\bar{v}$ , $\bar{v}$ , $\bar{u}$ ]	y, $\bar{y}+1/2, 3/4 [v, v, \bar{u}]$	$\bar{y}$ , $\bar{y}+1/2, 1/4 [\bar{v}, v, u]$
3/4, $\bar{y}$ , $\bar{y}+1/2 [\bar{u}$ , $\bar{v}$ ,v]	1/4,y, $\bar{y}+1/2 [u,v,v]$	1/4, $\bar{y}$ ,y+1/2 [u, $\bar{v}$ , $\bar{v}$ ]	3/4,y,y+1/2 [ $\bar{u}$ ,v, $\bar{v}$ ]
$\bar{y}+1/2, 3/4, \bar{y} [v, \bar{u}, \bar{v}]$	$\bar{y}+1/2, 1/4, y [v, u, v]$	y+1/2,1/4, $\bar{y}$ [ $\bar{v}$ ,u, $\bar{v}$ ]	y+1/2,3/4,y [ $\bar{v}$ , $\bar{u}$ ,v]
$\bar{y}$ , $\bar{y}+1/2, 3/4 [\bar{v}, v, \bar{u}]$	y, $\bar{y}+1/2, 1/4 [v, v, u]$	$\bar{y}$ ,y+1/2,1/4 [ $\bar{v}$ , $\bar{v}$ ,u]	y,y+1/2,3/4 [v, $\bar{v}$ , $\bar{u}$ ]

16	i	.3.	x,x,x [u,u,u]	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$
			$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
			$x+1/2, x+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, u]$	$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [u, u, u]$
			$x+1/2, \bar{x}+1/2, x+1/2 [\bar{u}, u, \bar{u}]$	$\bar{x}+1/2, x+1/2, x+1/2 [u, \bar{u}, \bar{u}]$
			$\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$	$x, x, \bar{x} [u, u, \bar{u}]$
			$x, \bar{x}, x [u, \bar{u}, u]$	$\bar{x}, x, x [\bar{u}, u, u]$
			$\bar{x}+1/2, \bar{x}+1/2, x+1/2 [u, u, \bar{u}]$	$x+1/2, x+1/2, x+1/2 [\bar{u}, \bar{u}, \bar{u}]$
			$\bar{x}+1/2, x+1/2, \bar{x}+1/2 [u, \bar{u}, u]$	$x+1/2, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, u, u]$

12	h	m'm'2..	x,1/2,0 [u,0,0]	$\bar{x}, 1/2, 0 [\bar{u}, 0, 0]$	0,x,1/2 [0,u,0]	0, $\bar{x}$ ,1/2 [0, $\bar{u}$ ,0]
			1/2,0,x [0,0,u]	1/2,0, $\bar{x}$ [0,0, $\bar{u}$ ]	0,x+1/2,1/2 [0, $\bar{u}$ ,0]	0, $\bar{x}+1/2, 1/2 [0, u, 0]$
			x+1/2,1/2,0 [ $\bar{u}$ ,0,0]	$\bar{x}+1/2, 1/2, 0 [u, 0, 0]$	1/2,0, $\bar{x}+1/2 [0, 0, u]$	1/2,0,x+1/2 [0,0, $\bar{u}$ ]

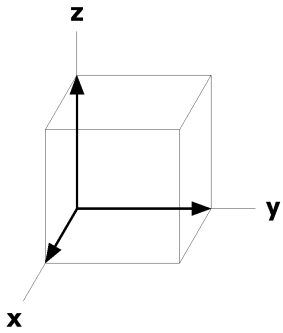
12	g	m'm'2..	x,0,1/2 [u,0,0]	$\bar{x}$ ,0,1/2 [ $\bar{u}$ ,0,0]	1/2,x,0 [0,u,0]	1/2, $\bar{x}$ ,0 [0, $\bar{u}$ ,0]
			0,1/2,x [0,0,u]	0,1/2, $\bar{x}$ [0,0, $\bar{u}$ ]	1/2,x+1/2,0 [0, $\bar{u}$ ,0]	1/2, $\bar{x}$ +1/2,0 [0,u,0]
			x+1/2,0,1/2 [ $\bar{u}$ ,0,0]	$\bar{x}$ +1/2,0,1/2 [u,0,0]	0,1/2, $\bar{x}$ +1/2 [0,0,u]	0,1/2,x+1/2 [0,0, $\bar{u}$ ]
12	f	m'm'2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0]	0,x,0 [0,u,0]	0, $\bar{x}$ ,0 [0, $\bar{u}$ ,0]
			0,0,x [0,0,u]	0,0, $\bar{x}$ [0,0, $\bar{u}$ ]	1/2,x+1/2,1/2 [0, $\bar{u}$ ,0]	1/2, $\bar{x}$ +1/2,1/2 [0,u,0]
			x+1/2,1/2,1/2 [ $\bar{u}$ ,0,0]	$\bar{x}$ +1/2,1/2,1/2 [0,u,0]	1/2,1/2, $\bar{x}$ +1/2 [0,0,u]	1/2,1/2,x+1/2 [0,0, $\bar{u}$ ]
8	e	.32'	1/4,1/4,1/4 [u,u,u]	3/4,3/4,1/4 [ $\bar{u}$ , $\bar{u}$ ,u]	3/4,1/4,3/4 [ $\bar{u}$ ,u, $\bar{u}$ ]	1/4,3/4,3/4 [u, $\bar{u}$ , $\bar{u}$ ]
			3/4,3/4,3/4 [ $\bar{u}$ , $\bar{u}$ , $\bar{u}$ ]	1/4,1/4,3/4 [u,u, $\bar{u}$ ]	1/4,3/4,1/4 [u, $\bar{u}$ ,u]	3/4,1/4,1/4 [ $\bar{u}$ ,u,u]
6	d	$\bar{4}m'.2'$	1/4,1/2,0 [u,0,0]	3/4,1/2,0 [ $\bar{u}$ ,0,0]	0,1/4,1/2 [0,u,0]	
			0,3/4,1/2 [0, $\bar{u}$ ,0]	1/2,0,1/4 [0,0,u]	1/2,0,3/4 [0,0, $\bar{u}$ ]	
6	c	$\bar{4}m'.2'$	1/4,0,1/2 [u,0,0]	3/4,0,1/2 [ $\bar{u}$ ,0,0]	1/2,1/4,0 [0,u,0]	
			1/2,3/4,0 [0, $\bar{u}$ ,0]	0,1/2,1/4 [0,0,u]	0,1/2,3/4 [0,0, $\bar{u}$ ]	
6	b	m'm'm'..	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	
			0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]	0,0,1/2 [0,0,0]	
2	a	m' $\bar{3}$ '.	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p4'm'm  
 $a^* = a$   $b^* = b$   
 Origin at 0,1/2,z

Along [1,1,1] p6mm  
 $a^* = (2a - b - c)/3$   $b^* = (-a + 2b - c)/3$   
 Origin at x,x,x

Along [1,1,0] p2mm1'  
 $a^* = c/2$   $b^* = -(-a + b)/2$   
 Origin at x,x,0



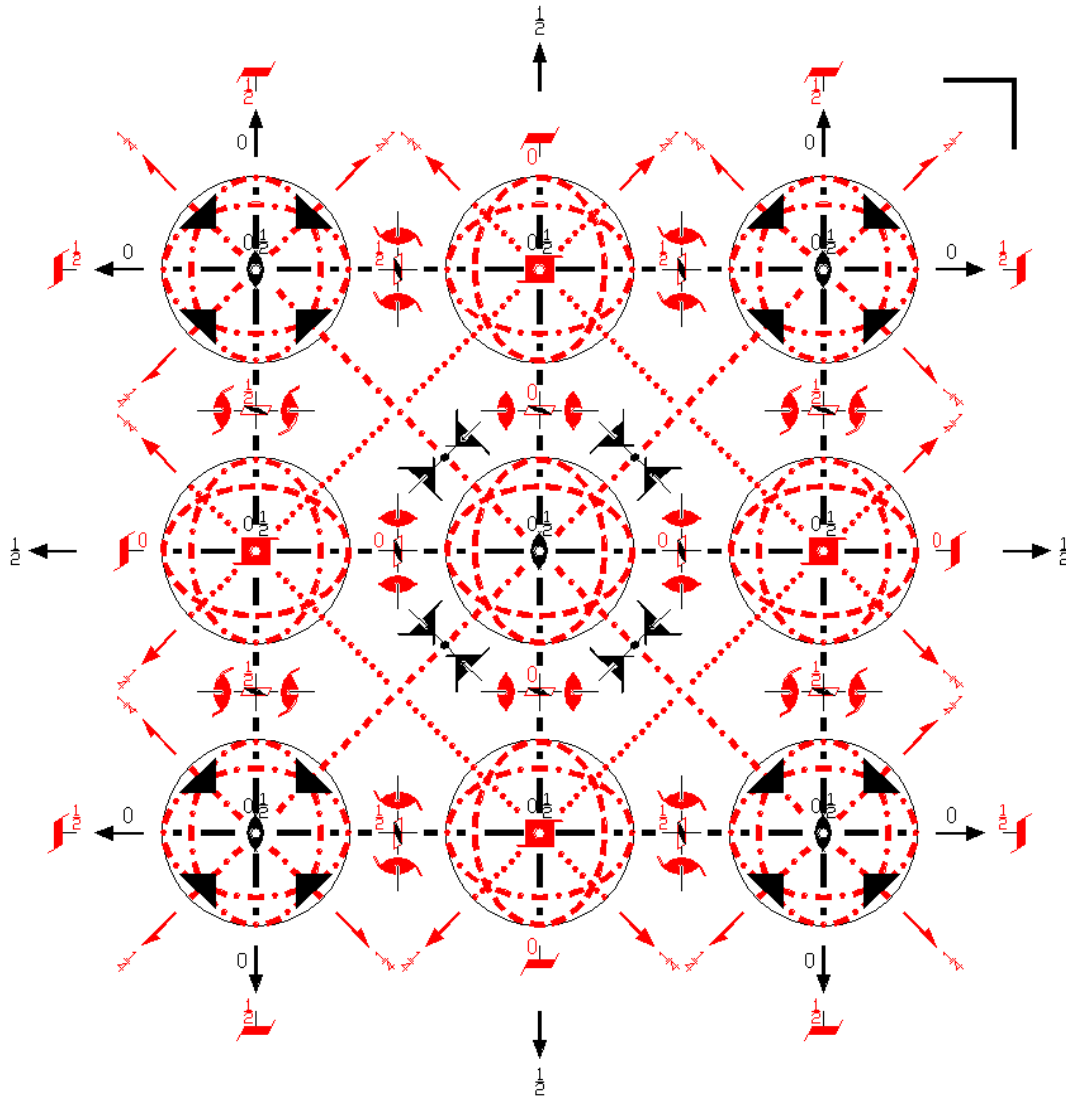
$Pm\bar{3}n'$

223.4.1609

$m\bar{3}n'$

$P4_2'/m\bar{3}2'/n'$

Cubic



**Origin** at center ( $m\bar{3}$ )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/4;$   $z \leq \min(x, 1/2-x, y, 1/2-y)$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $0,1/2,0$   $1/4,1/4,1/4$

**Symmetry Operations**

- (1) 1  
(1|0,0,0)
- (2) 2  $0,0,z$   
( $2_z$ |0,0,0)
- (3) 2  $0,y,0$   
( $2_y$ |0,0,0)
- (4) 2  $x,0,0$   
( $2_x$ |0,0,0)
- (5)  $3^+$   $x,x,x$   
( $3_{xyz}$ |0,0,0)
- (6)  $3^+$   $\bar{x},x,\bar{x}$   
( $3_{x\bar{y}\bar{z}}$ <sup>-1</sup>|0,0,0)
- (7)  $3^+$   $x,\bar{x},\bar{x}$   
( $3_{\bar{x}yz}$ <sup>-1</sup>|0,0,0)
- (8)  $3^+$   $\bar{x},\bar{x},x$   
( $3_{x\bar{y}\bar{z}}$ <sup>-1</sup>|0,0,0)
- (9)  $3^-$   $x,x,x$   
( $3_{xyz}$ <sup>-1</sup>|0,0,0)
- (10)  $3^-$   $x,\bar{x},\bar{x}$   
( $3_{\bar{x}yz}$ |0,0,0)
- (11)  $3^-$   $\bar{x},\bar{x},x$   
( $3_{x\bar{y}\bar{z}}$ |0,0,0)
- (12)  $3^-$   $\bar{x},x,\bar{x}$   
( $3_{x\bar{y}\bar{z}}$ |0,0,0)

(13) $2' (1/2, 1/2, 0) \ x, x, 1/4$ ( $2_{xy}   1/2, 1/2, 1/2$ )'	(14) $2' \ x, \bar{x} + 1/2, 1/4$ ( $2_{\bar{xy}}   1/2, 1/2, 1/2$ )'	(15) $4' \ (0, 0, 1/2) \ 1/2, 0, z$ ( $4_z^{-1}   1/2, 1/2, 1/2$ )'	(16) $4^+ \ (0, 0, 1/2) \ 0, 1/2, z$ ( $4_z   1/2, 1/2, 1/2$ )'
(17) $4' \ (1/2, 0, 0) \ x, 1/2, 0$ ( $4_x^{-1}   1/2, 1/2, 1/2$ )'	(18) $2' \ (0, 1/2, 1/2) \ 1/4, y, y$ ( $2_{yz}   1/2, 1/2, 1/2$ )'	(19) $2' \ 1/4, y + 1/2, \bar{y}$ ( $2_{\bar{yz}}   1/2, 1/2, 1/2$ )'	(20) $4^+ \ (1/2, 0, 0) \ x, 0, 1/2$ ( $4_x   1/2, 1/2, 1/2$ )'
(21) $4^+ \ (0, 1/2, 0) \ 1/2, y, 0$ ( $4_y   1/2, 1/2, 1/2$ )'	(22) $2' \ (1/2, 0, 1/2) \ x, 1/4, x$ ( $2_{xz}   1/2, 1/2, 1/2$ )'	(23) $4' \ (0, 1/2, 0) \ 0, y, 1/2$ ( $4_y^{-1}   1/2, 1/2, 1/2$ )'	(24) $2' \ \bar{x} + 1/2, 1/4, x$ ( $2_{\bar{xz}}   1/2, 1/2, 1/2$ )'
(25) $\bar{1} \ 0, 0, 0$ ( $\bar{1}   0, 0, 0$ )	(26) $m \ x, y, 0$ ( $m_z   0, 0, 0$ )	(27) $m \ x, 0, z$ ( $m_y   0, 0, 0$ )	(28) $m \ 0, y, z$ ( $m_x   0, 0, 0$ )
(29) $\bar{3}^+ \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}   0, 0, 0$ )	(30) $\bar{3}^+ \ \bar{x}, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}^{-1}   0, 0, 0$ )	(31) $\bar{3}^+ \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xy}z}^{-1}   0, 0, 0$ )	(32) $\bar{3}^+ \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{xy\bar{z}}^{-1}   0, 0, 0$ )
(33) $\bar{3}^- \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}^{-1}   0, 0, 0$ )	(34) $\bar{3}^- \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}   0, 0, 0$ )	(35) $\bar{3}^- \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{\bar{xy}z}   0, 0, 0$ )	(36) $\bar{3}^- \ \bar{x}, x, \bar{x}; 0, 0, 0$ ( $\bar{3}_{xy\bar{z}}   0, 0, 0$ )
(37) $c' \ (0, 0, 1/2) \ x + 1/2, \bar{x}, z$ ( $m_{xy}   1/2, 1/2, 12$ )'	(38) $n' \ (1/2, 1/2, 1/2) \ x, x, z$ ( $m_{\bar{xy}}   1/2, 1/2, 12$ )'	(39) $\bar{4}^- \ 0, 1/2, z; 0, 1/2, 1/4$ ( $\bar{4}_z^{-1}   1/2, 1/2, 12$ )'	(40) $\bar{4}^+ \ 1/2, 0, z; 1/2, 0, 1/4$ ( $\bar{4}_z   1/2, 1/2, 12$ )'
(41) $\bar{4}^- \ x, 0, 1/2; 1/4, 0, 1/2$ ( $\bar{4}_x^{-1}   1/2, 1/2, 12$ )'	(42) $a' \ (1/2, 0, 0) \ x, y + 1/2, \bar{y}$ ( $m_{yz}   1/2, 1/2, 12$ )'	(43) $n' \ (1/2, 1/2, 1/2) \ x, y, y$ ( $m_{\bar{yz}}   1/2, 1/2, 12$ )'	(44) $\bar{4}^+ \ x, 1/2, 0; 1/4, 1/2, 0$ ( $\bar{4}_x   1/2, 1/2, 12$ )'
(45) $\bar{4}^+ \ 0, y, 1/2; 0, 1/4, 1/2$ ( $\bar{4}_y   1/2, 1/2, 12$ )'	(46) $b' \ (0, 1/2, 0) \ \bar{x} + 1/2, y, x$ ( $m_{xz}   1/2, 1/2, 12$ )'	(47) $\bar{4}^- \ 1/2, y, 0; 1/2, 1/4, 0$ ( $\bar{4}_y^{-1}   1/2, 1/2, 12$ )'	(48) $n' \ (1/2, 1/2, 1/2) \ x, y, x$ ( $m_{\bar{xz}}   1/2, 1/2, 12$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

### Coordinates

48 | 1

(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$	(3) $\bar{x}, y, \bar{z} [\bar{u}, v, \bar{w}]$	(4) $x, \bar{y}, \bar{z} [u, \bar{v}, \bar{w}]$
(5) $z, x, y [w, u, v]$	(6) $z, \bar{x}, \bar{y} [w, \bar{u}, \bar{v}]$	(7) $\bar{z}, \bar{x}, y [w, \bar{u}, v]$	(8) $\bar{z}, x, \bar{y} [w, u, \bar{v}]$
(9) $y, z, x [v, w, u]$	(10) $\bar{y}, \bar{z}, \bar{x} [\bar{v}, \bar{w}, \bar{u}]$	(11) $y, \bar{z}, \bar{x} [v, \bar{w}, \bar{u}]$	(12) $\bar{y}, \bar{z}, x [\bar{v}, \bar{w}, u]$
(13) $y + 1/2, x + 1/2, \bar{z} + 1/2 [\bar{v}, \bar{u}, w]$	(14) $\bar{y} + 1/2, \bar{x} + 1/2, \bar{z} + 1/2 [v, u, w]$	(15) $y + 1/2, \bar{x} + 1/2, z + 1/2 [\bar{v}, u, \bar{w}]$	(16) $\bar{y} + 1/2, x + 1/2, z + 1/2 [v, \bar{u}, \bar{w}]$
(17) $x + 1/2, z + 1/2, \bar{y} + 1/2 [\bar{u}, \bar{w}, v]$	(18) $\bar{x} + 1/2, z + 1/2, y + 1/2 [u, \bar{w}, \bar{v}]$	(19) $\bar{x} + 1/2, \bar{z} + 1/2, \bar{y} + 1/2 [u, w, v]$	(20) $x + 1/2, \bar{z} + 1/2, y + 1/2 [\bar{u}, w, \bar{v}]$
(21) $z + 1/2, y + 1/2, \bar{x} + 1/2 [\bar{w}, \bar{v}, u]$	(22) $z + 1/2, \bar{y} + 1/2, x + 1/2 [w, \bar{v}, \bar{u}]$	(23) $\bar{z} + 1/2, y + 1/2, x + 1/2 [w, \bar{v}, u]$	(24) $\bar{z} + 1/2, \bar{y} + 1/2, \bar{x} + 1/2 [w, v, u]$
(25) $\bar{x}, \bar{y}, \bar{z} [u, v, w]$	(26) $x, y, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$	(27) $x, \bar{y}, z [u, v, \bar{w}]$	(28) $\bar{x}, y, z [u, \bar{v}, w]$
(29) $\bar{z}, \bar{x}, \bar{y} [w, u, v]$	(30) $\bar{z}, x, y [w, \bar{u}, \bar{v}]$	(31) $z, x, \bar{y} [\bar{w}, \bar{u}, \bar{v}]$	(32) $z, \bar{x}, y [w, u, \bar{v}]$
(33) $\bar{y}, \bar{z}, \bar{x} [v, w, u]$	(34) $y, \bar{z}, x [\bar{v}, \bar{w}, \bar{u}]$	(35) $\bar{y}, z, x [v, \bar{w}, u]$	(36) $y, z, \bar{x} [v, w, \bar{u}]$

(37)  $\bar{y}+1/2, \bar{x}+1/2, z+1/2 [\bar{v}, \bar{u}, w]$  (38)  $y+1/2, x+1/2, z+1/2 [v, u, w]$  (39)  $\bar{y}+1/2, x+1/2, \bar{z}+1/2 [\bar{v}, u, \bar{w}]$  (40)  $y+1/2, \bar{x}+1/2, \bar{z}+1/2 [v, \bar{u}, \bar{w}]$   
 (41)  $\bar{x}+1/2, \bar{z}+1/2, y+1/2 [\bar{u}, \bar{w}, v]$  (42)  $x+1/2, \bar{z}+1/2, \bar{y}+1/2 [u, \bar{w}, \bar{v}]$  (43)  $x+1/2, z+1/2, y+1/2 [u, w, v]$  (44)  $\bar{x}+1/2, z+1/2, \bar{y}+1/2 [\bar{u}, w, \bar{v}]$   
 (45)  $\bar{z}+1/2, \bar{y}+1/2, x+1/2 [\bar{w}, \bar{v}, u]$  (46)  $\bar{z}+1/2, y+1/2, \bar{x}+1/2 [\bar{w}, v, \bar{u}]$  (47)  $z+1/2, \bar{y}+1/2, \bar{x}+1/2 [w, \bar{v}, \bar{u}]$  (48)  $z+1/2, y+1/2, x+1/2 [w, v, u]$

24	k	m..	0,y,z [u,0,0]	0, $\bar{y}$ ,z [ $\bar{u}$ ,0,0]	0,y, $\bar{z}$ [ $\bar{u}$ ,0,0]	0, $\bar{y}$ , $\bar{z}$ [u,0,0]
			z,0,y [0,u,0]	z,0, $\bar{y}$ [0, $\bar{u}$ ,0]	$\bar{z}$ ,0,y [0, $\bar{u}$ ,0]	$\bar{z}$ ,0, $\bar{y}$ [0,u,0]
			y,z,0 [0,0,u]	$\bar{y}$ ,z,0 [0,0, $\bar{u}$ ]	y, $\bar{z}$ ,0 [0,0, $\bar{u}$ ]	$\bar{y}$ , $\bar{z}$ ,0 [0,0,u]
			$y+1/2, 1/2, \bar{z}+1/2 [0, \bar{u}, 0]$	$\bar{y}+1/2, 1/2, \bar{z}+1/2 [0, u, 0]$	$y+1/2, 1/2, z+1/2 [0, u, 0]$	$\bar{y}+1/2, 1/2, z+1/2 [0, \bar{u}, 0]$
			$1/2, z+1/2, \bar{y}+1/2 [\bar{u}, 0, 0]$	$1/2, z+1/2, y+1/2 [u, 0, 0]$	$1/2, \bar{z}+1/2, \bar{y}+1/2 [u, 0, 0]$	$1/2, \bar{z}+1/2, y+1/2 [\bar{u}, 0, 0]$
			$z+1/2, y+1/2, 1/2 [0, 0, u]$	$1/2+1/2, \bar{y}+1/2, 0 [0, 0, \bar{u}]$	$\bar{z}+1/2, y+1/2, 1/2 [0, 0, \bar{u}]$	$\bar{z}+1/2, \bar{y}+1/2, 1/2 [0, 0, u]$

24 j ..2'

1/4,y,y+1/2 [u,v, $\bar{v}$ ]	3/4, $\bar{y}$ ,y+1/2 [ $\bar{u}$ , $\bar{v}$ , $\bar{v}$ ]	3/4,y, $\bar{y}+1/2 [\bar{u}, v, v]$	1/4, $\bar{y}$ , $\bar{y}+1/2 [u, \bar{v}, v]$
y+1/2, 1/4,y [ $\bar{v}$ ,u,v]	y+1/2, 3/4, $\bar{y}$ [ $\bar{v}$ , $\bar{u}$ , $\bar{v}$ ]	$\bar{y}+1/2, 3/4,y [v, \bar{u}, v]$	$\bar{y}+1/2, 1/4, \bar{y} [v, u, \bar{v}]$
y,y+1/2, 1/4 [v, $\bar{v}$ ,u]	$\bar{y}$ ,y+1/2, 3/4 [ $\bar{v}$ , $\bar{v}$ , $\bar{u}$ ]	y, $\bar{y}+1/2, 3/4 [v, v, \bar{u}]$	$\bar{y}$ , $\bar{y}+1/2, 1/4 [\bar{v}, v, u]$
3/4, $\bar{y}$ , $\bar{y}+1/2 [u, v, \bar{v}]$	1/4,y, $\bar{y}+1/2 [\bar{u}, \bar{v}, \bar{v}]$	1/4, $\bar{y}$ ,y+1/2 [ $\bar{u}, v, v]$	3/4,y,y+1/2 [u, $\bar{v}$ ,v]
$\bar{y}+1/2, 3/4, \bar{y} [\bar{v}, u, v]$	$\bar{y}+1/2, 1/4, y [\bar{v}, \bar{u}, \bar{v}]$	y+1/2, 1/4, $\bar{y} [v, \bar{u}, v]$	y+1/2, 3/4, y [v, u, $\bar{v}$ ]
$\bar{y}$ , $\bar{y}+1/2, 3/4 [v, \bar{v}, u]$	y, $\bar{y}+1/2, 1/4 [\bar{v}, \bar{v}, \bar{u}]$	$\bar{y}$ ,y+1/2, 1/4 [v, v, $\bar{u}$ ]	y,y+1/2, 3/4 [ $\bar{v}$ , v, u]

16	i	.3.	x,x,x [u,u,u]	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$
			$\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
			$x+1/2, x+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, u]$	$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [u, u, u]$
			$x+1/2, \bar{x}+1/2, x+1/2 [\bar{u}, u, \bar{u}]$	$\bar{x}+1/2, x+1/2, x+1/2 [u, \bar{u}, \bar{u}]$
			$\bar{x}, \bar{x}, \bar{x} [u, u, u]$	$x, x, \bar{x} [\bar{u}, \bar{u}, u]$
			$x, \bar{x}, x [\bar{u}, u, \bar{u}]$	$\bar{x}, x, x [u, \bar{u}, \bar{u}]$
			$\bar{x}+1/2, \bar{x}+1/2, x+1/2 [\bar{u}, \bar{u}, u]$	$x+1/2, x+1/2, x+1/2 [u, u, u]$
			$\bar{x}+1/2, x+1/2, \bar{x}+1/2 [\bar{u}, u, \bar{u}]$	$x+1/2, \bar{x}+1/2, \bar{x}+1/2 [u, \bar{u}, \bar{u}]$

12	h	mm2..	x, 1/2, 0 [0,0,0]	$\bar{x}$ , 1/2, 0 [0,0,0]	0, x, 1/2 [0,0,0]	0, $\bar{x}$ , 1/2 [0,0,0]
			1/2, 0, x [0,0,0]	1/2, 0, $\bar{x}$ [0,0,0]	0, x+1/2, 1/2 [0,0,0]	0, $\bar{x}+1/2, 1/2 [0,0,0]$
			x+1/2, 1/2, 0 [0,0,0]	$\bar{x}+1/2, 1/2, 0 [0,0,0]$	1/2, 0, $\bar{x}+1/2 [0,0,0]$	1/2, 0, x+1/2 [0,0,0]

Continued

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Pm' $\bar{3}$ 'n

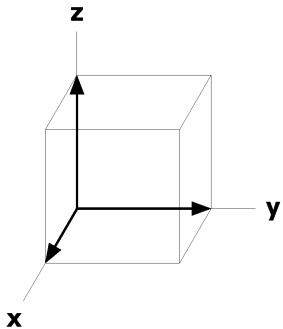
12	g	mm2..	x,0,1/2 [0,0,0]	$\bar{x}$ ,0,1/2 [0,0,0]	1/2,x,0 [0,0,0]	1/2, $\bar{x}$ ,0 [0,0,0]
			0,1/2,x [0,0,0]	0,1/2, $\bar{x}$ [0,0,0]	1/2,x+1/2,0 [0,0,0]	1/2, $\bar{x}$ +1/2,0 [0,0,0]
			x+1/2,0,1/2 [0,0,0]	$\bar{x}$ +1/2,0,1/2 [0,0,0]	0,1/2, $\bar{x}$ +1/2 [0,0,0]	0,1/2,x+1/2 [0,0,0]
12	f	mm2..	x,0,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x}$ ,0 [0,0,0]
			0,0,x [0,0,0]	0,0, $\bar{x}$ [0,0,0]	1/2,x+1/2,1/2 [0,0,0]	1/2, $\bar{x}$ +1/2,1/2 [0,0,0]
			x+1/2,1/2,1/2 [0,0,0]	$\bar{x}$ +1/2,1/2,1/2 [0,0,0]	1/2,1/2, $\bar{x}$ +1/2 [0,0,0]	1/2,1/2,x+1/2 [0,0,0]
8	e	.32'	1/4,1/4,1/4 [u,u,u]	3/4,3/4,1/4 [ $\bar{u}$ , $\bar{u}$ ,u]	3/4,1/4,3/4 [ $\bar{u}$ ,u, $\bar{u}$ ]	1/4,3/4,3/4 [u, $\bar{u}$ , $\bar{u}$ ]
			3/4,3/4,3/4 [u,u,u]	1/4,1/4,3/4 [ $\bar{u}$ , $\bar{u}$ ,u]	1/4,3/4,1/4 [ $\bar{u}$ ,u, $\bar{u}$ ]	3/4,1/4,1/4 [u, $\bar{u}$ , $\bar{u}$ ]
6	d	$\bar{4}$ 'm.2'	1/4,1/2,0 [0,0,0]	3/4,1/2,0 [0,0,0]	0,1/4,1/2 [0,0,0]	
			0,3/4,1/2 [0,0,0]	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]	
6	c	$\bar{4}$ 'm.2'	1/4,0,1/2 [0,0,0]	3/4,0,1/2 [0,0,0]	1/2,1/4,0 [0,0,0]	
			1/2,3/4,0 [0,0,0]	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	
6	b	mmm..	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	
			0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]	0,0,1/2 [0,0,0]	
2	a	m $\bar{3}$ .	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,1,1] p6'mm'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

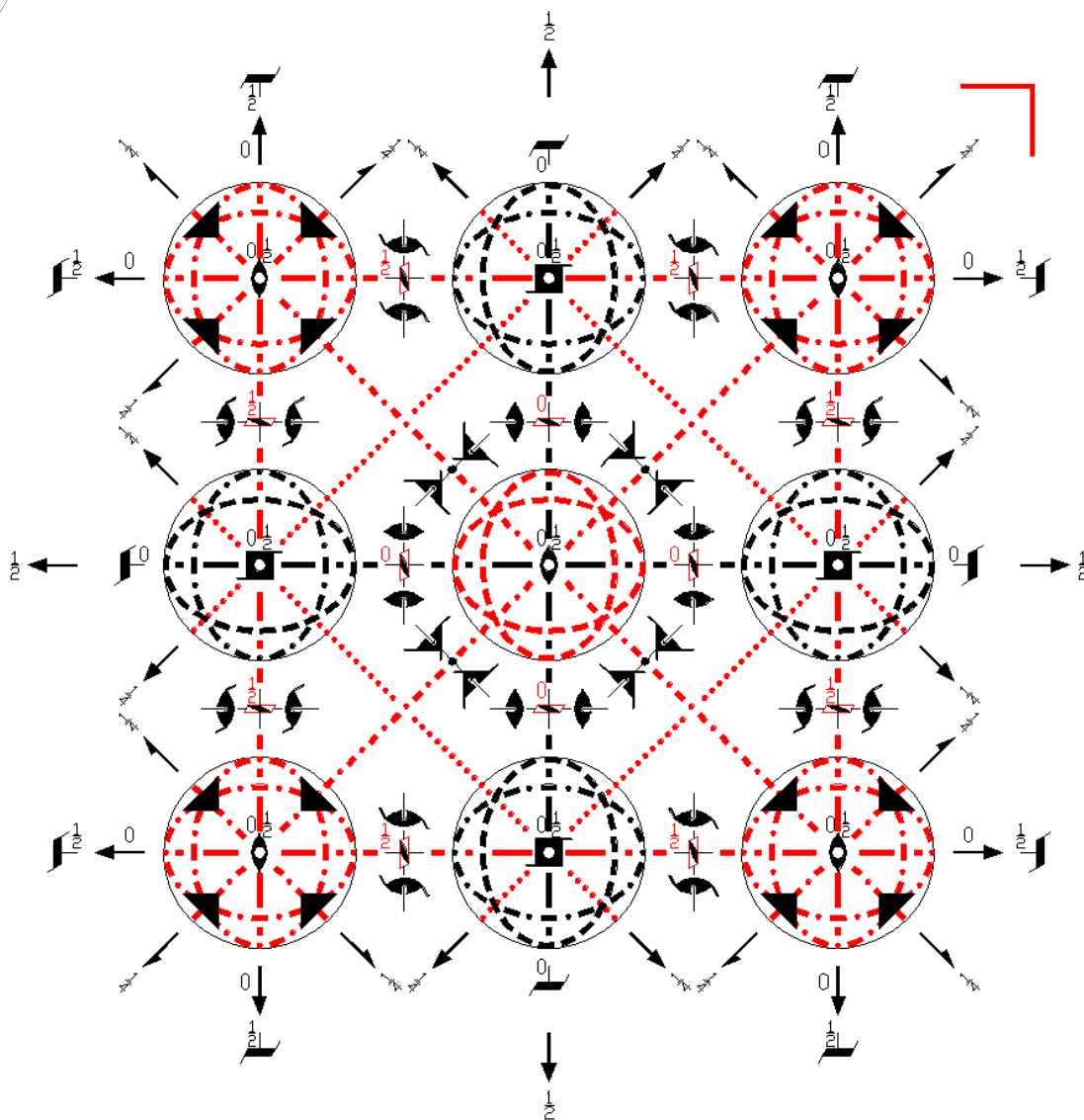
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



Pm $\bar{3}$ 'n'  
223.5.1610

m $\bar{3}$ 'n'  
P4<sub>2</sub>/m $\bar{3}$ '2/n'

Cubic



**Origin** at center (m $\bar{3}$ 'n')

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $z \leq \min(x, 1/2-x, y, 1/2-y)$

**Vertices** 0,0,0    1/2,0,0    1/2,1/2,0    0,1/2,0    1/4,1/4,1/4

**Symmetry Operations**

- |   |  |   |   |
|---|--|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)              | (12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)               |



(13) $2 (1/2, 1/2, 0) \ x, x, 1/4$ ( $2_{xy}   1/2, 1/2, 1/2$ )	(14) $2 \ x, \bar{x} + 1/2, 1/4$ ( $2_{\bar{xy}}   1/2, 1/2, 1/2$ )	(15) $4^- (0, 0, 1/2) \ 1/2, 0, z$ ( $4_z^{-1}   1/2, 1/2, 1/2$ )	(16) $4^+ (0, 0, 1/2) \ 0, 1/2, z$ ( $4_z   1/2, 1/2, 1/2$ )
(17) $4^- (1/2, 0, 0) \ x, 1/2, 0$ ( $4_x^{-1}   1/2, 1/2, 1/2$ )	(18) $2 (0, 1/2, 1/2) \ 1/4, y, y$ ( $2_{yz}   1/2, 1/2, 1/2$ )	(19) $2 \ 1/4, y + 1/2, \bar{y}$ ( $2_{\bar{yz}}   1/2, 1/2, 1/2$ )	(20) $4^+ (1/2, 0, 0) \ x, 0, 1/2$ ( $4_x   1/2, 1/2, 1/2$ )
(21) $4^+ (0, 1/2, 0) \ 1/2, y, 0$ ( $4_y   1/2, 1/2, 1/2$ )	(22) $2 (1/2, 0, 1/2) \ x, 1/4, x$ ( $2_{xz}   1/2, 1/2, 1/2$ )	(23) $4^- (0, 1/2, 0) \ 0, y, 1/2$ ( $4_y^{-1}   1/2, 1/2, 1/2$ )	(24) $2 \ \bar{x} + 1/2, 1/4, x$ ( $2_{\bar{xz}}   1/2, 1/2, 1/2$ )
(25) $\bar{1}^- \ 0, 0, 0$ ( $\bar{1}   0, 0, 0$ )'	(26) $m' \ x, y, 0$ ( $m_z   0, 0, 0$ )'	(27) $m' \ x, 0, z$ ( $m_y   0, 0, 0$ )'	(28) $m' \ 0, y, z$ ( $m_x   0, 0, 0$ )'
(29) $\bar{3}^+ \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}   0, 0, 0$ )'	(30) $\bar{3}^+ \ \bar{x}, x, \bar{x}; 0, 0, 0$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1}   0, 0, 0$ )'	(31) $\bar{3}^+ \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xy}\bar{z}}^{-1}   0, 0, 0$ )'	(32) $\bar{3}^+ \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{xy\bar{z}}^{-1}   0, 0, 0$ )'
(33) $\bar{3}^- \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}^{-1}   0, 0, 0$ )'	(34) $\bar{3}^- \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xy}\bar{z}}   0, 0, 0$ )'	(35) $\bar{3}^- \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{xy\bar{z}}   0, 0, 0$ )'	(36) $\bar{3}^- \ \bar{x}, x, \bar{x}; 0, 0, 0$ ( $\bar{3}_{x\bar{y}\bar{z}}   0, 0, 0$ )'
(37) $c' (0, 0, 1/2) \ x + 1/2, \bar{x}, z$ ( $m_{xy}   1/2, 1/2, 12$ )'	(38) $n' (1/2, 1/2, 1/2) \ x, x, z$ ( $m_{\bar{xy}}   1/2, 1/2, 12$ )'	(39) $\bar{4}^- \ 0, 1/2, z; 0, 1/2, 1/4$ ( $\bar{4}_z^{-1}   1/2, 1/2, 12$ )'	(40) $\bar{4}^+ \ 1/2, 0, z; 1/2, 0, 1/4$ ( $\bar{4}_z   1/2, 1/2, 12$ )'
(41) $\bar{4}^- \ x, 0, 1/2; 1/4, 0, 1/2$ ( $\bar{4}_x^{-1}   1/2, 1/2, 12$ )'	(42) $a' (1/2, 0, 0) \ x, y + 1/2, \bar{y}$ ( $m_{yz}   1/2, 1/2, 12$ )'	(43) $n' (1/2, 1/2, 1/2) \ x, y, y$ ( $m_{\bar{yz}}   1/2, 1/2, 12$ )'	(44) $\bar{4}^+ \ x, 1/2, 0; 1/4, 1/2, 0$ ( $\bar{4}_x   1/2, 1/2, 12$ )'
(45) $\bar{4}^+ \ 0, y, 1/2; 0, 1/4, 1/2$ ( $\bar{4}_y   1/2, 1/2, 12$ )'	(46) $b' (0, 1/2, 0) \ \bar{x} + 1/2, y, x$ ( $m_{xz}   1/2, 1/2, 12$ )'	(47) $\bar{4}^- \ 1/2, y, 0; 1/2, 1/4, 0$ ( $\bar{4}_y^{-1}   1/2, 1/2, 12$ )'	(48) $n' (1/2, 1/2, 1/2) \ x, y, x$ ( $m_{\bar{xz}}   1/2, 1/2, 12$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

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(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$	(3) $\bar{x}, y, \bar{z} [\bar{u}, v, \bar{w}]$	(4) $x, \bar{y}, \bar{z} [u, \bar{v}, \bar{w}]$
(5) $z, x, y [w, u, v]$	(6) $z, \bar{x}, \bar{y} [w, \bar{u}, \bar{v}]$	(7) $\bar{z}, \bar{x}, y [w, \bar{u}, v]$	(8) $\bar{z}, x, \bar{y} [w, u, \bar{v}]$
(9) $y, z, x [v, w, u]$	(10) $\bar{y}, \bar{z}, \bar{x} [\bar{v}, \bar{w}, \bar{u}]$	(11) $y, \bar{z}, \bar{x} [v, \bar{w}, \bar{u}]$	(12) $\bar{y}, \bar{z}, x [\bar{v}, \bar{w}, u]$
(13) $y + 1/2, x + 1/2, \bar{z} + 1/2 [v, u, \bar{w}]$	(14) $\bar{y} + 1/2, \bar{x} + 1/2, \bar{z} + 1/2 [\bar{v}, \bar{u}, \bar{w}]$	(15) $y + 1/2, \bar{x} + 1/2, z + 1/2 [v, \bar{u}, w]$	(16) $\bar{y} + 1/2, x + 1/2, z + 1/2 [\bar{v}, u, w]$
(17) $x + 1/2, z + 1/2, \bar{y} + 1/2 [u, w, \bar{v}]$	(18) $\bar{x} + 1/2, \bar{z} + 1/2, y + 1/2 [\bar{u}, w, v]$	(19) $\bar{x} + 1/2, \bar{z} + 1/2, \bar{y} + 1/2 [\bar{u}, \bar{w}, \bar{v}]$	(20) $x + 1/2, \bar{z} + 1/2, y + 1/2 [u, \bar{w}, v]$
(21) $z + 1/2, y + 1/2, \bar{x} + 1/2 [w, v, \bar{u}]$	(22) $z + 1/2, \bar{y} + 1/2, x + 1/2 [w, \bar{v}, u]$	(23) $\bar{z} + 1/2, y + 1/2, x + 1/2 [\bar{w}, v, u]$	(24) $\bar{z} + 1/2, \bar{y} + 1/2, \bar{x} + 1/2 [\bar{w}, \bar{v}, \bar{u}]$
(25) $\bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$	(26) $x, y, \bar{z} [u, v, \bar{w}]$	(27) $x, \bar{y}, z [u, \bar{v}, w]$	(28) $\bar{x}, y, z [\bar{u}, v, w]$
(29) $\bar{z}, \bar{x}, \bar{y} [\bar{w}, \bar{u}, \bar{v}]$	(30) $\bar{z}, x, y [\bar{w}, u, v]$	(31) $z, x, \bar{y} [w, u, \bar{v}]$	(32) $z, \bar{x}, y [w, \bar{u}, v]$
(33) $\bar{y}, \bar{z}, \bar{x} [\bar{v}, \bar{w}, \bar{u}]$	(34) $y, \bar{z}, x [v, \bar{w}, u]$	(35) $\bar{y}, z, x [\bar{v}, w, u]$	(36) $y, z, \bar{x} [v, w, \bar{u}]$

(37)  $\bar{y}+1/2, \bar{x}+1/2, z+1/2 [\bar{v}, \bar{u}, w]$  (38)  $y+1/2, x+1/2, z+1/2 [v, u, w]$  (39)  $\bar{y}+1/2, x+1/2, \bar{z}+1/2 [\bar{v}, u, \bar{w}]$  (40)  $y+1/2, \bar{x}+1/2, \bar{z}+1/2 [v, \bar{u}, \bar{w}]$   
 (41)  $\bar{x}+1/2, \bar{z}+1/2, y+1/2 [\bar{u}, \bar{w}, v]$  (42)  $x+1/2, \bar{z}+1/2, \bar{y}+1/2 [u, \bar{w}, \bar{v}]$  (43)  $x+1/2, z+1/2, y+1/2 [u, w, v]$  (44)  $\bar{x}+1/2, z+1/2, \bar{y}+1/2 [\bar{u}, w, \bar{v}]$   
 (45)  $\bar{z}+1/2, \bar{y}+1/2, x+1/2 [\bar{w}, \bar{v}, u]$  (46)  $\bar{z}+1/2, y+1/2, \bar{x}+1/2 [\bar{w}, v, \bar{u}]$  (47)  $z+1/2, \bar{y}+1/2, \bar{x}+1/2 [w, \bar{v}, \bar{u}]$  (48)  $z+1/2, y+1/2, x+1/2 [w, v, u]$

24	k	m'..	0,y,z [0,v,w]	0, $\bar{y}$ ,z [0, $\bar{v}$ ,w]	0,y, $\bar{z}$ [0,v, $\bar{w}$ ]	0, $\bar{y}$ , $\bar{z}$ [0, $\bar{v}$ , $\bar{w}$ ]
			z,0,y [w,0,v]	z,0, $\bar{y}$ [w,0, $\bar{v}$ ]	$\bar{z}$ ,0,y [w,0,v]	$\bar{z}$ ,0, $\bar{y}$ [w,0, $\bar{v}$ ]
			y,z,0 [v,w,0]	$\bar{y}$ ,z,0 [v,w,0]	y, $\bar{z}$ ,0 [v,w,0]	$\bar{y}$ , $\bar{z}$ ,0 [v,w,0]
			$y+1/2, 1/2, \bar{z}+1/2 [v, 0, \bar{w}]$	$\bar{y}+1/2, 1/2, \bar{z}+1/2 [\bar{v}, 0, \bar{w}]$	$y+1/2, 1/2, z+1/2 [v, 0, w]$	$\bar{y}+1/2, 1/2, z+1/2 [\bar{v}, 0, w]$
			$1/2, z+1/2, \bar{y}+1/2 [0, w, \bar{v}]$	$1/2, z+1/2, y+1/2 [0, w, v]$	$1/2, \bar{z}+1/2, \bar{y}+1/2 [0, \bar{w}, \bar{v}]$	$1/2, \bar{z}+1/2, y+1/2 [0, \bar{w}, v]$
			$z+1/2, y+1/2, 1/2 [w, v, 0]$	$1/2+1/2, \bar{y}+1/2, 0 [w, \bar{v}, 0]$	$\bar{z}+1/2, y+1/2, 1/2 [\bar{w}, v, 0]$	$\bar{z}+1/2, \bar{y}+1/2, 1/2 [\bar{w}, \bar{v}, 0]$

24 j ..2

1/4,y,y+1/2 [0,v,v]	3/4, $\bar{y}$ ,y+1/2 [0, $\bar{v}$ ,v]	3/4,y, $\bar{y}+1/2 [0,v,\bar{v}]$	1/4, $\bar{y}$ , $\bar{y}+1/2 [0,\bar{v},\bar{v}]$
y+1/2,1/4,y [v,0,v]	y+1/2,3/4, $\bar{y}$ [v,0, $\bar{v}$ ]	$\bar{y}+1/2, 3/4, y [\bar{v}, 0, v]$	$\bar{y}+1/2, 1/4, \bar{y} [\bar{v}, 0, \bar{v}]$
y,y+1/2,1/4 [v,v,0]	$\bar{y}$ ,y+1/2,3/4 [v,v,0]	y, $\bar{y}+1/2, 3/4 [v, \bar{v}, 0]$	$\bar{y}$ , $\bar{y}+1/2, 1/4 [v, \bar{v}, 0]$
3/4, $\bar{y}$ , $\bar{y}+1/2 [0,\bar{v},\bar{v}]$	1/4,y, $\bar{y}+1/2 [0,v,\bar{v}]$	1/4, $\bar{y}$ ,y+1/2 [0, $\bar{v}$ ,v]	3/4,y,y+1/2 [0,v,v]
$\bar{y}+1/2, 3/4, \bar{y} [\bar{v}, 0, \bar{v}]$	$\bar{y}+1/2, 1/4, y [\bar{v}, 0, v]$	y+1/2, 1/4, $\bar{y} [v, 0, \bar{v}]$	y+1/2, 3/4, y [v, 0, v]
$\bar{y}$ , $\bar{y}+1/2, 3/4 [v, \bar{v}, 0]$	y, $\bar{y}+1/2, 1/4 [v, \bar{v}, 0]$	$\bar{y}$ ,y+1/2, 1/4 [v,v,0]	y,y+1/2, 3/4 [v,v,0]

16	i	.3.	x,x,x [u,u,u]	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$
			$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
			$x+1/2, x+1/2, \bar{x}+1/2 [u, u, \bar{u}]$	$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, \bar{u}]$
			$x+1/2, \bar{x}+1/2, x+1/2 [u, \bar{u}, u]$	$\bar{x}+1/2, x+1/2, x+1/2 [\bar{u}, u, u]$
			$\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$	$x, x, \bar{x} [u, u, \bar{u}]$
			$x, \bar{x}, x [u, \bar{u}, u]$	$\bar{x}, x, x [\bar{u}, u, u]$
			$\bar{x}+1/2, \bar{x}+1/2, x+1/2 [\bar{u}, \bar{u}, u]$	$x+1/2, x+1/2, x+1/2 [u, u, u]$
			$\bar{x}+1/2, x+1/2, \bar{x}+1/2 [\bar{u}, u, \bar{u}]$	$x+1/2, \bar{x}+1/2, \bar{x}+1/2 [u, \bar{u}, \bar{u}]$

12	h	m'm'2..	x,1/2,0 [u,0,0]	$\bar{x}$ ,1/2,0 [ $\bar{u}$ ,0,0]	0,x,1/2 [0,u,0]	0, $\bar{x}$ ,1/2 [0, $\bar{u}$ ,0]
			1/2,0,x [0,0,u]	1/2,0, $\bar{x}$ [0,0, $\bar{u}$ ]	0,x+1/2,1/2 [0,u,0]	0, $\bar{x}+1/2, 1/2 [0,\bar{u},0]$
			x+1/2,1/2,0 [u,0,0]	$\bar{x}+1/2, 1/2, 0 [\bar{u}, 0, 0]$	1/2,0, $\bar{x}+1/2 [0,0,\bar{u}]$	1/2,0,x+1/2 [0,0,u]

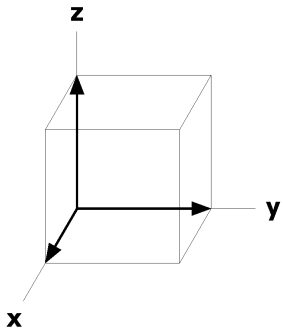
12	g	m'm'2..	x,0,1/2 [u,0,0]	$\bar{x}$ ,0,1/2 [ $\bar{u}$ ,0,0]	1/2,x,0 [0,u,0]	1/2, $\bar{x}$ ,0 [0, $\bar{u}$ ,0]
			0,1/2,x [0,0,u]	0,1/2, $\bar{x}$ [0,0, $\bar{u}$ ]	1/2,x+1/2,0 [0,u,0]	1/2, $\bar{x}$ +1/2,0 [0, $\bar{u}$ ,0]
			x+1/2,0,1/2 [u,0,0]	$\bar{x}$ +1/2,0,1/2 [ $\bar{u}$ ,0,0]	0,1/2, $\bar{x}$ +1/2 [0,0, $\bar{u}$ ]	0,1/2,x+1/2 [0,0,u]
12	f	m'm'2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0]	0,x,0 [0,u,0]	0, $\bar{x}$ ,0 [0, $\bar{u}$ ,0]
			0,0,x [0,0,u]	0,0, $\bar{x}$ [0,0, $\bar{u}$ ]	1/2,x+1/2,1/2 [0,u,0]	1/2, $\bar{x}$ +1/2,1/2 [0, $\bar{u}$ ,0]
			x+1/2,1/2,1/2 [u,0,0]	$\bar{x}$ +1/2,1/2,1/2 [ $\bar{u}$ ,0,0]	1/2,1/2, $\bar{x}$ +1/2 [0,0, $\bar{u}$ ]	1/2,1/2,x+1/2 [0,0,u]
8	e	.32	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]
			3/4,3/4,3/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
6	d	$\bar{4}$ 'm'.2	1/4,1/2,0 [0,0,0]	3/4,1/2,0 [0,0,0]		0,1/4,1/2 [0,0,0]
			0,3/4,1/2 [0,0,0]	1/2,0,1/4 [0,0,0]		1/2,0,3/4 [0,0,0]
6	c	$\bar{4}$ 'm'.2	1/4,0,1/2 [0,0,0]	3/4,0,1/2 [0,0,0]		1/2,1/4,0 [0,0,0]
			1/2,3/4,0 [0,0,0]	0,1/2,1/4 [0,0,0]		0,1/2,3/4 [0,0,0]
6	b	m'm'm'..	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]		1/2,1/2,0 [0,0,0]
			0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]		0,0,1/2 [0,0,0]
2	a	m' $\bar{3}$ '.	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = \mathbf{a}$   $\mathbf{b}^* = \mathbf{b}$   
 Origin at 0,1/2,z

Along [1,1,1] p6m'm'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

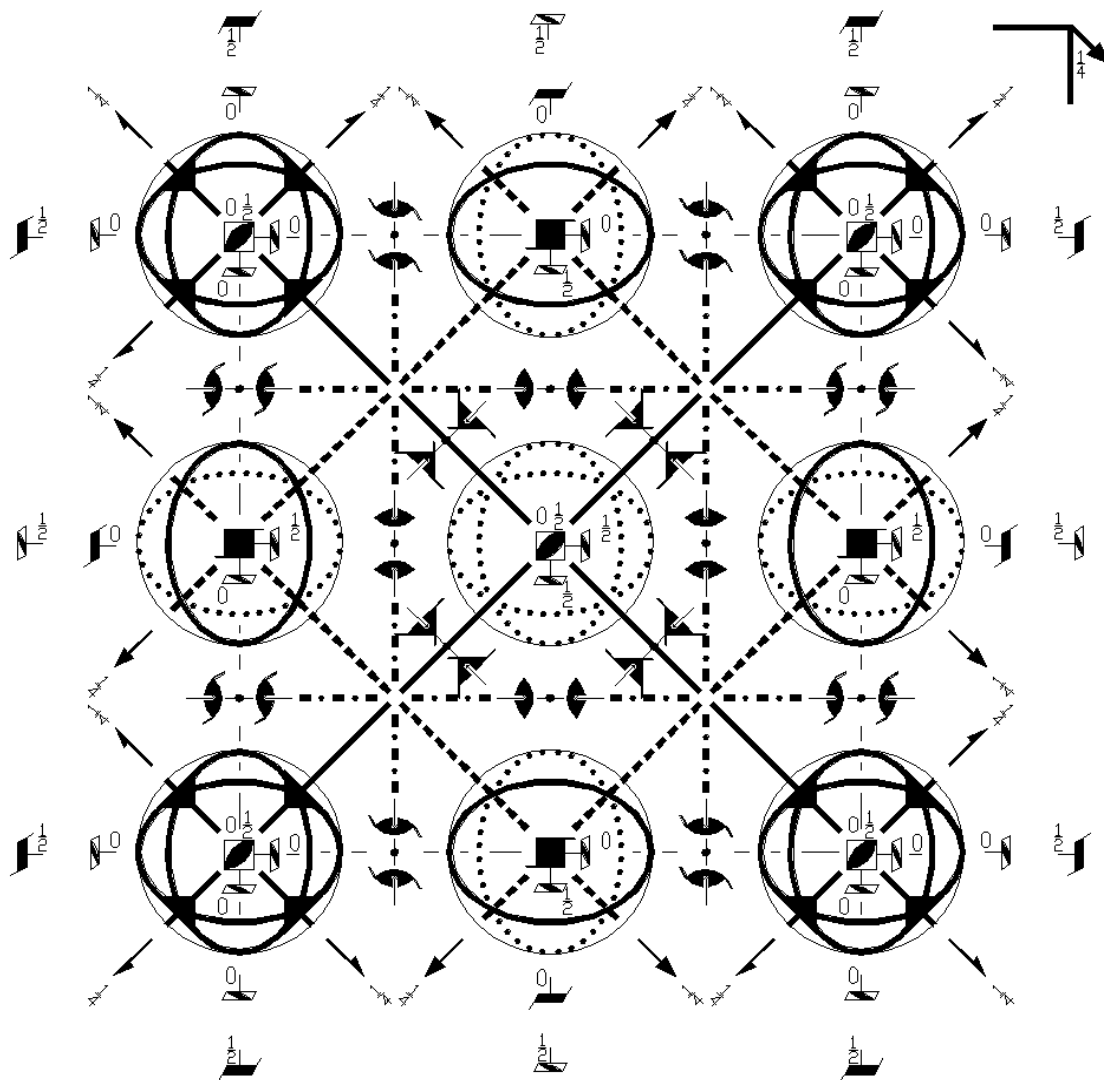
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$Pn\bar{3}m$   
224.1.1611

$m\bar{3}m$   
 $P4_2/n\bar{3}2/m$

Cubic



**Origin** at  $\bar{4}3m$ , at  $-1/4, -1/4, -1/4$  from center  $\bar{3}m$

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $-1/4 \leq z \leq 1/4$ ;  $y \leq x$ ;  $\max(x-1/2, -y) \leq z \leq \min(1/2-x, y)$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/4,1/4,1/4$   $1/4,1/4,-1/4$

### Symmetry Operations

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                  | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)        |

(13) $2 (1/2, 1/2, 0) \ x, x, 1/4$ ( $2_{xy}   1/2, 1/2, 1/2$ )	(14) $2 \ x, \bar{x}+1/2, 1/4$ ( $2_{\bar{xy}}   1/2, 1/2, 1/2$ )	(15) $4^- (0, 0, 1/2) \ 1/2, 0, z$ ( $4_z^{-1}   1/2, 1/2, 1/2$ )	(16) $4^+ (0, 0, 1/2) \ 0, 1/2, z$ ( $4_z   1/2, 1/2, 1/2$ )
(17) $4^- (1/2, 0, 0) \ x, 1/2, 0$ ( $4_x^{-1}   1/2, 1/2, 1/2$ )	(18) $2 (0, 1/2, 1/2) \ 1/4, y, y$ ( $2_{yz}   1/2, 1/2, 1/2$ )	(19) $2 \ 1/4, y+1/2, \bar{y}$ ( $2_{\bar{yz}}   1/2, 1/2, 1/2$ )	(20) $4^+ (1/2, 0, 0) \ x, 0, 1/2$ ( $4_x   1/2, 1/2, 1/2$ )
(21) $4^+ (0, 1/2, 0) \ 1/2, y, 0$ ( $4_y   1/2, 1/2, 1/2$ )	(22) $2 (1/2, 0, 1/2) \ x, 1/4, x$ ( $2_{xz}   1/2, 1/2, 1/2$ )	(23) $4^- (0, 1/2, 0) \ 0, y, 1/2$ ( $4_y^{-1}   1/2, 1/2, 1/2$ )	(24) $2 \ \bar{x}+1/2, 1/4, x$ ( $2_{\bar{xz}}   1/2, 1/2, 1/2$ )
(25) $\bar{1} \ 1/4, 1/4, 1/4$ ( $\bar{1}   1/2, 1/2, 1/2$ )	(26) $n (1/2, 1/2, 0) \ x, y, 1/4$ ( $m_z   1/2, 1/2, 1/2$ )	(27) $n (1/2, 0, 1/2) \ x, 1/4, z$ ( $m_y   1/2, 1/2, 1/2$ )	(28) $n (0, 1/2, 1/2) \ 1/4, y, z$ ( $m_x   1/2, 1/2, 1/2$ )
(29) $\bar{3}^+ \ x, x, x; 1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 1/2, 1/2$ )	(30) $\bar{3}^+ \ \bar{x}-1, x+1, \bar{x}; -1/4, 1/4, 3/4$ ( $\bar{3}_{x\bar{y}\bar{z}^{-1}}   1/2, 1/2, 1/2$ )	(31) $\bar{3}^+ \ x, \bar{x}+1, \bar{x}; 1/4, 3/4, -1/4$ ( $\bar{3}_{\bar{y}\bar{z}^{-1}}   1/2, 1/2, 1/2$ )	(32) $\bar{3}^+ \ \bar{x}+1, \bar{x}, x; 3/4, -1/4, 1/4$ ( $\bar{3}_{\bar{y}\bar{z}^{-1}}   1/2, 1/2, 1/2$ )
(33) $\bar{3}^- \ x, x, x; 1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(34) $\bar{3}^- \ x+1, \bar{x}-1, \bar{x}; 1/4, -1/4, 3/4$ ( $\bar{3}_{\bar{y}\bar{z}}   1/2, 1/2, 1/2$ )	(35) $\bar{3}^- \ \bar{x}, \bar{x}+1, x; -1/4, 3/4, 1/4$ ( $\bar{3}_{\bar{y}\bar{z}}   1/2, 1/2, 1/2$ )	(36) $\bar{3}^- \ \bar{x}+1, x, \bar{x}; 3/4, 1/4, -1/4$ ( $\bar{3}_{\bar{y}\bar{z}}   1/2, 1/2, 1/2$ )
(37) $m \ x, \bar{x}, z$ ( $m_{xy}   0, 0, 0$ )	(38) $m \ x, x, z$ ( $m_{\bar{xy}}   0, 0, 0$ )	(39) $\bar{4}^- \ 0, 0, z; 0, 0, 0$ ( $\bar{4}_z^{-1}   0, 0, 0$ )	(40) $\bar{4}^+ \ 0, 0, z; 0, 0, 0$ ( $\bar{4}_z   0, 0, 0$ )
(41) $\bar{4}^- \ x, 0, 0; 0, 0, 0$ ( $\bar{4}_x^{-1}   0, 0, 0$ )	(42) $m \ x, y, \bar{y}$ ( $m_{yz}   0, 0, 0$ )	(43) $m \ x, y, y$ ( $m_{\bar{yz}}   0, 0, 0$ )	(44) $\bar{4}^+ \ x, 0, 0; 0, 0, 0$ ( $\bar{4}_x   0, 0, 0$ )
(45) $\bar{4}^+ \ 0, y, 0; 0, 0, 0$ ( $\bar{4}_y   0, 0, 0$ )	(46) $m \ \bar{x}, y, x$ ( $m_{xz}   0, 0, 0$ )	(47) $\bar{4}^- \ 0, y, 0; 0, 0, 0$ ( $\bar{4}_y^{-1}   0, 0, 0$ )	(48) $m \ x, y, x$ ( $m_{\bar{xz}}   0, 0, 0$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

48 | 1

(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{x}, y, \bar{z} [\bar{u}, v, \bar{w}]$	(4) $x, \bar{y}, \bar{z} [u, \bar{v}, \bar{w}]$
(5) $z, x, y [w, u, v]$	(6) $z, \bar{x}, \bar{y} [w, \bar{u}, \bar{v}]$	(7) $\bar{z}, \bar{x}, y [\bar{w}, \bar{u}, v]$	(8) $\bar{z}, x, \bar{y} [\bar{w}, u, \bar{v}]$
(9) $y, z, x [v, w, u]$	(10) $\bar{y}, z, \bar{x} [\bar{v}, w, \bar{u}]$	(11) $y, \bar{z}, \bar{x} [v, \bar{w}, \bar{u}]$	(12) $\bar{y}, \bar{z}, x [\bar{v}, \bar{w}, u]$
(13) $y+1/2, x+1/2, \bar{z}+1/2 [v, u, \bar{w}]$	(14) $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2 [\bar{v}, \bar{u}, \bar{w}]$	(15) $y+1/2, \bar{x}+1/2, z+1/2 [v, \bar{u}, w]$	(16) $\bar{y}+1/2, x+1/2, z+1/2 [\bar{v}, u, w]$
(17) $x+1/2, z+1/2, \bar{y}+1/2 [u, w, \bar{v}]$	(18) $\bar{x}+1/2, z+1/2, y+1/2 [\bar{u}, w, v]$	(19) $\bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2 [\bar{u}, \bar{w}, \bar{v}]$	(20) $x+1/2, \bar{z}+1/2, y+1/2 [u, \bar{w}, v]$
(21) $z+1/2, y+1/2, \bar{x}+1/2 [w, v, \bar{u}]$	(22) $z+1/2, \bar{y}+1/2, x+1/2 [w, \bar{v}, u]$	(23) $\bar{z}+1/2, y+1/2, x+1/2 [\bar{w}, v, u]$	(24) $\bar{z}+1/2, \bar{y}+1/2, \bar{x}+1/2 [\bar{w}, \bar{v}, \bar{u}]$
(25) $\bar{x}+1/2, \bar{y}+1/2, \bar{z}+1/2 [u, v, w]$	(26) $x+1/2, y+1/2, \bar{z}+1/2 [\bar{u}, \bar{v}, \bar{w}]$	(27) $x+1/2, \bar{y}+1/2, z+1/2 [u, v, w]$	(28) $\bar{x}+1/2, y+1/2, z+1/2 [u, \bar{v}, \bar{w}]$
(29) $\bar{z}+1/2, \bar{x}+1/2, \bar{y}+1/2 [w, u, v]$	(30) $\bar{z}+1/2, x+1/2, y+1/2 [w, \bar{u}, \bar{v}]$	(31) $z+1/2, x+1/2, \bar{y}+1/2 [\bar{w}, \bar{u}, v]$	(32) $z+1/2, \bar{x}+1/2, y+1/2 [\bar{w}, u, \bar{v}]$
(33) $\bar{y}+1/2, \bar{z}+1/2, \bar{x}+1/2 [v, w, u]$	(34) $y+1/2, \bar{z}+1/2, x+1/2 [\bar{v}, w, \bar{u}]$	(35) $\bar{y}+1/2, z+1/2, x+1/2 [v, \bar{w}, \bar{u}]$	(36) $y+1/2, z+1/2, \bar{x}+1/2 [\bar{v}, w, u]$

(37) $\bar{y}, \bar{x}, z [v, u, \bar{w}]$	(38) $y, x, z [\bar{v}, \bar{u}, \bar{w}]$	(39) $\bar{y}, x, \bar{z} [v, \bar{u}, w]$	(40) $y, \bar{x}, \bar{z} [\bar{v}, u, w]$
(41) $\bar{x}, \bar{z}, y [u, w, \bar{v}]$	(42) $x, \bar{z}, y [\bar{u}, w, v]$	(43) $x, z, y [\bar{u}, \bar{w}, \bar{v}]$	(44) $\bar{x}, z, y [u, \bar{w}, v]$
(45) $\bar{z}, \bar{y}, x [w, v, \bar{u}]$	(46) $\bar{z}, y, \bar{x} [w, \bar{v}, u]$	(47) $z, \bar{y}, \bar{x} [\bar{w}, v, u]$	(48) $z, y, x [\bar{w}, \bar{v}, \bar{u}]$
24 k ..m			
$x, x, z [u, \bar{u}, 0]$	$\bar{x}, \bar{x}, z [\bar{u}, u, 0]$	$\bar{x}, x, \bar{z} [\bar{u}, \bar{u}, 0]$	$x, \bar{x}, \bar{z} [u, u, 0]$
$z, x, x [0, u, \bar{u}]$	$z, \bar{x}, \bar{x} [0, \bar{u}, u]$	$\bar{z}, \bar{x}, x [0, \bar{u}, \bar{u}]$	$\bar{z}, x, \bar{x} [0, u, u]$
$x, z, x [\bar{u}, 0, u]$	$\bar{x}, z, \bar{x} [u, 0, \bar{u}]$	$x, \bar{z}, \bar{x} [\bar{u}, 0, \bar{u}]$	$\bar{x}, \bar{z}, x [u, 0, u]$
$x+1/2, x+1/2, \bar{z}+1/2 [\bar{u}, u, 0]$	$\bar{x}+1/2, \bar{x}+1/2, \bar{z}+1/2 [u, \bar{u}, 0]$	$x+1/2, \bar{x}+1/2, z+1/2 [\bar{u}, \bar{u}, 0]$	$\bar{x}+1/2, x+1/2, z+1/2 [u, u, 0]$
$x+1/2, z+1/2, \bar{x}+1/2 [u, 0, u]$	$\bar{x}+1/2, z+1/2, x+1/2 [\bar{u}, 0, \bar{u}]$	$\bar{x}+1/2, \bar{z}+1/2, \bar{x}+1/2 [\bar{u}, 0, u]$	$x+1/2, \bar{z}+1/2, x+1/2 [u, 0, \bar{u}]$
$z+1/2, x+1/2, \bar{x}+1/2 [0, \bar{u}, \bar{u}]$	$z+1/2, \bar{x}+1/2, x+1/2 [0, u, u]$	$\bar{z}+1/2, x+1/2, x+1/2 [0, \bar{u}, u]$	$\bar{z}+1/2, \bar{x}+1/2, \bar{x}+1/2 [0, u, \bar{u}]$
24 j ..2			
$1/4, y, y+1/2 [0, v, v]$	$3/4, \bar{y}, y+1/2 [0, \bar{v}, v]$	$3/4, y, \bar{y}+1/2 [0, v, \bar{v}]$	$1/4, \bar{y}, \bar{y}+1/2 [0, \bar{v}, \bar{v}]$
$y+1/2, 1/4, y [v, 0, v]$	$y+1/2, 3/4, \bar{y} [v, 0, \bar{v}]$	$\bar{y}+1/2, 3/4, y [\bar{v}, 0, v]$	$\bar{y}+1/2, 1/4, \bar{y} [\bar{v}, 0, \bar{v}]$
$y, y+1/2, 1/4 [v, v, 0]$	$\bar{y}, y+1/2, 3/4 [\bar{v}, v, 0]$	$y, \bar{y}+1/2, 3/4 [v, \bar{v}, 0]$	$\bar{y}, \bar{y}+1/2, 1/4 [\bar{v}, \bar{v}, 0]$
$1/4, \bar{y}+1/2, \bar{y} [0, v, v]$	$3/4, y+1/2, \bar{y} [0, \bar{v}, v]$	$3/4, \bar{y}+1/2, y [0, v, \bar{v}]$	$1/4, y+1/2, \bar{y} [0, \bar{v}, \bar{v}]$
$\bar{y}, 1/4, \bar{y}+1/2 [v, 0, v]$	$\bar{y}, 3/4, y+1/2 [v, 0, \bar{v}]$	$y, 3/4, \bar{y}+1/2 [\bar{v}, 0, v]$	$y, 1/4, y+1/2 [\bar{v}, 0, \bar{v}]$
$\bar{y}+1/2, \bar{y}, 1/4 [v, v, 0]$	$y+1/2, \bar{y}, 3/4 [\bar{v}, v, 0]$	$\bar{y}+1/2, y, 3/4 [v, \bar{v}, 0]$	$y+1/2, y, 1/4 [\bar{v}, \bar{v}, 0]$
24 i ..2			
$1/4, y, \bar{y}+1/2 [0, \bar{v}, v]$	$3/4, \bar{y}, \bar{y}+1/2 [0, v, v]$	$3/4, y, y+1/2 [0, \bar{v}, \bar{v}]$	$1/4, \bar{y}, y+1/2 [0, v, \bar{v}]$
$\bar{y}+1/2, 1/4, y [v, 0, \bar{v}]$	$\bar{y}+1/2, 3/4, \bar{y} [v, 0, v]$	$y+1/2, 3/4, y [\bar{v}, 0, \bar{v}]$	$y+1/2, 1/4, \bar{y} [\bar{v}, 0, v]$
$y, \bar{y}+1/2, 1/4 [\bar{v}, v, 0]$	$\bar{y}, \bar{y}+1/2, 3/4 [v, v, 0]$	$y, y+1/2, 3/4 [\bar{v}, \bar{v}, 0]$	$\bar{y}, y+1/2, 1/4 [v, \bar{v}, 0]$
$1/4, \bar{y}+1/2, y [0, \bar{v}, v]$	$3/4, y+1/2, y [0, v, v]$	$3/4, \bar{y}+1/2, \bar{y} [0, v, \bar{v}]$	$1/4, y+1/2, \bar{y} [0, v, \bar{v}]$
$y, 1/4, \bar{y}+1/2 [v, 0, \bar{v}]$	$y, 3/4, y+1/2 [v, 0, v]$	$\bar{y}, 3/4, \bar{y}+1/2 [\bar{v}, 0, \bar{v}]$	$\bar{y}, 1/4, y+1/2 [\bar{v}, 0, v]$
$\bar{y}+1/2, y, 1/4 [\bar{v}, v, 0]$	$y+1/2, y, 3/4 [v, v, 0]$	$\bar{y}+1/2, \bar{y}, 3/4 [\bar{v}, \bar{v}, 0]$	$y+1/2, \bar{y}, 1/4 [v, \bar{v}, 0]$
24 h 2..			
$x, 0, 1/2 [u, 0, 0]$	$\bar{x}, 0, 1/2 [\bar{u}, 0, 0]$	$1/2, x, 0 [0, u, 0]$	$1/2, \bar{x}, 0 [0, \bar{u}, 0]$
$0, 1/2, x [0, 0, u]$	$0, 1/2, \bar{x} [0, 0, \bar{u}]$	$1/2, x+1/2, 0 [0, u, 0]$	$1/2, \bar{x}+1/2, 0 [0, \bar{u}, 0]$
$x+1/2, 0, 1/2 [u, 0, 0]$	$\bar{x}+1/2, 0, 1/2 [\bar{u}, 0, 0]$	$0, 1/2, \bar{x}+1/2 [0, 0, \bar{u}]$	$0, 1/2, x+1/2 [0, 0, u]$

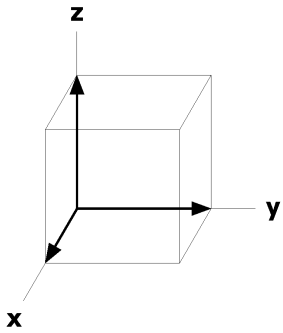
Continued			224.1.1611			Pn $\bar{3}m$		
			$\bar{x}+1/2, 1/2, 0$ [u,0,0]	$x+1/2, 1/2, 0$ [ $\bar{u}$ ,0,0]	$0, \bar{x}+1/2, 1/2$ [0,u,0]	$0, x+1/2, 1/2$ [0, $\bar{u}$ ,0]		
			$1/2, 0, \bar{x}+1/2$ [0,0,u]	$1/2, 0, x+1/2$ [0,0, $\bar{u}$ ]	$0, \bar{x}, 1/2$ [0,u,0]	$0, x, 1/2$ [0, $\bar{u}$ ,0]		
			$\bar{x}, 1/2, 0$ [u,0,0]	$x, 1/2, 0$ [ $\bar{u}$ ,0,0]	$1/2, 0, x$ [0,0, $\bar{u}$ ]	$1/2, 0, \bar{x}$ [0,0,u]		
12	g	2.mm	$x, 0, 0$ [0,0,0]	$\bar{x}, 0, 0$ [0,0,0]	$0, x, 0$ [0,0,0]	$0, \bar{x}, 0$ [0,0,0]		
			$0, 0, x$ [0,0,0]	$0, 0, \bar{x}$ [0,0,0]	$1/2, x+1/2, 1/2$ [0,0,0]	$1/2, \bar{x}+1/2, 1/2$ [0,0,0]		
			$x+1/2, 1/2, 1/2$ [0,0,0]	$\bar{x}+1/2, 1/2, 1/2$ [0,0,0]	$1/2, 1/2, \bar{x}+1/2$ [0,0,0]	$1/2, 1/2, x+1/2$ [0,0,0]		
12	f	2.22	$1/4, 0, 1/2$ [0,0,0]	$3/4, 0, 1/2$ [0,0,0]	$1/2, 1/4, 0$ [0,0,0]			
			$1/2, 3/4, 0$ [0,0,0]	$0, 1/2, 1/4$ [0,0,0]	$0, 1/2, 3/4$ [0,0,0]			
			$1/4, 1/2, 0$ [0,0,0]	$3/4, 1/2, 0$ [0,0,0]	$0, 1/4, 1/2$ [0,0,0]			
			$0, 3/4, 1/2$ [0,0,0]	$1/2, 0, 1/4$ [0,0,0]	$1/2, 0, 3/4$ [0,0,0]			
8	e	.3m	$x, x, x$ [0,0,0]	$\bar{x}, \bar{x}, x$ [0,0,0]				
			$\bar{x}, x, \bar{x}$ [0,0,0]	$x, \bar{x}, \bar{x}$ [0,0,0]				
			$x+1/2, x+1/2, \bar{x}+1/2$ [0,0,0]	$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2$ [0,0,0]				
			$x+1/2, \bar{x}+1/2, x+1/2$ [0,0,0]	$\bar{x}+1/2, x+1/2, x+1/2$ [0,0,0]				
6	d	$\bar{4}2.m$	$0, 1/2, 1/2$ [0,0,0]	$1/2, 0, 1/2$ [0,0,0]	$1/2, 1/2, 0$ [0,0,0]			
			$0, 1/2, 0$ [0,0,0]	$1/2, 0, 0$ [0,0,0]	$0, 0, 1/2$ [0,0,0]			
4	c	$\bar{3}m$	$3/4, 3/4, 3/4$ [0,0,0]	$1/4, 1/4, 3/4$ [0,0,0]	$1/4, 3/4, 1/4$ [0,0,0]	$3/4, 1/4, 1/4$ [0,0,0]		
4	b	$\bar{3}m$	$1/4, 1/4, 1/4$ [0,0,0]	$3/4, 3/4, 1/4$ [0,0,0]	$3/4, 1/4, 3/4$ [0,0,0]	$1/4, 3/4, 3/4$ [0,0,0]		
2	a	$\bar{4}3m$	$0, 0, 0$ [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]				

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,1,1] p6'm'm  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



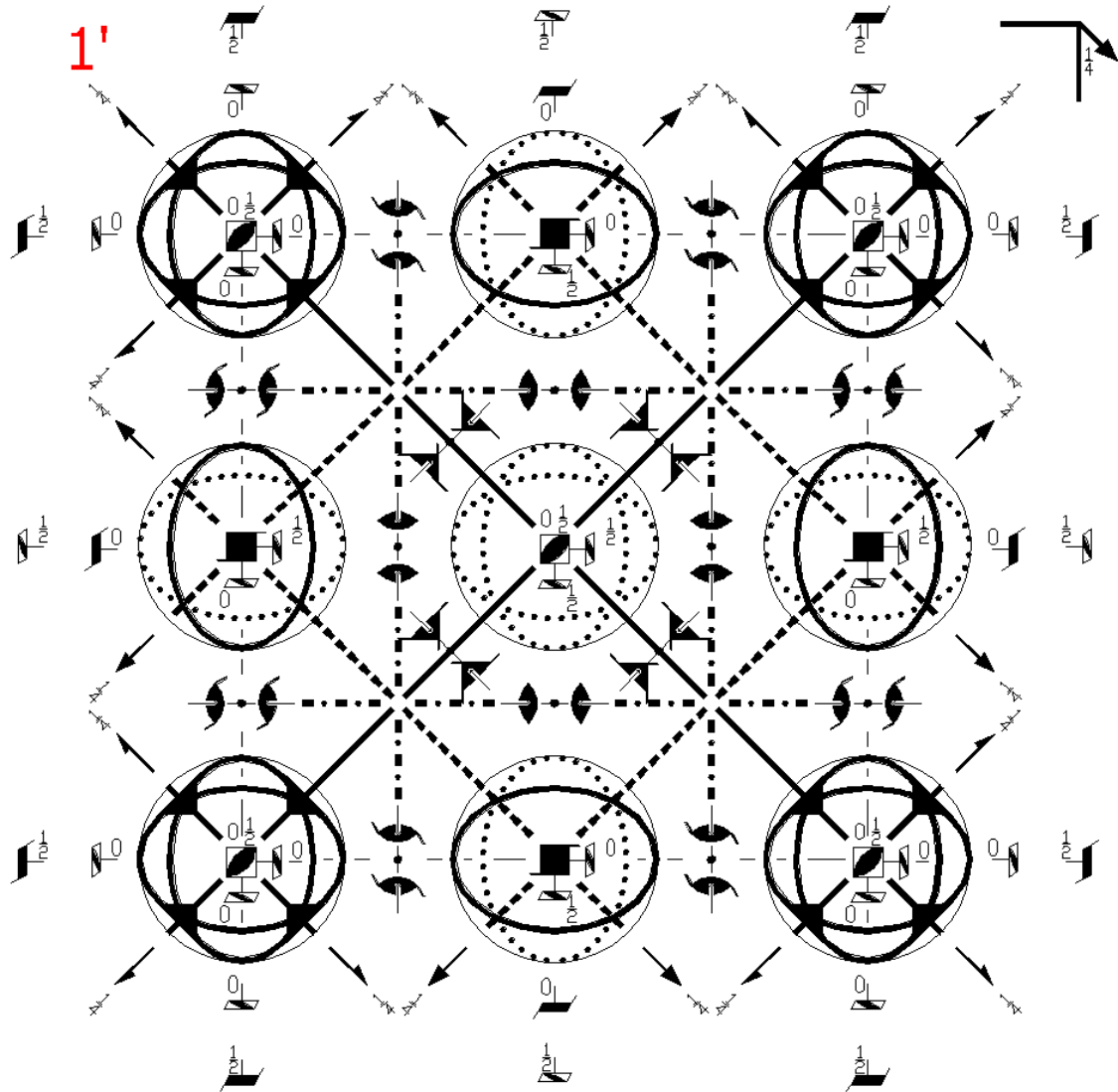
$Pn\bar{3}m1'$

224.2.1612

$m\bar{3}m1'$

$P4_2/n\bar{3}2/m1'$

Cubic



**Origin** at  $\bar{4}3m1'$ , at  $-1/4, -1/4, -1/4$  from center ( $\bar{3}m1'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; -1/4 \leq z \leq 1/4; y \leq x; \max(x-1/2, -y) \leq z \leq \min(1/2-x, y)$

**Vertices**  $0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/4,1/4,1/4 \quad 1/4,1/4,-1/4$

**Symmetry Operations**

For 1 + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                  | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)                   | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)                    |



(13) 2 (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)	(14) 2 x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)	(15) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)	(16) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)
(17) 4 <sup>-</sup> (1/2,0,0) x,1/2,0 (4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,1/2)	(18) 2 (0,1/2,1/2) 1/4,y,y (2 <sub>yz</sub>  1/2,1/2,1/2)	(19) 2 1/4,y+1/2, $\bar{y}$ (2 <sub><math>\bar{yz}</math></sub>  1/2,1/2,1/2)	(20) 4 <sup>+</sup> (1/2,0,0) x,0,1/2 (4 <sub>x</sub>  1/2,1/2,1/2)
(21) 4 <sup>+</sup> (0,1/2,0) 1/2,y,0 (4 <sub>y</sub>  1/2,1/2,1/2)	(22) 2 (1/2,0,1/2) x,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)	(23) 4 <sup>-</sup> (0,1/2,0) 0,y,1/2 (4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,1/2)	(24) 2 $\bar{x}$ +1/2,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)
(25) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$  1/2,1/2,1/2)	(26) n (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>  1/2,1/2,1/2)	(27) n (1/2,0,1/2) x,1/4,z (m <sub>y</sub>  1/2,1/2,1/2)	(28) n (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1/2)
(29) $\bar{3}^+$ x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}$  1/2,1/2,1/2)	(30) $\bar{3}^+$ $\bar{x}$ -1,x+1, $\bar{x}$ ; -1/4,1/4,3/4 ( $\bar{3}_{x\bar{y}z}$ <sup>-1</sup>  1/2,1/2,1/2)	(31) $\bar{3}^+$ x, $\bar{x}$ +1, $\bar{x}$ ; 1/4,3/4,-1/4 ( $\bar{3}_{x\bar{y}z}$ <sup>-1</sup>  1/2,1/2,1/2)	(32) $\bar{3}^+$ $\bar{x}$ +1, $\bar{x}$ ,x; 3/4,-1/4,1/4 ( $\bar{3}_{x\bar{y}z}$ <sup>-1</sup>  1/2,1/2,1/2)
(33) $\bar{3}^-$ x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,1/2,1/2)	(34) $\bar{3}^-$ x+1, $\bar{x}$ -1, $\bar{x}$ ; 1/4,-1/4,3/4 ( $\bar{3}_{x\bar{y}z}$  1/2,1/2,1/2)	(35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1,x; -1/4,3/4,1/4 ( $\bar{3}_{x\bar{y}z}$  1/2,1/2,1/2)	(36) $\bar{3}^-$ $\bar{x}$ +1,x, $\bar{x}$ ; 3/4,1/4,-1/4 ( $\bar{3}_{x\bar{y}z}$  1/2,1/2,1/2)
(37) m x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)	(38) m x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,0)	(39) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z$ <sup>-1</sup>  0,0,0)	(40) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)
(41) $\bar{4}^-$ x,0,0; 0,0,0 ( $\bar{4}_x$ <sup>-1</sup>  0,0,0)	(42) m x,y, $\bar{y}$ (m <sub>yz</sub>  0,0,0)	(43) m x,y,y (m <sub><math>\bar{yz}</math></sub>  0,0,0)	(44) $\bar{4}^+$ x,0,0; 0,0,0 ( $\bar{4}_x$  0,0,0)
(45) $\bar{4}^+$ 0,y,0; 0,0,0 ( $\bar{4}_y$  0,0,0)	(46) m $\bar{x}$ ,y,x (m <sub>xz</sub>  0,0,0)	(47) $\bar{4}^-$ 0,y,0; 0,0,0 ( $\bar{4}_y$ <sup>-1</sup>  0,0,0)	(48) m x,y,x (m <sub>xz</sub>  0,0,0)

## For 1' + set

(1) 1' (1 0,0,0)'	(2) 2' 0,0,z (2 <sub>z</sub>  0,0,0)'	(3) 2' 0,y,0 (2 <sub>y</sub>  0,0,0)'	(4) 2' x,0,0 (2 <sub>x</sub>  0,0,0)'
(5) 3 <sup>+</sup> x,x,x (3 <sub>xyz</sub>  0,0,0)'	(6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$ (3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0)'	(7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$ (3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0)'	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x (3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0)'
(9) 3 <sup>-</sup> x,x,x (3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)'	(10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$ (3 <sub>x<math>\bar{y}z</math></sub>  0,0,0)'	(11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x (3 <sub>x<math>\bar{y}z</math></sub>  0,0,0)'	(12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$ (3 <sub>x<math>\bar{y}z</math></sub>  0,0,0)'
13) 2' (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(14) 2' x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)'	(15) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(16) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)'
(17) 4 <sup>-</sup> (1/2,0,0) x,1/2,0 (4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(18) 2' (0,1/2,1/2) 1/4,y,y (2 <sub>yz</sub>  1/2,1/2,1/2)'	(19) 2' 1/4,y+1/2, $\bar{y}$ (2 <sub><math>\bar{yz}</math></sub>  1/2,1/2,1/2)'	(20) 4 <sup>+</sup> (1/2,0,0) x,0,1/2 (4 <sub>x</sub>  1/2,1/2,1/2)'
(21) 4 <sup>+</sup> (0,1/2,0) 1/2,y,0 (4 <sub>y</sub>  1/2,1/2,1/2)'	(22) 2' (1/2,0,1/2) x,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)'	(23) 4 <sup>-</sup> (0,1/2,0) 0,y,1/2 (4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(24) 2' $\bar{x}$ +1/2,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)'
(25) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$  1/2,1/2,1/2)'	(26) n' (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>  1/2,1/2,1/2)'	(27) n' (1/2,0,1/2) x,1/4,z (m <sub>y</sub>  1/2,1/2,1/2)'	(28) n' (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1/2)'
(29) $\bar{3}^+$ x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}$  1/2,1/2,1/2)'	(30) $\bar{3}^+$ $\bar{x}$ -1,x+1, $\bar{x}$ ; -1/4,1/4,3/4 ( $\bar{3}_{x\bar{y}z}$ <sup>-1</sup>  1/2,1/2,1/2)'	(31) $\bar{3}^+$ x, $\bar{x}$ +1, $\bar{x}$ ; 1/4,3/4,-1/4 ( $\bar{3}_{x\bar{y}z}$ <sup>-1</sup>  1/2,1/2,1/2)'	(32) $\bar{3}^+$ $\bar{x}$ +1, $\bar{x}$ ,x; 3/4,-1/4,1/4 ( $\bar{3}_{x\bar{y}z}$ <sup>-1</sup>  1/2,1/2,1/2)'
(33) $\bar{3}^-$ x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,1/2,1/2)'	(34) $\bar{3}^-$ x+1, $\bar{x}$ -1, $\bar{x}$ ; 1/4,-1/4,3/4 ( $\bar{3}_{x\bar{y}z}$  1/2,1/2,1/2)'	(35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1,x; -1/4,3/4,1/4 ( $\bar{3}_{x\bar{y}z}$  1/2,1/2,1/2)'	(36) $\bar{3}^-$ $\bar{x}$ +1,x, $\bar{x}$ ; 3/4,1/4,-1/4 ( $\bar{3}_{x\bar{y}z}$  1/2,1/2,1/2)'

Continued

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Pn $\bar{3}$ m1'

(37) $m' \quad x, \bar{x}, z$ ( $m_{xy}   0, 0, 0$ )'	(38) $m' \quad x, x, z$ ( $m_{\bar{xy}}   0, 0, 0$ )'	(39) $\bar{4}^- ' \quad 0, 0, z; 0, 0, 0$ ( $\bar{4}_z^{-1}   0, 0, 0$ )'	(40) $\bar{4}^+ ' \quad 0, 0, z; 0, 0, 0$ ( $\bar{4}_z   0, 0, 0$ )'
(41) $\bar{4}^- ' \quad x, 0, 0; 0, 0, 0$ ( $\bar{4}_x^{-1}   0, 0, 0$ )'	(42) $m' \quad x, y, \bar{y}$ ( $m_{yz}   0, 0, 0$ )'	(43) $m' \quad x, y, y$ ( $m_{\bar{yz}}   0, 0, 0$ )'	(44) $\bar{4}^+ ' \quad x, 0, 0; 0, 0, 0$ ( $\bar{4}_x   0, 0, 0$ )'
(45) $\bar{4}^+ ' \quad 0, y, 0; 0, 0, 0$ ( $\bar{4}_y   0, 0, 0$ )'	(46) $m' \quad \bar{x}, y, x$ ( $m_{xz}   0, 0, 0$ )'	(47) $\bar{4}^- ' \quad 0, y, 0; 0, 0, 0$ ( $\bar{4}_y^{-1}   0, 0, 0$ )'	(48) $m' \quad x, y, x$ ( $m_{\bar{xz}}   0, 0, 0$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25); 1'.

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

1 + 1' +

Continued

224.2.1612

Pn $\bar{3}$ m1'

48 l 11'

(1) $x, y, z [0, 0, 0]$	(2) $\bar{x}, \bar{y}, z [0, 0, 0]$	(3) $\bar{x}, y, \bar{z} [0, 0, 0]$	(4) $x, \bar{y}, \bar{z} [0, 0, 0]$
(5) $z, x, y [0, 0, 0]$	(6) $z, \bar{x}, \bar{y} [0, 0, 0]$	(7) $\bar{z}, \bar{x}, y [0, 0, 0]$	(8) $\bar{z}, x, \bar{y} [0, 0, 0]$
(9) $y, z, x [0, 0, 0]$	(10) $\bar{y}, z, \bar{x} [0, 0, 0]$	(11) $y, \bar{z}, \bar{x} [0, 0, 0]$	(12) $\bar{y}, \bar{z}, x [0, 0, 0]$
(13) $y+1/2, x+1/2, \bar{z}+1/2 [0, 0, 0]$	(14) $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2 [0, 0, 0]$	(15) $y+1/2, \bar{x}+1/2, z+1/2 [0, 0, 0]$	(16) $\bar{y}+1/2, x+1/2, z+1/2 [0, 0, 0]$
(17) $x+1/2, z+1/2, \bar{y}+1/2 [0, 0, 0]$	(18) $\bar{x}+1/2, z+1/2, y+1/2 [0, 0, 0]$	(19) $\bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2 [0, 0, 0]$	(20) $x+1/2, \bar{z}+1/2, y+1/2 [0, 0, 0]$
(21) $z+1/2, y+1/2, \bar{x}+1/2 [0, 0, 0]$	(22) $z+1/2, \bar{y}+1/2, x+1/2 [0, 0, 0]$	(23) $\bar{z}+1/2, y+1/2, x+1/2 [0, 0, 0]$	(24) $\bar{z}+1/2, \bar{y}+1/2, \bar{x}+1/2 [0, 0, 0]$
(25) $\bar{x}+1/2, \bar{y}+1/2, \bar{z}+1/2 [0, 0, 0]$	(26) $x+1/2, y+1/2, \bar{z}+1/2 [0, 0, 0]$	(27) $x+1/2, \bar{y}+1/2, z+1/2 [0, 0, 0]$	(28) $\bar{x}+1/2, y+1/2, z+1/2 [0, 0, 0]$
(29) $\bar{z}+1/2, \bar{x}+1/2, \bar{y}+1/2 [0, 0, 0]$	(30) $\bar{z}+1/2, x+1/2, y+1/2 [0, 0, 0]$	(31) $z+1/2, x+1/2, \bar{y}+1/2 [0, 0, 0]$	(32) $z+1/2, \bar{x}+1/2, y+1/2 [0, 0, 0]$
(33) $\bar{y}+1/2, \bar{z}+1/2, \bar{x}+1/2 [0, 0, 0]$	(34) $y+1/2, \bar{z}+1/2, x+1/2 [0, 0, 0]$	(35) $\bar{y}+1/2, z+1/2, x+1/2 [0, 0, 0]$	(36) $y+1/2, z+1/2, \bar{x}+1/2 [0, 0, 0]$
(37) $\bar{y}, \bar{x}, z [0, 0, 0]$	(38) $y, x, z [0, 0, 0]$	(39) $\bar{y}, x, \bar{z} [0, 0, 0]$	(40) $y, \bar{x}, \bar{z} [0, 0, 0]$
(41) $\bar{x}, \bar{z}, y [0, 0, 0]$	(42) $x, \bar{z}, \bar{y} [0, 0, 0]$	(43) $x, z, y [0, 0, 0]$	(44) $\bar{x}, z, \bar{y} [0, 0, 0]$
(45) $\bar{z}, \bar{y}, x [0, 0, 0]$	(46) $\bar{z}, y, \bar{x} [0, 0, 0]$	(47) $z, \bar{y}, \bar{x} [0, 0, 0]$	(48) $z, y, x [0, 0, 0]$

24 k ..m1'

$x, x, z [0, 0, 0]$	$\bar{x}, \bar{x}, z [0, 0, 0]$	$\bar{x}, x, \bar{z} [0, 0, 0]$	$x, \bar{x}, \bar{z} [0, 0, 0]$
$z, x, x [0, 0, 0]$	$z, \bar{x}, \bar{x} [0, 0, 0]$	$\bar{z}, \bar{x}, x [0, 0, 0]$	$\bar{z}, x, \bar{x} [0, 0, 0]$
$x, z, x [0, 0, 0]$	$\bar{x}, z, \bar{x} [0, 0, 0]$	$x, \bar{z}, \bar{x} [0, 0, 0]$	$\bar{x}, \bar{z}, x [0, 0, 0]$

$x+1/2, x+1/2, \bar{z}+1/2$ [0,0,0]	$\bar{x}+1/2, \bar{x}+1/2, \bar{z}+1/2$ [0,0,0]	$x+1/2, \bar{x}+1/2, z+1/2$ [0,0,0]	$\bar{x}+1/2, x+1/2, z+1/2$ [0,0,0]	
$x+1/2, z+1/2, \bar{x}+1/2$ [0,0,0]	$\bar{x}+1/2, z+1/2, x+1/2$ [0,0,0]	$\bar{x}+1/2, \bar{z}+1/2, \bar{x}+1/2$ [0,0,0]	$x+1/2, \bar{z}+1/2, x+1/2$ [0,0,0]	
$z+1/2, x+1/2, \bar{x}+1/2$ [0,0,0]	$z+1/2, \bar{x}+1/2, x+1/2$ [0,0,0]	$\bar{z}+1/2, x+1/2, x+1/2$ [0,0,0]	$\bar{z}+1/2, \bar{x}+1/2, \bar{x}+1/2$ [0,0,0]	
24 j ..21'				
$1/4, y, y+1/2$ [0,0,0]	$3/4, \bar{y}, y+1/2$ [0,0,0]	$3/4, y, \bar{y}+1/2$ [0,0,0]	$1/4, \bar{y}, \bar{y}+1/2$ [0,0,0]	
$y+1/2, 1/4, y$ [0,0,0]	$y+1/2, 3/4, \bar{y}$ [0,0,0]	$\bar{y}+1/2, 3/4, y$ [0,0,0]	$\bar{y}+1/2, 1/4, \bar{y}$ [0,0,0]	
$y, y+1/2, 1/4$ [0,0,0]	$\bar{y}, y+1/2, 3/4$ [0,0,0]	$y, \bar{y}+1/2, 3/4$ [0,0,0]	$\bar{y}, \bar{y}+1/2, 1/4$ [0,0,0]	
$1/4, \bar{y}+1/2, \bar{y}$ [0,0,0]	$3/4, y+1/2, \bar{y}$ [0,0,0]	$3/4, \bar{y}+1/2, y$ [0,0,0]	$1/4, y+1/2, y$ [0,0,0]	
$\bar{y}, 1/4, \bar{y}+1/2$ [0,0,0]	$\bar{y}, 3/4, y+1/2$ [0,0,0]	$y, 3/4, \bar{y}+1/2$ [0,0,0]	$y, 1/4, y+1/2$ [0,0,0]	
$\bar{y}+1/2, \bar{y}, 1/4$ [0,0,0]	$y+1/2, \bar{y}, 3/4$ [0,0,0]	$\bar{y}+1/2, y, 3/4$ [0,0,0]	$y+1/2, y, 1/4$ [0,0,0]	
24 i ..21'				
$1/4, y, \bar{y}+1/2$ [0,0,0]	$3/4, \bar{y}, \bar{y}+1/2$ [0,0,0]	$3/4, y, y+1/2$ [0,0,0]	$1/4, \bar{y}, y+1/2$ [0,0,0]	
$\bar{y}+1/2, 1/4, y$ [0,0,0]	$\bar{y}+1/2, 3/4, \bar{y}$ [0,0,0]	$y+1/2, 3/4, y$ [0,0,0]	$y+1/2, 1/4, \bar{y}$ [0,0,0]	
$y, \bar{y}+1/2, 1/4$ [0,0,0]	$\bar{y}, \bar{y}+1/2, 3/4$ [0,0,0]	$y, y+1/2, 3/4$ [0,0,0]	$\bar{y}, y+1/2, 1/4$ [0,0,0]	
$1/4, \bar{y}+1/2, y$ [0,0,0]	$3/4, y+1/2, y$ [0,0,0]	$3/4, \bar{y}+1/2, \bar{y}$ [0,0,0]	$1/4, y+1/2, \bar{y}$ [0,0,0]	
$y, 1/4, \bar{y}+1/2$ [0,0,0]	$y, 3/4, y+1/2$ [0,0,0]	$\bar{y}, 3/4, \bar{y}+1/2$ [0,0,0]	$\bar{y}, 1/4, y+1/2$ [0,0,0]	
$\bar{y}+1/2, y, 1/4$ [0,0,0]	$y+1/2, y, 3/4$ [0,0,0]	$\bar{y}+1/2, \bar{y}, 3/4$ [0,0,0]	$y+1/2, \bar{y}, 1/4$ [0,0,0]	
24 h 2..1'	$x, 0, 1/2$ [0,0,0]	$\bar{x}, 0, 1/2$ [0,0,0]	$1/2, x, 0$ [0,0,0]	$1/2, \bar{x}, 0$ [0,0,0]
	$0, 1/2, x$ [0,0,0]	$0, 1/2, \bar{x}$ [0,0,0]	$1/2, x+1/2, 0$ [0,0,0]	$1/2, \bar{x}+1/2, 0$ [0,0,0]
	$x+1/2, 0, 1/2$ [0,0,0]	$\bar{x}+1/2, 0, 1/2$ [0,0,0]	$0, 1/2, \bar{x}+1/2$ [0,0,0]	$0, 1/2, x+1/2$ [0,0,0]
	$\bar{x}+1/2, 1/2, 0$ [0,0,0]	$x+1/2, 1/2, 0$ [0,0,0]	$0, \bar{x}+1/2, 1/2$ [0,0,0]	$0, x+1/2, 1/2$ [0,0,0]
	$1/2, 0, \bar{x}+1/2$ [0,0,0]	$1/2, 0, x+1/2$ [0,0,0]	$0, \bar{x}, 1/2$ [0,0,0]	$0, x, 1/2$ [0,0,0]
	$\bar{x}, 1/2, 0$ [0,0,0]	$x, 1/2, 0$ [0,0,0]	$1/2, 0, x$ [0,0,0]	$1/2, 0, \bar{x}$ [0,0,0]
12 g 2.mm1'	$x, 0, 0$ [0,0,0]	$\bar{x}, 0, 0$ [0,0,0]	$0, x, 0$ [0,0,0]	$0, \bar{x}, 0$ [0,0,0]
	$0, 0, x$ [0,0,0]	$0, 0, \bar{x}$ [0,0,0]	$1/2, x+1/2, 1/2$ [0,0,0]	$1/2, \bar{x}+1/2, 1/2$ [0,0,0]
	$x+1/2, 1/2, 1/2$ [0,0,0]	$\bar{x}+1/2, 1/2, 1/2$ [0,0,0]	$1/2, 1/2, \bar{x}+1/2$ [0,0,0]	$1/2, 1/2, x+1/2$ [0,0,0]

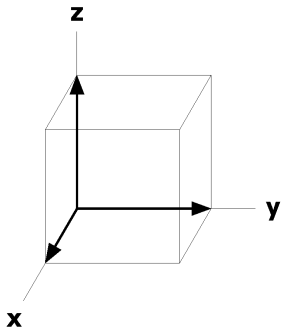
Continued		224.2.1612		Pn $\bar{3}$ m1'		
12	f	2.221'	1/4,0,1/2 [0,0,0]	3/4,0,1/2 [0,0,0]	1/2,1/4,0 [0,0,0]	
			1/2,3/4,0 [0,0,0]	0,1/2,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	
			1/4,1/2,0 [0,0,0]	3/4,1/2,0 [0,0,0]	0,1/4,1/2 [0,0,0]	
			0,3/4,1/2 [0,0,0]	1/2,0,1/4 [0,0,0]	1/2,0,3/4 [0,0,0]	
8	e	.3m1'	x,x,x [0,0,0]	$\bar{x},\bar{x},x$ [0,0,0]		
			$\bar{x},x,\bar{x}$ [0,0,0]	$x,\bar{x},\bar{x}$ [0,0,0]		
			$x+1/2,x+1/2,\bar{x}+1/2$ [0,0,0]	$\bar{x}+1/2,\bar{x}+1/2,\bar{x}+1/2$ [0,0,0]		
			$x+1/2,\bar{x}+1/2,x+1/2$ [0,0,0]	$\bar{x}+1/2,x+1/2,x+1/2$ [0,0,0]		
6	d	$\bar{4}2.m1'$	0,1/2,1/2 [0,0,0]	1/2,0,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]	
			0,1/2,0 [0,0,0]	1/2,0,0 [0,0,0]	0,0,1/2 [0,0,0]	
4	c	$\bar{3}m1'$	3/4,3/4,3/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]	3/4,1/4,1/4 [0,0,0]
4	b	$\bar{3}m1'$	1/4,1/4,1/4 [0,0,0]	3/4,3/4,1/4 [0,0,0]	3/4,1/4,3/4 [0,0,0]	1/4,3/4,3/4 [0,0,0]
2	a	$\bar{4}3m1'$	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,1,1] p6mm1'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/4



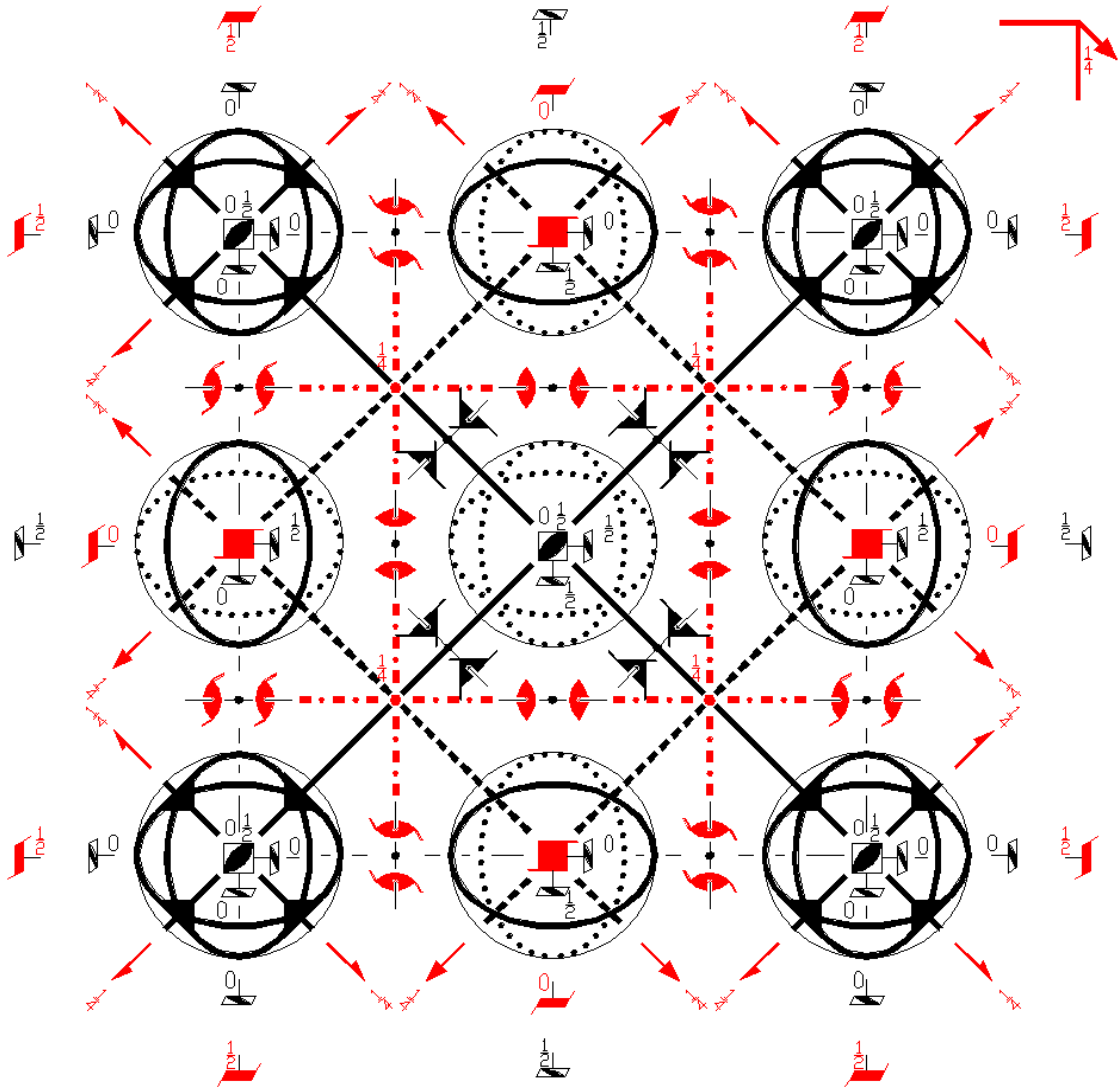
$Pn\bar{3}m$

224.3.1613

$m\bar{3}m$

$P4_2/n\bar{3}2'/m$

Cubic



**Origin** at  $\bar{4}3m$ , at  $-1/4, -1/4, -1/4$  from center ( $\bar{3}m$ )

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; -1/4 \leq z \leq 1/4; y \leq x; \max(x-1/2, -y) \leq z \leq \min(1/2-x, y)$

**Vertices**  $0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/4,1/4,1/4 \quad 1/4,1/4,-1/4$

**Symmetry Operations**

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)  | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}\bar{y}\bar{z}</math></sub>  0,0,0)              |

Continued

224.2.1612

Pn $\bar{3}m1'$ 

(13) $2'$ $(1/2, 1/2, 0)$ $x, x, 1/4$ $(2_{xy}   1/2, 1/2, 1/2)'$	(14) $2'$ $x, \bar{x}+1/2, 1/4$ $(2_{xy}   1/2, 1/2, 1/2)'$	(15) $4^-$ $(0, 0, 1/2)$ $1/2, 0, z$ $(4_z^{-1}   1/2, 1/2, 1/2)'$	(16) $4^+$ $(0, 0, 1/2)$ $0, 1/2, z$ $(4_z   1/2, 1/2, 1/2)'$
(17) $4^-$ $(1/2, 0, 0)$ $x, 1/2, 0$ $(4_x^{-1}   1/2, 1/2, 1/2)'$	(18) $2'$ $(0, 1/2, 1/2)$ $1/4, y, y$ $(2_{yz}   1/2, 1/2, 1/2)'$	(19) $2'$ $1/4, y+1/2, \bar{y}$ $(2_{yz}   1/2, 1/2, 1/2)'$	(20) $4^+$ $(1/2, 0, 0)$ $x, 0, 1/2$ $(4_x   1/2, 1/2, 1/2)'$
(21) $4^+$ $(0, 1/2, 0)$ $1/2, y, 0$ $(4_y   1/2, 1/2, 1/2)'$	(22) $2'$ $(1/2, 0, 1/2)$ $x, 1/4, x$ $(2_{xz}   1/2, 1/2, 1/2)'$	(23) $4^-$ $(0, 1/2, 0)$ $0, y, 1/2$ $(4_y^{-1}   1/2, 1/2, 1/2)'$	(24) $2'$ $\bar{x}+1/2, 1/4, x$ $(2_{xz}   1/2, 1/2, 1/2)'$
(25) $\bar{1}$ $1/4, 1/4, 1/4$ $(\bar{1}   1/2, 1/2, 1/2)'$	(26) $n'$ $(1/2, 1/2, 0)$ $x, y, 1/4$ $(m_z   1/2, 1/2, 1/2)'$	(27) $n'$ $(1/2, 0, 1/2)$ $x, 1/4, z$ $(m_y   1/2, 1/2, 1/2)'$	(28) $n'$ $(0, 1/2, 1/2)$ $1/4, y, z$ $(m_x   1/2, 1/2, 1/2)'$
(29) $\bar{3}^+$ $x, x, x; 1/4, 1/4, 1/4$ $(\bar{3}_{xyz}   1/2, 1/2, 1/2)'$	(30) $\bar{3}^+$ $\bar{x}-1, x+1, \bar{x}; -1/4, 1/4, 3/4$ $(\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2)'$	(31) $\bar{3}^+$ $x, \bar{x}+1, \bar{x}; 1/4, 3/4, -1/4$ $(\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2)'$	(32) $\bar{3}^+$ $\bar{x}+1, \bar{x}, x; 3/4, -1/4, 1/4$ $(\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2)'$
(33) $\bar{3}^-$ $x, x, x; 1/4, 1/4, 1/4$ $(\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2)'$	(34) $\bar{3}^-$ $x+1, \bar{x}-1, \bar{x}; 1/4, -1/4, 3/4$ $(\bar{3}_{xyz}   1/2, 1/2, 1/2)'$	(35) $\bar{3}^-$ $\bar{x}, \bar{x}+1, x; -1/4, 3/4, 1/4$ $(\bar{3}_{xyz}   1/2, 1/2, 1/2)'$	(36) $\bar{3}^-$ $\bar{x}+1, x, \bar{x}; 3/4, 1/4, -1/4$ $(\bar{3}_{xyz}   1/2, 1/2, 1/2)'$
(37) $m$ $x, \bar{x}, z$ $(m_{xy}   0, 0, 0)$	(38) $m$ $x, x, z$ $(m_{xy}   0, 0, 0)$	(39) $\bar{4}^-$ $0, 0, z; 0, 0, 0$ $(\bar{4}_z^{-1}   0, 0, 0)$	(40) $\bar{4}^+$ $0, 0, z; 0, 0, 0$ $(\bar{4}_z   0, 0, 0)$
(41) $\bar{4}^-$ $x, 0, 0; 0, 0, 0$ $(\bar{4}_x^{-1}   0, 0, 0)$	(42) $m$ $x, y, \bar{y}$ $(m_{yz}   0, 0, 0)$	(43) $m$ $x, y, y$ $(m_{yz}   0, 0, 0)$	(44) $\bar{4}^+$ $x, 0, 0; 0, 0, 0$ $(\bar{4}_x   0, 0, 0)$
(45) $\bar{4}^+$ $0, y, 0; 0, 0, 0$ $(\bar{4}_y   0, 0, 0)$	(46) $m$ $\bar{x}, y, x$ $(m_{xz}   0, 0, 0)$	(47) $\bar{4}^-$ $0, y, 0; 0, 0, 0$ $(\bar{4}_y^{-1}   0, 0, 0)$	(48) $m$ $x, y, x$ $(m_{xz}   0, 0, 0)$

**Generators selected** (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ; (2); (3); (5); (13); (25).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

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(1) $x, y, z$ $[u, v, w]$	(2) $\bar{x}, \bar{y}, z$ $[\bar{u}, \bar{v}, w]$	(3) $\bar{x}, y, \bar{z}$ $[\bar{u}, v, \bar{w}]$	(4) $x, \bar{y}, \bar{z}$ $[u, \bar{v}, \bar{w}]$
(5) $z, x, y$ $[w, u, v]$	(6) $z, \bar{x}, \bar{y}$ $[w, \bar{u}, \bar{v}]$	(7) $\bar{z}, \bar{x}, y$ $[\bar{w}, \bar{u}, v]$	(8) $\bar{z}, x, \bar{y}$ $[\bar{w}, u, \bar{v}]$
(9) $y, z, x$ $[v, w, u]$	(10) $\bar{y}, z, \bar{x}$ $[\bar{v}, w, \bar{u}]$	(11) $y, \bar{z}, \bar{x}$ $[v, \bar{w}, \bar{u}]$	(12) $\bar{y}, \bar{z}, x$ $[\bar{v}, \bar{w}, u]$
(13) $y+1/2, x+1/2, \bar{z}+1/2$ $[\bar{v}, \bar{u}, w]$	(14) $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2$ $[v, u, w]$	(15) $y+1/2, \bar{x}+1/2, z+1/2$ $[\bar{v}, u, \bar{w}]$	(16) $\bar{y}+1/2, x+1/2, z+1/2$ $[v, \bar{u}, \bar{w}]$
(17) $x+1/2, z+1/2, \bar{y}+1/2$ $[\bar{u}, \bar{w}, v]$	(18) $\bar{x}+1/2, z+1/2, y+1/2$ $[u, \bar{w}, \bar{v}]$	(19) $\bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2$ $[u, w, v]$	(20) $x+1/2, \bar{z}+1/2, y+1/2$ $[\bar{u}, w, \bar{v}]$
(21) $z+1/2, y+1/2, \bar{x}+1/2$ $[\bar{w}, \bar{v}, u]$	(22) $z+1/2, \bar{y}+1/2, x+1/2$ $[\bar{w}, v, \bar{u}]$	(23) $\bar{z}+1/2, y+1/2, x+1/2$ $[w, \bar{v}, \bar{u}]$	(24) $\bar{z}+1/2, \bar{y}+1/2, \bar{x}+1/2$ $[w, v, u]$
(25) $\bar{x}+1/2, \bar{y}+1/2, \bar{z}+1/2$ $[\bar{u}, \bar{v}, \bar{w}]$	(26) $x+1/2, y+1/2, \bar{z}+1/2$ $[u, v, \bar{w}]$	(27) $x+1/2, \bar{y}+1/2, z+1/2$ $[u, \bar{v}, w]$	(28) $\bar{x}+1/2, y+1/2, z+1/2$ $[\bar{u}, v, w]$
(29) $\bar{z}+1/2, \bar{x}+1/2, \bar{y}+1/2$ $[\bar{w}, \bar{u}, \bar{v}]$	(30) $\bar{z}+1/2, x+1/2, y+1/2$ $[\bar{w}, u, v]$	(31) $z+1/2, x+1/2, \bar{y}+1/2$ $[w, u, \bar{v}]$	(32) $z+1/2, \bar{x}+1/2, y+1/2$ $[w, \bar{u}, v]$
(33) $\bar{y}+1/2, \bar{z}+1/2, \bar{x}+1/2$ $[\bar{v}, \bar{w}, \bar{u}]$	(34) $y+1/2, \bar{z}+1/2, x+1/2$ $[v, \bar{w}, u]$	(35) $\bar{y}+1/2, z+1/2, x+1/2$ $[\bar{v}, w, u]$	(36) $y+1/2, z+1/2, \bar{x}+1/2$ $[v, w, \bar{u}]$

(37) $\bar{y}, \bar{x}, z$ [v,u, $\bar{w}$ ]	(38) $y, x, z$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(39) $\bar{y}, x, \bar{z}$ [v, $\bar{u}, w$ ]	(40) $y, \bar{x}, \bar{z}$ [ $\bar{v}, u, w$ ]
(41) $\bar{x}, \bar{z}, y$ [u,w, $\bar{v}$ ]	(42) $x, \bar{z}, y$ [ $\bar{u}, w, v$ ]	(43) $x, z, y$ [ $\bar{u}, \bar{w}, \bar{v}$ ]	(44) $\bar{x}, z, y$ [u, $\bar{w}, v$ ]
(45) $\bar{z}, \bar{y}, x$ [w,v, $\bar{u}$ ]	(46) $\bar{z}, y, x$ [w, $\bar{v}, u$ ]	(47) $z, \bar{y}, x$ [ $\bar{w}, v, u$ ]	(48) $z, y, x$ [ $\bar{w}, \bar{v}, \bar{u}$ ]
24 k ..m			
$x, x, z$ [u, $\bar{u}, 0$ ]	$\bar{x}, \bar{x}, z$ [ $\bar{u}, u, 0$ ]	$\bar{x}, x, \bar{z}$ [ $\bar{u}, \bar{u}, 0$ ]	$x, \bar{x}, \bar{z}$ [u,u,0]
$z, x, x$ [0,u, $\bar{u}$ ]	$z, \bar{x}, \bar{x}$ [0, $\bar{u}, u$ ]	$\bar{z}, \bar{x}, x$ [0, $\bar{u}, \bar{u}$ ]	$\bar{z}, x, \bar{x}$ [0,u,u]
$x, z, x$ [ $\bar{u}, 0, u$ ]	$\bar{x}, z, \bar{x}$ [u,0, $\bar{u}$ ]	$x, \bar{z}, \bar{x}$ [ $\bar{u}, 0, \bar{u}$ ]	$\bar{x}, \bar{z}, x$ [u,0,u]
$x+1/2, x+1/2, \bar{z}+1/2$ [u, $\bar{u}, 0$ ]	$\bar{x}+1/2, \bar{x}+1/2, \bar{z}+1/2$ [ $\bar{u}, u, 0$ ]	$x+1/2, \bar{x}+1/2, z+1/2$ [ $\bar{u}, \bar{u}, 0$ ]	$\bar{x}+1/2, x+1/2, z+1/2$ [u,u,0]
$x+1/2, z+1/2, \bar{x}+1/2$ [ $\bar{u}, 0, \bar{u}$ ]	$\bar{x}+1/2, z+1/2, x+1/2$ [u,0,u]	$\bar{x}+1/2, \bar{z}+1/2, \bar{x}+1/2$ [ $\bar{u}, 0, u$ ]	$x+1/2, \bar{z}+1/2, x+1/2$ [u,0, $\bar{u}$ ]
$z+1/2, x+1/2, \bar{x}+1/2$ [0,u,u]	$z+1/2, \bar{x}+1/2, x+1/2$ [0, $\bar{u}, \bar{u}$ ]	$\bar{z}+1/2, x+1/2, x+1/2$ [0,u, $\bar{u}$ ]	$\bar{z}+1/2, \bar{x}+1/2, \bar{x}+1/2$ [0, $\bar{u}, u$ ]
24 j ..2'			
$1/4, y, y+1/2$ [u,v, $\bar{v}$ ]	$3/4, \bar{y}, y+1/2$ [ $\bar{u}, \bar{v}, \bar{v}$ ]	$3/4, y, \bar{y}+1/2$ [ $\bar{u}, v, v$ ]	$1/4, \bar{y}, \bar{y}+1/2$ [u, $\bar{v}, v$ ]
$y+1/2, 1/4, y$ [ $\bar{v}, u, v$ ]	$y+1/2, 3/4, \bar{y}$ [ $\bar{v}, \bar{u}, \bar{v}$ ]	$\bar{y}+1/2, 3/4, y$ [v, $\bar{u}, v$ ]	$\bar{y}+1/2, 1/4, \bar{y}$ [v,u, $\bar{v}$ ]
$y, y+1/2, 1/4$ [v, $\bar{v}, u$ ]	$\bar{y}, y+1/2, 3/4$ [ $\bar{v}, \bar{v}, \bar{u}$ ]	$y, \bar{y}+1/2, 3/4$ [v,v, $\bar{u}$ ]	$\bar{y}, \bar{y}+1/2, 1/4$ [ $\bar{v}, v, u$ ]
$1/4, \bar{y}+1/2, \bar{y}$ [ $\bar{u}, \bar{v}, \bar{v}$ ]	$3/4, y+1/2, \bar{y}$ [u,v,v]	$3/4, \bar{y}+1/2, y$ [u, $\bar{v}, \bar{v}$ ]	$1/4, y+1/2, y$ [ $\bar{u}, v, \bar{v}$ ]
$\bar{y}, 1/4, \bar{y}+1/2$ [v, $\bar{u}, \bar{v}$ ]	$\bar{y}, 3/4, y+1/2$ [v,u,v]	$y, 3/4, \bar{y}+1/2$ [ $\bar{v}, u, \bar{v}$ ]	$y, 1/4, y+1/2$ [ $\bar{v}, \bar{u}, v$ ]
$\bar{y}+1/2, \bar{y}, 1/4$ [ $\bar{v}, v, \bar{u}$ ]	$y+1/2, \bar{y}, 3/4$ [v,v,u]	$\bar{y}+1/2, y, 3/4$ [ $\bar{v}, \bar{v}, u$ ]	$y+1/2, y, 1/4$ [v, $\bar{v}, \bar{u}$ ]
24 i ..2'			
$1/4, y, \bar{y}+1/2$ [u,v,v]	$3/4, \bar{y}, \bar{y}+1/2$ [ $\bar{u}, \bar{v}, \bar{v}$ ]	$3/4, y, y+1/2$ [ $\bar{u}, v, \bar{v}$ ]	$1/4, \bar{y}, y+1/2$ [u, $\bar{v}, \bar{v}$ ]
$\bar{y}+1/2, 1/4, y$ [v,u,v]	$\bar{y}+1/2, 3/4, \bar{y}$ [v, $\bar{u}, \bar{v}$ ]	$y+1/2, 3/4, y$ [ $\bar{v}, \bar{u}, v$ ]	$y+1/2, 1/4, \bar{y}$ [ $\bar{v}, u, \bar{v}$ ]
$y, \bar{y}+1/2, 1/4$ [v,v,u]	$\bar{y}, \bar{y}+1/2, 3/4$ [ $\bar{v}, v, \bar{u}$ ]	$y, y+1/2, 3/4$ [v, $\bar{v}, \bar{u}$ ]	$\bar{y}, y+1/2, 1/4$ [ $\bar{v}, \bar{v}, u$ ]
$1/4, \bar{y}+1/2, y$ [ $\bar{u}, \bar{v}, \bar{v}$ ]	$3/4, y+1/2, y$ [u,v, $\bar{v}$ ]	$3/4, \bar{y}+1/2, \bar{y}$ [u, $\bar{v}, v$ ]	$1/4, y+1/2, \bar{y}$ [ $\bar{u}, v, v$ ]
$y, 1/4, \bar{y}+1/2$ [ $\bar{v}, \bar{u}, \bar{v}$ ]	$y, 3/4, y+1/2$ [ $\bar{v}, u, v$ ]	$\bar{y}, 3/4, \bar{y}+1/2$ [v,u, $\bar{v}$ ]	$\bar{y}, 1/4, y+1/2$ [v, $\bar{u}, v$ ]
$\bar{y}+1/2, y, 1/4$ [ $\bar{v}, \bar{v}, \bar{u}$ ]	$y+1/2, y, 3/4$ [v, $\bar{v}, u$ ]	$\bar{y}+1/2, \bar{y}, 3/4$ [ $\bar{v}, v, u$ ]	$y+1/2, \bar{y}, 1/4$ [v,v, $\bar{u}$ ]
24 h 2..			
$x, 0, 1/2$ [u,0,0]	$\bar{x}, 0, 1/2$ [ $\bar{u}, 0, 0$ ]	$1/2, x, 0$ [0,u,0]	$1/2, \bar{x}, 0$ [0, $\bar{u}, 0$ ]
$0, 1/2, x$ [0,0,u]	$0, 1/2, \bar{x}$ [0,0, $\bar{u}$ ]	$1/2, x+1/2, 0$ [0, $\bar{u}, 0$ ]	$1/2, \bar{x}+1/2, 0$ [0,u,0]
$x+1/2, 0, 1/2$ [ $\bar{u}, 0, 0$ ]	$\bar{x}+1/2, 0, 1/2$ [u,0,0]	$0, 1/2, \bar{x}+1/2$ [0,0,u]	$0, 1/2, x+1/2$ [0,0, $\bar{u}$ ]

Continued			224.2.1612		Pn $\bar{3}m1'$	
			$\bar{x}+1/2, 1/2, 0$ [ $\bar{u}, 0, 0$ ]	$x+1/2, 1/2, 0$ [ $u, 0, 0$ ]	$0, \bar{x}+1/2, 1/2$ [ $0, \bar{u}, 0$ ]	$0, x+1/2, 1/2$ [ $0, u, 0$ ]
			$1/2, 0, \bar{x}+1/2$ [ $0, 0, \bar{u}$ ]	$1/2, 0, x+1/2$ [ $0, 0, u$ ]	$0, \bar{x}, 1/2$ [ $0, u, 0$ ]	$0, x, 1/2$ [ $0, \bar{u}, 0$ ]
			$\bar{x}, 1/2, 0$ [ $u, 0, 0$ ]	$x, 1/2, 0$ [ $\bar{u}, 0, 0$ ]	$1/2, 0, x$ [ $0, 0, \bar{u}$ ]	$1/2, 0, \bar{x}$ [ $0, 0, u$ ]
12	g	2.mm	$x, 0, 0$ [ $0, 0, 0$ ]	$\bar{x}, 0, 0$ [ $0, 0, 0$ ]	$0, x, 0$ [ $0, 0, 0$ ]	$0, \bar{x}, 0$ [ $0, 0, 0$ ]
			$0, 0, x$ [ $0, 0, 0$ ]	$0, 0, \bar{x}$ [ $0, 0, 0$ ]	$1/2, x+1/2, 1/2$ [ $0, 0, 0$ ]	$1/2, \bar{x}+1/2, 1/2$ [ $0, 0, 0$ ]
			$x+1/2, 1/2, 1/2$ [ $0, 0, 0$ ]	$\bar{x}+1/2, 1/2, 1/2$ [ $0, 0, 0$ ]	$1/2, 1/2, \bar{x}+1/2$ [ $0, 0, 0$ ]	$1/2, 1/2, x+1/2$ [ $0, 0, 0$ ]
12	f	2.2'2'	$1/4, 0, 1/2$ [ $u, 0, 0$ ]	$3/4, 0, 1/2$ [ $\bar{u}, 0, 0$ ]	$1/2, 1/4, 0$ [ $0, u, 0$ ]	
			$1/2, 3/4, 0$ [ $0, \bar{u}, 0$ ]	$0, 1/2, 1/4$ [ $0, 0, u$ ]	$0, 1/2, 3/4$ [ $0, 0, \bar{u}$ ]	
			$1/4, 1/2, 0$ [ $\bar{u}, 0, 0$ ]	$3/4, 1/2, 0$ [ $u, 0, 0$ ]	$0, 1/4, 1/2$ [ $0, \bar{u}, 0$ ]	
			$0, 3/4, 1/2$ [ $0, u, 0$ ]	$1/2, 0, 1/4$ [ $0, 0, \bar{u}$ ]	$1/2, 0, 3/4$ [ $0, 0, u$ ]	
8	e	.3m	$x, x, x$ [ $0, 0, 0$ ]	$\bar{x}, \bar{x}, x$ [ $0, 0, 0$ ]		
			$\bar{x}, x, \bar{x}$ [ $0, 0, 0$ ]	$x, \bar{x}, \bar{x}$ [ $0, 0, 0$ ]		
			$x+1/2, x+1/2, \bar{x}+1/2$ [ $0, 0, 0$ ]	$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2$ [ $0, 0, 0$ ]		
			$x+1/2, \bar{x}+1/2, x+1/2$ [ $0, 0, 0$ ]	$\bar{x}+1/2, x+1/2, x+1/2$ [ $0, 0, 0$ ]		
6	d	$\bar{4}2.m$	$0, 1/2, 1/2$ [ $0, 0, 0$ ]	$1/2, 0, 1/2$ [ $0, 0, 0$ ]	$1/2, 1/2, 0$ [ $0, 0, 0$ ]	
			$0, 1/2, 0$ [ $0, 0, 0$ ]	$1/2, 0, 0$ [ $0, 0, 0$ ]	$0, 0, 1/2$ [ $0, 0, 0$ ]	
4	c	$\bar{3}m$	$3/4, 3/4, 3/4$ [ $0, 0, 0$ ]	$1/4, 1/4, 3/4$ [ $0, 0, 0$ ]	$1/4, 3/4, 1/4$ [ $0, 0, 0$ ]	$3/4, 1/4, 1/4$ [ $0, 0, 0$ ]
4	b	$\bar{3}m$	$1/4, 1/4, 1/4$ [ $0, 0, 0$ ]	$3/4, 3/4, 1/4$ [ $0, 0, 0$ ]	$3/4, 1/4, 3/4$ [ $0, 0, 0$ ]	$1/4, 3/4, 3/4$ [ $0, 0, 0$ ]
2	a	$\bar{4}3m$	$0, 0, 0$ [ $0, 0, 0$ ]	$1/2, 1/2, 1/2$ [ $0, 0, 0$ ]		

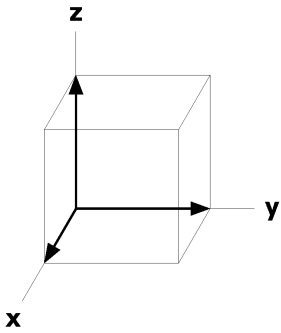
### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p4'mm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0, 0, z$

Along  $[1, 1, 1]$   $p6mm$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

Along  $[1, 1, 0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 1/4$

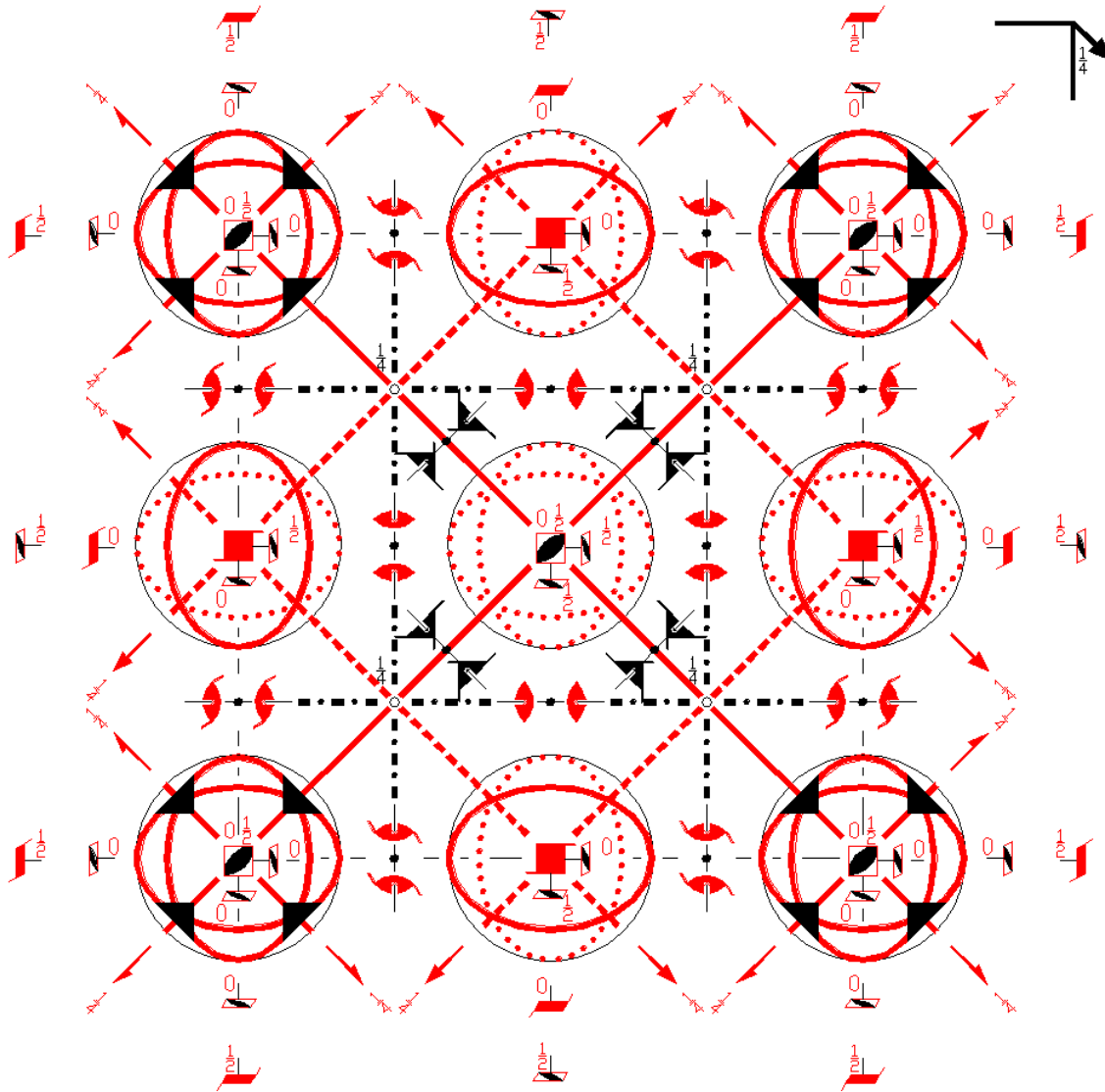




$Pn\bar{3}m'$   
224.4.1614

$m\bar{3}m'$   
 $P4_2'/n\bar{3}2'/m'$

Cubic



**Origin** at  $\bar{4}'3m'$ , at  $-1/4, -1/4, -1/4$  from center ( $\bar{3}m'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $-1/4 \leq z \leq 1/4$ ;  $y \leq x$ ;  $\max(x-1/2, -y) \leq z \leq \min(1/2-x, y)$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/4,1/4,1/4$   $1/4,1/4,-1/4$

**Symmetry Operations**

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)              |

(13) 2' (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(14) 2' x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(15) 4' ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(16) 4+ ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)'
(17) 4' ' (1/2,0,0) x,1/2,0 (4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(18) 2' (0,1/2,1/2) 1/4,y,y (2 <sub>yz</sub>  1/2,1/2,1/2)'	(19) 2' 1/4,y+1/2, $\bar{y}$ (2 <sub>yz</sub>  1/2,1/2,1/2)'	(20) 4+ ' (1/2,0,0) x,0,1/2 (4 <sub>x</sub>  1/2,1/2,1/2)'
(21) 4+ ' (0,1/2,0) 1/2,y,0 (4 <sub>y</sub>  1/2,1/2,1/2)'	(22) 2' (1/2,0,1/2) x,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)'	(23) 4' ' (0,1/2,0) 0,y,1/2 (4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(24) 2' $\bar{x}$ +1/2,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)'
(25) $\bar{1}$ 1/4,1/4,1/4 ( $\bar{1}$  1/2,1/2,1/2)	(26) n (1/2,1/2,0) x,y,1/4 (m <sub>z</sub>  1/2,1/2,1/2)	(27) n (1/2,0,1/2) x,1/4,z (m <sub>y</sub>  1/2,1/2,1/2)	(28) n (0,1/2,1/2) 1/4,y,z (m <sub>x</sub>  1/2,1/2,1/2)
(29) $\bar{3}^+$ x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}$  1/2,1/2,1/2)	(30) $\bar{3}^+$ $\bar{x}$ -1,x+1, $\bar{x}$ ; -1/4,1/4,3/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,1/2,1/2)	(31) $\bar{3}^+$ x, $\bar{x}$ +1, $\bar{x}$ ; 1/4,3/4,-1/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,1/2,1/2)	(32) $\bar{3}^+$ $\bar{x}$ +1, $\bar{x}$ ,x; 3/4,-1/4,1/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,1/2,1/2)
(33) $\bar{3}^-$ x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,1/2,1/2)	(34) $\bar{3}^-$ x+1, $\bar{x}$ -1, $\bar{x}$ ; 1/4,-1/4,3/4 ( $\bar{3}_{xyz}$  1/2,1/2,1/2)	(35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1,x; -1/4,3/4,1/4 ( $\bar{3}_{xyz}$  1/2,1/2,1/2)	(36) $\bar{3}^-$ $\bar{x}$ +1,x, $\bar{x}$ ; 3/4,1/4,-1/4 ( $\bar{3}_{xyz}$  1/2,1/2,1/2)
(37) m' x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)'	(38) m' x,x,z (m <sub>xy</sub>  0,0,0)'	(39) $\bar{4}^-$ ' 0,0,z; 0,0,0 ( $\bar{4}_z$ <sup>-1</sup>  0,0,0)'	(40) $\bar{4}^+$ ' 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'
(41) $\bar{4}^-$ ' x,0,0; 0,0,0 ( $\bar{4}_x$ <sup>-1</sup>  0,0,0)'	(42) m' x,y, $\bar{y}$ (m <sub>yz</sub>  0,0,0)'	(43) m' x,y,y (m <sub>yz</sub>  0,0,0)'	(44) $\bar{4}^+$ ' x,0,0; 0,0,0 ( $\bar{4}_x$  0,0,0)'
(45) $\bar{4}^+$ ' 0,y,0; 0,0,0 ( $\bar{4}_y$  0,0,0)'	(46) m' $\bar{x}$ ,y,x (m <sub>xz</sub>  0,0,0)'	(47) $\bar{4}^-$ ' 0,y,0; 0,0,0 ( $\bar{4}_y$ <sup>-1</sup>  0,0,0)'	(48) m' x,y,x (m <sub>xz</sub>  0,0,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

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(1) x,y,z [u,v,w]	(2) $\bar{x}$ , $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w]	(3) $\bar{x}$ ,y, $\bar{z}$ [ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x, $\bar{y}$ , $\bar{z}$ [u, $\bar{v}$ , $\bar{w}$ ]
(5) z,x,y [w,u,v]	(6) z, $\bar{x}$ , $\bar{y}$ [w, $\bar{u}$ , $\bar{v}$ ]	(7) $\bar{z}$ , $\bar{x}$ ,y [ $\bar{w}$ , $\bar{u}$ ,v]	(8) $\bar{z}$ ,x,y [ $\bar{w}$ ,u, $\bar{v}$ ]
(9) y,z,x [v,w,u]	(10) $\bar{y}$ ,z, $\bar{x}$ [ $\bar{v}$ ,w, $\bar{u}$ ]	(11) y, $\bar{z}$ , $\bar{x}$ [v, $\bar{w}$ , $\bar{u}$ ]	(12) $\bar{y}$ , $\bar{z}$ ,x [ $\bar{v}$ , $\bar{w}$ ,u]
(13) y+1/2,x+1/2, $\bar{z}$ +1/2 [ $\bar{v}$ , $\bar{u}$ ,w]	(14) $\bar{y}$ +1/2, $\bar{x}$ +1/2, $\bar{z}$ +1/2 [v,u,w]	(15) y+1/2, $\bar{x}$ +1/2,z+1/2 [ $\bar{v}$ ,u, $\bar{w}$ ]	(16) $\bar{y}$ +1/2,x+1/2,z+1/2 [v, $\bar{u}$ , $\bar{w}$ ]
(17) x+1/2,z+1/2, $\bar{y}$ +1/2 [ $\bar{u}$ , $\bar{w}$ ,v]	(18) $\bar{x}$ +1/2,z+1/2,y+1/2 [u, $\bar{w}$ , $\bar{v}$ ]	(19) $\bar{x}$ +1/2, $\bar{z}$ +1/2, $\bar{y}$ +1/2 [u,w,v]	(20) x+1/2, $\bar{z}$ +1/2,y+1/2 [ $\bar{u}$ ,w, $\bar{v}$ ]
(21) z+1/2,y+1/2, $\bar{x}$ +1/2 [ $\bar{w}$ , $\bar{v}$ ,u]	(22) z+1/2, $\bar{y}$ +1/2,x+1/2 [ $\bar{w}$ ,v, $\bar{u}$ ]	(23) $\bar{z}$ +1/2,y+1/2,x+1/2 [w, $\bar{v}$ , $\bar{u}$ ]	(24) $\bar{z}$ +1/2, $\bar{y}$ +1/2, $\bar{x}$ +1/2 [w,v,u]
(25) $\bar{x}$ +1/2, $\bar{y}$ +1/2, $\bar{z}$ +1/2 [u,v,w]	(26) x+1/2,y+1/2, $\bar{z}$ +1/2 [ $\bar{u}$ , $\bar{v}$ ,w]	(27) x+1/2, $\bar{y}$ +1/2,z+1/2 [ $\bar{u}$ ,v, $\bar{w}$ ]	(28) $\bar{x}$ +1/2,y+1/2,z+1/2 [u, $\bar{v}$ , $\bar{w}$ ]
(29) $\bar{z}$ +1/2, $\bar{x}$ +1/2, $\bar{y}$ +1/2 [w,u,v]	(30) $\bar{z}$ +1/2,x+1/2,y+1/2 [w, $\bar{u}$ , $\bar{v}$ ]	(31) z+1/2,x+1/2, $\bar{y}$ +1/2 [ $\bar{w}$ , $\bar{u}$ ,v]	(32) z+1/2, $\bar{x}$ +1/2,y+1/2 [ $\bar{w}$ ,u, $\bar{v}$ ]
(33) $\bar{y}$ +1/2, $\bar{z}$ +1/2, $\bar{x}$ +1/2 [v,w,u]	(34) y+1/2, $\bar{z}$ +1/2,x+1/2 [ $\bar{v}$ ,w, $\bar{u}$ ]	(35) $\bar{y}$ +1/2,z+1/2,x+1/2 [v, $\bar{w}$ , $\bar{u}$ ]	(36) y+1/2,z+1/2, $\bar{x}$ +1/2 [ $\bar{v}$ , $\bar{w}$ ,u]

(37) $\bar{y}, \bar{x}, z$ [ $\bar{v}, \bar{u}, w$ ]	(38) $y, x, z$ [ $v, u, w$ ]	(39) $\bar{y}, x, \bar{z}$ [ $\bar{v}, u, \bar{w}$ ]	(40) $y, \bar{x}, \bar{z}$ [ $v, \bar{u}, \bar{w}$ ]
(41) $\bar{x}, \bar{z}, y$ [ $\bar{u}, \bar{w}, v$ ]	(42) $x, \bar{z}, y$ [ $u, \bar{w}, v$ ]	(43) $x, z, y$ [ $u, w, v$ ]	(44) $\bar{x}, z, y$ [ $\bar{u}, w, \bar{v}$ ]
(45) $\bar{z}, \bar{y}, x$ [ $\bar{w}, \bar{v}, u$ ]	(46) $\bar{z}, y, x$ [ $w, v, u$ ]	(47) $z, \bar{y}, x$ [ $w, \bar{v}, u$ ]	(48) $z, y, x$ [ $w, v, u$ ]
24 k ..m'			
$x, x, z$ [ $u, u, w$ ]	$\bar{x}, \bar{x}, z$ [ $\bar{u}, \bar{u}, w$ ]	$\bar{x}, x, \bar{z}$ [ $\bar{u}, u, \bar{w}$ ]	$x, \bar{x}, \bar{z}$ [ $u, \bar{u}, \bar{w}$ ]
$z, x, x$ [ $w, u, u$ ]	$z, \bar{x}, \bar{x}$ [ $w, \bar{u}, \bar{u}$ ]	$\bar{z}, \bar{x}, x$ [ $\bar{w}, \bar{u}, u$ ]	$\bar{z}, x, \bar{x}$ [ $\bar{w}, u, \bar{u}$ ]
$x, z, x$ [ $u, w, u$ ]	$\bar{x}, z, \bar{x}$ [ $\bar{u}, w, \bar{u}$ ]	$x, \bar{z}, \bar{x}$ [ $u, \bar{w}, \bar{u}$ ]	$\bar{x}, \bar{z}, x$ [ $\bar{u}, \bar{w}, u$ ]
$x+1/2, x+1/2, \bar{z}+1/2$ [ $\bar{u}, \bar{u}, w$ ]	$\bar{x}+1/2, \bar{x}+1/2, \bar{z}+1/2$ [ $u, u, w$ ]	$x+1/2, \bar{x}+1/2, z+1/2$ [ $\bar{u}, u, \bar{w}$ ]	$\bar{x}+1/2, x+1/2, z+1/2$ [ $u, \bar{u}, \bar{w}$ ]
$x+1/2, z+1/2, \bar{x}+1/2$ [ $\bar{u}, \bar{w}, u$ ]	$\bar{x}+1/2, z+1/2, x+1/2$ [ $u, \bar{w}, \bar{u}$ ]	$\bar{x}+1/2, \bar{z}+1/2, \bar{x}+1/2$ [ $u, w, u$ ]	$x+1/2, \bar{z}+1/2, x+1/2$ [ $\bar{u}, w, \bar{u}$ ]
$z+1/2, x+1/2, \bar{x}+1/2$ [ $\bar{w}, \bar{u}, u$ ]	$z+1/2, \bar{x}+1/2, x+1/2$ [ $w, u, \bar{u}$ ]	$\bar{z}+1/2, x+1/2, x+1/2$ [ $w, \bar{u}, \bar{u}$ ]	$\bar{z}+1/2, \bar{x}+1/2, \bar{x}+1/2$ [ $w, u, u$ ]
24 j ..2'			
$1/4, y, y+1/2$ [ $u, v, \bar{v}$ ]	$3/4, \bar{y}, y+1/2$ [ $\bar{u}, \bar{v}, \bar{v}$ ]	$3/4, y, \bar{y}+1/2$ [ $\bar{u}, v, v$ ]	$1/4, \bar{y}, \bar{y}+1/2$ [ $u, \bar{v}, v$ ]
$y+1/2, 1/4, y$ [ $\bar{v}, u, v$ ]	$y+1/2, 3/4, \bar{y}$ [ $\bar{v}, \bar{u}, \bar{v}$ ]	$\bar{y}+1/2, 3/4, y$ [ $v, \bar{u}, v$ ]	$\bar{y}+1/2, 1/4, \bar{y}$ [ $v, u, \bar{v}$ ]
$y, y+1/2, 1/4$ [ $v, \bar{v}, u$ ]	$\bar{y}, y+1/2, 3/4$ [ $\bar{v}, \bar{v}, \bar{u}$ ]	$y, \bar{y}+1/2, 3/4$ [ $v, v, \bar{u}$ ]	$\bar{y}, \bar{y}+1/2, 1/4$ [ $\bar{v}, v, u$ ]
$1/4, \bar{y}+1/2, \bar{y}$ [ $u, v, \bar{v}$ ]	$3/4, y+1/2, \bar{y}$ [ $\bar{u}, \bar{v}, \bar{v}$ ]	$3/4, \bar{y}+1/2, \bar{y}$ [ $\bar{u}, v, v$ ]	$1/4, y+1/2, y$ [ $u, \bar{v}, v$ ]
$\bar{y}, 1/4, \bar{y}+1/2$ [ $\bar{v}, u, v$ ]	$\bar{y}, 3/4, y+1/2$ [ $\bar{v}, \bar{u}, \bar{v}$ ]	$y, 3/4, \bar{y}+1/2$ [ $v, \bar{u}, v$ ]	$y, 1/4, y+1/2$ [ $v, u, \bar{v}$ ]
$\bar{y}+1/2, \bar{y}, 1/4$ [ $v, \bar{v}, u$ ]	$y+1/2, \bar{y}, 3/4$ [ $\bar{v}, \bar{v}, \bar{u}$ ]	$\bar{y}+1/2, y, 3/4$ [ $v, v, \bar{u}$ ]	$y+1/2, y, 1/4$ [ $\bar{v}, v, u$ ]
24 i ..2'			
$1/4, y, \bar{y}+1/2$ [ $u, v, v$ ]	$3/4, \bar{y}, \bar{y}+1/2$ [ $\bar{u}, \bar{v}, v$ ]	$3/4, y, y+1/2$ [ $\bar{u}, v, \bar{v}$ ]	$1/4, \bar{y}, y+1/2$ [ $u, \bar{v}, \bar{v}$ ]
$\bar{y}+1/2, 1/4, y$ [ $v, u, v$ ]	$\bar{y}+1/2, 3/4, \bar{y}$ [ $v, \bar{u}, \bar{v}$ ]	$y+1/2, 3/4, y$ [ $\bar{v}, \bar{u}, v$ ]	$y+1/2, 1/4, \bar{y}$ [ $\bar{v}, u, \bar{v}$ ]
$y, \bar{y}+1/2, 1/4$ [ $v, v, u$ ]	$\bar{y}, \bar{y}+1/2, 3/4$ [ $\bar{v}, v, \bar{u}$ ]	$y, y+1/2, 3/4$ [ $v, \bar{v}, \bar{u}$ ]	$\bar{y}, y+1/2, 1/4$ [ $\bar{v}, \bar{v}, u$ ]
$1/4, \bar{y}+1/2, y$ [ $u, v, v$ ]	$3/4, y+1/2, y$ [ $\bar{u}, \bar{v}, v$ ]	$3/4, \bar{y}+1/2, \bar{y}$ [ $\bar{u}, v, \bar{v}$ ]	$1/4, y+1/2, \bar{y}$ [ $u, \bar{v}, \bar{v}$ ]
$y, 1/4, \bar{y}+1/2$ [ $v, u, v$ ]	$y, 3/4, y+1/2$ [ $v, \bar{u}, \bar{v}$ ]	$\bar{y}, 3/4, \bar{y}+1/2$ [ $\bar{v}, \bar{u}, v$ ]	$\bar{y}, 1/4, y+1/2$ [ $\bar{v}, u, \bar{v}$ ]
$\bar{y}+1/2, y, 1/4$ [ $v, v, u$ ]	$y+1/2, y, 3/4$ [ $\bar{v}, v, \bar{u}$ ]	$\bar{y}+1/2, \bar{y}, 3/4$ [ $v, \bar{v}, \bar{u}$ ]	$y+1/2, \bar{y}, 1/4$ [ $\bar{v}, \bar{v}, u$ ]
24 h 2..			
$x, 0, 1/2$ [ $u, 0, 0$ ]	$\bar{x}, 0, 1/2$ [ $\bar{u}, 0, 0$ ]	$1/2, x, 0$ [ $0, u, 0$ ]	$1/2, \bar{x}, 0$ [ $0, \bar{u}, 0$ ]
$0, 1/2, x$ [ $0, 0, u$ ]	$0, 1/2, \bar{x}$ [ $0, 0, \bar{u}$ ]	$1/2, x+1/2, 0$ [ $0, \bar{u}, 0$ ]	$1/2, \bar{x}+1/2, 0$ [ $0, u, 0$ ]
$x+1/2, 0, 1/2$ [ $\bar{u}, 0, 0$ ]	$\bar{x}+1/2, 0, 1/2$ [ $u, 0, 0$ ]	$0, 1/2, \bar{x}+1/2$ [ $0, 0, u$ ]	$0, 1/2, x+1/2$ [ $0, 0, \bar{u}$ ]

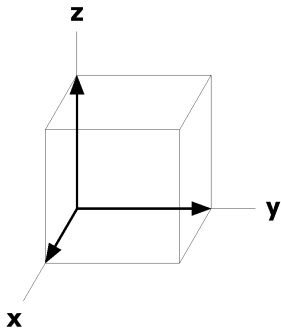
Continued		224.2.1612		Pn $\bar{3}$ m1'		
		$\bar{x}+1/2, 1/2, 0$ [u,0,0]	$x+1/2, 1/2, 0$ [ $\bar{u}$ ,0,0]	$0, \bar{x}+1/2, 1/2$ [0,u,0]	$0, x+1/2, 1/2$ [0, $\bar{u}$ ,0]	
		$1/2, 0, \bar{x}+1/2$ [0,0,u]	$1/2, 0, x+1/2$ [0,0, $\bar{u}$ ]	$0, \bar{x}, 1/2$ [0, $\bar{u}$ ,0]	$0, x, 1/2$ [0,u,0]	
		$\bar{x}, 1/2, 0$ [ $\bar{u}$ ,0,0]	$x, 1/2, 0$ [u,0,0]	$1/2, 0, x$ [0,0,u]	$1/2, 0, \bar{x}$ [0,0, $\bar{u}$ ]	
12	g	2.m'm'	$x, 0, 0$ [u,0,0]	$\bar{x}, 0, 0$ [ $\bar{u}$ ,0,0]	$0, x, 0$ [0,u,0]	$0, \bar{x}, 0$ [0, $\bar{u}$ ,0]
			$0, 0, x$ [0,0,u]	$0, 0, \bar{x}$ [0,0, $\bar{u}$ ]	$1/2, x+1/2, 1/2$ [0, $\bar{u}$ ,0]	$1/2, \bar{x}+1/2, 1/2$ [0,u,0]
			$x+1/2, 1/2, 1/2$ [ $\bar{u}$ ,0,0]	$\bar{x}+1/2, 1/2, 1/2$ [u,0,0]	$1/2, 1/2, \bar{x}+1/2$ [0,0,u]	$1/2, 1/2, x+1/2$ [0,0, $\bar{u}$ ]
12	f	2.2'2'	$1/4, 0, 1/2$ [u,0,0]	$3/4, 0, 1/2$ [ $\bar{u}$ ,0,0]	$1/2, 1/4, 0$ [0,u,0]	
			$1/2, 3/4, 0$ [0, $\bar{u}$ ,0]	$0, 1/2, 1/4$ [0,0,u]	$0, 1/2, 3/4$ [0,0, $\bar{u}$ ]	
			$1/4, 1/2, 0$ [u,0,0]	$3/4, 1/2, 0$ [ $\bar{u}$ ,0,0]	$0, 1/4, 1/2$ [0,u,0]	
			$0, 3/4, 1/2$ [0, $\bar{u}$ ,0]	$1/2, 0, 1/4$ [0,0,u]	$1/2, 0, 3/4$ [0,0, $\bar{u}$ ]	
8	e	.3m'	$x, x, x$ [u,u,u]	$\bar{x}, \bar{x}, x$ [ $\bar{u}$ , $\bar{u}$ ,u]		
			$\bar{x}, x, \bar{x}$ [ $\bar{u}$ ,u, $\bar{u}$ ]	$x, \bar{x}, \bar{x}$ [u, $\bar{u}$ , $\bar{u}$ ]		
			$x+1/2, x+1/2, \bar{x}+1/2$ [ $\bar{u}$ , $\bar{u}$ ,u]	$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2$ [u,u,u]		
			$x+1/2, \bar{x}+1/2, x+1/2$ [ $\bar{u}$ ,u, $\bar{u}$ ]	$\bar{x}+1/2, x+1/2, x+1/2$ [u, $\bar{u}$ , $\bar{u}$ ]		
6	d	$\bar{4}'2.m'$	$0, 1/2, 1/2$ [0,0,0]	$1/2, 0, 1/2$ [0,0,0]	$1/2, 1/2, 0$ [0,0,0]	
			$0, 1/2, 0$ [0,0,0]	$1/2, 0, 0$ [0,0,0]	$0, 0, 1/2$ [0,0,0]	
4	c	$\bar{3}m'$	$3/4, 3/4, 3/4$ [u,u,u]	$1/4, 1/4, 3/4$ [ $\bar{u}$ , $\bar{u}$ ,u]	$1/4, 3/4, 1/4$ [ $\bar{u}$ ,u, $\bar{u}$ ]	$3/4, 1/4, 1/4$ [u, $\bar{u}$ , $\bar{u}$ ]
4	b	$\bar{3}m'$	$1/4, 1/4, 1/4$ [u,u,u]	$3/4, 3/4, 1/4$ [ $\bar{u}$ , $\bar{u}$ ,u]	$3/4, 1/4, 3/4$ [ $\bar{u}$ ,u, $\bar{u}$ ]	$1/4, 3/4, 3/4$ [u, $\bar{u}$ , $\bar{u}$ ]
2	a	$\bar{4}'3m'$	$0, 0, 0$ [0,0,0]	$1/2, 1/2, 1/2$ [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,1,1] p6'mm'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = -(-\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/4



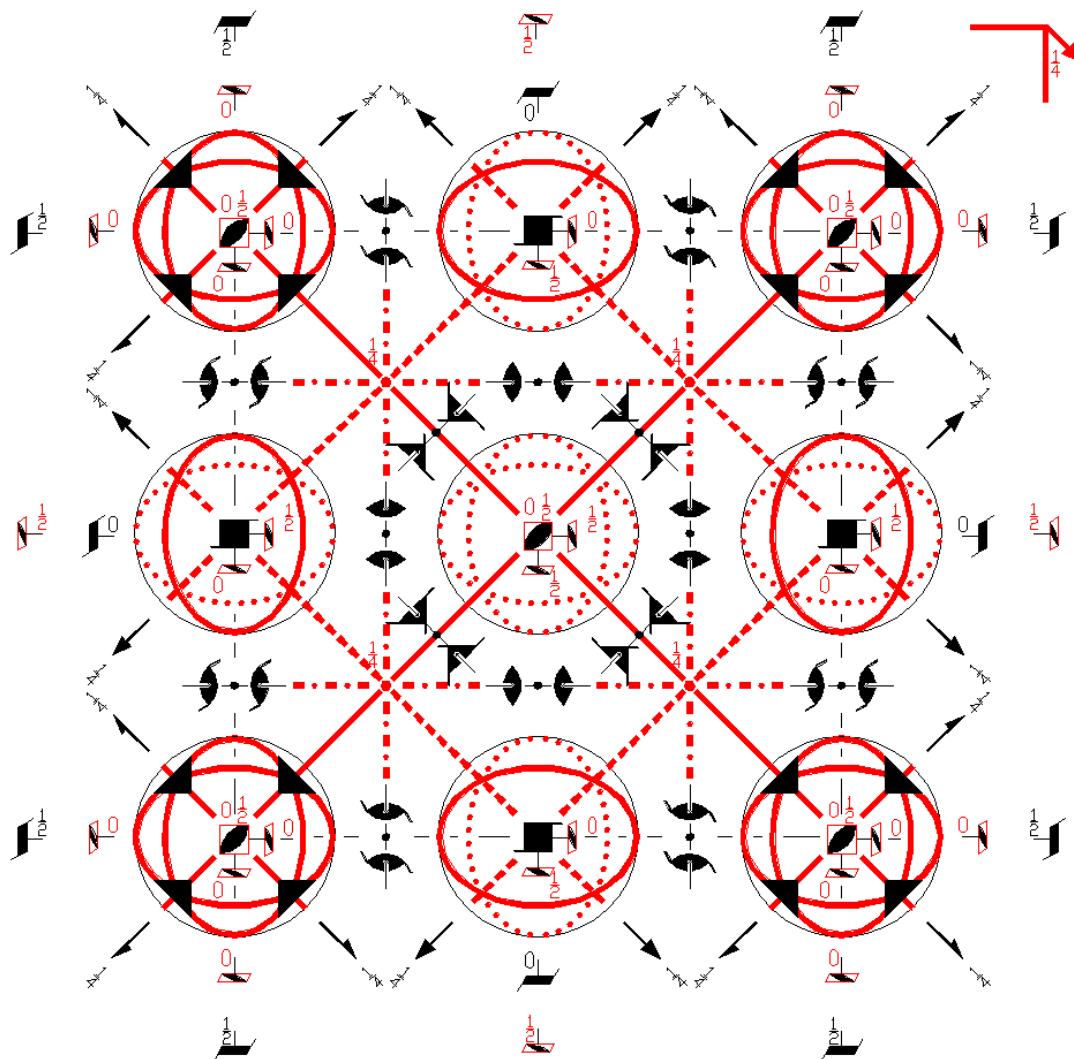
$Pn\bar{3}m'$

224.5.1615

$m\bar{3}m'$

$P4_2/n\bar{3}'2/m'$

Cubic



Origin at  $\bar{4}'3m'$ , at  $-1/4, -1/4, -1/4$  from center ( $\bar{3}'m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; -1/4 \leq z \leq 1/4; y \leq x; \max(x-1/2, -y) \leq z \leq \min(1/2-x, y)$

Vertices  $0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/4,1/4,1/4 \quad 1/4,1/4,-1/4$

**Symmetry Operations**

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                  | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  0,0,0)              |

(13) $2 (1/2, 1/2, 0) \ x, x, 1/4$ ( $2_{xy}   1/2, 1/2, 1/2$ )	(14) $2 \ x, \bar{x} + 1/2, 1/4$ ( $2_{\bar{xy}}   1/2, 1/2, 1/2$ )	(15) $4^- (0, 0, 1/2) \ 1/2, 0, z$ ( $4_z^{-1}   1/2, 1/2, 1/2$ )	(16) $4^+ (0, 0, 1/2) \ 0, 1/2, z$ ( $4_z   1/2, 1/2, 1/2$ )
(17) $4^- (1/2, 0, 0) \ x, 1/2, 0$ ( $4_x^{-1}   1/2, 1/2, 1/2$ )	(18) $2 (0, 1/2, 1/2) \ 1/4, y, y$ ( $2_{yz}   1/2, 1/2, 1/2$ )	(19) $2 \ 1/4, y + 1/2, \bar{y}$ ( $2_{\bar{yz}}   1/2, 1/2, 1/2$ )	(20) $4^+ (1/2, 0, 0) \ x, 0, 1/2$ ( $4_x   1/2, 1/2, 1/2$ )
(21) $4^+ (0, 1/2, 0) \ 1/2, y, 0$ ( $4_y   1/2, 1/2, 1/2$ )	(22) $2 (1/2, 0, 1/2) \ x, 1/4, x$ ( $2_{xz}   1/2, 1/2, 1/2$ )	(23) $4^- (0, 1/2, 0) \ 0, y, 1/2$ ( $4_y^{-1}   1/2, 1/2, 1/2$ )	(24) $2 \ \bar{x} + 1/2, 1/4, x$ ( $2_{\bar{xz}}   1/2, 1/2, 1/2$ )
(25) $\bar{1} \ 1/4, 1/4, 1/4$ ( $\bar{1}   1/2, 1/2, 1/2$ )'	(26) $n' (1/2, 1/2, 0) \ x, y, 1/4$ ( $m_z   1/2, 1/2, 1/2$ )'	(27) $n' (1/2, 0, 1/2) \ x, 1/4, z$ ( $m_y   1/2, 1/2, 1/2$ )'	(28) $n' (0, 1/2, 1/2) \ 1/4, y, z$ ( $m_x   1/2, 1/2, 1/2$ )'
(29) $\bar{3}^+ \ x, x, x; 1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 1/2, 1/2$ )'	(30) $\bar{3}^+ \ \bar{x} - 1, \bar{x} + 1, \bar{x}; -1/4, 1/4, 3/4$ ( $\bar{3}_{\bar{xyz}^{-1}}   1/2, 1/2, 1/2$ )'	(31) $\bar{3}^+ \ x, \bar{x} + 1, \bar{x}; 1/4, 3/4, -1/4$ ( $\bar{3}_{\bar{xyz}^{-1}}   1/2, 1/2, 1/2$ )'	(32) $\bar{3}^+ \ \bar{x} + 1, \bar{x}, \bar{x}; 3/4, -1/4, 1/4$ ( $\bar{3}_{\bar{xyz}^{-1}}   1/2, 1/2, 1/2$ )'
(33) $\bar{3}^- \ x, x, x; 1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2$ )'	(34) $\bar{3}^- \ \bar{x} + 1, \bar{x} - 1, \bar{x}; 1/4, -1/4, 3/4$ ( $\bar{3}_{\bar{xyz}}   1/2, 1/2, 1/2$ )'	(35) $\bar{3}^- \ \bar{x}, \bar{x} + 1, \bar{x}; -1/4, 3/4, 1/4$ ( $\bar{3}_{\bar{xyz}}   1/2, 1/2, 1/2$ )'	(36) $\bar{3}^- \ \bar{x} + 1, \bar{x}, \bar{x}; 3/4, 1/4, -1/4$ ( $\bar{3}_{\bar{xyz}}   1/2, 1/2, 1/2$ )'
(37) $m' \ x, \bar{x}, z$ ( $m_{xy}   0, 0, 0$ )'	(38) $m' \ x, x, z$ ( $m_{\bar{xy}}   0, 0, 0$ )'	(39) $\bar{4}^- \ 0, 0, z; 0, 0, 0$ ( $\bar{4}_z^{-1}   0, 0, 0$ )'	(40) $\bar{4}^+ \ 0, 0, z; 0, 0, 0$ ( $\bar{4}_z   0, 0, 0$ )'
(41) $\bar{4}^- \ x, 0, 0; 0, 0, 0$ ( $\bar{4}_x^{-1}   0, 0, 0$ )'	(42) $m' \ x, y, \bar{y}$ ( $m_{yz}   0, 0, 0$ )'	(43) $m' \ x, y, y$ ( $m_{\bar{yz}}   0, 0, 0$ )'	(44) $\bar{4}^+ \ x, 0, 0; 0, 0, 0$ ( $\bar{4}_x   0, 0, 0$ )'
(45) $\bar{4}^+ \ 0, y, 0; 0, 0, 0$ ( $\bar{4}_y   0, 0, 0$ )'	(46) $m' \ \bar{x}, y, x$ ( $m_{xz}   0, 0, 0$ )'	(47) $\bar{4}^- \ 0, y, 0; 0, 0, 0$ ( $\bar{4}_y^{-1}   0, 0, 0$ )'	(48) $m' \ x, y, x$ ( $m_{\bar{xz}}   0, 0, 0$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

48 | 1

(1) $x, y, z [u, v, w]$	(2) $\bar{x}, \bar{y}, z [\bar{u}, \bar{v}, w]$	(3) $\bar{x}, y, \bar{z} [\bar{u}, v, \bar{w}]$	(4) $x, \bar{y}, \bar{z} [u, \bar{v}, \bar{w}]$
(5) $z, x, y [w, u, v]$	(6) $z, \bar{x}, \bar{y} [w, \bar{u}, \bar{v}]$	(7) $\bar{z}, \bar{x}, y [\bar{w}, \bar{u}, v]$	(8) $\bar{z}, x, \bar{y} [\bar{w}, u, \bar{v}]$
(9) $y, z, x [v, w, u]$	(10) $\bar{y}, z, \bar{x} [\bar{v}, w, \bar{u}]$	(11) $y, \bar{z}, \bar{x} [v, \bar{w}, \bar{u}]$	(12) $\bar{y}, \bar{z}, x [\bar{v}, \bar{w}, u]$
(13) $y + 1/2, x + 1/2, \bar{z} + 1/2 [v, u, \bar{w}]$	(14) $\bar{y} + 1/2, \bar{x} + 1/2, \bar{z} + 1/2 [\bar{v}, \bar{u}, \bar{w}]$	(15) $y + 1/2, \bar{x} + 1/2, z + 1/2 [v, \bar{u}, w]$	(16) $\bar{y} + 1/2, x + 1/2, z + 1/2 [\bar{v}, u, w]$
(17) $x + 1/2, z + 1/2, \bar{y} + 1/2 [u, w, \bar{v}]$	(18) $\bar{x} + 1/2, z + 1/2, y + 1/2 [\bar{u}, w, v]$	(19) $\bar{x} + 1/2, \bar{z} + 1/2, \bar{y} + 1/2 [\bar{u}, \bar{w}, \bar{v}]$	(20) $x + 1/2, \bar{z} + 1/2, y + 1/2 [u, \bar{w}, v]$
(21) $z + 1/2, y + 1/2, \bar{x} + 1/2 [w, v, \bar{u}]$	(22) $z + 1/2, \bar{y} + 1/2, x + 1/2 [w, \bar{v}, u]$	(23) $\bar{z} + 1/2, y + 1/2, x + 1/2 [\bar{w}, v, u]$	(24) $\bar{z} + 1/2, \bar{y} + 1/2, \bar{x} + 1/2 [\bar{w}, \bar{v}, \bar{u}]$
(25) $\bar{x} + 1/2, \bar{y} + 1/2, \bar{z} + 1/2 [\bar{u}, \bar{v}, \bar{w}]$	(26) $x + 1/2, y + 1/2, \bar{z} + 1/2 [u, v, \bar{w}]$	(27) $x + 1/2, \bar{y} + 1/2, z + 1/2 [u, \bar{v}, w]$	(28) $\bar{x} + 1/2, y + 1/2, z + 1/2 [\bar{u}, v, w]$
(29) $\bar{z} + 1/2, \bar{x} + 1/2, \bar{y} + 1/2 [\bar{w}, \bar{u}, \bar{v}]$	(30) $\bar{z} + 1/2, x + 1/2, y + 1/2 [\bar{w}, u, v]$	(31) $z + 1/2, x + 1/2, \bar{y} + 1/2 [w, u, \bar{v}]$	(32) $z + 1/2, \bar{x} + 1/2, y + 1/2 [w, \bar{u}, v]$
(33) $\bar{y} + 1/2, \bar{z} + 1/2, \bar{x} + 1/2 [\bar{v}, \bar{w}, \bar{u}]$	(34) $y + 1/2, \bar{z} + 1/2, x + 1/2 [v, \bar{w}, u]$	(35) $\bar{y} + 1/2, z + 1/2, x + 1/2 [\bar{v}, w, u]$	(36) $y + 1/2, z + 1/2, \bar{x} + 1/2 [v, w, \bar{u}]$

(37) $\bar{y}, \bar{x}, z [\bar{v}, \bar{u}, w]$	(38) $y, x, z [v, u, w]$	(39) $\bar{y}, x, \bar{z} [\bar{v}, u, \bar{w}]$	(40) $y, \bar{x}, \bar{z} [v, \bar{u}, \bar{w}]$
(41) $\bar{x}, \bar{z}, y [\bar{u}, \bar{w}, v]$	(42) $x, \bar{z}, y [u, \bar{w}, v]$	(43) $x, z, y [u, w, v]$	(44) $\bar{x}, \bar{z}, y [\bar{u}, \bar{w}, \bar{v}]$
(45) $\bar{z}, \bar{y}, x [\bar{w}, \bar{v}, u]$	(46) $\bar{z}, y, x [\bar{w}, v, u]$	(47) $z, \bar{y}, x [w, \bar{v}, u]$	(48) $z, y, x [w, v, u]$
24 k ..m'			
$x, x, z [u, u, w]$	$\bar{x}, \bar{x}, z [\bar{u}, \bar{u}, w]$	$\bar{x}, x, \bar{z} [\bar{u}, u, \bar{w}]$	$x, \bar{x}, \bar{z} [u, \bar{u}, \bar{w}]$
$z, x, x [w, u, u]$	$z, \bar{x}, \bar{x} [w, \bar{u}, \bar{u}]$	$\bar{z}, \bar{x}, x [\bar{w}, \bar{u}, u]$	$\bar{z}, x, \bar{x} [\bar{w}, u, \bar{u}]$
$x, z, x [u, w, u]$	$\bar{x}, z, \bar{x} [\bar{u}, w, \bar{u}]$	$x, \bar{z}, \bar{x} [u, \bar{w}, \bar{u}]$	$\bar{x}, \bar{z}, x [\bar{u}, \bar{w}, u]$
$x+1/2, x+1/2, \bar{z}+1/2 [u, u, \bar{w}]$	$\bar{x}+1/2, \bar{x}+1/2, \bar{z}+1/2 [\bar{u}, \bar{u}, \bar{w}]$	$x+1/2, \bar{x}+1/2, z+1/2 [u, \bar{u}, w]$	$\bar{x}+1/2, x+1/2, z+1/2 [\bar{u}, u, w]$
$x+1/2, z+1/2, \bar{x}+1/2 [u, w, \bar{u}]$	$\bar{x}+1/2, z+1/2, x+1/2 [\bar{u}, w, u]$	$\bar{x}+1/2, \bar{z}+1/2, \bar{x}+1/2 [\bar{u}, \bar{w}, \bar{u}]$	$x+1/2, \bar{z}+1/2, x+1/2 [u, \bar{w}, u]$
$z+1/2, x+1/2, \bar{x}+1/2 [w, u, \bar{u}]$	$z+1/2, \bar{x}+1/2, x+1/2 [w, \bar{u}, u]$	$\bar{z}+1/2, x+1/2, x+1/2 [\bar{w}, u, u]$	$\bar{z}+1/2, \bar{x}+1/2, \bar{x}+1/2 [\bar{w}, \bar{u}, \bar{u}]$
24 j ..2			
$1/4, y, y+1/2 [0, v, v]$	$3/4, \bar{y}, y+1/2 [0, \bar{v}, v]$	$3/4, y, \bar{y}+1/2 [0, v, \bar{v}]$	$1/4, \bar{y}, \bar{y}+1/2 [0, \bar{v}, \bar{v}]$
$y+1/2, 1/4, y [v, 0, v]$	$y+1/2, 3/4, \bar{y} [v, 0, \bar{v}]$	$\bar{y}+1/2, 3/4, y [\bar{v}, 0, v]$	$\bar{y}+1/2, 1/4, \bar{y} [\bar{v}, 0, \bar{v}]$
$y, y+1/2, 1/4 [v, v, 0]$	$\bar{y}, y+1/2, 3/4 [\bar{v}, v, 0]$	$y, \bar{y}+1/2, 3/4 [v, \bar{v}, 0]$	$\bar{y}, \bar{y}+1/2, 1/4 [\bar{v}, \bar{v}, 0]$
$1/4, \bar{y}+1/2, \bar{y} [0, \bar{v}, \bar{v}]$	$3/4, y+1/2, \bar{y} [0, v, \bar{v}]$	$3/4, \bar{y}+1/2, y [0, \bar{v}, v]$	$1/4, y+1/2, \bar{y} [0, v, v]$
$\bar{y}, 1/4, \bar{y}+1/2 [\bar{v}, 0, \bar{v}]$	$\bar{y}, 3/4, y+1/2 [\bar{v}, 0, v]$	$y, 3/4, \bar{y}+1/2 [v, 0, \bar{v}]$	$y, 1/4, y+1/2 [v, 0, v]$
$\bar{y}+1/2, \bar{y}, 1/4 [\bar{v}, \bar{v}, 0]$	$y+1/2, \bar{y}, 3/4 [v, \bar{v}, 0]$	$\bar{y}+1/2, y, 3/4 [\bar{v}, v, 0]$	$y+1/2, y, 1/4 [v, v, 0]$
24 i ..2			
$1/4, y, \bar{y}+1/2 [0, \bar{v}, v]$	$3/4, \bar{y}, \bar{y}+1/2 [0, v, v]$	$3/4, y, y+1/2 [0, \bar{v}, \bar{v}]$	$1/4, \bar{y}, y+1/2 [0, v, \bar{v}]$
$\bar{y}+1/2, 1/4, y [v, 0, \bar{v}]$	$\bar{y}+1/2, 3/4, \bar{y} [v, 0, v]$	$y+1/2, 3/4, y [\bar{v}, 0, \bar{v}]$	$y+1/2, 1/4, \bar{y} [\bar{v}, 0, v]$
$y, \bar{y}+1/2, 1/4 [\bar{v}, v, 0]$	$\bar{y}, \bar{y}+1/2, 3/4 [v, v, 0]$	$y, y+1/2, 3/4 [\bar{v}, \bar{v}, 0]$	$\bar{y}, y+1/2, 1/4 [v, \bar{v}, 0]$
$1/4, \bar{y}+1/2, y [0, v, \bar{v}]$	$3/4, y+1/2, y [0, \bar{v}, \bar{v}]$	$3/4, \bar{y}+1/2, \bar{y} [0, v, v]$	$1/4, y+1/2, \bar{y} [0, \bar{v}, v]$
$y, 1/4, \bar{y}+1/2 [\bar{v}, 0, v]$	$y, 3/4, y+1/2 [\bar{v}, 0, \bar{v}]$	$\bar{y}, 3/4, \bar{y}+1/2 [v, 0, \bar{v}]$	$\bar{y}, 1/4, y+1/2 [v, 0, v]$
$\bar{y}+1/2, y, 1/4 [v, \bar{v}, 0]$	$y+1/2, y, 3/4 [v, \bar{v}, 0]$	$\bar{y}+1/2, \bar{y}, 3/4 [v, v, 0]$	$y+1/2, \bar{y}, 1/4 [\bar{v}, v, 0]$
24 h 2..			
$x, 0, 1/2 [u, 0, 0]$	$\bar{x}, 0, 1/2 [\bar{u}, 0, 0]$	$1/2, x, 0 [0, u, 0]$	$1/2, \bar{x}, 0 [0, \bar{u}, 0]$
$0, 1/2, x [0, 0, u]$	$0, 1/2, \bar{x} [0, 0, \bar{u}]$	$1/2, x+1/2, 0 [0, u, 0]$	$1/2, \bar{x}+1/2, 0 [0, \bar{u}, 0]$
$x+1/2, 0, 1/2 [u, 0, 0]$	$\bar{x}+1/2, 0, 1/2 [\bar{u}, 0, 0]$	$0, 1/2, \bar{x}+1/2 [0, 0, \bar{u}]$	$0, 1/2, x+1/2 [0, 0, u]$

Continued

224.5.1615

Pn'3'm'

			$\bar{x}+1/2, 1/2, 0$ [ $\bar{u}, 0, 0$ ]	$x+1/2, 1/2, 0$ [ $u, 0, 0$ ]	$0, \bar{x}+1/2, 1/2$ [ $0, \bar{u}, 0$ ]	$0, x+1/2, 1/2$ [ $0, u, 0$ ]
			$1/2, 0, \bar{x}+1/2$ [ $0, 0, \bar{u}$ ]	$1/2, 0, x+1/2$ [ $0, 0, u$ ]	$0, \bar{x}, 1/2$ [ $0, \bar{u}, 0$ ]	$0, x, 1/2$ [ $0, u, 0$ ]
			$\bar{x}, 1/2, 0$ [ $\bar{u}, 0, 0$ ]	$x, 1/2, 0$ [ $u, 0, 0$ ]	$1/2, 0, x$ [ $0, 0, u$ ]	$1/2, 0, \bar{x}$ [ $0, 0, \bar{u}$ ]
12	g	2.m'm'	$x, 0, 0$ [ $u, 0, 0$ ]	$\bar{x}, 0, 0$ [ $\bar{u}, 0, 0$ ]	$0, x, 0$ [ $0, u, 0$ ]	$0, \bar{x}, 0$ [ $0, \bar{u}, 0$ ]
			$0, 0, x$ [ $0, 0, u$ ]	$0, 0, \bar{x}$ [ $0, 0, \bar{u}$ ]	$1/2, x+1/2, 1/2$ [ $0, u, 0$ ]	$1/2, \bar{x}+1/2, 1/2$ [ $0, \bar{u}, 0$ ]
			$x+1/2, 1/2, 1/2$ [ $u, 0, 0$ ]	$\bar{x}+1/2, 1/2, 1/2$ [ $\bar{u}, 0, 0$ ]	$1/2, 1/2, \bar{x}+1/2$ [ $0, 0, \bar{u}$ ]	$1/2, 1/2, x+1/2$ [ $0, 0, u$ ]
12	f	2.22	$1/4, 0, 1/2$ [ $0, 0, 0$ ]	$3/4, 0, 1/2$ [ $0, 0, 0$ ]	$1/2, 1/4, 0$ [ $0, 0, 0$ ]	
			$1/2, 3/4, 0$ [ $0, 0, 0$ ]	$0, 1/2, 1/4$ [ $0, 0, 0$ ]	$0, 1/2, 3/4$ [ $0, 0, 0$ ]	
			$1/4, 1/2, 0$ [ $0, 0, 0$ ]	$3/4, 1/2, 0$ [ $0, 0, 0$ ]	$0, 1/4, 1/2$ [ $0, 0, 0$ ]	
			$0, 3/4, 1/2$ [ $0, 0, 0$ ]	$1/2, 0, 1/4$ [ $0, 0, 0$ ]	$1/2, 0, 3/4$ [ $0, 0, 0$ ]	
8	e	.3m'	$x, x, x$ [ $u, u, u$ ]	$\bar{x}, \bar{x}, \bar{x}$ [ $\bar{u}, \bar{u}, \bar{u}$ ]		
			$\bar{x}, x, \bar{x}$ [ $\bar{u}, u, \bar{u}$ ]	$x, \bar{x}, x$ [ $u, \bar{u}, u$ ]		
			$x+1/2, x+1/2, \bar{x}+1/2$ [ $u, u, \bar{u}$ ]	$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2$ [ $\bar{u}, \bar{u}, \bar{u}$ ]		
			$x+1/2, \bar{x}+1/2, x+1/2$ [ $u, \bar{u}, u$ ]	$\bar{x}+1/2, x+1/2, x+1/2$ [ $\bar{u}, u, u$ ]		
6	d	$\bar{4}'2.m'$	$0, 1/2, 1/2$ [ $0, 0, 0$ ]	$1/2, 0, 1/2$ [ $0, 0, 0$ ]	$1/2, 1/2, 0$ [ $0, 0, 0$ ]	
			$0, 1/2, 0$ [ $0, 0, 0$ ]	$1/2, 0, 0$ [ $0, 0, 0$ ]	$0, 0, 1/2$ [ $0, 0, 0$ ]	
4	c	$\bar{3}'m'$	$3/4, 3/4, 3/4$ [ $0, 0, 0$ ]	$1/4, 1/4, 3/4$ [ $0, 0, 0$ ]	$1/4, 3/4, 1/4$ [ $0, 0, 0$ ]	$3/4, 1/4, 1/4$ [ $0, 0, 0$ ]
4	b	$\bar{3}'m'$	$1/4, 1/4, 1/4$ [ $0, 0, 0$ ]	$3/4, 3/4, 1/4$ [ $0, 0, 0$ ]	$3/4, 1/4, 3/4$ [ $0, 0, 0$ ]	$1/4, 3/4, 3/4$ [ $0, 0, 0$ ]
2	a	$\bar{4}'3m'$	$0, 0, 0$ [ $0, 0, 0$ ]	$1/2, 1/2, 1/2$ [ $0, 0, 0$ ]		

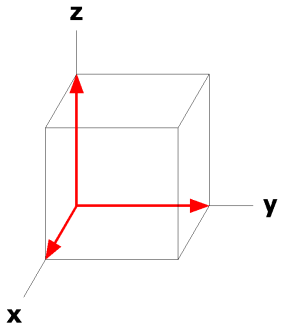
**Symmetry of Special Projections**

Along  $[0, 0, 1]$  p4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0, 0, z$

Along  $[1, 1, 1]$  p6m'm'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

Along  $[1, 1, 0]$  p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 1/4$

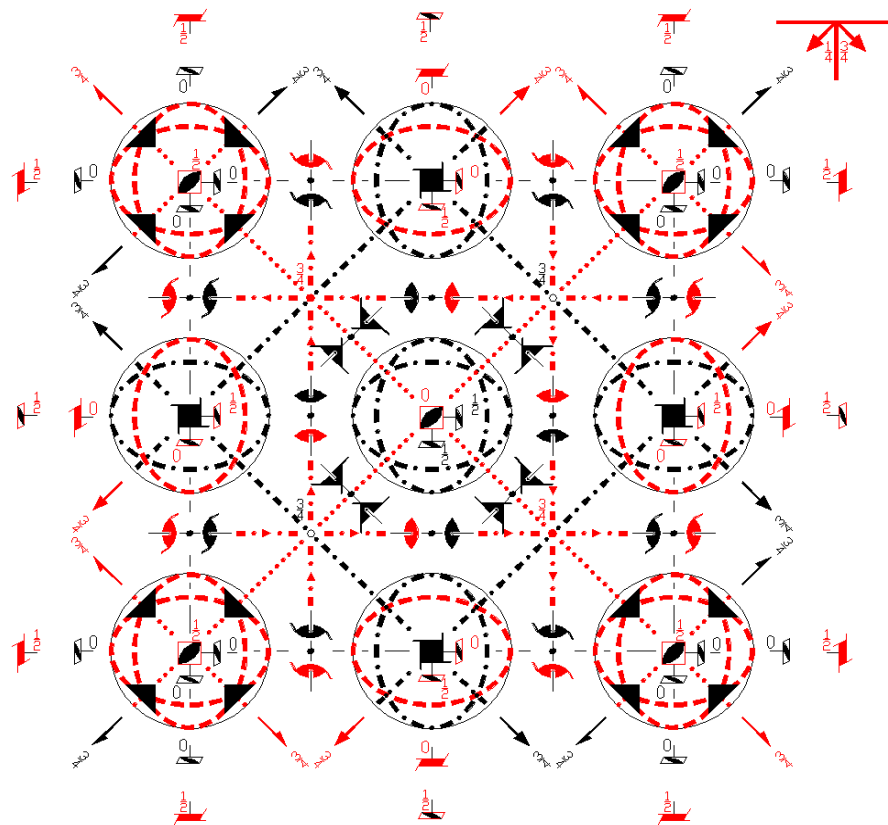
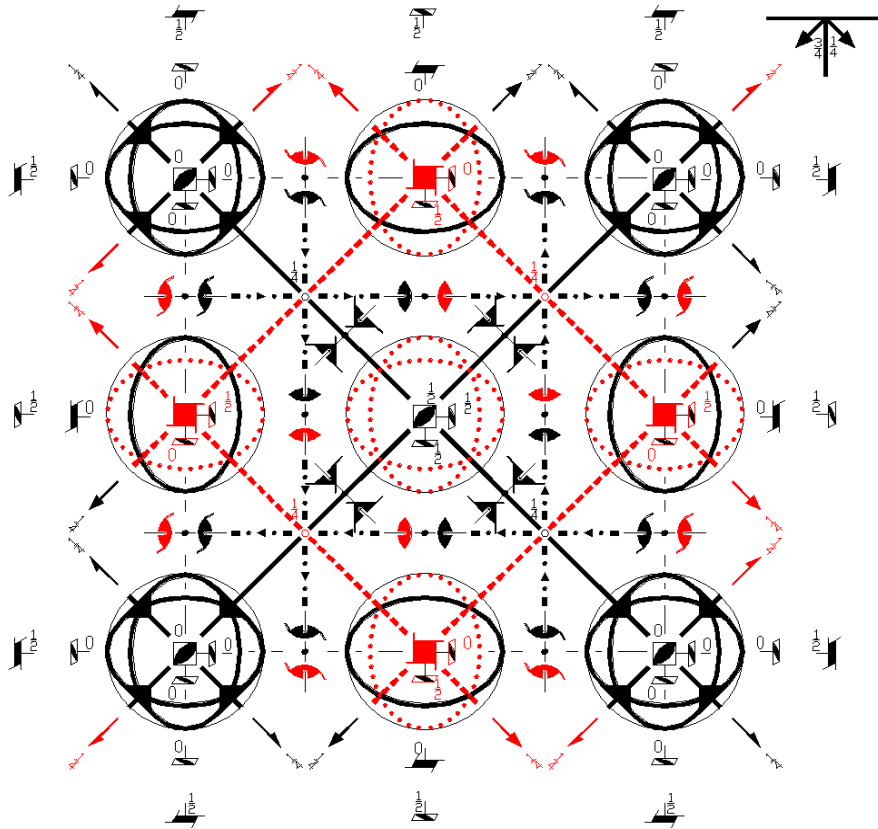




$P_F n\bar{3}m$   
224.6.1616

$n\bar{3}m1'$   
 $P_F 4_2/n\bar{3}2/m$

Cubic



**Origin** at  $\bar{4}3m$ , at  $-1/4, -1/4, -1/4$  from center ( $\bar{3}m$ )

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; -1/4 \leq z \leq 1/4; y \leq x; \max(x-1/2, -y) \leq z \leq \min(1/2-x, y)$

Vertices  $0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/4,1/4,1/4 \quad 1/4,1/4,-1/4$

### Symmetry Operations

For  $(0,0,0)$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) $1$<br>$(1 0,0,0)$  | (2) $2$ $0,0,z$<br>$(2_z 0,0,0)$   | (3) $2$ $0,y,0$<br>$(2_y 0,0,0)$   | (4) $2$ $x,0,0$<br>$(2_x 0,0,0)$   |
| (5) $3^+$ $x,x,x$<br>$(3_{xyz} 0,0,0)$                                      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>$(3_{x\bar{y}z}^{-1} 0,0,0)$                                      | (7) $3^+$ $x,\bar{x},\bar{x}$<br>$(3_{x\bar{y}z}^{-1} 0,0,0)$                                    | (8) $3^+$ $\bar{x},\bar{x},x$<br>$(3_{x\bar{y}z}^{-1} 0,0,0)$                                    |
| (9) $3^-$ $x,x,x$<br>$(3_{xyz}^{-1} 0,0,0)$                                 | (10) $3^-$ $x,\bar{x},\bar{x}$<br>$(3_{x\bar{y}z} 0,0,0)$  | (11) $3^-$ $\bar{x},\bar{x},x$<br>$(3_{x\bar{y}z} 0,0,0)$  | (12) $3^-$ $\bar{x},x,\bar{x}$<br>$(3_{x\bar{y}z} 0,0,0)$  |
| (13) $2$ $(1/2,1/2,0)$ $x,x,1/4$<br>$(2_{xy} 1/2,1/2,1/2)$                  | (14) $2$ $x,\bar{x}+1/2,1/4$<br>$(2_{\bar{xy}} 1/2,1/2,1/2)$                                       | (15) $4^-$ $(0,0,1/2)$ $1/2,0,z$<br>$(4_z^{-1} 1/2,1/2,1/2)$                                     | (16) $4^+$ $(0,0,1/2)$ $0,1/2,z$<br>$(4_z 1/2,1/2,1/2)$  |
| (17) $4^-$ $(1/2,0,0)$ $x,1/2,0$<br>$(4_x^{-1} 1/2,1/2,1/2)$                | (18) $2$ $(0,1/2,1/2)$ $1/4,y,y$<br>$(2_{yz} 1/2,1/2,1/2)$   | (19) $2$ $1/4,y+1/2,\bar{y}$<br>$(2_{yz} 1/2,1/2,1/2)$   | (20) $4^+$ $(1/2,0,0)$ $x,0,1/2$<br>$(4_x 1/2,1/2,1/2)$  |
| (21) $4^+$ $(0,1/2,0)$ $1/2,y,0$<br>$(4_y 1/2,1/2,1/2)$                     | (22) $2$ $(1/2,0,1/2)$ $x,1/4,x$<br>$(2_{xz} 1/2,1/2,1/2)$   | (23) $4^-$ $(0,1/2,0)$ $0,y,1/2$<br>$(4_y^{-1} 1/2,1/2,1/2)$                                     | (24) $2$ $\bar{x}+1/2,1/4,x$<br>$(2_{xz} 1/2,1/2,1/2)$   |
| (25) $\bar{1}$ $1/4,1/4,1/4$<br>$(\bar{1} 1/2,1/2,1/2)$                     | (26) $n$ $(1/2,1/2,0)$ $x,y,1/4$<br>$(m_z 1/2,1/2,1/2)$  | (27) $n$ $(1/2,0,1/2)$ $x,1/4,z$<br>$(m_y 1/2,1/2,1/2)$  | (28) $n$ $(0,1/2,1/2)$ $1/4,y,z$<br>$(m_x 1/2,1/2,1/2)$  |
| (29) $\bar{3}^+$ $x,x,x; 1/4,1/4,1/4$<br>$(\bar{3}_{xyz} 1/2,1/2,1/2)$      | (30) $\bar{3}^+$ $\bar{x}-1,x+1,\bar{x}; -1/4,1/4,3/4$<br>$(\bar{3}_{x\bar{y}z}^{-1} 1/2,1/2,1/2)$ | (31) $\bar{3}^+$ $x,\bar{x}+1,\bar{x}; 1/4,3/4,-1/4$<br>$(\bar{3}_{x\bar{y}z}^{-1} 1/2,1/2,1/2)$ | (32) $\bar{3}^+$ $\bar{x}+1,\bar{x},x; 3/4,-1/4,1/4$<br>$(\bar{3}_{x\bar{y}z}^{-1} 1/2,1/2,1/2)$ |
| (33) $\bar{3}^-$ $x,x,x; 1/4,1/4,1/4$<br>$(\bar{3}_{xyz}^{-1} 1/2,1/2,1/2)$ | (34) $\bar{3}^-$ $x+1,\bar{x}-1,\bar{x}; 1/4,-1/4,3/4$<br>$(\bar{3}_{x\bar{y}z} 1/2,1/2,1/2)$      | (35) $\bar{3}^-$ $\bar{x},\bar{x}+1,x; -1/4,3/4,1/4$<br>$(\bar{3}_{x\bar{y}z} 1/2,1/2,1/2)$      | (36) $\bar{3}^-$ $\bar{x}+1,x,\bar{x}; 3/4,1/4,-1/4$<br>$(\bar{3}_{x\bar{y}z} 1/2,1/2,1/2)$      |
| (37) $m$ $x,\bar{x},z$<br>$(m_{xy} 0,0,0)$                                  | (38) $m$ $x,x,z$<br>$(m_{\bar{xy}} 0,0,0)$   | (39) $\bar{4}^-$ $0,0,z; 0,0,0$<br>$(\bar{4}_z^{-1} 0,0,0)$                                      | (40) $\bar{4}^+$ $0,0,z; 0,0,0$<br>$(\bar{4}_z 0,0,0)$   |
| (41) $\bar{4}^-$ $x,0,0; 0,0,0$<br>$(\bar{4}_x^{-1} 0,0,0)$                 | (42) $m$ $x,y,\bar{y}$<br>$(m_{yz} 0,0,0)$   | (43) $m$ $x,y,y$<br>$(m_{\bar{yz}} 0,0,0)$   | (44) $\bar{4}^+$ $x,0,0; 0,0,0$<br>$(\bar{4}_x 0,0,0)$   |
| (45) $\bar{4}^+$ $0,y,0; 0,0,0$<br>$(\bar{4}_y 0,0,0)$                      | (46) $m$ $\bar{x},y,x$<br>$(m_{xz} 0,0,0)$   | (47) $\bar{4}^-$ $0,y,0; 0,0,0$<br>$(\bar{4}_y^{-1} 0,0,0)$                                      | (48) $m$ $x,y,x$<br>$(m_{xz} 0,0,0)$   |

For  $(1,0,0)'$  + set

- |   |   |   |  |
|---|---|---|--|
| (1) $t'$ $(1,0,0)$<br>$(1 1,0,0)'$                                      | (2) $2'$ $1/2,0,z$<br>$(2_z 1,0,0)'$  | (3) $2'$ $1/2,y,0$<br>$(2_y 1,0,0)'$  | (4) $2'$ $(1,0,0)$ $x,0,0$<br>$(2_x 1,0,0)'$   |
| (5) $3^+$ $(1/3,1/3,1/3)$<br>$x+2/3,x+1/3,x$<br>$(3_{xyz} 1,0,0)'$      | (6) $3^+$ $(1/3,-1/3,1/3)$<br>$\bar{x}+2/3,x-1/3,\bar{x}$<br>$(3_{x\bar{y}z}^{-1} 1,0,0)'$    | (7) $3^+$ $(1/3,-1/3,-1/3)$<br>$x+2/3,x-1/3,\bar{x}$<br>$(3_{x\bar{y}z}^{-1} 1,0,0)'$ | (8) $3^+$ $(1/3,1/3,-1/3)$<br>$\bar{x}+2/3,\bar{x}-1/3,x$<br>$(3_{x\bar{y}z}^{-1} 1,0,0)'$ |
| (9) $3^-$ $(1/3,1/3,1/3)$<br>$x+1/3,x-1/3,x$<br>$(3_{xyz}^{-1} 1,0,0)'$ | (10) $3^-$ $(1/3,-1/3,-1/3)$<br>$\bar{x}+1/3,\bar{x}+1/3,\bar{x}$<br>$(3_{x\bar{y}z} 1,0,0)'$ | (11) $3^-$ $(1/3,1/3,-1/3)$<br>$x+1/3,\bar{x}-1/3,x$<br>$(3_{x\bar{y}z} 1,0,0)'$      | (12) $3^-$ $(1/3,-1/3,1/3)$<br>$\bar{x}+1/3,x+1/3,\bar{x}$<br>$(3_{x\bar{y}z} 1,0,0)'$     |

(13) $2' \quad x+1/2, x, 1/4$ $(2_{xy}   3/2, 1/2, 1/2)'$	(14) $2' \quad (1/2, 1/2, 0) \quad x, \bar{x}, 1/4$ $(2_{\bar{xy}}   3/2, 1/2, 1/2)'$	(15) $4' \quad (0, 0, 1/2) \quad 1, -1/2, z$ $(4_z^{-1}   3/2, 1/2, 1/2)'$	(16) $4^+ \quad (0, 0, 1/2) \quad 1/2, 1, z$ $(4_z   3/2, 1/2, 1/2)'$
(17) $4' \quad (3/2, 0, 0) \quad x, 1/2, 0$ $(4_x^{-1}   3/2, 1/2, 1/2)'$	(18) $2' \quad (0, 1/2, 1/2) \quad 3/4, y, y$ $(2_{yz}   3/2, 1/2, 1/2)'$	(19) $2' \quad 3/4, y+1/2, \bar{y}$ $(2_{\bar{yz}}   3/2, 1/2, 1/2)'$	(20) $4^+ \quad (3/2, 0, 0) \quad x, 0, 1/2$ $(4_x   3/2, 1/2, 1/2)'$
(21) $4^+ \quad (0, 1/2, 0) \quad 1, y, -1/2$ $(4_y   3/2, 1/2, 1/2)'$	(22) $2' \quad x+1/2, 1/4, x$ $(2_{xz}   3/2, 1/2, 1/2)'$	(23) $4' \quad (0, 1/2, 0) \quad 1/2, y, 1$ $(4_y^{-1}   3/2, 1/2, 1/2)'$	(24) $2' \quad (1/2, 0, -1/2) \quad \bar{x}+1, 1/4, x$ $(2_{\bar{xz}}   3/2, 1/2, 1/2)'$
(25) $\bar{1} \quad 3/4, 1/4, 1/4$ $(\bar{1}   3/2, 1/2, 1/2)'$	(26) $n' \quad (3/2, 1/2, 0) \quad x, y, 1/4$ $(m_z   3/2, 1/2, 1/2)'$	(27) $n' \quad (3/2, 0, 1/2) \quad x, 1/4, z$ $(m_y   3/2, 1/2, 1/2)'$	(28) $n' \quad (0, 1/2, 1/2) \quad 3/4, y, z$ $(m_x   3/2, 1/2, 1/2)'$
(29) $\bar{3}^+ \quad x, x-1, x;$ $3/4, 1/4, 3/4$ $(\bar{3}_{xyz}   3/2, 1/2, 1/2)'$	(30) $\bar{3}^+ \quad \bar{x}-1, x-2, \bar{x};$ $1/4, 3/4, 5/4$ $(\bar{3}_{\bar{xyz}}^{-1}   3/2, 1/2, 1/2)'$	(31) $\bar{3}^+ \quad x, \bar{x}+2, \bar{x};$ $3/4, 5/4, -3/4$ $(\bar{3}_{\bar{xyz}}^{-1}   3/2, 1/2, 1/2)'$	(32) $\bar{3}^+ \quad \bar{x}+1, \bar{x}-1, x;$ $5/4, -3/4, -1/4$ $(\bar{3}_{\bar{xyz}}^{-1}   3/2, 1/2, 1/2)'$
(33) $\bar{3}^- \quad x+1, x+1, x;$ $3/4, 3/4, -1/4$ $(\bar{3}_{xyz}^{-1}   3/2, 1/2, 1/2)'$	(34) $\bar{3}^- \quad x+2, \bar{x}-2, \bar{x};$ $3/4, -3/4, 5/4$ $(\bar{3}_{\bar{xyz}}   3/2, 1/2, 1/2)'$	(35) $\bar{3}^- \quad \bar{x}+1, \bar{x}+2, x;$ $1/4, 5/4, 3/4$ $(\bar{3}_{\bar{yz}}   3/2, 1/2, 1/2)'$	(36) $\bar{3}^- \quad \bar{x}+2, x-1, \bar{x};$ $5/4, -1/4, -3/4$ $(\bar{3}_{\bar{xyz}}   3/2, 1/2, 1/2)'$
(37) $g' \quad (1/2, -1/2, 0) \quad x+1/2, \bar{x}, z$ $(m_{xy}   1, 0, 0)'$	(38) $g' \quad (1/2, 1/2, 0) \quad x+1/2, x, z$ $(m_{\bar{xy}}   1, 0, 0)'$	(39) $\bar{4}^- \quad 1/2, 1/2, z; \quad 1/2, 1/2, 0$ $(\bar{4}_z^{-1}   1, 0, 0)'$	(40) $\bar{4}^+ \quad 1/2, -1/2, z; \quad 1/2, -1/2, 0$ $(\bar{4}_z   1, 0, 0)'$
(41) $\bar{4}^- \quad x+1/2, 0, 0; \quad 1/2, 0, 0$ $(\bar{4}_x^{-1}   1, 0, 0)'$	(42) $a' \quad (1, 0, 0) \quad x, y, \bar{y}$ $(m_{yz}   1, 0, 0)'$	(43) $a' \quad (1, 0, 0) \quad x, y, y$ $(m_{\bar{yz}}   1, 0, 0)'$	(44) $\bar{4}^+ \quad x+1/2, 0, 0; \quad 1/2, 0, 0$ $(\bar{4}_x   1, 0, 0)'$
(45) $\bar{4}^+ \quad 1/2, y, 1/2; \quad 1/2, 0, 1/2$ $(\bar{4}_y   1, 0, 0)'$	(46) $g' \quad (1/2, 0, -1/2) \quad \bar{x}+1/2, y, x$ $(m_{xz}   1, 0, 0)'$	(47) $\bar{4}^- \quad 1/2, y, -1/2; \quad 0, 0, 0$ $(\bar{4}_y^{-1}   1, 0, 0)'$	(48) $g' \quad (1/2, 0, 1/2) \quad x+1/2, y, x$ $(m_{\bar{xz}}   1, 0, 0)'$

**Generators selected** (1);  $t'(1, 0, 0)$ ;  $t'(0, 1, 0)$ ;  $t'(0, 0, 1)$ ; (2); (3); (5); (13); (25).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

Coordinates

96		1	(0, 0, 0) +	(1, 0, 0)' +							
(1)	$x, y, z$	$[u, v, w]$	(2)	$\bar{x}, \bar{y}, z$	$[\bar{u}, \bar{v}, w]$	(3)	$\bar{x}, \bar{y}, \bar{z}$	$[\bar{u}, \bar{v}, \bar{w}]$	(4)	$x, \bar{y}, \bar{z}$	$[u, \bar{v}, \bar{w}]$
(5)	$z, x, y$	$[w, u, v]$	(6)	$z, \bar{x}, \bar{y}$	$[w, \bar{u}, \bar{v}]$	(7)	$\bar{z}, \bar{x}, y$	$[\bar{w}, \bar{u}, v]$	(8)	$\bar{z}, x, \bar{y}$	$[\bar{w}, u, \bar{v}]$
(9)	$y, z, x$	$[v, w, u]$	(10)	$\bar{y}, z, \bar{x}$	$[\bar{v}, w, \bar{u}]$	(11)	$y, \bar{z}, \bar{x}$	$[v, \bar{w}, \bar{u}]$	(12)	$\bar{y}, z, x$	$[\bar{v}, w, u]$
(13)	$y+1/2, x+1/2, \bar{z}+1/2$	$[v, u, \bar{w}]$	(14)	$\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2$	$[\bar{v}, \bar{u}, \bar{w}]$	(15)	$y+1/2, \bar{x}+1/2, z+1/2$	$[v, \bar{u}, w]$	(16)	$\bar{y}+1/2, x+1/2, z+1/2$	$[\bar{v}, u, w]$
(17)	$x+1/2, z+1/2, \bar{y}+1/2$	$[u, w, \bar{v}]$	(18)	$\bar{x}+1/2, z+1/2, y+1/2$	$[\bar{u}, w, v]$	(19)	$\bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2$	$[\bar{u}, \bar{w}, \bar{v}]$	(20)	$x+1/2, \bar{z}+1/2, y+1/2$	$[u, \bar{w}, v]$
(21)	$z+1/2, y+1/2, \bar{x}+1/2$	$[w, v, \bar{u}]$	(22)	$z+1/2, \bar{y}+1/2, x+1/2$	$[w, \bar{v}, u]$	(23)	$\bar{z}+1/2, y+1/2, x+1/2$	$[\bar{w}, v, u]$	(24)	$\bar{z}+1/2, \bar{y}+1/2, \bar{x}+1/2$	$[\bar{w}, \bar{v}, \bar{u}]$
(25)	$\bar{x}+1/2, \bar{y}+1/2, \bar{z}+1/2$	$[u, v, w]$	(26)	$x+1/2, y+1/2, \bar{z}+1/2$	$[\bar{u}, \bar{v}, w]$	(27)	$x+1/2, \bar{y}+1/2, z+1/2$	$[u, v, \bar{w}]$	(28)	$\bar{x}+1/2, y+1/2, z+1/2$	$[u, \bar{v}, \bar{w}]$
(29)	$\bar{z}+1/2, \bar{x}+1/2, \bar{y}+1/2$	$[w, u, v]$	(30)	$\bar{z}+1/2, x+1/2, y+1/2$	$[w, \bar{u}, \bar{v}]$	(31)	$z+1/2, x+1/2, \bar{y}+1/2$	$[\bar{w}, \bar{u}, v]$	(32)	$z+1/2, \bar{x}+1/2, y+1/2$	$[\bar{w}, u, \bar{v}]$
(33)	$\bar{y}+1/2, \bar{z}+1/2, \bar{x}+1/2$	$[v, w, u]$	(34)	$y+1/2, \bar{z}+1/2, x+1/2$	$[\bar{v}, w, \bar{u}]$	(35)	$\bar{y}+1/2, z+1/2, x+1/2$	$[v, \bar{w}, \bar{u}]$	(36)	$y+1/2, z+1/2, \bar{x}+1/2$	$[\bar{v}, w, u]$

(37) $\bar{y}, \bar{x}, z [v, u, \bar{w}]$	(38) $y, x, z [\bar{v}, \bar{u}, \bar{w}]$	(39) $\bar{y}, x, \bar{z} [v, \bar{u}, w]$	(40) $y, \bar{x}, \bar{z} [\bar{v}, u, w]$
(41) $\bar{x}, \bar{z}, y [u, w, \bar{v}]$	(42) $x, \bar{z}, \bar{y} [\bar{u}, w, v]$	(43) $x, z, y [\bar{u}, \bar{w}, \bar{v}]$	(44) $\bar{x}, z, \bar{y} [u, \bar{w}, v]$
(45) $\bar{z}, \bar{y}, x [w, v, \bar{u}]$	(46) $\bar{z}, y, \bar{x} [w, \bar{v}, u]$	(47) $z, \bar{y}, \bar{x} [\bar{w}, v, u]$	(48) $z, y, x [\bar{w}, \bar{v}, \bar{u}]$
48 k ..m			
$x, x, z [u, \bar{u}, 0]$	$\bar{x}, \bar{x}, z [\bar{u}, u, 0]$	$\bar{x}, x, \bar{z} [\bar{u}, \bar{u}, 0]$	$x, \bar{x}, \bar{z} [u, u, 0]$
$z, x, x [0, u, \bar{u}]$	$z, \bar{x}, \bar{x} [0, \bar{u}, u]$	$\bar{z}, \bar{x}, x [0, \bar{u}, \bar{u}]$	$\bar{z}, x, \bar{x} [0, u, u]$
$x, z, x [\bar{u}, 0, u]$	$\bar{x}, z, \bar{x} [u, 0, \bar{u}]$	$x, \bar{z}, \bar{x} [\bar{u}, 0, \bar{u}]$	$\bar{x}, \bar{z}, x [u, 0, u]$
$x+1/2, x+1/2, \bar{z}+1/2 [\bar{u}, u, 0]$	$\bar{x}+1/2, \bar{x}+1/2, \bar{z}+1/2 [u, \bar{u}, 0]$	$x+1/2, \bar{x}+1/2, z+1/2 [\bar{u}, \bar{u}, 0]$	$\bar{x}+1/2, x+1/2, z+1/2 [u, u, 0]$
$x+1/2, z+1/2, \bar{x}+1/2 [u, 0, u]$	$\bar{x}+1/2, z+1/2, x+1/2 [\bar{u}, 0, \bar{u}]$	$\bar{x}+1/2, \bar{z}+1/2, \bar{x}+1/2 [\bar{u}, 0, u]$	$x+1/2, \bar{z}+1/2, x+1/2 [u, 0, \bar{u}]$
$z+1/2, x+1/2, \bar{x}+1/2 [0, \bar{u}, \bar{u}]$	$z+1/2, \bar{x}+1/2, x+1/2 [0, u, u]$	$\bar{z}+1/2, x+1/2, x+1/2 [0, \bar{u}, u]$	$\bar{z}+1/2, \bar{x}+1/2, \bar{x}+1/2 [0, u, \bar{u}]$
48 j ..2'			
$1/4, y, y+1/2 [u, v, \bar{v}]$	$3/4, \bar{y}, y+1/2 [u, v, v]$	$3/4, y, \bar{y}+1/2 [\bar{u}, v, v]$	$1/4, \bar{y}, \bar{y}+1/2 [\bar{u}, v, \bar{v}]$
$y+1/2, 1/4, y [\bar{v}, u, v]$	$y+1/2, 3/4, \bar{y} [v, u, v]$	$\bar{y}+1/2, 3/4, y [v, \bar{u}, v]$	$\bar{y}+1/2, 1/4, \bar{y} [\bar{v}, \bar{u}, v]$
$y, y+1/2, 1/4 [v, \bar{v}, u]$	$\bar{y}, y+1/2, 3/4 [v, v, u]$	$y, \bar{y}+1/2, 3/4 [v, v, \bar{u}]$	$\bar{y}, \bar{y}+1/2, 1/4 [v, \bar{v}, \bar{u}]$
$1/4, \bar{y}+1/2, \bar{y} [u, v, \bar{v}]$	$3/4, y+1/2, \bar{y} [\bar{u}, \bar{v}, \bar{v}]$	$3/4, \bar{y}+1/2, y [u, \bar{v}, v]$	$1/4, y+1/2, y [\bar{u}, v, \bar{v}]$
$\bar{y}, 1/4, \bar{y}+1/2 [\bar{v}, u, v]$	$\bar{y}, 3/4, y+1/2 [\bar{v}, \bar{u}, \bar{v}]$	$y, 3/4, \bar{y}+1/2 [\bar{v}, u, \bar{v}]$	$y, 1/4, y+1/2 [\bar{v}, \bar{u}, v]$
$\bar{y}+1/2, \bar{y}, 1/4 [v, \bar{v}, u]$	$y+1/2, \bar{y}, 3/4 [\bar{v}, \bar{v}, \bar{u}]$	$\bar{y}+1/2, y, 3/4 [\bar{v}, \bar{v}, u]$	$y+1/2, y, 1/4 [v, \bar{v}, \bar{u}]$
48 i ..2			
$1/4, y, \bar{y}+1/2 [0, \bar{v}, v]$	$3/4, \bar{y}, \bar{y}+1/2 [0, \bar{v}, \bar{v}]$	$3/4, y, y+1/2 [0, \bar{v}, \bar{v}]$	$1/4, \bar{y}, y+1/2 [0, \bar{v}, v]$
$\bar{y}+1/2, 1/4, y [v, 0, \bar{v}]$	$\bar{y}+1/2, 3/4, \bar{y} [\bar{v}, 0, \bar{v}]$	$y+1/2, 3/4, y [\bar{v}, 0, \bar{v}]$	$y+1/2, 1/4, \bar{y} [v, 0, \bar{v}]$
$y, \bar{y}+1/2, 1/4 [\bar{v}, v, 0]$	$\bar{y}, \bar{y}+1/2, 3/4 [\bar{v}, \bar{v}, 0]$	$y, y+1/2, 3/4 [\bar{v}, \bar{v}, 0]$	$\bar{y}, y+1/2, 1/4 [\bar{v}, v, 0]$
$1/4, \bar{y}+1/2, y [0, \bar{v}, v]$	$3/4, y+1/2, y [0, v, v]$	$3/4, \bar{y}+1/2, \bar{y} [0, v, v]$	$1/4, y+1/2, \bar{y} [0, \bar{v}, v]$
$\bar{y}, 1/4, y+1/2 [v, 0, \bar{v}]$	$y, 3/4, y+1/2 [v, 0, v]$	$\bar{y}, 3/4, \bar{y}+1/2 [v, 0, v]$	$\bar{y}, 1/4, y+1/2 [v, 0, \bar{v}]$
$\bar{y}+1/2, y, 1/4 [\bar{v}, v, 0]$	$y+1/2, y, 3/4 [v, v, 0]$	$\bar{y}+1/2, \bar{y}, 3/4 [v, v, 0]$	$y+1/2, \bar{y}, 1/4 [\bar{v}, v, 0]$
48 h 2'..			
$x, 0, 1/2 [0, v, w]$	$\bar{x}, 0, 1/2 [0, \bar{v}, w]$	$1/2, x, 0 [w, 0, v]$	$1/2, \bar{x}, 0 [w, 0, \bar{v}]$
$0, 1/2, x [v, w, 0]$	$0, 1/2, \bar{x} [\bar{v}, w, 0]$	$1/2, x+1/2, 0 [v, 0, \bar{w}]$	$1/2, \bar{x}+1/2, 0 [\bar{v}, 0, \bar{w}]$
$x+1/2, 0, 1/2 [0, \bar{w}, v]$	$\bar{x}+1/2, 0, 1/2 [0, \bar{w}, \bar{v}]$	$0, 1/2, \bar{x}+1/2 [\bar{w}, \bar{v}, 0]$	$0, 1/2, x+1/2 [\bar{w}, v, 0]$

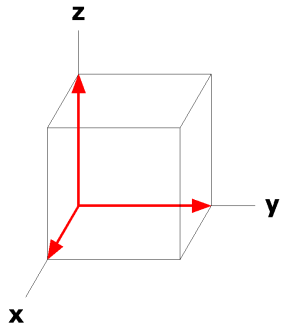
Continued			224.6.1616			$P_F n\bar{3}m$		
			$\bar{x}+1/2, 1/2, 0 [0, v, w]$	$x+1/2, 1/2, 0 [0, \bar{v}, w]$	$0, \bar{x}+1/2, 1/2 [w, 0, v]$	$0, x+1/2, 1/2 [w, 0, \bar{v}]$		
			$1/2, 0, \bar{x}+1/2 [v, w, 0]$	$1/2, 0, x+1/2 [\bar{v}, w, 0]$	$0, \bar{x}, 1/2 [v, 0, \bar{w}]$	$0, x, 1/2 [\bar{v}, 0, \bar{w}]$		
			$\bar{x}, 1/2, 0 [0, \bar{w}, v]$	$x, 1/2, 0 [0, \bar{w}, \bar{v}]$	$1/2, 0, x [\bar{w}, \bar{v}, 0]$	$1/2, 0, \bar{x} [\bar{w}, v, 0]$		
24	g	2.mm	$x, 0, 0 [0, 0, 0]$	$\bar{x}, 0, 0 [0, 0, 0]$	$0, x, 0 [0, 0, 0]$	$0, \bar{x}, 0 [0, 0, 0]$		
			$0, 0, x [0, 0, 0]$	$0, 0, \bar{x} [0, 0, 0]$	$1/2, x+1/2, 1/2 [0, 0, 0]$	$1/2, \bar{x}+1/2, 1/2 [0, 0, 0]$		
			$x+1/2, 1/2, 1/2 [0, 0, 0]$	$\bar{x}+1/2, 1/2, 1/2 [0, 0, 0]$	$1/2, 1/2, \bar{x}+1/2 [0, 0, 0]$	$1/2, 1/2, x+1/2 [0, 0, 0]$		
24	f	2'.2'2	$1/4, 0, 1/2 [0, \bar{v}, v]$	$3/4, 0, 1/2 [0, \bar{v}, \bar{v}]$	$1/2, 1/4, 0 [v, 0, \bar{v}]$			
			$1/2, 3/4, 0 [\bar{v}, 0, \bar{v}]$	$0, 1/2, 1/4 [\bar{v}, v, 0]$	$0, 1/2, 3/4 [\bar{v}, \bar{v}, 0]$			
			$1/4, 1/2, 0 [0, \bar{v}, v]$	$3/4, 1/2, 0 [0, v, v]$	$0, 1/4, 1/2 [v, 0, \bar{v}]$			
			$0, 3/4, 1/2 [v, 0, v]$	$1/2, 0, 1/4 [\bar{v}, v, 0]$	$1/2, 0, 3/4 [v, v, 0]$			
16	e	.3m	$x, x, x [0, 0, 0]$	$\bar{x}, \bar{x}, x [0, 0, 0]$				
			$\bar{x}, x, \bar{x} [0, 0, 0]$	$x, \bar{x}, \bar{x} [0, 0, 0]$				
			$x+1/2, x+1/2, \bar{x}+1/2 [0, 0, 0]$	$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [0, 0, 0]$				
			$x+1/2, \bar{x}+1/2, x+1/2 [0, 0, 0]$	$\bar{x}+1/2, x+1/2, x+1/2 [0, 0, 0]$				
12	d	$\bar{4}'2'.m$	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$			
			$0, 1/2, 0 [0, 0, 0]$	$1/2, 0, 0 [0, 0, 0]$	$0, 0, 1/2 [0, 0, 0]$			
8	c	$\bar{3}'m$	$3/4, 3/4, 3/4 [0, 0, 0]$	$1/4, 1/4, 3/4 [0, 0, 0]$	$1/4, 3/4, 1/4 [0, 0, 0]$	$3/4, 1/4, 1/4 [0, 0, 0]$		
8	b	$\bar{3}m$	$1/4, 1/4, 1/4 [0, 0, 0]$	$3/4, 3/4, 1/4 [0, 0, 0]$	$3/4, 1/4, 3/4 [0, 0, 0]$	$1/4, 3/4, 3/4 [0, 0, 0]$		
4	a	$\bar{4}3m$	$0, 0, 0 [0, 0, 0]$	$1/2, 1/2, 1/2 [0, 0, 0]$				

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0, 0, z$

Along  $[1, 1, 1]$   $p6mm1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

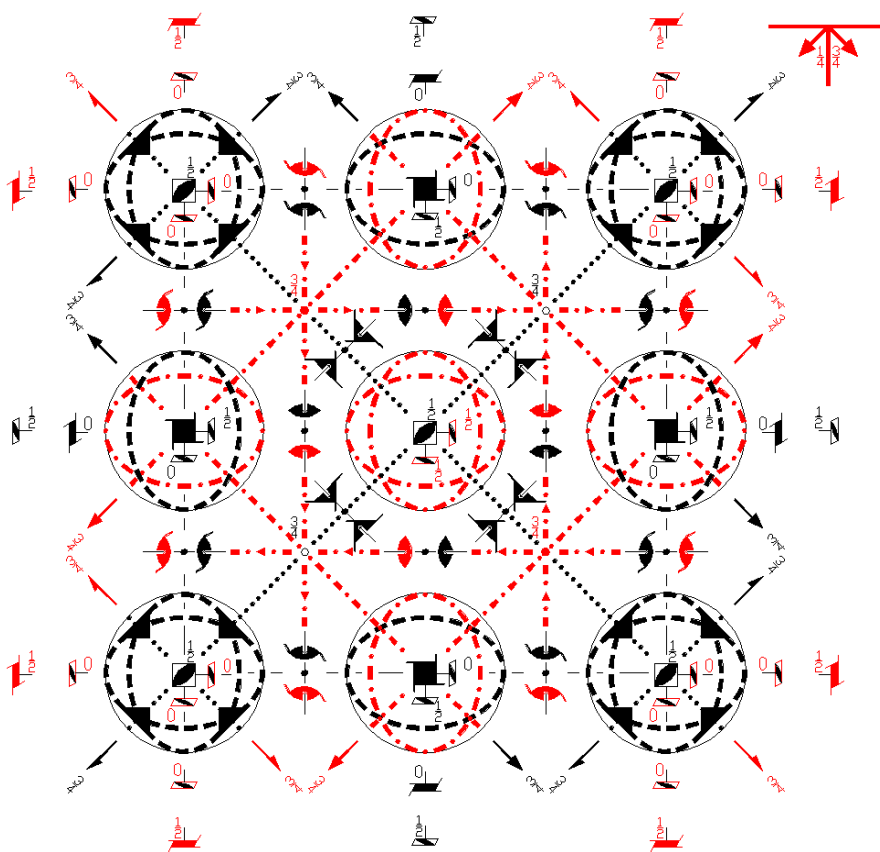
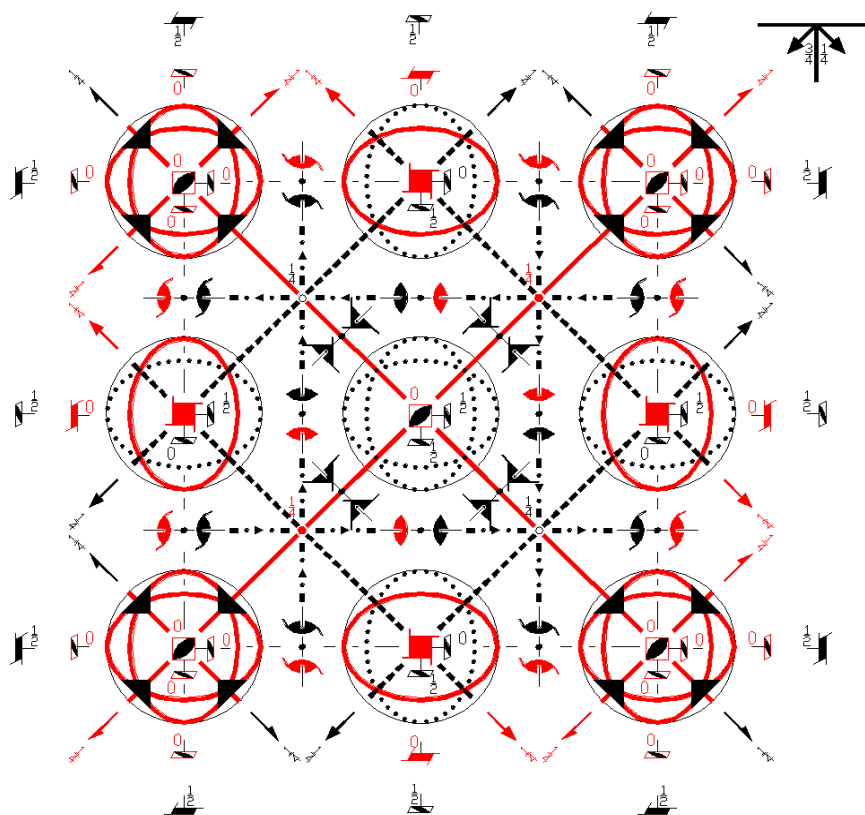
Along  $[1, 1, 0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 1/4$



$P_F n\bar{3}m'$   
224.7.1617

$n\bar{3}m1'$   
 $P_F 4_2'/n\bar{3}2'/m'$

Cubic



**Origin** at  $\bar{4}'3m'$ , at  $-1/4, -1/4, -1/4$  from center ( $\bar{3}m'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad -1/4 \leq z \leq 1/4; \quad y \leq x; \quad \max(x-1/2, -y) \leq z \leq \min(1/2-x, y)$

Vertices  $0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/4,1/4,1/4 \quad 1/4,1/4,-1/4$

### Symmetry Operations

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                   | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0)          | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0)  | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0)  |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)                     | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)                      | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)                | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)               |
| (13) 2' (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'                          | (14) 2' x, $\bar{x}+1/2,1/4$<br>(2 <sub><math>\bar{x}y</math></sub>  1/2,1/2,1/2)'                            | (15) 4 <sup>-</sup> ' (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'                | (16) 4 <sup>+</sup> ' (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>  1/2,1/2,1/2)'                             |
| (17) 4 <sup>-</sup> ' (1/2,0,0) x,1/2,0<br>(4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,1/2)' | (18) 2' (0,1/2,1/2) 1/4,y,y<br>(2 <sub>yz</sub>  1/2,1/2,1/2)'  | (19) 2' 1/4,y+1/2, $\bar{y}$<br>(2 <sub>yz</sub>  1/2,1/2,1/2)'  | (20) 4 <sup>+</sup> ' (1/2,0,0) x,0,1/2<br>(4 <sub>x</sub>  1/2,1/2,1/2)'                             |
| (21) 4 <sup>+</sup> ' (0,1/2,0) 1/2,y,0<br>(4 <sub>y</sub>  1/2,1/2,1/2)'               | (22) 2' (1/2,0,1/2) x,1/4,x<br>(2 <sub>zx</sub>  1/2,1/2,1/2)'  | (23) 4 <sup>-</sup> ' (0,1/2,0) 0,y,1/2<br>(4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,1/2)'                | (24) 2' $\bar{x}+1/2,1/4,x$<br>(2 <sub><math>\bar{z}x</math></sub>  1/2,1/2,1/2)'                     |
| (25) $\bar{1}$ 1/4,1/4,1/4<br>( $\bar{1}$  1/2,1/2,1/2)                                 | (26) n (1/2,1/2,0) x,y,1/4<br>(m <sub>z</sub>  1/2,1/2,1/2)   | (27) n (1/2,0,1/2) x,1/4,z<br>(m <sub>y</sub>  1/2,1/2,1/2)  | (28) n (0,1/2,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,1/2)   |
| (29) $\bar{3}^+$ x,x,x; 1/4,1/4,1/4<br>( $\bar{3}_{xyz}$  1/2,1/2,1/2)                  | (30) $\bar{3}^+$ $\bar{x}-1,x+1,\bar{x}; -1/4,1/4,3/4$<br>( $\bar{3}_{\bar{x}yz}$ <sup>-1</sup>  1/2,1/2,1/2) | (31) $\bar{3}^+$ x, $\bar{x}+1,\bar{x}; 1/4,3/4,-1/4$<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,1/2,1/2) | (32) $\bar{3}^+$ $\bar{x}+1,\bar{x},x; 3/4,-1/4,1/4$<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,1/2,1/2) |
| (33) $\bar{3}^-$ x,x,x; 1/4,1/4,1/4<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,1/2,1/2)    | (34) $\bar{3}^-$ x+1, $\bar{x}-1,\bar{x}; 1/4,-1/4,3/4$<br>( $\bar{3}_{xyz}$  1/2,1/2,1/2)                    | (35) $\bar{3}^-$ $\bar{x},\bar{x}+1,x; -1/4,3/4,1/4$<br>( $\bar{3}_{xyz}$  1/2,1/2,1/2)                | (36) $\bar{3}^-$ $\bar{x}+1,x,\bar{x}; 3/4,1/4,-1/4$<br>( $\bar{3}_{xyz}$  1/2,1/2,1/2)               |
| (37) m' x, $\bar{x},z$<br>(m <sub>xy</sub>  0,0,0)'                                     | (38) m' x,x,z<br>(m <sub><math>\bar{x}y</math></sub>  0,0,0)'   | (39) $\bar{4}^-$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z$ <sup>-1</sup>  0,0,0)'                                | (40) $\bar{4}^+$ ' 0,0,z; 0,0,0<br>( $\bar{4}_z$  0,0,0)'   |
| (41) $\bar{4}^-$ ' x,0,0; 0,0,0<br>( $\bar{4}_x$ <sup>-1</sup>  0,0,0)'                 | (42) m' x,y, $\bar{y}$<br>(m <sub>yz</sub>  0,0,0)'   | (43) m' x,y,y<br>(m <sub><math>\bar{y}z</math></sub>  0,0,0)'  | (44) $\bar{4}^+$ ' x,0,0; 0,0,0<br>( $\bar{4}_x$  0,0,0)'   |
| (45) $\bar{4}^+$ ' 0,y,0; 0,0,0<br>( $\bar{4}_y$  0,0,0)'                               | (46) m' $\bar{x},y,x$<br>(m <sub><math>\bar{z}x</math></sub>  0,0,0)'   | (47) $\bar{4}^-$ ' 0,y,0; 0,0,0<br>( $\bar{4}_y$ <sup>-1</sup>  0,0,0)'                                | (48) m' x,y,x<br>(m <sub><math>\bar{z}x</math></sub>  0,0,0)'   |

For (1,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) $\bar{t}$ (1,0,0)<br>( $\bar{1}$  1,0,0)'   | (2) 2' 1/2,0,z<br>(2 <sub>z</sub>  1,0,0)'  | (3) 2' 1/2,y,0<br>(2 <sub>y</sub>  1,0,0)'   | (4) 2' (1,0,0) x,0,0<br>(2 <sub>x</sub>  1,0,0)'  |
| (5) 3 <sup>+</sup> ' (1/3,1/3,1/3)<br>x+2/3,x+1/3,x<br>(3 <sub>xyz</sub>  1,0,0)'               | (6) 3 <sup>+</sup> ' (1/3,-1/3,1/3)<br>x+2/3,x-1/3,x<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  1,0,0)' | (7) 3 <sup>+</sup> ' (1/3,-1/3,-1/3)<br>x+2/3,x-1/3,x<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  1,0,0)' | (8) 3 <sup>+</sup> ' (1/3,1/3,-1/3)<br>x+2/3,x-1/3,x<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  1,0,0)' |
| (9) 3 <sup>-</sup> ' (1/3,1/3,1/3)<br>x+1/3,x-1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1,0,0)' | (10) 3 <sup>-</sup> ' (1/3,-1/3,-1/3)<br>x+1/3,x+1/3,x<br>(3 <sub><math>\bar{x}yz</math></sub>  1,0,0)'             | (11) 3 <sup>-</sup> ' (1/3,1/3,-1/3)<br>x+1/3,x-1/3,x<br>(3 <sub><math>\bar{x}yz</math></sub>  1,0,0)'               | (12) 3 <sup>-</sup> ' (1/3,-1/3,1/3)<br>x+1/3,x+1/3,x<br>(3 <sub><math>\bar{x}yz</math></sub>  1,0,0)'              |

(13) $2 \quad x+1/2, x, 1/4$ ( $2_{xy}   3/2, 1/2, 1/2$ )	(14) $2 \quad (1/2, 1/2, 0) \quad x, \bar{x}, 1/4$ ( $2_{\bar{xy}}   3/2, 1/2, 1/2$ )	(15) $4^- \quad (0, 0, 1/2) \quad 1, -1/2, z$ ( $4_z^-   3/2, 1/2, 1/2$ )	(16) $4^+ \quad (0, 0, 1/2) \quad 1/2, 1, z$ ( $4_z   3/2, 1/2, 1/2$ )
(17) $4^- \quad (3/2, 0, 0) \quad x, 1/2, 0$ ( $4_x^-   3/2, 1/2, 1/2$ )	(18) $2 \quad (0, 1/2, 1/2) \quad 3/4, y, y$ ( $2_{yz}   3/2, 1/2, 1/2$ )	(19) $2 \quad 3/4, y+1/2, \bar{y}$ ( $2_{\bar{yz}}   3/2, 1/2, 1/2$ )	(20) $4^+ \quad (3/2, 0, 0) \quad x, 0, 1/2$ ( $4_x   3/2, 1/2, 1/2$ )
(21) $4^+ \quad (0, 1/2, 0) \quad 1, y, -1/2$ ( $4_y   3/2, 1/2, 1/2$ )	(22) $2 \quad x+1/2, 1/4, x$ ( $2_{xz}   3/2, 1/2, 1/2$ )	(23) $4^- \quad (0, 1/2, 0) \quad 1/2, y, 1$ ( $4_y^-   3/2, 1/2, 1/2$ )	(24) $2 \quad (1/2, 0, -1/2) \quad \bar{x}+1, 1/4, x$ ( $2_{\bar{xz}}   3/2, 1/2, 1/2$ )
(25) $\bar{1} \quad 3/4, 1/4, 1/4$ ( $\bar{1}   3/2, 1/2, 1/2$ )'	(26) $n' \quad (3/2, 1/2, 0) \quad x, y, 1/4$ ( $m_z   3/2, 1/2, 1/2$ )'	(27) $n' \quad (3/2, 0, 1/2) \quad x, 1/4, z$ ( $m_y   3/2, 1/2, 1/2$ )'	(28) $n' \quad (0, 1/2, 1/2) \quad 3/4, y, z$ ( $m_x   3/2, 1/2, 1/2$ )'
(29) $\bar{3}^+ \quad x, x-1, x;$ $3/4, 1/4, 3/4$ ( $\bar{3}_{xyz}   3/2, 1/2, 1/2$ )'	(30) $\bar{3}^+ \quad \bar{x}-1, x-2, \bar{x};$ $1/4, 3/4, 5/4$ ( $\bar{3}_{\bar{xyz}}^{-1}   3/2, 1/2, 1/2$ )'	(31) $\bar{3}^+ \quad x, \bar{x}+2, \bar{x};$ $3/4, 5/4, -3/4$ ( $\bar{3}_{\bar{yz}}^{-1}   3/2, 1/2, 1/2$ )'	(32) $\bar{3}^+ \quad \bar{x}+1, \bar{x}-1, x;$ $5/4, -3/4, -1/4$ ( $\bar{3}_{\bar{yz}}^{-1}   3/2, 1/2, 1/2$ )'
(33) $\bar{3}^- \quad x+1, x+1, x;$ $3/4, 3/4, -1/4$ ( $\bar{3}_{xyz}^{-1}   3/2, 1/2, 1/2$ )'	(34) $\bar{3}^- \quad x+2, \bar{x}-2, \bar{x};$ $3/4, -3/4, 5/4$ ( $\bar{3}_{\bar{xyz}}   3/2, 1/2, 1/2$ )'	(35) $\bar{3}^- \quad \bar{x}+1, \bar{x}+2, x;$ $1/4, 5/4, 3/4$ ( $\bar{3}_{\bar{yz}}   3/2, 1/2, 1/2$ )'	(36) $\bar{3}^- \quad \bar{x}+2, x-1, \bar{x};$ $5/4, -1/4, -3/4$ ( $\bar{3}_{\bar{xyz}}   3/2, 1/2, 1/2$ )'
(37) $g \quad (1/2, -1/2, 0) \quad x+1/2, \bar{x}, z$ ( $m_{xy}   1, 0, 0$ )	(38) $g \quad (1/2, 1/2, 0) \quad x+1/2, x, z$ ( $m_{\bar{xy}}   1, 0, 0$ )	(39) $\bar{4}^- \quad 1/2, 1/2, z; 1/2, 1/2, 0$ ( $\bar{4}_z^-   1, 0, 0$ )	(40) $\bar{4}^+ \quad 1/2, -1/2, z; 1/2, -1/2, 0$ ( $\bar{4}_z   1, 0, 0$ )
(41) $\bar{4}^- \quad x+1/2, 0, 0; 1/2, 0, 0$ ( $\bar{4}_x^-   1, 0, 0$ )	(42) $a \quad (1, 0, 0) \quad x, y, \bar{y}$ ( $m_{yz}   1, 0, 0$ )	(43) $a \quad (1, 0, 0) \quad x, y, y$ ( $m_{\bar{yz}}   1, 0, 0$ )	(44) $\bar{4}^+ \quad x+1/2, 0, 0; 1/2, 0, 0$ ( $\bar{4}_x   1, 0, 0$ )
(45) $\bar{4}^+ \quad 1/2, y, 1/2; 1/2, 0, 1/2$ ( $\bar{4}_y   1, 0, 0$ )	(46) $g \quad (1/2, 0, -1/2) \quad \bar{x}+1/2, y, x$ ( $m_{xz}   1, 0, 0$ )	(47) $\bar{4}^- \quad 1/2, y, -1/2; 0, 0, 0$ ( $\bar{4}_y^-   1, 0, 0$ )	(48) $g \quad (1/2, 0, 1/2) \quad x+1/2, y, x$ ( $m_{\bar{xz}}   1, 0, 0$ )

**Generators selected** (1);  $t'(1, 0, 0)$ ;  $t'(0, 1, 0)$ ;  $t'(0, 0, 1)$ ; (2); (3); (5); (13); (25).

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

96		1	(0,0,0) +	(1,0,0)' +							
(1)	$x, y, z$	$[u, v, w]$	(2)	$\bar{x}, \bar{y}, z$	$[\bar{u}, \bar{v}, w]$	(3)	$\bar{x}, y, \bar{z}$	$[\bar{u}, v, \bar{w}]$	(4)	$x, \bar{y}, \bar{z}$	$[u, \bar{v}, \bar{w}]$
(5)	$z, x, y$	$[w, u, v]$	(6)	$z, \bar{x}, \bar{y}$	$[w, \bar{u}, \bar{v}]$	(7)	$\bar{z}, \bar{x}, y$	$[\bar{w}, \bar{u}, v]$	(8)	$\bar{z}, x, \bar{y}$	$[\bar{w}, u, \bar{v}]$
(9)	$y, z, x$	$[v, w, u]$	(10)	$\bar{y}, z, \bar{x}$	$[\bar{v}, w, \bar{u}]$	(11)	$y, \bar{z}, \bar{x}$	$[v, \bar{w}, \bar{u}]$	(12)	$\bar{y}, z, x$	$[\bar{v}, w, u]$
(13)	$y+1/2, x+1/2, \bar{z}+1/2$	$[\bar{v}, \bar{u}, w]$	(14)	$\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2$	$[v, u, w]$	(15)	$y+1/2, \bar{x}+1/2, z+1/2$	$[\bar{v}, u, \bar{w}]$	(16)	$\bar{y}+1/2, x+1/2, z+1/2$	$[v, \bar{u}, \bar{w}]$
(17)	$x+1/2, z+1/2, \bar{y}+1/2$	$[\bar{u}, \bar{w}, v]$	(18)	$\bar{x}+1/2, z+1/2, y+1/2$	$[u, \bar{w}, \bar{v}]$	(19)	$\bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2$	$[u, w, v]$	(20)	$x+1/2, \bar{z}+1/2, y+1/2$	$[\bar{u}, w, \bar{v}]$
(21)	$z+1/2, y+1/2, \bar{x}+1/2$	$[\bar{w}, \bar{v}, u]$	(22)	$z+1/2, \bar{y}+1/2, x+1/2$	$[\bar{w}, v, \bar{u}]$	(23)	$\bar{z}+1/2, y+1/2, x+1/2$	$[w, \bar{v}, \bar{u}]$	(24)	$\bar{z}+1/2, \bar{y}+1/2, \bar{x}+1/2$	$[w, v, u]$
(25)	$\bar{x}+1/2, \bar{y}+1/2, \bar{z}+1/2$	$[u, v, w]$	(26)	$x+1/2, y+1/2, \bar{z}+1/2$	$[\bar{u}, \bar{v}, w]$	(27)	$x+1/2, \bar{y}+1/2, z+1/2$	$[\bar{u}, v, \bar{w}]$	(28)	$\bar{x}+1/2, y+1/2, z+1/2$	$[u, \bar{v}, \bar{w}]$
(29)	$\bar{z}+1/2, \bar{x}+1/2, \bar{y}+1/2$	$[w, u, v]$	(30)	$\bar{z}+1/2, x+1/2, y+1/2$	$[w, \bar{u}, \bar{v}]$	(31)	$z+1/2, x+1/2, \bar{y}+1/2$	$[\bar{w}, \bar{u}, v]$	(32)	$z+1/2, \bar{x}+1/2, y+1/2$	$[\bar{w}, u, \bar{v}]$
(33)	$\bar{y}+1/2, \bar{z}+1/2, \bar{x}+1/2$	$[v, w, u]$	(34)	$y+1/2, \bar{z}+1/2, x+1/2$	$[\bar{v}, w, \bar{u}]$	(35)	$\bar{y}+1/2, z+1/2, x+1/2$	$[v, \bar{w}, \bar{u}]$	(36)	$y+1/2, z+1/2, \bar{x}+1/2$	$[\bar{v}, w, u]$



(37) $\bar{y}, \bar{x}, z [\bar{v}, \bar{u}, w]$	(38) $y, x, z [v, u, w]$	(39) $\bar{y}, x, \bar{z} [\bar{v}, u, \bar{w}]$	(40) $y, \bar{x}, \bar{z} [v, \bar{u}, \bar{w}]$
(41) $\bar{x}, \bar{z}, y [\bar{u}, \bar{w}, v]$	(42) $x, \bar{z}, y [u, \bar{w}, \bar{v}]$	(43) $x, z, y [u, w, v]$	(44) $\bar{x}, z, y [\bar{u}, w, \bar{v}]$
(45) $\bar{z}, \bar{y}, x [\bar{w}, \bar{v}, u]$	(46) $\bar{z}, y, x [\bar{w}, v, \bar{u}]$	(47) $z, \bar{y}, x [w, \bar{v}, \bar{u}]$	(48) $z, y, x [w, v, u]$
48 k ..m'			
$x, x, z [u, u, w]$	$\bar{x}, \bar{x}, z [\bar{u}, \bar{u}, w]$	$\bar{x}, x, \bar{z} [\bar{u}, u, \bar{w}]$	$x, \bar{x}, \bar{z} [u, \bar{u}, \bar{w}]$
$z, x, x [w, u, u]$	$z, \bar{x}, \bar{x} [\bar{w}, \bar{u}, \bar{u}]$	$\bar{z}, \bar{x}, x [\bar{w}, \bar{u}, u]$	$\bar{z}, x, \bar{x} [\bar{w}, u, \bar{u}]$
$x, z, x [u, w, u]$	$\bar{x}, z, \bar{x} [\bar{u}, w, \bar{u}]$	$x, \bar{z}, \bar{x} [u, w, \bar{u}]$	$\bar{x}, \bar{z}, x [\bar{u}, \bar{w}, u]$
$x+1/2, x+1/2, \bar{z}+1/2 [\bar{u}, \bar{u}, w]$	$\bar{x}+1/2, \bar{x}+1/2, \bar{z}+1/2 [u, u, w]$	$x+1/2, \bar{x}+1/2, z+1/2 [\bar{u}, u, \bar{w}]$	$\bar{x}+1/2, x+1/2, z+1/2 [u, \bar{u}, \bar{w}]$
$x+1/2, z+1/2, \bar{x}+1/2 [\bar{u}, \bar{w}, u]$	$\bar{x}+1/2, z+1/2, x+1/2 [u, \bar{w}, \bar{u}]$	$\bar{x}+1/2, \bar{z}+1/2, \bar{x}+1/2 [u, w, u]$	$x+1/2, \bar{z}+1/2, x+1/2 [\bar{u}, w, \bar{u}]$
$z+1/2, x+1/2, \bar{x}+1/2 [\bar{w}, \bar{u}, u]$	$z+1/2, \bar{x}+1/2, x+1/2 [\bar{w}, u, \bar{u}]$	$\bar{z}+1/2, x+1/2, x+1/2 [w, \bar{u}, \bar{u}]$	$\bar{z}+1/2, \bar{x}+1/2, \bar{x}+1/2 [w, u, u]$
48 j ..2			
$1/4, y, y+1/2 [0, v, v]$	$3/4, \bar{y}, y+1/2 [0, v, \bar{v}]$	$3/4, y, \bar{y}+1/2 [0, v, \bar{v}]$	$1/4, \bar{y}, \bar{y}+1/2 [0, v, v]$
$y+1/2, 1/4, y [v, 0, v]$	$y+1/2, 3/4, \bar{y} [\bar{v}, 0, v]$	$\bar{y}+1/2, 3/4, y [\bar{v}, 0, v]$	$\bar{y}+1/2, 1/4, \bar{y} [v, 0, v]$
$y, y+1/2, 1/4 [v, v, 0]$	$\bar{y}, y+1/2, 3/4 [v, \bar{v}, 0]$	$y, \bar{y}+1/2, 3/4 [v, \bar{v}, 0]$	$\bar{y}, \bar{y}+1/2, 1/4 [v, v, 0]$
$1/4, \bar{y}+1/2, \bar{y} [0, v, v]$	$3/4, y+1/2, \bar{y} [0, \bar{v}, v]$	$3/4, \bar{y}+1/2, y [0, \bar{v}, v]$	$1/4, y+1/2, y [0, v, v]$
$\bar{y}, 1/4, \bar{y}+1/2 [v, 0, v]$	$\bar{y}, 3/4, y+1/2 [v, 0, \bar{v}]$	$y, 3/4, \bar{y}+1/2 [v, 0, \bar{v}]$	$y, 1/4, y+1/2 [v, 0, v]$
$\bar{y}+1/2, \bar{y}, 1/4 [v, v, 0]$	$y+1/2, \bar{y}, 3/4 [\bar{v}, v, 0]$	$\bar{y}+1/2, y, 3/4 [\bar{v}, v, 0]$	$y+1/2, y, 1/4 [v, v, 0]$
48 i ..2'			
$1/4, y, \bar{y}+1/2 [u, v, v]$	$3/4, \bar{y}, \bar{y}+1/2 [u, v, \bar{v}]$	$3/4, y, y+1/2 [\bar{u}, v, \bar{v}]$	$1/4, \bar{y}, y+1/2 [\bar{u}, v, v]$
$\bar{y}+1/2, 1/4, y [v, u, v]$	$\bar{y}+1/2, 3/4, \bar{y} [\bar{v}, u, v]$	$y+1/2, 3/4, y [\bar{v}, \bar{u}, v]$	$y+1/2, 1/4, \bar{y} [v, \bar{u}, v]$
$y, \bar{y}+1/2, 1/4 [v, v, u]$	$\bar{y}, \bar{y}+1/2, 3/4 [v, \bar{v}, u]$	$y, y+1/2, 3/4 [v, \bar{v}, \bar{u}]$	$\bar{y}, y+1/2, 1/4 [v, v, \bar{u}]$
$1/4, \bar{y}+1/2, y [u, v, v]$	$3/4, y+1/2, y [\bar{u}, \bar{v}, v]$	$3/4, \bar{y}+1/2, \bar{y} [u, \bar{v}, v]$	$1/4, y+1/2, \bar{y} [\bar{u}, v, v]$
$\bar{y}, 1/4, y+1/2 [v, u, v]$	$y, 3/4, y+1/2 [v, \bar{u}, \bar{v}]$	$\bar{y}, 3/4, \bar{y}+1/2 [v, u, \bar{v}]$	$\bar{y}, 1/4, y+1/2 [v, \bar{u}, v]$
$\bar{y}+1/2, y, 1/4 [v, v, u]$	$y+1/2, y, 3/4 [\bar{v}, v, \bar{u}]$	$\bar{y}+1/2, \bar{y}, 3/4 [\bar{v}, v, u]$	$y+1/2, \bar{y}, 1/4 [v, v, \bar{u}]$
48 h 2'..			
$x, 0, 1/2 [0, v, w]$	$\bar{x}, 0, 1/2 [0, \bar{v}, w]$	$1/2, x, 0 [w, 0, v]$	$1/2, \bar{x}, 0 [w, 0, \bar{v}]$
$0, 1/2, x [v, w, 0]$	$0, 1/2, \bar{x} [\bar{v}, w, 0]$	$1/2, x+1/2, 0 [\bar{v}, 0, w]$	$1/2, \bar{x}+1/2, 0 [v, 0, w]$
$x+1/2, 0, 1/2 [0, w, \bar{v}]$	$\bar{x}+1/2, 0, 1/2 [0, w, v]$	$0, 1/2, \bar{x}+1/2 [w, v, 0]$	$0, 1/2, x+1/2 [w, \bar{v}, 0]$

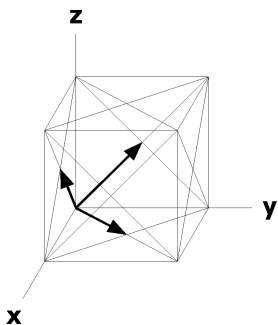
Continued		224.7.1617		$P_6 n\bar{3}m'$		
		$\bar{x}+1/2, 1/2, 0 [0, v, w]$	$x+1/2, 1/2, 0 [0, \bar{v}, w]$	$0, \bar{x}+1/2, 1/2 [w, 0, v]$	$0, x+1/2, 1/2 [w, 0, \bar{v}]$	
		$1/2, 0, \bar{x}+1/2 [v, w, 0]$	$1/2, 0, x+1/2 [\bar{v}, w, 0]$	$0, \bar{x}, 1/2 [\bar{v}, 0, w]$	$0, x, 1/2 [v, 0, w]$	
		$\bar{x}, 1/2, 0 [0, w, \bar{v}]$	$x, 1/2, 0 [0, w, v]$	$1/2, 0, x [w, v, 0]$	$1/2, 0, \bar{x} [w, \bar{v}, 0]$	
24	g	2.m'm'	$x, 0, 0 [u, 0, 0]$	$\bar{x}, 0, 0 [\bar{u}, 0, 0]$	$0, x, 0 [0, u, 0]$	$0, \bar{x}, 0 [0, \bar{u}, 0]$
			$0, 0, x [0, 0, u]$	$0, 0, \bar{x} [0, 0, \bar{u}]$	$1/2, x+1/2, 1/2 [0, \bar{u}, 0]$	$1/2, \bar{x}+1/2, 1/2 [0, u, 0]$
			$x+1/2, 1/2, 1/2 [\bar{u}, 0, 0]$	$\bar{x}+1/2, 1/2, 1/2 [u, 0, 0]$	$1/2, 1/2, \bar{x}+1/2 [0, 0, u]$	$1/2, 1/2, x+1/2 [0, 0, \bar{u}]$
24	f	2'.22'	$1/4, 0, 1/2 [0, v, v]$	$3/4, 0, 1/2 [0, v, \bar{v}]$	$1/2, 1/4, 0 [v, 0, v]$	
			$1/2, 3/4, 0 [\bar{v}, 0, v]$	$0, 1/2, 1/4 [v, v, 0]$	$0, 1/2, 3/4 [v, \bar{v}, 0]$	
			$1/4, 1/2, 0 [0, v, v]$	$3/4, 1/2, 0 [0, \bar{v}, v]$	$0, 1/4, 1/2 [v, 0, v]$	
			$0, 3/4, 1/2 [v, 0, \bar{v}]$	$1/2, 0, 1/4 [v, v, 0]$	$1/2, 0, 3/4 [\bar{v}, v, 0]$	
16	e	.3m'	$x, x, x [u, u, u]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$		
			$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$		
			$x+1/2, x+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, u]$	$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [u, u, u]$		
			$x+1/2, \bar{x}+1/2, x+1/2 [\bar{u}, u, \bar{u}]$	$\bar{x}+1/2, x+1/2, x+1/2 [u, \bar{u}, \bar{u}]$		
12	d	$\bar{4}2'.m'$	$0, 1/2, 1/2 [u, 0, 0]$	$1/2, 0, 1/2 [0, u, 0]$	$1/2, 1/2, 0 [0, 0, u]$	
			$0, 1/2, 0 [0, u, 0]$	$1/2, 0, 0 [u, 0, 0]$	$0, 0, 1/2 [0, 0, u]$	
8	c	$\bar{3}m'$	$3/4, 3/4, 3/4 [0, 0, 0]$	$1/4, 1/4, 3/4 [0, 0, 0]$	$1/4, 3/4, 1/4 [0, 0, 0]$	$3/4, 1/4, 1/4 [0, 0, 0]$
8	b	$\bar{3}m'$	$1/4, 1/4, 1/4 [u, u, u]$	$3/4, 3/4, 1/4 [\bar{u}, \bar{u}, u]$	$3/4, 1/4, 3/4 [\bar{u}, u, \bar{u}]$	$1/4, 3/4, 3/4 [u, \bar{u}, \bar{u}]$
4	a	$\bar{4}3m'$	$0, 0, 0 [0, 0, 0]$	$1/2, 1/2, 1/2 [0, 0, 0]$		

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0, 0, z$

Along  $[1, 1, 1]$   $p6mm1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

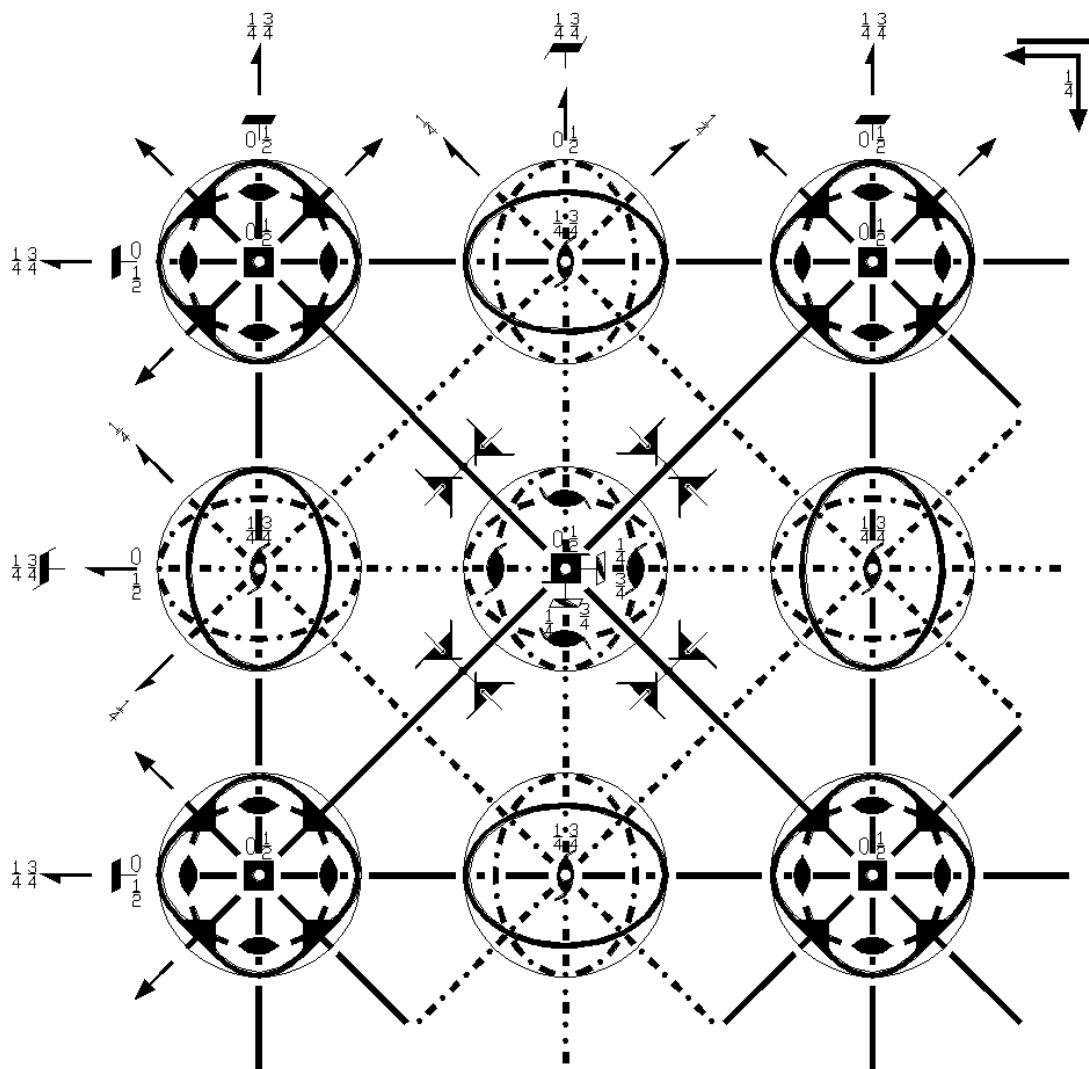
Along  $[1, 1, 0]$   $p_6c_2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x-1/4, x+1/4, 1/4$



$Fm\bar{3}m$   
225.1.1618

$m\bar{3}m$   
 $F4/m\bar{3}2/m$

Cubic



**Origin** at center ( $m\bar{3}m$ )

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/4$ ;  $y \leq \min(x, 1/2-x)$ ;  $z \leq y$

**Vertices** 0,0,0      1/2,0,0      1/4,1/4,0      1/4,1/4,1/4

**Symmetry Operations**

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                         | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)    | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)      | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)     |

(13) $2 \ x,x,0$ ( $2_{xy} 0,0,0$ )	(14) $2 \ x,\bar{x},0$ ( $2_{\bar{xy}} 0,0,0$ )	(15) $4^- \ 0,0,z$ ( $4_z^{-1} 0,0,0$ )	(16) $4^+ \ 0,0,z$ ( $4_z 0,0,0$ )
(17) $4^- \ x,0,0$ ( $4_x^{-1} 0,0,0$ )	(18) $2 \ 0,y,y$ ( $2_{yz} 0,0,0$ )	(19) $2 \ 0,y,\bar{y}$ ( $2_{\bar{yz}} 0,0,0$ )	(20) $4^+ \ x,0,0$ ( $4_x 0,0,0$ )
(21) $4^+ \ 0,y,0$ ( $4_y 0,0,0$ )	(22) $2 \ x,0,x$ ( $2_{xz} 0,0,0$ )	(23) $4^- \ 0,y,0$ ( $4_y^{-1} 0,0,0$ )	(24) $2 \ \bar{x},0,x$ ( $2_{\bar{xz}} 0,0,0$ )
(25) $\bar{1} \ 0,0,0$ ( $\bar{1} 0,0,0$ )	(26) $m \ x,y,0$ ( $m_z 0,0,0$ )	(27) $m \ x,0,z$ ( $m_y 0,0,0$ )	(28) $m \ 0,y,z$ ( $m_x 0,0,0$ )
(29) $\bar{3}^+ \ x,x,x; 0,0,0$ ( $\bar{3}_{xyz} 0,0,0$ )	(30) $\bar{3}^+ \ \bar{x},\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{xyz}}^{-1} 0,0,0$ )	(31) $\bar{3}^+ \ x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{xy}z}^{-1} 0,0,0$ )	(32) $\bar{3}^+ \ \bar{x},\bar{x},x; 0,0,0$ ( $\bar{3}_{xy\bar{z}}^{-1} 0,0,0$ )
(33) $\bar{3}^- \ x,x,x; 0,0,0$ ( $\bar{3}_{xyz}^{-1} 0,0,0$ )	(34) $\bar{3}^- \ x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{xyz}} 0,0,0$ )	(35) $\bar{3}^- \ \bar{x},\bar{x},x; 0,0,0$ ( $\bar{3}_{\bar{xy}z}^{-1} 0,0,0$ )	(36) $\bar{3}^- \ \bar{x},x,\bar{x}; 0,0,0$ ( $\bar{3}_{x\bar{y}z}^{-1} 0,0,0$ )
(37) $m \ x,\bar{x},z$ ( $m_{xy} 0,0,0$ )	(38) $m \ x,x,z$ ( $m_{\bar{xy}} 0,0,0$ )	(39) $\bar{4}^- \ 0,0,z; 0,0,0$ ( $\bar{4}_z^{-1} 0,0,0$ )	(40) $\bar{4}^+ \ 0,0,z; 0,0,0$ ( $\bar{4}_z 0,0,0$ )
(41) $\bar{4}^- \ x,0,0; 0,0,0$ ( $\bar{4}_x^{-1} 0,0,0$ )	(42) $m \ x,y,\bar{y}$ ( $m_{yz} 0,0,0$ )	(43) $m \ x,y,y$ ( $m_{\bar{yz}} 0,0,0$ )	(44) $\bar{4}^+ \ x,0,0; 0,0,0$ ( $\bar{4}_x 0,0,0$ )
(45) $\bar{4}^+ \ 0,y,0; 0,0,0$ ( $\bar{4}_y 0,0,0$ )	(46) $m \ \bar{x},y,x$ ( $m_{xz} 0,0,0$ )	(47) $\bar{4}^- \ 0,y,0; 0,0,0$ ( $\bar{4}_y^{-1} 0,0,0$ )	(48) $m \ x,y,x$ ( $m_{\bar{xz}} 0,0,0$ )

For (0,1/2,1/2) + set

(1) $t \ (0,1/2,1/2)$ ( $\bar{1} 0,1/2,1/2$ )	(2) $2 \ (0,0,1/2) \ 0,1/4,z$ ( $2_z 0,1/2,1/2$ )	(3) $2 \ (0,1/2,0) \ 0,y,1/4$ ( $2_y 0,1/2,1/2$ )	(4) $2 \ x,1/4,1/4$ ( $2_x 0,1/2,1/2$ )
(5) $3^+ \ (1/3,1/3,1/3)$ $x-1/3,x-1/6,x$ ( $3_{xyz} 0,1/2,1/2$ )	(6) $3^+ \ \bar{x},x+1/2,\bar{x}$ ( $3_{\bar{xyz}}^{-1} 0,1/2,1/2$ )	(7) $3^+ \ (-1/3,1/3,1/3)$ $x+1/3,\bar{x}-1/6,\bar{x}$ ( $3_{\bar{xyz}}^{-1} 0,1/2,1/2$ )	(8) $3^+ \ \bar{x},\bar{x}+1/2,x$ ( $3_{xy\bar{z}}^{-1} 0,1/2,1/2$ )
(9) $3^- \ (1/3,1/3,1/3)$ $x-1/6,x+1/6,x$ ( $3_{xyz}^{-1} 0,1/2,1/2$ )	(10) $3^- \ (-1/3,1/3,1/3)$ $x+1/6,\bar{x}+1/6,\bar{x}$ ( $3_{\bar{xyz}} 0,1/2,1/2$ )	(11) $3^- \ \bar{x}+1/2,\bar{x}+1/2,x$ ( $3_{xy\bar{z}} 0,1/2,1/2$ )	(12) $3^- \ \bar{x}-1/2,x+1/2,\bar{x}$ ( $3_{x\bar{y}z}^{-1} 0,1/2,1/2$ )
(13) $2 \ (1/4,1/4,0) \ x,x+1/4,1/4$ ( $2_{xy} 0,1/2,1/2$ )	(14) $2 \ (-1/4,1/4,0) \ x,\bar{x}+1/4,1/4$ ( $2_{\bar{xy}} 0,1/2,1/2$ )	(15) $4^- \ (0,0,1/2) \ 1/4,1/4,z$ ( $4_z^{-1} 0,1/2,1/2$ )	(16) $4^+ \ (0,0,1/2) \ -1/4,1/4,z$ ( $4_z 0,1/2,1/2$ )
(17) $4^- \ x,1/2,0$ ( $4_x^{-1} 0,1/2,1/2$ )	(18) $2 \ (0,1/2,1/2) \ 0,y,y$ ( $2_{yz} 0,1/2,1/2$ )	(19) $2 \ 0,y+1/2,\bar{y}$ ( $2_{\bar{yz}} 0,1/2,1/2$ )	(20) $4^+ \ x,0,1/2$ ( $4_x 0,1/2,1/2$ )
(21) $4^+ \ (0,1/2,0) \ 1/4,y,1/4$ ( $4_y 0,1/2,1/2$ )	(22) $2 \ (1/4,0,1/4) \ x-1/4,1/4,x$ ( $2_{xz} 0,1/2,1/2$ )	(23) $4^- \ (0,1/2,0) \ -1/4,y,1/4$ ( $4_y^{-1} 0,1/2,1/2$ )	(24) $2 \ (-1/4,0,1/4)\bar{x}+1/4,1/4,x$ ( $2_{\bar{xz}} 0,1/2,1/2$ )
(25) $\bar{1} \ 0,1/4,1/4$ ( $\bar{1} 0,1/2,1/2$ )	(26) $b \ (0,1/2,0) \ x,y,1/4$ ( $m_z 0,1/2,1/2$ )	(27) $c \ (0,0,1/2) \ x,1/4,z$ ( $m_y 0,1/2,1/2$ )	(28) $n \ (0,1/2,1/2) \ 0,y,z$ ( $m_x 0,1/2,1/2$ )
(29) $\bar{3}^+ \ x,x+1/2,x;$ $0,1/2,0$ ( $\bar{3}_{xyz} 0,1/2,1/2$ )	(30) $\bar{3}^+ \ \bar{x}-1,x+1/2,\bar{x};$ $-1/2,0,1/2$ ( $\bar{3}_{\bar{xyz}}^{-1} 0,1/2,1/2$ )	(31) $\bar{3}^+ \ x,\bar{x}+1/2,\bar{x};$ $0,1/2,0$ ( $\bar{3}_{\bar{xy}z}^{-1} 0,1/2,1/2$ )	(32) $\bar{3}^+ \ \bar{x}-1,\bar{x}+1/2,x;$ $1/2,0,1/2$ ( $\bar{3}_{xy\bar{z}}^{-1} 0,1/2,1/2$ )

- |  |   |  |   |
|--|---|--|---|
| (33) $\bar{3}^-$ $x-1/2, x-1/2, x;$<br>0,0,1/2<br>( $\bar{3}_{xyz}^{-1}   0, 1/2, 1/2$ ) | (34) $\bar{3}^-$ $x+1/2, \bar{x}-1/2, \bar{x};$<br>0,0,1/2<br>( $\bar{3}_{\bar{xyz}}   0, 1/2, 1/2$ ) | (35) $\bar{3}^-$ $\bar{x}-1/2, \bar{x}+1/2, x;$<br>-1/2,1/2,0<br>( $\bar{3}_{\bar{xyz}}   0, 1/2, 1/2$ ) | (36) $\bar{3}^-$ $\bar{x}+1/2, x+1/2, \bar{x};$<br>1/2,1/2,0<br>( $\bar{3}_{\bar{xyz}}   0, 1/2, 1/2$ ) |
| (37) $g$ (-1/4,1/4,1/2) $x+1/4, \bar{x}, z$<br>( $m_{xy}   0, 1/2, 1/2$ )                | (38) $g$ (1/4,1/4,1/2) $x-1/4, x, z$<br>( $m_{\bar{xy}}   0, 1/2, 1/2$ )                              | (39) $\bar{4}^-$ -1/4,1/4,z; -1/4,1/4,1/4<br>( $\bar{4}_z^{-1}   0, 1/2, 1/2$ )                          | (40) $\bar{4}^+$ 1/4,1/4,z; 1/4,1/4,1/4<br>( $\bar{4}_z   0, 1/2, 1/2$ )                                |
| (41) $\bar{4}^-$ $x, 0, 1/2; 0, 0, 1/2$<br>( $\bar{4}_x^{-1}   0, 1/2, 1/2$ )            | (42) $m$ $x, y+1/2, \bar{y}$<br>( $m_{yz}   0, 1/2, 1/2$ )  | (43) $g$ (0,1/2,1/2) $x, y, y$<br>( $m_{\bar{yz}}   0, 1/2, 1/2$ )                                       | (44) $\bar{4}^+$ $x, 1/2, 0; 0, 1/2, 0$<br>( $\bar{4}_x   0, 1/2, 1/2$ )                                |
| (45) $\bar{4}^+$ -1/4,y,1/4; -1/4,1/4,1/4<br>( $\bar{4}_y   0, 1/2, 1/2$ )               | (46) $g$ (-1/4,1/2,1/4) $\bar{x}+1/4, y, x$<br>( $m_{xz}   0, 1/2, 1/2$ )                             | (47) $\bar{4}^-$ 1/4,y,1/4; 1/4,1/4,1/4<br>( $\bar{4}_y^{-1}   0, 1/2, 1/2$ )                            | (48) $g$ (1/4,1/2,1/4) $x-1/4, y, x$<br>( $m_{\bar{xz}}   0, 1/2, 1/2$ )                                |

For (1/2,0,1/2) + set

- |   |  |  |   |
|---|--|--|---|
| (1) $t$ (1/2,0,1/2)<br>( $1   1/2, 0, 1/2$ )  | (2) $2$ (0,0,1/2) 1/4,0,z<br>( $2_z   1/2, 0, 1/2$ )   | (3) $2$ 1/4,y,1/4<br>( $2_y   1/2, 0, 1/2$ )   | (4) $2$ (1/2,0,0) $x, 0, 1/2$<br>( $2_x   1/2, 0, 1/2$ )  |
| (5) $3^+$ (1/3,1/3,1/3)<br>$x+1/6, x-1/6, x$<br>( $3_{xyz}   1/2, 0, 1/2$ )           | (6) $3^+$ (1/3,-1/3,1/3)<br>$x+1/6, x+1/6, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ )              | (7) $3^+$ $x+1/2, \bar{x}-1/2, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ )                            | (8) $3^+$ $\bar{x}+1/2, \bar{x}+1/2, x$<br>( $3_{xyz}^{-1}   1/2, 0, 1/2$ )                                   |
| (9) $3^-$ (1/3,1/3,1/3)<br>$x-1/6, x-1/3, x$<br>( $3_{xyz}^{-1}   1/2, 0, 1/2$ )      | (10) $3^-$ $x+1/2, \bar{x}, \bar{x}$<br>( $3_{\bar{xyz}}   1/2, 0, 1/2$ )                                  | (11) $3^-$ $\bar{x}+1/2, \bar{x}, x$<br>( $3_{\bar{xyz}}   1/2, 0, 1/2$ )                                    | (12) $3^-$ (1/3,-1/3,1/3)<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>( $3_{\bar{xyz}}   1/2, 0, 1/2$ )               |
| (13) $2$ (1/4,1/4,0) $x, x-1/4, 1/4$<br>( $2_{xy}   1/2, 0, 1/2$ )                    | (14) $2$ (1/4,-1/4,0) $x, \bar{x}+1/4, 1/4$<br>( $2_{\bar{xy}}   1/2, 0, 1/2$ )                            | (15) $4^-$ (0,0,1/2) 1/4,-1/4,z<br>( $\bar{4}_z^{-1}   1/2, 0, 1/2$ )  | (16) $4^+$ (0,0,1/2) 1/4,1/4,z<br>( $\bar{4}_z   1/2, 0, 1/2$ )   |
| (17) $4^-$ (1/2,0,0) $x, 1/4, 1/4$<br>( $\bar{4}_x^{-1}   1/2, 0, 1/2$ )              | (18) $2$ (0,1/4,1/4) 1/4,y-1/4,y<br>( $2_{yz}   1/2, 0, 1/2$ )   | (19) $2$ (0,-1/2,1/2) 1/4,y+1/4, $\bar{y}$<br>( $2_{\bar{yz}}   1/2, 0, 1/2$ )                               | (20) $4^+$ (1/2,0,0) $x, -1/4, 1/4$<br>( $\bar{4}_x   1/2, 0, 1/2$ )  |
| (21) $4^+$ 1/2,y,0<br>( $\bar{4}_y   1/2, 0, 1/2$ )                                   | (22) $2$ (1/2,0,1/2) $x, 0, x$<br>( $2_{xz}   1/2, 0, 1/2$ )   | (23) $4^-$ 0,y,1/2<br>( $\bar{4}_y^{-1}   1/2, 0, 1/2$ )   | (24) $2$ $\bar{x}+1/2, 0, x$<br>( $2_{\bar{xz}}   1/2, 0, 1/2$ )  |
| (25) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}   1/2, 0, 1/2$ )                               | (26) $a$ (1/2,0,0) $x, y, 1/4$<br>( $m_z   1/2, 0, 1/2$ )  | (27) $n$ (1/2,0,1/2) $x, 0, z$<br>( $m_y   1/2, 0, 1/2$ )  | (28) $c$ (0,0,1/2) 1/4,y,z<br>( $m_x   1/2, 0, 1/2$ )   |
| (29) $\bar{3}^+$ $x-1/2, x-1/2, x;$<br>0,0,1/2<br>( $\bar{3}_{xyz}   1/2, 0, 1/2$ )   | (30) $\bar{3}^+$ $\bar{x}-1/2, x+1/2, \bar{x};$<br>0,0,1/2<br>( $\bar{3}_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ ) | (31) $\bar{3}^+$ $x+1/2, \bar{x}+1/2, \bar{x};$<br>1/2,1/2,0<br>( $\bar{3}_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ ) | (32) $\bar{3}^+$ $\bar{x}+1/2, \bar{x}-1/2, x;$<br>1/2,-1/2,0<br>( $\bar{3}_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ ) |
| (33) $\bar{3}^-$ $x+1/2, x, x;$<br>1/2,0,0<br>( $\bar{3}_{xyz}^{-1}   1/2, 0, 1/2$ )  | (34) $\bar{3}^-$ $x+1/2, \bar{x}-1, \bar{x};$<br>0,-1/2,1/2<br>( $\bar{3}_{\bar{xyz}}   1/2, 0, 1/2$ )     | (35) $\bar{3}^-$ $\bar{x}+1/2, \bar{x}+1, x;$<br>0,1/2,1/2<br>( $\bar{3}_{\bar{xyz}}   1/2, 0, 1/2$ )        | (36) $\bar{3}^-$ $\bar{x}+1/2, x, \bar{x};$<br>1/2,0,0<br>( $\bar{3}_{\bar{xyz}}   1/2, 0, 1/2$ )             |
| (37) $g$ (1/4,-1/4,1/2) $x+1/4, \bar{x}, z$<br>( $m_{xy}   1/2, 0, 1/2$ )             | (38) $g$ (1/4,1/4,1/2) $x+1/4, x, z$<br>( $m_{\bar{xy}}   1/2, 0, 1/2$ )                                   | (39) $\bar{4}^-$ 1/4,1/4,z; 1/4,1/4,1/4<br>( $\bar{4}_z^{-1}   1/2, 0, 1/2$ )                                | (40) $\bar{4}^+$ 1/4,-1/4,z; 1/4,-1/4,1/4<br>( $\bar{4}_z   1/2, 0, 1/2$ )                                    |
| (41) $\bar{4}^-$ $x, -1/4, 1/4; 1/4, -1/4, 1/4$<br>( $\bar{4}_x^{-1}   1/2, 0, 1/2$ ) | (42) $g$ (1/2,-1/4,1/4) $x, y+1/4, \bar{y}$<br>( $m_{yz}   1/2, 0, 1/2$ )                                  | (43) $g$ (1/2,1/4,1/4) $x, y-1/4, y$<br>( $m_{\bar{yz}}   1/2, 0, 1/2$ )                                     | (44) $\bar{4}^+$ $x, 1/4, 1/4; 1/4, 1/4, 1/4$<br>( $\bar{4}_x   1/2, 0, 1/2$ )                                |
| (45) $\bar{4}^+$ 0,y,1/2; 0,0,1/2<br>( $\bar{4}_y   1/2, 0, 1/2$ )                    | (46) $m$ $\bar{x}+1/2, y, x$<br>( $m_{xz}   1/2, 0, 1/2$ )   | (47) $\bar{4}^-$ 1/2,y,0; 1/2,0,0<br>( $\bar{4}_y^{-1}   1/2, 0, 1/2$ )                                      | (48) $g$ (1/2,0,1/2) $x, y, x$<br>( $m_{\bar{xz}}   1/2, 0, 1/2$ )  |

For (1/2,1/2,0) + set

(1) $t$ (1/2,1/2,0) (1   1/2,1/2,0)	(2) $2$ 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,0)	(3) $2$ (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)	(4) $2$ (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)
(5) $3^+$ (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) $3^+$ $\bar{x}$ +1/2,x, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(7) $3^+$ x+1/2, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(8) $3^+$ (1/3,1/3,-1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)
(9) $3^-$ (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) $3^-$ x, $\bar{x}$ +1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)	(11) $3^-$ (1/3,1/3,-1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub>   1/2,1/2,0)	(12) $3^-$ $\bar{x}$ , x+1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)
(13) $2$ (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)	(14) $2$ x, $\bar{x}$ +1/2,0 (2 <sub>xy</sub>   1/2,1/2,0)	(15) $4^-$ 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,0)	(16) $4^+$ 0,1/2,z (4 <sub>z</sub>   1/2,1/2,0)
(17) $4^-$ (1/2,0,0) x,1/4,-1/4 (4 <sub>x</sub> <sup>-1</sup>   1/2,1/2,0)	(18) $2$ (0,1/4,1/4) 1/4,y+1/4,y (2 <sub>yz</sub>   1/2,1/2,0)	(19) $2$ (0,1/4,-1/4) 1/4,y+1/4, $\bar{y}$ (2 <sub>yz</sub>   1/2,1/2,0)	(20) $4^+$ (1/2,0,0) x,1/4,1/4 (4 <sub>x</sub>   1/2,1/2,0)
(21) $4^+$ (0,1/2,0) 1/4,y,-1/4 (4 <sub>y</sub>   1/2,1/2,0)	(22) $2$ (1/4,0,1/4) x+1/4,1/4,x (2 <sub>xz</sub>   1/2,1/2,0)	(23) $4^-$ (0,1/2,0) 1/4,y,1/4 (4 <sub>y</sub> <sup>-1</sup>   1/2,1/2,0)	(24) $2$ (1/4,0,-1/4) $\bar{x}$ +1/4,1/4,x (2 <sub>xz</sub>   1/2,1/2,0)
(25) $\bar{1}$ 1/4,1/4,0 (1   1/2,1/2,0)	(26) $n$ (1/2,1/2,0) x,y,0 (m <sub>z</sub>   1/2,1/2,0)	(27) $a$ (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)	(28) $b$ (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)
(29) $\bar{3}^+$ x+1/2,x,x; 1/2,0,0 (3 <sub>xyz</sub>   1/2,1/2,0)	(30) $\bar{3}^+$ $\bar{x}$ -1/2,x+1, $\bar{x}$ ; 0,1/2,1/2 (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(31) $\bar{3}^+$ x-1/2, $\bar{x}$ +1, $\bar{x}$ ; 0,1/2,-1/2 (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(32) $\bar{3}^+$ $\bar{x}$ +1/2, $\bar{x}$ ,x; 1/2,0,0 (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)
(33) $\bar{3}^-$ x,x+1/2,x; 0,1/2,0 (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(34) $\bar{3}^-$ x+1, $\bar{x}$ -1/2, $\bar{x}$ ; 1/2,0,1/2 (3 <sub>xyz</sub>   1/2,1/2,0)	(35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1/2,x; 0,1/2,0 (3 <sub>xyz</sub>   1/2,1/2,0)	(36) $\bar{3}^-$ $\bar{x}$ +1,x-1/2, $\bar{x}$ ; 1/2,0,-1/2 (3 <sub>xyz</sub>   1/2,1/2,0)
(37) $m$ x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,0)	(38) $g$ (1/2,1/2,0) x,x,z (m <sub>xy</sub>   1/2,1/2,0)	(39) $\bar{4}^-$ 0,1/2,z; 0,1/2,0 (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,0)	(40) $\bar{4}^+$ 1/2,0,z; 1/2,0,0 (4 <sub>z</sub>   1/2,1/2,0)
(41) $\bar{4}^-$ x,1/4,1/4; 1/4,1/4,1/4 (4 <sub>x</sub> <sup>-1</sup>   1/2,1/2,0)	(42) $g$ (1/2,1/4,-1/4) x,y+1/4, $\bar{y}$ (m <sub>yz</sub>   1/2,1/2,0)	(43) $g$ (1/2,1/4,1/4) x,y+1/4,y (m <sub>yz</sub>   1/2,1/2,0)	(44) $\bar{4}^+$ x,1/4,-1/4; 1/4,1/4,-1/4 (4 <sub>x</sub>   1/2,1/2,0)
(45) $\bar{4}^+$ 1/4,y,1/4; 1/4,1/4,1/4 (4 <sub>y</sub>   1/2,1/2,0)	(46) $g$ (1/4,1/2,-1/4) $\bar{x}$ +1/4,y,x (m <sub>xz</sub>   1/2,1/2,0)	(47) $\bar{4}^-$ 1/4,y,-1/4; 1/4,1/4,-1/4 (4 <sub>y</sub> <sup>-1</sup>   1/2,1/2,0)	(48) $g$ (1/4,1/2,1/4) x+1/4,y,x (m <sub>xz</sub>   1/2,1/2,0)

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

## Positions

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

192		1	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +					
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}$ , $\bar{y}$ ,z	[ $\bar{u}$ , $\bar{v}$ ,w]	(3)	$\bar{x}$ ,y,z	[ $\bar{u}$ ,v,w]	(4)	x, $\bar{y}$ ,z	[u, $\bar{v}$ ,w]
(5)	z,x,y	[w,u,v]	(6)	z, $\bar{x}$ , $\bar{y}$	[w, $\bar{u}$ , $\bar{v}$ ]	(7)	$\bar{z}$ ,x,y	[ $\bar{w}$ ,u,v]	(8)	$\bar{z}$ ,x, $\bar{y}$	[ $\bar{w}$ ,u, $\bar{v}$ ]

(9)	$y,z,x$	$[v,w,u]$	(10)	$\bar{y},z,\bar{x}$	$[\bar{v},w,\bar{u}]$	(11)	$y,\bar{z},\bar{x}$	$[v,\bar{w},\bar{u}]$	(12)	$\bar{y},\bar{z},x$	$[\bar{v},\bar{w},u]$
(13)	$y,x,\bar{z}$	$[v,u,\bar{w}]$	(14)	$\bar{y},\bar{x},z$	$[\bar{v},\bar{u},w]$	(15)	$y,\bar{x},z$	$[v,\bar{u},w]$	(16)	$\bar{y},x,z$	$[\bar{v},u,w]$
(17)	$x,z,\bar{y}$	$[u,w,\bar{v}]$	(18)	$\bar{x},z,y$	$[\bar{u},w,\bar{v}]$	(19)	$\bar{x},z,\bar{y}$	$[\bar{u},\bar{w},\bar{v}]$	(20)	$x,\bar{z},y$	$[u,\bar{w},\bar{v}]$
(21)	$z,y,\bar{x}$	$[w,v,\bar{u}]$	(22)	$z,\bar{y},x$	$[w,\bar{v},u]$	(23)	$\bar{z},y,x$	$[\bar{w},v,u]$	(24)	$\bar{z},\bar{y},\bar{x}$	$[\bar{w},\bar{v},\bar{u}]$
(25)	$\bar{x},\bar{y},z$	$[u,v,w]$	(26)	$x,y,\bar{z}$	$[\bar{u},\bar{v},w]$	(27)	$x,\bar{y},z$	$[\bar{u},v,\bar{w}]$	(28)	$\bar{x},y,z$	$[u,\bar{v},\bar{w}]$
(29)	$\bar{z},\bar{x},\bar{y}$	$[w,u,v]$	(30)	$\bar{z},x,y$	$[w,\bar{u},\bar{v}]$	(31)	$z,x,\bar{y}$	$[\bar{w},\bar{u},v]$	(32)	$z,\bar{x},y$	$[\bar{w},u,\bar{v}]$
(33)	$\bar{y},\bar{z},\bar{x}$	$[v,w,u]$	(34)	$y,\bar{z},x$	$[\bar{v},w,\bar{u}]$	(35)	$\bar{y},z,x$	$[v,\bar{w},\bar{u}]$	(36)	$y,z,\bar{x}$	$[\bar{v},\bar{w},u]$
(37)	$\bar{y},\bar{x},z$	$[v,u,\bar{w}]$	(38)	$y,x,z$	$[\bar{v},\bar{u},\bar{w}]$	(39)	$\bar{y},x,z$	$[v,\bar{u},w]$	(40)	$y,\bar{x},z$	$[\bar{v},u,\bar{w}]$
(41)	$\bar{x},\bar{z},y$	$[u,w,\bar{v}]$	(42)	$x,\bar{z},\bar{y}$	$[\bar{u},w,\bar{v}]$	(43)	$x,z,y$	$[\bar{u},\bar{w},\bar{v}]$	(44)	$\bar{x},z,\bar{y}$	$[u,\bar{w},\bar{v}]$
(45)	$\bar{z},\bar{y},x$	$[w,v,\bar{u}]$	(46)	$\bar{z},y,\bar{x}$	$[w,\bar{v},u]$	(47)	$z,\bar{y},\bar{x}$	$[\bar{w},v,u]$	(48)	$z,y,x$	$[\bar{w},\bar{v},\bar{u}]$
96	k	..m	$x,x,z$	$[u,\bar{u},0]$	$\bar{x},\bar{x},z$	$[\bar{u},u,0]$	$\bar{x},x,\bar{z}$	$[\bar{u},\bar{u},0]$	$x,\bar{x},z$	$[u,u,0]$	
			$z,x,x$	$[0,u,\bar{u}]$	$z,\bar{x},\bar{x}$	$[0,\bar{u},u]$	$\bar{z},\bar{x},x$	$[0,u,\bar{u}]$	$\bar{z},x,\bar{x}$	$[0,u,u]$	
			$x,z,x$	$[\bar{u},0,u]$	$\bar{x},z,\bar{x}$	$[u,0,\bar{u}]$	$x,\bar{z},\bar{x}$	$[\bar{u},0,\bar{u}]$	$\bar{x},z,x$	$[u,0,u]$	
			$x,x,\bar{z}$	$[\bar{u},u,0]$	$\bar{x},\bar{x},\bar{z}$	$[u,\bar{u},0]$	$x,\bar{x},z$	$[\bar{u},\bar{u},0]$	$\bar{x},x,z$	$[u,u,0]$	
			$x,z,\bar{x}$	$[u,0,u]$	$\bar{x},z,x$	$[\bar{u},0,\bar{u}]$	$\bar{x},\bar{z},\bar{x}$	$[\bar{u},0,u]$	$x,\bar{z},x$	$[u,0,\bar{u}]$	
			$z,x,\bar{x}$	$[0,\bar{u},\bar{u}]$	$z,\bar{x},x$	$[0,u,u]$	$\bar{z},x,x$	$[0,\bar{u},u]$	$\bar{z},\bar{x},\bar{x}$	$[0,u,\bar{u}]$	
96	j	m..	$0,y,z$	$[u,0,0]$	$0,\bar{y},z$	$[\bar{u},0,0]$	$0,y,\bar{z}$	$[\bar{u},0,0]$	$0,\bar{y},z$	$[u,0,0]$	
			$z,0,y$	$[0,u,0]$	$z,0,\bar{y}$	$[0,\bar{u},0]$	$\bar{z},0,y$	$[0,\bar{u},0]$	$\bar{z},0,\bar{y}$	$[0,u,0]$	
			$y,z,0$	$[0,0,u]$	$\bar{y},z,0$	$[0,0,\bar{u}]$	$y,\bar{z},0$	$[0,0,\bar{u}]$	$\bar{y},z,0$	$[0,0,u]$	
			$y,0,\bar{z}$	$[0,u,0]$	$\bar{y},0,\bar{z}$	$[0,\bar{u},0]$	$y,0,z$	$[0,\bar{u},0]$	$\bar{y},0,z$	$[0,u,0]$	
			$0,z,\bar{y}$	$[u,0,0]$	$0,z,y$	$[\bar{u},0,0]$	$0,\bar{z},\bar{y}$	$[\bar{u},0,0]$	$0,\bar{z},y$	$[u,0,0]$	
			$z,y,0$	$[0,0,\bar{u}]$	$z,\bar{y},0$	$[0,0,u]$	$\bar{z},y,0$	$[0,0,u]$	$\bar{z},\bar{y},0$	$[0,0,\bar{u}]$	
48	i	m.m2	$1/2,y,y$	$[0,0,0]$	$1/2,\bar{y},y$	$[0,0,0]$	$1/2,y,\bar{y}$	$[0,0,0]$	$1/2,\bar{y},\bar{y}$	$[0,0,0]$	
			$y,1/2,y$	$[0,0,0]$	$y,1/2,\bar{y}$	$[0,0,0]$	$\bar{y},1/2,y$	$[0,0,0]$	$\bar{y},1/2,\bar{y}$	$[0,0,0]$	
			$y,y,1/2$	$[0,0,0]$	$\bar{y},y,1/2$	$[0,0,0]$	$y,\bar{y},1/2$	$[0,0,0]$	$\bar{y},\bar{y},1/2$	$[0,0,0]$	
48	h	m.m2	$0,y,y$	$[0,0,0]$	$0,\bar{y},y$	$[0,0,0]$	$0,y,\bar{y}$	$[0,0,0]$	$0,\bar{y},\bar{y}$	$[0,0,0]$	
			$y,0,y$	$[0,0,0]$	$y,0,\bar{y}$	$[0,0,0]$	$\bar{y},0,y$	$[0,0,0]$	$\bar{y},0,\bar{y}$	$[0,0,0]$	
			$y,y,0$	$[0,0,0]$	$\bar{y},y,0$	$[0,0,0]$	$y,\bar{y},0$	$[0,0,0]$	$\bar{y},\bar{y},0$	$[0,0,0]$	

Continued		225.1.1618		Fm $\bar{3}$ m		
48	g	2.mm	x,1/4,1/4 [0,0,0] 1/4,1/4,x [0,0,0] x,1/4,3/4 [0,0,0]	$\bar{x}$ ,3/4,1/4 [0,0,0] 3/4,1/4, $\bar{x}$ [0,0,0] $\bar{x}$ ,1/4,1/4 [0,0,0]	1/4,x,1/4 [0,0,0] 1/4,x,3/4 [0,0,0] 1/4,1/4, $\bar{x}$ [0,0,0]	1/4, $\bar{x}$ ,3/4 [0,0,0] 3/4, $\bar{x}$ ,3/4 [0,0,0] 1/4,3/4,x [0,0,0]
32	f	.3m	x,x,x [0,0,0] x,x, $\bar{x}$ [0,0,0]	$\bar{x}$ , $\bar{x}$ ,x [0,0,0] $\bar{x}$ , $\bar{x}$ , $\bar{x}$ [0,0,0]	$\bar{x}$ ,x, $\bar{x}$ [0,0,0] x, $\bar{x}$ ,x [0,0,0]	x, $\bar{x}$ , $\bar{x}$ [0,0,0] $\bar{x}$ ,x,x [0,0,0]
24	e	4m.m	x,0,0 [0,0,0] 0, $\bar{x}$ ,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0] 0,0,x [0,0,0]	0,x,0 [0,0,0] 0,0, $\bar{x}$ [0,0,0]	
24	d	m.mm	0,1/4,1/4 [0,0,0] 1/4,0,3/4 [0,0,0]	0,3/4,1/4 [0,0,0] 1/4,1/4,0 [0,0,0]	1/4,0,1/4 [0,0,0] 3/4,1/4,0 [0,0,0]	
8	c	$\bar{4}$ 3m	1/4,1/4,1/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]		
4	b	m $\bar{3}$ m	1/2,1/2,1/2 [0,0,0]			
4	a	m $\bar{3}$ m	0,0,0 [0,0,0]			

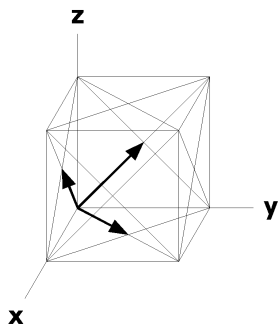
### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,1,1] p6'm'm  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

Along [1,1,0] c2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0





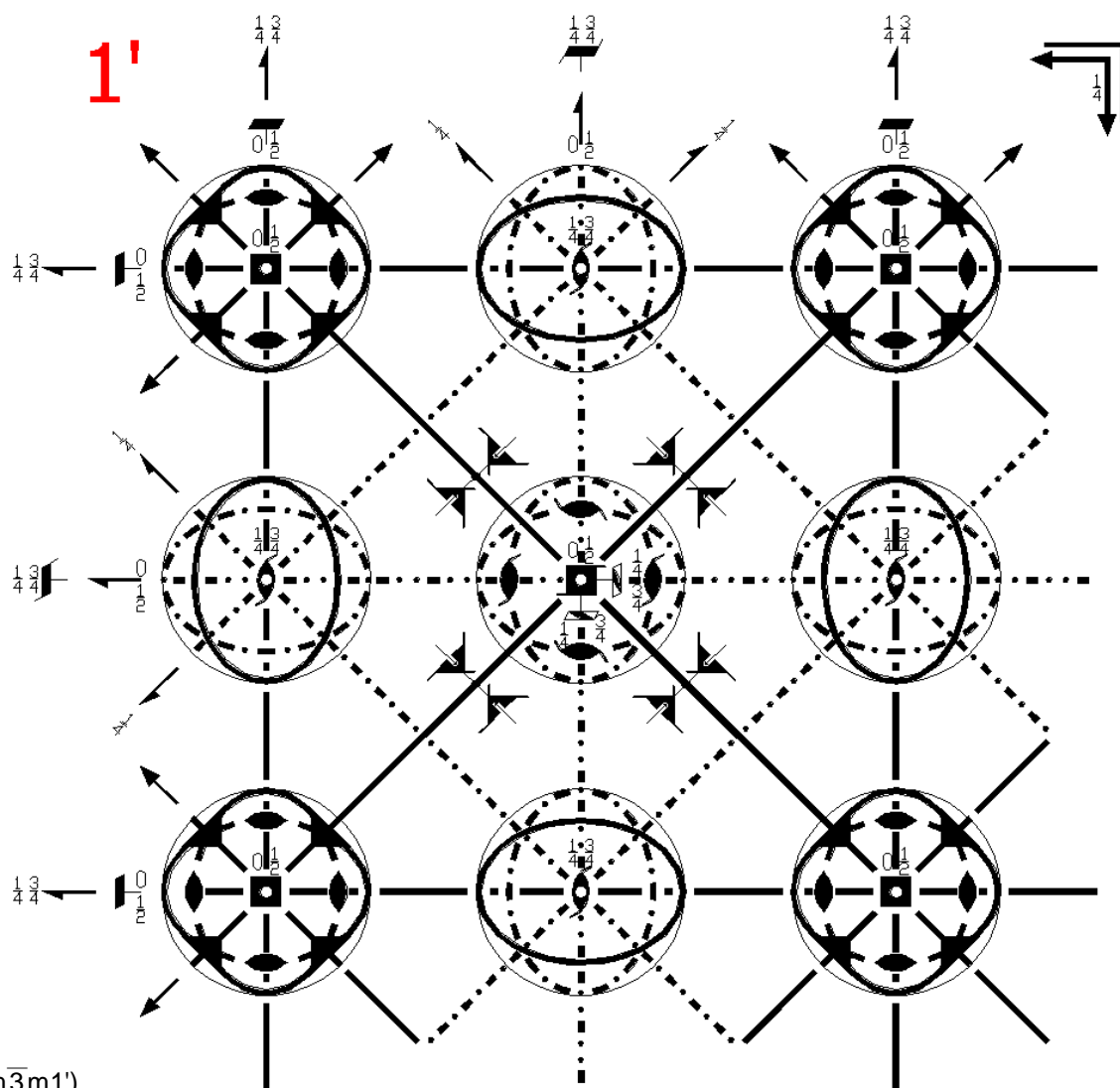
Fm $\bar{3}m1'$

225.2.1619

m $\bar{3}m1'$

F4/m $\bar{3}2/m1'$

Cubic



Origin at center (m $\bar{3}m1'$ )

<b>Asymmetric unit</b>	$0 \leq x \leq 1/2;$	$0 \leq y \leq 1/4;$	$0 \leq z \leq 1/4;$	$y \leq \min(x, 1/2-x);$	$z \leq y$
Vertices	0,0,0	1/2,0,0	1/4,1/4,0	1/4,1/4,1/4	

**Symmetry Operations**

For (0,0,0) + set

- |   |  |   |  |
|---|--|---|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math><sup>-1</sup> 0,0,0)</sub> | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)      | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math><sup>-1</sup> 0,0,0)</sub> |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)           | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0) | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)            |

(13) $2 \ x,x,0$ ( $2_{xy} 0,0,0$ )	(14) $2 \ x,\bar{x},0$ ( $2_{\bar{xy}} 0,0,0$ )	(15) $4^- \ 0,0,z$ ( $4_z^{-1} 0,0,0$ )	(16) $4^+ \ 0,0,z$ ( $4_z 0,0,0$ )
(17) $4^- \ x,0,0$ ( $4_x^{-1} 0,0,0$ )	(18) $2 \ 0,y,y$ ( $2_{yz} 0,0,0$ )	(19) $2 \ 0,y,\bar{y}$ ( $2_{\bar{yz}} 0,0,0$ )	(20) $4^+ \ x,0,0$ ( $4_x 0,0,0$ )
(21) $4^+ \ 0,y,0$ ( $4_y 0,0,0$ )	(22) $2 \ x,0,x$ ( $2_{xz} 0,0,0$ )	(23) $4^- \ 0,y,0$ ( $4_y^{-1} 0,0,0$ )	(24) $2 \ \bar{x},0,x$ ( $2_{\bar{xz}} 0,0,0$ )
(25) $\bar{1} \ 0,0,0$ ( $\bar{1} 0,0,0$ )	(26) $m \ x,y,0$ ( $m_z 0,0,0$ )	(27) $m \ x,0,z$ ( $m_y 0,0,0$ )	(28) $m \ 0,y,z$ ( $m_x 0,0,0$ )
(29) $\bar{3}^+ \ x,x,x; 0,0,0$ ( $\bar{3}_{xyz} 0,0,0$ )	(30) $\bar{3}^+ \ \bar{x},\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{xyz}}^{-1} 0,0,0$ )	(31) $\bar{3}^+ \ x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{xyz}}^{-1} 0,0,0$ )	(32) $\bar{3}^+ \ \bar{x},\bar{x},x; 0,0,0$ ( $\bar{3}_{xyz}^{-1} 0,0,0$ )
(33) $\bar{3}^- \ x,x,x; 0,0,0$ ( $\bar{3}_{xyz}^{-1} 0,0,0$ )	(34) $\bar{3}^- \ x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{xyz}} 0,0,0$ )	(35) $\bar{3}^- \ \bar{x},\bar{x},x; 0,0,0$ ( $\bar{3}_{\bar{xyz}} 0,0,0$ )	(36) $\bar{3}^- \ \bar{x},x,\bar{x}; 0,0,0$ ( $\bar{3}_{xyz}^{-1} 0,0,0$ )
(37) $m \ x,\bar{x},z$ ( $m_{xy} 0,0,0$ )	(38) $m \ x,x,z$ ( $m_{\bar{xy}} 0,0,0$ )	(39) $\bar{4}^- \ 0,0,z; 0,0,0$ ( $\bar{4}_z^{-1} 0,0,0$ )	(40) $\bar{4}^+ \ 0,0,z; 0,0,0$ ( $\bar{4}_z 0,0,0$ )
(41) $\bar{4}^- \ x,0,0; 0,0,0$ ( $\bar{4}_x^{-1} 0,0,0$ )	(42) $m \ x,y,\bar{y}$ ( $m_{yz} 0,0,0$ )	(43) $m \ x,y,y$ ( $m_{\bar{yz}} 0,0,0$ )	(44) $\bar{4}^+ \ x,0,0; 0,0,0$ ( $\bar{4}_x 0,0,0$ )
(45) $\bar{4}^+ \ 0,y,0; 0,0,0$ ( $\bar{4}_y 0,0,0$ )	(46) $m \ \bar{x},y,x$ ( $m_{xz} 0,0,0$ )	(47) $\bar{4}^- \ 0,y,0; 0,0,0$ ( $\bar{4}_y^{-1} 0,0,0$ )	(48) $m \ x,y,x$ ( $m_{\bar{xz}} 0,0,0$ )

For (0,1/2,1/2) + set

(1) $t \ (0,1/2,1/2)$ ( $1 0,1/2,1/2$ )	(2) $2 \ (0,0,1/2) \ 0,1/4,z$ ( $2_z 0,1/2,1/2$ )	(3) $2 \ (0,1/2,0) \ 0,y,1/4$ ( $2_y 0,1/2,1/2$ )	(4) $2 \ x,1/4,1/4$ ( $2_x 0,1/2,1/2$ )
(5) $3^+ \ (1/3,1/3,1/3)$ $x-1/3,x-1/6,x$ ( $3_{xyz} 0,1/2,1/2$ )	(6) $3^+ \ \bar{x},x+1/2,\bar{x}$ ( $3_{\bar{xyz}}^{-1} 0,1/2,1/2$ )	(7) $3^+ \ (-1/3,1/3,1/3)$ $x+1/3,\bar{x}-1/6,\bar{x}$ ( $3_{\bar{xyz}}^{-1} 0,1/2,1/2$ )	(8) $3^+ \ \bar{x},\bar{x}+1/2,x$ ( $3_{xyz}^{-1} 0,1/2,1/2$ )
(9) $3^- \ (1/3,1/3,1/3)$ $x-1/6,x+1/6,x$ ( $3_{xyz}^{-1} 0,1/2,1/2$ )	(10) $3^- \ (-1/3,1/3,1/3)$ $x+1/6,\bar{x}+1/6,\bar{x}$ ( $3_{\bar{xyz}} 0,1/2,1/2$ )	(11) $3^- \ \bar{x}+1/2,\bar{x}+1/2,x$ ( $3_{\bar{yz}} 0,1/2,1/2$ )	(12) $3^- \ \bar{x}-1/2,x+1/2,\bar{x}$ ( $3_{xyz} 0,1/2,1/2$ )
(13) $2 \ (1/4,1/4,0) \ x,x+1/4,1/4$ ( $2_{xy} 0,1/2,1/2$ )	(14) $2 \ (-1/4,1/4,0) \ x,\bar{x}+1/4,1/4$ ( $2_{\bar{xy}} 0,1/2,1/2$ )	(15) $4^- \ (0,0,1/2) \ 1/4,1/4,z$ ( $4_z^{-1} 0,1/2,1/2$ )	(16) $4^+ \ (0,0,1/2) \ -1/4,1/4,z$ ( $4_z 0,1/2,1/2$ )
(17) $4^- \ x,1/2,0$ ( $4_x^{-1} 0,1/2,1/2$ )	(18) $2 \ (0,1/2,1/2) \ 0,y,y$ ( $2_{yz} 0,1/2,1/2$ )	(19) $2 \ 0,y+1/2,\bar{y}$ ( $2_{\bar{yz}} 0,1/2,1/2$ )	(20) $4^+ \ x,0,1/2$ ( $4_x 0,1/2,1/2$ )
(21) $4^+ \ (0,1/2,0) \ 1/4,y,1/4$ ( $4_y 0,1/2,1/2$ )	(22) $2 \ (1/4,0,1/4) \ x-1/4,1/4,x$ ( $2_{xz} 0,1/2,1/2$ )	(23) $4^- \ (0,1/2,0) \ -1/4,y,1/4$ ( $4_y^{-1} 0,1/2,1/2$ )	(24) $2 \ (-1/4,0,1/4)\bar{x}+1/4,1/4,x$ ( $2_{\bar{xz}} 0,1/2,1/2$ )
(25) $\bar{1} \ 0,1/4,1/4$ ( $\bar{1} 0,1/2,1/2$ )	(26) $b \ (0,1/2,0) \ x,y,1/4$ ( $m_z 0,1/2,1/2$ )	(27) $c \ (0,0,1/2) \ x,1/4,z$ ( $m_y 0,1/2,1/2$ )	(28) $n \ (0,1/2,1/2) \ 0,y,z$ ( $m_x 0,1/2,1/2$ )
(29) $\bar{3}^+ \ x,x+1/2,x;$ $0,1/2,0$ ( $\bar{3}_{xyz} 0,1/2,1/2$ )	(30) $\bar{3}^+ \ \bar{x}-1,x+1/2,\bar{x};$ $-1/2,0,1/2$ ( $\bar{3}_{\bar{xyz}}^{-1} 0,1/2,1/2$ )	(31) $\bar{3}^+ \ x,\bar{x}+1/2,\bar{x};$ $0,1/2,0$ ( $\bar{3}_{xyz}^{-1} 0,1/2,1/2$ )	(32) $\bar{3}^+ \ \bar{x}-1,\bar{x}+1/2,x;$ $1/2,0,1/2$ ( $\bar{3}_{xyz}^{-1} 0,1/2,1/2$ )

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| (33) $\bar{3}^-$ $x-1/2, x-1/2, x;$<br>0,0,1/2<br>( $\bar{3}_{xyz}^{-1}   0, 1/2, 1/2$ ) | (34) $\bar{3}^-$ $x+1/2, \bar{x}-1/2, \bar{x};$<br>0,0,1/2<br>( $\bar{3}_{\bar{xyz}}   0, 1/2, 1/2$ ) | (35) $\bar{3}^-$ $\bar{x}-1/2, \bar{x}+1/2, x;$<br>-1/2,1/2,0<br>( $\bar{3}_{\bar{xyz}}   0, 1/2, 1/2$ ) | (36) $\bar{3}^-$ $\bar{x}+1/2, x+1/2, \bar{x};$<br>1/2,1/2,0<br>( $\bar{3}_{\bar{xyz}}   0, 1/2, 1/2$ ) |
| (37) $g$ (-1/4,1/4,1/2) $x+1/4, \bar{x}, z$<br>( $m_{xy}   0, 1/2, 1/2$ )                | (38) $g$ (1/4,1/4,1/2) $x-1/4, x, z$<br>( $m_{\bar{xy}}   0, 1/2, 1/2$ )                              | (39) $\bar{4}^-$ -1/4,1/4,z; -1/4,1/4,1/4<br>( $\bar{4}_z^{-1}   0, 1/2, 1/2$ )                          | (40) $\bar{4}^+$ 1/4,1/4,z; 1/4,1/4,1/4<br>( $\bar{4}_z   0, 1/2, 1/2$ )                                |
| (41) $\bar{4}^-$ $x, 0, 1/2; 0, 0, 1/2$<br>( $\bar{4}_x^{-1}   0, 1/2, 1/2$ )            | (42) $m$ $x, y+1/2, \bar{y}$<br>( $m_{yz}   0, 1/2, 1/2$ )  | (43) $g$ (0,1/2,1/2) $x, y, y$<br>( $m_{\bar{yz}}   0, 1/2, 1/2$ )                                       | (44) $\bar{4}^+$ $x, 1/2, 0; 0, 1/2, 0$<br>( $\bar{4}_x   0, 1/2, 1/2$ )                                |
| (45) $\bar{4}^+$ -1/4,y,1/4; -1/4,1/4,1/4<br>( $\bar{4}_y   0, 1/2, 1/2$ )               | (46) $g$ (-1/4,1/2,1/4) $\bar{x}+1/4, y, x$<br>( $m_{xz}   0, 1/2, 1/2$ )                             | (47) $\bar{4}^-$ 1/4,y,1/4; 1/4,1/4,1/4<br>( $\bar{4}_y^{-1}   0, 1/2, 1/2$ )                            | (48) $g$ (1/4,1/2,1/4) $x-1/4, y, x$<br>( $m_{\bar{xz}}   0, 1/2, 1/2$ )                                |

For (1/2,0,1/2) + set

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|---|--|--|---|
| (1) $t$ (1/2,0,1/2)<br>( $1   1/2, 0, 1/2$ )  | (2) $2$ (0,0,1/2) 1/4,0,z<br>( $2_z   1/2, 0, 1/2$ )   | (3) $2$ 1/4,y,1/4<br>( $2_y   1/2, 0, 1/2$ )   | (4) $2$ (1/2,0,0) $x, 0, 1/2$<br>( $2_x   1/2, 0, 1/2$ )  |
| (5) $3^+$ (1/3,1/3,1/3)<br>$x+1/6, x-1/6, x$<br>( $3_{xyz}   1/2, 0, 1/2$ )           | (6) $3^+$ (1/3,-1/3,1/3)<br>$x+1/6, x+1/6, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ )              | (7) $3^+$ $x+1/2, \bar{x}-1/2, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ )                            | (8) $3^+$ $\bar{x}+1/2, \bar{x}+1/2, x$<br>( $3_{xyz}^{-1}   1/2, 0, 1/2$ )                                   |
| (9) $3^-$ (1/3,1/3,1/3)<br>$x-1/6, x-1/3, x$<br>( $3_{xyz}^{-1}   1/2, 0, 1/2$ )      | (10) $3^-$ $x+1/2, \bar{x}, \bar{x}$<br>( $3_{\bar{xyz}}   1/2, 0, 1/2$ )                                  | (11) $3^-$ $\bar{x}+1/2, \bar{x}, x$<br>( $3_{\bar{xyz}}   1/2, 0, 1/2$ )                                    | (12) $3^-$ (1/3,-1/3,1/3)<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>( $3_{\bar{xyz}}   1/2, 0, 1/2$ )               |
| (13) $2$ (1/4,1/4,0) $x, x-1/4, 1/4$<br>( $2_{xy}   1/2, 0, 1/2$ )                    | (14) $2$ (1/4,-1/4,0) $x, \bar{x}+1/4, 1/4$<br>( $2_{\bar{xy}}   1/2, 0, 1/2$ )                            | (15) $4^-$ (0,0,1/2) 1/4,-1/4,z<br>( $\bar{4}_z^{-1}   1/2, 0, 1/2$ )  | (16) $4^+$ (0,0,1/2) 1/4,1/4,z<br>( $\bar{4}_z   1/2, 0, 1/2$ )   |
| (17) $4^-$ (1/2,0,0) $x, 1/4, 1/4$<br>( $\bar{4}_x^{-1}   1/2, 0, 1/2$ )              | (18) $2$ (0,1/4,1/4) 1/4,y-1/4,y<br>( $2_{yz}   1/2, 0, 1/2$ )   | (19) $2$ (0,-1/2,1/2) 1/4,y+1/4, $\bar{y}$<br>( $2_{\bar{yz}}   1/2, 0, 1/2$ )                               | (20) $4^+$ (1/2,0,0) $x, -1/4, 1/4$<br>( $\bar{4}_x   1/2, 0, 1/2$ )  |
| (21) $4^+$ 1/2,y,0<br>( $\bar{4}_y   1/2, 0, 1/2$ )                                   | (22) $2$ (1/2,0,1/2) $x, 0, x$<br>( $2_{xz}   1/2, 0, 1/2$ )   | (23) $4^-$ 0,y,1/2<br>( $\bar{4}_y^{-1}   1/2, 0, 1/2$ )   | (24) $2$ $\bar{x}+1/2, 0, x$<br>( $2_{\bar{xz}}   1/2, 0, 1/2$ )  |
| (25) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}   1/2, 0, 1/2$ )                               | (26) $a$ (1/2,0,0) $x, y, 1/4$<br>( $m_z   1/2, 0, 1/2$ )  | (27) $n$ (1/2,0,1/2) $x, 0, z$<br>( $m_y   1/2, 0, 1/2$ )  | (28) $c$ (0,0,1/2) 1/4,y,z<br>( $m_x   1/2, 0, 1/2$ )   |
| (29) $\bar{3}^+$ $x-1/2, x-1/2, x;$<br>0,0,1/2<br>( $\bar{3}_{xyz}   1/2, 0, 1/2$ )   | (30) $\bar{3}^+$ $\bar{x}-1/2, x+1/2, \bar{x};$<br>0,0,1/2<br>( $\bar{3}_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ ) | (31) $\bar{3}^+$ $x+1/2, \bar{x}+1/2, \bar{x};$<br>1/2,1/2,0<br>( $\bar{3}_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ ) | (32) $\bar{3}^+$ $\bar{x}+1/2, \bar{x}-1/2, x;$<br>1/2,-1/2,0<br>( $\bar{3}_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ ) |
| (33) $\bar{3}^-$ $x+1/2, x, x;$<br>1/2,0,0<br>( $\bar{3}_{xyz}^{-1}   1/2, 0, 1/2$ )  | (34) $\bar{3}^-$ $x+1/2, \bar{x}-1, \bar{x};$<br>0,-1/2,1/2<br>( $\bar{3}_{\bar{xyz}}   1/2, 0, 1/2$ )     | (35) $\bar{3}^-$ $\bar{x}+1/2, \bar{x}+1, x;$<br>0,1/2,1/2<br>( $\bar{3}_{\bar{xyz}}   1/2, 0, 1/2$ )        | (36) $\bar{3}^-$ $\bar{x}+1/2, x, \bar{x};$<br>1/2,0,0<br>( $\bar{3}_{\bar{xyz}}   1/2, 0, 1/2$ )             |
| (37) $g$ (1/4,-1/4,1/2) $x+1/4, \bar{x}, z$<br>( $m_{xy}   1/2, 0, 1/2$ )             | (38) $g$ (1/4,1/4,1/2) $x+1/4, x, z$<br>( $m_{\bar{xy}}   1/2, 0, 1/2$ )                                   | (39) $\bar{4}^-$ 1/4,1/4,z; 1/4,1/4,1/4<br>( $\bar{4}_z^{-1}   1/2, 0, 1/2$ )                                | (40) $\bar{4}^+$ 1/4,-1/4,z; 1/4,-1/4,1/4<br>( $\bar{4}_z   1/2, 0, 1/2$ )                                    |
| (41) $\bar{4}^-$ $x, -1/4, 1/4; 1/4, -1/4, 1/4$<br>( $\bar{4}_x^{-1}   1/2, 0, 1/2$ ) | (42) $g$ (1/2,-1/4,1/4) $x, y+1/4, \bar{y}$<br>( $m_{yz}   1/2, 0, 1/2$ )                                  | (43) $g$ (1/2,1/4,1/4) $x, y-1/4, y$<br>( $m_{\bar{yz}}   1/2, 0, 1/2$ )                                     | (44) $\bar{4}^+$ $x, 1/4, 1/4; 1/4, 1/4, 1/4$<br>( $\bar{4}_x   1/2, 0, 1/2$ )                                |
| (45) $\bar{4}^+$ 0,y,1/2; 0,0,1/2<br>( $\bar{4}_y   1/2, 0, 1/2$ )                    | (46) $m$ $\bar{x}+1/2, y, x$<br>( $m_{xz}   1/2, 0, 1/2$ )   | (47) $\bar{4}^-$ 1/2,y,0; 1/2,0,0<br>( $\bar{4}_y^{-1}   1/2, 0, 1/2$ )                                      | (48) $g$ (1/2,0,1/2) $x, y, x$<br>( $m_{\bar{xz}}   1/2, 0, 1/2$ )  |

## For (1/2,1/2,0) + set

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|--|---|---|---|
| (1) $t$ (1/2,1/2,0)<br>(1   1/2,1/2,0)   | (2) $2$ 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)   | (3) $2$ (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)   | (4) $2$ (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)   |
| (5) $3^+$ (1/3,1/3,1/3)<br>x+1/6,x+1/3,x<br>(3 <sub>xyz</sub>   1/2,1/2,0)               | (6) $3^+$ $\bar{x}$ +1/2,x, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)                         | (7) $3^+$ x+1/2, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)                          | (8) $3^+$ (1/3,1/3,-1/3)<br>x+1/6,x+1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)                 |
| (9) $3^-$ (1/3,1/3,1/3)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0) | (10) $3^-$ x, $\bar{x}$ +1/2, $\bar{x}$<br>(3 <sub>xyz</sub>   1/2,1/2,0)                                     | (11) $3^-$ (1/3,1/3,-1/3)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub>   1/2,1/2,0)                                    | (12) $3^-$ $\bar{x}$ ,x+1/2, $\bar{x}$<br>(3 <sub>xyz</sub>   1/2,1/2,0)                                  |
| (13) $2$ (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>   1/2,1/2,0)                              | (14) $2$ x, $\bar{x}$ +1/2,0<br>(2 <sub>xy</sub>   1/2,1/2,0)   | (15) $4^-$ 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,0)  | (16) $4^+$ 0,1/2,z<br>(4 <sub>z</sub>   1/2,1/2,0)  |
| (17) $4^-$ (1/2,0,0) x,1/4,-1/4<br>(4 <sub>x</sub> <sup>-1</sup>   1/2,1/2,0)            | (18) $2$ (0,1/4,1/4) 1/4,y+1/4,y<br>(2 <sub>yz</sub>   1/2,1/2,0)   | (19) $2$ (0,1/4,-1/4) 1/4,y+1/4, $\bar{y}$<br>(2 <sub>yz</sub>   1/2,1/2,0)                                     | (20) $4^+$ (1/2,0,0) x,1/4,1/4<br>(4 <sub>x</sub>   1/2,1/2,0)  |
| (21) $4^+$ (0,1/2,0) 1/4,y,-1/4<br>(4 <sub>y</sub>   1/2,1/2,0)                          | (22) $2$ (1/4,0,1/4) x+1/4,1/4,x<br>(2 <sub>xz</sub>   1/2,1/2,0)   | (23) $4^-$ (0,1/2,0) 1/4,y,1/4<br>(4 <sub>y</sub> <sup>-1</sup>   1/2,1/2,0)                                    | (24) $2$ (1/4,0,-1/4) $\bar{x}$ +1/4,1/4,x<br>(2 <sub>xz</sub>   1/2,1/2,0)                               |
| (25) $\bar{1}$ 1/4,1/4,0<br>(1   1/2,1/2,0)  | (26) $n$ (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>   1/2,1/2,0)  | (27) $a$ (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0)  | (28) $b$ (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)  |
| (29) $\bar{3}^+$ x+1/2,x,x;<br>1/2,0,0<br>(3 <sub>xyz</sub>   1/2,1/2,0)                 | (30) $\bar{3}^+$ $\bar{x}$ -1/2,x+1, $\bar{x}$ ;<br>0,1/2,1/2<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0) | (31) $\bar{3}^+$ x-1/2, $\bar{x}$ +1, $\bar{x}$ ;<br>0,1/2,-1/2<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0) | (32) $\bar{3}^+$ $\bar{x}$ +1/2, $\bar{x}$ ,x;<br>1/2,0,0<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0) |
| (33) $\bar{3}^-$ x,x+1/2,x;<br>0,1/2,0<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)   | (34) $\bar{3}^-$ x+1, $\bar{x}$ -1/2, $\bar{x}$ ;<br>1/2,0,1/2<br>(3 <sub>xyz</sub>   1/2,1/2,0)              | (35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1/2,x;<br>0,1/2,0<br>(3 <sub>xyz</sub>   1/2,1/2,0)                     | (36) $\bar{3}^-$ $\bar{x}$ +1,x-1/2, $\bar{x}$ ;<br>1/2,0,-1/2<br>(3 <sub>xyz</sub>   1/2,1/2,0)          |
| (37) $m$ x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>   1/2,1/2,0)                            | (38) $g$ (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>   1/2,1/2,0)   | (39) $\bar{4}^-$ 0,1/2,z; 0,1/2,0<br>(4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,0)                                 | (40) $\bar{4}^+$ 1/2,0,z; 1/2,0,0<br>(4 <sub>z</sub>   1/2,1/2,0)   |
| (41) $\bar{4}^-$ x,1/4,1/4; 1/4,1/4,1/4<br>(4 <sub>x</sub> <sup>-1</sup>   1/2,1/2,0)    | (42) $g$ (1/2,1/4,-1/4) x,y+1/4, $\bar{y}$<br>(m <sub>yz</sub>   1/2,1/2,0)                                   | (43) $g$ (1/2,1/4,1/4) x,y+1/4,y<br>(m <sub>yz</sub>   1/2,1/2,0)   | (44) $\bar{4}^+$ x,1/4,-1/4; 1/4,1/4,-1/4<br>(4 <sub>x</sub>   1/2,1/2,0)                                 |
| (45) $\bar{4}^+$ 1/4,y,1/4; 1/4,1/4,1/4<br>(4 <sub>y</sub>   1/2,1/2,0)                  | (46) $g$ (1/4,1/2,-1/4) $\bar{x}$ +1/4,y,x<br>(m <sub>xz</sub>   1/2,1/2,0)                                   | (47) $\bar{4}^-$ 1/4,y,-1/4; 1/4,1/4,-1/4<br>(4 <sub>y</sub> <sup>-1</sup>   1/2,1/2,0)                         | (48) $g$ (1/4,1/2,1/4) x+1/4,y,x<br>(m <sub>xz</sub>   1/2,1/2,0)   |

## For (0,0,0)' + set

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|--|--|---|---|
| (1) $1'$<br>(1   0,0,0)'                                       | (2) $2'$ 0,0,z<br>(2 <sub>z</sub>   0,0,0)'                                      | (3) $2'$ 0,y,0<br>(2 <sub>y</sub>   0,0,0)'                                       | (4) $2'$ x,0,0<br>(2 <sub>x</sub>   0,0,0)'                                       |
| (5) $3^+$ ' x,x,x<br>(3 <sub>xyz</sub>   0,0,0)'               | (6) $3^+$ ' $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   0,0,0)' | (7) $3^+$ ' x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   0,0,0)' | (8) $3^+$ ' $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   0,0,0)' |
| (9) $3^-$ ' x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   0,0,0)' | (10) $3^-$ ' x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub>   0,0,0)'             | (11) $3^-$ ' $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>xyz</sub>   0,0,0)'              | (12) $3^-$ ' $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub>xyz</sub>   0,0,0)'               |
| (13) $2'$ x,x,0<br>(2 <sub>xy</sub>   0,0,0)'                  | (14) $2'$ x, $\bar{x}$ ,0<br>(2 <sub>xy</sub>   0,0,0)'                          | (15) $4^-$ ' 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>   0,0,0)'                     | (16) $4^+$ ' 0,0,z<br>(4 <sub>z</sub>   0,0,0)'                                   |
| (17) $4^-$ ' x,0,0<br>(4 <sub>x</sub> <sup>-1</sup>   0,0,0)'  | (18) $2'$ 0,y,y<br>(2 <sub>yz</sub>   0,0,0)'                                    | (19) $2'$ 0,y, $\bar{y}$<br>(2 <sub>yz</sub>   0,0,0)'                            | (20) $4^+$ ' x,0,0<br>(4 <sub>x</sub>   0,0,0)'                                   |

(21) $4^+ ' 0,y,0$ ( $4_y   0,0,0$ )'	(22) $2' x,0,x$ ( $2_{xz}   0,0,0$ )'	(23) $4^- ' 0,y,0$ ( $4_y^{-1}   0,0,0$ )'	(24) $2' \bar{x},0,x$ ( $2_{\bar{z}}   0,0,0$ )'
(25) $\bar{1}' 0,0,0$ ( $\bar{1}   0,0,0$ )'	(26) $m' x,y,0$ ( $m_z   0,0,0$ )'	(27) $m' x,0,z$ ( $m_y   0,0,0$ )'	(28) $m' 0,y,z$ ( $m_x   0,0,0$ )'
(29) $\bar{3}^+ ' x,x,x; 0,0,0$ ( $\bar{3}_{xyz}   0,0,0$ )'	(30) $\bar{3}^+ ' \bar{x},x,\bar{x}; 0,0,0$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1}   0,0,0$ )'	(31) $\bar{3}^+ ' x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{y}\bar{z}}^{-1}   0,0,0$ )'	(32) $\bar{3}^+ ' \bar{x},\bar{x},x; 0,0,0$ ( $\bar{3}_{\bar{y}\bar{z}}^{-1}   0,0,0$ )'
(33) $\bar{3}^- ' x,x,x; 0,0,0$ ( $\bar{3}_{xyz}^{-1}   0,0,0$ )'	(34) $\bar{3}^- ' x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{y}\bar{z}}   0,0,0$ )'	(35) $\bar{3}^- ' \bar{x},\bar{x},x; 0,0,0$ ( $\bar{3}_{\bar{y}\bar{z}}   0,0,0$ )'	(36) $\bar{3}^- ' \bar{x},x,\bar{x}; 0,0,0$ ( $\bar{3}_{x\bar{y}\bar{z}}   0,0,0$ )'
(37) $m' x,\bar{x},z$ ( $m_{xy}   0,0,0$ )'	(38) $m' x,x,z$ ( $m_{\bar{xy}}   0,0,0$ )'	(39) $\bar{4}^- ' 0,0,z; 0,0,0$ ( $\bar{4}_z^{-1}   0,0,0$ )'	(40) $\bar{4}^+ ' 0,0,z; 0,0,0$ ( $\bar{4}_z   0,0,0$ )'
(41) $\bar{4}^- ' x,0,0; 0,0,0$ ( $\bar{4}_x^{-1}   0,0,0$ )'	(42) $m' x,y,\bar{y}$ ( $m_{yz}   0,0,0$ )'	(43) $m' x,y,y$ ( $m_{\bar{yz}}   0,0,0$ )'	(44) $\bar{4}^+ ' x,0,0; 0,0,0$ ( $\bar{4}_x   0,0,0$ )'
(45) $\bar{4}^+ ' 0,y,0; 0,0,0$ ( $\bar{4}_y   0,0,0$ )'	(46) $m' \bar{x},y,x$ ( $m_{xz}   0,0,0$ )'	(47) $\bar{4}^- ' 0,y,0; 0,0,0$ ( $\bar{4}_y^{-1}   0,0,0$ )'	(48) $m' x,y,x$ ( $m_{\bar{z}}   0,0,0$ )'

## For (0,1/2,1/2)' + set

(1) $t' (0,1/2,1/2)$ ( $\bar{1}   0,1/2,1/2$ )'	(2) $2' (0,0,1/2) 0,1/4,z$ ( $2_z   0,1/2,1/2$ )'	(3) $2' (0,1/2,0) 0,y,1/4$ ( $2_y   0,1/2,1/2$ )'	(4) $2' x,1/4,1/4$ ( $2_x   0,1/2,1/2$ )'
(5) $3^+ ' (1/3,1/3,1/3)$ $x-1/3,x-1/6,x$ ( $3_{xyz}   0,1/2,1/2$ )'	(6) $3^+ ' \bar{x},x+1/2,\bar{x}$ ( $3_{x\bar{y}\bar{z}}^{-1}   0,1/2,1/2$ )'	(7) $3^+ ' (-1/3,1/3,1/3)$ $x+1/3,x-1/6,\bar{x}$ ( $3_{\bar{y}\bar{z}}^{-1}   0,1/2,1/2$ )'	(8) $3^+ ' \bar{x},\bar{x}+1/2,x$ ( $3_{x\bar{y}\bar{z}}^{-1}   0,1/2,1/2$ )'
(9) $3^- ' (1/3,1/3,1/3)$ $x-1/6,x+1/6,x$ ( $3_{xyz}^{-1}   0,1/2,1/2$ )'	(10) $3^- ' (-1/3,1/3,1/3)$ $x+1/6,x+1/6,\bar{x}$ ( $3_{\bar{y}\bar{z}}   0,1/2,1/2$ )'	(11) $3^- ' \bar{x}+1/2,\bar{x}+1/2,x$ ( $3_{x\bar{y}\bar{z}}   0,1/2,1/2$ )'	(12) $3^- ' \bar{x}-1/2,x+1/2,\bar{x}$ ( $3_{x\bar{y}\bar{z}}   0,1/2,1/2$ )'
(13) $2' (1/4,1/4,0) x,x+1/4,1/4$ ( $2_{xy}   0,1/2,1/2$ )'	(14) $2' (-1/4,1/4,0) x,\bar{x}+1/4,1/4$ ( $2_{\bar{xy}}   0,1/2,1/2$ )'	(15) $4^- ' (0,0,1/2) 1/4,1/4,z$ ( $4_z^{-1}   0,1/2,1/2$ )'	(16) $4^+ ' (0,0,1/2) -1/4,1/4,z$ ( $4_z   0,1/2,1/2$ )'
(17) $4^- ' x,1/2,0$ ( $4_x^{-1}   0,1/2,1/2$ )'	(18) $2' (0,1/2,1/2) 0,y,y$ ( $2_{yz}   0,1/2,1/2$ )'	(19) $2' 0,y+1/2,\bar{y}$ ( $2_{\bar{yz}}   0,1/2,1/2$ )'	(20) $4^+ ' x,0,1/2$ ( $4_x   0,1/2,1/2$ )'
(21) $4^+ ' (0,1/2,0) 1/4,y,1/4$ ( $4_y   0,1/2,1/2$ )'	(22) $2' (1/4,0,1/4) x-1/4,1/4,x$ ( $2_{xz}   0,1/2,1/2$ )'	(23) $4^- ' (0,1/2,0) -1/4,y,1/4$ ( $4_y^{-1}   0,1/2,1/2$ )'	(24) $2' (-1/4,0,1/4)\bar{x}+1/4,1/4,x$ ( $2_{\bar{z}}   0,1/2,1/2$ )'
(25) $\bar{1}' 0,1/4,1/4$ ( $\bar{1}   0,1/2,1/2$ )'	(26) $b' (0,1/2,0) x,y,1/4$ ( $m_z   0,1/2,1/2$ )'	(27) $c' (0,0,1/2) x,1/4,z$ ( $m_y   0,1/2,1/2$ )'	(28) $n' (0,1/2,1/2) 0,y,z$ ( $m_x   0,1/2,1/2$ )'
(29) $\bar{3}^+ ' x,x+1/2,x;$ $0,1/2,0$ ( $\bar{3}_{xyz}   0,1/2,1/2$ )'	(30) $\bar{3}^+ ' \bar{x}-1,x+1/2,\bar{x};$ $-1/2,0,1/2$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1}   0,1/2,1/2$ )'	(31) $\bar{3}^+ ' x,\bar{x}+1/2,\bar{x};$ $0,1/2,0$ ( $\bar{3}_{\bar{y}\bar{z}}^{-1}   0,1/2,1/2$ )'	(32) $\bar{3}^+ ' \bar{x}-1,\bar{x}+1/2,x;$ $1/2,0,1/2$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1}   0,1/2,1/2$ )'
(33) $\bar{3}^- ' x-1/2,x-1/2,x;$ $0,0,1/2$ ( $\bar{3}_{xyz}^{-1}   0,1/2,1/2$ )'	(34) $\bar{3}^- ' x+1/2,\bar{x}-1/2,\bar{x};$ $0,0,1/2$ ( $\bar{3}_{\bar{y}\bar{z}}   0,1/2,1/2$ )'	(35) $\bar{3}^- ' \bar{x}-1/2,\bar{x}+1/2,x;$ $-1/2,1/2,0$ ( $\bar{3}_{x\bar{y}\bar{z}}   0,1/2,1/2$ )'	(36) $\bar{3}^- ' \bar{x}+1/2,x+1/2,\bar{x};$ $1/2,1/2,0$ ( $\bar{3}_{x\bar{y}\bar{z}}   0,1/2,1/2$ )'
(37) $g' (-1/4,1/4,1/2) x+1/4,\bar{x},z$ ( $m_{xy}   0,1/2,1/2$ )'	(38) $g' (1/4,1/4,1/2) x-1/4,x,z$ ( $m_{\bar{xy}}   0,1/2,1/2$ )'	(39) $\bar{4}^- ' -1/4,1/4,z; -1/4,1/4,1/4$ ( $\bar{4}_z^{-1}   0,1/2,1/2$ )'	(40) $\bar{4}^+ ' 1/4,1/4,z; 1/4,1/4,1/4$ ( $\bar{4}_z   0,1/2,1/2$ )'

- (41)  $\bar{4}^- ' x, 0, 1/2; 0, 0, 1/2$   
( $\bar{4}_x^{-1} | 0, 1/2, 1/2$ )'
- (42)  $m' x, y+1/2, \bar{y}$   
( $m_{yz} | 0, 1/2, 1/2$ )'
- (43)  $g' (0, 1/2, 1/2) x, y, y$   
( $m_{\bar{y}z} | 0, 1/2, 1/2$ )'
- (44)  $\bar{4}^+ ' x, 1/2, 0; 0, 1/2, 0$   
( $\bar{4}_x | 0, 1/2, 1/2$ )'
- (45)  $\bar{4}^+ ' -1/4, y, 1/4; -1/4, 1/4, 1/4$   
( $\bar{4}_y | 0, 1/2, 1/2$ )'
- (46)  $g' (-1/4, 1/2, 1/4) \bar{x}+1/4, y, x$   
( $m_{xz} | 0, 1/2, 1/2$ )'
- (47)  $\bar{4}^- ' 1/4, y, 1/4; 1/4, 1/4, 1/4$   
( $\bar{4}_y^{-1} | 0, 1/2, 1/2$ )'
- (48)  $g' (1/4, 1/2, 1/4) x-1/4, y, x$   
( $m_{\bar{x}z} | 0, 1/2, 1/2$ )'

For (1/2, 0, 1/2)' + set

- (1)  $t' (1/2, 0, 1/2)$   
( $1 | 1/2, 0, 1/2$ )'
- (2)  $2' (0, 0, 1/2) 1/4, 0, z$   
( $2_z | 1/2, 0, 1/2$ )'
- (3)  $2' 1/4, y, 1/4$   
( $2_y | 1/2, 0, 1/2$ )'
- (4)  $2' (1/2, 0, 0) x, 0, 1/2$   
( $2_x | 1/2, 0, 1/2$ )'
- (5)  $3^+ ' (1/3, 1/3, 1/3)$   
 $x+1/6, x-1/6, x$   
( $3_{xyz} | 1/2, 0, 1/2$ )'
- (6)  $3^+ ' (1/3, -1/3, 1/3)$   
 $\bar{x}+1/6, x+1/6, \bar{x}$   
( $3_{x\bar{y}z}^{-1} | 1/2, 0, 1/2$ )'
- (7)  $3^+ ' x+1/2, \bar{x}-1/2, \bar{x}$   
( $3_{\bar{y}z}^{-1} | 1/2, 0, 1/2$ )'
- (8)  $3^+ ' \bar{x}+1/2, \bar{x}+1/2, x$   
( $3_{x\bar{y}\bar{z}}^{-1} | 1/2, 0, 1/2$ )'
- (9)  $3^- ' (1/3, 1/3, 1/3)$   
 $x-1/6, x-1/3, x$   
( $3_{xyz}^{-1} | 1/2, 0, 1/2$ )'
- (10)  $3^- ' x+1/2, \bar{x}, \bar{x}$   
( $3_{\bar{y}z} | 1/2, 0, 1/2$ )'
- (11)  $3^- ' \bar{x}+1/2, \bar{x}, x$   
( $3_{x\bar{y}\bar{z}} | 1/2, 0, 1/2$ )'
- (12)  $3^- ' (1/3, -1/3, 1/3)$   
 $\bar{x}-1/6, x+1/3, \bar{x}$   
( $3_{x\bar{y}z} | 1/2, 0, 1/2$ )'
- (13)  $2' (1/4, 1/4, 0) x, x-1/4, 1/4$   
( $2_{xy} | 1/2, 0, 1/2$ )'
- (14)  $2' (1/4, -1/4, 0) x, \bar{x}+1/4, 1/4$   
( $2_{\bar{xy}} | 1/2, 0, 1/2$ )'
- (15)  $4^- ' (0, 0, 1/2) 1/4, -1/4, z$   
( $4_z^{-1} | 1/2, 0, 1/2$ )'
- (16)  $4^+ ' (0, 0, 1/2) 1/4, 1/4, z$   
( $4_z | 1/2, 0, 1/2$ )'
- (17)  $4^- ' (1/2, 0, 0) x, 1/4, 1/4$   
( $4_x^{-1} | 1/2, 0, 1/2$ )'
- (18)  $2' (0, 1/4, 1/4) 1/4, y-1/4, y$   
( $2_{yz} | 1/2, 0, 1/2$ )'
- (19)  $2' (0, -1/2, 1/2) 1/4, y+1/4, \bar{y}$   
( $2_{\bar{y}z} | 1/2, 0, 1/2$ )'
- (20)  $4^+ ' (1/2, 0, 0) x, -1/4, 1/4$   
( $4_x | 1/2, 0, 1/2$ )'
- (21)  $4^+ ' 1/2, y, 0$   
( $4_y | 1/2, 0, 1/2$ )'
- (22)  $2' (1/2, 0, 1/2) x, 0, x$   
( $2_{xz} | 1/2, 0, 1/2$ )'
- (23)  $4^- ' 0, y, 1/2$   
( $4_y^{-1} | 1/2, 0, 1/2$ )'
- (24)  $2' \bar{x}+1/2, 0, x$   
( $2_{\bar{x}z} | 1/2, 0, 1/2$ )'
- (25)  $\bar{1} ' 1/4, 0, 1/4$   
( $\bar{1} | 1/2, 0, 1/2$ )'
- (26)  $a' (1/2, 0, 0) x, y, 1/4$   
( $m_z | 1/2, 0, 1/2$ )'
- (27)  $n' (1/2, 0, 1/2) x, 0, z$   
( $m_y | 1/2, 0, 1/2$ )'
- (28)  $c' (0, 0, 1/2) 1/4, y, z$   
( $m_x | 1/2, 0, 1/2$ )'
- (29)  $\bar{3}^+ ' x-1/2, x-1/2, x;$   
 $0, 0, 1/2$   
( $\bar{3}_{xyz} | 1/2, 0, 1/2$ )'
- (30)  $\bar{3}^+ ' \bar{x}-1/2, x+1/2, \bar{x};$   
 $0, 0, 1/2$   
( $\bar{3}_{x\bar{y}z}^{-1} | 1/2, 0, 1/2$ )'
- (31)  $\bar{3}^+ ' x+1/2, \bar{x}+1/2, \bar{x};$   
 $1/2, 1/2, 0$   
( $\bar{3}_{\bar{y}z}^{-1} | 1/2, 0, 1/2$ )'
- (32)  $\bar{3}^+ ' \bar{x}+1/2, \bar{x}-1/2, x;$   
 $1/2, -1/2, 0$   
( $\bar{3}_{x\bar{y}\bar{z}}^{-1} | 1/2, 0, 1/2$ )'
- (33)  $\bar{3}^- ' x+1/2, x, x;$   
 $1/2, 0, 0$   
( $\bar{3}_{xyz}^{-1} | 1/2, 0, 1/2$ )'
- (34)  $\bar{3}^- ' x+1/2, \bar{x}-1, \bar{x};$   
 $0, -1/2, 1/2$   
( $\bar{3}_{\bar{y}z} | 1/2, 0, 1/2$ )'
- (35)  $\bar{3}^- ' \bar{x}+1/2, \bar{x}+1, x;$   
 $0, 1/2, 1/2$   
( $\bar{3}_{x\bar{y}\bar{z}} | 1/2, 0, 1/2$ )'
- (36)  $\bar{3}^- ' \bar{x}+1/2, x, \bar{x};$   
 $1/2, 0, 0$   
( $\bar{3}_{x\bar{y}z} | 1/2, 0, 1/2$ )'
- (37)  $g' (1/4, -1/4, 1/2) x+1/4, \bar{x}, z$   
( $m_{xy} | 1/2, 0, 1/2$ )'
- (38)  $g' (1/4, 1/4, 1/2) x+1/4, x, z$   
( $m_{\bar{xy}} | 1/2, 0, 1/2$ )'
- (39)  $\bar{4}^- ' 1/4, 1/4, z; 1/4, 1/4, 1/4$   
( $\bar{4}_z^{-1} | 1/2, 0, 1/2$ )'
- (40)  $\bar{4}^+ ' 1/4, -1/4, z; 1/4, -1/4, 1/4$   
( $\bar{4}_z | 1/2, 0, 1/2$ )'
- (41)  $\bar{4}^- ' x, -1/4, 1/4; 1/4, -1/4, 1/4$   
( $\bar{4}_x^{-1} | 1/2, 0, 1/2$ )'
- (42)  $g' (1/2, -1/4, 1/4) x, y+1/4, \bar{y}$   
( $m_{yz} | 1/2, 0, 1/2$ )'
- (43)  $g' (1/2, 1/4, 1/4) x, y-1/4, y$   
( $m_{\bar{y}z} | 1/2, 0, 1/2$ )'
- (44)  $\bar{4}^+ ' x, 1/4, 1/4; 1/4, 1/4, 1/4$   
( $\bar{4}_x | 1/2, 0, 1/2$ )'
- (45)  $\bar{4}^+ ' 0, y, 1/2; 0, 0, 1/2$   
( $\bar{4}_y | 1/2, 0, 1/2$ )'
- (46)  $m' \bar{x}+1/2, y, x$   
( $m_{xz} | 1/2, 0, 1/2$ )'
- (47)  $\bar{4}^- ' 1/2, y, 0; 1/2, 0, 0$   
( $\bar{4}_y^{-1} | 1/2, 0, 1/2$ )'
- (48)  $g' (1/2, 0, 1/2) x, y, x$   
( $m_{\bar{x}z} | 1/2, 0, 1/2$ )'

For (1/2, 1/2, 0)' + set

- (1)  $t' (1/2, 1/2, 0)$   
( $1 | 1/2, 1/2, 0$ )'
- (2)  $2' 1/4, 1/4, z$   
( $2_z | 1/2, 1/2, 0$ )'
- (3)  $2' (0, 1/2, 0) 1/4, y, 0$   
( $2_y | 1/2, 1/2, 0$ )'
- (4)  $2' (1/2, 0, 0) x, 1/4, 0$   
( $2_x | 1/2, 1/2, 0$ )'
- (5)  $3^+ ' (1/3, 1/3, 1/3)$   
 $x+1/6, x+1/3, x$   
( $3_{xyz} | 1/2, 1/2, 0$ )'
- (6)  $3^+ ' \bar{x}+1/2, x, \bar{x}$   
( $3_{x\bar{y}z}^{-1} | 1/2, 1/2, 0$ )'
- (7)  $3^+ ' x+1/2, \bar{x}, \bar{x}$   
( $3_{\bar{y}z}^{-1} | 1/2, 1/2, 0$ )'
- (8)  $3^+ ' (1/3, 1/3, -1/3)$   
 $\bar{x}+1/6, \bar{x}+1/3, \bar{x}$   
( $3_{x\bar{y}\bar{z}}^{-1} | 1/2, 1/2, 0$ )'

(9) $3^-$ ' (1/3,1/3,1/3) x+1/3,x+1/6,x ( $3_{xyz}^{-1}$   1/2,1/2,0)'	(10) $3^-$ ' x, $\bar{x}$ +1/2, $\bar{x}$ ( $3_{\bar{xyz}}$   1/2,1/2,0)'	(11) $3^-$ ' (1/3,1/3,-1/3) x+1/3,x+1/6,x ( $3_{xy\bar{z}}$   1/2,1/2,0)'	(12) $3^-$ ' $\bar{x}$ ,x+1/2, $\bar{x}$ ( $3_{xy\bar{z}}$   1/2,1/2,0)'
(13) $2'$ (1/2,1/2,0) x,x,0 ( $2_{xy}$   1/2,1/2,0)'	(14) $2'$ x, $\bar{x}$ +1/2,0 ( $2_{\bar{xy}}$   1/2,1/2,0)'	(15) $4^-$ ' 1/2,0,z ( $4_z^{-1}$   1/2,1/2,0)'	(16) $4^+$ ' 0,1/2,z ( $4_z$   1/2,1/2,0)'
(17) $4^-$ ' (1/2,0,0) x,1/4,-1/4 ( $4_x^{-1}$   1/2,1/2,0)'	(18) $2'$ (0,1/4,1/4) 1/4,y+1/4,y ( $2_{yz}$   1/2,1/2,0)'	(19) $2'$ (0,1/4,-1/4) 1/4,y+1/4, $\bar{y}$ ( $2_{yz}$   1/2,1/2,0)'	(20) $4^+$ ' (1/2,0,0) x,1/4,1/4 ( $4_x$   1/2,1/2,0)'
(21) $4^+$ ' (0,1/2,0) 1/4,y,-1/4 ( $4_y$   1/2,1/2,0)'	(22) $2'$ (1/4,0,1/4) x+1/4,1/4,x ( $2_{xz}$   1/2,1/2,0)'	(23) $4^-$ ' (0,1/2,0) 1/4,y,1/4 ( $4_y^{-1}$   1/2,1/2,0)'	(24) $2'$ (1/4,0,-1/4) $\bar{x}$ +1/4,1/4,x ( $2_{xz}$   1/2,1/2,0)'
(25) $\bar{1}$ ' 1/4,1/4,0 ( $\bar{1}$   1/2,1/2,0)'	(26) n' (1/2,1/2,0) x,y,0 ( $m_z$   1/2,1/2,0)'	(27) a' (1/2,0,0) x,1/4,z ( $m_y$   1/2,1/2,0)'	(28) b' (0,1/2,0) 1/4,y,z ( $m_x$   1/2,1/2,0)'
(29) $\bar{3}^+$ ' x+1/2,x,x; 1/2,0,0 ( $\bar{3}_{xyz}$   1/2,1/2,0)'	(30) $\bar{3}^+$ ' $\bar{x}$ -1/2,x+1, $\bar{x}$ ; 0,1/2,1/2 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0)'	(31) $\bar{3}^+$ ' x-1/2, $\bar{x}$ +1, $\bar{x}$ ; 0,1/2,-1/2 ( $\bar{3}_{xy\bar{z}}$   1/2,1/2,0)'	(32) $\bar{3}^+$ ' $\bar{x}$ +1/2, $\bar{x}$ ,x; 1/2,0,0 ( $\bar{3}_{xy\bar{z}}$   1/2,1/2,0)'
(33) $\bar{3}^-$ ' x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xy\bar{z}}$   1/2,1/2,0)'	(34) $\bar{3}^-$ ' x+1, $\bar{x}$ -1/2, $\bar{x}$ ; 1/2,0,1/2 ( $\bar{3}_{xyz}$   1/2,1/2,0)'	(35) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ +1/2,x; 0,1/2,0 ( $\bar{3}_{xy\bar{z}}$   1/2,1/2,0)'	(36) $\bar{3}^-$ ' $\bar{x}$ +1,x-1/2, $\bar{x}$ ; 1/2,0,-1/2 ( $\bar{3}_{xyz}$   1/2,1/2,0)'
(37) m' x+1/2, $\bar{x}$ ,z ( $m_{xy}$   1/2,1/2,0)'	(38) g' (1/2,1/2,0) x,x,z ( $m_{\bar{xy}}$   1/2,1/2,0)'	(39) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,0 ( $\bar{4}_z^{-1}$   1/2,1/2,0)'	(40) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,0 ( $\bar{4}_z$   1/2,1/2,0)'
(41) $\bar{4}^-$ ' x,1/4,1/4; 1/4,1/4,1/4 ( $\bar{4}_x^{-1}$   1/2,1/2,0)'	(42) g' (1/2,1/4,-1/4) x,y+1/4, $\bar{y}$ ( $m_{yz}$   1/2,1/2,0)'	(43) g' (1/2,1/4,1/4) x,y+1/4,y ( $m_{\bar{yz}}$   1/2,1/2,0)'	(44) $\bar{4}^+$ ' x,1/4,-1/4; 1/4,1/4,-1/4 ( $\bar{4}_x$   1/2,1/2,0)'
(45) $\bar{4}^+$ ' 1/4,y,1/4; 1/4,1/4,1/4 ( $\bar{4}_y$   1/2,1/2,0)'	(46) g' (1/4,1/2,-1/4) $\bar{x}$ +1/4,y,x ( $m_{xz}$   1/2,1/2,0)'	(47) $\bar{4}^-$ ' 1/4,y,-1/4; 1/4,1/4,-1/4 ( $\bar{4}_y^{-1}$   1/2,1/2,0)'	(48) g' (1/4,1/2,1/4) x+1/4,y,x ( $m_{\bar{xz}}$   1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25); 1'.

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

### Coordinates

(0,0,0) + (0,1/2,1/2,) + (1/2,0,1/2) + (1/2,1/2,0) +  
(0,0,0)' + (0,1/2,1/2,)' + (1/2,0,1/2)' + (1/2,1/2,0)'

192 | 11'

(1) x,y,z [0,0,0]	(2) $\bar{x}$ , $\bar{y}$ ,z [0,0,0]	(3) $\bar{x}$ ,y, $\bar{z}$ [0,0,0]	(4) x, $\bar{y}$ , $\bar{z}$ [0,0,0]
(5) z,x,y [0,0,0]	(6) z, $\bar{x}$ , $\bar{y}$ [0,0,0]	(7) $\bar{z}$ , $\bar{x}$ ,y [0,0,0]	(8) $\bar{z}$ ,x, $\bar{y}$ [0,0,0]
(9) y,z,x [0,0,0]	(10) $\bar{y}$ ,z, $\bar{x}$ [0,0,0]	(11) y, $\bar{z}$ , $\bar{x}$ [0,0,0]	(12) $\bar{y}$ , $\bar{z}$ ,x [0,0,0]
(13) y,x, $\bar{z}$ [0,0,0]	(14) $\bar{y}$ , $\bar{x}$ , $\bar{z}$ [0,0,0]	(15) y, $\bar{x}$ ,z [0,0,0]	(16) $\bar{y}$ ,x,z [0,0,0]
(17) x,z, $\bar{y}$ [0,0,0]	(18) $\bar{x}$ ,z,y [0,0,0]	(19) $\bar{x}$ , $\bar{z}$ , $\bar{y}$ [0,0,0]	(20) x, $\bar{z}$ ,y [0,0,0]
(21) z,y, $\bar{x}$ [0,0,0]	(22) z, $\bar{y}$ ,x [0,0,0]	(23) $\bar{z}$ ,y,x [0,0,0]	(24) $\bar{z}$ , $\bar{y}$ , $\bar{x}$ [0,0,0]

(25)	$\bar{x}, \bar{y}, \bar{z}$	[0,0,0]	(26)	$x, y, \bar{z}$	[0,0,0]	(27)	$x, \bar{y}, z$	[0,0,0]	(28)	$\bar{x}, y, z$	[0,0,0]
(29)	$\bar{z}, \bar{x}, \bar{y}$	[0,0,0]	(30)	$\bar{z}, x, y$	[0,0,0]	(31)	$z, x, \bar{y}$	[0,0,0]	(32)	$z, \bar{x}, y$	[0,0,0]
(33)	$\bar{y}, \bar{z}, \bar{x}$	[0,0,0]	(34)	$y, \bar{z}, x$	[0,0,0]	(35)	$\bar{y}, z, x$	[0,0,0]	(36)	$y, z, \bar{x}$	[0,0,0]
(37)	$\bar{y}, \bar{x}, z$	[0,0,0]	(38)	$y, x, z$	[0,0,0]	(39)	$\bar{y}, x, \bar{z}$	[0,0,0]	(40)	$y, \bar{x}, \bar{z}$	[0,0,0]
(41)	$\bar{x}, \bar{z}, y$	[0,0,0]	(42)	$x, \bar{z}, \bar{y}$	[0,0,0]	(43)	$x, z, y$	[0,0,0]	(44)	$\bar{x}, z, \bar{y}$	[0,0,0]
(45)	$\bar{z}, \bar{y}, x$	[0,0,0]	(46)	$\bar{z}, y, \bar{x}$	[0,0,0]	(47)	$z, \bar{y}, \bar{x}$	[0,0,0]	(48)	$z, y, x$	[0,0,0]
96	k	..m1'	$x, x, z$	[0,0,0]	$\bar{x}, \bar{x}, z$	[0,0,0]	$\bar{x}, x, \bar{z}$	[0,0,0]	$x, \bar{x}, \bar{z}$	[0,0,0]	
			$z, x, x$	[0,0,0]	$z, \bar{x}, \bar{x}$	[0,0,0]	$\bar{z}, \bar{x}, x$	[0,0,0]	$\bar{z}, x, \bar{x}$	[0,0,0]	
			$x, z, x$	[0,0,0]	$\bar{x}, z, \bar{x}$	[0,0,0]	$x, \bar{z}, \bar{x}$	[0,0,0]	$\bar{x}, \bar{z}, x$	[0,0,0]	
			$x, x, \bar{z}$	[0,0,0]	$\bar{x}, \bar{x}, \bar{z}$	[0,0,0]	$x, \bar{x}, z$	[0,0,0]	$\bar{x}, x, z$	[0,0,0]	
			$x, z, \bar{x}$	[0,0,0]	$\bar{x}, z, x$	[0,0,0]	$\bar{x}, \bar{z}, \bar{x}$	[0,0,0]	$x, \bar{z}, x$	[0,0,0]	
			$z, x, \bar{x}$	[0,0,0]	$z, \bar{x}, x$	[0,0,0]	$\bar{z}, x, x$	[0,0,0]	$\bar{z}, \bar{x}, \bar{x}$	[0,0,0]	
96	j	m..1'	$0, y, z$	[0,0,0]	$0, \bar{y}, z$	[0,0,0]	$0, y, \bar{z}$	[0,0,0]	$0, \bar{y}, \bar{z}$	[0,0,0]	
			$z, 0, y$	[0,0,0]	$z, 0, \bar{y}$	[0,0,0]	$\bar{z}, 0, y$	[0,0,0]	$\bar{z}, 0, \bar{y}$	[0,0,0]	
			$y, z, 0$	[0,0,0]	$\bar{y}, z, 0$	[0,0,0]	$y, \bar{z}, 0$	[0,0,0]	$\bar{y}, \bar{z}, 0$	[0,0,0]	
			$y, 0, \bar{z}$	[0,0,0]	$\bar{y}, 0, \bar{z}$	[0,0,0]	$y, 0, z$	[0,0,0]	$\bar{y}, 0, z$	[0,0,0]	
			$0, z, \bar{y}$	[0,0,0]	$0, z, y$	[0,0,0]	$0, \bar{z}, \bar{y}$	[0,0,0]	$0, \bar{z}, y$	[0,0,0]	
			$z, y, 0$	[0,0,0]	$z, \bar{y}, 0$	[0,0,0]	$\bar{z}, y, 0$	[0,0,0]	$\bar{z}, \bar{y}, 0$	[0,0,0]	
48	i	m.m21'	$1/2, y, y$	[0,0,0]	$1/2, \bar{y}, y$	[0,0,0]	$1/2, y, \bar{y}$	[0,0,0]	$1/2, \bar{y}, \bar{y}$	[0,0,0]	
			$y, 1/2, y$	[0,0,0]	$y, 1/2, \bar{y}$	[0,0,0]	$\bar{y}, 1/2, y$	[0,0,0]	$\bar{y}, 1/2, \bar{y}$	[0,0,0]	
			$y, y, 1/2$	[0,0,0]	$\bar{y}, y, 1/2$	[0,0,0]	$y, \bar{y}, 1/2$	[0,0,0]	$\bar{y}, \bar{y}, 1/2$	[0,0,0]	
48	h	m.m21'	$0, y, y$	[0,0,0]	$0, \bar{y}, y$	[0,0,0]	$0, y, \bar{y}$	[0,0,0]	$0, \bar{y}, \bar{y}$	[0,0,0]	
			$y, 0, y$	[0,0,0]	$y, 0, \bar{y}$	[0,0,0]	$\bar{y}, 0, y$	[0,0,0]	$\bar{y}, 0, \bar{y}$	[0,0,0]	
			$y, y, 0$	[0,0,0]	$\bar{y}, y, 0$	[0,0,0]	$y, \bar{y}, 0$	[0,0,0]	$\bar{y}, \bar{y}, 0$	[0,0,0]	
48	g	2.mm1'	$x, 1/4, 1/4$	[0,0,0]	$\bar{x}, 3/4, 1/4$	[0,0,0]	$1/4, x, 1/4$	[0,0,0]	$1/4, \bar{x}, 3/4$	[0,0,0]	
			$1/4, 1/4, x$	[0,0,0]	$3/4, 1/4, \bar{x}$	[0,0,0]	$1/4, x, 3/4$	[0,0,0]	$3/4, \bar{x}, 3/4$	[0,0,0]	
			$x, 1/4, 3/4$	[0,0,0]	$\bar{x}, 1/4, 1/4$	[0,0,0]	$1/4, 1/4, \bar{x}$	[0,0,0]	$1/4, 3/4, x$	[0,0,0]	
32	f	.3m1'	$x, x, x$	[0,0,0]	$\bar{x}, \bar{x}, x$	[0,0,0]	$\bar{x}, x, \bar{x}$	[0,0,0]	$x, \bar{x}, \bar{x}$	[0,0,0]	
			$x, x, \bar{x}$	[0,0,0]	$\bar{x}, \bar{x}, \bar{x}$	[0,0,0]	$x, \bar{x}, x$	[0,0,0]	$\bar{x}, x, x$	[0,0,0]	



Continued

225.2.1619

 $Fm\bar{3}m1'$ 

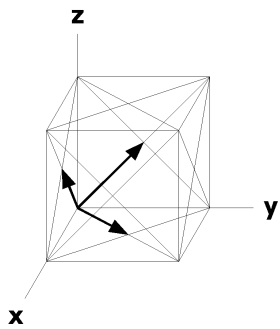
24	e	$4m.m1'$ $x,0,0$ $[0,0,0]$	$\bar{x},0,0$ $[0,0,0]$	$0,x,0$ $[0,0,0]$
		$0,\bar{x},0$ $[0,0,0]$	$0,0,x$ $[0,0,0]$	$0,0,\bar{x}$ $[0,0,0]$
24	d	$m.mm1'$ $0,1/4,1/4$ $[0,0,0]$	$0,3/4,1/4$ $[0,0,0]$	$1/4,0,1/4$ $[0,0,0]$
		$1/4,0,3/4$ $[0,0,0]$	$1/4,1/4,0$ $[0,0,0]$	$3/4,1/4,0$ $[0,0,0]$
8	c	$\bar{4}3m1'$ $1/4,1/4,1/4$ $[0,0,0]$	$1/4,1/4,3/4$ $[0,0,0]$	
4	b	$m\bar{3}m1'$ $1/2,1/2,1/2$ $[0,0,0]$		
4	a	$m\bar{3}m1'$ $0,0,0$ $[0,0,0]$		

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p6mm1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at  $x,x,x$

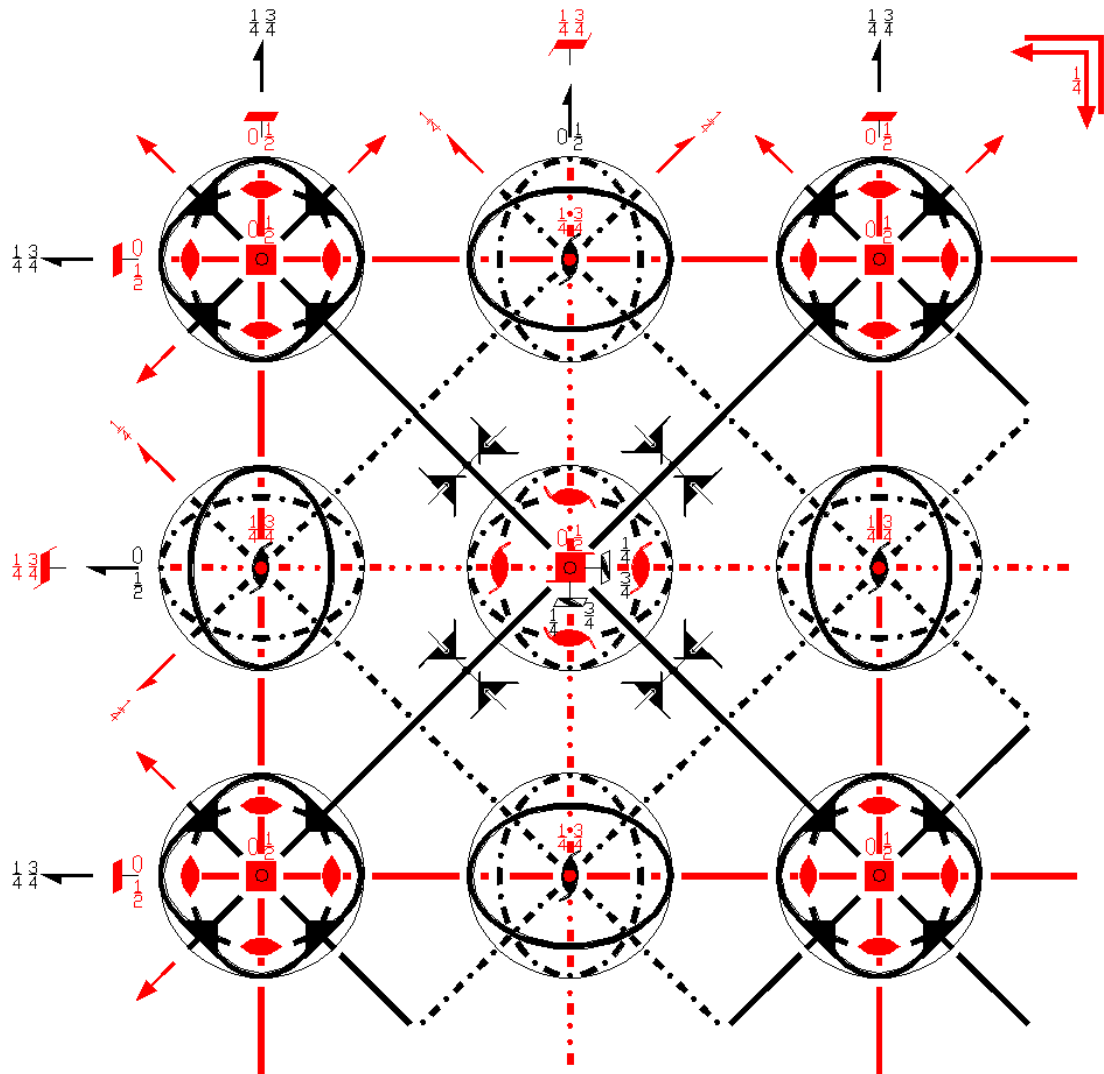
Along  $[1,1,0]$   $c2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x,x,0$



$Fm\bar{3}'m$   
225.3.1620

$m\bar{3}'m$   
 $F4'/m\bar{3}'2'/m$

Cubic



**Origin** at center ( $m\bar{3}'m$ )

<b>Asymmetric unit</b>	$0 \leq x \leq 1/2;$	$0 \leq y \leq 1/4;$	$0 \leq z \leq 1/4;$	$y \leq \min(x, 1/2-x);$	$z \leq y$
Vertices	0,0,0	1/2,0,0	1/4,1/4,0	1/4,1/4,1/4	

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)              | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub>xyz<sup>-1</sup></sub>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz<sup>-1</sup></sub>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz<sup>-1</sup></sub>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz<sup>-1</sup></sub>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)            | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub>xyz</sub>  0,0,0)              | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)             |

(13) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(14) 2' x, $\bar{x}$ ,0 (2 <sub>xy</sub>  0,0,0)'	(15) 4' 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'	(16) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)'
(17) 4' x,0,0 (4 <sub>x</sub> <sup>-1</sup>  0,0,0)'	(18) 2' 0,y,y (2 <sub>yz</sub>  0,0,0)'	(19) 2' 0,y, $\bar{y}$ (2 <sub>yz</sub>  0,0,0)'	(20) 4 <sup>+</sup> x,0,0 (4 <sub>x</sub>  0,0,0)'
(21) 4 <sup>+</sup> 0,y,0 (4 <sub>y</sub>  0,0,0)'	(22) 2' x,0,x (2 <sub>xz</sub>  0,0,0)'	(23) 4' 0,y,0 (4 <sub>y</sub> <sup>-1</sup>  0,0,0)'	(24) 2' $\bar{x}$ ,0,x (2 <sub>xz</sub>  0,0,0)'
(25) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)'	(26) m' x,y,0 (m <sub>z</sub>  0,0,0)'	(27) m' x,0,z (m <sub>y</sub>  0,0,0)'	(28) m' 0,y,z (m <sub>x</sub>  0,0,0)'
(29) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'	(30) $\bar{3}^+$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(31) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(32) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'
(33) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(34) $\bar{3}^-$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'	(35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'	(36) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'
(37) m x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)	(38) m x,x,z (m <sub>xy</sub>  0,0,0)	(39) $\bar{4}$ 0,0,z; 0,0,0 ( $\bar{4}_z$ <sup>-1</sup>  0,0,0)	(40) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)
(41) $\bar{4}$ x,0,0; 0,0,0 ( $\bar{4}_x$ <sup>-1</sup>  0,0,0)	(42) m x,y, $\bar{y}$ (m <sub>yz</sub>  0,0,0)	(43) m x,y,y (m <sub>yz</sub>  0,0,0)	(44) $\bar{4}^+$ x,0,0; 0,0,0 ( $\bar{4}_x$  0,0,0)
(45) $\bar{4}^+$ 0,y,0; 0,0,0 ( $\bar{4}_y$  0,0,0)	(46) m $\bar{x}$ ,y,x (m <sub>xz</sub>  0,0,0)	(47) $\bar{4}$ 0,y,0; 0,0,0 ( $\bar{4}_y$ <sup>-1</sup>  0,0,0)	(48) m x,y,x (m <sub>xz</sub>  0,0,0)

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2) (1 0,1/2,1/2)	(2) 2 (0,0,1/2) 0,1/4,z (2 <sub>z</sub>  0,1/2,1/2)	(3) 2 (0,1/2,0) 0,y,1/4 (2 <sub>y</sub>  0,1/2,1/2)	(4) 2 x,1/4,1/4 (2 <sub>x</sub>  0,1/2,1/2)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x-1/3,x-1/6,x (3 <sub>xyz</sub>  0,1/2,1/2)	(6) 3 <sup>+</sup> $\bar{x}$ ,x+1/2, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(7) 3 <sup>+</sup> (-1/3,1/3,1/3) x+1/3, $\bar{x}$ -1/6, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ +1/2,x (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x-1/6,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(10) 3 <sup>-</sup> (-1/3,1/3,1/3) x+1/6, $\bar{x}$ +1/6, $\bar{x}$ (3 <sub>xyz</sub>  0,1/2,1/2)	(11) 3 <sup>-</sup> $\bar{x}$ +1/2, $\bar{x}$ +1/2,x (3 <sub>xyz</sub>  0,1/2,1/2)	(12) 3 <sup>-</sup> $\bar{x}$ -1/2,x+1/2, $\bar{x}$ (3 <sub>xyz</sub>  0,1/2,1/2)
(13) 2' (1/4,1/4,0) x,x+1/4,1/4 (2 <sub>xy</sub>  0,1/2,1/2)'	(14) 2' (-1/4,1/4,0) x, $\bar{x}$ +1/4,1/4 (2 <sub>xy</sub>  0,1/2,1/2)'	(15) 4' (0,0,1/2) 1/4,1/4,z (4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/2)'	(16) 4 <sup>+</sup> (0,0,1/2) -1/4,1/4,z (4 <sub>z</sub>  0,1/2,1/2)'
(17) 4' x,1/2,0 (4 <sub>x</sub> <sup>-1</sup>  0,1/2,1/2)'	(18) 2' (0,1/2,1/2) 0,y,y (2 <sub>yz</sub>  0,1/2,1/2)'	(19) 2' 0,y+1/2, $\bar{y}$ (2 <sub>yz</sub>  0,1/2,1/2)'	(20) 4 <sup>+</sup> x,0,1/2 (4 <sub>x</sub>  0,1/2,1/2)'
(21) 4 <sup>+</sup> (0,1/2,0) 1/4,y,1/4 (4 <sub>y</sub>  0,1/2,1/2)'	(22) 2' (1/4,0,1/4) x-1/4,1/4,x (2 <sub>xz</sub>  0,1/2,1/2)'	(23) 4' (0,1/2,0) -1/4,y,1/4 (4 <sub>y</sub> <sup>-1</sup>  0,1/2,1/2)'	(24) 2' (-1/4,0,1/4) $\bar{x}$ +1/4,1/4,x (2 <sub>xz</sub>  0,1/2,1/2)'
(25) $\bar{1}$ 0,1/4,1/4 ( $\bar{1}$  0,1/2,1/2)'	(26) b' (0,1/2,0) x,y,1/4 (m <sub>z</sub>  0,1/2,1/2)'	(27) c' (0,0,1/2) x,1/4,z (m <sub>y</sub>  0,1/2,1/2)'	(28) n' (0,1/2,1/2) 0,y,z (m <sub>x</sub>  0,1/2,1/2)'
(29) $\bar{3}^+$ x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$  0,1/2,1/2)'	(30) $\bar{3}^+$ $\bar{x}$ -1,x+1/2, $\bar{x}$ ; -1/2,0,1/2 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,1/2,1/2)'	(31) $\bar{3}^+$ x, $\bar{x}$ +1/2, $\bar{x}$ ; 0,1/2,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,1/2,1/2)'	(32) $\bar{3}^+$ $\bar{x}$ -1, $\bar{x}$ +1/2,x; 1/2,0,1/2 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,1/2,1/2)'

- |   |  |  |   |
|---|--|--|---|
| (33) $\bar{3}^-$ ' x-1/2,x-1/2,x;<br>0,0,1/2<br>( $\bar{3}_{xyz}^{-1}$  0,1/2,1/2)' | (34) $\bar{3}^-$ ' x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ;<br>0,0,1/2<br>( $\bar{3}_{\bar{xyz}}$  0,1/2,1/2)' | (35) $\bar{3}^-$ ' $\bar{x}$ -1/2, $\bar{x}$ +1/2, x;<br>-1/2,1/2,0<br>( $\bar{3}_{\bar{yz}}$  0,1/2,1/2)' | (36) $\bar{3}^-$ ' $\bar{x}$ +1/2, x+1/2, $\bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{\bar{yz}}$  0,1/2,1/2)' |
| (37) g (-1/4,1/4,1/2) x+1/4, $\bar{x}$ ,z<br>( $m_{xy}$  0,1/2,1/2)                 | (38) g (1/4,1/4,1/2) x-1/4,x,z<br>( $m_{\bar{xy}}$  0,1/2,1/2)   | (39) $\bar{4}^-$ -1/4,1/4,z; -1/4,1/4,1/4<br>( $\bar{4}_z^{-1}$  0,1/2,1/2)                                | (40) $\bar{4}^+$ 1/4,1/4,z; 1/4,1/4,1/4<br>( $\bar{4}_z$  0,1/2,1/2)                                      |
| (41) $\bar{4}^-$ x,0,1/2; 0,0,1/2<br>( $\bar{4}_x^{-1}$  0,1/2,1/2)                 | (42) m x,y+1/2, $\bar{y}$<br>( $m_{yz}$  0,1/2,1/2)  | (43) g (0,1/2,1/2) x,y,y<br>( $m_{\bar{yz}}$  0,1/2,1/2)   | (44) $\bar{4}^+$ x,1/2,0; 0,1/2,0<br>( $\bar{4}_x$  0,1/2,1/2)  |
| (45) $\bar{4}^+$ -1/4,y,1/4; -1/4,1/4,1/4<br>( $\bar{4}_y$  0,1/2,1/2)              | (46) g (-1/4,1/2,1/4) $\bar{x}$ +1/4,y,x<br>( $m_{xz}$  0,1/2,1/2)                                       | (47) $\bar{4}^-$ 1/4,y,1/4; 1/4,1/4,1/4<br>( $\bar{4}_y^{-1}$  0,1/2,1/2)                                  | (48) g (1/4,1/2,1/4) x-1/4,y,x<br>( $m_{\bar{xz}}$  0,1/2,1/2)  |

For (1/2,0,1/2) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,0,1/2)<br>(1 1/2,0,1/2)  | (2) 2 (0,0,1/2) 1/4,0,z<br>( $2_z$  1/2,0,1/2)   | (3) 2 1/4,y,1/4<br>( $2_y$  1/2,0,1/2)   | (4) 2 (1/2,0,0) x,0,1/2<br>( $2_x$  1/2,0,1/2)   |
| (5) $3^+$ (1/3,1/3,1/3)<br>x+1/6,x-1/6,x<br>( $3_{xyz}$  1/2,0,1/2)             | (6) $3^+$ (1/3,-1/3,1/3)<br>x+1/6,x+1/6, $\bar{x}$<br>( $3_{\bar{xyz}}^{-1}$  1/2,0,1/2)                     | (7) $3^+$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$<br>( $3_{\bar{yz}}^{-1}$  1/2,0,1/2)                                | (8) $3^+$ $\bar{x}$ +1/2, $\bar{x}$ +1/2,x<br>( $3_{\bar{yz}}^{-1}$  1/2,0,1/2)                                |
| (9) $3^-$ (1/3,1/3,1/3)<br>x-1/6,x-1/3,x<br>( $3_{xyz}^{-1}$  1/2,0,1/2)        | (10) $3^-$ x+1/2, $\bar{x}$ , $\bar{x}$<br>( $3_{\bar{yz}}$  1/2,0,1/2)                                      | (11) $3^-$ $\bar{x}$ +1/2, $\bar{x}$ , x<br>( $3_{\bar{yz}}$  1/2,0,1/2)                                       | (12) $3^-$ (1/3,-1/3,1/3)<br>$\bar{x}$ -1/6, x+1/3, $\bar{x}$<br>( $3_{\bar{yz}}$  1/2,0,1/2)                  |
| (13) $2'$ (1/4,1/4,0) x,x-1/4,1/4<br>( $2_{xy}$  1/2,0,1/2)'                    | (14) $2'$ (1/4,-1/4,0) x, $\bar{x}$ +1/4,1/4<br>( $2_{\bar{xy}}$  1/2,0,1/2)'                                | (15) $4^-$ ' (0,0,1/2) 1/4,-1/4,z<br>( $4_z^{-1}$  1/2,0,1/2)'   | (16) $4^+$ ' (0,0,1/2) 1/4,1/4,z<br>( $4_z$  1/2,0,1/2)'   |
| (17) $4^-$ ' (1/2,0,0) x,1/4,1/4<br>( $4_x^{-1}$  1/2,0,1/2)'                   | (18) $2'$ (0,1/4,1/4) 1/4,y-1/4,y<br>( $2_{yz}$  1/2,0,1/2)'   | (19) $2'$ (0,-1/2,1/2) 1/4,y+1/4, $\bar{y}$<br>( $2_{\bar{yz}}$  1/2,0,1/2)'                                   | (20) $4^+$ ' (1/2,0,0) x,-1/4,1/4<br>( $4_x$  1/2,0,1/2)'  |
| (21) $4^+$ ' 1/2,y,0<br>( $4_y$  1/2,0,1/2)'                                    | (22) $2'$ (1/2,0,1/2) x,0,x<br>( $2_{xz}$  1/2,0,1/2)'   | (23) $4^-$ ' 0,y,1/2<br>( $4_y^{-1}$  1/2,0,1/2)'  | (24) $2'$ $\bar{x}$ +1/2,0,x<br>( $2_{\bar{xz}}$  1/2,0,1/2)'  |
| (25) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$  1/2,0,1/2)'                            | (26) a' (1/2,0,0) x,y,1/4<br>( $m_z$  1/2,0,1/2)'  | (27) n' (1/2,0,1/2) x,0,z<br>( $m_y$  1/2,0,1/2)'  | (28) c' (0,0,1/2) 1/4,y,z<br>( $m_x$  1/2,0,1/2)'  |
| (29) $\bar{3}^+$ ' x-1/2,x-1/2,x;<br>0,0,1/2<br>( $\bar{3}_{xyz}$  1/2,0,1/2)'  | (30) $\bar{3}^+$ ' $\bar{x}$ -1/2,x+1/2, $\bar{x}$ ;<br>0,0,1/2<br>( $\bar{3}_{\bar{xyz}}^{-1}$  1/2,0,1/2)' | (31) $\bar{3}^+$ ' x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{\bar{yz}}^{-1}$  1/2,0,1/2)' | (32) $\bar{3}^+$ ' $\bar{x}$ +1/2, $\bar{x}$ -1/2,x;<br>1/2,-1/2,0<br>( $\bar{3}_{\bar{yz}}^{-1}$  1/2,0,1/2)' |
| (33) $\bar{3}^-$ ' x+1/2,x,x;<br>1/2,0,0<br>( $\bar{3}_{xyz}^{-1}$  1/2,0,1/2)' | (34) $\bar{3}^-$ ' x+1/2, $\bar{x}$ -1, $\bar{x}$ ;<br>0,-1/2,1/2<br>( $\bar{3}_{\bar{yz}}$  1/2,0,1/2)'     | (35) $\bar{3}^-$ ' $\bar{x}$ +1/2, $\bar{x}$ +1, x;<br>0,1/2,1/2<br>( $\bar{3}_{\bar{yz}}$  1/2,0,1/2)'        | (36) $\bar{3}^-$ ' $\bar{x}$ +1/2, x, $\bar{x}$ ;<br>1/2,0,0<br>( $\bar{3}_{\bar{yz}}$  1/2,0,1/2)'            |
| (37) g (1/4,-1/4,1/2) x+1/4, $\bar{x}$ ,z<br>( $m_{xy}$  1/2,0,1/2)             | (38) g (1/4,1/4,1/2) x+1/4,x,z<br>( $m_{\bar{xy}}$  1/2,0,1/2)   | (39) $\bar{4}^-$ 1/4,1/4,z; 1/4,1/4,1/4<br>( $\bar{4}_z^{-1}$  1/2,0,1/2)                                      | (40) $\bar{4}^+$ 1/4,-1/4,z; 1/4,-1/4,1/4<br>( $\bar{4}_z$  1/2,0,1/2)   |
| (41) $\bar{4}^-$ x,-1/4,1/4; 1/4,-1/4,1/4<br>( $\bar{4}_x^{-1}$  1/2,0,1/2)     | (42) g (1/2,-1/4,1/4) x,y+1/4, $\bar{y}$<br>( $m_{yz}$  1/2,0,1/2)   | (43) g (1/2,1/4,1/4) x,y-1/4,y<br>( $m_{\bar{yz}}$  1/2,0,1/2)   | (44) $\bar{4}^+$ x,1/4,1/4; 1/4,1/4,1/4<br>( $\bar{4}_x$  1/2,0,1/2)   |
| (45) $\bar{4}^+$ 0,y,1/2; 0,0,1/2<br>( $\bar{4}_y$  1/2,0,1/2)                  | (46) m $\bar{x}$ +1/2,y,x<br>( $m_{xz}$  1/2,0,1/2)  | (47) $\bar{4}^-$ 1/2,y,0; 1/2,0,0<br>( $\bar{4}_y^{-1}$  1/2,0,1/2)  | (48) g (1/2,0,1/2) x,y,x<br>( $m_{\bar{xz}}$  1/2,0,1/2)   |

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (1   1/2,1/2,0)	(2) 2 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,0)	(3) 2 (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)	(4) 2 (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) 3 <sup>+</sup> $\bar{x}$ +1/2,x, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(7) 3 <sup>+</sup> x+1/2, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(8) 3 <sup>+</sup> (1/3,1/3,-1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) 3 <sup>-</sup> x, $\bar{x}$ +1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)	(11) 3 <sup>-</sup> (1/3,1/3,-1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub>   1/2,1/2,0)	(12) 3 <sup>-</sup> $\bar{x}$ ,x+1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)
(13) 2' (1/2,1/2,0) x,x,0 (2 <sub>xy</sub>   1/2,1/2,0)'	(14) 2' x, $\bar{x}$ +1/2,0 (2 <sub>xy</sub>   1/2,1/2,0)'	(15) 4' 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,0)'	(16) 4' 0,1/2,z (4 <sub>z</sub>   1/2,1/2,0)'
(17) 4' 1/2,0,0 x,1/4,-1/4 (4 <sub>x</sub> <sup>-1</sup>   1/2,1/2,0)'	(18) 2' (0,1/4,1/4) 1/4,y+1/4,y (2 <sub>yz</sub>   1/2,1/2,0)'	(19) 2' (0,1/4,-1/4) 1/4,y+1/4, $\bar{y}$ (2 <sub>yz</sub>   1/2,1/2,0)'	(20) 4' 1/2,0,0 x,1/4,1/4 (4 <sub>x</sub>   1/2,1/2,0)'
(21) 4' 1/2,0,0 1/4,y,-1/4 (4 <sub>y</sub>   1/2,1/2,0)'	(22) 2' (1/4,0,1/4) x+1/4,1/4,x (2 <sub>xz</sub>   1/2,1/2,0)'	(23) 4' 1/2,0,0 1/4,y,1/4 (4 <sub>y</sub> <sup>-1</sup>   1/2,1/2,0)'	(24) 2' (1/4,0,-1/4) $\bar{x}$ +1/4,1/4,x (2 <sub>xz</sub>   1/2,1/2,0)'
(25) $\bar{1}$ ' 1/4,1/4,0 ( $\bar{1}$   1/2,1/2,0)'	(26) n' (1/2,1/2,0) x,y,0 (m <sub>z</sub>   1/2,1/2,0)'	(27) a' (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)'	(28) b' (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)'
(29) $\bar{3}^+$ ' x+1/2,x,x; 1/2,0,0 ( $\bar{3}_{xyz}$   1/2,1/2,0)'	(30) $\bar{3}^+$ ' $\bar{x}$ -1/2,x+1, $\bar{x}$ ; 0,1/2,1/2 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)'	(31) $\bar{3}^+$ ' x-1/2, $\bar{x}$ +1, $\bar{x}$ ; 0,1/2,-1/2 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)'	(32) $\bar{3}^+$ ' $\bar{x}$ +1/2, $\bar{x}$ ,x; 1/2,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)'
(33) $\bar{3}^-$ ' x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)'	(34) $\bar{3}^-$ ' x+1, $\bar{x}$ -1/2, $\bar{x}$ ; 1/2,0,1/2 ( $\bar{3}_{xyz}$   1/2,1/2,0)'	(35) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ +1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$   1/2,1/2,0)'	(36) $\bar{3}^-$ ' $\bar{x}$ +1,x-1/2, $\bar{x}$ ; 1/2,0,-1/2 ( $\bar{3}_{xyz}$   1/2,1/2,0)'
(37) m x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   1/2,1/2,0)	(38) g (1/2,1/2,0) x,x,z (m <sub>xy</sub>   1/2,1/2,0)	(39) $\bar{4}^-$ 0,1/2,z; 0,1/2,0 ( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,0)	(40) $\bar{4}^+$ 1/2,0,z; 1/2,0,0 ( $\bar{4}_z$   1/2,1/2,0)
(41) $\bar{4}^-$ x,1/4,1/4; 1/4,1/4,1/4 ( $\bar{4}_x$ <sup>-1</sup>   1/2,1/2,0)	(42) g (1/2,1/4,-1/4) x,y+1/4, $\bar{y}$ (m <sub>yz</sub>   1/2,1/2,0)	(43) g (1/2,1/4,1/4) x,y+1/4,y (m <sub>yz</sub>   1/2,1/2,0)	(44) $\bar{4}^+$ x,1/4,-1/4; 1/4,1/4,-1/4 ( $\bar{4}_x$   1/2,1/2,0)
(45) $\bar{4}^+$ 1/4,y,1/4; 1/4,1/4,1/4 ( $\bar{4}_y$   1/2,1/2,0)	(46) g (1/4,1/2,-1/4) $\bar{x}$ +1/4,y,x (m <sub>xz</sub>   1/2,1/2,0)	(47) $\bar{4}^-$ 1/4,y,-1/4; 1/4,1/4,-1/4 ( $\bar{4}_y$ <sup>-1</sup>   1/2,1/2,0)	(48) g (1/4,1/2,1/4) x+1/4,y,x (m <sub>xz</sub>   1/2,1/2,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

192		1	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +					
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	[ $\bar{u},\bar{v},w$ ]	(3)	$\bar{x},y,z$	[ $\bar{u},v,w$ ]	(4)	x, $\bar{y},z$	[u, $\bar{v},w$ ]
(5)	z,x,y	[w,u,v]	(6)	z, $\bar{x},\bar{y}$	[w, $\bar{u},\bar{v}$ ]	(7)	$\bar{z},x,y$	[ $\bar{w},u,v$ ]	(8)	$\bar{z},x,\bar{y}$	[ $\bar{w},u,\bar{v}$ ]

(9)	$y,z,x [v,w,u]$	(10)	$\bar{y},z,\bar{x} [\bar{v},w,\bar{u}]$	(11)	$y,\bar{z},\bar{x} [v,\bar{w},\bar{u}]$	(12)	$\bar{y},\bar{z},x [\bar{v},\bar{w},u]$
(13)	$y,x,\bar{z} [\bar{v},\bar{u},w]$	(14)	$\bar{y},\bar{x},\bar{z} [v,u,w]$	(15)	$y,\bar{x},z [\bar{v},u,\bar{w}]$	(16)	$\bar{y},x,z [v,\bar{u},\bar{w}]$
(17)	$x,z,\bar{y} [\bar{u},\bar{w},v]$	(18)	$\bar{x},z,y [u,\bar{w},\bar{v}]$	(19)	$\bar{x},\bar{z},\bar{y} [u,w,v]$	(20)	$x,\bar{z},y [\bar{u},w,\bar{v}]$
(21)	$z,y,\bar{x} [\bar{w},\bar{v},u]$	(22)	$z,\bar{y},x [\bar{w},v,\bar{u}]$	(23)	$\bar{z},y,x [w,\bar{v},\bar{u}]$	(24)	$\bar{z},\bar{y},\bar{x} [w,v,u]$
(25)	$\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$	(26)	$x,y,\bar{z} [u,v,\bar{w}]$	(27)	$x,\bar{y},z [u,\bar{v},w]$	(28)	$\bar{x},y,z [\bar{u},v,w]$
(29)	$\bar{z},\bar{x},\bar{y} [\bar{w},\bar{u},\bar{v}]$	(30)	$\bar{z},x,y [\bar{w},u,v]$	(31)	$z,x,\bar{y} [w,u,\bar{v}]$	(32)	$z,\bar{x},y [w,\bar{u},v]$
(33)	$\bar{y},\bar{z},\bar{x} [\bar{v},\bar{w},\bar{u}]$	(34)	$y,\bar{z},x [v,\bar{w},u]$	(35)	$\bar{y},z,x [v,w,\bar{u}]$	(36)	$y,z,\bar{x} [v,w,\bar{u}]$
(37)	$\bar{y},\bar{x},z [v,u,\bar{w}]$	(38)	$y,x,z [\bar{v},\bar{u},\bar{w}]$	(39)	$\bar{y},x,\bar{z} [v,\bar{u},w]$	(40)	$y,\bar{x},z [\bar{v},u,w]$
(41)	$\bar{x},\bar{z},y [u,w,\bar{v}]$	(42)	$x,\bar{z},\bar{y} [\bar{u},w,v]$	(43)	$x,z,y [\bar{u},\bar{w},\bar{v}]$	(44)	$\bar{x},z,\bar{y} [u,\bar{w},v]$
(45)	$\bar{z},\bar{y},x [w,v,\bar{u}]$	(46)	$\bar{z},y,\bar{x} [w,\bar{v},u]$	(47)	$z,\bar{y},\bar{x} [\bar{w},v,u]$	(48)	$z,y,x [\bar{w},\bar{v},\bar{u}]$
96	k ..m	$x,x,z [u,\bar{u},0]$	$\bar{x},\bar{x},z [\bar{u},u,0]$	$\bar{x},x,\bar{z} [\bar{u},\bar{u},0]$	$x,\bar{x},z [u,u,0]$		
		$z,x,x [0,u,\bar{u}]$	$z,\bar{x},x [0,\bar{u},u]$	$\bar{z},\bar{x},x [0,\bar{u},\bar{u}]$	$\bar{z},x,x [0,u,u]$		
		$x,z,x [\bar{u},0,u]$	$\bar{x},z,\bar{x} [u,0,\bar{u}]$	$x,\bar{z},\bar{x} [\bar{u},0,\bar{u}]$	$\bar{x},z,x [u,0,u]$		
		$x,x,\bar{z} [u,\bar{u},0]$	$\bar{x},\bar{x},\bar{z} [\bar{u},u,0]$	$x,\bar{x},z [u,u,0]$	$\bar{x},x,z [\bar{u},\bar{u},0]$		
		$x,z,\bar{x} [\bar{u},0,\bar{u}]$	$\bar{x},z,x [u,0,u]$	$\bar{x},\bar{z},\bar{x} [u,0,\bar{u}]$	$x,\bar{z},x [\bar{u},0,u]$		
		$z,x,\bar{x} [0,u,u]$	$z,\bar{x},x [0,\bar{u},\bar{u}]$	$\bar{z},x,x [0,u,\bar{u}]$	$\bar{z},\bar{x},x [0,\bar{u},u]$		
96	j m'..	$0,y,z [0,v,w]$	$0,\bar{y},z [0,\bar{v},w]$	$0,y,\bar{z} [0,v,\bar{w}]$	$0,\bar{y},z [0,\bar{v},\bar{w}]$		
		$z,0,y [w,0,v]$	$z,0,\bar{y} [w,0,\bar{v}]$	$\bar{z},0,y [\bar{w},0,v]$	$\bar{z},0,\bar{y} [\bar{w},0,\bar{v}]$		
		$y,z,0 [v,w,0]$	$\bar{y},z,0 [\bar{v},w,0]$	$y,\bar{z},0 [v,\bar{w},0]$	$\bar{y},z,0 [\bar{v},\bar{w},0]$		
		$y,0,\bar{z} [\bar{v},0,w]$	$\bar{y},0,\bar{z} [v,0,w]$	$y,0,z [\bar{v},0,\bar{w}]$	$\bar{y},0,z [v,0,\bar{w}]$		
		$0,z,\bar{y} [0,\bar{w},v]$	$0,z,y [0,\bar{w},\bar{v}]$	$0,\bar{z},\bar{y} [0,w,v]$	$0,\bar{z},y [0,w,\bar{v}]$		
		$z,y,0 [\bar{w},\bar{v},0]$	$z,\bar{y},0 [\bar{w},v,0]$	$\bar{z},y,0 [w,\bar{v},0]$	$\bar{z},\bar{y},0 [w,v,0]$		
48	i m'.m2'	$1/2,y,y [0,\bar{v},w]$	$1/2,\bar{y},y [0,v,w]$	$1/2,y,\bar{y} [0,\bar{v},\bar{w}]$	$1/2,\bar{y},y [0,v,\bar{w}]$		
		$y,1/2,y [w,0,\bar{v}]$	$y,1/2,\bar{y} [w,0,v]$	$\bar{y},1/2,y [\bar{w},0,\bar{v}]$	$\bar{y},1/2,\bar{y} [\bar{w},0,v]$		
		$y,y,1/2 [\bar{v},w,0]$	$\bar{y},y,1/2 [v,w,0]$	$y,\bar{y},1/2 [\bar{v},\bar{w},0]$	$\bar{y},\bar{y},1/2 [v,\bar{w},0]$		
48	h m'.m2'	$0,y,y [0,\bar{v},w]$	$0,\bar{y},y [0,v,w]$	$0,y,\bar{y} [0,\bar{v},\bar{w}]$	$0,\bar{y},y [0,v,\bar{w}]$		
		$y,0,y [w,0,\bar{v}]$	$y,0,\bar{y} [w,0,v]$	$\bar{y},0,y [\bar{w},0,\bar{v}]$	$\bar{y},0,\bar{y} [\bar{w},0,v]$		
		$y,y,0 [\bar{v},w,0]$	$\bar{y},y,0 [v,w,0]$	$y,\bar{y},0 [\bar{v},\bar{w},0]$	$\bar{y},\bar{y},0 [v,\bar{w},0]$		

Continued

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Fm $\bar{3}$ 'm

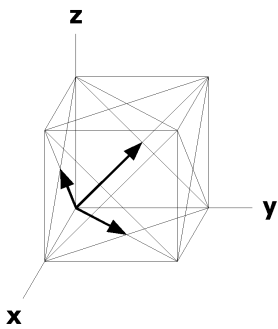
48	g	2.mm	x,1/4,1/4 [0,0,0]	$\bar{x}$ ,3/4,1/4 [0,0,0]	1/4,x,1/4 [0,0,0]	1/4, $\bar{x}$ ,3/4 [0,0,0]
			1/4,1/4,x [0,0,0]	3/4,1/4, $\bar{x}$ [0,0,0]	1/4,x,3/4 [0,0,0]	3/4, $\bar{x}$ ,3/4 [0,0,0]
			x,1/4,3/4 [0,0,0]	$\bar{x}$ ,1/4,1/4 [0,0,0]	1/4,1/4, $\bar{x}$ [0,0,0]	1/4,3/4,x [0,0,0]
32	f	.3m	x,x,x [0,0,0]	$\bar{x}$ , $\bar{x}$ ,x [0,0,0]	$\bar{x}$ ,x, $\bar{x}$ [0,0,0]	x, $\bar{x}$ , $\bar{x}$ [0,0,0]
			x,x, $\bar{x}$ [0,0,0]	$\bar{x}$ , $\bar{x}$ , $\bar{x}$ [0,0,0]	x, $\bar{x}$ ,x [0,0,0]	$\bar{x}$ ,x,x [0,0,0]
24	e	4'm'.m	x,0,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0]	0,x,0 [0,0,0]	
			0, $\bar{x}$ ,0 [0,0,0]	0,0,x [0,0,0]	0,0, $\bar{x}$ [0,0,0]	
24	d	m'.mm	0,1/4,1/4 [0,0,0]	0,3/4,1/4 [0,0,0]	1/4,0,1/4 [0,0,0]	
			1/4,0,3/4 [0,0,0]	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]	
8	c	$\bar{4}$ 3m	1/4,1/4,1/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]		
4	b	m' $\bar{3}$ 'm	1/2,1/2,1/2 [0,0,0]			
4	a	m' $\bar{3}$ 'm	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4'm'm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,1,1] p6mm  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

Along [1,1,0] c2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



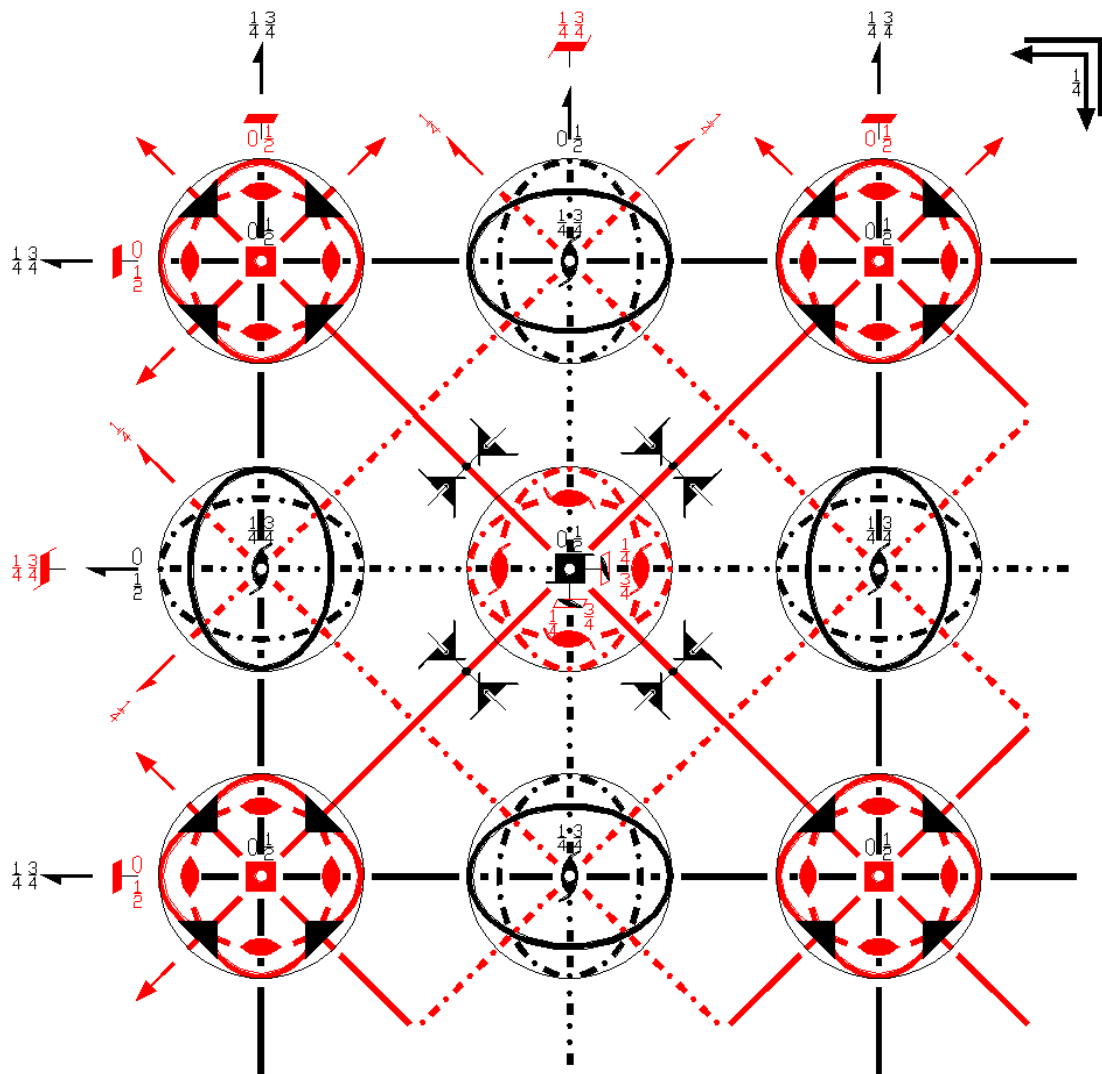
Fm $\bar{3}$ m'

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m $\bar{3}$ m'

F4'/m $\bar{3}$ 2'/m'

Cubic



**Origin** at center (m $\bar{3}$ m')

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/4$ ;  $y \leq \min(x, 1/2-x)$ ;  $z \leq y$

**Vertices** 0,0,0      1/2,0,0      1/4,1/4,0      1/4,1/4,1/4

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                  | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)              | (12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)               |



(13) 2' x,x,0 (2 <sub>xy</sub>  0,0,0)'	(14) 2' x, $\bar{x}$ ,0 (2 <sub>xy</sub>  0,0,0)'	(15) 4' 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)'	(16) 4' 0,0,z (4 <sub>z</sub>  0,0,0)'
(17) 4' x,0,0 (4 <sub>x</sub> <sup>-1</sup>  0,0,0)'	(18) 2' 0,y,y (2 <sub>yz</sub>  0,0,0)'	(19) 2' 0,y, $\bar{y}$ (2 <sub>yz</sub>  0,0,0)'	(20) 4' x,0,0 (4 <sub>x</sub>  0,0,0)'
(21) 4' 0,y,0 (4 <sub>y</sub>  0,0,0)'	(22) 2' x,0,x (2 <sub>xz</sub>  0,0,0)'	(23) 4' 0,y,0 (4 <sub>y</sub> <sup>-1</sup>  0,0,0)'	(24) 2' $\bar{x}$ ,0,x (2 <sub>xz</sub>  0,0,0)'
(25) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(26) m x,y,0 (m <sub>z</sub>  0,0,0)	(27) m x,0,z (m <sub>y</sub>  0,0,0)	(28) m 0,y,z (m <sub>x</sub>  0,0,0)
(29) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)	(30) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)	(31) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)	(32) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)
(33) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)	(34) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)	(35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)	(36) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)
(37) m' x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)'	(38) m' x,x,z (m <sub>xy</sub>  0,0,0)'	(39) $\bar{4}^-$ 0,0,z; 0,0,0 ( $\bar{4}_z$ <sup>-1</sup>  0,0,0)'	(40) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'
(41) $\bar{4}^-$ x,0,0; 0,0,0 ( $\bar{4}_x$ <sup>-1</sup>  0,0,0)'	(42) m' x,y, $\bar{y}$ (m <sub>yz</sub>  0,0,0)'	(43) m' x,y,y (m <sub>yz</sub>  0,0,0)'	(44) $\bar{4}^+$ x,0,0; 0,0,0 ( $\bar{4}_x$  0,0,0)'
(45) $\bar{4}^+$ 0,y,0; 0,0,0 ( $\bar{4}_y$  0,0,0)'	(46) m' $\bar{x}$ ,y,x (m <sub>xz</sub>  0,0,0)'	(47) $\bar{4}^-$ 0,y,0; 0,0,0 ( $\bar{4}_y$ <sup>-1</sup>  0,0,0)'	(48) m' x,y,x (m <sub>xz</sub>  0,0,0)'

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2) (1 0,1/2,1/2)	(2) 2 (0,0,1/2) 0,1/4,z (2 <sub>z</sub>  0,1/2,1/2)	(3) 2 (0,1/2,0) 0,y,1/4 (2 <sub>y</sub>  0,1/2,1/2)	(4) 2 x,1/4,1/4 (2 <sub>x</sub>  0,1/2,1/2)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x-1/3,x-1/6,x (3 <sub>xyz</sub>  0,1/2,1/2)	(6) 3 <sup>+</sup> $\bar{x}$ ,x+1/2, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(7) 3 <sup>+</sup> (-1/3,1/3,1/3) x+1/3, $\bar{x}$ -1/6, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ +1/2,x (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x-1/6,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(10) 3 <sup>-</sup> (-1/3,1/3,1/3) x+1/6, $\bar{x}$ +1/6, $\bar{x}$ (3 <sub>xyz</sub>  0,1/2,1/2)	(11) 3 <sup>-</sup> $\bar{x}$ +1/2, $\bar{x}$ +1/2,x (3 <sub>xyz</sub>  0,1/2,1/2)	(12) 3 <sup>-</sup> $\bar{x}$ -1/2,x+1/2, $\bar{x}$ (3 <sub>xyz</sub>  0,1/2,1/2)
(13) 2' (1/4,1/4,0) x,x+1/4,1/4 (2 <sub>xy</sub>  0,1/2,1/2)'	(14) 2' (-1/4,1/4,0) x, $\bar{x}$ +1/4,1/4 (2 <sub>xy</sub>  0,1/2,1/2)'	(15) 4' (0,0,1/2) 1/4,1/4,z (4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/2)'	(16) 4' (0,0,1/2) -1/4,1/4,z (4 <sub>z</sub>  0,1/2,1/2)'
(17) 4' x,1/2,0 (4 <sub>x</sub> <sup>-1</sup>  0,1/2,1/2)'	(18) 2' (0,1/2,1/2) 0,y,y (2 <sub>yz</sub>  0,1/2,1/2)'	(19) 2' 0,y+1/2, $\bar{y}$ (2 <sub>yz</sub>  0,1/2,1/2)'	(20) 4' x,0,1/2 (4 <sub>x</sub>  0,1/2,1/2)'
(21) 4' (0,1/2,0) 1/4,y,1/4 (4 <sub>y</sub>  0,1/2,1/2)'	(22) 2' (1/4,0,1/4) x-1/4,1/4,x (2 <sub>xz</sub>  0,1/2,1/2)'	(23) 4' (0,1/2,0) -1/4,y,1/4 (4 <sub>y</sub> <sup>-1</sup>  0,1/2,1/2)'	(24) 2' (-1/4,0,1/4) $\bar{x}$ +1/4,1/4,x (2 <sub>xz</sub>  0,1/2,1/2)'
(25) $\bar{1}$ 0,1/4,1/4 ( $\bar{1}$  0,1/2,1/2)	(26) b (0,1/2,0) x,y,1/4 (m <sub>z</sub>  0,1/2,1/2)	(27) c (0,0,1/2) x,1/4,z (m <sub>y</sub>  0,1/2,1/2)	(28) n (0,1/2,1/2) 0,y,z (m <sub>x</sub>  0,1/2,1/2)
(29) $\bar{3}^+$ x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$  0,1/2,1/2)	(30) $\bar{3}^+$ $\bar{x}$ -1,x+1/2, $\bar{x}$ ; -1/2,0,1/2 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,1/2,1/2)	(31) $\bar{3}^+$ x, $\bar{x}$ +1/2, $\bar{x}$ ; 0,1/2,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,1/2,1/2)	(32) $\bar{3}^+$ $\bar{x}$ -1, $\bar{x}$ +1/2,x; 1/2,0,1/2 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,1/2,1/2)

- (33)  $\bar{3}^-$   $x-1/2, x-1/2, x;$   
0,0,1/2  
( $\bar{3}_{xyz}^{-1} | 0, 1/2, 1/2$ )'
- (34)  $\bar{3}^-$   $x+1/2, \bar{x}-1/2, \bar{x};$   
0,0,1/2  
( $\bar{3}_{\bar{xyz}} | 0, 1/2, 1/2$ )'
- (35)  $\bar{3}^-$   $\bar{x}-1/2, \bar{x}+1/2, x;$   
-1/2,1/2,0  
( $\bar{3}_{\bar{xyz}} | 0, 1/2, 1/2$ )'
- (36)  $\bar{3}^-$   $\bar{x}+1/2, x+1/2, \bar{x};$   
1/2,1/2,0  
( $\bar{3}_{\bar{xyz}} | 0, 1/2, 1/2$ )'
- (37)  $g'$   $(-1/4, 1/4, 1/2)$   $x+1/4, \bar{x}, z$  (38)  $g'$   $(1/4, 1/4, 1/2)$   $x-1/4, x, z$  (39)  $\bar{4}^-$   $-1/4, 1/4, z;$   $-1/4, 1/4, 1/4$  (40)  $\bar{4}^+$   $1/4, 1/4, z;$   $1/4, 1/4, 1/4$   
( $m_{xy} | 0, 1/2, 1/2$ )' ( $m_{\bar{xy}} | 0, 1/2, 1/2$ )' ( $\bar{4}_z^{-1} | 0, 1/2, 1/2$ )' ( $\bar{4}_z^+ | 0, 1/2, 1/2$ )'
- (41)  $\bar{4}^-$   $x, 0, 1/2; 0, 0, 1/2$  (42)  $m'$   $x, y+1/2, \bar{y}$   
( $\bar{4}_x^{-1} | 0, 1/2, 1/2$ )' ( $m_{yz} | 0, 1/2, 1/2$ )'
- (43)  $g'$   $(0, 1/2, 1/2)$   $x, y, y$  (44)  $\bar{4}^+$   $x, 1/2, 0; 0, 1/2, 0$   
( $m_{yz} | 0, 1/2, 1/2$ )' ( $\bar{4}_x^+ | 0, 1/2, 1/2$ )'
- (45)  $\bar{4}^+$   $-1/4, y, 1/4; -1/4, 1/4, 1/4$  (46)  $g'$   $(-1/4, 1/2, 1/4)$   $\bar{x}+1/4, y, x$  (47)  $\bar{4}^-$   $1/4, y, 1/4; 1/4, 1/4, 1/4$  (48)  $g'$   $(1/4, 1/2, 1/4)$   $x-1/4, y, x$   
( $\bar{4}_y^+ | 0, 1/2, 1/2$ )' ( $m_{xz} | 0, 1/2, 1/2$ )' ( $\bar{4}_y^{-1} | 0, 1/2, 1/2$ )' ( $m_{\bar{xz}} | 0, 1/2, 1/2$ )'

For (1/2,0,1/2) + set

- (1)  $t$   $(1/2, 0, 1/2)$   
( $1 | 1/2, 0, 1/2$ )'
- (2)  $2$   $(0, 0, 1/2)$   $1/4, 0, z$   
( $2_z | 1/2, 0, 1/2$ )'
- (3)  $2$   $1/4, y, 1/4$   
( $2_y | 1/2, 0, 1/2$ )'
- (4)  $2$   $(1/2, 0, 0)$   $x, 0, 1/2$   
( $2_x | 1/2, 0, 1/2$ )'
- (5)  $3^+$   $(1/3, 1/3, 1/3)$   
 $x+1/6, x-1/6, x$   
( $3_{xyz} | 1/2, 0, 1/2$ )'
- (6)  $3^+$   $(1/3, -1/3, 1/3)$   
 $x+1/6, x+1/6, \bar{x}$   
( $3_{\bar{xyz}}^{-1} | 1/2, 0, 1/2$ )'
- (7)  $3^+$   $x+1/2, \bar{x}-1/2, \bar{x}$   
( $3_{\bar{xyz}}^{-1} | 1/2, 0, 1/2$ )'
- (8)  $3^+$   $\bar{x}+1/2, \bar{x}+1/2, x$   
( $3_{xyz}^{-1} | 1/2, 0, 1/2$ )'
- (9)  $3^-$   $(1/3, 1/3, 1/3)$   
 $x-1/6, x-1/3, x$   
( $3_{xyz}^{-1} | 1/2, 0, 1/2$ )'
- (10)  $3^-$   $x+1/2, \bar{x}, \bar{x}$   
( $3_{\bar{xyz}} | 1/2, 0, 1/2$ )'
- (11)  $3^-$   $\bar{x}+1/2, \bar{x}, x$   
( $3_{\bar{xyz}} | 1/2, 0, 1/2$ )'
- (12)  $3^-$   $(1/3, -1/3, 1/3)$   
 $\bar{x}-1/6, x+1/3, \bar{x}$   
( $3_{\bar{xyz}} | 1/2, 0, 1/2$ )'
- (13)  $2'$   $(1/4, 1/4, 0)$   $x, x-1/4, 1/4$  (14)  $2'$   $(1/4, -1/4, 0)$   $x, \bar{x}+1/4, 1/4$  (15)  $4^-$   $(0, 0, 1/2)$   $1/4, -1/4, z$  (16)  $4^+$   $(0, 0, 1/2)$   $1/4, 1/4, z$   
( $2_{xy} | 1/2, 0, 1/2$ )' ( $2_{\bar{xy}} | 1/2, 0, 1/2$ )' ( $4_z^{-1} | 1/2, 0, 1/2$ )' ( $4_z^+ | 1/2, 0, 1/2$ )'
- (17)  $4^-$   $(1/2, 0, 0)$   $x, 1/4, 1/4$  (18)  $2'$   $(0, 1/4, 1/4)$   $1/4, y-1/4, y$  (19)  $2'$   $(0, -1/2, 1/2)$   $1/4, y+1/4, \bar{y}$  (20)  $4^+$   $(1/2, 0, 0)$   $x, -1/4, 1/4$   
( $4_x^{-1} | 1/2, 0, 1/2$ )' ( $2_{yz} | 1/2, 0, 1/2$ )' ( $2_{\bar{yz}} | 1/2, 0, 1/2$ )' ( $4_x^+ | 1/2, 0, 1/2$ )'
- (21)  $4^+$   $1/2, y, 0$  (22)  $2'$   $(1/2, 0, 1/2)$   $x, 0, x$  (23)  $4^-$   $0, y, 1/2$  (24)  $2'$   $\bar{x}+1/2, 0, x$   
( $4_y^+ | 1/2, 0, 1/2$ )' ( $2_{xz} | 1/2, 0, 1/2$ )' ( $4_y^{-1} | 1/2, 0, 1/2$ )' ( $2_{\bar{xz}} | 1/2, 0, 1/2$ )'
- (25)  $\bar{1}$   $1/4, 0, 1/4$  (26)  $a$   $(1/2, 0, 0)$   $x, y, 1/4$  (27)  $n$   $(1/2, 0, 1/2)$   $x, 0, z$  (28)  $c$   $(0, 0, 1/2)$   $1/4, y, z$   
( $\bar{1} | 1/2, 0, 1/2$ )' ( $m_z | 1/2, 0, 1/2$ )' ( $m_y | 1/2, 0, 1/2$ )' ( $m_x | 1/2, 0, 1/2$ )'
- (29)  $\bar{3}^+$   $x-1/2, x-1/2, x;$   
0,0,1/2  
( $\bar{3}_{xyz} | 1/2, 0, 1/2$ )'
- (30)  $\bar{3}^+$   $\bar{x}-1/2, x+1/2, \bar{x};$   
0,0,1/2  
( $\bar{3}_{\bar{xyz}}^{-1} | 1/2, 0, 1/2$ )'
- (31)  $\bar{3}^+$   $x+1/2, \bar{x}+1/2, \bar{x};$   
1/2,1/2,0  
( $\bar{3}_{\bar{xyz}}^{-1} | 1/2, 0, 1/2$ )'
- (32)  $\bar{3}^+$   $\bar{x}+1/2, \bar{x}-1/2, x;$   
1/2,-1/2,0  
( $\bar{3}_{\bar{xyz}}^{-1} | 1/2, 0, 1/2$ )'
- (33)  $\bar{3}^-$   $x+1/2, x, x;$   
1/2,0,0  
( $\bar{3}_{xyz}^{-1} | 1/2, 0, 1/2$ )'
- (34)  $\bar{3}^-$   $x+1/2, \bar{x}-1, \bar{x};$   
0,-1/2,1/2  
( $\bar{3}_{\bar{xyz}} | 1/2, 0, 1/2$ )'
- (35)  $\bar{3}^-$   $\bar{x}+1/2, \bar{x}+1, x;$   
0,1/2,1/2  
( $\bar{3}_{\bar{xyz}} | 1/2, 0, 1/2$ )'
- (36)  $\bar{3}^-$   $\bar{x}+1/2, x, \bar{x};$   
1/2,0,0  
( $\bar{3}_{\bar{xyz}} | 1/2, 0, 1/2$ )'
- (37)  $g'$   $(1/4, -1/4, 1/2)$   $x+1/4, \bar{x}, z$  (38)  $g'$   $(1/4, 1/4, 1/2)$   $x+1/4, x, z$  (39)  $\bar{4}^-$   $1/4, 1/4, z;$   $1/4, 1/4, 1/4$  (40)  $\bar{4}^+$   $1/4, -1/4, z;$   $1/4, -1/4, 1/4$   
( $m_{xy} | 1/2, 0, 1/2$ )' ( $m_{\bar{xy}} | 1/2, 0, 1/2$ )' ( $\bar{4}_z^{-1} | 1/2, 0, 1/2$ )' ( $\bar{4}_z^+ | 1/2, 0, 1/2$ )'
- (41)  $\bar{4}^-$   $x, -1/4, 1/4; 1/4, -1/4, 1/4$  (42)  $g'$   $(1/2, -1/4, 1/4)$   $x, y+1/4, \bar{y}$  (43)  $g'$   $(1/2, 1/4, 1/4)$   $x, y-1/4, y$  (44)  $\bar{4}^+$   $x, 1/4, 1/4; 1/4, 1/4, 1/4$   
( $\bar{4}_x^{-1} | 1/2, 0, 1/2$ )' ( $m_{yz} | 1/2, 0, 1/2$ )' ( $m_{\bar{yz}} | 1/2, 0, 1/2$ )' ( $\bar{4}_x^+ | 1/2, 0, 1/2$ )'
- (45)  $\bar{4}^+$   $0, y, 1/2; 0, 0, 1/2$  (46)  $m'$   $\bar{x}+1/2, y, x$  (47)  $\bar{4}^-$   $1/2, y, 0; 1/2, 0, 0$  (48)  $g'$   $(1/2, 0, 1/2)$   $x, y, x$   
( $\bar{4}_y^+ | 1/2, 0, 1/2$ )' ( $m_{xz} | 1/2, 0, 1/2$ )' ( $\bar{4}_y^{-1} | 1/2, 0, 1/2$ )' ( $m_{\bar{xz}} | 1/2, 0, 1/2$ )'

For (1/2,1/2,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t$ (1/2,1/2,0)<br>(1   1/2,1/2,0)   | (2) $2$ 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)   | (3) $2$ (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)   | (4) $2$ (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)   |
| (5) $3^+$ (1/3,1/3,1/3)<br>x+1/6,x+1/3,x<br>(3 <sub>xyz</sub>   1/2,1/2,0)               | (6) $3^+$ $\bar{x}$ +1/2,x, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)                         | (7) $3^+$ x+1/2, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)                          | (8) $3^+$ (1/3,1/3,-1/3)<br>x+1/6,x+1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)                 |
| (9) $3^-$ (1/3,1/3,1/3)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0) | (10) $3^-$ x, $\bar{x}$ +1/2, $\bar{x}$<br>(3 <sub>xyz</sub>   1/2,1/2,0)                                     | (11) $3^-$ (1/3,1/3,-1/3)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub>   1/2,1/2,0)                                    | (12) $3^-$ $\bar{x}$ ,x+1/2, $\bar{x}$<br>(3 <sub>xyz</sub>   1/2,1/2,0)                                  |
| (13) $2'$ (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>   1/2,1/2,0)'                            | (14) $2'$ x, $\bar{x}$ +1/2,0<br>(2 <sub>xy</sub>   1/2,1/2,0)'   | (15) $4^-$ 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,0)'   | (16) $4^+$ 0,1/2,z<br>(4 <sub>z</sub>   1/2,1/2,0)'   |
| (17) $4^-$ (1/2,0,0) x,1/4,-1/4<br>(4 <sub>x</sub> <sup>-1</sup>   1/2,1/2,0)'           | (18) $2'$ (0,1/4,1/4) 1/4,y+1/4,y<br>(2 <sub>yz</sub>   1/2,1/2,0)'   | (19) $2'$ (0,1/4,-1/4) 1/4,y+1/4, $\bar{y}$<br>(2 <sub>yz</sub>   1/2,1/2,0)'                                   | (20) $4^+$ (1/2,0,0) x,1/4,1/4<br>(4 <sub>x</sub>   1/2,1/2,0)'   |
| (21) $4^+$ (0,1/2,0) 1/4,y,-1/4<br>(4 <sub>y</sub>   1/2,1/2,0)'                         | (22) $2'$ (1/4,0,1/4) x+1/4,1/4,x<br>(2 <sub>xz</sub>   1/2,1/2,0)'   | (23) $4^-$ (0,1/2,0) 1/4,y,1/4<br>(4 <sub>y</sub> <sup>-1</sup>   1/2,1/2,0)'                                   | (24) $2'$ (1/4,0,-1/4) $\bar{x}$ +1/4,1/4,x<br>(2 <sub>xz</sub>   1/2,1/2,0)'                             |
| (25) $\bar{1}$ 1/4,1/4,0<br>(1   1/2,1/2,0)  | (26) $n$ (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>   1/2,1/2,0)  | (27) $a$ (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0)  | (28) $b$ (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)  |
| (29) $\bar{3}^+$ x+1/2,x,x;<br>1/2,0,0<br>(3 <sub>xyz</sub>   1/2,1/2,0)                 | (30) $\bar{3}^+$ $\bar{x}$ -1/2,x+1, $\bar{x}$ ;<br>0,1/2,1/2<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0) | (31) $\bar{3}^+$ x-1/2, $\bar{x}$ +1, $\bar{x}$ ;<br>0,1/2,-1/2<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0) | (32) $\bar{3}^+$ $\bar{x}$ +1/2, $\bar{x}$ ,x;<br>1/2,0,0<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0) |
| (33) $\bar{3}^-$ x,x+1/2,x;<br>0,1/2,0<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)   | (34) $\bar{3}^-$ x+1, $\bar{x}$ -1/2, $\bar{x}$ ;<br>1/2,0,1/2<br>(3 <sub>xyz</sub>   1/2,1/2,0)              | (35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1/2,x;<br>0,1/2,0<br>(3 <sub>xyz</sub>   1/2,1/2,0)                     | (36) $\bar{3}^-$ $\bar{x}$ +1,x-1/2, $\bar{x}$ ;<br>1/2,0,-1/2<br>(3 <sub>xyz</sub>   1/2,1/2,0)          |
| (37) $m'$ x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>   1/2,1/2,0)'                          | (38) $g'$ (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>   1/2,1/2,0)'   | (39) $\bar{4}^-$ 0,1/2,z; 0,1/2,0<br>(4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,0)'                                | (40) $\bar{4}^+$ 1/2,0,z; 1/2,0,0<br>(4 <sub>z</sub>   1/2,1/2,0)'  |
| (41) $\bar{4}^-$ x,1/4,1/4; 1/4,1/4,1/4<br>(4 <sub>x</sub> <sup>-1</sup>   1/2,1/2,0)'   | (42) $g'$ (1/2,1/4,-1/4) x,y+1/4, $\bar{y}$<br>(m <sub>yz</sub>   1/2,1/2,0)'                                 | (43) $g'$ (1/2,1/4,1/4) x,y+1/4,y<br>(m <sub>yz</sub>   1/2,1/2,0)'   | (44) $\bar{4}^+$ x,1/4,-1/4; 1/4,1/4,-1/4<br>(4 <sub>x</sub>   1/2,1/2,0)'                                |
| (45) $\bar{4}^+$ 1/4,y,1/4; 1/4,1/4,1/4<br>(4 <sub>y</sub>   1/2,1/2,0)'                 | (46) $g'$ (1/4,1/2,-1/4) $\bar{x}$ +1/4,y,x<br>(m <sub>xz</sub>   1/2,1/2,0)'                                 | (47) $\bar{4}^-$ 1/4,y,-1/4; 1/4,1/4,-1/4<br>(4 <sub>y</sub> <sup>-1</sup>   1/2,1/2,0)'                        | (48) $g'$ (1/4,1/2,1/4) x+1/4,y,x<br>(m <sub>xz</sub>   1/2,1/2,0)'                                       |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

- |     |       |         |           |                          |                             |               |                         |                             |
|-----|-------|---------|-----------|--------------------------|-----------------------------|---------------|-------------------------|-----------------------------|
| 192 |       | 1       | (0,0,0) + | (0,1/2,1/2) +            | (1/2,0,1/2) +               | (1/2,1/2,0) + |                         |                             |
| (1) | x,y,z | [u,v,w] | (2)       | $\bar{x}$ , $\bar{y}$ ,z | [ $\bar{u}$ , $\bar{v}$ ,w] | (3)           | $\bar{x}$ ,y,z          | [ $\bar{u}$ ,v,w]           |
| (5) | z,x,y | [w,u,v] | (6)       | z, $\bar{x}$ , $\bar{y}$ | [w, $\bar{u}$ , $\bar{v}$ ] | (7)           | $\bar{z}$ ,x,y          | [ $\bar{w}$ ,u,v]           |
|     |       |         |           |                          |                             | (8)           | $\bar{z}$ ,x, $\bar{y}$ | [ $\bar{w}$ ,u, $\bar{v}$ ] |

(9)	$y,z,x [v,w,u]$	(10)	$\bar{y},z,\bar{x} [\bar{v},w,\bar{u}]$	(11)	$y,\bar{z},\bar{x} [v,\bar{w},\bar{u}]$	(12)	$\bar{y},\bar{z},x [\bar{v},\bar{w},u]$
(17)	$x,z,\bar{y} [\bar{u},\bar{w},v]$	(18)	$\bar{x},z,y [u,\bar{w},\bar{v}]$	(19)	$\bar{x},\bar{z},\bar{y} [u,w,v]$	(20)	$x,\bar{z},y [\bar{u},w,\bar{v}]$
(21)	$z,y,\bar{x} [\bar{w},\bar{v},u]$	(22)	$z,\bar{y},x [\bar{w},v,\bar{u}]$	(23)	$\bar{z},y,x [w,\bar{v},\bar{u}]$	(24)	$\bar{z},\bar{y},\bar{x} [w,v,u]$
(25)	$\bar{x},\bar{y},\bar{z} [u,v,w]$	(26)	$x,y,\bar{z} [\bar{u},\bar{v},w]$	(27)	$x,\bar{y},z [\bar{u},v,\bar{w}]$	(28)	$\bar{x},y,z [u,\bar{v},\bar{w}]$
(29)	$\bar{z},\bar{x},\bar{y} [w,u,v]$	(30)	$\bar{z},x,y [w,\bar{u},\bar{v}]$	(31)	$z,x,\bar{y} [\bar{w},\bar{u},v]$	(32)	$z,\bar{x},y [\bar{w},u,\bar{v}]$
(33)	$\bar{y},\bar{z},\bar{x} [v,w,u]$	(34)	$y,\bar{z},x [\bar{v},w,\bar{u}]$	(35)	$\bar{y},z,x [v,\bar{w},\bar{u}]$	(36)	$y,z,\bar{x} [\bar{v},\bar{w},u]$
(37)	$\bar{y},\bar{x},z [\bar{v},\bar{u},w]$	(38)	$y,x,z [v,u,w]$	(39)	$\bar{y},x,\bar{z} [\bar{v},u,\bar{w}]$	(40)	$y,\bar{x},z [v,\bar{u},\bar{w}]$
(41)	$\bar{x},\bar{z},y [\bar{u},\bar{w},v]$	(42)	$x,\bar{z},\bar{y} [u,\bar{w},\bar{v}]$	(43)	$x,z,y [u,w,v]$	(44)	$\bar{x},z,\bar{y} [\bar{u},w,\bar{v}]$
(45)	$\bar{z},\bar{y},x [\bar{w},\bar{v},u]$	(46)	$\bar{z},y,\bar{x} [\bar{w},v,\bar{u}]$	(47)	$z,\bar{y},\bar{x} [w,\bar{v},\bar{u}]$	(48)	$z,y,x [w,v,u]$
96	k	..m'	$x,x,z [u,u,w]$	$\bar{x},\bar{x},z [\bar{u},\bar{u},w]$	$\bar{x},x,\bar{z} [\bar{u},u,\bar{w}]$	$x,\bar{x},z [u,\bar{u},\bar{w}]$	
			$z,x,x [w,u,u]$	$z,\bar{x},\bar{x} [w,\bar{u},\bar{u}]$	$\bar{z},\bar{x},x [\bar{w},\bar{u},u]$	$\bar{z},x,\bar{x} [\bar{w},u,\bar{u}]$	
			$x,z,x [u,w,u]$	$\bar{x},z,\bar{x} [\bar{u},w,\bar{u}]$	$x,\bar{z},\bar{x} [u,w,\bar{u}]$	$\bar{x},\bar{z},x [\bar{u},\bar{w},u]$	
			$x,x,\bar{z} [\bar{u},\bar{u},w]$	$\bar{x},\bar{x},\bar{z} [u,u,w]$	$x,\bar{x},z [\bar{u},u,\bar{w}]$	$\bar{x},x,z [u,\bar{u},\bar{w}]$	
			$x,z,\bar{x} [\bar{u},\bar{w},u]$	$\bar{x},z,x [u,\bar{w},\bar{u}]$	$\bar{x},\bar{z},\bar{x} [u,w,u]$	$x,\bar{z},x [\bar{u},w,\bar{u}]$	
			$z,x,\bar{x} [\bar{w},\bar{u},u]$	$z,\bar{x},x [\bar{w},u,\bar{u}]$	$\bar{z},x,x [w,\bar{u},\bar{u}]$	$\bar{z},\bar{x},\bar{x} [w,u,u]$	
96	j	m..	$0,y,z [u,0,0]$	$0,\bar{y},z [\bar{u},0,0]$	$0,y,\bar{z} [\bar{u},0,0]$	$0,\bar{y},z [u,0,0]$	
			$z,0,y [0,u,0]$	$z,0,\bar{y} [0,\bar{u},0]$	$\bar{z},0,y [0,\bar{u},0]$	$\bar{z},0,\bar{y} [0,u,0]$	
			$y,z,0 [0,0,u]$	$\bar{y},z,0 [0,0,\bar{u}]$	$y,\bar{z},0 [0,0,\bar{u}]$	$\bar{y},z,0 [0,0,u]$	
			$y,0,\bar{z} [0,\bar{u},0]$	$\bar{y},0,\bar{z} [0,u,0]$	$y,0,z [0,u,0]$	$\bar{y},0,z [0,\bar{u},0]$	
			$0,z,\bar{y} [\bar{u},0,0]$	$0,z,y [u,0,0]$	$0,\bar{z},\bar{y} [u,0,0]$	$0,\bar{z},y [\bar{u},0,0]$	
			$z,y,0 [0,0,u]$	$z,\bar{y},0 [0,0,\bar{u}]$	$\bar{z},y,0 [0,0,\bar{u}]$	$\bar{z},\bar{y},0 [0,0,u]$	
48	i	m.m'2'	$1/2,y,y [u,0,0]$	$1/2,\bar{y},y [\bar{u},0,0]$	$1/2,y,\bar{y} [\bar{u},0,0]$	$1/2,\bar{y},\bar{y} [u,0,0]$	
			$y,1/2,y [0,u,0]$	$y,1/2,\bar{y} [0,\bar{u},0]$	$\bar{y},1/2,y [0,\bar{u},0]$	$\bar{y},1/2,\bar{y} [0,u,0]$	
			$y,y,1/2 [0,0,u]$	$\bar{y},y,1/2 [0,0,\bar{u}]$	$y,\bar{y},1/2 [0,0,\bar{u}]$	$\bar{y},\bar{y},1/2 [0,0,u]$	
48	h	m.m'2'	$0,y,y [u,0,0]$	$0,\bar{y},y [\bar{u},0,0]$	$0,y,\bar{y} [\bar{u},0,0]$	$0,\bar{y},\bar{y} [u,0,0]$	
			$y,0,y [0,u,0]$	$y,0,\bar{y} [0,\bar{u},0]$	$\bar{y},0,y [0,\bar{u},0]$	$\bar{y},0,\bar{y} [0,u,0]$	
			$y,y,0 [0,0,u]$	$\bar{y},y,0 [0,0,\bar{u}]$	$y,\bar{y},0 [0,0,\bar{u}]$	$\bar{y},\bar{y},0 [0,0,u]$	

Continued

225.4.1621

Fm $\bar{3}$ m'

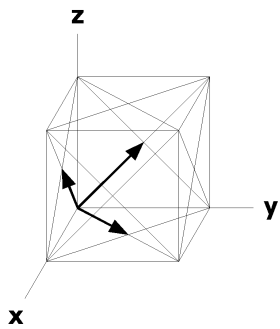
48	g	2.m'm'	x,1/4,1/4 [u,0,0] 1/4,1/4,x [0,0,u] x,1/4,3/4 [ $\bar{u}$ ,0,0]	$\bar{x}$ ,3/4,1/4 [ $\bar{u}$ ,0,0] 3/4,1/4, $\bar{x}$ [0,0, $\bar{u}$ ] $\bar{x}$ ,1/4,1/4 [u,0,0]	1/4,x,1/4 [0,u,0] 1/4,x,3/4 [0, $\bar{u}$ ,0] 1/4,1/4, $\bar{x}$ [0,0,u]	1/4, $\bar{x}$ ,3/4 [0, $\bar{u}$ ,0] 3/4, $\bar{x}$ ,3/4 [0,u,0] 1/4,3/4,x [0,0, $\bar{u}$ ]
32	f	.3m'	x,x,x [u,u,u] x,x, $\bar{x}$ [ $\bar{u}$ , $\bar{u}$ ,u]	$\bar{x}$ , $\bar{x}$ ,x [ $\bar{u}$ , $\bar{u}$ ,u] $\bar{x}$ , $\bar{x}$ , $\bar{x}$ [u,u,u]	$\bar{x}$ ,x, $\bar{x}$ [ $\bar{u}$ ,u, $\bar{u}$ ] x, $\bar{x}$ ,x [ $\bar{u}$ ,u, $\bar{u}$ ]	x, $\bar{x}$ , $\bar{x}$ [u, $\bar{u}$ , $\bar{u}$ ] $\bar{x}$ ,x,x [u, $\bar{u}$ , $\bar{u}$ ]
24	e	4'm.m'	x,0,0 [0,0,0] 0, $\bar{x}$ ,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0] 0,0,x [0,0,0]	0,x,0 [0,0,0] 0,0, $\bar{x}$ [0,0,0]	
24	d	m.m'm'	0,1/4,1/4 [u,0,0] 1/4,0,3/4 [0, $\bar{u}$ ,0]	0,3/4,1/4 [ $\bar{u}$ ,0,0] 1/4,1/4,0 [0,0,u]	1/4,0,1/4 [0,u,0] 3/4,1/4,0 [0,0, $\bar{u}$ ]	
8	c	$\bar{4}$ '3m'	1/4,1/4,1/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]		
4	b	m $\bar{3}$ m'	1/2,1/2,1/2 [0,0,0]			
4	a	m $\bar{3}$ m'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,1,1] p6'mm'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

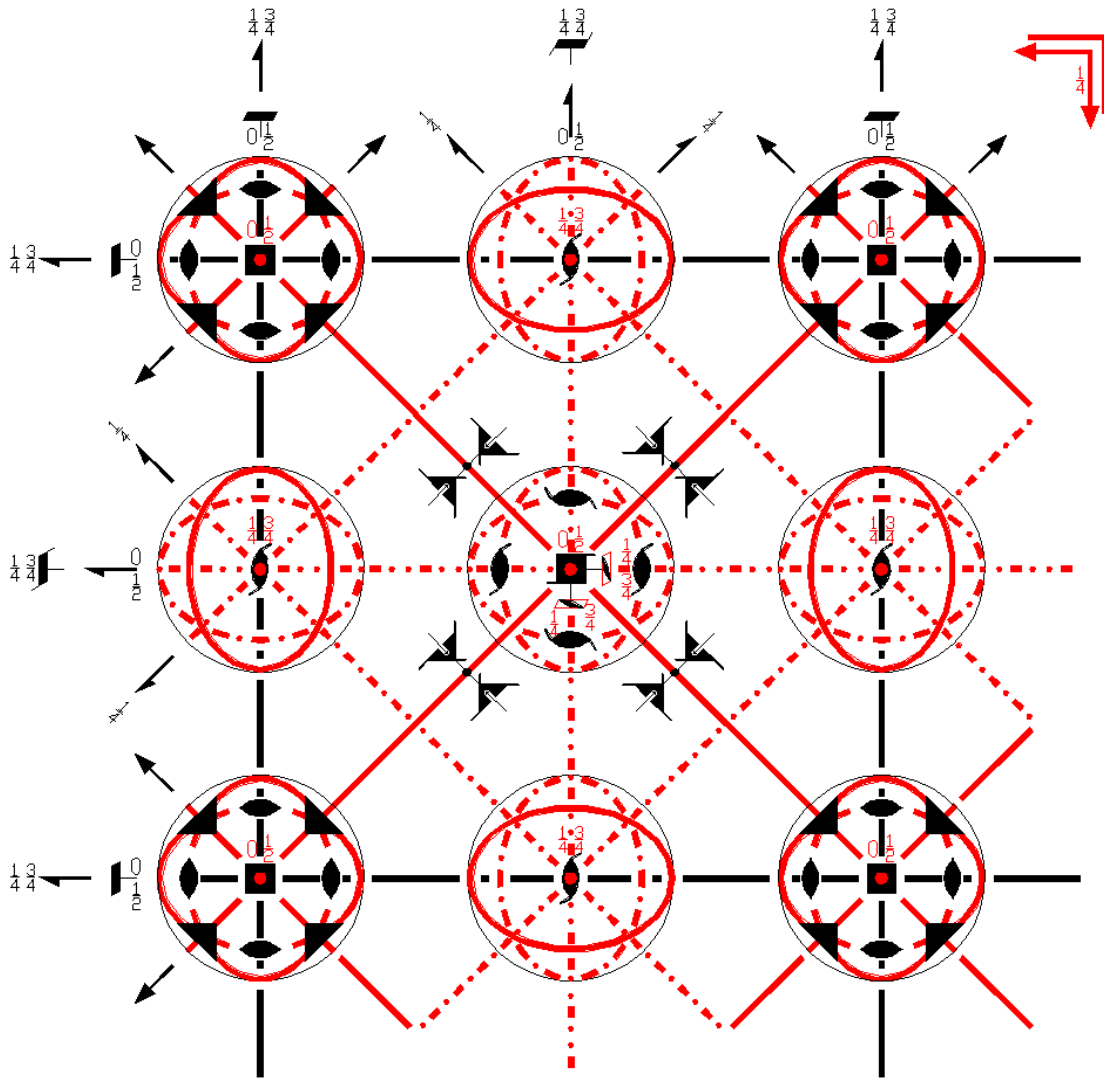
Along [1,1,0] c2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,0



Fm $\bar{3}$ 'm'  
225.5.1622

m $\bar{3}$ 'm'  
F4/m $\bar{3}$ '2/m'

Cubic



**Origin** at center (m $\bar{3}$ 'm')

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/4$ ;  $y \leq \min(x, 1/2-x)$ ;  $z \leq y$   
**Vertices** 0,0,0      1/2,0,0      1/4,1/4,0      1/4,1/4,1/4

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                  | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)              | (12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)               |

(13) 2 x,x,0 (2 <sub>xy</sub>  0,0,0)	(14) 2 x, $\bar{x}$ ,0 (2 <sub><math>\bar{xy}</math></sub>  0,0,0)	(15) 4 <sup>-</sup> 0,0,z (4 <sub>z</sub> <sup>-1</sup>  0,0,0)	(16) 4 <sup>+</sup> 0,0,z (4 <sub>z</sub>  0,0,0)
(17) 4 <sup>-</sup> x,0,0 (4 <sub>x</sub> <sup>-1</sup>  0,0,0)	(18) 2 0,y,y (2 <sub>yz</sub>  0,0,0)	(19) 2 0,y, $\bar{y}$ (2 <sub><math>\bar{yz}</math></sub>  0,0,0)	(20) 4 <sup>+</sup> x,0,0 (4 <sub>x</sub>  0,0,0)
(21) 4 <sup>+</sup> 0,y,0 (4 <sub>y</sub>  0,0,0)	(22) 2 x,0,x (2 <sub>xz</sub>  0,0,0)	(23) 4 <sup>-</sup> 0,y,0 (4 <sub>y</sub> <sup>-1</sup>  0,0,0)	(24) 2 $\bar{x}$ ,0,x (2 <sub><math>\bar{xz}</math></sub>  0,0,0)
(25) $\bar{1}$ ' 0,0,0 ( $\bar{1}$  0,0,0)'	(26) m' x,y,0 (m <sub>z</sub>  0,0,0)'	(27) m' x,0,z (m <sub>y</sub>  0,0,0)'	(28) m' 0,y,z (m <sub>x</sub>  0,0,0)'
(29) $\bar{3}^+$ ' x,x,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'	(30) $\bar{3}^+$ ' $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0)'	(31) $\bar{3}^+$ ' x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0)'	(32) $\bar{3}^+$ ' $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0)'
(33) $\bar{3}^-$ ' x,x,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(34) $\bar{3}^-$ ' x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)'	(35) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)'	(36) $\bar{3}^-$ ' $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)'
(37) m' x, $\bar{x}$ ,z (m <sub>xy</sub>  0,0,0)'	(38) m' x,x,z (m <sub><math>\bar{xy}</math></sub>  0,0,0)'	(39) $\bar{4}^-$ ' 0,0,z; 0,0,0 ( $\bar{4}_z$ <sup>-1</sup>  0,0,0)'	(40) $\bar{4}^+$ ' 0,0,z; 0,0,0 ( $\bar{4}_z$  0,0,0)'
(41) $\bar{4}^-$ ' x,0,0; 0,0,0 ( $\bar{4}_x$ <sup>-1</sup>  0,0,0)'	(42) m' x,y, $\bar{y}$ (m <sub>yz</sub>  0,0,0)'	(43) m' x,y,y (m <sub><math>\bar{yz}</math></sub>  0,0,0)'	(44) $\bar{4}^+$ ' x,0,0; 0,0,0 ( $\bar{4}_x$  0,0,0)'
(45) $\bar{4}^+$ ' 0,y,0; 0,0,0 ( $\bar{4}_y$  0,0,0)'	(46) m' $\bar{x}$ ,y,x (m <sub>xz</sub>  0,0,0)'	(47) $\bar{4}^-$ ' 0,y,0; 0,0,0 ( $\bar{4}_y$ <sup>-1</sup>  0,0,0)'	(48) m' x,y,x (m <sub><math>\bar{xz}</math></sub>  0,0,0)'

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2) (1 0,1/2,1/2)	(2) 2 (0,0,1/2) 0,1/4,z (2 <sub>z</sub>  0,1/2,1/2)	(3) 2 (0,1/2,0) 0,y,1/4 (2 <sub>y</sub>  0,1/2,1/2)	(4) 2 x,1/4,1/4 (2 <sub>x</sub>  0,1/2,1/2)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x-1/3,x-1/6,x (3 <sub>xyz</sub>  0,1/2,1/2)	(6) 3 <sup>+</sup> $\bar{x}$ ,x+1/2, $\bar{x}$ (3 <sub><math>\bar{y}\bar{z}</math></sub> <sup>-1</sup>  0,1/2,1/2)	(7) 3 <sup>+</sup> (-1/3,1/3,1/3) x+1/3,x-1/6, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ +1/2,x (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x-1/6,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(10) 3 <sup>-</sup> (-1/3,1/3,1/3) x+1/6, $\bar{x}$ +1/6, $\bar{x}$ (3 <sub>xyz</sub>  0,1/2,1/2)	(11) 3 <sup>-</sup> $\bar{x}$ +1/2, $\bar{x}$ +1/2,x (3 <sub><math>\bar{y}\bar{z}</math></sub>  0,1/2,1/2)	(12) 3 <sup>-</sup> $\bar{x}$ -1/2,x+1/2, $\bar{x}$ (3 <sub>xyz</sub>  0,1/2,1/2)
(13) 2 (1/4,1/4,0) x,x+1/4,1/4 (2 <sub>xy</sub>  0,1/2,1/2)	(14) 2 (-1/4,1/4,0) x, $\bar{x}$ +1/4,1/4 (2 <sub><math>\bar{xy}</math></sub>  0,1/2,1/2)	(15) 4 <sup>-</sup> (0,0,1/2) 1/4,1/4,z (4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/2)	(16) 4 <sup>+</sup> (0,0,1/2) -1/4,1/4,z (4 <sub>z</sub>  0,1/2,1/2)
(17) 4 <sup>-</sup> x,1/2,0 (4 <sub>x</sub> <sup>-1</sup>  0,1/2,1/2)	(18) 2 (0,1/2,1/2) 0,y,y (2 <sub>yz</sub>  0,1/2,1/2)	(19) 2 0,y+1/2, $\bar{y}$ (2 <sub><math>\bar{yz}</math></sub>  0,1/2,1/2)	(20) 4 <sup>+</sup> x,0,1/2 (4 <sub>x</sub>  0,1/2,1/2)
(21) 4 <sup>+</sup> (0,1/2,0) 1/4,y,1/4 (4 <sub>y</sub>  0,1/2,1/2)	(22) 2 (1/4,0,1/4) x-1/4,1/4,x (2 <sub>xz</sub>  0,1/2,1/2)	(23) 4 <sup>-</sup> (0,1/2,0) -1/4,y,1/4 (4 <sub>y</sub> <sup>-1</sup>  0,1/2,1/2)	(24) 2 (-1/4,0,1/4) $\bar{x}$ +1/4,1/4,x (2 <sub><math>\bar{xz}</math></sub>  0,1/2,1/2)
(25) $\bar{1}$ ' 0,1/4,1/4 ( $\bar{1}$  0,1/2,1/2)'	(26) b' (0,1/2,0) x,y,1/4 (m <sub>z</sub>  0,1/2,1/2)'	(27) c' (0,0,1/2) x,1/4,z (m <sub>y</sub>  0,1/2,1/2)'	(28) n' (0,1/2,1/2) 0,y,z (m <sub>x</sub>  0,1/2,1/2)'
(29) $\bar{3}^+$ ' x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$  0,1/2,1/2)'	(30) $\bar{3}^+$ ' $\bar{x}$ -1,x+1/2, $\bar{x}$ ; -1/2,0,1/2 ( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,1/2,1/2)'	(31) $\bar{3}^+$ ' x, $\bar{x}$ +1/2, $\bar{x}$ ; 0,1/2,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,1/2,1/2)'	(32) $\bar{3}^+$ ' $\bar{x}$ -1, $\bar{x}$ +1/2,x; 1/2,0,1/2 ( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,1/2,1/2)'

- (33)  $\bar{3}^-$  ' x-1/2,x-1/2,x;  
0,0,1/2  
( $\bar{3}_{xyz}^{-1}$ |0,1/2,1/2)'
- (34)  $\bar{3}^-$  ' x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ;  
0,0,1/2  
( $\bar{3}_{\bar{xyz}}$ |0,1/2,1/2)'
- (35)  $\bar{3}^-$  '  $\bar{x}$ -1/2, $\bar{x}$ +1/2, x;  
-1/2,1/2,0  
( $\bar{3}_{\bar{yz}}$ |0,1/2,1/2)'
- (36)  $\bar{3}^-$  '  $\bar{x}$ +1/2, x+1/2, $\bar{x}$ ;  
1/2,1/2,0  
( $\bar{3}_{\bar{yz}}$ |0,1/2,1/2)'
- (37)  $g'$  (-1/4,1/4,1/2) x+1/4, $\bar{x}$ ,z (38)  $g'$  (1/4,1/4,1/2) x-1/4,x,z (39)  $\bar{4}^-$  ' -1/4,1/4,z; -1/4,1/4,1/4 (40)  $\bar{4}^+$  ' 1/4,1/4,z; 1/4,1/4,1/4  
( $m_{xy}$ |0,1/2,1/2)' ( $m_{\bar{xy}}$ |0,1/2,1/2)' ( $\bar{4}_z^{-1}$ |0,1/2,1/2)' ( $\bar{4}_z$ |0,1/2,1/2)'
- (41)  $\bar{4}^-$  ' x,0,1/2; 0,0,1/2 (42)  $m'$  x,y+1/2, $\bar{y}$   
( $\bar{4}_x^{-1}$ |0,1/2,1/2)' ( $m_{yz}$ |0,1/2,1/2)'
- (43)  $g'$  (0,1/2,1/2) x,y,y (44)  $\bar{4}^+$  ' x,1/2,0; 0,1/2,0  
( $m_{yz}$ |0,1/2,1/2)' ( $\bar{4}_x$ |0,1/2,1/2)'
- (45)  $\bar{4}^+$  ' -1/4,y,1/4; -1/4,1/4,1/4 (46)  $g'$  (-1/4,1/2,1/4)  $\bar{x}$ +1/4,y,x (47)  $\bar{4}^-$  ' 1/4,y,1/4; 1/4,1/4,1/4 (48)  $g'$  (1/4,1/2,1/4) x-1/4,y,x  
( $\bar{4}_y$ |0,1/2,1/2)' ( $m_{xz}$ |0,1/2,1/2)' ( $\bar{4}_y^{-1}$ |0,1/2,1/2)' ( $m_{\bar{xz}}$ |0,1/2,1/2)'

For (1/2,0,1/2) + set

- (1)  $t$  (1/2,0,1/2)  
(1|1/2,0,1/2)
- (2) 2 (0,0,1/2) 1/4,0,z  
( $2_z$ |1/2,0,1/2)
- (3) 2 1/4,y,1/4  
( $2_y$ |1/2,0,1/2)
- (4) 2 (1/2,0,0) x,0,1/2  
( $2_x$ |1/2,0,1/2)
- (5)  $3^+$  (1/3,1/3,1/3)  
x+1/6,x-1/6,x  
( $3_{xyz}$ |1/2,0,1/2)
- (6)  $3^+$  (1/3,-1/3,1/3)  
x+1/6,x+1/6, $\bar{x}$   
( $3_{\bar{xyz}}^{-1}$ |1/2,0,1/2)
- (7)  $3^+$  x+1/2, $\bar{x}$ -1/2, $\bar{x}$   
( $3_{\bar{yz}}^{-1}$ |1/2,0,1/2)
- (8)  $3^+$   $\bar{x}$ +1/2, $\bar{x}$ +1/2,x  
( $3_{\bar{yz}}^{-1}$ |1/2,0,1/2)
- (9)  $3^-$  (1/3,1/3,1/3)  
x-1/6,x-1/3,x  
( $3_{xyz}^{-1}$ |1/2,0,1/2)
- (10)  $3^-$  x+1/2, $\bar{x}$ , $\bar{x}$   
( $3_{\bar{yz}}$ |1/2,0,1/2)
- (11)  $3^-$   $\bar{x}$ +1/2, $\bar{x}$ , x  
( $3_{\bar{yz}}$ |1/2,0,1/2)
- (12)  $3^-$  (1/3,-1/3,1/3)  
 $\bar{x}$ -1/6, x+1/3, $\bar{x}$   
( $3_{\bar{yz}}$ |1/2,0,1/2)
- (13) 2 (1/4,1/4,0) x,x-1/4,1/4 (14) 2 (1/4,-1/4,0) x, $\bar{x}$ +1/4,1/4 (15)  $4^-$  (0,0,1/2) 1/4,-1/4,z  
( $2_{xy}$ |1/2,0,1/2) ( $2_{\bar{xy}}$ |1/2,0,1/2) ( $\bar{4}_z^{-1}$ |1/2,0,1/2) ( $\bar{4}_z$ |1/2,0,1/2)
- (17)  $4^-$  (1/2,0,0) x,1/4,1/4 (18) 2 (0,1/4,1/4) 1/4,y-1/4,y (19) 2 (0,-1/2,1/2) 1/4,y+1/4, $\bar{y}$  (20)  $4^+$  (1/2,0,0) x,-1/4,1/4  
( $4_x^{-1}$ |1/2,0,1/2) ( $2_{yz}$ |1/2,0,1/2) ( $2_{\bar{yz}}$ |1/2,0,1/2) ( $4_x$ |1/2,0,1/2)
- (21)  $4^+$  1/2,y,0 (22) 2 (1/2,0,1/2) x,0,x (23)  $4^-$  0,y,1/2 (24) 2  $\bar{x}$ +1/2,0,x  
( $4_y$ |1/2,0,1/2) ( $2_{xz}$ |1/2,0,1/2) ( $4_y^{-1}$ |1/2,0,1/2) ( $2_{\bar{xz}}$ |1/2,0,1/2)
- (25)  $\bar{1}^-$  1/4,0,1/4 (26)  $a'$  (1/2,0,0) x,y,1/4 (27)  $n'$  (1/2,0,1/2) x,0,z (28)  $c'$  (0,0,1/2) 1/4,y,z  
( $\bar{1}$ |1/2,0,1/2)' ( $m_z$ |1/2,0,1/2)' ( $m_y$ |1/2,0,1/2)' ( $m_x$ |1/2,0,1/2)'
- (29)  $\bar{3}^+$  ' x-1/2,x-1/2,x;  
0,0,1/2  
( $\bar{3}_{xyz}$ |1/2,0,1/2)'
- (30)  $\bar{3}^+$  '  $\bar{x}$ -1/2,x+1/2, $\bar{x}$ ;  
0,0,1/2  
( $\bar{3}_{\bar{xyz}}^{-1}$ |1/2,0,1/2)'
- (31)  $\bar{3}^+$  ' x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ;  
1/2,1/2,0  
( $\bar{3}_{\bar{yz}}^{-1}$ |1/2,0,1/2)'
- (32)  $\bar{3}^+$  '  $\bar{x}$ +1/2, $\bar{x}$ -1/2,x;  
1/2,-1/2,0  
( $\bar{3}_{\bar{yz}}^{-1}$ |1/2,0,1/2)'
- (33)  $\bar{3}^-$  ' x+1/2,x,x;  
1/2,0,0  
( $\bar{3}_{xyz}^{-1}$ |1/2,0,1/2)'
- (34)  $\bar{3}^-$  ' x+1/2, $\bar{x}$ -1, $\bar{x}$ ;  
0,-1/2,1/2  
( $\bar{3}_{\bar{yz}}$ |1/2,0,1/2)'
- (35)  $\bar{3}^-$  '  $\bar{x}$ +1/2, $\bar{x}$ +1, x;  
0,1/2,1/2  
( $\bar{3}_{\bar{yz}}$ |1/2,0,1/2)'
- (36)  $\bar{3}^-$  '  $\bar{x}$ +1/2, x, $\bar{x}$ ;  
1/2,0,0  
( $\bar{3}_{\bar{yz}}$ |1/2,0,1/2)'
- (37)  $g'$  (1/4,-1/4,1/2) x+1/4, $\bar{x}$ ,z (38)  $g'$  (1/4,1/4,1/2) x+1/4,x,z (39)  $\bar{4}^-$  ' 1/4,1/4,z; 1/4,1/4,1/4 (40)  $\bar{4}^+$  ' 1/4,-1/4,z; 1/4,-1/4,1/4  
( $m_{xy}$ |1/2,0,1/2)' ( $m_{\bar{xy}}$ |1/2,0,1/2)' ( $\bar{4}_z^{-1}$ |1/2,0,1/2)' ( $\bar{4}_z$ |1/2,0,1/2)'
- (41)  $\bar{4}^-$  ' x,-1/4,1/4; 1/4,-1/4,1/4 (42)  $g'$  (1/2,-1/4,1/4) x,y+1/4, $\bar{y}$  (43)  $g'$  (1/2,1/4,1/4) x,y-1/4,y (44)  $\bar{4}^+$  ' x,1/4,1/4; 1/4,1/4,1/4  
( $\bar{4}_x^{-1}$ |1/2,0,1/2)' ( $m_{yz}$ |1/2,0,1/2)' ( $m_{\bar{yz}}$ |1/2,0,1/2)' ( $\bar{4}_x$ |1/2,0,1/2)'
- (45)  $\bar{4}^+$  ' 0,y,1/2; 0,0,1/2 (46)  $m'$   $\bar{x}$ +1/2,y,x (47)  $\bar{4}^-$  ' 1/2,y,0; 1/2,0,0 (48)  $g'$  (1/2,0,1/2) x,y,x  
( $\bar{4}_y$ |1/2,0,1/2)' ( $m_{xz}$ |1/2,0,1/2)' ( $\bar{4}_y^{-1}$ |1/2,0,1/2)' ( $m_{\bar{xz}}$ |1/2,0,1/2)'



For (1/2,1/2,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,0)<br>(1   1/2,1/2,0)  | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)  | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)  | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)  |
| (5) 3 <sup>+</sup> (1/3,1/3,1/3)<br>x+1/6,x+1/3,x<br>(3 <sub>xyz</sub>   1/2,1/2,0)               | (6) 3 <sup>+</sup> $\bar{x}$ +1/2,x, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)                   | (7) 3 <sup>+</sup> x+1/2, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)                    | (8) 3 <sup>+</sup> (1/3,1/3,-1/3)<br>x+1/6,x+1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)           |
| (9) 3 <sup>-</sup> (1/3,1/3,1/3)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0) | (10) 3 <sup>-</sup> x, $\bar{x}$ +1/2, $\bar{x}$<br>(3 <sub>xyz</sub>   1/2,1/2,0)                               | (11) 3 <sup>-</sup> (1/3,1/3,-1/3)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub>   1/2,1/2,0)                              | (12) 3 <sup>-</sup> $\bar{x}$ ,x+1/2, $\bar{x}$<br>(3 <sub>xyz</sub>   1/2,1/2,0)                            |
| (13) 2 (1/2,1/2,0) x,x,0<br>(2 <sub>xy</sub>   1/2,1/2,0)   | (14) 2 x, $\bar{x}$ +1/2,0<br>(2 <sub>xy</sub>   1/2,1/2,0)  | (15) 4 <sup>-</sup> 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,0)  | (16) 4 <sup>+</sup> 0,1/2,z<br>(4 <sub>z</sub>   1/2,1/2,0)  |
| (17) 4 <sup>-</sup> (1/2,0,0) x,1/4,-1/4<br>(4 <sub>x</sub> <sup>-1</sup>   1/2,1/2,0)            | (18) 2 (0,1/4,1/4) 1/4,y+1/4,y<br>(2 <sub>yz</sub>   1/2,1/2,0)  | (19) 2 (0,1/4,-1/4) 1/4,y+1/4, $\bar{y}$<br>(2 <sub>yz</sub>   1/2,1/2,0)  | (20) 4 <sup>+</sup> (1/2,0,0) x,1/4,1/4<br>(4 <sub>x</sub>   1/2,1/2,0)                                      |
| (21) 4 <sup>+</sup> (0,1/2,0) 1/4,y,-1/4<br>(4 <sub>y</sub>   1/2,1/2,0)                          | (22) 2 (1/4,0,1/4) x+1/4,1/4,x<br>(2 <sub>xz</sub>   1/2,1/2,0)  | (23) 4 <sup>-</sup> (0,1/2,0) 1/4,y,1/4<br>(4 <sub>y</sub> <sup>-1</sup>   1/2,1/2,0)                              | (24) 2 (1/4,0,-1/4) $\bar{x}$ +1/4,1/4,x<br>(2 <sub>xz</sub>   1/2,1/2,0)                                    |
| (25) $\bar{1}$ ' 1/4,1/4,0<br>( $\bar{1}$   1/2,1/2,0)'   | (26) n' (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>   1/2,1/2,0)'   | (27) a' (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0)'   | (28) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)'   |
| (29) $\bar{3}^+$ ' x+1/2,x,x;<br>1/2,0,0<br>( $\bar{3}_{xyz}$   1/2,1/2,0)'                       | (30) $\bar{3}^+$ ' $\bar{x}$ -1/2,x+1, $\bar{x}$ ;<br>0,1/2,1/2<br>( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)' | (31) $\bar{3}^+$ ' x-1/2, $\bar{x}$ +1, $\bar{x}$ ;<br>0,1/2,-1/2<br>( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)' | (32) $\bar{3}^+$ ' $\bar{x}$ +1/2, $\bar{x}$ ,x;<br>1/2,0,0<br>( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)' |
| (33) $\bar{3}^-$ ' x,x+1/2,x;<br>0,1/2,0<br>( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)'         | (34) $\bar{3}^-$ ' x+1, $\bar{x}$ -1/2, $\bar{x}$ ;<br>1/2,0,1/2<br>( $\bar{3}_{xyz}$   1/2,1/2,0)'              | (35) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ +1/2,x;<br>0,1/2,0<br>( $\bar{3}_{xyz}$   1/2,1/2,0)'                     | (36) $\bar{3}^-$ ' $\bar{x}$ +1,x-1/2, $\bar{x}$ ;<br>1/2,0,-1/2<br>( $\bar{3}_{xyz}$   1/2,1/2,0)'          |
| (37) m' x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>   1/2,1/2,0)'                                     | (38) g' (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>   1/2,1/2,0)'  | (39) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,0<br>( $\bar{4}_z$ <sup>-1</sup>   1/2,1/2,0)'                                   | (40) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,0<br>( $\bar{4}_z$   1/2,1/2,0)'   |
| (41) $\bar{4}^-$ ' x,1/4,1/4; 1/4,1/4,1/4<br>( $\bar{4}_x$ <sup>-1</sup>   1/2,1/2,0)'            | (42) g' (1/2,1/4,-1/4) x,y+1/4, $\bar{y}$<br>(m <sub>yz</sub>   1/2,1/2,0)'                                      | (43) g' (1/2,1/4,1/4) x,y+1/4,y<br>(m <sub>yz</sub>   1/2,1/2,0)'  | (44) $\bar{4}^+$ ' x,1/4,-1/4; 1/4,1/4,-1/4<br>( $\bar{4}_x$   1/2,1/2,0)'                                   |
| (45) $\bar{4}^+$ ' 1/4,y,1/4; 1/4,1/4,1/4<br>( $\bar{4}_y$   1/2,1/2,0)'                          | (46) g' (1/4,1/2,-1/4) $\bar{x}$ +1/4,y,x<br>(m <sub>xz</sub>   1/2,1/2,0)'                                      | (47) $\bar{4}^-$ ' 1/4,y,-1/4; 1/4,1/4,-1/4<br>( $\bar{4}_y$ <sup>-1</sup>   1/2,1/2,0)'                           | (48) g' (1/4,1/2,1/4) x+1/4,y,x<br>(m <sub>xz</sub>   1/2,1/2,0)'  |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

- |     |       |         |           |                      |                         |               |               |                   |     |                     |                         |
|-----|-------|---------|-----------|----------------------|-------------------------|---------------|---------------|-------------------|-----|---------------------|-------------------------|
| 192 |       | 1       | (0,0,0) + | (0,1/2,1/2) +        | (1/2,0,1/2) +           | (1/2,1/2,0) + |               |                   |     |                     |                         |
| (1) | x,y,z | [u,v,w] | (2)       | $\bar{x},\bar{y},z$  | [ $\bar{u},\bar{v},w$ ] | (3)           | $\bar{x},y,z$ | [ $\bar{u},v,w$ ] | (4) | x, $\bar{y},z$      | [u, $\bar{v},w$ ]       |
| (5) | z,x,y | [w,u,v] | (6)       | z, $\bar{x},\bar{y}$ | [w, $\bar{u},\bar{v}$ ] | (7)           | $\bar{z},x,y$ | [ $\bar{w},u,v$ ] | (8) | $\bar{z},x,\bar{y}$ | [ $\bar{w},u,\bar{v}$ ] |

(9)	$y,z,x [v,w,u]$	(10)	$\bar{y},z,\bar{x} [\bar{v},w,\bar{u}]$	(11)	$y,\bar{z},\bar{x} [v,\bar{w},\bar{u}]$	(12)	$\bar{y},\bar{z},x [\bar{v},\bar{w},u]$	
(13)	$y,x,\bar{z} [v,u,\bar{w}]$	(14)	$\bar{y},\bar{x},\bar{z} [\bar{v},\bar{u},\bar{w}]$	(15)	$y,\bar{x},z [v,\bar{u},w]$	(16)	$\bar{y},x,z [\bar{v},u,w]$	
(17)	$x,z,\bar{y} [u,w,\bar{v}]$	(18)	$\bar{x},z,y [\bar{u},w,\bar{v}]$	(19)	$\bar{x},z,\bar{y} [\bar{u},\bar{w},\bar{v}]$	(20)	$x,\bar{z},y [u,\bar{w},\bar{v}]$	
(21)	$z,y,\bar{x} [w,v,\bar{u}]$	(22)	$z,\bar{y},x [w,\bar{v},\bar{u}]$	(23)	$\bar{z},y,x [\bar{w},v,u]$	(24)	$\bar{z},\bar{y},\bar{x} [\bar{w},\bar{v},\bar{u}]$	
(25)	$\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$	(26)	$x,y,\bar{z} [u,v,\bar{w}]$	(27)	$x,\bar{y},z [u,\bar{v},w]$	(28)	$\bar{x},y,z [\bar{u},v,w]$	
(29)	$\bar{z},\bar{x},\bar{y} [\bar{w},\bar{u},\bar{v}]$	(30)	$\bar{z},x,y [\bar{w},u,v]$	(31)	$z,x,\bar{y} [w,u,\bar{v}]$	(32)	$z,\bar{x},y [w,\bar{u},\bar{v}]$	
(33)	$\bar{y},\bar{z},\bar{x} [\bar{v},\bar{w},\bar{u}]$	(34)	$y,\bar{z},x [v,\bar{w},u]$	(35)	$\bar{y},z,x [v,w,\bar{u}]$	(36)	$y,z,\bar{x} [v,w,\bar{u}]$	
(37)	$\bar{y},\bar{x},z [\bar{v},\bar{u},w]$	(38)	$y,x,z [v,u,w]$	(39)	$\bar{y},x,z [\bar{v},u,\bar{w}]$	(40)	$y,\bar{x},z [v,\bar{u},\bar{w}]$	
(41)	$\bar{x},\bar{z},y [\bar{u},\bar{w},\bar{v}]$	(42)	$x,\bar{z},\bar{y} [u,\bar{w},\bar{v}]$	(43)	$x,z,y [u,w,v]$	(44)	$\bar{x},z,\bar{y} [\bar{u},w,\bar{v}]$	
(45)	$\bar{z},\bar{y},x [\bar{w},\bar{v},u]$	(46)	$\bar{z},y,\bar{x} [\bar{w},v,\bar{u}]$	(47)	$z,\bar{y},\bar{x} [w,\bar{v},\bar{u}]$	(48)	$z,y,x [w,v,u]$	
96	k ..m'	$x,x,z [u,u,w]$	$\bar{x},\bar{x},z [\bar{u},\bar{u},w]$	$\bar{x},x,\bar{z} [\bar{u},u,\bar{w}]$	$x,\bar{x},z [u,\bar{u},\bar{w}]$	$z,x,x [w,u,u]$	$\bar{z},\bar{x},x [\bar{w},\bar{u},\bar{u}]$	$\bar{z},x,x [w,\bar{u},\bar{u}]$
		$x,z,x [u,w,u]$	$\bar{x},z,\bar{x} [\bar{u},w,\bar{u}]$	$x,\bar{z},\bar{x} [u,\bar{w},\bar{u}]$	$\bar{x},z,x [u,\bar{w},\bar{u}]$	$x,x,\bar{z} [u,u,\bar{w}]$	$\bar{x},x,z [\bar{u},\bar{u},\bar{w}]$	$\bar{x},x,z [u,\bar{u},\bar{w}]$
		$x,x,\bar{z} [u,u,\bar{w}]$	$\bar{x},\bar{x},\bar{z} [\bar{u},\bar{u},\bar{w}]$	$x,\bar{x},z [u,\bar{u},w]$	$\bar{x},x,z [u,\bar{u},w]$	$x,z,\bar{x} [u,w,\bar{u}]$	$\bar{x},z,\bar{x} [\bar{u},\bar{w},\bar{u}]$	$\bar{x},z,x [u,\bar{w},\bar{u}]$
		$x,z,\bar{x} [u,w,\bar{u}]$	$\bar{x},z,x [\bar{u},w,u]$	$\bar{x},z,\bar{x} [\bar{u},\bar{w},\bar{u}]$	$x,\bar{z},x [u,\bar{w},\bar{u}]$	$z,x,\bar{x} [w,u,\bar{u}]$	$\bar{z},\bar{x},x [\bar{w},\bar{u},\bar{u}]$	$\bar{z},x,x [w,\bar{u},\bar{u}]$
		$z,x,\bar{x} [w,u,\bar{u}]$	$\bar{z},\bar{x},x [\bar{w},\bar{u},\bar{u}]$	$\bar{z},x,x [w,\bar{u},u]$	$\bar{z},x,x [w,\bar{u},u]$	$z,x,\bar{x} [w,u,\bar{u}]$	$\bar{z},\bar{x},x [\bar{w},\bar{u},\bar{u}]$	$\bar{z},x,x [w,\bar{u},\bar{u}]$
96	j m'..	$0,y,z [0,v,w]$	$0,\bar{y},z [0,\bar{v},w]$	$0,y,\bar{z} [0,v,\bar{w}]$	$0,\bar{y},z [0,\bar{v},\bar{w}]$	$z,0,y [w,0,v]$	$\bar{z},0,y [\bar{w},0,v]$	$\bar{z},0,y [w,0,\bar{v}]$
		$y,z,0 [v,w,0]$	$\bar{y},z,0 [\bar{v},w,0]$	$y,\bar{z},0 [v,\bar{w},0]$	$\bar{y},z,0 [\bar{v},\bar{w},0]$	$y,0,\bar{z} [v,0,\bar{w}]$	$\bar{y},0,z [v,0,w]$	$\bar{y},0,z [v,0,\bar{w}]$
		$0,z,\bar{y} [0,w,\bar{v}]$	$0,z,y [0,w,v]$	$0,\bar{z},\bar{y} [0,\bar{w},\bar{v}]$	$0,\bar{z},y [0,\bar{w},v]$	$0,z,y [0,w,\bar{v}]$	$0,\bar{z},y [0,\bar{w},\bar{v}]$	$0,\bar{z},y [0,w,\bar{v}]$
		$z,y,0 [w,v,0]$	$\bar{z},\bar{y},0 [\bar{w},\bar{v},0]$	$\bar{z},y,0 [w,\bar{v},0]$	$\bar{z},y,0 [\bar{w},v,0]$	$z,y,0 [w,v,0]$	$\bar{z},y,0 [\bar{w},\bar{v},0]$	$\bar{z},y,0 [w,\bar{v},0]$
48	i m'.m'2	$1/2,y,y [0,v,v]$	$1/2,\bar{y},y [0,\bar{v},v]$	$1/2,y,\bar{y} [0,v,\bar{v}]$	$1/2,\bar{y},y [0,\bar{v},\bar{v}]$	$y,1/2,y [v,0,v]$	$\bar{y},1/2,y [\bar{v},0,\bar{v}]$	$\bar{y},1/2,y [v,0,\bar{v}]$
		$y,y,1/2 [v,v,0]$	$\bar{y},y,1/2 [\bar{v},v,0]$	$y,\bar{y},1/2 [v,\bar{v},0]$	$\bar{y},\bar{y},1/2 [\bar{v},\bar{v},0]$	$0,z,\bar{y} [0,w,\bar{v}]$	$0,\bar{z},y [0,\bar{w},\bar{v}]$	$0,\bar{z},y [0,w,\bar{v}]$
48	h m'.m'2	$0,y,y [0,v,v]$	$0,\bar{y},y [0,\bar{v},v]$	$0,y,\bar{y} [0,v,\bar{v}]$	$0,\bar{y},y [0,\bar{v},\bar{v}]$	$y,0,y [v,0,v]$	$\bar{y},0,y [\bar{v},0,\bar{v}]$	$\bar{y},0,y [v,0,\bar{v}]$
		$y,y,0 [v,v,0]$	$\bar{y},y,0 [\bar{v},v,0]$	$y,\bar{y},0 [v,\bar{v},0]$	$\bar{y},\bar{y},0 [\bar{v},\bar{v},0]$	$z,y,0 [w,v,0]$	$\bar{z},y,0 [\bar{w},v,0]$	$\bar{z},y,0 [w,\bar{v},0]$

Continued

225.5.1622

Fm' $\bar{3}$ 'm'

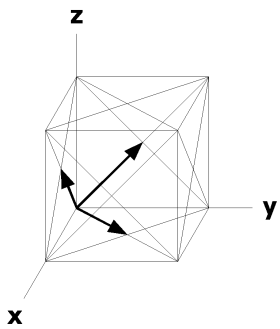
48	g	2.m'm'	x,1/4,1/4 [u,0,0]	$\bar{x}$ ,3/4,1/4 [ $\bar{u}$ ,0,0]	1/4,x,1/4 [0,u,0]	1/4, $\bar{x}$ ,3/4 [0, $\bar{u}$ ,0]
			1/4,1/4,x [0,0,u]	3/4,1/4, $\bar{x}$ [0,0, $\bar{u}$ ]	1/4,x,3/4 [0,u,0]	3/4, $\bar{x}$ ,3/4 [0, $\bar{u}$ ,0]
			x,1/4,3/4 [u,0,0]	$\bar{x}$ ,1/4,1/4 [ $\bar{u}$ ,0,0]	1/4,1/4, $\bar{x}$ [0,0, $\bar{u}$ ]	1/4,3/4,x [0,0,u]
32	f	.3m'	x,x,x [u,u,u]	$\bar{x}$ , $\bar{x}$ ,x [ $\bar{u}$ , $\bar{u}$ ,u]	$\bar{x}$ ,x, $\bar{x}$ [ $\bar{u}$ ,u, $\bar{u}$ ]	x, $\bar{x}$ , $\bar{x}$ [u, $\bar{u}$ , $\bar{u}$ ]
			x,x, $\bar{x}$ [u,u, $\bar{u}$ ]	$\bar{x}$ , $\bar{x}$ , $\bar{x}$ [ $\bar{u}$ , $\bar{u}$ , $\bar{u}$ ]	x, $\bar{x}$ ,x [u, $\bar{u}$ ,u]	$\bar{x}$ ,x,x [ $\bar{u}$ ,u,u]
24	e	4m'.m'	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0]	0,x,0 [0,u,0]	
			0, $\bar{x}$ ,0 [0, $\bar{u}$ ,0]	0,0,x [0,0,u]	0,0, $\bar{x}$ [0,0, $\bar{u}$ ]	
24	d	m'.m'm'	0,1/4,1/4 [0,0,0]	0,3/4,1/4 [0,0,0]	1/4,0,1/4 [0,0,0]	
			1/4,0,3/4 [0,0,0]	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]	
8	c	$\bar{4}$ '3m'	1/4,1/4,1/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]		
4	b	m' $\bar{3}$ 'm'	1/2,1/2,1/2 [0,0,0]			
4	a	m' $\bar{3}$ 'm'	0,0,0 [0,0,0]			

**Symmetry of Special Projections**

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,1,1] p6m'm'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

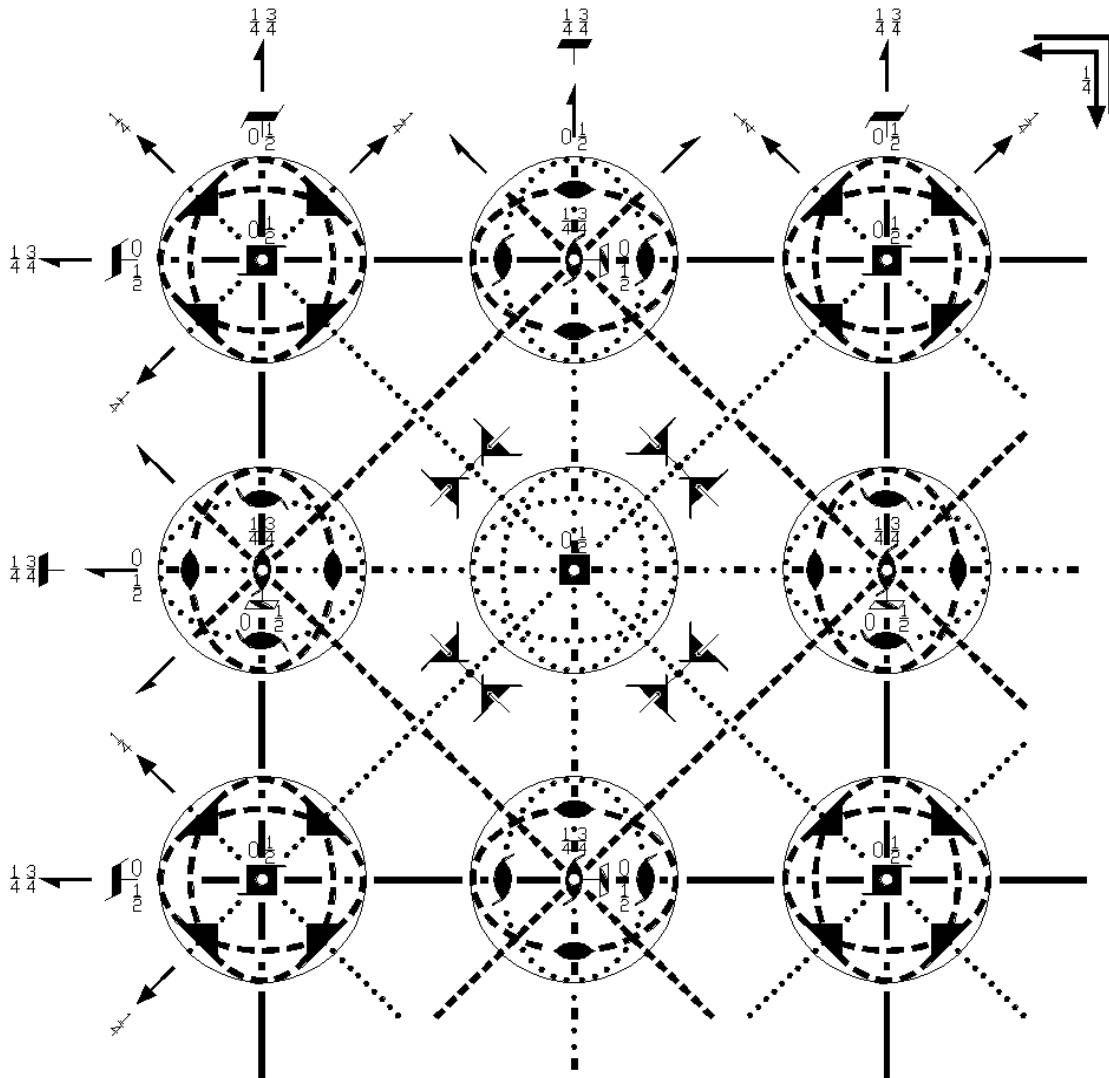
Along [1,1,0] c2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,0



$Fm\bar{3}c$   
226.1.1623

$m\bar{3}m$   
 $F4/m\bar{3}2/c$

Cubic



**Origin** at center ( $m\bar{3}$ )

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/4$ ;  $y \leq \min(x, 1/2-x)$ ;  $z \leq y$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/4,1/4,0$   $1/4,1/4,1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)   | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)   | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)   |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)               | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0) | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0) | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0) |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}$ <sup>-1</sup>  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)              | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)              | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)              |

(13) 2 (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)	(14) 2 x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)	(15) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)	(16) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)
(17) 4 <sup>-</sup> (1/2,0,0) x,1/2,0 (4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,1/2)	(18) 2 (0,1/2,1/2) 1/4,y,y (2 <sub>yz</sub>  1/2,1/2,1/2)	(19) 2 1/4,y+1/2, $\bar{y}$ (2 <sub><math>\bar{yz}</math></sub>  1/2,1/2,1/2)	(20) 4 <sup>+</sup> (1/2,0,0) x,0,1/2 (4 <sub>x</sub>  1/2,1/2,1/2)
(21) 4 <sup>+</sup> (0,1/2,0) 1/2,y,0 (4 <sub>y</sub>  1/2,1/2,1/2)	(22) 2 (1/2,0,1/2) x,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)	(23) 4 <sup>-</sup> (0,1/2,0) 0,y,1/2 (4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,1/2)	(24) 2 $\bar{x}$ +1/2,1/4,x (2 <sub><math>\bar{xz}</math></sub>  1/2,1/2,1/2)
(25) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(26) m x,y,0 (m <sub>z</sub>  0,0,0)	(27) m x,0,z (m <sub>y</sub>  0,0,0)	(28) m 0,y,z (m <sub>x</sub>  0,0,0)
(29) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)	(30) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{\bar{xyz}}$ <sup>-1</sup>  0,0,0)	(31) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{\bar{xyz}}$ <sup>-1</sup>  0,0,0)	(32) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)
(33) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)	(34) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{\bar{xyz}}$  0,0,0)	(35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{\bar{xyz}}$  0,0,0)	(36) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)
(37) c (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,1/2)	(38) n (1/2,1/2,1/2) x,x,z (m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)	(39) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>  1/2,1/2,1/2)	(40) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$  1/2,1/2,1/2)
(41) $\bar{4}^-$ x,0,1/2; 1/4,0,1/2 ( $\bar{4}_x$ <sup>-1</sup>  1/2,1/2,1/2)	(42) a (1/2,0,0) x,y+1/2, $\bar{y}$ (m <sub>yz</sub>  1/2,1/2,1/2)	(43) n (1/2,1/2,1/2) x,y,y (m <sub><math>\bar{yz}</math></sub>  1/2,1/2,1/2)	(44) $\bar{4}^+$ x,1/2,0; 1/4,1/2,0 ( $\bar{4}_x$  1/2,1/2,1/2)
(45) $\bar{4}^+$ 0,y,1/2; 0,1/4,1/2 ( $\bar{4}_y$  1/2,1/2,1/2)	(46) b (0,1/2,0) $\bar{x}$ +1/2,y,x (m <sub>xz</sub>  1/2,1/2,1/2)	(47) $\bar{4}^-$ 1/2,y,0; 1/2,1/4,0 ( $\bar{4}_y$ <sup>-1</sup>  1/2,1/2,1/2)	(48) n (1/2,1/2,1/2) x,y,x (m <sub><math>\bar{xz}</math></sub>  1/2,1/2,1/2)

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2) ( $\bar{1}$  0,1/2,1/2)	(2) 2 (0,0,1/2) 0,1/4,z (2 <sub>z</sub>  0,1/2,1/2)	(3) 2 (0,1/2,0) 0,y,1/4 (2 <sub>y</sub>  0,1/2,1/2)	(4) 2 x,1/4,1/4 (2 <sub>x</sub>  0,1/2,1/2)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x-1/3,x-1/6,x (3 <sub>xyz</sub>  0,1/2,1/2)	(6) 3 <sup>+</sup> $\bar{x}$ ,x+1/2, $\bar{x}$ (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,1/2,1/2)	(7) 3 <sup>+</sup> (-1/3,1/3,1/3) x+1/3, $\bar{x}$ -1/6, $\bar{x}$ (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,1/2,1/2)	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ +1/2,x (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,1/2,1/2)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x-1/6,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(10) 3 <sup>-</sup> (-1/3,1/3,1/3) x+1/6, $\bar{x}$ +1/6, $\bar{x}$ (3 <sub>xyz</sub>  0,1/2,1/2)	(11) 3 <sup>-</sup> $\bar{x}$ +1/2, $\bar{x}$ +1/2,x (3 <sub><math>\bar{xyz}</math></sub>  0,1/2,1/2)	(12) 3 <sup>-</sup> $\bar{x}$ -1/2,x+1/2, $\bar{x}$ (3 <sub><math>\bar{xyz}</math></sub>  0,1/2,1/2)
(13) 2 (1/4,1/4,0) x,x-1/4,0 (2 <sub>xy</sub>  1/2,0,0)	(14) 2 (1/4,-1/4,0) x, $\bar{x}$ +1/4,0 (2 <sub><math>\bar{xy}</math></sub>  1/2,0,0)	(15) 4 <sup>-</sup> 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>  1/2,0,0)	(16) 4 <sup>+</sup> 1/4,1/4,z (4 <sub>z</sub>  1/2,0,0)
(17) 4 <sup>-</sup> (1/2,0,0) x,0,0 (4 <sub>x</sub> <sup>-1</sup>  1/2,0,0)	(18) 2 1/4,y,y (2 <sub>yz</sub>  1/2,0,0)	(19) 2 1/4,y, $\bar{y}$ (2 <sub><math>\bar{yz}</math></sub>  1/2,0,0)	(20) 4 <sup>+</sup> (1/2,0,0) x,0,0 (4 <sub>x</sub>  1/2,0,0)
(21) 4 <sup>+</sup> 1/4,y,-1/4 (4 <sub>y</sub>  1/2,0,0)	(22) 2 (1/4,0,1/4) x+1/4,0,x (2 <sub>xz</sub>  1/2,0,0)	(23) 4 <sup>-</sup> 1/4,y,1/4 (4 <sub>y</sub> <sup>-1</sup>  1/2,0,0)	(24) 2 (1/4,0,-1/4) $\bar{x}$ +1/4,0,x (2 <sub><math>\bar{xz}</math></sub>  1/2,0,0)
(25) $\bar{1}$ 0,1/4,1/4 ( $\bar{1}$  0,1/2,1/2)	(26) b (0,1/2,0) x,y,1/4 (m <sub>z</sub>  0,1/2,1/2)	(27) c (0,0,1/2) x,1/4,z (m <sub>y</sub>  0,1/2,1/2)	(28) n (0,1/2,1/2) 0,y,z (m <sub>x</sub>  0,1/2,1/2)
(29) $\bar{3}^+$ x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$  0,1/2,1/2)	(30) $\bar{3}^+$ $\bar{x}$ -1,x+1/2, $\bar{x}$ ; -1/2,0,1/2 ( $\bar{3}_{\bar{xyz}}$ <sup>-1</sup>  0,1/2,1/2)	(31) $\bar{3}^+$ x, $\bar{x}$ +1/2, $\bar{x}$ ; 0,1/2,0 ( $\bar{3}_{\bar{xyz}}$ <sup>-1</sup>  0,1/2,1/2)	(32) $\bar{3}^+$ $\bar{x}$ -1, $\bar{x}$ +1/2,x; 1/2,0,1/2 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,1/2,1/2)

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| (33) $\bar{3}^-$ $x-1/2, x-1/2, x;$<br>0,0,1/2<br>( $\bar{3}_{xyz}^{-1}   0, 1/2, 1/2$ ) | (34) $\bar{3}^-$ $x+1/2, \bar{x}-1/2, \bar{x};$<br>0,0,1/2<br>( $\bar{3}_{\bar{xyz}}   0, 1/2, 1/2$ ) | (35) $\bar{3}^-$ $\bar{x}-1/2, \bar{x}+1/2, x;$<br>-1/2,1/2,0<br>( $\bar{3}_{\bar{xyz}}   0, 1/2, 1/2$ ) | (36) $\bar{3}^-$ $\bar{x}+1/2, x+1/2, \bar{x};$<br>1/2,1/2,0<br>( $\bar{3}_{\bar{xyz}}   0, 1/2, 1/2$ ) |
| (37) g (1/4, -1/4, 0) $x+1/4, \bar{x}, z$<br>( $m_{xy}   1/2, 0, 0$ )                    | (38) g (1/4, 1/4, 0) $x+1/4, x, z$<br>( $m_{\bar{xy}}   1/2, 0, 0$ )                                  | (39) $\bar{4}^-$ 1/4, 1/4, z; 1/4, 1/4, 0<br>( $\bar{4}_z^{-1}   1/2, 0, 0$ )                            | (40) $\bar{4}^+$ 1/4, -1/4, z; 1/4, -1/4, 0<br>( $\bar{4}_z   1/2, 0, 0$ )                              |
| (41) $\bar{4}^-$ $x, 0, 0; 1/4, 0, 0$<br>( $\bar{4}_x^{-1}   1/2, 0, 0$ )                | (42) a (1/2, 0, 0) $x, y, \bar{y}$<br>( $m_{yz}   1/2, 0, 0$ )  | (43) a (1/2, 0, 0) $x, y, y$<br>( $m_{\bar{yz}}   1/2, 0, 0$ )   | (44) $\bar{4}^+$ $x, 0, 0; 1/4, 0, 0$<br>( $\bar{4}_x   1/2, 0, 0$ )                                    |
| (45) $\bar{4}^+$ 1/4, y, 1/4; 1/4, 0, 1/4<br>( $\bar{4}_y   1/2, 0, 0$ )                 | (46) g (1/4, 0, -1/4) $\bar{x}+1/4, y, x$<br>( $m_{xz}   1/2, 0, 0$ )                                 | (47) $\bar{4}^-$ 1/4, y, -1/4; 1/4, 0, -1/4<br>( $\bar{4}_y^{-1}   1/2, 0, 0$ )                          | (48) g (1/4, 0, 1/4) $x+1/4, y, x$<br>( $m_{\bar{xz}}   1/2, 0, 0$ )                                    |

For (1/2, 0, 1/2) + set

- |  |  |  |   |
|--|--|--|---|
| (1) t (1/2, 0, 1/2)<br>( $1   1/2, 0, 1/2$ )   | (2) 2 (0, 0, 1/2) 1/4, 0, z<br>( $2_z   1/2, 0, 1/2$ )   | (3) 2 1/4, y, 1/4<br>( $2_y   1/2, 0, 1/2$ )   | (4) 2 (1/2, 0, 0) $x, 0, 1/4$<br>( $2_x   1/2, 0, 1/2$ )  |
| (5) $3^+$ (1/3, 1/3, 1/3)<br>$x+1/6, x-1/6, x$<br>( $3_{xyz}   1/2, 0, 1/2$ )        | (6) $3^+$ (1/3, -1/3, 1/3)<br>$x+1/6, x+1/6, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ )            | (7) $3^+$ $x+1/2, \bar{x}-1/2, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ )                            | (8) $3^+$ $\bar{x}+1/2, \bar{x}+1/2, x$<br>( $3_{xyz}^{-1}   1/2, 0, 1/2$ )                                   |
| (9) $3^-$ (1/3, 1/3, 1/3)<br>$x-1/6, x-1/3, x$<br>( $3_{xyz}^{-1}   1/2, 0, 1/2$ )   | (10) $3^-$ $x+1/2, \bar{x}, \bar{x}$<br>( $3_{\bar{xyz}}   1/2, 0, 1/2$ )                                  | (11) $3^-$ $\bar{x}+1/2, \bar{x}, x$<br>( $3_{\bar{xyz}}   1/2, 0, 1/2$ )                                    | (12) $3^-$ (1/3, -1/3, 1/3)<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>( $3_{\bar{xyz}}   1/2, 0, 1/2$ )             |
| (13) 2 (1/4, 1/4, 0) $x, x+1/4, 0$<br>( $2_{xy}   0, 1/2, 0$ )                       | (14) 2 (-1/4, 1/4, 0) $x, \bar{x}+1/4, 0$<br>( $2_{\bar{xy}}   0, 1/2, 0$ )                                | (15) $4^-$ 1/4, 1/4, z<br>( $\bar{4}_z^{-1}   0, 1/2, 0$ )   | (16) $4^+$ -1/4, 1/4, z<br>( $\bar{4}_z   0, 1/2, 0$ )  |
| (17) $4^-$ $x, 1/4, -1/4$<br>( $\bar{4}_x^{-1}   0, 1/2, 0$ )                        | (18) 2 (0, 1/4, 1/4) $0, y+1/4, y$<br>( $2_{yz}   0, 1/2, 0$ )   | (19) 2 (0, 1/4, -1/4) $0, y+1/4, \bar{y}$<br>( $2_{\bar{yz}}   0, 1/2, 0$ )                                  | (20) $4^+$ $x, 1/4, 1/4$<br>( $\bar{4}_x   0, 1/2, 0$ )   |
| (21) $4^+$ (0, 1/2, 0) $0, y, 0$<br>( $\bar{4}_y   0, 1/2, 0$ )                      | (22) 2 $x, 1/4, x$<br>( $2_{xz}   0, 1/2, 0$ )   | (23) $4^-$ (0, 1/2, 0) $0, y, 0$<br>( $\bar{4}_y^{-1}   0, 1/2, 0$ )   | (24) 2 $\bar{x}, 1/4, x$<br>( $2_{\bar{xz}}   0, 1/2, 0$ )  |
| (25) $\bar{1}$ 1/4, 0, 1/4<br>( $\bar{1}   1/2, 0, 1/2$ )                            | (26) a (1/2, 0, 0) $x, y, 1/4$<br>( $m_z   1/2, 0, 1/2$ )  | (27) n (1/2, 0, 1/2) $x, 0, z$<br>( $m_y   1/2, 0, 1/2$ )  | (28) c (0, 0, 1/2) 1/4, y, z<br>( $m_x   1/2, 0, 1/2$ )   |
| (29) $\bar{3}^+$ $x-1/2, x-1/2, x;$<br>0,0,1/2<br>( $\bar{3}_{xyz}   1/2, 0, 1/2$ )  | (30) $\bar{3}^+$ $\bar{x}-1/2, x+1/2, \bar{x};$<br>0,0,1/2<br>( $\bar{3}_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ ) | (31) $\bar{3}^+$ $x+1/2, \bar{x}+1/2, \bar{x};$<br>1/2,1/2,0<br>( $\bar{3}_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ ) | (32) $\bar{3}^+$ $\bar{x}+1/2, \bar{x}-1/2, x;$<br>1/2,-1/2,0<br>( $\bar{3}_{\bar{xyz}}^{-1}   1/2, 0, 1/2$ ) |
| (33) $\bar{3}^-$ $x+1/2, x, x;$<br>1/2,0,0<br>( $\bar{3}_{xyz}^{-1}   1/2, 0, 1/2$ ) | (34) $\bar{3}^-$ $x+1/2, \bar{x}-1, \bar{x};$<br>0,-1/2,1/2<br>( $\bar{3}_{\bar{xyz}}   1/2, 0, 1/2$ )     | (35) $\bar{3}^-$ $\bar{x}+1/2, \bar{x}+1, x;$<br>0,1/2,1/2<br>( $\bar{3}_{\bar{xyz}}   1/2, 0, 1/2$ )        | (36) $\bar{3}^-$ $\bar{x}+1/2, x, \bar{x};$<br>1/2,0,0<br>( $\bar{3}_{\bar{xyz}}   1/2, 0, 1/2$ )             |
| (37) g (-1/4, 1/4, 0) $x+1/4, \bar{x}, z$<br>( $m_{xy}   0, 1/2, 0$ )                | (38) g (1/4, 1/4, 0) $x-1/4, x, z$<br>( $m_{\bar{xy}}   0, 1/2, 0$ )                                       | (39) $\bar{4}^-$ -1/4, 1/4, z; -1/4, 1/4, 0<br>( $\bar{4}_z^{-1}   0, 1/2, 0$ )                              | (40) $\bar{4}^+$ 1/4, 1/4, z; 1/4, 1/4, 0<br>( $\bar{4}_z   0, 1/2, 0$ )                                      |
| (41) $\bar{4}^-$ $x, 1/4, 1/4; 0, 1/4, 1/4$<br>( $\bar{4}_x^{-1}   0, 1/2, 0$ )      | (42) g (0, 1/4, -1/4) $x, y+1/4, \bar{y}$<br>( $m_{yz}   0, 1/2, 0$ )                                      | (43) g (0, 1/4, 1/4) $x, y+1/4, y$<br>( $m_{\bar{yz}}   0, 1/2, 0$ )   | (44) $\bar{4}^+$ $x, 1/4, -1/4; 0, 1/4, -1/4$<br>( $\bar{4}_x   0, 1/2, 0$ )                                  |
| (45) $\bar{4}^+$ $0, y, 0; 0, 1/4, 0$<br>( $\bar{4}_y   0, 1/2, 0$ )                 | (46) b (0, 1/2, 0) $\bar{x}, y, x$<br>( $m_{xz}   0, 1/2, 0$ )   | (47) $\bar{4}^-$ $0, y, 0; 0, 1/4, 0$<br>( $\bar{4}_y^{-1}   0, 1/2, 0$ )                                    | (48) b (0, 1/2, 0) $x, y, x$<br>( $m_{\bar{xz}}   0, 1/2, 0$ )  |

## For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (1   1/2,1/2,0)	(2) 2 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,0)	(3) 2 (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)	(4) 2 (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) 3 <sup>+</sup> $\bar{x}$ +1/2,x, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(7) 3 <sup>+</sup> x+1/2, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(8) 3 <sup>+</sup> (1/3,1/3,-1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) 3 <sup>-</sup> x, $\bar{x}$ +1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)	(11) 3 <sup>-</sup> (1/3,1/3,-1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub>   1/2,1/2,0)	(12) 3 <sup>-</sup> $\bar{x}$ , x+1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)
(13) 2 x,x,1/4 (2 <sub>xy</sub>   0,0,1/2)	(14) 2 x, $\bar{x}$ ,1/4 (2 <sub>xy</sub>   0,0,1/2)	(15) 4 <sup>-</sup> (0,0,1/2) 0,0,z (4 <sub>z</sub> <sup>-1</sup>   0,0,1/2)	(16) 4 <sup>+</sup> (0,0,1/2) 0,0,z (4 <sub>z</sub>   0,0,1/2)
(17) 4 <sup>-</sup> x,1/4,1/4 (4 <sub>x</sub> <sup>-1</sup>   0,0,1/2)	(18) 2 (0,1/4,1/4) 0,y-1/4,y (2 <sub>yz</sub>   0,0,1/2)	(19) 2 (0,-1/4,1/4) 0,y+1/4, $\bar{y}$ (2 <sub>yz</sub>   0,0,1/2)	(20) 4 <sup>+</sup> x,-1/4,1/4 (4 <sub>x</sub>   0,0,1/2)
(21) 4 <sup>+</sup> 1/4,y,1/4 (4 <sub>y</sub>   0,0,1/2)	(22) 2 (1/4,0,1/4) x-1/4,0,x (2 <sub>xz</sub>   0,0,1/2)	(23) 4 <sup>-</sup> -1/4,y,1/4 (4 <sub>y</sub> <sup>-1</sup>   0,0,1/2)	(24) 2 (-1/4,0,1/4) $\bar{x}$ +1/4,0,x (2 <sub>xz</sub>   0,0,1/2)
(25) $\bar{1}$ 1/4,1/4,0 ( $\bar{1}$   1/2,1/2,0)	(26) n (1/2,1/2,0) x,y,0 (m <sub>z</sub>   1/2,1/2,0)	(27) a (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)	(28) b (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)
(29) $\bar{3}^+$ x+1/2,x,x; 1/2,0,0 ( $\bar{3}_{xyz}$   1/2,1/2,0)	(30) $\bar{3}^+$ $\bar{x}$ -1/2,x+1, $\bar{x}$ ; 0,1/2,1/2 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)	(31) $\bar{3}^+$ x-1/2, $\bar{x}$ +1, $\bar{x}$ ; 0,1/2,-1/2 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)	(32) $\bar{3}^+$ $\bar{x}$ +1/2, $\bar{x}$ ,x; 1/2,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)
(33) $\bar{3}^-$ x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)	(34) $\bar{3}^-$ x+1, $\bar{x}$ -1/2, $\bar{x}$ ; 1/2,0,1/2 ( $\bar{3}_{xyz}$   1/2,1/2,0)	(35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$   1/2,1/2,0)	(36) $\bar{3}^-$ $\bar{x}$ +1,x-1/2, $\bar{x}$ ; 1/2,0,-1/2 ( $\bar{3}_{xyz}$   1/2,1/2,0)
(37) c (0,0,1/2) x, $\bar{x}$ ,z (m <sub>xy</sub>   0,0,1/2)	(38) c (0,0,1/2) x,x,z (m <sub>xy</sub>   0,0,1/2)	(39) $\bar{4}^-$ 0,0,z; 0,0,1/4 ( $\bar{4}_z$ <sup>-1</sup>   0,0,1/2)	(40) $\bar{4}^+$ 0,0,z; 0,0,1/4 ( $\bar{4}_z$   0,0,1/2)
(41) $\bar{4}^-$ x,-1/4,1/4; 0,-1/4,1/4 ( $\bar{4}_x$ <sup>-1</sup>   0,0,1/2)	(42) g (0,-1/4,1/4) x,y+1/4, $\bar{y}$ (m <sub>yz</sub>   0,0,1/2)	(43) g (0,1/4,1/4) x,y-1/4,y (m <sub>yz</sub>   0,0,1/2)	(44) $\bar{4}^+$ x,1/4,1/4; 0,1/4,1/4 ( $\bar{4}_x$   0,0,1/2)
(45) $\bar{4}^+$ -1/4,y,1/4; -1/4,0,1/4 ( $\bar{4}_y$   0,0,1/2)	(46) g (-1/4,0,1/4) $\bar{x}$ +1/4,y,x (m <sub>xz</sub>   0,0,1/2)	(47) $\bar{4}^-$ 1/4,y,1/4; 1/4,0,1/4 ( $\bar{4}_y$ <sup>-1</sup>   0,0,1/2)	(48) g (1/4,0,1/4) x-1/4,y,x (m <sub>xz</sub>   0,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

192	j	1	(0,0,0) +	(0,1/2,1/2,) +	(1/2,0,1/2) +	(1/2,1/2,0) +					
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}$ , $\bar{y}$ ,z	[ $\bar{u}$ , $\bar{v}$ ,w]	(3)	$\bar{x}$ ,y,z	[ $\bar{u}$ ,v, $\bar{w}$ ]	(4)	x, $\bar{y}$ ,z	[u, $\bar{v}$ , $\bar{w}$ ]
(5)	z,x,y	[w,u,v]	(6)	z, $\bar{x}$ , $\bar{y}$	[w, $\bar{u}$ , $\bar{v}$ ]	(7)	$\bar{z}$ ,x,y	[ $\bar{w}$ ,u,v]	(8)	$\bar{z}$ ,x, $\bar{y}$	[ $\bar{w}$ ,u, $\bar{v}$ ]

(9) $y, z, x [v, w, u]$	(10) $\bar{y}, z, \bar{x} [\bar{v}, w, \bar{u}]$	(11) $y, \bar{z}, \bar{x} [v, \bar{w}, \bar{u}]$	(12) $\bar{y}, \bar{z}, x [\bar{v}, \bar{w}, u]$
(13) $y+1/2, x+1/2, \bar{z}+1/2 [v, u, \bar{w}]$	(14) $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2 [\bar{v}, \bar{u}, \bar{w}]$	(15) $y+1/2, \bar{x}+1/2, z+1/2 [v, \bar{u}, w]$	(16) $\bar{y}+1/2, x+1/2, z+1/2 [\bar{v}, u, w]$
(17) $x+1/2, z+1/2, \bar{y}+1/2 [u, w, \bar{v}]$	(18) $\bar{x}+1/2, z+1/2, y+1/2 [\bar{u}, w, v]$	(19) $\bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2 [\bar{u}, \bar{w}, \bar{v}]$	(20) $x+1/2, \bar{z}+1/2, y+1/2 [u, \bar{w}, v]$
(21) $z+1/2, y+1/2, \bar{x}+1/2 [w, v, \bar{u}]$	(22) $z+1/2, \bar{y}+1/2, x+1/2 [w, \bar{v}, u]$	(23) $\bar{z}+1/2, y+1/2, x+1/2 [\bar{w}, v, u]$	(24) $\bar{z}+1/2, \bar{y}+1/2, \bar{x}+1/2 [\bar{w}, \bar{v}, \bar{u}]$
(25) $\bar{x}, \bar{y}, \bar{z} [u, v, w]$	(26) $x, y, \bar{z} [\bar{u}, \bar{v}, w]$	(27) $x, \bar{y}, z [\bar{u}, v, \bar{w}]$	(28) $\bar{x}, y, z [u, \bar{v}, \bar{w}]$
(29) $\bar{z}, \bar{x}, \bar{y} [w, u, v]$	(30) $\bar{z}, x, y [w, \bar{u}, \bar{v}]$	(31) $z, x, \bar{y} [\bar{w}, \bar{u}, v]$	(32) $z, \bar{x}, y [\bar{w}, u, \bar{v}]$
(33) $\bar{y}, \bar{z}, \bar{x} [v, w, u]$	(34) $y, \bar{z}, x [\bar{v}, w, \bar{u}]$	(35) $\bar{y}, z, x [v, \bar{w}, \bar{u}]$	(36) $y, z, \bar{x} [\bar{v}, \bar{w}, u]$
(37) $\bar{y}+1/2, \bar{x}+1/2, z+1/2 [v, u, \bar{w}]$	(38) $y+1/2, x+1/2, z+1/2 [\bar{v}, \bar{u}, \bar{w}]$	(39) $\bar{y}+1/2, x+1/2, \bar{z}+1/2 [v, \bar{u}, w]$	(40) $y+1/2, \bar{x}+1/2, \bar{z}+1/2 [\bar{v}, u, w]$
(41) $\bar{x}+1/2, \bar{z}+1/2, y+1/2 [u, w, \bar{v}]$	(42) $x+1/2, \bar{z}+1/2, \bar{y}+1/2 [\bar{u}, w, v]$	(43) $x+1/2, z+1/2, y+1/2 [\bar{u}, \bar{w}, \bar{v}]$	(44) $\bar{x}+1/2, z+1/2, \bar{y}+1/2 [u, \bar{w}, v]$
(45) $\bar{z}+1/2, \bar{y}+1/2, x+1/2 [w, v, \bar{u}]$	(46) $\bar{z}+1/2, y+1/2, \bar{x}+1/2 [w, \bar{v}, u]$	(47) $z+1/2, \bar{y}+1/2, \bar{x}+1/2 [\bar{w}, v, u]$	(48) $z+1/2, y+1/2, x+1/2 [\bar{w}, \bar{v}, \bar{u}]$

96 i m..

$0, y, z [u, 0, 0]$	$0, \bar{y}, z [\bar{u}, 0, 0]$	$0, y, \bar{z} [\bar{u}, 0, 0]$	$0, \bar{y}, \bar{z} [u, 0, 0]$
$z, 0, y [0, u, 0]$	$z, 0, \bar{y} [0, \bar{u}, 0]$	$\bar{z}, 0, y [0, \bar{u}, 0]$	$\bar{z}, 0, \bar{y} [0, u, 0]$
$y, z, 0 [0, 0, u]$	$\bar{y}, z, 0 [0, 0, \bar{u}]$	$y, \bar{z}, 0 [0, 0, \bar{u}]$	$\bar{y}, \bar{z}, 0 [0, 0, u]$
$y+1/2, 1/2, \bar{z}+1/2 [0, u, 0]$	$\bar{y}+1/2, 1/2, \bar{z}+1/2 [0, \bar{u}, 0]$	$y+1/2, 1/2, z+1/2 [0, \bar{u}, 0]$	$\bar{y}+1/2, 1/2, z+1/2 [0, u, 0]$
$1/2, z+1/2, \bar{y}+1/2 [u, 0, 0]$	$1/2, z+1/2, y+1/2 [\bar{u}, 0, 0]$	$1/2, \bar{z}+1/2, \bar{y}+1/2 [\bar{u}, 0, 0]$	$1/2, \bar{z}+1/2, y+1/2 [u, 0, 0]$
$z+1/2, y+1/2, 1/2 [0, 0, \bar{u}]$	$z+1/2, \bar{y}+1/2, 1/2 [0, 0, u]$	$\bar{z}+1/2, y+1/2, 1/2 [0, 0, u]$	$\bar{z}+1/2, \bar{y}+1/2, 1/2 [0, 0, \bar{u}]$
96 h ..2	$1/4, y, y [0, v, v]$	$3/4, \bar{y}, y [0, \bar{v}, v]$	$3/4, y, \bar{y} [0, v, \bar{v}]$
	$y, 1/4, y [v, 0, v]$	$y, 3/4, \bar{y} [v, 0, \bar{v}]$	$\bar{y}, 3/4, y [v, 0, v]$
	$y, y, 1/4 [v, v, 0]$	$\bar{y}, y, 3/4 [v, v, 0]$	$y, \bar{y}, 3/4 [v, v, 0]$
	$3/4, \bar{y}, \bar{y} [0, v, v]$	$1/4, y, \bar{y} [0, \bar{v}, v]$	$1/4, \bar{y}, y [0, v, \bar{v}]$
	$\bar{y}, 3/4, \bar{y} [v, 0, v]$	$\bar{y}, 1/4, y [v, 0, \bar{v}]$	$y, 1/4, \bar{y} [v, 0, v]$
	$\bar{y}, \bar{y}, 3/4 [v, v, 0]$	$y, \bar{y}, 1/4 [v, v, 0]$	$y, y, 3/4 [v, v, 0]$

64 g .3.

$x, x, x [u, u, u]$	$\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$	$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
$x+1/2, x+1/2, \bar{x}+1/2 [u, u, \bar{u}]$	$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, \bar{u}]$	$x+1/2, \bar{x}+1/2, x+1/2 [u, \bar{u}, u]$	$\bar{x}+1/2, x+1/2, x+1/2 [\bar{u}, u, \bar{u}]$
$\bar{x}, \bar{x}, \bar{x} [u, u, u]$	$x, x, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$	$x, \bar{x}, x [\bar{u}, u, \bar{u}]$	$\bar{x}, x, x [u, \bar{u}, \bar{u}]$
$\bar{x}+1/2, \bar{x}+1/2, x+1/2 [u, u, \bar{u}]$	$x+1/2, x+1/2, x+1/2 [\bar{u}, \bar{u}, \bar{u}]$	$\bar{x}+1/2, x+1/2, \bar{x}+1/2 [u, \bar{u}, u]$	$x+1/2, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, u, \bar{u}]$



Continued

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Fm $\bar{3}$ c

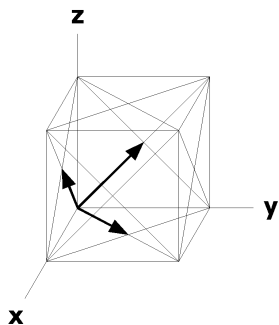
48	f	4..	x,1/4,1/4 [u,0,0]	$\bar{x}$ ,3/4,1/4 [ $\bar{u}$ ,0,0]	1/4,x,1/4 [0,u,0]	1/4, $\bar{x}$ ,3/4 [0, $\bar{u}$ ,0]
			1/4,1/4,x [0,0,u]	3/4,1/4, $\bar{x}$ [0,0, $\bar{u}$ ]	$\bar{x}$ ,3/4,3/4 [u,0,0]	x,1/4,3/4 [ $\bar{u}$ ,0,0]
			3/4, $\bar{x}$ ,3/4 [0,u,0]	3/4,x,1/4 [0, $\bar{u}$ ,0]	3/4,3/4, $\bar{x}$ [0,0,u]	1/4,3/4,x [0,0, $\bar{u}$ ]
48	e	mm2..	x,0,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x}$ ,0 [0,0,0]
			0,0,x [0,0,0]	0,0, $\bar{x}$ [0,0,0]	1/2,x+1/2,1/2 [0,0,0]	1/2, $\bar{x}$ +1/2,1/2 [0,0,0]
			x+1/2,1/2,1/2 [0,0,0]	$\bar{x}$ +1/2,1/2,1/2 [0,0,0]	1/2,1/2, $\bar{x}$ +1/2 [0,0,0]	1/2,1/2,x+1/2 [0,0,0]
24	d	4/m..	0,1/4,1/4 [u,0,0]	0,3/4,1/4 [ $\bar{u}$ ,0,0]	1/4,0,1/4 [0,u,0]	
			1/4,0,3/4 [0, $\bar{u}$ ,0]	1/4,1/4,0 [0,0,u]	3/4,1/4,0 [0,0, $\bar{u}$ ]	
24	c	$\bar{4}$ m.2	1/4,0,0 [0,0,0]	3/4,0,0 [0,0,0]	0,1/4,0 [0,0,0]	
			0,3/4,0 [0,0,0]	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]	
8	b	$m\bar{3}$ .	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
8	a	432	1/4,1/4,1/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]		

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,1,1] p6'm'm  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/4$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



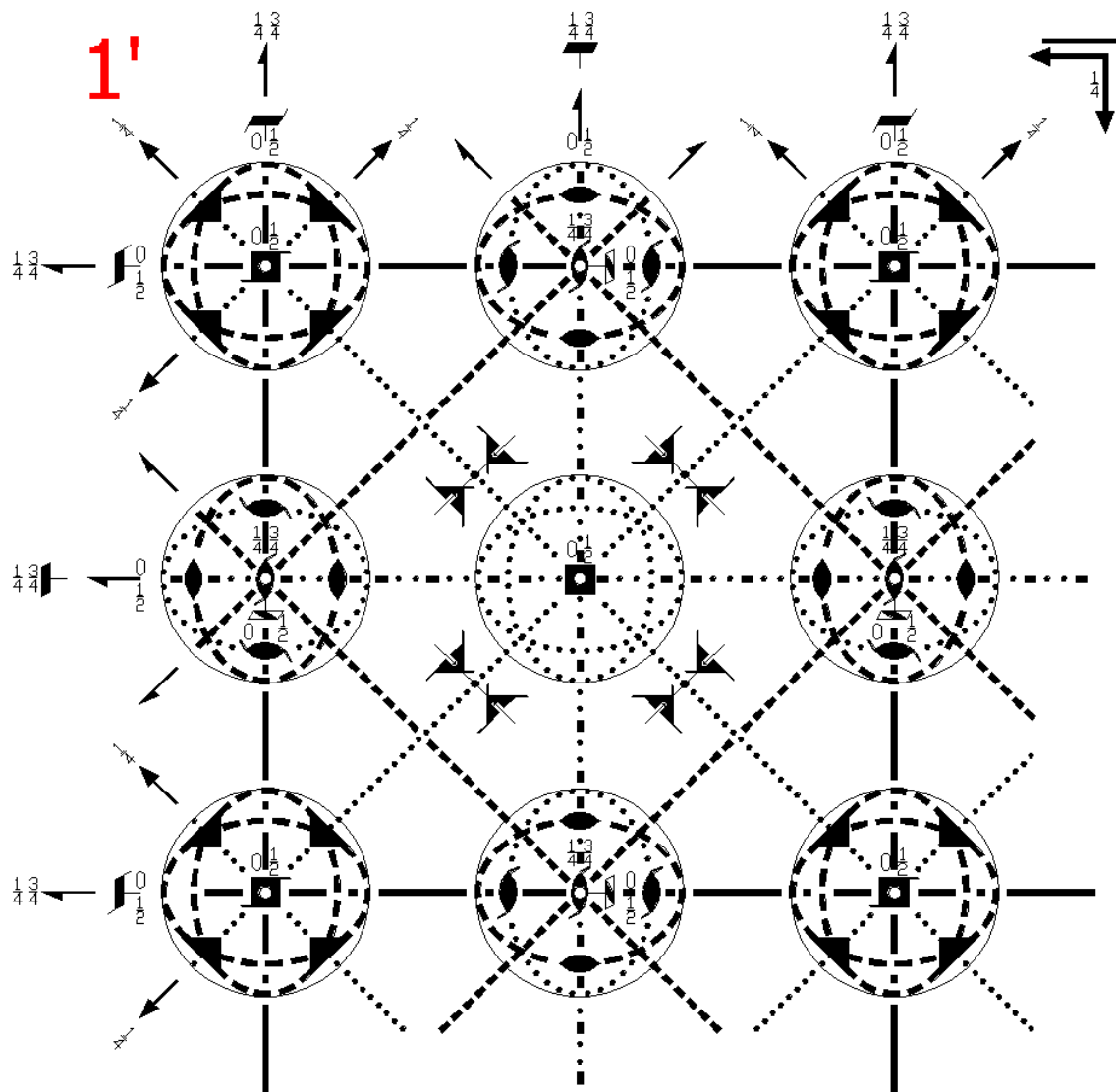
Fm $\bar{3}$ c1'

226.2.1624

m $\bar{3}$ m1'

F4/m $\bar{3}$ 2/c1'

Cubic



Origin at center (m $\bar{3}$ 1')

<b>Asymmetric unit</b>	$0 \leq x \leq 1/2;$	$0 \leq y \leq 1/4;$	$0 \leq z \leq 1/4;$	$y \leq \min(x, 1/2-x);$	$z \leq y$
Vertices	0,0,0	1/2,0,0	1/4,1/4,0	1/4,1/4,1/4	

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |   |
|---|--|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)             | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)                                      | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0) | (12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0)               |

(13) 2 (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)	(14) 2 x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)	(15) 4 <sup>-</sup> (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)	(16) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)
(17) 4 <sup>-</sup> (1/2,0,0) x,1/2,0 (4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,1/2)	(18) 2 (0,1/2,1/2) 1/4,y,y (2 <sub>yz</sub>  1/2,1/2,1/2)	(19) 2 1/4,y+1/2, $\bar{y}$ (2 <sub><math>\bar{yz}</math></sub>  1/2,1/2,1/2)	(20) 4 <sup>+</sup> (1/2,0,0) x,0,1/2 (4 <sub>x</sub>  1/2,1/2,1/2)
(21) 4 <sup>+</sup> (0,1/2,0) 1/2,y,0 (4 <sub>y</sub>  1/2,1/2,1/2)	(22) 2 (1/2,0,1/2) x,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)	(23) 4 <sup>-</sup> (0,1/2,0) 0,y,1/2 (4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,1/2)	(24) 2 $\bar{x}$ +1/2,1/4,x (2 <sub><math>\bar{xz}</math></sub>  1/2,1/2,1/2)
(25) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(26) m x,y,0 (m <sub>z</sub>  0,0,0)	(27) m x,0,z (m <sub>y</sub>  0,0,0)	(28) m 0,y,z (m <sub>x</sub>  0,0,0)
(29) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)	(30) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{\bar{xyz}}$ <sup>-1</sup>  0,0,0)	(31) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{\bar{xyz}}$ <sup>-1</sup>  0,0,0)	(32) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)
(33) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)	(34) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{\bar{xyz}}$  0,0,0)	(35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{\bar{xyz}}$  0,0,0)	(36) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)
(37) c (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,1/2)	(38) n (1/2,1/2,1/2) x,x,z (m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)	(39) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>  1/2,1/2,1/2)	(40) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$  1/2,1/2,1/2)
(41) $\bar{4}^-$ x,0,1/2; 1/4,0,1/2 ( $\bar{4}_x$ <sup>-1</sup>  1/2,1/2,1/2)	(42) a (1/2,0,0) x,y+1/2, $\bar{y}$ (m <sub>yz</sub>  1/2,1/2,1/2)	(43) n (1/2,1/2,1/2) x,y,y (m <sub><math>\bar{yz}</math></sub>  1/2,1/2,1/2)	(44) $\bar{4}^+$ x,1/2,0; 1/4,1/2,0 ( $\bar{4}_x$  1/2,1/2,1/2)
(45) $\bar{4}^+$ 0,y,1/2; 0,1/4,1/2 ( $\bar{4}_y$  1/2,1/2,1/2)	(46) b (0,1/2,0) $\bar{x}$ +1/2,y,x (m <sub>xz</sub>  1/2,1/2,1/2)	(47) $\bar{4}^-$ 1/2,y,0; 1/2,1/4,0 ( $\bar{4}_y$ <sup>-1</sup>  1/2,1/2,1/2)	(48) n (1/2,1/2,1/2) x,y,x (m <sub><math>\bar{xz}</math></sub>  1/2,1/2,1/2)

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2) ( $\bar{1}$  0,1/2,1/2)	(2) 2 (0,0,1/2) 0,1/4,z (2 <sub>z</sub>  0,1/2,1/2)	(3) 2 (0,1/2,0) 0,y,1/4 (2 <sub>y</sub>  0,1/2,1/2)	(4) 2 x,1/4,1/4 (2 <sub>x</sub>  0,1/2,1/2)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x-1/3,x-1/6,x (3 <sub>xyz</sub>  0,1/2,1/2)	(6) 3 <sup>+</sup> $\bar{x}$ ,x+1/2, $\bar{x}$ (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,1/2,1/2)	(7) 3 <sup>+</sup> (-1/3,1/3,1/3) x+1/3, $\bar{x}$ -1/6, $\bar{x}$ (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,1/2,1/2)	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ +1/2,x (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,1/2,1/2)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x-1/6,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(10) 3 <sup>-</sup> (-1/3,1/3,1/3) x+1/6, $\bar{x}$ +1/6, $\bar{x}$ (3 <sub>xyz</sub>  0,1/2,1/2)	(11) 3 <sup>-</sup> $\bar{x}$ +1/2, $\bar{x}$ +1/2,x (3 <sub><math>\bar{xyz}</math></sub>  0,1/2,1/2)	(12) 3 <sup>-</sup> $\bar{x}$ -1/2,x+1/2, $\bar{x}$ (3 <sub>xyz</sub>  0,1/2,1/2)
(13) 2 (1/4,1/4,0) x,x-1/4,0 (2 <sub>xy</sub>  1/2,0,0)	(14) 2 (1/4,-1/4,0) x, $\bar{x}$ +1/4,0 (2 <sub><math>\bar{xy}</math></sub>  1/2,0,0)	(15) 4 <sup>-</sup> 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>  1/2,0,0)	(16) 4 <sup>+</sup> 1/4,1/4,z (4 <sub>z</sub>  1/2,0,0)
(17) 4 <sup>-</sup> (1/2,0,0) x,0,0 (4 <sub>x</sub> <sup>-1</sup>  1/2,0,0)	(18) 2 1/4,y,y (2 <sub>yz</sub>  1/2,0,0)	(19) 2 1/4,y, $\bar{y}$ (2 <sub><math>\bar{yz}</math></sub>  1/2,0,0)	(20) 4 <sup>+</sup> (1/2,0,0) x,0,0 (4 <sub>x</sub>  1/2,0,0)
(21) 4 <sup>+</sup> 1/4,y,-1/4 (4 <sub>y</sub>  1/2,0,0)	(22) 2 (1/4,0,1/4) x+1/4,0,x (2 <sub>xz</sub>  1/2,0,0)	(23) 4 <sup>-</sup> 1/4,y,1/4 (4 <sub>y</sub> <sup>-1</sup>  1/2,0,0)	(24) 2 (1/4,0,-1/4) $\bar{x}$ +1/4,0,x (2 <sub><math>\bar{xz}</math></sub>  1/2,0,0)
(25) $\bar{1}$ 0,1/4,1/4 ( $\bar{1}$  0,1/2,1/2)	(26) b (0,1/2,0) x,y,1/4 (m <sub>z</sub>  0,1/2,1/2)	(27) c (0,0,1/2) x,1/4,z (m <sub>y</sub>  0,1/2,1/2)	(28) n (0,1/2,1/2) 0,y,z (m <sub>x</sub>  0,1/2,1/2)
(29) $\bar{3}^+$ x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$  0,1/2,1/2)	(30) $\bar{3}^+$ $\bar{x}$ -1,x+1/2, $\bar{x}$ ; -1/2,0,1/2 ( $\bar{3}_{\bar{xyz}}$ <sup>-1</sup>  0,1/2,1/2)	(31) $\bar{3}^+$ x, $\bar{x}$ +1/2, $\bar{x}$ ; 0,1/2,0 ( $\bar{3}_{\bar{xyz}}$ <sup>-1</sup>  0,1/2,1/2)	(32) $\bar{3}^+$ $\bar{x}$ -1, $\bar{x}$ +1/2,x; 1/2,0,1/2 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,1/2,1/2)

(33) $\bar{3}^-$ x-1/2,x-1/2,x; 0,0,1/2 ( $\bar{3}_{xyz}^{-1}$  0,1/2,1/2)	(34) $\bar{3}^-$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ; 0,0,1/2 ( $\bar{3}_{\bar{xyz}}$  0,1/2,1/2)	(35) $\bar{3}^-$ $\bar{x}$ -1/2, $\bar{x}$ +1/2, x; -1/2,1/2,0 ( $\bar{3}_{\bar{yz}}$  0,1/2,1/2)	(36) $\bar{3}^-$ $\bar{x}$ +1/2, x+1/2, $\bar{x}$ ; 1/2,1/2,0 ( $\bar{3}_{\bar{yz}}$  0,1/2,1/2)
(37) g (1/4,-1/4,0) x+1/4, $\bar{x}$ ,z ( $m_{xy}$  1/2,0,0)	(38) g (1/4,1/4,0) x+1/4,x,z ( $m_{\bar{xy}}$  1/2,0,0)	(39) $\bar{4}^-$ 1/4,1/4,z; 1/4,1/4,0 ( $\bar{4}_z^{-1}$  1/2,0,0)	(40) $\bar{4}^+$ 1/4,-1/4,z; 1/4,-1/4,0 ( $\bar{4}_z$  1/2,0,0)
(41) $\bar{4}^-$ x,0,0; 1/4,0,0 ( $\bar{4}_x^{-1}$  1/2,0,0)	(42) a (1/2,0,0) x,y, $\bar{y}$ ( $m_{yz}$  1/2,0,0)	(43) a (1/2,0,0) x,y,y ( $m_{\bar{yz}}$  1/2,0,0)	(44) $\bar{4}^+$ x,0,0; 1/4,0,0 ( $\bar{4}_x$  1/2,0,0)
(45) $\bar{4}^+$ 1/4,y,1/4; 1/4,0,1/4 ( $\bar{4}_y$  1/2,0,0)	(46) g (1/4,0,-1/4) $\bar{x}$ +1/4,y,x ( $m_{xz}$  1/2,0,0)	(47) $\bar{4}^-$ 1/4,y,-1/4; 1/4,0,-1/4 ( $\bar{4}_y^{-1}$  1/2,0,0)	(48) g (1/4,0,1/4) x+1/4,y,x ( $m_{\bar{xz}}$  1/2,0,0)

For (1/2,0,1/2) + set

(1) t (1/2,0,1/2) (1 1/2,0,1/2)	(2) 2 (0,0,1/2) 1/4,0,z (2 $_z$  1/2,0,1/2)	(3) 2 1/4,y,1/4 (2 $_y$  1/2,0,1/2)	(4) 2 (1/2,0,0) x,0,1/4 (2 $_x$  1/2,0,1/2)
(5) $3^+$ (1/3,1/3,1/3) x+1/6,x-1/6,x ( $3_{xyz}$  1/2,0,1/2)	(6) $3^+$ (1/3,-1/3,1/3) x+1/6,x+1/6, $\bar{x}$ ( $3_{\bar{xyz}^{-1}}$  1/2,0,1/2)	(7) $3^+$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ( $3_{\bar{yz}^{-1}}$  1/2,0,1/2)	(8) $3^+$ $\bar{x}$ +1/2, $\bar{x}$ +1/2,x ( $3_{\bar{yz}^{-1}}$  1/2,0,1/2)
(9) $3^-$ (1/3,1/3,1/3) x-1/6,x-1/3,x ( $3_{xyz}^{-1}$  1/2,0,1/2)	(10) $3^-$ x+1/2, $\bar{x}$ , $\bar{x}$ ( $3_{\bar{yz}}$  1/2,0,1/2)	(11) $3^-$ $\bar{x}$ +1/2, $\bar{x}$ , x ( $3_{\bar{yz}}$  1/2,0,1/2)	(12) $3^-$ (1/3,-1/3,1/3) $\bar{x}$ -1/6, x+1/3, $\bar{x}$ ( $3_{\bar{yz}}$  1/2,0,1/2)
(13) 2 (1/4,1/4,0) x,x+1/4,0 (2 $_{xy}$  0,1/2,0)	(14) 2 (-1/4,1/4,0) x, $\bar{x}$ +1/4,0 (2 $_{\bar{xy}}$  0,1/2,0)	(15) $4^-$ 1/4,1/4,z ( $4_z^{-1}$  0,1/2,0)	(16) $4^+$ -1/4,1/4,z ( $4_z$  0,1/2,0)
(17) $4^-$ x,1/4,-1/4 ( $4_x^{-1}$  0,1/2,0)	(18) 2 (0,1/4,1/4) 0,y+1/4,y (2 $_{yz}$  0,1/2,0)	(19) 2 (0,1/4,-1/4) 0,y+1/4, $\bar{y}$ (2 $_{\bar{yz}}$  0,1/2,0)	(20) $4^+$ x,1/4,1/4 ( $4_x$  0,1/2,0)
(21) $4^+$ (0,1/2,0) 0,y,0 ( $4_y$  0,1/2,0)	(22) 2 x,1/4,x (2 $_{xz}$  0,1/2,0)	(23) $4^-$ (0,1/2,0) 0,y,0 ( $4_y^{-1}$  0,1/2,0)	(24) 2 $\bar{x}$ ,1/4,x (2 $_{\bar{xz}}$  0,1/2,0)
(25) $\bar{1}$ 1/4,0,1/4 ( $\bar{1}$  1/2,0,1/2)	(26) a (1/2,0,0) x,y,1/4 ( $m_z$  1/2,0,1/2)	(27) n (1/2,0,1/2) x,0,z ( $m_y$  1/2,0,1/2)	(28) c (0,0,1/2) 1/4,y,z ( $m_x$  1/2,0,1/2)
(29) $\bar{3}^+$ x-1/2,x-1/2,x; 0,0,1/2 ( $\bar{3}_{xyz}$  1/2,0,1/2)	(30) $\bar{3}^+$ $\bar{x}$ -1/2,x+1/2, $\bar{x}$ ; 0,0,1/2 ( $\bar{3}_{\bar{xyz}^{-1}}$  1/2,0,1/2)	(31) $\bar{3}^+$ x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ; 1/2,1/2,0 ( $\bar{3}_{\bar{yz}^{-1}}$  1/2,0,1/2)	(32) $\bar{3}^+$ $\bar{x}$ +1/2, $\bar{x}$ -1/2,x; 1/2,-1/2,0 ( $\bar{3}_{\bar{yz}^{-1}}$  1/2,0,1/2)
(33) $\bar{3}^-$ x+1/2,x,x; 1/2,0,0 ( $\bar{3}_{xyz}^{-1}$  1/2,0,1/2)	(34) $\bar{3}^-$ x+1/2, $\bar{x}$ -1, $\bar{x}$ ; 0,-1/2,1/2 ( $\bar{3}_{\bar{yz}}$  1/2,0,1/2)	(35) $\bar{3}^-$ $\bar{x}$ +1/2, $\bar{x}$ +1, x; 0,1/2,1/2 ( $\bar{3}_{\bar{yz}}$  1/2,0,1/2)	(36) $\bar{3}^-$ $\bar{x}$ +1/2, x, $\bar{x}$ ; 1/2,0,0 ( $\bar{3}_{\bar{yz}}$  1/2,0,1/2)
(37) g (-1/4,1/4,0) x+1/4, $\bar{x}$ ,z ( $m_{xy}$  0,1/2,0)	(38) g (1/4,1/4,0) x-1/4,x,z ( $m_{\bar{xy}}$  0,1/2,0)	(39) $\bar{4}^-$ -1/4,1/4,z; -1/4,1/4,0 ( $\bar{4}_z^{-1}$  0,1/2,0)	(40) $\bar{4}^+$ 1/4,1/4,z; 1/4,1/4,0 ( $\bar{4}_z$  0,1/2,0)
(41) $\bar{4}^-$ x,1/4,1/4; 0,1/4,1/4 ( $\bar{4}_x^{-1}$  0,1/2,0)	(42) g (0,1/4,-1/4) x,y+1/4, $\bar{y}$ ( $m_{yz}$  0,1/2,0)	(43) g (0,1/4,1/4) x,y+1/4,y ( $m_{\bar{yz}}$  0,1/2,0)	(44) $\bar{4}^+$ x,1/4,-1/4; 0,1/4,-1/4 ( $\bar{4}_x$  0,1/2,0)
(45) $\bar{4}^+$ 0,y,0; 0,1/4,0 ( $\bar{4}_y$  0,1/2,0)	(46) b (0,1/2,0) $\bar{x}$ ,y,x ( $m_{xz}$  0,1/2,0)	(47) $\bar{4}^-$ 0,y,0; 0,1/4,0 ( $\bar{4}_y^{-1}$  0,1/2,0)	(48) b (0,1/2,0) x,y,x ( $m_{\bar{xz}}$  0,1/2,0)

## For (1/2,1/2,0) + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t$ (1/2,1/2,0)<br>(1   1/2,1/2,0)   | (2) $2$ 1/4,1/4,z<br>(2 <sub>z</sub>   1/2,1/2,0)   | (3) $2$ (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>   1/2,1/2,0)   | (4) $2$ (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>   1/2,1/2,0)   |
| (5) $3^+$ (1/3,1/3,1/3)<br>x+1/6,x+1/3,x<br>(3 <sub>xyz</sub>   1/2,1/2,0)               | (6) $3^+$ $\bar{x}$ +1/2,x, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)                         | (7) $3^+$ x+1/2, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)                          | (8) $3^+$ (1/3,1/3,-1/3)<br>x+1/6,x+1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)                 |
| (9) $3^-$ (1/3,1/3,1/3)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0) | (10) $3^-$ x, $\bar{x}$ +1/2, $\bar{x}$<br>(3 <sub>xyz</sub>   1/2,1/2,0)                                     | (11) $3^-$ (1/3,1/3,-1/3)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub>   1/2,1/2,0)                                    | (12) $3^-$ $\bar{x}$ ,x+1/2, $\bar{x}$<br>(3 <sub>xyz</sub>   1/2,1/2,0)                                  |
| (13) $2$ x,x,1/4<br>(2 <sub>xy</sub>   0,0,1/2)  | (14) $2$ x, $\bar{x}$ ,1/4<br>(2 <sub>xy</sub>   0,0,1/2)   | (15) $4^-$ (0,0,1/2) 0,0,z<br>(4 <sub>z</sub> <sup>-1</sup>   0,0,1/2)  | (16) $4^+$ (0,0,1/2) 0,0,z<br>(4 <sub>z</sub>   0,0,1/2)  |
| (17) $4^-$ x,1/4,1/4<br>(4 <sub>x</sub> <sup>-1</sup>   0,0,1/2)                         | (18) $2$ (0,1/4,1/4) 0,y-1/4,y<br>(2 <sub>yz</sub>   0,0,1/2)   | (19) $2$ (0,-1/4,1/4) 0,y+1/4, $\bar{y}$<br>(2 <sub>yz</sub>   0,0,1/2)   | (20) $4^+$ x,-1/4,1/4<br>(4 <sub>x</sub>   0,0,1/2)   |
| (21) $4^+$ 1/4,y,1/4<br>(4 <sub>y</sub>   0,0,1/2)                                       | (22) $2$ (1/4,0,1/4) x-1/4,0,x<br>(2 <sub>xz</sub>   0,0,1/2)   | (23) $4^-$ -1/4,y,1/4<br>(4 <sub>y</sub> <sup>-1</sup>   0,0,1/2)   | (24) $2$ (-1/4,0,1/4) $\bar{x}$ +1/4,0,x<br>(2 <sub>xz</sub>   0,0,1/2)                                   |
| (25) $\bar{1}$ 1/4,1/4,0<br>(1   1/2,1/2,0)  | (26) $n$ (1/2,1/2,0) x,y,0<br>(m <sub>z</sub>   1/2,1/2,0)  | (27) $a$ (1/2,0,0) x,1/4,z<br>(m <sub>y</sub>   1/2,1/2,0)  | (28) $b$ (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>   1/2,1/2,0)  |
| (29) $\bar{3}^+$ x+1/2,x,x;<br>1/2,0,0<br>(3 <sub>xyz</sub>   1/2,1/2,0)                 | (30) $\bar{3}^+$ $\bar{x}$ -1/2,x+1, $\bar{x}$ ;<br>0,1/2,1/2<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0) | (31) $\bar{3}^+$ x-1/2, $\bar{x}$ +1, $\bar{x}$ ;<br>0,1/2,-1/2<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0) | (32) $\bar{3}^+$ $\bar{x}$ +1/2, $\bar{x}$ ,x;<br>1/2,0,0<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0) |
| (33) $\bar{3}^-$ x,x+1/2,x;<br>0,1/2,0<br>(3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)   | (34) $\bar{3}^-$ x+1, $\bar{x}$ -1/2, $\bar{x}$ ;<br>1/2,0,1/2<br>(3 <sub>xyz</sub>   1/2,1/2,0)              | (35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ +1/2,x;<br>0,1/2,0<br>(3 <sub>xyz</sub>   1/2,1/2,0)                     | (36) $\bar{3}^-$ $\bar{x}$ +1,x-1/2, $\bar{x}$ ;<br>1/2,0,-1/2<br>(3 <sub>xyz</sub>   1/2,1/2,0)          |
| (37) $c$ (0,0,1/2) x, $\bar{x}$ ,z<br>(m <sub>xy</sub>   0,0,1/2)                        | (38) $c$ (0,0,1/2) x,x,z<br>(m <sub>xy</sub>   0,0,1/2)   | (39) $\bar{4}^-$ 0,0,z; 0,0,1/4<br>(4 <sub>z</sub> <sup>-1</sup>   0,0,1/2)                                     | (40) $\bar{4}^+$ 0,0,z; 0,0,1/4<br>(4 <sub>z</sub>   0,0,1/2)   |
| (41) $\bar{4}^-$ x,-1/4,1/4; 0,-1/4,1/4<br>(4 <sub>x</sub> <sup>-1</sup>   0,0,1/2)      | (42) $g$ (0,-1/4,1/4) x,y+1/4, $\bar{y}$<br>(m <sub>yz</sub>   0,0,1/2)                                       | (43) $g$ (0,1/4,1/4) x,y-1/4,y<br>(m <sub>yz</sub>   0,0,1/2)   | (44) $\bar{4}^+$ x,1/4,1/4; 0,1/4,1/4<br>(4 <sub>x</sub>   0,0,1/2)                                       |
| (45) $\bar{4}^+$ -1/4,y,1/4; -1/4,0,1/4<br>(4 <sub>y</sub>   0,0,1/2)                    | (46) $g$ (-1/4,0,1/4) $\bar{x}$ +1/4,y,x<br>(m <sub>xz</sub>   0,0,1/2)                                       | (47) $\bar{4}^-$ 1/4,y,1/4; 1/4,0,1/4<br>(4 <sub>y</sub> <sup>-1</sup>   0,0,1/2)                               | (48) $g$ (1/4,0,1/4) x-1/4,y,x<br>(m <sub>xz</sub>   0,0,1/2)   |

## For (0,0,0)' + set

- |   |  |   |   |
|---|--|---|---|
| (1) $1'$<br>(1   0,0,0)'  | (2) $2'$ 0,0,z<br>(2 <sub>z</sub>   0,0,0)'                                      | (3) $2'$ 0,y,0<br>(2 <sub>y</sub>   0,0,0)'                                       | (4) $2'$ x,0,0<br>(2 <sub>x</sub>   0,0,0)'                                       |
| (5) $3^+$ ' x,x,x<br>(3 <sub>xyz</sub>   0,0,0)'                                | (6) $3^+$ ' $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   0,0,0)' | (7) $3^+$ ' x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>   0,0,0)' | (8) $3^+$ ' $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   0,0,0)' |
| (9) $3^-$ ' x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>   0,0,0)'                  | (10) $3^-$ ' x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub>   0,0,0)'             | (11) $3^-$ ' $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>xyz</sub>   0,0,0)'              | (12) $3^-$ ' $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub>xyz</sub>   0,0,0)'               |
| (13) $2'$ (1/2,1/2,0) x,x,1/4<br>(2 <sub>xy</sub>   1/2,1/2,1/2)'               | (14) $2'$ x, $\bar{x}$ +1/2,1/4<br>(2 <sub>xy</sub>   1/2,1/2,1/2)'              | (15) $4^-$ ' (0,0,1/2) 1/2,0,z<br>(4 <sub>z</sub> <sup>-1</sup>   1/2,1/2,1/2)'   | (16) $4^+$ ' (0,0,1/2) 0,1/2,z<br>(4 <sub>z</sub>   1/2,1/2,1/2)'                 |
| (17) $4^-$ ' (1/2,0,0) x,1/2,0<br>(4 <sub>x</sub> <sup>-1</sup>   1/2,1/2,1/2)' | (18) $2'$ (0,1/2,1/2) 1/4,y,y<br>(2 <sub>yz</sub>   1/2,1/2,1/2)'                | (19) $2'$ 1/4,y+1/2, $\bar{y}$<br>(2 <sub>yz</sub>   1/2,1/2,1/2)'                | (20) $4^+$ ' (1/2,0,0) x,0,1/2<br>(4 <sub>x</sub>   1/2,1/2,1/2)'                 |

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|--|--|---|---|
| (21) $4^+ ' (0, 1/2, 0) \ 1/2, y, 0$<br>( $4_y   1/2, 1/2, 1/2$ )'                     | (22) $2' (1/2, 0, 1/2) \ x, 1/4, x$<br>( $2_{xz}   1/2, 1/2, 1/2$ )'                                   | (23) $4^- ' (0, 1/2, 0) \ 0, y, 1/2$<br>( $4_y^{-1}   1/2, 1/2, 1/2$ )'                               | (24) $2' \ \bar{x} + 1/2, 1/4, x$<br>( $2_{\bar{z}}   1/2, 1/2, 1/2$ )'                               |
| (25) $\bar{1}' \ 0, 0, 0$<br>( $\bar{1}   0, 0, 0$ )'                                  | (26) $m' \ x, y, 0$<br>( $m_z   0, 0, 0$ )'  | (27) $m' \ x, 0, z$<br>( $m_y   0, 0, 0$ )'   | (28) $m' \ 0, y, z$<br>( $m_x   0, 0, 0$ )'   |
| (29) $\bar{3}^+ ' \ x, x, x; \ 0, 0, 0$<br>( $\bar{3}_{xyz}   0, 0, 0$ )'              | (30) $\bar{3}^+ ' \ \bar{x}, x, \bar{x}; \ 0, 0, 0$<br>( $\bar{3}_{x\bar{y}\bar{z}}^{-1}   0, 0, 0$ )' | (31) $\bar{3}^+ ' \ x, \bar{x}, \bar{x}; \ 0, 0, 0$<br>( $\bar{3}_{\bar{y}\bar{z}}^{-1}   0, 0, 0$ )' | (32) $\bar{3}^+ ' \ \bar{x}, \bar{x}, x; \ 0, 0, 0$<br>( $\bar{3}_{\bar{y}\bar{z}}^{-1}   0, 0, 0$ )' |
| (33) $\bar{3}^- ' \ x, x, x; \ 0, 0, 0$<br>( $\bar{3}_{xyz}^{-1}   0, 0, 0$ )'         | (34) $\bar{3}^- ' \ x, \bar{x}, \bar{x}; \ 0, 0, 0$<br>( $\bar{3}_{\bar{y}\bar{z}}   0, 0, 0$ )'       | (35) $\bar{3}^- ' \ \bar{x}, \bar{x}, x; \ 0, 0, 0$<br>( $\bar{3}_{\bar{y}\bar{z}}   0, 0, 0$ )'      | (36) $\bar{3}^- ' \ \bar{x}, x, \bar{x}; \ 0, 0, 0$<br>( $\bar{3}_{\bar{y}\bar{z}}   0, 0, 0$ )'      |
| (37) $c' (0, 0, 1/2) \ x + 1/2, \bar{x}, z$<br>( $m_{xy}   1/2, 1/2, 1/2$ )'           | (38) $n' (1/2, 1/2, 1/2) \ x, x, z$<br>( $m_{\bar{xy}}   1/2, 1/2, 1/2$ )'                             | (39) $\bar{4}^- ' \ 0, 1/2, z; \ 0, 1/2, 1/4$<br>( $\bar{4}_z^{-1}   1/2, 1/2, 1/2$ )'                | (40) $\bar{4}^+ ' \ 1/2, 0, z; \ 1/2, 0, 1/4$<br>( $\bar{4}_z   1/2, 1/2, 1/2$ )'                     |
| (41) $\bar{4}^- ' \ x, 0, 1/2; \ 1/4, 0, 1/2$<br>( $\bar{4}_x^{-1}   1/2, 1/2, 1/2$ )' | (42) $a' (1/2, 0, 0) \ x, y + 1/2, \bar{y}$<br>( $m_{yz}   1/2, 1/2, 1/2$ )'                           | (43) $n' (1/2, 1/2, 1/2) \ x, y, y$<br>( $m_{\bar{yz}}   1/2, 1/2, 1/2$ )'                            | (44) $\bar{4}^+ ' \ x, 1/2, 0; \ 1/4, 1/2, 0$<br>( $\bar{4}_x   1/2, 1/2, 1/2$ )'                     |
| (45) $\bar{4}^+ ' \ 0, y, 1/2; \ 0, 1/4, 1/2$<br>( $\bar{4}_y   1/2, 1/2, 1/2$ )'      | (46) $b' (0, 1/2, 0) \ \bar{x} + 1/2, y, x$<br>( $m_{xz}   1/2, 1/2, 1/2$ )'                           | (47) $\bar{4}^- ' \ 1/2, y, 0; \ 1/2, 1/4, 0$<br>( $\bar{4}_y^{-1}   1/2, 1/2, 1/2$ )'                | (48) $n' (1/2, 1/2, 1/2) \ x, y, x$<br>( $m_{\bar{z}}   1/2, 1/2, 1/2$ )'                             |

For (0, 1/2, 1/2)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t' (0, 1/2, 1/2)$<br>( $\bar{1}   0, 1/2, 1/2$ )'  | (2) $2' (0, 0, 1/2) \ 0, 1/4, z$<br>( $2_z   0, 1/2, 1/2$ )'   | (3) $2' (0, 1/2, 0) \ 0, y, 1/4$<br>( $2_y   0, 1/2, 1/2$ )'   | (4) $2' \ x, 1/4, 1/4$<br>( $2_x   0, 1/2, 1/2$ )'   |
| (5) $3^+ ' (1/3, 1/3, 1/3)$<br>$x - 1/3, x - 1/6, x$<br>( $3_{xyz}   0, 1/2, 1/2$ )'                | (6) $3^+ ' \ \bar{x}, x + 1/2, \bar{x}$<br>( $3_{x\bar{y}\bar{z}}^{-1}   0, 1/2, 1/2$ )'                                     | (7) $3^+ ' (-1/3, 1/3, 1/3)$<br>$x + 1/3, x - 1/6, \bar{x}$<br>( $3_{\bar{y}\bar{z}}^{-1}   0, 1/2, 1/2$ )'              | (8) $3^+ ' \ \bar{x}, \bar{x} + 1/2, x$<br>( $3_{x\bar{y}\bar{z}}^{-1}   0, 1/2, 1/2$ )'                                   |
| (9) $3^- ' (1/3, 1/3, 1/3)$<br>$x - 1/6, x + 1/6, x$<br>( $3_{xyz}^{-1}   0, 1/2, 1/2$ )'           | (10) $3^- ' (-1/3, 1/3, 1/3)$<br>$x + 1/6, x + 1/6, \bar{x}$<br>( $3_{\bar{y}\bar{z}}   0, 1/2, 1/2$ )'                      | (11) $3^- ' \ \bar{x} + 1/2, \bar{x} + 1/2, x$<br>( $3_{x\bar{y}\bar{z}}   0, 1/2, 1/2$ )'                               | (12) $3^- ' \ \bar{x} - 1/2, x + 1/2, \bar{x}$<br>( $3_{\bar{y}\bar{z}}   0, 1/2, 1/2$ )'                                  |
| (13) $2' (1/4, 1/4, 0) \ x, x - 1/4, 0$<br>( $2_{xy}   1/2, 0, 0$ )'                                | (14) $2' (1/4, -1/4, 0) \ x, \bar{x} + 1/4, 0$<br>( $2_{\bar{xy}}   1/2, 0, 0$ )'  | (15) $4^- ' \ 1/4, -1/4, z$<br>( $4_z^{-1}   1/2, 0, 0$ )'   | (16) $4^+ ' \ 1/4, 1/4, z$<br>( $4_z   1/2, 0, 0$ )'   |
| (17) $4^- ' (1/2, 0, 0) \ x, 0, 0$<br>( $4_x^{-1}   1/2, 0, 0$ )'                                   | (18) $2' \ 1/4, y, y$<br>( $2_{yz}   1/2, 0, 0$ )'   | (19) $2' \ 1/4, y, \bar{y}$<br>( $2_{\bar{yz}}   1/2, 0, 0$ )'   | (20) $4^+ ' (1/2, 0, 0) \ x, 0, 0$<br>( $4_x   1/2, 0, 0$ )'   |
| (21) $4^+ ' \ 1/4, y, -1/4$<br>( $4_y   1/2, 0, 0$ )'   | (22) $2' (1/4, 0, 1/4) \ x + 1/4, 0, x$<br>( $2_{xz}   1/2, 0, 0$ )'   | (23) $4^- ' \ 1/4, y, 1/4$<br>( $4_y^{-1}   1/2, 0, 0$ )'  | (24) $2' (1/4, 0, -1/4) \ \bar{x} + 1/4, 0, x$<br>( $2_{\bar{z}}   1/2, 0, 0$ )'   |
| (25) $\bar{1}' \ 0, 1/4, 1/4$<br>( $\bar{1}   0, 1/2, 1/2$ )'                                       | (26) $b' (0, 1/2, 0) \ x, y, 1/4$<br>( $m_z   0, 1/2, 1/2$ )'  | (27) $c' (0, 0, 1/2) \ x, 1/4, z$<br>( $m_y   0, 1/2, 1/2$ )'  | (28) $n' (0, 1/2, 1/2) \ 0, y, z$<br>( $m_x   0, 1/2, 1/2$ )'  |
| (29) $\bar{3}^+ ' \ x, x + 1/2, x;$<br>$0, 1/2, 0$<br>( $\bar{3}_{xyz}   0, 1/2, 1/2$ )'            | (30) $\bar{3}^+ ' \ \bar{x} - 1, x + 1/2, \bar{x};$<br>$-1/2, 0, 1/2$<br>( $\bar{3}_{x\bar{y}\bar{z}}^{-1}   0, 1/2, 1/2$ )' | (31) $\bar{3}^+ ' \ x, \bar{x} + 1/2, \bar{x};$<br>$0, 1/2, 0$<br>( $\bar{3}_{\bar{y}\bar{z}}^{-1}   0, 1/2, 1/2$ )'     | (32) $\bar{3}^+ ' \ \bar{x} - 1, \bar{x} + 1/2, x;$<br>$1/2, 0, 1/2$<br>( $\bar{3}_{\bar{y}\bar{z}}^{-1}   0, 1/2, 1/2$ )' |
| (33) $\bar{3}^- ' \ x - 1/2, x - 1/2, x;$<br>$0, 0, 1/2$<br>( $\bar{3}_{xyz}^{-1}   0, 1/2, 1/2$ )' | (34) $\bar{3}^- ' \ x + 1/2, \bar{x} - 1/2, \bar{x};$<br>$0, 0, 1/2$<br>( $\bar{3}_{\bar{y}\bar{z}}   0, 1/2, 1/2$ )'        | (35) $\bar{3}^- ' \ \bar{x} - 1/2, \bar{x} + 1/2, x;$<br>$-1/2, 1/2, 0$<br>( $\bar{3}_{\bar{y}\bar{z}}   0, 1/2, 1/2$ )' | (36) $\bar{3}^- ' \ \bar{x} + 1/2, x + 1/2, \bar{x};$<br>$1/2, 1/2, 0$<br>( $\bar{3}_{\bar{y}\bar{z}}   0, 1/2, 1/2$ )'    |
| (37) $g' (1/4, -1/4, 0) \ x + 1/4, \bar{x}, z$<br>( $m_{xy}   1/2, 0, 0$ )'                         | (38) $g' (1/4, 1/4, 0) \ x + 1/4, x, z$<br>( $m_{\bar{xy}}   1/2, 0, 0$ )'   | (39) $\bar{4}^- ' \ 1/4, 1/4, z; \ 1/4, 1/4, 0$<br>( $\bar{4}_z^{-1}   1/2, 0, 0$ )'                                     | (40) $\bar{4}^+ ' \ 1/4, -1/4, z; \ 1/4, -1/4, 0$<br>( $\bar{4}_z   1/2, 0, 0$ )'  |

- (41)  $\bar{4}^- ' x,0,0; 1/4,0,0$   
( $\bar{4}_x^{-1} | 1/2,0,0$ )'
- (42)  $a' (1/2,0,0) x,y,\bar{y}$   
( $m_{yz} | 1/2,0,0$ )'
- (43)  $a' (1/2,0,0) x,y,y$   
( $m_{\bar{y}z} | 1/2,0,0$ )'
- (44)  $\bar{4}^+ ' x,0,0; 1/4,0,0$   
( $\bar{4}_x | 1/2,0,0$ )'
- (45)  $\bar{4}^+ ' 1/4,y,1/4; 1/4,0,1/4$   
( $\bar{4}_y | 1/2,0,0$ )'
- (46)  $g' (1/4,0,-1/4) \bar{x}+1/4,y,x$   
( $m_{xz} | 1/2,0,0$ )'
- (47)  $\bar{4}^- ' 1/4,y,-1/4; 1/4,0,-1/4$   
( $\bar{4}_y^{-1} | 1/2,0,0$ )'
- (48)  $g' (1/4,0,1/4) x+1/4,y,x$   
( $m_{\bar{x}z} | 1/2,0,0$ )'
- For (1/2,0,1/2)' + set
- (1)  $t' (1/2,0,1/2)$   
( $1 | 1/2,0,1/2$ )'
- (2)  $2' (0,0,1/2) 1/4,0,z$   
( $2_z | 1/2,0,1/2$ )'
- (3)  $2' 1/4,y,1/4$   
( $2_y | 1/2,0,1/2$ )'
- (4)  $2' (1/2,0,0) x,0,1/4$   
( $2_x | 1/2,0,1/2$ )'
- (5)  $3^+ ' (1/3,1/3,1/3)$   
 $x+1/6,x-1/6,x$   
( $3_{xyz} | 1/2,0,1/2$ )'
- (6)  $3^+ ' (1/3,-1/3,1/3)$   
 $\bar{x}+1/6,x+1/6,\bar{x}$   
( $3_{x\bar{y}z}^{-1} | 1/2,0,1/2$ )'
- (7)  $3^+ ' x+1/2,\bar{x}-1/2,\bar{x}$   
( $3_{\bar{y}z}^{-1} | 1/2,0,1/2$ )'
- (8)  $3^+ ' \bar{x}+1/2,\bar{x}+1/2,x$   
( $3_{xy\bar{z}}^{-1} | 1/2,0,1/2$ )'
- (9)  $3^- ' (1/3,1/3,1/3)$   
 $x-1/6,x-1/3,x$   
( $3_{xyz}^{-1} | 1/2,0,1/2$ )'
- (10)  $3^- ' x+1/2,\bar{x},\bar{x}$   
( $3_{\bar{y}z} | 1/2,0,1/2$ )'
- (11)  $3^- ' \bar{x}+1/2,\bar{x},x$   
( $3_{xy\bar{z}} | 1/2,0,1/2$ )'
- (12)  $3^- ' (1/3,-1/3,1/3)$   
 $\bar{x}-1/6,x+1/3,\bar{x}$   
( $3_{x\bar{y}z} | 1/2,0,1/2$ )'
- (13)  $2' (1/4,1/4,0) x,x+1/4,0$   
( $2_{xy} | 0,1/2,0$ )'
- (14)  $2' (-1/4,1/4,0) x,\bar{x}+1/4,0$   
( $2_{\bar{xy}} | 0,1/2,0$ )'
- (15)  $4^- ' 1/4,1/4,z$   
( $4_z^{-1} | 0,1/2,0$ )'
- (16)  $4^+ ' -1/4,1/4,z$   
( $4_z | 0,1/2,0$ )'
- (17)  $4^- ' x,1/4,-1/4$   
( $4_x^{-1} | 0,1/2,0$ )'
- (18)  $2' (0,1/4,1/4) 0,y+1/4,y$   
( $2_{yz} | 0,1/2,0$ )'
- (19)  $2' (0,1/4,-1/4) 0,y+1/4,\bar{y}$   
( $2_{\bar{y}z} | 0,1/2,0$ )'
- (20)  $4^+ ' x,1/4,1/4$   
( $4_x | 0,1/2,0$ )'
- (21)  $4^+ ' (0,1/2,0) 0,y,0$   
( $4_y | 0,1/2,0$ )'
- (22)  $2' x,1/4,x$   
( $2_{xz} | 0,1/2,0$ )'
- (23)  $4^- ' (0,1/2,0) 0,y,0$   
( $4_y^{-1} | 0,1/2,0$ )'
- (24)  $2' \bar{x},1/4,x$   
( $2_{\bar{x}z} | 0,1/2,0$ )'
- (25)  $\bar{1} ' 1/4,0,1/4$   
( $\bar{1} | 1/2,0,1/2$ )'
- (26)  $a' (1/2,0,0) x,y,1/4$   
( $m_z | 1/2,0,1/2$ )'
- (27)  $n' (1/2,0,1/2) x,0,z$   
( $m_y | 1/2,0,1/2$ )'
- (28)  $c' (0,0,1/2) 1/4,y,z$   
( $m_x | 1/2,0,1/2$ )'
- (29)  $\bar{3}^+ ' x-1/2,x-1/2,x;$   
 $0,0,1/2$   
( $\bar{3}_{xyz} | 1/2,0,1/2$ )'
- (30)  $\bar{3}^+ ' \bar{x}-1/2,x+1/2,\bar{x};$   
 $0,0,1/2$   
( $\bar{3}_{x\bar{y}z}^{-1} | 1/2,0,1/2$ )'
- (31)  $\bar{3}^+ ' x+1/2,\bar{x}+1/2,\bar{x};$   
 $1/2,1/2,0$   
( $\bar{3}_{\bar{y}z}^{-1} | 1/2,0,1/2$ )'
- (32)  $\bar{3}^+ ' \bar{x}+1/2,\bar{x}-1/2,x;$   
 $1/2,-1/2,0$   
( $\bar{3}_{xy\bar{z}}^{-1} | 1/2,0,1/2$ )'
- (33)  $\bar{3}^- ' x+1/2,x,x;$   
 $1/2,0,0$   
( $\bar{3}_{xyz}^{-1} | 1/2,0,1/2$ )'
- (34)  $\bar{3}^- ' x+1/2,\bar{x}-1,\bar{x};$   
 $0,-1/2,1/2$   
( $\bar{3}_{\bar{y}z} | 1/2,0,1/2$ )'
- (35)  $\bar{3}^- ' \bar{x}+1/2,\bar{x}+1,x;$   
 $0,1/2,1/2$   
( $\bar{3}_{xy\bar{z}} | 1/2,0,1/2$ )'
- (36)  $\bar{3}^- ' \bar{x}+1/2,x,\bar{x};$   
 $1/2,0,0$   
( $\bar{3}_{x\bar{y}z} | 1/2,0,1/2$ )'
- (37)  $g' (-1/4,1/4,0) x+1/4,\bar{x},z$   
( $m_{xy} | 0,1/2,0$ )'
- (38)  $g' (1/4,1/4,0) x-1/4,x,z$   
( $m_{\bar{xy}} | 0,1/2,0$ )'
- (39)  $\bar{4}^- ' -1/4,1/4,z; -1/4,1/4,0$   
( $\bar{4}_z^{-1} | 0,1/2,0$ )'
- (40)  $\bar{4}^+ ' 1/4,1/4,z; 1/4,1/4,0$   
( $\bar{4}_z | 0,1/2,0$ )'
- (41)  $\bar{4}^- ' x,1/4,1/4; 0,1/4,1/4$   
( $\bar{4}_x^{-1} | 0,1/2,0$ )'
- (42)  $g' (0,1/4,-1/4) x,y+1/4,\bar{y}$   
( $m_{yz} | 0,1/2,0$ )'
- (43)  $g' (0,1/4,1/4) x,y+1/4,y$   
( $m_{\bar{y}z} | 0,1/2,0$ )'
- (44)  $\bar{4}^+ ' x,1/4,-1/4; 0,1/4,-1/4$   
( $\bar{4}_x | 0,1/2,0$ )'
- (45)  $\bar{4}^+ ' 0,y,0; 0,1/4,0$   
( $\bar{4}_y | 0,1/2,0$ )'
- (46)  $b' (0,1/2,0) \bar{x},y,x$   
( $m_{xz} | 0,1/2,0$ )'
- (47)  $\bar{4}^- ' 0,y,0; 0,1/4,0$   
( $\bar{4}_y^{-1} | 0,1/2,0$ )'
- (48)  $b' (0,1/2,0) x,y,x$   
( $m_{\bar{x}z} | 0,1/2,0$ )'

For (1/2,1/2,0)' + set

- (1)  $t' (1/2,1/2,0)$   
( $1 | 1/2,1/2,0$ )'
- (2)  $2' 1/4,1/4,z$   
( $2_z | 1/2,1/2,0$ )'
- (3)  $2' (0,1/2,0) 1/4,y,0$   
( $2_y | 1/2,1/2,0$ )'
- (4)  $2' (1/2,0,0) x,1/4,0$   
( $2_x | 1/2,1/2,0$ )'
- (5)  $3^+ ' (1/3,1/3,1/3)$   
 $x+1/6,x+1/3,x$   
( $3_{xyz} | 1/2,1/2,0$ )'
- (6)  $3^+ ' \bar{x}+1/2,x,\bar{x}$   
( $3_{x\bar{y}z}^{-1} | 1/2,1/2,0$ )'
- (7)  $3^+ ' x+1/2,\bar{x},\bar{x}$   
( $3_{\bar{y}z}^{-1} | 1/2,1/2,0$ )'
- (8)  $3^+ ' (1/3,1/3,-1/3)$   
 $\bar{x}+1/6,\bar{x}+1/3,\bar{x}$   
( $3_{xy\bar{z}}^{-1} | 1/2,1/2,0$ )'

(9) $3^-$ ' (1/3,1/3,1/3) x+1/3,x+1/6,x ( $3_{xyz}^{-1}$   1/2,1/2,0)'	(10) $3^-$ ' x, $\bar{x}$ +1/2, $\bar{x}$ ( $3_{xyz}^{-1}$   1/2,1/2,0)'	(11) $3^-$ ' (1/3,1/3,-1/3) x+1/3, $\bar{x}$ +1/6, x ( $3_{xyz}^{-1}$   1/2,1/2,0)'	(12) $3^-$ ' $\bar{x}$ , x+1/2, $\bar{x}$ ( $3_{xyz}^{-1}$   1/2,1/2,0)'
(13) $2'$ x,x,1/4 ( $2_{xy}$   0,0,1/2)'	(14) $2'$ x, $\bar{x}$ ,1/4 ( $2_{xy}$   0,0,1/2)'	(15) $4^-$ ' (0,0,1/2) 0,0,z ( $4_z^{-1}$   0,0,1/2)'	(16) $4^+$ ' (0,0,1/2) 0,0,z ( $4_z$   0,0,1/2)'
(17) $4^-$ ' x,1/4,1/4 ( $4_x^{-1}$   0,0,1/2)'	(18) $2'$ (0,1/4,1/4) 0,y-1/4,y ( $2_{yz}$   0,0,1/2)'	(19) $2'$ (0,-1/4,1/4) 0,y+1/4, $\bar{y}$ ( $2_{yz}$   0,0,1/2)'	(20) $4^+$ ' x,-1/4,1/4 ( $4_x$   0,0,1/2)'
(21) $4^+$ ' 1/4,y,1/4 ( $4_y$   0,0,1/2)'	(22) $2'$ (1/4,0,1/4) x-1/4,0,x ( $2_{xz}$   0,0,1/2)'	(23) $4^-$ ' -1/4,y,1/4 ( $4_y^{-1}$   0,0,1/2)'	(24) $2'$ (-1/4,0,1/4) $\bar{x}$ +1/4,0,x ( $2_{xz}$   0,0,1/2)'
(25) $\bar{1}$ ' 1/4,1/4,0 ( $\bar{1}$   1/2,1/2,0)'	(26) n' (1/2,1/2,0) x,y,0 ( $m_z$   1/2,1/2,0)'	(27) a' (1/2,0,0) x,1/4,z ( $m_y$   1/2,1/2,0)'	(28) b' (0,1/2,0) 1/4,y,z ( $m_x$   1/2,1/2,0)'
(29) $\bar{3}^+$ ' x+1/2,x,x; 1/2,0,0 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0)'	(30) $\bar{3}^+$ ' $\bar{x}$ -1/2,x+1, $\bar{x}$ ; 0,1/2,1/2 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0)'	(31) $\bar{3}^+$ ' x-1/2, $\bar{x}$ +1, $\bar{x}$ ; 0,1/2,-1/2 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0)'	(32) $\bar{3}^+$ ' $\bar{x}$ +1/2, $\bar{x}$ ,x; 1/2,0,0 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0)'
(33) $\bar{3}^-$ ' x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0)'	(34) $\bar{3}^-$ ' x+1, $\bar{x}$ -1/2, $\bar{x}$ ; 1/2,0,1/2 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0)'	(35) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ +1/2, x; 0,1/2,0 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0)'	(36) $\bar{3}^-$ ' $\bar{x}$ +1, x-1/2, $\bar{x}$ ; 1/2,0,-1/2 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,0)'
(37) c' (0,0,1/2) x, $\bar{x}$ ,z ( $m_{xy}$   0,0,1/2)'	(38) c' (0,0,1/2) x,x,z ( $m_{xy}$   0,0,1/2)'	(39) $\bar{4}^-$ ' 0,0,z; 0,0,1/4 ( $\bar{4}_z^{-1}$   0,0,1/2)'	(40) $\bar{4}^+$ ' 0,0,z; 0,0,1/4 ( $\bar{4}_z$   0,0,1/2)'
(41) $\bar{4}^-$ ' x,-1/4,1/4; 0,-1/4,1/4 ( $\bar{4}_x^{-1}$   0,0,1/2)'	(42) g' (0,-1/4,1/4) x,y+1/4, $\bar{y}$ ( $m_{yz}$   0,0,1/2)'	(43) g' (0,1/4,1/4) x,y-1/4,y ( $m_{yz}$   0,0,1/2)'	(44) $\bar{4}^+$ ' x,1/4,1/4; 0,1/4,1/4 ( $\bar{4}_x$   0,0,1/2)'
(45) $\bar{4}^+$ ' -1/4,y,1/4; -1/4,0,1/4 ( $\bar{4}_y$   0,0,1/2)'	(46) g' (-1/4,0,1/4) $\bar{x}$ +1/4,y,x ( $m_{xz}$   0,0,1/2)'	(47) $\bar{4}^-$ ' 1/4,y,1/4; 1/4,0,1/4 ( $\bar{4}_y^{-1}$   0,0,1/2)'	(48) g' (1/4,0,1/4) x-1/4,y,x ( $m_{xz}$   0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25); 1'.

### Positions

### Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

192	j	11'	(0,0,0) + (0,0,0)'	(0,1/2,1/2,) + (0,1/2,1/2,)'	(1/2,0,1/2) + (1/2,0,1/2)'	(1/2,1/2,0) + (1/2,1/2,0)'	
(1)	x,y,z [0,0,0]	(2)	$\bar{x}$ , $\bar{y}$ ,z [0,0,0]	(3)	$\bar{x}$ ,y, $\bar{z}$ [0,0,0]	(4)	x, $\bar{y}$ , $\bar{z}$ [0,0,0]
(5)	z,x,y [0,0,0]	(6)	z, $\bar{x}$ , $\bar{y}$ [0,0,0]	(7)	$\bar{z}$ , $\bar{x}$ ,y [0,0,0]	(8)	$\bar{z}$ ,x, $\bar{y}$ [0,0,0]
(9)	y,z,x [0,0,0]	(10)	$\bar{y}$ ,z, $\bar{x}$ [0,0,0]	(11)	y, $\bar{z}$ , $\bar{x}$ [0,0,0]	(12)	$\bar{y}$ , $\bar{z}$ ,x [0,0,0]
(13)	y+1/2,x+1/2, $\bar{z}$ +1/2 [0,0,0]	(14)	$\bar{y}$ +1/2, $\bar{x}$ +1/2, $\bar{z}$ +1/2 [0,0,0]	(15)	y+1/2, $\bar{x}$ +1/2,z+1/2 [0,0,0]	(16)	$\bar{y}$ +1/2,x+1/2,z+1/2 [0,0,0]
(17)	x+1/2,z+1/2, $\bar{y}$ +1/2 [0,0,0]	(18)	$\bar{x}$ +1/2,z+1/2,y+1/2 [0,0,0]	(19)	$\bar{x}$ +1/2, $\bar{z}$ +1/2, $\bar{y}$ +1/2 [0,0,0]	(20)	x+1/2, $\bar{z}$ +1/2,y+1/2 [0,0,0]
(21)	z+1/2,y+1/2, $\bar{x}$ +1/2 [0,0,0]	(22)	z+1/2, $\bar{y}$ +1/2,x+1/2 [0,0,0]	(23)	$\bar{z}$ +1/2,y+1/2,x+1/2 [0,0,0]	(24)	$\bar{z}$ +1/2, $\bar{y}$ +1/2, $\bar{x}$ +1/2 [0,0,0]



(25) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]	(26) $x, y, \bar{z}$ [0,0,0]	(27) $x, \bar{y}, z$ [0,0,0]	(28) $\bar{x}, y, z$ [0,0,0]
(29) $\bar{z}, \bar{x}, \bar{y}$ [0,0,0]	(30) $\bar{z}, x, y$ [0,0,0]	(31) $z, x, \bar{y}$ [0,0,0]	(32) $z, \bar{x}, y$ [0,0,0]
(33) $\bar{y}, \bar{z}, \bar{x}$ [0,0,0]	(34) $y, \bar{z}, x$ [0,0,0]	(35) $\bar{y}, z, x$ [0,0,0]	(36) $y, z, \bar{x}$ [0,0,0]
(37) $\bar{y}+1/2, \bar{x}+1/2, z+1/2$ [0,0,0]	(38) $y+1/2, x+1/2, z+1/2$ [0,0,0]	(39) $\bar{y}+1/2, x+1/2, \bar{z}+1/2$ [0,0,0]	(40) $y+1/2, \bar{x}+1/2, \bar{z}+1/2$ [0,0,0]
(41) $\bar{x}+1/2, \bar{z}+1/2, y+1/2$ [0,0,0]	(42) $x+1/2, \bar{z}+1/2, \bar{y}+1/2$ [0,0,0]	(43) $x+1/2, z+1/2, y+1/2$ [0,0,0]	(44) $\bar{x}+1/2, z+1/2, \bar{y}+1/2$ [0,0,0]
(45) $\bar{z}+1/2, \bar{y}+1/2, x+1/2$ [0,0,0]	(46) $\bar{z}+1/2, y+1/2, \bar{x}+1/2$ [0,0,0]	(47) $z+1/2, \bar{y}+1/2, \bar{x}+1/2$ [0,0,0]	(48) $z+1/2, y+1/2, x+1/2$ [p

96 i m..1'

0,y,z [0,0,0]	0, $\bar{y}$ ,z [0,0,0]	0,y, $\bar{z}$ [0,0,0]	0, $\bar{y}$ , $\bar{z}$ [0,0,0]
z,0,y [0,0,0]	z,0, $\bar{y}$ [0,0,0]	$\bar{z}$ ,0,y [0,0,0]	$\bar{z}$ ,0, $\bar{y}$ [0,0,0]
y,z,0 [0,0,0]	$\bar{y}$ ,z,0 [0,0,0]	y, $\bar{z}$ ,0 [0,0,0]	$\bar{y}$ , $\bar{z}$ ,0 [0,0,0]
y+1/2,1/2, $\bar{z}+1/2$ [0,0,0]	$\bar{y}+1/2,1/2,\bar{z}+1/2$ [0,0,0]	y+1/2,1/2,z+1/2 [0,0,0]	$\bar{y}+1/2,1/2,z+1/2$ [0,0,0]
1/2,z+1/2, $\bar{y}+1/2$ [0,0,0]	1/2,z+1/2,y+1/2 [0,0,0]	1/2, $\bar{z}+1/2,\bar{y}+1/2$ [0,0,0]	1/2, $\bar{z}+1/2,y+1/2$ [0,0,0]
z+1/2,y+1/2,1/2 [0,0,0]	z+1/2, $\bar{y}+1/2,1/2$ [0,0,0]	$\bar{z}+1/2,y+1/2,1/2$ [0,0,0]	$\bar{z}+1/2,\bar{y}+1/2,1/2$ [0,0,0]

96 h ..21'	1/4,y,y [0,0,0]	3/4, $\bar{y}$ ,y [0,0,0]	3/4,y, $\bar{y}$ [0,0,0]	1/4, $\bar{y}$ , $\bar{y}$ [0,0,0]
	y,1/4,y [0,0,0]	y,3/4, $\bar{y}$ [0,0,0]	$\bar{y}$ ,3/4,y [0,0,0]	$\bar{y}$ ,1/4, $\bar{y}$ [0,0,0]
	y,y,1/4 [0,0,0]	$\bar{y}$ ,y,3/4 [0,0,0]	y, $\bar{y}$ ,3/4 [0,0,0]	$\bar{y}$ , $\bar{y}$ ,1/4 [0,0,0]
	3/4, $\bar{y}$ , $\bar{y}$ [0,0,0]	1/4,y, $\bar{y}$ [0,0,0]	1/4, $\bar{y}$ ,y [0,0,0]	3/4,y,y [0,0,0]
	$\bar{y}$ ,3/4, $\bar{y}$ [0,0,0]	$\bar{y}$ ,1/4,y [0,0,0]	y,1/4, $\bar{y}$ [0,0,0]	$\bar{y}$ ,3/4,y [0,0,0]
	$\bar{y}$ , $\bar{y}$ ,3/4 [0,0,0]	y, $\bar{y}$ ,1/4 [0,0,0]	$\bar{y}$ ,y,1/4 [0,0,0]	y,y,3/4 [0,0,0]

64 g .3.1'

x,x,x [0,0,0]	$\bar{x}, \bar{x}, x$ [0,0,0]	$\bar{x}, x, \bar{x}$ [0,0,0]	x, $\bar{x}, \bar{x}$ [0,0,0]
x+1/2,x+1/2, $\bar{x}+1/2$ [0,0,0]	$\bar{x}+1/2,\bar{x}+1/2,\bar{x}+1/2$ [0,0,0]	x+1/2, $\bar{x}+1/2,x+1/2$ [0,0,0]	$\bar{x}+1/2,x+1/2,x+1/2$ [0,0,0]
$\bar{x}, \bar{x}, \bar{x}$ [0,0,0]	x,x, $\bar{x}$ [0,0,0]	x, $\bar{x}, x$ [0,0,0]	$\bar{x}, x, x$ [0,0,0]
$\bar{x}+1/2,\bar{x}+1/2,x+1/2$ [0,0,0]	x+1/2,x+1/2,x+1/2 [0,0,0]	$\bar{x}+1/2,x+1/2,\bar{x}+1/2$ [0,0,0]	x+1/2, $\bar{x}+1/2,\bar{x}+1/2$ [0,0,0]
48 f 4..1'	x,1/4,1/4 [0,0,0]	$\bar{x}$ ,3/4,1/4 [0,0,0]	1/4,x,1/4 [0,0,0]
	1/4,1/4,x [0,0,0]	3/4,1/4, $\bar{x}$ [0,0,0]	$\bar{x}$ ,3/4,3/4 [0,0,0]
	3/4, $\bar{x}$ ,3/4 [0,0,0]	3/4,x,1/4 [0,0,0]	3/4,3/4, $\bar{x}$ [0,0,0]
			1/4,3/4,x [0,0,0]

Continued

226.2.1624

Fm $\bar{3}$ c1'

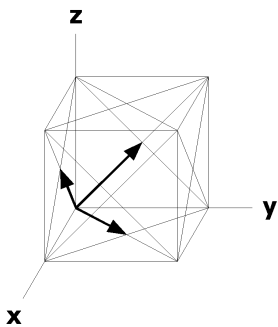
48	e	mm2..1'	x,0,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x}$ ,0 [0,0,0]
			0,0,x [0,0,0]	0,0, $\bar{x}$ [0,0,0]	1/2,x+1/2,1/2 [0,0,0]	1/2, $\bar{x}$ +1/2,1/2 [0,0,0]
			x+1/2,1/2,1/2 [0,0,0]	$\bar{x}$ +1/2,1/2,1/2 [0,0,0]	1/2,1/2, $\bar{x}$ +1/2 [0,0,0]	1/2,1/2,x+1/2 [0,0,0]
24	d	4/m..1'	0,1/4,1/4 [0,0,0]	0,3/4,1/4 [0,0,0]		1/4,0,1/4 [0,0,0]
			1/4,0,3/4 [0,0,0]	1/4,1/4,0 [0,0,0]		3/4,1/4,0 [0,0,0]
24	c	$\bar{4}$ m.21'	1/4,0,0 [0,0,0]	3/4,0,0 [0,0,0]		0,1/4,0 [0,0,0]
			0,3/4,0 [0,0,0]	0,0,1/4 [0,0,0]		0,0,3/4 [0,0,0]
8	b	$m\bar{3}$ .1'	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
8	a	4321'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,1,1] p6mm1'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

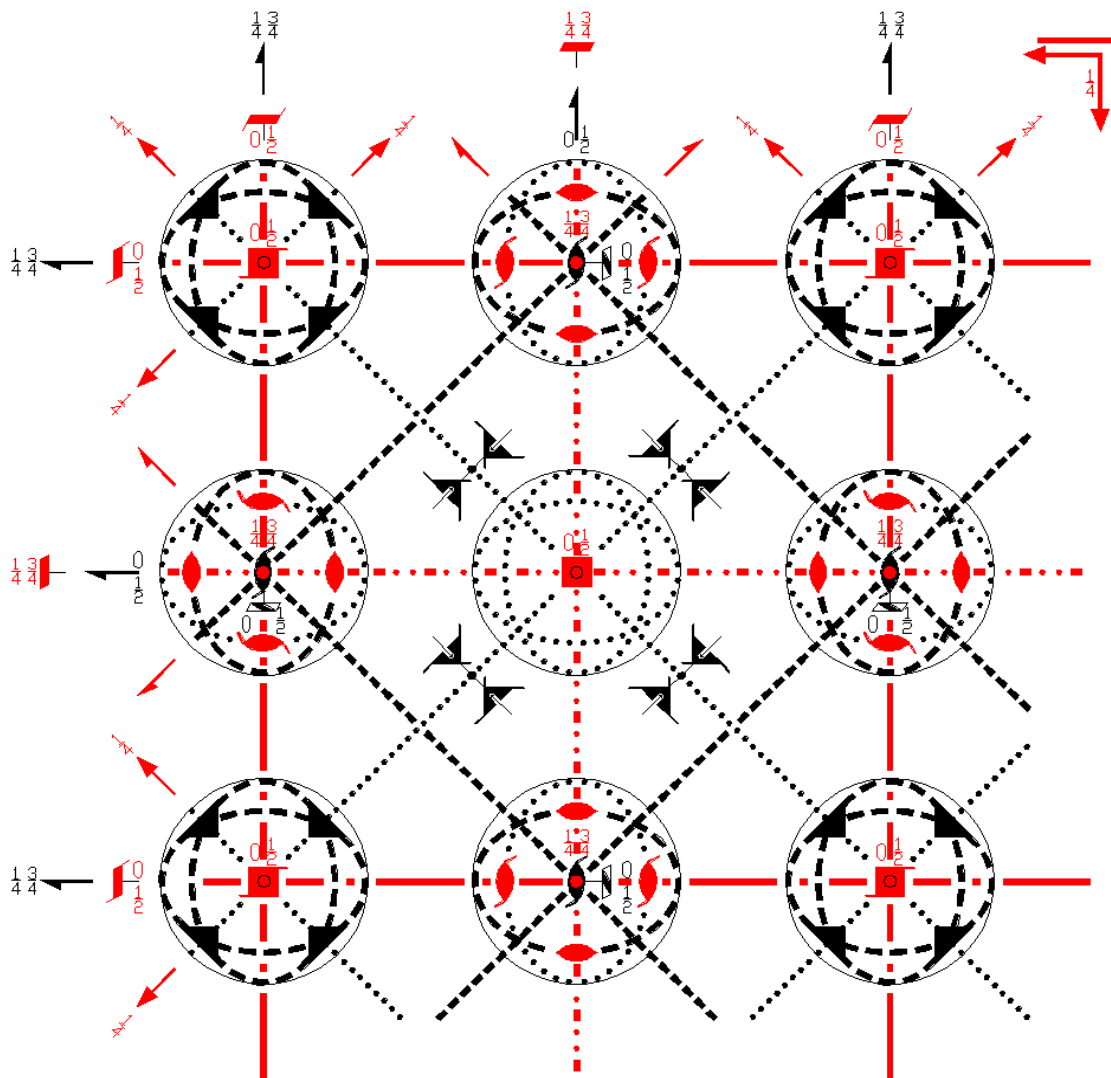
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/4$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



Fm $\bar{3}$ 'c  
226.3.1625

m $\bar{3}$ 'm  
F4'/m $\bar{3}$ '2'/c

Cubic



**Origin** at center (m $\bar{3}$ 'c)

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/4$ ;  $y \leq \min(x, 1/2-x)$ ;  $z \leq y$

**Vertices** 0,0,0      1/2,0,0      1/4,1/4,0      1/4,1/4,1/4

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                  | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)               | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)              |

(13) 2' (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(14) 2' x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(15) 4' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(16) 4 <sup>+</sup> (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)'
(17) 4' (1/2,0,0) x,1/2,0 (4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(18) 2' (0,1/2,1/2) 1/4,y,y (2 <sub>yz</sub>  1/2,1/2,1/2)'	(19) 2' 1/4,y+1/2, $\bar{y}$ (2 <sub>yz</sub>  1/2,1/2,1/2)'	(20) 4 <sup>+</sup> (1/2,0,0) x,0,1/2 (4 <sub>x</sub>  1/2,1/2,1/2)'
(21) 4 <sup>+</sup> (0,1/2,0) 1/2,y,0 (4 <sub>y</sub>  1/2,1/2,1/2)'	(22) 2' (1/2,0,1/2) x,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)'	(23) 4' (0,1/2,0) 0,y,1/2 (4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(24) 2' $\bar{x}$ +1/2,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)'
(25) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)'	(26) m' x,y,0 (m <sub>z</sub>  0,0,0)'	(27) m' x,0,z (m <sub>y</sub>  0,0,0)'	(28) m' 0,y,z (m <sub>x</sub>  0,0,0)'
(29) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'	(30) $\bar{3}^+$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(31) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(32) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'
(33) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(34) $\bar{3}^-$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'	(35) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'	(36) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'
(37) c (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,1/2)	(38) n (1/2,1/2,1/2) x,x,z (m <sub>xy</sub>  1/2,1/2,1/2)	(39) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>  1/2,1/2,1/2)	(40) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$  1/2,1/2,1/2)
(41) $\bar{4}^-$ x,0,1/2; 1/4,0,1/2 ( $\bar{4}_x$ <sup>-1</sup>  1/2,1/2,1/2)	(42) a (1/2,0,0) x,y+1/2, $\bar{y}$ (m <sub>yz</sub>  1/2,1/2,1/2)	(43) n (1/2,1/2,1/2) x,y,y (m <sub>yz</sub>  1/2,1/2,1/2)	(44) $\bar{4}^+$ x,1/2,0; 1/4,1/2,0 ( $\bar{4}_x$  1/2,1/2,1/2)
(45) $\bar{4}^+$ 0,y,1/2; 0,1/4,1/2 ( $\bar{4}_y$  1/2,1/2,1/2)	(46) b (0,1/2,0) $\bar{x}$ +1/2,y,x (m <sub>xz</sub>  1/2,1/2,1/2)	(47) $\bar{4}^-$ 1/2,y,0; 1/2,1/4,0 ( $\bar{4}_y$ <sup>-1</sup>  1/2,1/2,1/2)	(48) n (1/2,1/2,1/2) x,y,x (m <sub>xz</sub>  1/2,1/2,1/2)

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2) ( $\bar{1}$  0,1/2,1/2)	(2) 2 (0,0,1/2) 0,1/4,z (2 <sub>z</sub>  0,1/2,1/2)	(3) 2 (0,1/2,0) 0,y,1/4 (2 <sub>y</sub>  0,1/2,1/2)	(4) 2 x,1/4,1/4 (2 <sub>x</sub>  0,1/2,1/2)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x-1/3,x-1/6,x (3 <sub>xyz</sub>  0,1/2,1/2)	(6) 3 <sup>+</sup> $\bar{x}$ ,x+1/2, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(7) 3 <sup>+</sup> (-1/3,1/3,1/3) x+1/3, $\bar{x}$ -1/6, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ +1/2,x (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x-1/6,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(10) 3 <sup>-</sup> (-1/3,1/3,1/3) x+1/6, $\bar{x}$ +1/6, $\bar{x}$ (3 <sub>xyz</sub>  0,1/2,1/2)	(11) 3 <sup>-</sup> $\bar{x}$ +1/2, $\bar{x}$ +1/2,x (3 <sub>xyz</sub>  0,1/2,1/2)	(12) 3 <sup>-</sup> $\bar{x}$ -1/2,x+1/2, $\bar{x}$ (3 <sub>xyz</sub>  0,1/2,1/2)
(13) 2' (1/4,1/4,0) x,x-1/4,0 (2 <sub>xy</sub>  1/2,0,0)'	(14) 2' (1/4,-1/4,0) x, $\bar{x}$ +1/4,0 (2 <sub>xy</sub>  1/2,0,0)'	(15) 4' (1/4,-1/4,z) (4 <sub>z</sub> <sup>-1</sup>  1/2,0,0)'	(16) 4 <sup>+</sup> (1/4,1/4,z) (4 <sub>z</sub>  1/2,0,0)'
(17) 4' (1/2,0,0) x,0,0 (4 <sub>x</sub> <sup>-1</sup>  1/2,0,0)'	(18) 2' 1/4,y,y (2 <sub>yz</sub>  1/2,0,0)'	(19) 2' 1/4,y, $\bar{y}$ (2 <sub>yz</sub>  1/2,0,0)'	(20) 4 <sup>+</sup> (1/2,0,0) x,0,0 (4 <sub>x</sub>  1/2,0,0)'
(21) 4 <sup>+</sup> (1/4,y,-1/4) (4 <sub>y</sub>  1/2,0,0)'	(22) 2' (1/4,0,1/4) x+1/4,0,x (2 <sub>xz</sub>  1/2,0,0)'	(23) 4' (1/4,y,1/4) (4 <sub>y</sub> <sup>-1</sup>  1/2,0,0)'	(24) 2' (1/4,0,-1/4) $\bar{x}$ +1/4,0,x (2 <sub>xz</sub>  1/2,0,0)'
(25) $\bar{1}$ 0,1/4,1/4 ( $\bar{1}$  0,1/2,1/2)'	(26) b' (0,1/2,0) x,y,1/4 (m <sub>z</sub>  0,1/2,1/2)'	(27) c' (0,0,1/2) x,1/4,z (m <sub>y</sub>  0,1/2,1/2)'	(28) n' (0,1/2,1/2) 0,y,z (m <sub>x</sub>  0,1/2,1/2)'
(29) $\bar{3}^+$ x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$  0,1/2,1/2)'	(30) $\bar{3}^+$ $\bar{x}$ -1,x+1/2, $\bar{x}$ ; -1/2,0,1/2 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,1/2,1/2)'	(31) $\bar{3}^+$ x, $\bar{x}$ +1/2, $\bar{x}$ ; 0,1/2,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,1/2,1/2)'	(32) $\bar{3}^+$ $\bar{x}$ -1, $\bar{x}$ +1/2,x; 1/2,0,1/2 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,1/2,1/2)'

- |   |  |   |  |
|---|--|---|--|
| (33) $\bar{3}^-$ ' x-1/2,x-1/2,x;<br>0,0,1/2<br>( $\bar{3}_{xyz}^{-1}$  0,1/2,1/2)' | (34) $\bar{3}^-$ ' x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ;<br>0,0,1/2<br>( $\bar{3}_{xyz}$  0,1/2,1/2)' | (35) $\bar{3}^-$ ' $\bar{x}$ -1/2, $\bar{x}$ +1/2, x;<br>-1/2,1/2,0<br>( $\bar{3}_{xyz}$  0,1/2,1/2)' | (36) $\bar{3}^-$ ' $\bar{x}$ +1/2, x+1/2, $\bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{xyz}$  0,1/2,1/2)' |
| (37) g (1/4,-1/4,0) x+1/4, $\bar{x}$ ,z<br>( $m_{xy}$  1/2,0,0)                     | (38) g (1/4,1/4,0) x+1/4,x,z<br>( $m_{xy}$  1/2,0,0)   | (39) $\bar{4}^-$ 1/4,1/4,z; 1/4,1/4,0<br>( $\bar{4}_z^{-1}$  1/2,0,0)                                 | (40) $\bar{4}^+$ 1/4,-1/4,z; 1/4,-1/4,0<br>( $\bar{4}_z$  1/2,0,0)                                   |
| (41) $\bar{4}^-$ x,0,0; 1/4,0,0<br>( $\bar{4}_x^{-1}$  1/2,0,0)                     | (42) a (1/2,0,0) x,y, $\bar{y}$<br>( $m_{yz}$  1/2,0,0)  | (43) a (1/2,0,0) x,y,y<br>( $m_{yz}$  1/2,0,0)  | (44) $\bar{4}^+$ x,0,0; 1/4,0,0<br>( $\bar{4}_x$  1/2,0,0)   |
| (45) $\bar{4}^+$ 1/4,y,1/4; 1/4,0,1/4<br>( $\bar{4}_y$  1/2,0,0)                    | (46) g (1/4,0,-1/4) $\bar{x}$ +1/4,y,x<br>( $m_{xz}$  1/2,0,0)                                     | (47) $\bar{4}^-$ 1/4,y,-1/4; 1/4,0,-1/4<br>( $\bar{4}_y^{-1}$  1/2,0,0)                               | (48) g (1/4,0,1/4) x+1/4,y,x<br>( $m_{xz}$  1/2,0,0)   |

For (1/2,0,1/2) + set

- |  |  |   |   |
|--|--|---|---|
| (1) t (1/2,0,1/2)<br>(1 1/2,0,1/2)   | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)  | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>  1/2,0,1/2)  |
| (5) 3 <sup>+</sup> (1/3,1/3,1/3)<br>x+1/6,x-1/6,x<br>(3 <sub>xyz</sub>  1/2,0,1/2)               | (6) 3 <sup>+</sup> (1/3,-1/3,1/3)<br>x+1/6,x+1/6, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) | (7) 3 <sup>+</sup> x+1/2, $\bar{x}$ -1/2, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2)        | (8) 3 <sup>+</sup> $\bar{x}$ +1/2, $\bar{x}$ +1/2,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2)        |
| (9) 3 <sup>-</sup> (1/3,1/3,1/3)<br>x-1/6,x-1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) | (10) 3 <sup>-</sup> x+1/2, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub>  1/2,0,1/2)                          | (11) 3 <sup>-</sup> $\bar{x}$ +1/2, $\bar{x}$ , x<br>(3 <sub>xyz</sub>  1/2,0,1/2)                        | (12) 3 <sup>-</sup> (1/3,-1/3,1/3)<br>$\bar{x}$ -1/6, x+1/3, $\bar{x}$<br>(3 <sub>xyz</sub>  1/2,0,1/2)   |
| (13) 2' (1/4,1/4,0) x,x+1/4,0<br>(2 <sub>xy</sub>  0,1/2,0)'                                     | (14) 2' (-1/4,1/4,0) x, $\bar{x}$ +1/4,0<br>(2 <sub>xy</sub>  0,1/2,0)'                                    | (15) 4 <sup>-</sup> ' 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,0)'                               | (16) 4 <sup>+</sup> ' -1/4,1/4,z<br>(4 <sub>z</sub>  0,1/2,0)'  |
| (17) 4 <sup>-</sup> ' x,1/4,-1/4<br>(4 <sub>x</sub> <sup>-1</sup>  0,1/2,0)'                     | (18) 2' (0,1/4,1/4) 0,y+1/4,y<br>(2 <sub>yz</sub>  0,1/2,0)'   | (19) 2' (0,1/4,-1/4) 0,y+1/4, $\bar{y}$<br>(2 <sub>yz</sub>  0,1/2,0)'                                    | (20) 4 <sup>+</sup> ' x,1/4,1/4<br>(4 <sub>x</sub>  0,1/2,0)'   |
| (21) 4 <sup>+</sup> ' (0,1/2,0) 0,y,0<br>(4 <sub>y</sub>  0,1/2,0)'                              | (22) 2' x,1/4,x<br>(2 <sub>xz</sub>  0,1/2,0)'   | (23) 4 <sup>-</sup> ' (0,1/2,0) 0,y,0<br>(4 <sub>y</sub> <sup>-1</sup>  0,1/2,0)'                         | (24) 2' $\bar{x}$ ,1/4,x<br>(2 <sub>xz</sub>  0,1/2,0)'   |
| (25) $\bar{1}^-$ 1/4,0,1/4<br>( $\bar{1}$  1/2,0,1/2)'   | (26) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)'  | (27) n' (1/2,0,1/2) x,0,z<br>(m <sub>y</sub>  1/2,0,1/2)'   | (28) c' (0,0,1/2) 1/4,y,z<br>(m <sub>x</sub>  1/2,0,1/2)'   |
| (29) $\bar{3}^+$ ' x-1/2,x-1/2,x;<br>0,0,1/2<br>( $\bar{3}_{xyz}$  1/2,0,1/2)'                   | (30) $\bar{3}^+$ ' $\bar{x}$ -1/2,x+1/2, $\bar{x}$ ;<br>0,0,1/2<br>( $\bar{3}_{xyz}^{-1}$  1/2,0,1/2)'     | (31) $\bar{3}^+$ ' x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{xyz}^{-1}$  1/2,0,1/2)' | (32) $\bar{3}^+$ ' $\bar{x}$ +1/2, $\bar{x}$ -1/2,x;<br>1/2,-1/2,0<br>( $\bar{3}_{xyz}^{-1}$  1/2,0,1/2)' |
| (33) $\bar{3}^-$ ' x+1/2,x,x;<br>1/2,0,0<br>( $\bar{3}_{xyz}^{-1}$  1/2,0,1/2)'                  | (34) $\bar{3}^-$ ' x+1/2, $\bar{x}$ -1, $\bar{x}$ ;<br>0,-1/2,1/2<br>( $\bar{3}_{xyz}$  1/2,0,1/2)'        | (35) $\bar{3}^-$ ' $\bar{x}$ +1/2, $\bar{x}$ +1, x;<br>0,1/2,1/2<br>( $\bar{3}_{xyz}$  1/2,0,1/2)'        | (36) $\bar{3}^-$ ' $\bar{x}$ +1/2, x, $\bar{x}$ ;<br>1/2,0,0<br>( $\bar{3}_{xyz}$  1/2,0,1/2)'            |
| (37) g (-1/4,1/4,0) x+1/4, $\bar{x}$ ,z<br>( $m_{xy}$  0,1/2,0)                                  | (38) g (1/4,1/4,0) x-1/4,x,z<br>( $m_{xy}$  0,1/2,0)   | (39) $\bar{4}^-$ -1/4,1/4,z; -1/4,1/4,0<br>( $\bar{4}_z^{-1}$  0,1/2,0)                                   | (40) $\bar{4}^+$ 1/4,1/4,z; 1/4,1/4,0<br>( $\bar{4}_z$  0,1/2,0)  |
| (41) $\bar{4}^-$ x,1/4,1/4; 0,1/4,1/4<br>( $\bar{4}_x^{-1}$  0,1/2,0)                            | (42) g (0,1/4,-1/4) x,y+1/4, $\bar{y}$<br>( $m_{yz}$  0,1/2,0)   | (43) g (0,1/4,1/4) x,y+1/4,y<br>( $m_{yz}$  0,1/2,0)  | (44) $\bar{4}^+$ x,1/4,-1/4; 0,1/4,-1/4<br>( $\bar{4}_x$  0,1/2,0)  |
| (45) $\bar{4}^+$ 0,y,0; 0,1/4,0<br>( $\bar{4}_y$  0,1/2,0)                                       | (46) b (0,1/2,0) $\bar{x}$ ,y,x<br>( $m_{xz}$  0,1/2,0)  | (47) $\bar{4}^-$ 0,y,0; 0,1/4,0<br>( $\bar{4}_y^{-1}$  0,1/2,0)   | (48) b (0,1/2,0) x,y,x<br>( $m_{xz}$  0,1/2,0)  |

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (1   1/2,1/2,0)	(2) 2 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,0)	(3) 2 (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)	(4) 2 (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) 3 <sup>+</sup> $\bar{x}$ +1/2,x, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(7) 3 <sup>+</sup> x+1/2, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(8) 3 <sup>+</sup> (1/3,1/3,-1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) 3 <sup>-</sup> x, $\bar{x}$ +1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)	(11) 3 <sup>-</sup> (1/3,1/3,-1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub>   1/2,1/2,0)	(12) 3 <sup>-</sup> $\bar{x}$ , x+1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)
(13) 2' x,x,1/4 (2 <sub>xy</sub>   0,0,1/2)'	(14) 2' x, $\bar{x}$ ,1/4 (2 <sub>xy</sub>   0,0,1/2)'	(15) 4' (0,0,1/2) 0,0,z (4 <sub>z</sub> <sup>-1</sup>   0,0,1/2)'	(16) 4' (0,0,1/2) 0,0,z (4 <sub>z</sub>   0,0,1/2)'
(17) 4' x,1/4,1/4 (4 <sub>x</sub> <sup>-1</sup>   0,0,1/2)'	(18) 2' (0,1/4,1/4) 0,y-1/4,y (2 <sub>yz</sub>   0,0,1/2)'	(19) 2' (0,-1/4,1/4) 0,y+1/4, $\bar{y}$ (2 <sub>yz</sub>   0,0,1/2)'	(20) 4' x,-1/4,1/4 (4 <sub>x</sub>   0,0,1/2)'
(21) 4' 1/4,y,1/4 (4 <sub>y</sub>   0,0,1/2)'	(22) 2' (1/4,0,1/4) x-1/4,0,x (2 <sub>xz</sub>   0,0,1/2)'	(23) 4' -1/4,y,1/4 (4 <sub>y</sub> <sup>-1</sup>   0,0,1/2)'	(24) 2' (-1/4,0,1/4) $\bar{x}$ +1/4,0,x (2 <sub>xz</sub>   0,0,1/2)'
(25) $\bar{1}$ ' 1/4,1/4,0 ( $\bar{1}$   1/2,1/2,0)'	(26) n' (1/2,1/2,0) x,y,0 (m <sub>z</sub>   1/2,1/2,0)'	(27) a' (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)'	(28) b' (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)'
(29) $\bar{3}$ <sup>+</sup> x+1/2,x,x; 1/2,0,0 ( $\bar{3}$ <sub>xyz</sub>   1/2,1/2,0)'	(30) $\bar{3}$ <sup>+</sup> $\bar{x}$ -1/2,x+1, $\bar{x}$ ; 0,1/2,1/2 ( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)'	(31) $\bar{3}$ <sup>+</sup> x-1/2, $\bar{x}$ +1, $\bar{x}$ ; 0,1/2,-1/2 ( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)'	(32) $\bar{3}$ <sup>+</sup> $\bar{x}$ +1/2, $\bar{x}$ ,x; 1/2,0,0 ( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)'
(33) $\bar{3}$ <sup>-</sup> x,x+1/2,x; 0,1/2,0 ( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)'	(34) $\bar{3}$ <sup>-</sup> x+1, $\bar{x}$ -1/2, $\bar{x}$ ; 1/2,0,1/2 ( $\bar{3}$ <sub>xyz</sub>   1/2,1/2,0)'	(35) $\bar{3}$ <sup>-</sup> $\bar{x}$ , $\bar{x}$ +1/2,x; 0,1/2,0 ( $\bar{3}$ <sub>xyz</sub>   1/2,1/2,0)'	(36) $\bar{3}$ <sup>-</sup> $\bar{x}$ +1,x-1/2, $\bar{x}$ ; 1/2,0,-1/2 ( $\bar{3}$ <sub>xyz</sub>   1/2,1/2,0)'
(37) c (0,0,1/2) x, $\bar{x}$ ,z (m <sub>xy</sub>   0,0,1/2)	(38) c (0,0,1/2) x,x,z (m <sub>xy</sub>   0,0,1/2)	(39) $\bar{4}$ ' 0,0,z; 0,0,1/4 ( $\bar{4}$ <sub>z</sub> <sup>-1</sup>   0,0,1/2)	(40) $\bar{4}$ <sup>+</sup> 0,0,z; 0,0,1/4 ( $\bar{4}$ <sub>z</sub>   0,0,1/2)
(41) $\bar{4}$ ' x,-1/4,1/4; 0,-1/4,1/4 ( $\bar{4}$ <sub>x</sub> <sup>-1</sup>   0,0,1/2)	(42) g (0,-1/4,1/4) x,y+1/4, $\bar{y}$ (m <sub>yz</sub>   0,0,1/2)	(43) g (0,1/4,1/4) x,y-1/4,y (m <sub>yz</sub>   0,0,1/2)	(44) $\bar{4}$ <sup>+</sup> x,1/4,1/4; 0,1/4,1/4 ( $\bar{4}$ <sub>x</sub>   0,0,1/2)
(45) $\bar{4}$ <sup>+</sup> -1/4,y,1/4; -1/4,0,1/4 ( $\bar{4}$ <sub>y</sub>   0,0,1/2)	(46) g (-1/4,0,1/4) $\bar{x}$ +1/4,y,x (m <sub>xz</sub>   0,0,1/2)	(47) $\bar{4}$ ' 1/4,y,1/4; 1/4,0,1/4 ( $\bar{4}$ <sub>y</sub> <sup>-1</sup>   0,0,1/2)	(48) g (1/4,0,1/4) x-1/4,y,x (m <sub>xz</sub>   0,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

192	j	1	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +					
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}$ , $\bar{y}$ ,z	[ $\bar{u}$ , $\bar{v}$ ,w]	(3)	$\bar{x}$ ,y,z	[ $\bar{u}$ ,v, $\bar{w}$ ]	(4)	x, $\bar{y}$ ,z	[u, $\bar{v}$ , $\bar{w}$ ]
(5)	z,x,y	[w,u,v]	(6)	z, $\bar{x}$ , $\bar{y}$	[w, $\bar{u}$ , $\bar{v}$ ]	(7)	$\bar{z}$ ,x,y	[ $\bar{w}$ ,u,v]	(8)	$\bar{z}$ ,x, $\bar{y}$	[ $\bar{w}$ ,u, $\bar{v}$ ]

- (9)  $y, z, x [v, w, u]$  (10)  $\bar{y}, z, \bar{x} [\bar{v}, w, \bar{u}]$  (11)  $y, \bar{z}, \bar{x} [v, \bar{w}, \bar{u}]$  (12)  $\bar{y}, \bar{z}, x [\bar{v}, \bar{w}, u]$   
 (13)  $y+1/2, x+1/2, \bar{z}+1/2 [\bar{v}, \bar{u}, w]$  (14)  $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2 [v, u, w]$  (15)  $y+1/2, \bar{x}+1/2, z+1/2 [\bar{v}, u, \bar{w}]$  (16)  $\bar{y}+1/2, x+1/2, z+1/2 [v, \bar{u}, \bar{w}]$   
 (17)  $x+1/2, z+1/2, \bar{y}+1/2 [\bar{u}, \bar{w}, v]$  (18)  $\bar{x}+1/2, z+1/2, y+1/2 [u, \bar{w}, \bar{v}]$  (19)  $\bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2 [u, w, v]$  (20)  $x+1/2, \bar{z}+1/2, y+1/2 [\bar{u}, w, \bar{v}]$   
 (21)  $z+1/2, y+1/2, \bar{x}+1/2 [\bar{w}, \bar{v}, u]$  (22)  $z+1/2, \bar{y}+1/2, x+1/2 [\bar{w}, v, \bar{u}]$  (23)  $\bar{z}+1/2, y+1/2, x+1/2 [w, \bar{v}, \bar{u}]$  (24)  $\bar{z}+1/2, \bar{y}+1/2, \bar{x}+1/2 [w, v, u]$   
 (25)  $\bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$  (26)  $x, y, \bar{z} [u, v, \bar{w}]$  (27)  $x, \bar{y}, z [u, \bar{v}, w]$  (28)  $\bar{x}, y, z [\bar{u}, v, w]$   
 (29)  $\bar{z}, \bar{x}, \bar{y} [\bar{w}, \bar{u}, \bar{v}]$  (30)  $\bar{z}, x, y [\bar{w}, u, v]$  (31)  $z, x, \bar{y} [w, u, \bar{v}]$  (32)  $z, \bar{x}, y [w, \bar{u}, v]$   
 (33)  $\bar{y}, \bar{z}, \bar{x} [\bar{v}, \bar{w}, \bar{u}]$  (34)  $y, \bar{z}, x [v, \bar{w}, u]$  (35)  $\bar{y}, z, x [\bar{v}, w, u]$  (36)  $y, z, \bar{x} [v, w, \bar{u}]$   
 (37)  $\bar{y}+1/2, \bar{x}+1/2, z+1/2 [v, u, \bar{w}]$  (38)  $y+1/2, x+1/2, z+1/2 [\bar{v}, \bar{u}, \bar{w}]$  (39)  $\bar{y}+1/2, x+1/2, \bar{z}+1/2 [v, \bar{u}, w]$  (40)  $y+1/2, \bar{x}+1/2, \bar{z}+1/2 [\bar{v}, u, w]$   
 (41)  $\bar{x}+1/2, \bar{z}+1/2, y+1/2 [u, w, \bar{v}]$  (42)  $x+1/2, \bar{z}+1/2, \bar{y}+1/2 [\bar{u}, w, v]$  (43)  $x+1/2, z+1/2, y+1/2 [\bar{u}, \bar{w}, \bar{v}]$  (44)  $\bar{x}+1/2, z+1/2, \bar{y}+1/2 [u, \bar{w}, \bar{v}]$   
 (45)  $\bar{z}+1/2, \bar{y}+1/2, x+1/2 [w, v, \bar{u}]$  (46)  $\bar{z}+1/2, y+1/2, \bar{x}+1/2 [w, \bar{v}, u]$  (47)  $z+1/2, \bar{y}+1/2, \bar{x}+1/2 [\bar{w}, v, u]$  (48)  $z+1/2, y+1/2, x+1/2 [\bar{w}, \bar{v}, \bar{u}]$

96 i m'..

- $0, y, z [0, v, w]$   $0, \bar{y}, z [0, \bar{v}, w]$   $0, y, \bar{z} [0, v, \bar{w}]$   $0, \bar{y}, \bar{z} [0, \bar{v}, \bar{w}]$   
 $z, 0, y [w, 0, v]$   $z, 0, \bar{y} [w, 0, \bar{v}]$   $\bar{z}, 0, y [\bar{w}, 0, v]$   $\bar{z}, 0, \bar{y} [\bar{w}, 0, \bar{v}]$   
 $y, z, 0 [v, w, 0]$   $\bar{y}, z, 0 [\bar{v}, w, 0]$   $y, \bar{z}, 0 [v, \bar{w}, 0]$   $\bar{y}, \bar{z}, 0 [\bar{v}, \bar{w}, 0]$   
 $y+1/2, 1/2, \bar{z}+1/2 [\bar{v}, 0, w]$   $\bar{y}+1/2, 1/2, \bar{z}+1/2 [v, 0, w]$   $y+1/2, 1/2, z+1/2 [\bar{v}, 0, \bar{w}]$   $\bar{y}+1/2, 1/2, z+1/2 [v, 0, \bar{w}]$   
 $1/2, z+1/2, \bar{y}+1/2 [0, \bar{w}, v]$   $1/2, z+1/2, y+1/2 [0, \bar{w}, \bar{v}]$   $1/2, \bar{z}+1/2, \bar{y}+1/2 [0, w, v]$   $1/2, \bar{z}+1/2, y+1/2 [0, w, \bar{v}]$   
 $z+1/2, y+1/2, 1/2 [\bar{w}, \bar{v}, 0]$   $z+1/2, \bar{y}+1/2, 1/2 [\bar{w}, v, 0]$   $\bar{z}+1/2, y+1/2, 1/2 [w, \bar{v}, 0]$   $\bar{z}+1/2, \bar{y}+1/2, 1/2 [w, v, 0]$

- 96 h ..2'  $1/4, y, y [u, v, \bar{v}]$   $3/4, \bar{y}, y [\bar{u}, \bar{v}, \bar{v}]$   $3/4, y, \bar{y} [\bar{u}, v, v]$   $1/4, \bar{y}, \bar{y} [u, \bar{v}, \bar{v}]$   
 $y, 1/4, y [\bar{v}, u, v]$   $y, 3/4, \bar{y} [\bar{v}, \bar{u}, \bar{v}]$   $\bar{y}, 3/4, y [v, \bar{u}, v]$   $\bar{y}, 1/4, \bar{y} [v, u, \bar{v}]$   
 $y, y, 1/4 [v, \bar{v}, u]$   $\bar{y}, y, 3/4 [\bar{v}, \bar{v}, \bar{u}]$   $y, \bar{y}, 3/4 [v, v, \bar{u}]$   $\bar{y}, \bar{y}, 1/4 [\bar{v}, v, u]$   
 $3/4, \bar{y}, \bar{y} [\bar{u}, \bar{v}, v]$   $1/4, y, \bar{y} [u, v, v]$   $1/4, \bar{y}, y [u, \bar{v}, \bar{v}]$   $3/4, y, y [\bar{u}, v, \bar{v}]$   
 $\bar{y}, 3/4, y [v, \bar{u}, \bar{v}]$   $\bar{y}, 1/4, y [v, u, v]$   $y, 1/4, \bar{y} [\bar{v}, u, \bar{v}]$   $y, 3/4, y [v, \bar{u}, v]$   
 $\bar{y}, \bar{y}, 3/4 [\bar{v}, v, \bar{u}]$   $y, \bar{y}, 1/4 [v, v, u]$   $\bar{y}, y, 1/4 [\bar{v}, \bar{v}, u]$   $y, y, 3/4 [v, \bar{v}, \bar{u}]$

64 g .3.

- $x, x, x [u, u, u]$   $\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$   $\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$   $x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$   
 $x+1/2, x+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, u]$   $\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [u, u, u]$   $x+1/2, \bar{x}+1/2, x+1/2 [\bar{u}, u, \bar{u}]$   $\bar{x}+1/2, x+1/2, x+1/2 [u, \bar{u}, \bar{u}]$   
 $\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$   $x, x, \bar{x} [u, u, \bar{u}]$   $x, \bar{x}, x [u, \bar{u}, u]$   $\bar{x}, x, x [\bar{u}, u, u]$   
 $\bar{x}+1/2, \bar{x}+1/2, x+1/2 [u, u, \bar{u}]$   $x+1/2, x+1/2, x+1/2 [\bar{u}, \bar{u}, \bar{u}]$   $\bar{x}+1/2, x+1/2, \bar{x}+1/2 [u, \bar{u}, u]$   $x+1/2, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, u, u]$

Continued

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Fm $\bar{3}$ 'c

48	f	4'..	x,1/4,1/4 [0,0,0]	$\bar{x}$ ,3/4,1/4 [0,0,0]	1/4,x,1/4 [0,0,0]	1/4, $\bar{x}$ ,3/4 [0,0,0]
			1/4,1/4,x [0,0,0]	3/4,1/4, $\bar{x}$ [0,0,0]	$\bar{x}$ ,3/4,3/4 [0,0,0]	x,1/4,3/4 [0,0,0]
			3/4, $\bar{x}$ ,3/4 [0,0,0]	3/4,x,1/4 [0,0,0]	3/4,3/4, $\bar{x}$ [0,0,0]	1/4,3/4,x [0,0,0]
48	e	m'm'2..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0]	0,x,0 [0,u,0]	0, $\bar{x}$ ,0 [0, $\bar{u}$ ,0]
			0,0,x [0,0,u]	0,0, $\bar{x}$ [0,0, $\bar{u}$ ]	1/2,x+1/2,1/2 [0, $\bar{u}$ ,0]	1/2, $\bar{x}$ +1/2,1/2 [0,u,0]
			x+1/2,1/2,1/2 [ $\bar{u}$ ,0,0]	$\bar{x}$ +1/2,1/2,1/2 [u,0,0]	1/2,1/2, $\bar{x}$ +1/2 [0,0,u]	1/2,1/2,x+1/2 [0,0, $\bar{u}$ ]
24	d	4'/m'..	0,1/4,1/4 [0,0,0]	0,3/4,1/4 [0,0,0]	1/4,0,1/4 [0,0,0]	
			1/4,0,3/4 [0,0,0]	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]	
24	c	$\bar{4}$ m'.2'	1/4,0,0 [u,0,0]	3/4,0,0 [ $\bar{u}$ ,0,0]	0,1/4,0 [0,u,0]	
			0,3/4,0 [0, $\bar{u}$ ,0]	0,0,1/4 [0,0,u]	0,0,3/4 [0,0, $\bar{u}$ ]	
8	b	m' $\bar{3}$ '.	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
8	a	4'32'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]		

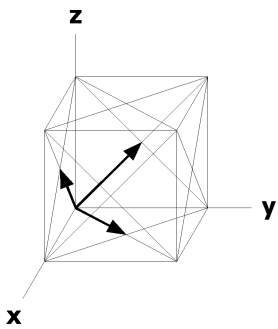
### Symmetry of Special Projections

Along [0,0,1] p4'm'm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,1,1] p6mm  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/4$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0





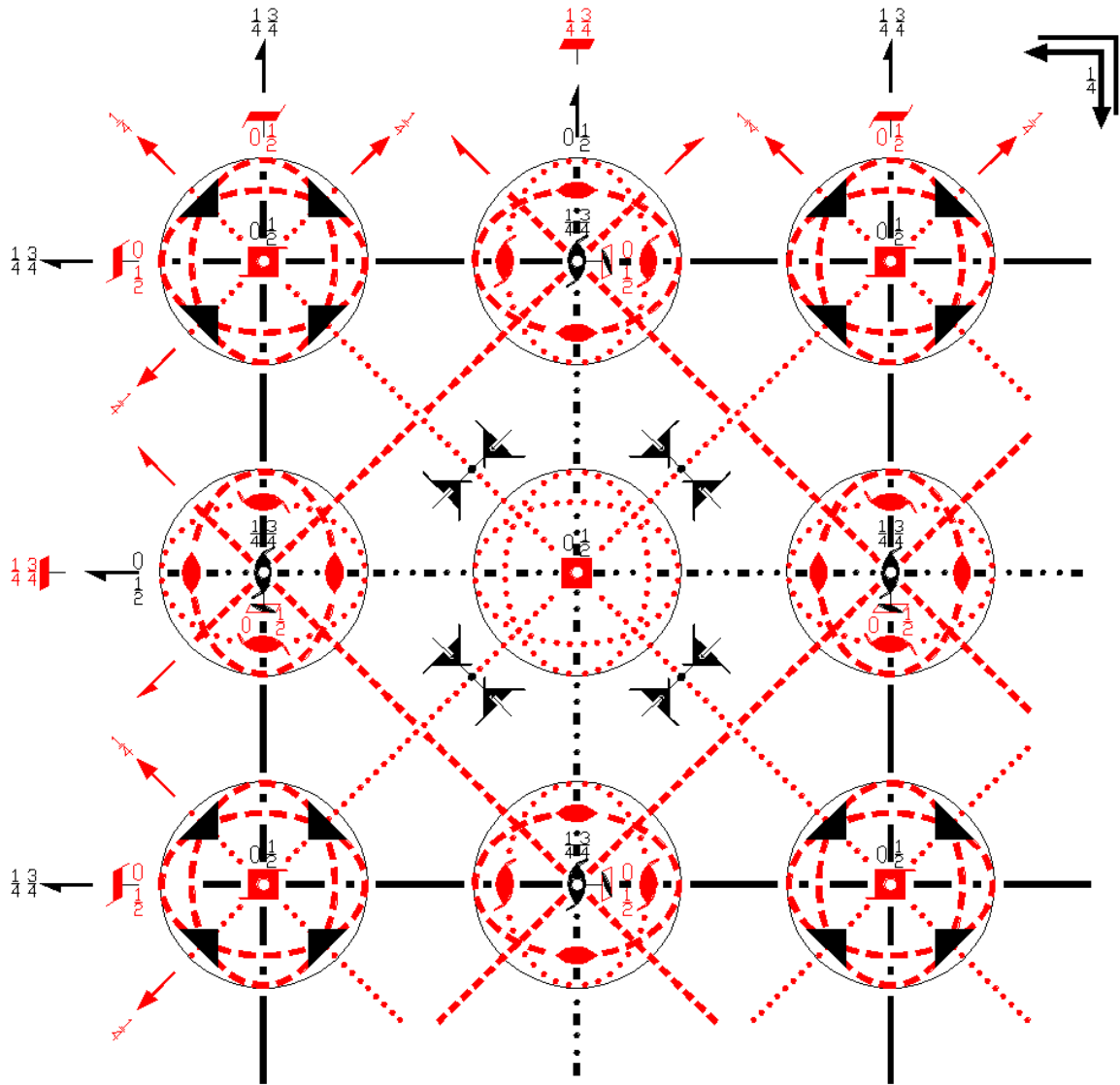
Fm $\bar{3}$ c'

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m $\bar{3}$ m'

F4'/m $\bar{3}$ 2'/c'

Cubic



**Origin** at center (m $\bar{3}$ )

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/4$ ;  $y \leq \min(x, 1/2-x)$ ;  $z \leq y$

**Vertices** 0,0,0      1/2,0,0      1/4,1/4,0      1/4,1/4,1/4

**Symmetry Operations**

For (0,0,0) + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                  | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz</math></sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)             | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)              | (12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)               |

(13) 2' (1/2,1/2,0) x,x,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(14) 2' x, $\bar{x}$ +1/2,1/4 (2 <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)'	(15) 4' ' (0,0,1/2) 1/2,0,z (4 <sub>z</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(16) 4+ ' (0,0,1/2) 0,1/2,z (4 <sub>z</sub>  1/2,1/2,1/2)'
(17) 4' ' (1/2,0,0) x,1/2,0 (4 <sub>x</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(18) 2' (0,1/2,1/2) 1/4,y,y (2 <sub>yz</sub>  1/2,1/2,1/2)'	(19) 2' 1/4,y+1/2, $\bar{y}$ (2 <sub><math>\bar{yz}</math></sub>  1/2,1/2,1/2)'	(20) 4+ ' (1/2,0,0) x,0,1/2 (4 <sub>x</sub>  1/2,1/2,1/2)'
(21) 4+ ' (0,1/2,0) 1/2,y,0 (4 <sub>y</sub>  1/2,1/2,1/2)'	(22) 2' (1/2,0,1/2) x,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)'	(23) 4' ' (0,1/2,0) 0,y,1/2 (4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,1/2)'	(24) 2' $\bar{x}$ +1/2,1/4,x (2 <sub><math>\bar{xz}</math></sub>  1/2,1/2,1/2)'
(25) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(26) m x,y,0 (m <sub>z</sub>  0,0,0)	(27) m x,0,z (m <sub>y</sub>  0,0,0)	(28) m 0,y,z (m <sub>x</sub>  0,0,0)
(29) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)	(30) $\bar{3}^+$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0)	(31) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0)	(32) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,0,0)
(33) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)	(34) $\bar{3}^-$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)	(35) $\bar{3}^-$ x, $\bar{x}$ ,x; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)	(36) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0 ( $\bar{3}_{x\bar{y}\bar{z}}$  0,0,0)
(37) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/2,1/2,1/2)'	(38) n' (1/2,1/2,1/2) x,x,z (m <sub><math>\bar{xy}</math></sub>  1/2,1/2,1/2)'	(39) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z$ <sup>-1</sup>  1/2,1/2,1/2)'	(40) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$  1/2,1/2,1/2)'
(41) $\bar{4}^-$ ' x,0,1/2; 1/4,0,1/2 ( $\bar{4}_x$ <sup>-1</sup>  1/2,1/2,1/2)'	(42) a' (1/2,0,0) x,y+1/2, $\bar{y}$ (m <sub>yz</sub>  1/2,1/2,1/2)'	(43) n' (1/2,1/2,1/2) x,y,y (m <sub><math>\bar{yz}</math></sub>  1/2,1/2,1/2)'	(44) $\bar{4}^+$ ' x,1/2,0; 1/4,1/2,0 ( $\bar{4}_x$  1/2,1/2,1/2)'
(45) $\bar{4}^+$ ' 0,y,1/2; 0,1/4,1/2 ( $\bar{4}_y$  1/2,1/2,1/2)'	(46) b' (0,1/2,0) $\bar{x}$ +1/2,y,x (m <sub>xz</sub>  1/2,1/2,1/2)'	(47) $\bar{4}^-$ ' 1/2,y,0; 1/2,1/4,0 ( $\bar{4}_y$ <sup>-1</sup>  1/2,1/2,1/2)'	(48) n' (1/2,1/2,1/2) x,y,x (m $\bar{xz}$  1/2,1/2,1/2)'

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2) ( $\bar{1}$  0,1/2,1/2)	(2) 2 (0,0,1/2) 0,1/4,z (2 <sub>z</sub>  0,1/2,1/2)	(3) 2 (0,1/2,0) 0,y,1/4 (2 <sub>y</sub>  0,1/2,1/2)	(4) 2 x,1/4,1/4 (2 <sub>x</sub>  0,1/2,1/2)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x-1/3,x-1/6,x (3 <sub>xyz</sub>  0,1/2,1/2)	(6) 3 <sup>+</sup> $\bar{x}$ ,x+1/2, $\bar{x}$ (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,1/2,1/2)	(7) 3 <sup>+</sup> (-1/3,1/3,1/3) x+1/3,x-1/6,x (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,1/2,1/2)	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ +1/2,x (3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  0,1/2,1/2)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x-1/6,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(10) 3 <sup>-</sup> (-1/3,1/3,1/3) x+1/6,x+1/6,x (3 <sub>xyz</sub>  0,1/2,1/2)	(11) 3 <sup>-</sup> $\bar{x}$ +1/2, $\bar{x}$ +1/2,x (3 <sub><math>\bar{xyz}</math></sub>  0,1/2,1/2)	(12) 3 <sup>-</sup> $\bar{x}$ -1/2,x+1/2, $\bar{x}$ (3 <sub><math>\bar{xyz}</math></sub>  0,1/2,1/2)
(13) 2' (1/4,1/4,0) x,x-1/4,0 (2 <sub>xy</sub>  1/2,0,0)'	(14) 2' (1/4,-1/4,0) x, $\bar{x}$ +1/4,0 (2 <sub><math>\bar{xy}</math></sub>  1/2,0,0)'	(15) 4' ' 1/4,-1/4,z (4 <sub>z</sub> <sup>-1</sup>  1/2,0,0)'	(16) 4+ ' 1/4,1/4,z (4 <sub>z</sub>  1/2,0,0)'
(17) 4' ' (1/2,0,0) x,0,0 (4 <sub>x</sub> <sup>-1</sup>  1/2,0,0)'	(18) 2' 1/4,y,y (2 <sub>yz</sub>  1/2,0,0)'	(19) 2' 1/4,y, $\bar{y}$ (2 <sub><math>\bar{yz}</math></sub>  1/2,0,0)'	(20) 4+ ' (1/2,0,0) x,0,0 (4 <sub>x</sub>  1/2,0,0)'
(21) 4+ ' 1/4,y,-1/4 (4 <sub>y</sub>  1/2,0,0)'	(22) 2' (1/4,0,1/4) x+1/4,0,x (2 <sub>xz</sub>  1/2,0,0)'	(23) 4' ' 1/4,y,1/4 (4 <sub>y</sub> <sup>-1</sup>  1/2,0,0)'	(24) 2' (1/4,0,-1/4) $\bar{x}$ +1/4,0,x (2 <sub><math>\bar{xz}</math></sub>  1/2,0,0)'
(25) $\bar{1}$ 0,1/4,1/4 ( $\bar{1}$  0,1/2,1/2)	(26) b (0,1/2,0) x,y,1/4 (m <sub>z</sub>  0,1/2,1/2)	(27) c (0,0,1/2) x,1/4,z (m <sub>y</sub>  0,1/2,1/2)	(28) n (0,1/2,1/2) 0,y,z (m <sub>x</sub>  0,1/2,1/2)
(29) $\bar{3}^+$ x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$  0,1/2,1/2)	(30) $\bar{3}^+$ $\bar{x}$ -1,x+1/2, $\bar{x}$ ; -1/2,0,1/2 ( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,1/2,1/2)	(31) $\bar{3}^+$ x, $\bar{x}$ +1/2, $\bar{x}$ ; 0,1/2,0 ( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,1/2,1/2)	(32) $\bar{3}^+$ $\bar{x}$ -1, $\bar{x}$ +1/2,x; 1/2,0,1/2 ( $\bar{3}_{x\bar{y}\bar{z}}$ <sup>-1</sup>  0,1/2,1/2)

(33) $\bar{3}^-$ $x-1/2, x-1/2, x;$ 0,0,1/2 ( $\bar{3}_{xyz}^{-1}$   0,1/2,1/2)	(34) $\bar{3}^-$ $x+1/2, \bar{x}-1/2, \bar{x};$ 0,0,1/2 ( $\bar{3}_{\bar{xyz}}$   0,1/2,1/2)	(35) $\bar{3}^-$ $\bar{x}-1/2, \bar{x}+1/2, x;$ -1/2,1/2,0 ( $\bar{3}_{\bar{xyz}}$   0,1/2,1/2)	(36) $\bar{3}^-$ $\bar{x}+1/2, x+1/2, \bar{x};$ 1/2,1/2,0 ( $\bar{3}_{\bar{xyz}}$   0,1/2,1/2)
(37) $g'$ (1/4,-1/4,0) $x+1/4, \bar{x}, z$ ( $m_{xy}$   1/2,0,0)'	(38) $g'$ (1/4,1/4,0) $x+1/4, x, z$ ( $m_{\bar{xy}}$   1/2,0,0)'	(39) $\bar{4}^-$ 1/4,1/4,z; 1/4,1/4,0 ( $\bar{4}_z^{-1}$   1/2,0,0)'	(40) $\bar{4}^+$ 1/4,-1/4,z; 1/4,-1/4,0 ( $\bar{4}_z$   1/2,0,0)'
(41) $\bar{4}^-$ $x, 0, 0;$ 1/4,0,0 ( $\bar{4}_x^{-1}$   1/2,0,0)'	(42) $a'$ (1/2,0,0) $x, y, \bar{y}$ ( $m_{yz}$   1/2,0,0)'	(43) $a'$ (1/2,0,0) $x, y, y$ ( $m_{\bar{yz}}$   1/2,0,0)'	(44) $\bar{4}^+$ $x, 0, 0;$ 1/4,0,0 ( $\bar{4}_x$   1/2,0,0)'
(45) $\bar{4}^+$ 1/4,y,1/4; 1/4,0,1/4 ( $\bar{4}_y$   1/2,0,0)'	(46) $g'$ (1/4,0,-1/4) $\bar{x}+1/4, y, x$ ( $m_{xz}$   1/2,0,0)'	(47) $\bar{4}^-$ 1/4,y,-1/4; 1/4,0,-1/4 ( $\bar{4}_y^{-1}$   1/2,0,0)'	(48) $g'$ (1/4,0,1/4) $x+1/4, y, x$ ( $m_{\bar{xz}}$   1/2,0,0)'

For (1/2,0,1/2) + set

(1) $t$ (1/2,0,1/2) (1   1/2,0,1/2)	(2) 2 (0,0,1/2) 1/4,0,z (2 $_z$   1/2,0,1/2)	(3) 2 1/4,y,1/4 (2 $_y$   1/2,0,1/2)	(4) 2 (1/2,0,0) $x, 0, 1/4$ (2 $_x$   1/2,0,1/2)
(5) $3^+$ (1/3,1/3,1/3) $x+1/6, x-1/6, x$ ( $3_{xyz}$   1/2,0,1/2)	(6) $3^+$ (1/3,-1/3,1/3) $x+1/6, x+1/6, \bar{x}$ ( $3_{\bar{xyz}^{-1}}$   1/2,0,1/2)	(7) $3^+$ $x+1/2, \bar{x}-1/2, \bar{x}$ ( $3_{\bar{xyz}^{-1}}$   1/2,0,1/2)	(8) $3^+$ $\bar{x}+1/2, \bar{x}+1/2, x$ ( $3_{\bar{xyz}^{-1}}$   1/2,0,1/2)
(9) $3^-$ (1/3,1/3,1/3) $x-1/6, x-1/3, x$ ( $3_{xyz}^{-1}$   1/2,0,1/2)	(10) $3^-$ $x+1/2, \bar{x}, \bar{x}$ ( $3_{\bar{xyz}}$   1/2,0,1/2)	(11) $3^-$ $\bar{x}+1/2, \bar{x}, x$ ( $3_{\bar{xyz}}$   1/2,0,1/2)	(12) $3^-$ (1/3,-1/3,1/3) $\bar{x}-1/6, x+1/3, \bar{x}$ ( $3_{\bar{xyz}}$   1/2,0,1/2)
(13) 2' (1/4,1/4,0) $x, x+1/4, 0$ (2 $_{xy}$   0,1/2,0)'	(14) 2' (-1/4,1/4,0) $x, \bar{x}+1/4, 0$ (2 $_{\bar{xy}}$   0,1/2,0)'	(15) $4^-$ 1/4,1/4,z ( $4_z^{-1}$   0,1/2,0)'	(16) $4^+$ -1/4,1/4,z ( $4_z$   0,1/2,0)'
(17) $4^-$ $x, 1/4, -1/4$ ( $4_x^{-1}$   0,1/2,0)'	(18) 2' (0,1/4,1/4) 0,y+1/4,y (2 $_{yz}$   0,1/2,0)'	(19) 2' (0,1/4,-1/4) 0,y+1/4, $\bar{y}$ (2 $_{\bar{yz}}$   0,1/2,0)'	(20) $4^+$ $x, 1/4, 1/4$ ( $4_x$   0,1/2,0)'
(21) $4^+$ (0,1/2,0) 0,y,0 ( $4_y$   0,1/2,0)'	(22) 2' $x, 1/4, x$ (2 $_{xz}$   0,1/2,0)'	(23) $4^-$ (0,1/2,0) 0,y,0 ( $4_y^{-1}$   0,1/2,0)'	(24) 2' $\bar{x}, 1/4, x$ (2 $_{\bar{xz}}$   0,1/2,0)'
(25) $\bar{1}$ 1/4,0,1/4 ( $\bar{1}$   1/2,0,1/2)	(26) $a$ (1/2,0,0) $x, y, 1/4$ ( $m_z$   1/2,0,1/2)	(27) $n$ (1/2,0,1/2) $x, 0, z$ ( $m_y$   1/2,0,1/2)	(28) $c$ (0,0,1/2) 1/4,y,z ( $m_x$   1/2,0,1/2)
(29) $\bar{3}^+$ $x-1/2, x-1/2, x;$ 0,0,1/2 ( $\bar{3}_{xyz}$   1/2,0,1/2)	(30) $\bar{3}^+$ $\bar{x}-1/2, x+1/2, \bar{x};$ 0,0,1/2 ( $\bar{3}_{\bar{xyz}^{-1}}$   1/2,0,1/2)	(31) $\bar{3}^+$ $x+1/2, \bar{x}+1/2, \bar{x};$ 1/2,1/2,0 ( $\bar{3}_{\bar{xyz}^{-1}}$   1/2,0,1/2)	(32) $\bar{3}^+$ $\bar{x}+1/2, \bar{x}-1/2, x;$ 1/2,-1/2,0 ( $\bar{3}_{\bar{xyz}^{-1}}$   1/2,0,1/2)
(33) $\bar{3}^-$ $x+1/2, x, x;$ 1/2,0,0 ( $\bar{3}_{xyz}^{-1}$   1/2,0,1/2)	(34) $\bar{3}^-$ $x+1/2, \bar{x}-1, \bar{x};$ 0,-1/2,1/2 ( $\bar{3}_{\bar{xyz}}$   1/2,0,1/2)	(35) $\bar{3}^-$ $\bar{x}+1/2, \bar{x}+1, x;$ 0,1/2,1/2 ( $\bar{3}_{\bar{xyz}}$   1/2,0,1/2)	(36) $\bar{3}^-$ $\bar{x}+1/2, x, \bar{x};$ 1/2,0,0 ( $\bar{3}_{\bar{xyz}}$   1/2,0,1/2)
(37) $g'$ (-1/4,1/4,0) $x+1/4, \bar{x}, z$ ( $m_{xy}$   0,1/2,0)'	(38) $g'$ (1/4,1/4,0) $x-1/4, x, z$ ( $m_{\bar{xy}}$   0,1/2,0)'	(39) $\bar{4}^-$ -1/4,1/4,z; -1/4,1/4,0 ( $\bar{4}_z^{-1}$   0,1/2,0)'	(40) $\bar{4}^+$ 1/4,1/4,z; 1/4,1/4,0 ( $\bar{4}_z$   0,1/2,0)'
(41) $\bar{4}^-$ $x, 1/4, 1/4;$ 0,1/4,1/4 ( $\bar{4}_x^{-1}$   0,1/2,0)'	(42) $g'$ (0,1/4,-1/4) $x, y+1/4, \bar{y}$ ( $m_{yz}$   0,1/2,0)'	(43) $g'$ (0,1/4,1/4) $x, y+1/4, y$ ( $m_{\bar{yz}}$   0,1/2,0)'	(44) $\bar{4}^+$ $x, 1/4, -1/4;$ 0,1/4,-1/4 ( $\bar{4}_x$   0,1/2,0)'
(45) $\bar{4}^+$ 0,y,0; 0,1/4,0 ( $\bar{4}_y$   0,1/2,0)'	(46) $b'$ (0,1/2,0) $\bar{x}, y, x$ ( $m_{xz}$   0,1/2,0)'	(47) $\bar{4}^-$ 0,y,0; 0,1/4,0 ( $\bar{4}_y^{-1}$   0,1/2,0)'	(48) $b'$ (0,1/2,0) $x, y, x$ ( $m_{\bar{xz}}$   0,1/2,0)'

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (1   1/2,1/2,0)	(2) 2 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,0)	(3) 2 (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)	(4) 2 (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) 3 <sup>+</sup> $\bar{x}$ +1/2,x, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(7) 3 <sup>+</sup> x+1/2, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(8) 3 <sup>+</sup> (1/3,1/3,-1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) 3 <sup>-</sup> x, $\bar{x}$ +1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)	(11) 3 <sup>-</sup> (1/3,1/3,-1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub>   1/2,1/2,0)	(12) 3 <sup>-</sup> $\bar{x}$ , x+1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)
(13) 2' x,x,1/4 (2 <sub>xy</sub>   0,0,1/2)'	(14) 2' x, $\bar{x}$ ,1/4 (2 <sub>xy</sub>   0,0,1/2)'	(15) 4' (0,0,1/2) 0,0,z (4 <sub>z</sub> <sup>-1</sup>   0,0,1/2)'	(16) 4' (0,0,1/2) 0,0,z (4 <sub>z</sub>   0,0,1/2)'
(17) 4' x,1/4,1/4 (4 <sub>x</sub> <sup>-1</sup>   0,0,1/2)'	(18) 2' (0,1/4,1/4) 0,y-1/4,y (2 <sub>yz</sub>   0,0,1/2)'	(19) 2' (0,-1/4,1/4) 0,y+1/4, $\bar{y}$ (2 <sub>yz</sub>   0,0,1/2)'	(20) 4' x,-1/4,1/4 (4 <sub>x</sub>   0,0,1/2)'
(21) 4' 1/4,y,1/4 (4 <sub>y</sub>   0,0,1/2)'	(22) 2' (1/4,0,1/4) x-1/4,0,x (2 <sub>xz</sub>   0,0,1/2)'	(23) 4' -1/4,y,1/4 (4 <sub>y</sub> <sup>-1</sup>   0,0,1/2)'	(24) 2' (-1/4,0,1/4) $\bar{x}$ +1/4,0,x (2 <sub>xz</sub>   0,0,1/2)'
(25) $\bar{1}$ 1/4,1/4,0 ( $\bar{1}$   1/2,1/2,0)	(26) n (1/2,1/2,0) x,y,0 (m <sub>z</sub>   1/2,1/2,0)	(27) a (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)	(28) b (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)
(29) 3 <sup>+</sup> x+1/2,x,x; 1/2,0,0 (3 <sub>xyz</sub>   1/2,1/2,0)	(30) 3 <sup>+</sup> $\bar{x}$ -1/2,x+1, $\bar{x}$ ; 0,1/2,1/2 (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(31) 3 <sup>+</sup> x-1/2, $\bar{x}$ +1, $\bar{x}$ ; 0,1/2,-1/2 (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(32) 3 <sup>+</sup> $\bar{x}$ +1/2, $\bar{x}$ ,x; 1/2,0,0 (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)
(33) 3 <sup>-</sup> x,x+1/2,x; 0,1/2,0 (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(34) 3 <sup>-</sup> x+1, $\bar{x}$ -1/2, $\bar{x}$ ; 1/2,0,1/2 (3 <sub>xyz</sub>   1/2,1/2,0)	(35) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ +1/2,x; 0,1/2,0 (3 <sub>xyz</sub>   1/2,1/2,0)	(36) 3 <sup>-</sup> $\bar{x}$ +1,x-1/2, $\bar{x}$ ; 1/2,0,-1/2 (3 <sub>xyz</sub>   1/2,1/2,0)
(37) c' (0,0,1/2) x, $\bar{x}$ ,z (m <sub>xy</sub>   0,0,1/2)'	(38) c' (0,0,1/2) x,x,z (m <sub>xy</sub>   0,0,1/2)'	(39) 4' (0,0,z; 0,0,1/4) (4 <sub>z</sub> <sup>-1</sup>   0,0,1/2)'	(40) 4' (0,0,z; 0,0,1/4) (4 <sub>z</sub>   0,0,1/2)'
(41) 4' x,-1/4,1/4; 0,-1/4,1/4 (4 <sub>x</sub> <sup>-1</sup>   0,0,1/2)'	(42) g' (0,-1/4,1/4) x,y+1/4, $\bar{y}$ (m <sub>yz</sub>   0,0,1/2)'	(43) g' (0,1/4,1/4) x,y-1/4,y (m <sub>yz</sub>   0,0,1/2)'	(44) 4' x,1/4,1/4; 0,1/4,1/4 (4 <sub>x</sub>   0,0,1/2)'
(45) 4' -1/4,y,1/4; -1/4,0,1/4 (4 <sub>y</sub>   0,0,1/2)'	(46) g' (-1/4,0,1/4) $\bar{x}$ +1/4,y,x (m <sub>xz</sub>   0,0,1/2)'	(47) 4' 1/4,y,1/4; 1/4,0,1/4 (4 <sub>y</sub> <sup>-1</sup>   0,0,1/2)'	(48) g' (1/4,0,1/4) x-1/4,y,x (m <sub>xz</sub>   0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

192	j	1	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +					
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	[ $\bar{u},\bar{v},w$ ]	(3)	$\bar{x},y,z$	[ $\bar{u},v,w$ ]	(4)	x, $\bar{y},z$	[u, $\bar{v},w$ ]
(5)	z,x,y	[w,u,v]	(6)	z, $\bar{x},\bar{y}$	[w, $\bar{u},\bar{v}$ ]	(7)	$\bar{z},\bar{x},y$	[ $\bar{w},\bar{u},v$ ]	(8)	$\bar{z},x,y$	[ $\bar{w},u,v$ ]

(9) $y, z, x [v, w, u]$	(10) $\bar{y}, z, \bar{x} [\bar{v}, w, \bar{u}]$	(11) $y, \bar{z}, \bar{x} [v, \bar{w}, \bar{u}]$	(12) $\bar{y}, \bar{z}, x [\bar{v}, \bar{w}, u]$
(13) $y+1/2, x+1/2, \bar{z}+1/2 [\bar{v}, \bar{u}, w]$	(14) $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2 [v, u, w]$	(15) $y+1/2, \bar{x}+1/2, z+1/2 [\bar{v}, u, \bar{w}]$	(16) $\bar{y}+1/2, x+1/2, z+1/2 [v, \bar{u}, \bar{w}]$
(17) $x+1/2, z+1/2, \bar{y}+1/2 [\bar{u}, \bar{w}, v]$	(18) $\bar{x}+1/2, z+1/2, y+1/2 [u, \bar{w}, \bar{v}]$	(19) $\bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2 [u, w, v]$	(20) $x+1/2, \bar{z}+1/2, y+1/2 [\bar{u}, w, \bar{v}]$
(21) $z+1/2, y+1/2, \bar{x}+1/2 [\bar{w}, \bar{v}, u]$	(22) $z+1/2, \bar{y}+1/2, x+1/2 [\bar{w}, v, \bar{u}]$	(23) $\bar{z}+1/2, y+1/2, x+1/2 [w, \bar{v}, \bar{u}]$	(24) $\bar{z}+1/2, \bar{y}+1/2, \bar{x}+1/2 [w, v, u]$
(25) $\bar{x}, \bar{y}, \bar{z} [u, v, w]$	(26) $x, y, \bar{z} [\bar{u}, \bar{v}, w]$	(27) $x, \bar{y}, z [\bar{u}, v, \bar{w}]$	(28) $\bar{x}, y, z [u, \bar{v}, \bar{w}]$
(29) $\bar{z}, \bar{x}, \bar{y} [w, u, v]$	(30) $\bar{z}, x, y [w, \bar{u}, \bar{v}]$	(31) $z, x, \bar{y} [\bar{w}, \bar{u}, v]$	(32) $z, \bar{x}, y [\bar{w}, u, \bar{v}]$
(33) $\bar{y}, \bar{z}, \bar{x} [v, w, u]$	(34) $y, \bar{z}, x [\bar{v}, w, \bar{u}]$	(35) $\bar{y}, z, x [v, \bar{w}, \bar{u}]$	(36) $y, z, \bar{x} [\bar{v}, \bar{w}, u]$
(37) $\bar{y}+1/2, \bar{x}+1/2, z+1/2 [\bar{v}, \bar{u}, w]$	(38) $y+1/2, x+1/2, z+1/2 [v, u, w]$	(39) $\bar{y}+1/2, x+1/2, \bar{z}+1/2 [\bar{v}, u, \bar{w}]$	(40) $y+1/2, \bar{x}+1/2, \bar{z}+1/2 [v, \bar{u}, \bar{w}]$
(41) $\bar{x}+1/2, \bar{z}+1/2, y+1/2 [\bar{u}, \bar{w}, v]$	(42) $x+1/2, \bar{z}+1/2, \bar{y}+1/2 [u, \bar{w}, \bar{v}]$	(43) $x+1/2, z+1/2, y+1/2 [u, w, v]$	(44) $\bar{x}+1/2, z+1/2, \bar{y}+1/2 [\bar{u}, w, \bar{v}]$
(45) $\bar{z}+1/2, \bar{y}+1/2, x+1/2 [\bar{w}, \bar{v}, u]$	(46) $\bar{z}+1/2, y+1/2, \bar{x}+1/2 [\bar{w}, v, \bar{u}]$	(47) $z+1/2, \bar{y}+1/2, \bar{x}+1/2 [w, \bar{v}, \bar{u}]$	(48) $z+1/2, y+1/2, x+1/2 [w, v, u]$

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$0, y, z [u, 0, 0]$	$0, \bar{y}, z [\bar{u}, 0, 0]$	$0, y, \bar{z} [\bar{u}, 0, 0]$	$0, \bar{y}, \bar{z} [u, 0, 0]$
$z, 0, y [0, u, 0]$	$z, 0, \bar{y} [0, \bar{u}, 0]$	$\bar{z}, 0, y [0, \bar{u}, 0]$	$\bar{z}, 0, \bar{y} [0, u, 0]$
$y, z, 0 [0, 0, u]$	$\bar{y}, z, 0 [0, 0, \bar{u}]$	$y, \bar{z}, 0 [0, 0, \bar{u}]$	$\bar{y}, \bar{z}, 0 [0, 0, u]$
$y+1/2, 1/2, \bar{z}+1/2 [0, \bar{u}, 0]$	$\bar{y}+1/2, 1/2, \bar{z}+1/2 [0, u, 0]$	$y+1/2, 1/2, z+1/2 [0, u, 0]$	$\bar{y}+1/2, 1/2, z+1/2 [0, \bar{u}, 0]$
$1/2, z+1/2, \bar{y}+1/2 [\bar{u}, 0, 0]$	$1/2, z+1/2, y+1/2 [u, 0, 0]$	$1/2, \bar{z}+1/2, \bar{y}+1/2 [u, 0, 0]$	$1/2, \bar{z}+1/2, y+1/2 [\bar{u}, 0, 0]$
$z+1/2, y+1/2, 1/2 [0, 0, u]$	$z+1/2, \bar{y}+1/2, 1/2 [0, 0, \bar{u}]$	$\bar{z}+1/2, y+1/2, 1/2 [0, 0, \bar{u}]$	$\bar{z}+1/2, \bar{y}+1/2, 1/2 [0, 0, u]$

96 h ..2'	$1/4, y, y [u, v, \bar{v}]$	$3/4, \bar{y}, y [\bar{u}, \bar{v}, \bar{v}]$	$3/4, y, \bar{y} [\bar{u}, v, v]$	$1/4, \bar{y}, \bar{y} [u, \bar{v}, \bar{v}]$
	$y, 1/4, y [\bar{v}, u, v]$	$y, 3/4, \bar{y} [\bar{v}, \bar{u}, \bar{v}]$	$\bar{y}, 3/4, y [v, \bar{u}, v]$	$\bar{y}, 1/4, \bar{y} [v, u, \bar{v}]$
	$y, y, 1/4 [v, \bar{v}, u]$	$\bar{y}, y, 3/4 [\bar{v}, \bar{v}, \bar{u}]$	$y, \bar{y}, 3/4 [v, v, \bar{u}]$	$\bar{y}, \bar{y}, 1/4 [v, v, u]$
	$3/4, \bar{y}, \bar{y} [u, v, \bar{v}]$	$1/4, y, \bar{y} [\bar{u}, \bar{v}, \bar{v}]$	$1/4, \bar{y}, y [\bar{u}, v, v]$	$3/4, y, y [u, \bar{v}, v]$
	$\bar{y}, 3/4, y [\bar{v}, u, v]$	$\bar{y}, 1/4, y [\bar{v}, \bar{u}, \bar{v}]$	$y, 1/4, \bar{y} [v, \bar{u}, v]$	$y, 3/4, y [v, u, \bar{v}]$
	$\bar{y}, \bar{y}, 3/4 [v, \bar{v}, u]$	$y, \bar{y}, 1/4 [\bar{v}, \bar{v}, \bar{u}]$	$\bar{y}, y, 1/4 [v, v, \bar{u}]$	$y, y, 3/4 [\bar{v}, v, u]$

64 g .3.

$x, x, x [u, u, u]$	$\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$	$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
$x+1/2, x+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, u]$	$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [u, u, u]$	$x+1/2, \bar{x}+1/2, x+1/2 [\bar{u}, u, \bar{u}]$	$\bar{x}+1/2, x+1/2, x+1/2 [u, \bar{u}, \bar{u}]$
$\bar{x}, \bar{x}, \bar{x} [u, u, u]$	$x, x, \bar{x} [\bar{u}, \bar{u}, u]$	$x, \bar{x}, x [\bar{u}, u, \bar{u}]$	$\bar{x}, x, x [u, \bar{u}, \bar{u}]$
$\bar{x}+1/2, \bar{x}+1/2, x+1/2 [\bar{u}, \bar{u}, u]$	$x+1/2, x+1/2, x+1/2 [u, u, u]$	$\bar{x}+1/2, x+1/2, \bar{x}+1/2 [\bar{u}, u, \bar{u}]$	$x+1/2, \bar{x}+1/2, \bar{x}+1/2 [u, \bar{u}, \bar{u}]$

Continued

226.4.1626

Fm $\bar{3}$ c'

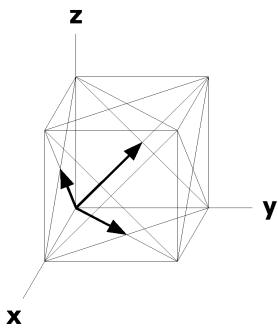
48	f	4'..	x,1/4,1/4 [0,0,0]	$\bar{x}$ ,3/4,1/4 [0,0,0]	1/4,x,1/4 [0,0,0]	1/4, $\bar{x}$ ,3/4 [0,0,0]
			1/4,1/4,x [0,0,0]	3/4,1/4, $\bar{x}$ [0,0,0]	$\bar{x}$ ,3/4,3/4 [0,0,0]	x,1/4,3/4 [0,0,0]
			3/4, $\bar{x}$ ,3/4 [0,0,0]	3/4,x,1/4 [0,0,0]	3/4,3/4, $\bar{x}$ [0,0,0]	1/4,3/4,x [0,0,0]
48	e	mm2..	x,0,0 [0,0,0]	$\bar{x}$ ,0,0 [0,0,0]	0,x,0 [0,0,0]	0, $\bar{x}$ ,0 [0,0,0]
			0,0,x [0,0,0]	0,0, $\bar{x}$ [0,0,0]	1/2,x+1/2,1/2 [0,0,0]	1/2, $\bar{x}$ +1/2,1/2 [0,0,0]
			x+1/2,1/2,1/2 [0,0,0]	$\bar{x}$ +1/2,1/2,1/2 [0,0,0]	1/2,1/2, $\bar{x}$ +1/2 [0,0,0]	1/2,1/2,x+1/2 [0,0,0]
24	d	4'/m..	0,1/4,1/4 [0,0,0]	0,3/4,1/4 [0,0,0]	1/4,0,1/4 [0,0,0]	
			1/4,0,3/4 [0,0,0]	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]	
24	c	$\bar{4}$ 'm.2'	1/4,0,0 [0,0,0]	3/4,0,0 [0,0,0]	0,1/4,0 [0,0,0]	
			0,3/4,0 [0,0,0]	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]	
8	b	m $\bar{3}$ .	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
8	a	4'32'	1/4,1/4,1/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,1,1] p6'mm'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

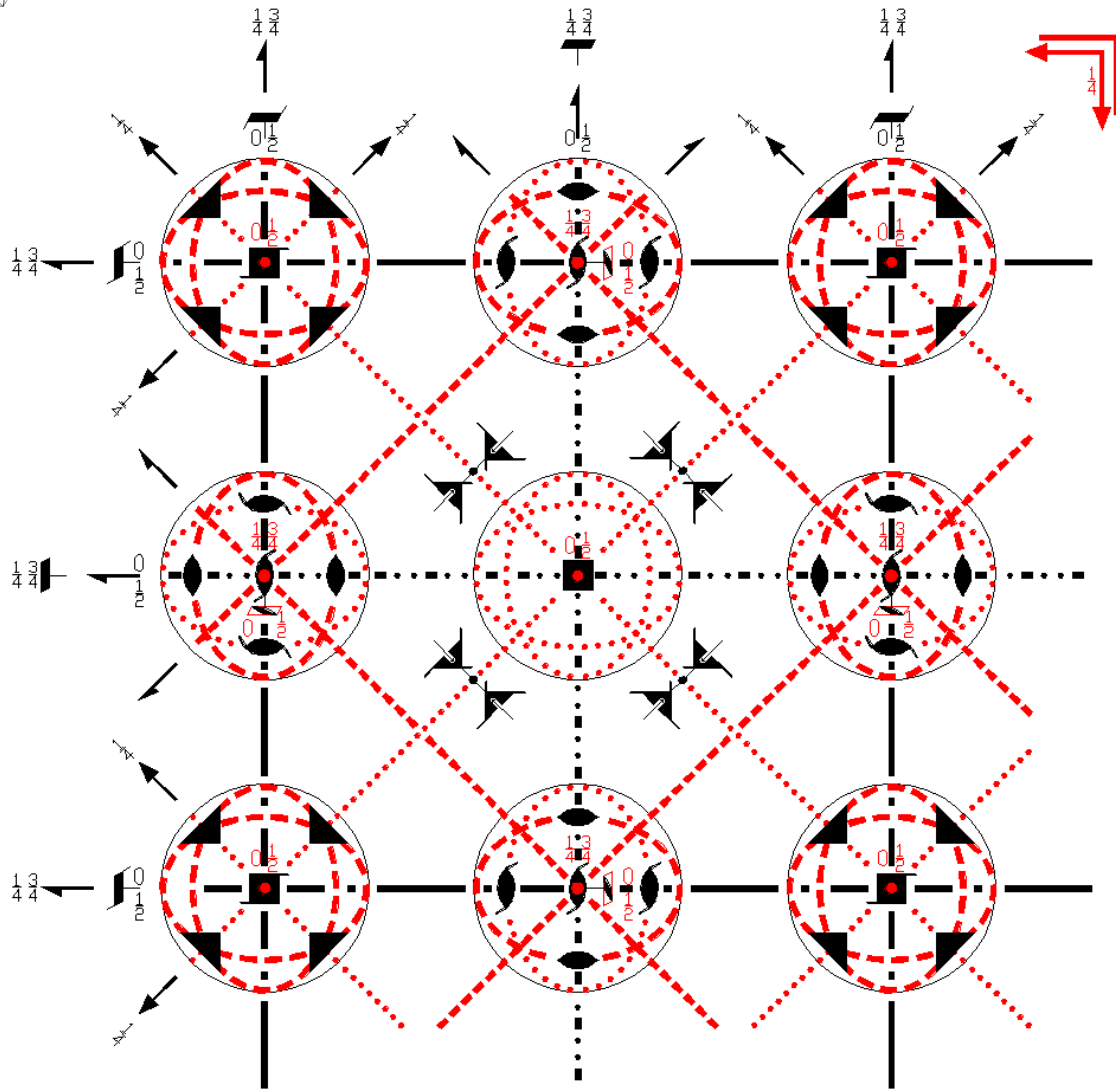
Along [1,1,0] p2'mm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/4$   
 Origin at x,x,0



Fm $\bar{3}$ 'c'  
226.5.1627

m $\bar{3}$ 'm'  
F4/m $\bar{3}$ '2/c'

Cubic



**Origin** at center (m $\bar{3}$ '')

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/4$ ;  $0 \leq z \leq 1/4$ ;  $y \leq \min(x, 1/2-x)$ ;  $z \leq y$

**Vertices** 0,0,0      1/2,0,0      1/4,1/4,0      1/4,1/4,1/4

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |   |
|---|--|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)             | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub> <sup>-1</sup>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)                                      | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub><math>\bar{xy}\bar{z}</math></sub>  0,0,0) | (12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)  |

(13) $2 (1/2, 1/2, 0) \ x, x, 1/4$ ( $2_{xy}   1/2, 1/2, 1/2$ )	(14) $2 \ x, \bar{x} + 1/2, 1/4$ ( $2_{\bar{xy}}   1/2, 1/2, 1/2$ )	(15) $4^- (0, 0, 1/2) \ 1/2, 0, z$ ( $4_z^{-1}   1/2, 1/2, 1/2$ )	(16) $4^+ (0, 0, 1/2) \ 0, 1/2, z$ ( $4_z   1/2, 1/2, 1/2$ )
(17) $4^- (1/2, 0, 0) \ x, 1/2, 0$ ( $4_x^{-1}   1/2, 1/2, 1/2$ )	(18) $2 (0, 1/2, 1/2) \ 1/4, y, y$ ( $2_{yz}   1/2, 1/2, 1/2$ )	(19) $2 \ 1/4, y + 1/2, \bar{y}$ ( $2_{\bar{yz}}   1/2, 1/2, 1/2$ )	(20) $4^+ (1/2, 0, 0) \ x, 0, 1/2$ ( $4_x   1/2, 1/2, 1/2$ )
(21) $4^+ (0, 1/2, 0) \ 1/2, y, 0$ ( $4_y   1/2, 1/2, 1/2$ )	(22) $2 (1/2, 0, 1/2) \ x, 1/4, x$ ( $2_{xz}   1/2, 1/2, 1/2$ )	(23) $4^- (0, 1/2, 0) \ 0, y, 1/2$ ( $4_y^{-1}   1/2, 1/2, 1/2$ )	(24) $2 \ \bar{x} + 1/2, 1/4, x$ ( $2_{\bar{xz}}   1/2, 1/2, 1/2$ )
(25) $\bar{1}^+ \ 0, 0, 0$ ( $\bar{1}   0, 0, 0$ )'	(26) $m' \ x, y, 0$ ( $m_z   0, 0, 0$ )'	(27) $m' \ x, 0, z$ ( $m_y   0, 0, 0$ )'	(28) $m' \ 0, y, z$ ( $m_x   0, 0, 0$ )'
(29) $\bar{3}^+ \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}   0, 0, 0$ )'	(30) $\bar{3}^+ \ \bar{x}, x, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xy}\bar{z}}^{-1}   0, 0, 0$ )'	(31) $\bar{3}^+ \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}^{-1}   0, 0, 0$ )'	(32) $\bar{3}^+ \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{\bar{xy}\bar{z}}^{-1}   0, 0, 0$ )'
(33) $\bar{3}^- \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}^{-1}   0, 0, 0$ )'	(34) $\bar{3}^- \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}   0, 0, 0$ )'	(35) $\bar{3}^- \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}   0, 0, 0$ )'	(36) $\bar{3}^- \ \bar{x}, x, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}   0, 0, 0$ )'
(37) $c' (0, 0, 1/2) \ x + 1/2, \bar{x}, z$ ( $m_{xy}   1/2, 1/2, 1/2$ )'	(38) $n' (1/2, 1/2, 1/2) \ x, x, z$ ( $m_{\bar{xy}}   1/2, 1/2, 1/2$ )'	(39) $\bar{4}^- \ 0, 1/2, z; 0, 1/2, 1/4$ ( $\bar{4}_z^{-1}   1/2, 1/2, 1/2$ )'	(40) $\bar{4}^+ \ 1/2, 0, z; 1/2, 0, 1/4$ ( $\bar{4}_z   1/2, 1/2, 1/2$ )'
(41) $\bar{4}^- \ x, 0, 1/2; 1/4, 0, 1/2$ ( $\bar{4}_x^{-1}   1/2, 1/2, 1/2$ )'	(42) $a' (1/2, 0, 0) \ x, y + 1/2, \bar{y}$ ( $m_{yz}   1/2, 1/2, 1/2$ )'	(43) $n' (1/2, 1/2, 1/2) \ x, y, y$ ( $m_{\bar{yz}}   1/2, 1/2, 1/2$ )'	(44) $\bar{4}^+ \ x, 1/2, 0; 1/4, 1/2, 0$ ( $\bar{4}_x   1/2, 1/2, 1/2$ )'
(45) $\bar{4}^+ \ 0, y, 1/2; 0, 1/4, 1/2$ ( $\bar{4}_y   1/2, 1/2, 1/2$ )'	(46) $b' (0, 1/2, 0) \ \bar{x} + 1/2, y, x$ ( $m_{xz}   1/2, 1/2, 1/2$ )'	(47) $\bar{4}^- \ 1/2, y, 0; 1/2, 1/4, 0$ ( $\bar{4}_y^{-1}   1/2, 1/2, 1/2$ )'	(48) $n' (1/2, 1/2, 1/2) \ x, y, x$ ( $m_{\bar{xz}}   1/2, 1/2, 1/2$ )'

For (0, 1/2, 1/2) + set

(1) $t (0, 1/2, 1/2)$ ( $1   0, 1/2, 1/2$ )	(2) $2 (0, 0, 1/2) \ 0, 1/4, z$ ( $2_z   0, 1/2, 1/2$ )	(3) $2 (0, 1/2, 0) \ 0, y, 1/4$ ( $2_y   0, 1/2, 1/2$ )	(4) $2 \ x, 1/4, 1/4$ ( $2_x   0, 1/2, 1/2$ )
(5) $3^+ (1/3, 1/3, 1/3)$ $x - 1/3, x - 1/6, x$ ( $3_{xyz}   0, 1/2, 1/2$ )	(6) $3^+ \ \bar{x}, x + 1/2, \bar{x}$ ( $3_{\bar{xyz}}^{-1}   0, 1/2, 1/2$ )	(7) $3^+ (-1/3, 1/3, 1/3)$ $x + 1/3, x - 1/6, x$ ( $3_{\bar{xyz}}^{-1}   0, 1/2, 1/2$ )	(8) $3^+ \ \bar{x}, \bar{x} + 1/2, x$ ( $3_{\bar{xyz}}^{-1}   0, 1/2, 1/2$ )
(9) $3^- (1/3, 1/3, 1/3)$ $x - 1/6, x + 1/6, x$ ( $3_{xyz}^{-1}   0, 1/2, 1/2$ )	(10) $3^- (-1/3, 1/3, 1/3)$ $x + 1/6, \bar{x} + 1/6, \bar{x}$ ( $3_{\bar{xyz}}   0, 1/2, 1/2$ )	(11) $3^- \ \bar{x} + 1/2, \bar{x} + 1/2, x$ ( $3_{\bar{xyz}}   0, 1/2, 1/2$ )	(12) $3^- \ \bar{x} - 1/2, x + 1/2, \bar{x}$ ( $3_{\bar{xyz}}   0, 1/2, 1/2$ )
(13) $2 (1/4, 1/4, 0) \ x, x - 1/4, 0$ ( $2_{xy}   1/2, 0, 0$ )	(14) $2 (1/4, -1/4, 0) \ x, \bar{x} + 1/4, 0$ ( $2_{\bar{xy}}   1/2, 0, 0$ )	(15) $4^- \ 1/4, -1/4, z$ ( $4_z^{-1}   1/2, 0, 0$ )	(16) $4^+ \ 1/4, 1/4, z$ ( $4_z   1/2, 0, 0$ )
(17) $4^- (1/2, 0, 0) \ x, 0, 0$ ( $4_x^{-1}   1/2, 0, 0$ )	(18) $2 \ 1/4, y, y$ ( $2_{yz}   1/2, 0, 0$ )	(19) $2 \ 1/4, y, \bar{y}$ ( $2_{\bar{yz}}   1/2, 0, 0$ )	(20) $4^+ (1/2, 0, 0) \ x, 0, 0$ ( $4_x   1/2, 0, 0$ )
(21) $4^+ \ 1/4, y, -1/4$ ( $4_y   1/2, 0, 0$ )	(22) $2 (1/4, 0, 1/4) \ x + 1/4, 0, x$ ( $2_{xz}   1/2, 0, 0$ )	(23) $4^- \ 1/4, y, 1/4$ ( $4_y^{-1}   1/2, 0, 0$ )	(24) $2 (1/4, 0, -1/4) \ \bar{x} + 1/4, 0, x$ ( $2_{\bar{xz}}   1/2, 0, 0$ )
(25) $\bar{1}^+ \ 0, 1/4, 1/4$ ( $\bar{1}   0, 1/2, 1/2$ )'	(26) $b' (0, 1/2, 0) \ x, y, 1/4$ ( $m_z   0, 1/2, 1/2$ )'	(27) $c' (0, 0, 1/2) \ x, 1/4, z$ ( $m_y   0, 1/2, 1/2$ )'	(28) $n' (0, 1/2, 1/2) \ 0, y, z$ ( $m_x   0, 1/2, 1/2$ )'
(29) $\bar{3}^+ \ x, x + 1/2, x;$ $0, 1/2, 0$ ( $\bar{3}_{xyz}   0, 1/2, 1/2$ )'	(30) $\bar{3}^+ \ \bar{x} - 1, x + 1/2, \bar{x};$ $-1/2, 0, 1/2$ ( $\bar{3}_{\bar{xyz}}^{-1}   0, 1/2, 1/2$ )'	(31) $\bar{3}^+ \ x, \bar{x} + 1/2, \bar{x};$ $0, 1/2, 0$ ( $\bar{3}_{\bar{xyz}}^{-1}   0, 1/2, 1/2$ )'	(32) $\bar{3}^+ \ \bar{x} - 1, \bar{x} + 1/2, x;$ $1/2, 0, 1/2$ ( $\bar{3}_{\bar{xyz}}^{-1}   0, 1/2, 1/2$ )'



- |   |  |   |  |
|---|--|---|--|
| (33) $\bar{3}^-$ ' x-1/2,x-1/2,x;<br>0,0,1/2<br>( $\bar{3}_{xyz}^{-1}$  0,1/2,1/2)' | (34) $\bar{3}^-$ ' x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ;<br>0,0,1/2<br>( $\bar{3}_{\bar{xyz}}$  0,1/2,1/2)' | (35) $\bar{3}^-$ ' $\bar{x}$ -1/2, $\bar{x}$ +1/2, x;<br>-1/2,1/2,0<br>( $\bar{3}_{xyz}$  0,1/2,1/2)' | (36) $\bar{3}^-$ ' $\bar{x}$ +1/2, x+1/2, $\bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{\bar{xyz}}$  0,1/2,1/2)' |
| (37) g' (1/4,-1/4,0) x+1/4, $\bar{x}$ ,z<br>( $m_{xy}$  1/2,0,0)'                   | (38) g' (1/4,1/4,0) x+1/4,x,z<br>( $m_{\bar{xy}}$  1/2,0,0)'   | (39) $\bar{4}^-$ ' 1/4,1/4,z; 1/4,1/4,0<br>( $\bar{4}_z^{-1}$  1/2,0,0)'                              | (40) $\bar{4}^+$ ' 1/4,-1/4,z; 1/4,-1/4,0<br>( $\bar{4}_z$  1/2,0,0)'                                      |
| (41) $\bar{4}^-$ ' x,0,0; 1/4,0,0<br>( $\bar{4}_x^{-1}$  1/2,0,0)'                  | (42) a' (1/2,0,0) x,y, $\bar{y}$<br>( $m_{yz}$  1/2,0,0)'  | (43) a' (1/2,0,0) x,y,y<br>( $m_{\bar{yz}}$  1/2,0,0)'  | (44) $\bar{4}^+$ ' x,0,0; 1/4,0,0<br>( $\bar{4}_x$  1/2,0,0)'  |
| (45) $\bar{4}^+$ ' 1/4,y,1/4; 1/4,0,1/4<br>( $\bar{4}_y$  1/2,0,0)'                 | (46) g' (1/4,0,-1/4) $\bar{x}$ +1/4,y,x<br>( $m_{xz}$  1/2,0,0)'   | (47) $\bar{4}^-$ ' 1/4,y,-1/4; 1/4,0,-1/4<br>( $\bar{4}_y^{-1}$  1/2,0,0)'                            | (48) g' (1/4,0,1/4) x+1/4,y,x<br>( $m_{\bar{xz}}$  1/2,0,0)'   |

For (1/2,0,1/2) + set

- |  |   |   |  |
|--|---|---|--|
| (1) t (1/2,0,1/2)<br>(1 1/2,0,1/2)   | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)  | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)  | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>  1/2,0,1/2)   |
| (5) 3 <sup>+</sup> (1/3,1/3,1/3)<br>x+1/6,x-1/6,x<br>(3 <sub>xyz</sub>  1/2,0,1/2)               | (6) 3 <sup>+</sup> (1/3,-1/3,1/3)<br>x+1/6,x+1/6, $\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,0,1/2) | (7) 3 <sup>+</sup> x+1/2, $\bar{x}$ -1/2, $\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub> <sup>-1</sup>  1/2,0,1/2) | (8) 3 <sup>+</sup> $\bar{x}$ +1/2, $\bar{x}$ +1/2,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2)                         |
| (9) 3 <sup>-</sup> (1/3,1/3,1/3)<br>x-1/6,x-1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) | (10) 3 <sup>-</sup> x+1/2, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub>  1/2,0,1/2)   | (11) 3 <sup>-</sup> $\bar{x}$ +1/2, $\bar{x}$ , x<br>(3 <sub><math>\bar{xyz}</math></sub>  1/2,0,1/2)                 | (12) 3 <sup>-</sup> (1/3,-1/3,1/3)<br>$\bar{x}$ -1/6, x+1/3, $\bar{x}$<br>(3 <sub><math>\bar{xyz}</math></sub>  1/2,0,1/2) |
| (13) 2 (1/4,1/4,0) x,x+1/4,0<br>(2 <sub>xy</sub>  0,1/2,0)                                       | (14) 2 (-1/4,1/4,0) x, $\bar{x}$ +1/4,0<br>(2 <sub><math>\bar{xy}</math></sub>  0,1/2,0)                                      | (15) 4 <sup>-</sup> 1/4,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,0)  | (16) 4 <sup>+</sup> -1/4,1/4,z<br>(4 <sub>z</sub>  0,1/2,0)  |
| (17) 4 <sup>-</sup> x,1/4,-1/4<br>(4 <sub>x</sub> <sup>-1</sup>  0,1/2,0)                        | (18) 2 (0,1/4,1/4) 0,y+1/4,y<br>(2 <sub>yz</sub>  0,1/2,0)  | (19) 2 (0,1/4,-1/4) 0,y+1/4, $\bar{y}$<br>(2 <sub><math>\bar{yz}</math></sub>  0,1/2,0)                               | (20) 4 <sup>+</sup> x,1/4,1/4<br>(4 <sub>x</sub>  0,1/2,0)   |
| (21) 4 <sup>+</sup> (0,1/2,0) 0,y,0<br>(4 <sub>y</sub>  0,1/2,0)                                 | (22) 2 x,1/4,x<br>(2 <sub>xz</sub>  0,1/2,0)  | (23) 4 <sup>-</sup> (0,1/2,0) 0,y,0<br>(4 <sub>y</sub> <sup>-1</sup>  0,1/2,0)  | (24) 2 $\bar{x}$ ,1/4,x<br>(2 <sub><math>\bar{xz}</math></sub>  0,1/2,0)   |
| (25) $\bar{1}^-$ 1/4,0,1/4<br>( $\bar{1}$  1/2,0,1/2)'   | (26) a' (1/2,0,0) x,y,1/4<br>( $m_z$  1/2,0,1/2)'   | (27) n' (1/2,0,1/2) x,0,z<br>( $m_y$  1/2,0,1/2)'   | (28) c' (0,0,1/2) 1/4,y,z<br>( $m_x$  1/2,0,1/2)'  |
| (29) $\bar{3}^+$ ' x-1/2,x-1/2,x;<br>0,0,1/2<br>( $\bar{3}_{xyz}$  1/2,0,1/2)'                   | (30) $\bar{3}^+$ ' $\bar{x}$ -1/2,x+1/2, $\bar{x}$ ;<br>0,0,1/2<br>( $\bar{3}_{\bar{xyz}}$ <sup>-1</sup>  1/2,0,1/2)'         | (31) $\bar{3}^+$ ' x+1/2, $\bar{x}$ +1/2, $\bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,0,1/2)'    | (32) $\bar{3}^+$ ' $\bar{x}$ +1/2, $\bar{x}$ -1/2,x;<br>1/2,-1/2,0<br>( $\bar{3}_{\bar{xyz}}$ <sup>-1</sup>  1/2,0,1/2)'   |
| (33) $\bar{3}^-$ ' x+1/2,x,x;<br>1/2,0,0<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,0,1/2)'         | (34) $\bar{3}^-$ ' x+1/2, $\bar{x}$ -1, $\bar{x}$ ;<br>0,-1/2,1/2<br>( $\bar{3}_{\bar{xyz}}$  1/2,0,1/2)'                     | (35) $\bar{3}^-$ ' $\bar{x}$ +1/2, $\bar{x}$ +1, x;<br>0,1/2,1/2<br>( $\bar{3}_{xyz}$  1/2,0,1/2)'                    | (36) $\bar{3}^-$ ' $\bar{x}$ +1/2, x, $\bar{x}$ ;<br>1/2,0,0<br>( $\bar{3}_{\bar{xyz}}$  1/2,0,1/2)'                       |
| (37) g' (-1/4,1/4,0) x+1/4, $\bar{x}$ ,z<br>( $m_{xy}$  0,1/2,0)'                                | (38) g' (1/4,1/4,0) x-1/4,x,z<br>( $m_{\bar{xy}}$  0,1/2,0)'  | (39) $\bar{4}^-$ ' -1/4,1/4,z; -1/4,1/4,0<br>( $\bar{4}_z^{-1}$  0,1/2,0)'  | (40) $\bar{4}^+$ ' 1/4,1/4,z; 1/4,1/4,0<br>( $\bar{4}_z$  0,1/2,0)'  |
| (41) $\bar{4}^-$ ' x,1/4,1/4; 0,1/4,1/4<br>( $\bar{4}_x^{-1}$  0,1/2,0)'                         | (42) g' (0,1/4,-1/4) x,y+1/4, $\bar{y}$<br>( $m_{yz}$  0,1/2,0)'  | (43) g' (0,1/4,1/4) x,y+1/4,y<br>( $m_{\bar{yz}}$  0,1/2,0)'  | (44) $\bar{4}^+$ ' x,1/4,-1/4; 0,1/4,-1/4<br>( $\bar{4}_x$  0,1/2,0)'  |
| (45) $\bar{4}^+$ ' 0,y,0; 0,1/4,0<br>( $\bar{4}_y$  0,1/2,0)'                                    | (46) b' (0,1/2,0) $\bar{x}$ ,y,x<br>( $m_{xz}$  0,1/2,0)'   | (47) $\bar{4}^-$ ' 0,y,0; 0,1/4,0<br>( $\bar{4}_y^{-1}$  0,1/2,0)'  | (48) b' (0,1/2,0) x,y,x<br>( $m_{\bar{xz}}$  0,1/2,0)'   |

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (1   1/2,1/2,0)	(2) 2 1/4,1/4,z (2 <sub>z</sub>   1/2,1/2,0)	(3) 2 (0,1/2,0) 1/4,y,0 (2 <sub>y</sub>   1/2,1/2,0)	(4) 2 (1/2,0,0) x,1/4,0 (2 <sub>x</sub>   1/2,1/2,0)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) 3 <sup>+</sup> $\bar{x}$ +1/2,x, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(7) 3 <sup>+</sup> x+1/2, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(8) 3 <sup>+</sup> (1/3,1/3,-1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) 3 <sup>-</sup> x, $\bar{x}$ +1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)	(11) 3 <sup>-</sup> (1/3,1/3,-1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub>   1/2,1/2,0)	(12) 3 <sup>-</sup> $\bar{x}$ , x+1/2, $\bar{x}$ (3 <sub>xyz</sub>   1/2,1/2,0)
(13) 2 x,x,1/4 (2 <sub>xy</sub>   0,0,1/2)	(14) 2 x, $\bar{x}$ ,1/4 (2 <sub>xy</sub>   0,0,1/2)	(15) 4 <sup>-</sup> (0,0,1/2) 0,0,z (4 <sub>z</sub> <sup>-1</sup>   0,0,1/2)	(16) 4 <sup>+</sup> (0,0,1/2) 0,0,z (4 <sub>z</sub>   0,0,1/2)
(17) 4 <sup>-</sup> x,1/4,1/4 (4 <sub>x</sub> <sup>-1</sup>   0,0,1/2)	(18) 2 (0,1/4,1/4) 0,y-1/4,y (2 <sub>yz</sub>   0,0,1/2)	(19) 2 (0,-1/4,1/4) 0,y+1/4, $\bar{y}$ (2 <sub>yz</sub>   0,0,1/2)	(20) 4 <sup>+</sup> x,-1/4,1/4 (4 <sub>x</sub>   0,0,1/2)
(21) 4 <sup>+</sup> 1/4,y,1/4 (4 <sub>y</sub>   0,0,1/2)	(22) 2 (1/4,0,1/4) x-1/4,0,x (2 <sub>xz</sub>   0,0,1/2)	(23) 4 <sup>-</sup> -1/4,y,1/4 (4 <sub>y</sub> <sup>-1</sup>   0,0,1/2)	(24) 2 (-1/4,0,1/4) $\bar{x}$ +1/4,0,x (2 <sub>xz</sub>   0,0,1/2)
(25) $\bar{1}$ ' 1/4,1/4,0 ( $\bar{1}$   1/2,1/2,0)'	(26) n' (1/2,1/2,0) x,y,0 (m <sub>z</sub>   1/2,1/2,0)'	(27) a' (1/2,0,0) x,1/4,z (m <sub>y</sub>   1/2,1/2,0)'	(28) b' (0,1/2,0) 1/4,y,z (m <sub>x</sub>   1/2,1/2,0)'
(29) $\bar{3}^+$ ' x+1/2,x,x; 1/2,0,0 ( $\bar{3}_{xyz}$   1/2,1/2,0)'	(30) $\bar{3}^+$ ' $\bar{x}$ -1/2,x+1, $\bar{x}$ ; 0,1/2,1/2 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)'	(31) $\bar{3}^+$ ' x-1/2, $\bar{x}$ +1, $\bar{x}$ ; 0,1/2,-1/2 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)'	(32) $\bar{3}^+$ ' $\bar{x}$ +1/2, $\bar{x}$ ,x; 1/2,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)'
(33) $\bar{3}^-$ ' x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)'	(34) $\bar{3}^-$ ' x+1, $\bar{x}$ -1/2, $\bar{x}$ ; 1/2,0,1/2 ( $\bar{3}_{xyz}$   1/2,1/2,0)'	(35) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ +1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$   1/2,1/2,0)'	(36) $\bar{3}^-$ ' $\bar{x}$ +1,x-1/2, $\bar{x}$ ; 1/2,0,-1/2 ( $\bar{3}_{xyz}$   1/2,1/2,0)'
(37) c' (0,0,1/2) x, $\bar{x}$ ,z (m <sub>xy</sub>   0,0,1/2)'	(38) c' (0,0,1/2) x,x,z (m <sub>xy</sub>   0,0,1/2)'	(39) $\bar{4}^-$ ' 0,0,z; 0,0,1/4 ( $\bar{4}_z$ <sup>-1</sup>   0,0,1/2)'	(40) $\bar{4}^+$ ' 0,0,z; 0,0,1/4 ( $\bar{4}_z$   0,0,1/2)'
(41) $\bar{4}^-$ ' x,-1/4,1/4; 0,-1/4,1/4 ( $\bar{4}_x$ <sup>-1</sup>   0,0,1/2)'	(42) g' (0,-1/4,1/4) x,y+1/4, $\bar{y}$ (m <sub>yz</sub>   0,0,1/2)'	(43) g' (0,1/4,1/4) x,y-1/4,y (m <sub>yz</sub>   0,0,1/2)'	(44) $\bar{4}^+$ ' x,1/4,1/4; 0,1/4,1/4 ( $\bar{4}_x$   0,0,1/2)'
(45) $\bar{4}^+$ ' -1/4,y,1/4; -1/4,0,1/4 ( $\bar{4}_y$   0,0,1/2)'	(46) g' (-1/4,0,1/4) $\bar{x}$ +1/4,y,x (m <sub>xz</sub>   0,0,1/2)'	(47) $\bar{4}^-$ ' 1/4,y,1/4; 1/4,0,1/4 ( $\bar{4}_y$ <sup>-1</sup>   0,0,1/2)'	(48) g' (1/4,0,1/4) x-1/4,y,x (m <sub>xz</sub>   0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

192	j	1	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +					
(1)	x,y,z	[u,v,w]	(2)	$\bar{x},\bar{y},z$	[ $\bar{u},\bar{v},w$ ]	(3)	$\bar{x},y,z$	[ $\bar{u},v,w$ ]	(4)	x, $\bar{y},z$	[u, $\bar{v},w$ ]
(5)	z,x,y	[w,u,v]	(6)	z, $\bar{x},\bar{y}$	[w, $\bar{u},\bar{v}$ ]	(7)	$\bar{z},x,y$	[ $\bar{w},u,v$ ]	(8)	$\bar{z},x,\bar{y}$	[ $\bar{w},u,\bar{v}$ ]

- (9)  $y, z, x [v, w, u]$  (10)  $\bar{y}, z, \bar{x} [\bar{v}, w, \bar{u}]$  (11)  $y, \bar{z}, \bar{x} [v, \bar{w}, \bar{u}]$  (12)  $\bar{y}, \bar{z}, x [\bar{v}, \bar{w}, u]$   
 (13)  $y+1/2, x+1/2, \bar{z}+1/2 [v, u, \bar{w}]$  (14)  $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2 [\bar{v}, \bar{u}, \bar{w}]$  (15)  $y+1/2, \bar{x}+1/2, z+1/2 [v, \bar{u}, w]$  (16)  $\bar{y}+1/2, x+1/2, z+1/2 [\bar{v}, u, w]$   
 (17)  $x+1/2, z+1/2, \bar{y}+1/2 [u, w, \bar{v}]$  (18)  $\bar{x}+1/2, z+1/2, y+1/2 [\bar{u}, w, v]$  (19)  $\bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2 [\bar{u}, \bar{w}, \bar{v}]$  (20)  $x+1/2, \bar{z}+1/2, y+1/2 [u, \bar{w}, v]$   
 (21)  $z+1/2, y+1/2, \bar{x}+1/2 [w, v, \bar{u}]$  (22)  $z+1/2, \bar{y}+1/2, x+1/2 [w, \bar{v}, u]$  (23)  $\bar{z}+1/2, y+1/2, x+1/2 [\bar{w}, v, u]$  (24)  $\bar{z}+1/2, \bar{y}+1/2, \bar{x}+1/2 [\bar{w}, \bar{v}, \bar{u}]$   
 (25)  $\bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$  (26)  $x, y, \bar{z} [u, v, \bar{w}]$  (27)  $x, \bar{y}, z [u, \bar{v}, w]$  (28)  $\bar{x}, y, z [\bar{u}, v, w]$   
 (29)  $\bar{z}, \bar{x}, \bar{y} [\bar{w}, \bar{u}, \bar{v}]$  (30)  $\bar{z}, x, y [\bar{w}, u, v]$  (31)  $z, x, \bar{y} [w, u, \bar{v}]$  (32)  $z, \bar{x}, y [w, \bar{u}, v]$   
 (33)  $\bar{y}, \bar{z}, \bar{x} [\bar{v}, \bar{w}, \bar{u}]$  (34)  $y, \bar{z}, x [v, \bar{w}, u]$  (35)  $\bar{y}, z, x [\bar{v}, w, u]$  (36)  $y, z, \bar{x} [v, w, \bar{u}]$   
 (37)  $\bar{y}+1/2, \bar{x}+1/2, z+1/2 [\bar{v}, \bar{u}, w]$  (38)  $y+1/2, x+1/2, z+1/2 [v, u, w]$  (39)  $\bar{y}+1/2, x+1/2, \bar{z}+1/2 [\bar{v}, u, \bar{w}]$  (40)  $y+1/2, \bar{x}+1/2, \bar{z}+1/2 [v, \bar{u}, \bar{w}]$   
 (41)  $\bar{x}+1/2, \bar{z}+1/2, y+1/2 [\bar{u}, \bar{w}, v]$  (42)  $x+1/2, \bar{z}+1/2, \bar{y}+1/2 [u, \bar{w}, \bar{v}]$  (43)  $x+1/2, z+1/2, y+1/2 [u, w, v]$  (44)  $\bar{x}+1/2, z+1/2, \bar{y}+1/2 [\bar{u}, w, \bar{v}]$   
 (45)  $\bar{z}+1/2, \bar{y}+1/2, x+1/2 [\bar{w}, \bar{v}, u]$  (46)  $\bar{z}+1/2, y+1/2, \bar{x}+1/2 [\bar{w}, v, \bar{u}]$  (47)  $z+1/2, \bar{y}+1/2, \bar{x}+1/2 [w, \bar{v}, \bar{u}]$  (48)  $z+1/2, y+1/2, x+1/2 [w, v, u]$

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- $0, y, z [0, v, w]$   $0, \bar{y}, z [0, \bar{v}, w]$   $0, y, \bar{z} [0, v, \bar{w}]$   $0, \bar{y}, \bar{z} [0, \bar{v}, \bar{w}]$   
 $z, 0, y [w, 0, v]$   $z, 0, \bar{y} [w, 0, \bar{v}]$   $\bar{z}, 0, y [\bar{w}, 0, v]$   $\bar{z}, 0, \bar{y} [\bar{w}, 0, \bar{v}]$   
 $y, z, 0 [v, w, 0]$   $\bar{y}, z, 0 [\bar{v}, w, 0]$   $y, \bar{z}, 0 [v, \bar{w}, 0]$   $\bar{y}, \bar{z}, 0 [\bar{v}, \bar{w}, 0]$   
 $y+1/2, 1/2, \bar{z}+1/2 [v, 0, \bar{w}]$   $\bar{y}+1/2, 1/2, \bar{z}+1/2 [\bar{v}, 0, \bar{w}]$   $y+1/2, 1/2, z+1/2 [v, 0, w]$   $\bar{y}+1/2, 1/2, z+1/2 [\bar{v}, 0, w]$   
 $1/2, z+1/2, \bar{y}+1/2 [0, w, \bar{v}]$   $1/2, z+1/2, y+1/2 [0, w, v]$   $1/2, \bar{z}+1/2, \bar{y}+1/2 [0, \bar{w}, \bar{v}]$   $1/2, \bar{z}+1/2, y+1/2 [0, \bar{w}, v]$   
 $z+1/2, y+1/2, 1/2 [w, v, 0]$   $z+1/2, \bar{y}+1/2, 1/2 [w, \bar{v}, 0]$   $\bar{z}+1/2, y+1/2, 1/2 [\bar{w}, v, 0]$   $\bar{z}+1/2, \bar{y}+1/2, 1/2 [\bar{w}, \bar{v}, 0]$
- 96 h ..2
- $1/4, y, y [0, v, v]$   $3/4, \bar{y}, y [0, \bar{v}, v]$   $3/4, y, \bar{y} [0, v, \bar{v}]$   $1/4, \bar{y}, \bar{y} [0, \bar{v}, \bar{v}]$   
 $y, 1/4, y [v, 0, v]$   $y, 3/4, \bar{y} [v, 0, \bar{v}]$   $\bar{y}, 3/4, y [\bar{v}, 0, v]$   $\bar{y}, 1/4, \bar{y} [\bar{v}, 0, \bar{v}]$   
 $y, y, 1/4 [v, v, 0]$   $\bar{y}, y, 3/4 [\bar{v}, v, 0]$   $y, \bar{y}, 3/4 [v, \bar{v}, 0]$   $\bar{y}, \bar{y}, 1/4 [\bar{v}, \bar{v}, 0]$   
 $3/4, \bar{y}, \bar{y} [0, \bar{v}, \bar{v}]$   $1/4, y, \bar{y} [0, v, \bar{v}]$   $1/4, \bar{y}, y [0, \bar{v}, v]$   $3/4, y, y [0, v, v]$   
 $\bar{y}, 3/4, y [\bar{v}, 0, \bar{v}]$   $\bar{y}, 1/4, y [\bar{v}, 0, v]$   $y, 1/4, \bar{y} [v, 0, \bar{v}]$   $y, 3/4, y [v, 0, v]$   
 $\bar{y}, \bar{y}, 3/4 [\bar{v}, \bar{v}, 0]$   $y, \bar{y}, 1/4 [v, \bar{v}, 0]$   $\bar{y}, y, 1/4 [\bar{v}, v, 0]$   $y, y, 3/4 [v, v, 0]$

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- $x, x, x [u, u, u]$   $\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$   $\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$   $x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$   
 $x+1/2, x+1/2, \bar{x}+1/2 [u, u, \bar{u}]$   $\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, \bar{u}]$   $x+1/2, \bar{x}+1/2, x+1/2 [u, \bar{u}, u]$   $\bar{x}+1/2, x+1/2, x+1/2 [\bar{u}, u, \bar{u}]$   
 $\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$   $x, x, \bar{x} [u, u, \bar{u}]$   $x, \bar{x}, x [u, \bar{u}, u]$   $\bar{x}, x, x [\bar{u}, u, \bar{u}]$   
 $\bar{x}+1/2, \bar{x}+1/2, x+1/2 [\bar{u}, \bar{u}, u]$   $x+1/2, x+1/2, x+1/2 [u, u, u]$   $\bar{x}+1/2, x+1/2, \bar{x}+1/2 [\bar{u}, u, \bar{u}]$   $x+1/2, \bar{x}+1/2, \bar{x}+1/2 [u, \bar{u}, \bar{u}]$

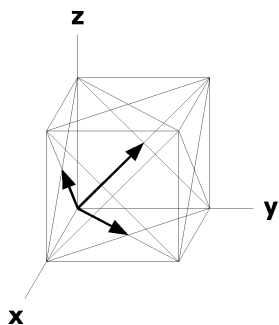
48	f	4..	x,1/4,1/4 [u,0,0]	$\bar{x}$ ,3/4,1/4 [ $\bar{u}$ ,0,0]	1/4,x,1/4 [0,u,0]	1/4, $\bar{x}$ ,3/4 [0, $\bar{u}$ ,0]
			1/4,1/4,x [0,0,u]	3/4,1/4, $\bar{x}$ [0,0, $\bar{u}$ ]	$\bar{x}$ ,3/4,3/4 [ $\bar{u}$ ,0,0]	x,1/4,3/4 [u,0,0]
			3/4, $\bar{x}$ ,3/4 [0, $\bar{u}$ ,0]	3/4,x,1/4 [0,u,0]	3/4,3/4, $\bar{x}$ [0,0, $\bar{u}$ ]	1/4,3/4,x [0,0,u]
48	e	m' $\bar{2}$ ..	x,0,0 [u,0,0]	$\bar{x}$ ,0,0 [ $\bar{u}$ ,0,0]	0,x,0 [0,u,0]	0, $\bar{x}$ ,0 [0, $\bar{u}$ ,0]
			0,0,x [0,0,u]	0,0, $\bar{x}$ [0,0, $\bar{u}$ ]	1/2,x+1/2,1/2 [0,u,0]	1/2, $\bar{x}$ +1/2,1/2 [0, $\bar{u}$ ,0]
			x+1/2,1/2,1/2 [u,0,0]	$\bar{x}$ +1/2,1/2,1/2 [ $\bar{u}$ ,0,0]	1/2,1/2, $\bar{x}$ +1/2 [0,0, $\bar{u}$ ]	1/2,1/2,x+1/2 [0,0,u]
24	d	4/m'..	0,1/4,1/4 [0,0,0]	0,3/4,1/4 [0,0,0]	1/4,0,1/4 [0,0,0]	
			1/4,0,3/4 [0,0,0]	1/4,1/4,0 [0,0,0]	3/4,1/4,0 [0,0,0]	
24	c	$\bar{4}$ 'm'.2	1/4,0,0 [0,0,0]	3/4,0,0 [0,0,0]	0,1/4,0 [0,0,0]	
			0,3/4,0 [0,0,0]	0,0,1/4 [0,0,0]	0,0,3/4 [0,0,0]	
8	b	m' $\bar{3}$ '.	0,0,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]		
8	a	432	1/4,1/4,1/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]		

### Symmetry of Special Projections

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 0,0,z

Along [1,1,1] p6m'm'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

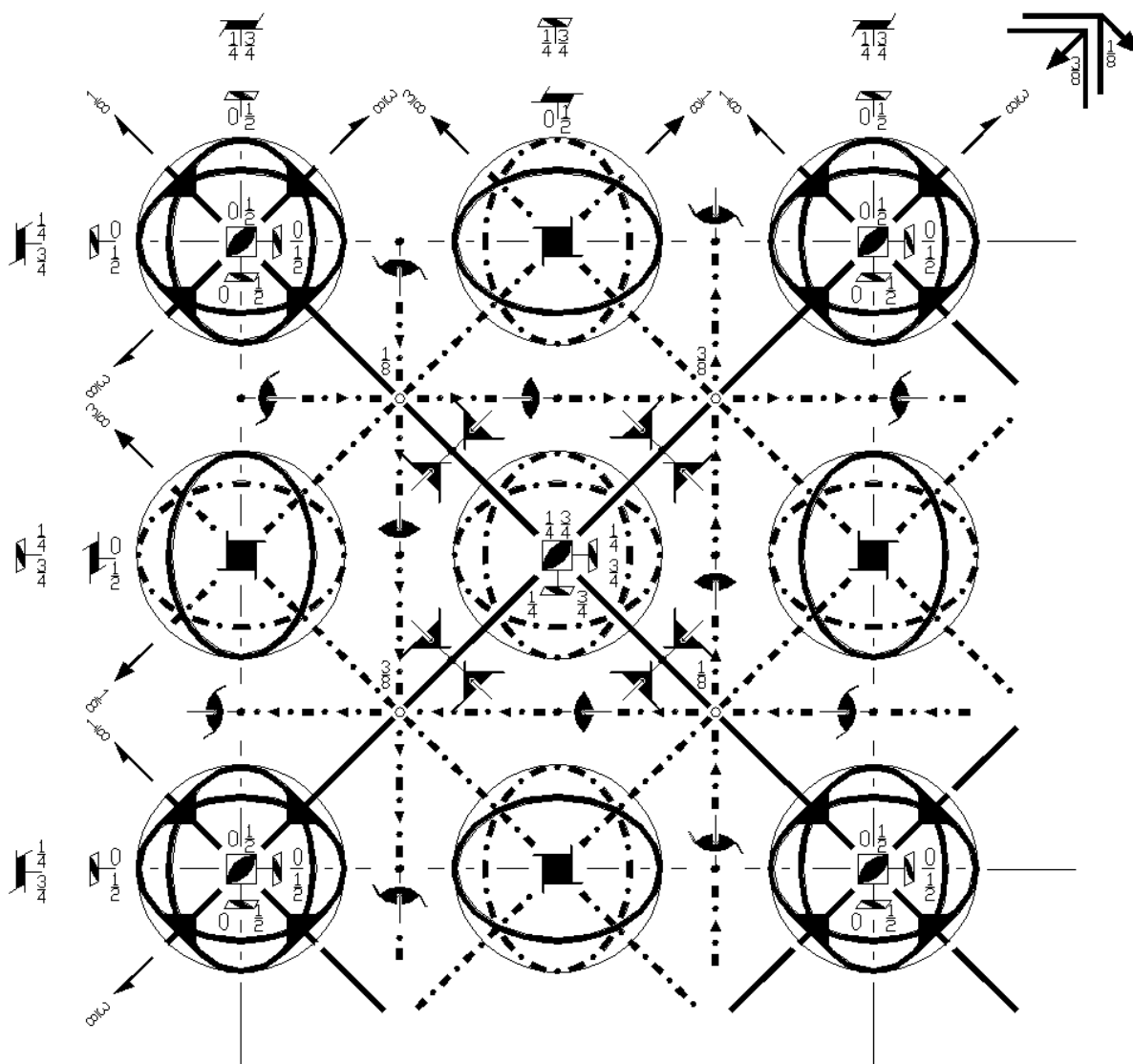
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/4$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$Fd\bar{3}m$   
227.1.1628

$m\bar{3}m$   
 $F4_1/d\bar{3}2/m$

Cubic



Origin at  $\bar{4}3m$ , at  $-1/8, -1/8, -1/8$  from center ( $\bar{3}m$ )

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/8$ ;  $-1/8 \leq z \leq 1/8$ ;  $y \leq \min(1/2-x, x)$ ;  $-y \leq z \leq y$

Vertices  $0,0,0$   $1/2,0,0$   $3/8,1/8,1/8$   $1/8,1/8,1/8$   $3/8,1/8,-1/8$   $1/8,1/8,-1/8$

### Symmetry Operations

For  $(0,0,0)$  + set

- |   |  |  |   |
|---|--|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)   | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)   | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>  1/2,0,1/2)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> (1/3,-1/3,1/3)<br>x+1/6,x+1/6,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) | (7) 3 <sup>+</sup> (-1/3,1/3,1/3)<br>x+1/3,x-1/6,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2) | (8) 3 <sup>+</sup> (1/3,1/3,-1/3)<br>x+1/6,x+1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x,x̄+1/2,x̄<br>(3 <sub>xyz</sub>  1/2,1/2,0)                                   | (11) 3 <sup>-</sup> x̄+1/2,x̄,x<br>(3 <sub>xy</sub>  1/2,0,1/2)                                    | (12) 3 <sup>-</sup> x̄-1/2,x+1/2,x̄<br>(3 <sub>xy</sub>  0,1/2,1/2)                               |

- (13)  $2 (1/2, 1/2, 0) \ x, x-1/4, 3/8$   
 $(2_{xy} | 3/4, 1/4, 3/4)$
- (17)  $4^- (3/4, 0, 0) \ x, 1/2, 1/4$   
 $(4_x^{-1} | 3/4, 1/4, 3/4)$
- (21)  $4^+ (0, 1/4, 0) \ 3/4, y, 0$   
 $(4_y | 3/4, 1/4, 3/4)$
- (25)  $\bar{1} \ 1/8, 1/8, 1/8$   
 $(\bar{1} | 1/4, 1/4, 1/4)$
- (29)  $\bar{3}^+ \ x, x, x;$   
 $1/8, 1/8, 1/8$   
 $(\bar{3}_{xyz} | 1/4, 1/4, 1/4)$
- (33)  $\bar{3}^- \ x, x, x;$   
 $1/8, 1/8, 1/8$   
 $(\bar{3}_{xyz}^{-1} | 1/4, 1/4, 1/4)$
- (37)  $g (1/4, -1/4, 1/2) \ x+1/4, \bar{x}, z$   
 $(m_{xy} | 1/2, 0, 1/2)$
- (41)  $\bar{4}^- \ x, -1/4, 1/4; \ 1/4, -1/4, 1/4$   
 $(\bar{4}_x^{-1} | 1/2, 0, 1/2)$
- (45)  $\bar{4}^+ \ 0, y, 1/2; \ 0, 0, 1/2$   
 $(\bar{4}_y | 1/2, 0, 1/2)$
- (14)  $2 \ x, \bar{x}+1/4, 1/8$   
 $(2_{xy} | 1/4, 1/4, 1/4)$
- (18)  $2 (0, 1/2, 1/2) \ 3/8, y+1/4, y$   
 $(2_{yz} | 3/4, 3/4, 1/4)$
- (22)  $2 (1/2, 0, 1/2) \ x-1/4, 3/8, x$   
 $(2_{xz} | 1/4, 3/4, 3/4)$
- (26)  $d (1/4, 3/4, 0) \ x, y, 3/8$   
 $(m_z | 1/4, 3/4, 3/4)$
- (30)  $\bar{3}^+ \ \bar{x}-1, x+1, \bar{x};$   
 $-1/8, 1/8, 7/8$   
 $(\bar{3}_{xyz}^{-1} | 3/4, 1/4, 3/4)$
- (34)  $\bar{3}^- \ x+3/2, \bar{x}-1, \bar{x};$   
 $5/8, -1/8, 7/8$   
 $(\bar{3}_{xyz} | 3/4, 3/4, 1/4)$
- (38)  $m \ x, x, z$   
 $(m_{xy} | 0, 0, 0)$
- (42)  $g (1/2, 1/4, -1/4) \ x, y+1/4, \bar{y}$   
 $(m_{yz} | 1/2, 1/2, 0)$
- (46)  $g (-1/4, 1/2, 1/4) \ \bar{x}+1/4, y, x$   
 $(m_{xz} | 0, 1/2, 1/2)$
- (15)  $4^- (0, 0, 3/4) \ 1/2, 1/4, z$   
 $(4_z^{-1} | 1/4, 3/4, 3/4)$
- (19)  $2 \ 1/8, y+1/4, \bar{y}$   
 $(2_{yz} | 1/4, 1/4, 1/4)$
- (23)  $4^- (0, 3/4, 0) \ 1/4, y, 1/2$   
 $(4_y^{-1} | 3/4, 3/4, 1/4)$
- (27)  $d (3/4, 0, 1/4) \ x, 3/8, z$   
 $(m_y | 3/4, 3/4, 1/4)$
- (31)  $\bar{3}^+ \ x, \bar{x}+1, \bar{x};$   
 $1/8, 7/8, -1/8$   
 $(\bar{3}_{xyz}^{-1} | 1/4, 3/4, 3/4)$
- (35)  $\bar{3}^- \ \bar{x}+1/2, \bar{x}+3/2, x;$   
 $-1/8, 7/8, 5/8$   
 $(\bar{3}_{xyz} | 3/4, 1/4, 3/4)$
- (39)  $\bar{4}^- \ -1/4, 1/4, z; \ -1/4, 1/4, 1/4$   
 $(\bar{4}_z^{-1} | 0, 1/2, 1/2)$
- (43)  $m \ x, y, y$   
 $(m_{yz} | 0, 0, 0)$
- (47)  $\bar{4}^- \ 1/4, y, -1/4; \ 1/4, 1/4, -1/4$   
 $(\bar{4}_y^{-1} | 1/2, 1/2, 0)$
- (16)  $4^+ (0, 0, 1/4) \ 0, 3/4, z$   
 $(4_z | 3/4, 3/4, 1/4)$
- (20)  $4^+ (1/4, 0, 0) \ x, 0, 3/4$   
 $(4_x | 1/4, 3/4, 3/4)$
- (24)  $2 \ \bar{x}+1/4, 1/8, x$   
 $(2_{xz} | 1/4, 1/4, 1/4)$
- (28)  $d (0, 1/4, 3/4) \ 3/8, y, z$   
 $(m_x | 3/4, 1/4, 3/4)$
- (32)  $\bar{3}^+ \ \bar{x}+1, \bar{x}, x;$   
 $7/8, -1/8, 1/8$   
 $(\bar{3}_{xyz}^{-1} | 3/4, 3/4, 1/4)$
- (36)  $\bar{3}^- \ \bar{x}+1, x+1/2, \bar{x};$   
 $7/8, 5/8, -1/8$   
 $(\bar{3}_{xyz} | 1/4, 3/4, 3/4)$
- (40)  $\bar{4}^+ \ 1/2, 0, z; \ 1/2, 0, 0$   
 $(\bar{4}_z | 1/2, 1/2, 0)$
- (44)  $\bar{4}^+ \ x, 1/2, 0; \ 0, 1/2, 0$   
 $(\bar{4}_x | 0, 1/2, 1/2)$
- (48)  $m \ x, y, x$   
 $(m_{xz} | 0, 0, 0)$

For (0, 1/2, 1/2) + set

- (1)  $t (0, 1/2, 1/2)$   
 $(1 | 0, 1/2, 1/2)$
- (5)  $3^+ (1/3, 1/3, 1/3)$   
 $x-1/3, x-1/6, x$   
 $(3_{xyz} | 0, 1/2, 1/2)$
- (9)  $3^- (1/3, 1/3, 1/3)$   
 $x-1/6, x+1/6, x$   
 $(3_{xyz}^{-1} | 0, 1/2, 1/2)$
- (13)  $2 (3/4, 3/4, 0) \ x, x, 1/8$   
 $(2_{xy} | 3/4, 3/4, 1/4)$
- (17)  $4^- (3/4, 0, 0) \ x, 1/2, -1/4$   
 $(4_x^{-1} | 3/4, 3/4, 1/4)$
- (21)  $4^+ (0, 3/4, 0) \ 1/2, y, -1/4$   
 $(4_y | 3/4, 3/4, 1/4)$
- (25)  $\bar{1} \ 1/8, 3/8, 3/8$   
 $(\bar{1} | 1/4, 3/4, 3/4)$
- (29)  $\bar{3}^+ \ x, x+1/2, x;$   
 $1/8, 5/8, 1/8$   
 $(\bar{3}_{xyz} | 1/4, 3/4, 3/4)$
- (2)  $2 \ 0, 0, z$   
 $(2_z | 0, 0, 0)$
- (6)  $3^+ \ \bar{x}+1/2, x, \bar{x}$   
 $(3_{xyz}^{-1} | 1/2, 1/2, 0)$
- (10)  $3^- \ x+1/2, \bar{x}, \bar{x}$   
 $(3_{xyz} | 1/2, 0, 1/2)$
- (14)  $2 (-1/4, 1/4, 0) \ x, \bar{x}+1/2, 3/8$   
 $(2_{xy} | 1/4, 3/4, 3/4)$
- (18)  $2 (0, 1/2, 1/2) \ 3/8, y-1/4, y$   
 $(2_{yz} | 3/4, 1/4, 3/4)$
- (22)  $2 (1/4, 0, 1/4) \ x, 1/8, x$   
 $(2_{xz} | 1/4, 1/4, 1/4)$
- (26)  $d (1/4, 1/4, 0) \ x, y, 1/8$   
 $(m_z | 1/4, 1/4, 1/4)$
- (30)  $\bar{3}^+ \ \bar{x}-1, x+3/2, \bar{x};$   
 $-1/8, 5/8, 7/8$   
 $(\bar{3}_{xyz}^{-1} | 3/4, 3/4, 1/4)$
- (3)  $2 \ 1/4, y, 1/4$   
 $(2_y | 1/2, 0, 1/2)$
- (7)  $3^+ \ x, \bar{x}, \bar{x}$   
 $(3_{xyz}^{-1} | 0, 0, 0)$
- (11)  $3^- (1/3, 1/3, -1/3)$   
 $x+1/3, x+1/6, x$   
 $(3_{xyz} | 1/2, 1/2, 0)$
- (15)  $4^- (0, 0, 1/4) \ 1/4, 0, z$   
 $(4_z^{-1} | 1/4, 1/4, 1/4)$
- (19)  $2 \ 1/8, y+3/4, \bar{y}$   
 $(2_{yz} | 1/4, 3/4, 3/4)$
- (23)  $4^- (0, 1/4, 0) \ 0, y, 3/4$   
 $(4_y^{-1} | 3/4, 1/4, 3/4)$
- (27)  $d (3/4, 0, 3/4) \ x, 1/8, z$   
 $(m_y | 3/4, 1/4, 3/4)$
- (31)  $\bar{3}^+ \ x, \bar{x}+1/2, \bar{x};$   
 $1/8, 3/8, -1/8$   
 $(\bar{3}_{xyz}^{-1} | 1/4, 1/4, 1/4)$
- (4)  $2 (1/2, 0, 0) \ x, 1/4, 0$   
 $(2_x | 1/2, 1/2, 0)$
- (8)  $3^+ \ \bar{x}+1/2, \bar{x}+1/2, x$   
 $(3_{xyz}^{-1} | 1/2, 0, 1/2)$
- (12)  $3^- \ \bar{x}, x, \bar{x}$   
 $(3_{xyz} | 0, 0, 0)$
- (16)  $4^+ (0, 0, 3/4) \ 1/4, 1/2, z$   
 $(4_z | 3/4, 1/4, 3/4)$
- (20)  $4^+ (1/4, 0, 0) \ x, 0, 1/4$   
 $(4_x | 1/4, 1/4, 1/4)$
- (24)  $2 (-1/4, 0, 1/4) \ \bar{x}+1/2, 3/8, x$   
 $(2_{xz} | 1/4, 3/4, 3/4)$
- (28)  $d (0, 3/4, 1/4) \ 3/8, y, z$   
 $(m_x | 3/4, 3/4, 1/4)$
- (32)  $\bar{3}^+ \ \bar{x}+1, \bar{x}-1/2, x;$   
 $7/8, -5/8, 1/8$   
 $(\bar{3}_{xyz}^{-1} | 3/4, 1/4, 3/4)$

- (33)  $\bar{3}^-$   $x-1/2, x-1/2, x;$   
 $1/8, 1/8, 5/8$   
 $(\bar{3}_{xyz}^{-1} | 1/4, 3/4, 3/4)$
- (34)  $\bar{3}^-$   $x+1, \bar{x}-3/2, \bar{x};$   
 $1/8, -5/8, 7/8$   
 $(\bar{3}_{\bar{xyz}} | 3/4, 1/4, 3/4)$
- (35)  $\bar{3}^-$   $\bar{x}, \bar{x}+1, x;$   
 $-1/8, 7/8, 1/8$   
 $(\bar{3}_{\bar{xyz}} | 3/4, 3/4, 1/4)$
- (36)  $\bar{3}^-$   $\bar{x}+1/2, x, \bar{x};$   
 $3/8, 1/8, -1/8$   
 $(\bar{3}_{\bar{xyz}} | 1/4, 1/4, 1/4)$
- (37)  $m$   $x+1/2, \bar{x}, z$   
 $(m_{xy} | 1/2, 1/2, 0)$
- (38)  $g$   $(1/4, 1/4, 1/2)$   $x-1/4, x, z$   
 $(m_{\bar{xy}} | 0, 1/2, 1/2)$
- (39)  $\bar{4}^-$   $0, 0, z; 0, 0, 0$   
 $(\bar{4}_z^{-1} | 0, 0, 0)$
- (40)  $\bar{4}^+$   $1/4, -1/4, z; 1/4, -1/4, 1/4$   
 $(\bar{4}_z | 1/2, 0, 1/2)$
- (41)  $\bar{4}^-$   $x, 1/4, 1/4; 1/4, 1/4, 1/4$   
 $(\bar{4}_x^{-1} | 1/2, 1/2, 0)$
- (42)  $g$   $(1/2, -1/4, 1/4)$   $x, y+1/4, \bar{y}$   
 $(m_{yz} | 1/2, 0, 1/2)$
- (43)  $g$   $(0, 1/2, 1/2)$   $x, y, y$   
 $(m_{\bar{yz}} | 0, 1/2, 1/2)$
- (44)  $\bar{4}^+$   $x, 0, 0; 0, 0, 0$   
 $(\bar{4}_x | 0, 0, 0)$
- (45)  $\bar{4}^+$   $1/4, y, 1/4; 1/4, 1/4, 1/4$   
 $(\bar{4}_y | 1/2, 1/2, 0)$
- (46)  $m$   $\bar{x}, y, x$   
 $(m_{xz} | 0, 0, 0)$
- (47)  $\bar{4}^-$   $1/2, y, 0; 1/2, 0, 0$   
 $(\bar{4}_y^{-1} | 1/2, 0, 1/2)$
- (48)  $g$   $(1/4, 1/2, 1/4)$   $x-1/4, y, x$   
 $(m_{\bar{xz}} | 0, 1/2, 1/2)$

For  $(1/2, 0, 1/2)$  + set

- (1)  $t$   $(1/2, 0, 1/2)$   
 $(1 | 1/2, 0, 1/2)$
- (2)  $2$   $1/4, 1/4, z$   
 $(2_z | 1/2, 1/2, 0)$
- (3)  $2$   $(0, 1/2, 0)$   $0, y, 1/4$   
 $(2_y | 0, 1/2, 1/2)$
- (4)  $2$   $x, 0, 0$   
 $(2_x | 0, 0, 0)$
- (5)  $3^+$   $(1/3, 1/3, 1/3)$   
 $x+1/6, x-1/6, x$   
 $(3_{xyz} | 1/2, 0, 1/2)$
- (6)  $3^+$   $\bar{x}, x, \bar{x}$   
 $(3_{\bar{xyz}}^{-1} | 0, 0, 0)$
- (7)  $3^+$   $x+1/2, \bar{x}, \bar{x}$   
 $(3_{\bar{xyz}}^{-1} | 1/2, 1/2, 0)$
- (8)  $3^+$   $\bar{x}, \bar{x}+1/2, x$   
 $(3_{xyz}^{-1} | 0, 1/2, 1/2)$
- (9)  $3^-$   $(1/3, 1/3, 1/3)$   
 $x-1/6, x-1/3, x$   
 $(3_{xyz}^{-1} | 1/2, 0, 1/2)$
- (10)  $3^-$   $(-1/3, 1/3, 1/3)$   
 $x+1/6, \bar{x}+1/6, \bar{x}$   
 $(3_{\bar{xyz}} | 0, 1/2, 1/2)$
- (11)  $3^-$   $\bar{x}, \bar{x}, x$   
 $(3_{\bar{yz}} | 0, 0, 0)$
- (12)  $3^-$   $\bar{x}, x+1/2, \bar{x}$   
 $(3_{\bar{yz}} | 1/2, 1/2, 0)$
- (13)  $2$   $(1/4, 1/4, 0)$   $x, x, 1/8$   
 $(2_{xy} | 1/4, 1/4, 1/4)$
- (14)  $2$   $(1/4, -1/4, 0)$   $x, \bar{x}+1/2, 3/8$   
 $(2_{\bar{xy}} | 3/4, 1/4, 3/4)$
- (15)  $4^-$   $(0, 0, 1/4)$   $3/4, 0, z$   
 $(4_z^{-1} | 3/4, 3/4, 1/4)$
- (16)  $4^+$   $(0, 0, 3/4)$   $-1/4, 1/2, z$   
 $(4_z | 1/4, 3/4, 3/4)$
- (17)  $4^-$   $(1/4, 0, 0)$   $x, 1/4, 0$   
 $(4_x^{-1} | 1/4, 1/4, 1/4)$
- (18)  $2$   $(0, 3/4, 3/4)$   $1/8, y, y$   
 $(2_{yz} | 1/4, 3/4, 3/4)$
- (19)  $2$   $(0, -1/4, 1/4)$   $3/8, y+1/2, \bar{y}$   
 $(2_{\bar{yz}} | 3/4, 1/4, 3/4)$
- (20)  $4^+$   $(3/4, 0, 0)$   $x, 1/4, 1/2$   
 $(4_x | 3/4, 3/4, 1/4)$
- (21)  $4^+$   $(0, 1/4, 0)$   $1/4, y, 0$   
 $(4_y | 1/4, 1/4, 1/4)$
- (22)  $2$   $(1/2, 0, 1/2)$   $x+1/4, 3/8, x$   
 $(2_{xz} | 3/4, 3/4, 1/4)$
- (23)  $4^-$   $(0, 3/4, 0)$   $-1/4, y, 1/2$   
 $(4_y^{-1} | 1/4, 3/4, 3/4)$
- (24)  $2$   $\bar{x}+3/4, 1/8, x$   
 $(2_{\bar{xz}} | 3/4, 1/4, 3/4)$
- (25)  $\bar{1}$   $3/8, 1/8, 3/8$   
 $(\bar{1} | 3/4, 1/4, 3/4)$
- (26)  $d$   $(3/4, 3/4, 0)$   $x, y, 1/8$   
 $(m_z | 3/4, 3/4, 1/4)$
- (27)  $d$   $(1/4, 0, 3/4)$   $x, 3/8, z$   
 $(m_y | 1/4, 3/4, 3/4)$
- (28)  $d$   $(0, 1/4, 1/4)$   $1/8, y, z$   
 $(m_x | 1/4, 1/4, 1/4)$
- (29)  $\bar{3}^+$   $x-1/2, x-1/2, x;$   
 $1/8, 1/8, 5/8$   
 $(\bar{3}_{xyz} | 3/4, 1/4, 3/4)$
- (30)  $\bar{3}^+$   $\bar{x}-1/2, x+1/2, \bar{x};$   
 $-1/8, 1/8, 3/8$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 1/4, 1/4, 1/4)$
- (31)  $\bar{3}^+$   $x-1/2, \bar{x}+3/2, \bar{x};$   
 $1/8, 7/8, -5/8$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 3/4, 3/4, 1/4)$
- (32)  $\bar{3}^+$   $\bar{x}+3/2, \bar{x}+1/2, x;$   
 $7/8, -1/8, 5/8$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 1/4, 3/4, 3/4)$
- (33)  $\bar{3}^-$   $x+1/2, x, x;$   
 $5/8, 1/8, 1/8$   
 $(\bar{3}_{xyz}^{-1} | 3/4, 1/4, 3/4)$
- (34)  $\bar{3}^-$   $x+1, \bar{x}-1, \bar{x};$   
 $1/8, -1/8, 7/8$   
 $(\bar{3}_{\bar{xyz}} | 1/4, 3/4, 3/4)$
- (35)  $\bar{3}^-$   $\bar{x}, \bar{x}+1/2, x;$   
 $-1/8, 3/8, 1/8$   
 $(\bar{3}_{\bar{yz}} | 1/4, 1/4, 1/4)$
- (36)  $\bar{3}^-$   $\bar{x}+3/2, x-1/2, \bar{x};$   
 $7/8, 1/8, -5/8$   
 $(\bar{3}_{\bar{yz}} | 3/4, 3/4, 1/4)$
- (37)  $m$   $x, \bar{x}, z$   
 $(m_{xy} | 0, 0, 0)$
- (38)  $g$   $(1/4, 1/4, 1/2)$   $x+1/4, x, z$   
 $(m_{\bar{xy}} | 1/2, 0, 1/2)$
- (39)  $\bar{4}^-$   $0, 1/2, z; 0, 1/2, 0$   
 $(\bar{4}_z^{-1} | 1/2, 1/2, 0)$
- (40)  $\bar{4}^+$   $1/4, 1/4, z; 1/4, 1/4, 1/4$   
 $(\bar{4}_z | 0, 1/2, 1/2)$
- (41)  $\bar{4}^-$   $x, 0, 0; 0, 0, 0$   
 $(\bar{4}_x^{-1} | 0, 0, 0)$
- (42)  $m$   $x, y+1/2, \bar{y}$   
 $(m_{yz} | 0, 1/2, 1/2)$
- (43)  $g$   $(1/2, 1/4, 1/4)$   $x, y-1/4, y$   
 $(m_{\bar{yz}} | 1/2, 0, 1/2)$
- (44)  $\bar{4}^+$   $x, 1/4, -1/4; 1/4, 1/4, -1/4$   
 $(\bar{4}_x | 1/2, 1/2, 0)$
- (45)  $\bar{4}^+$   $0, y, 0; 0, 0, 0$   
 $(\bar{4}_y | 0, 0, 0)$
- (46)  $g$   $(1/4, 1/2, -1/4)$   $\bar{x}+1/4, y, x$   
 $(m_{xz} | 1/2, 1/2, 0)$
- (47)  $\bar{4}^-$   $1/4, y, 1/4; 1/4, 1/4, 1/4$   
 $(\bar{4}_y^{-1} | 0, 1/2, 1/2)$
- (48)  $g$   $(1/2, 0, 1/2)$   $x, y, x$   
 $(m_{\bar{xz}} | 1/2, 0, 1/2)$

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (1   1/2,1/2,0)	(2) 2 (0,0,1/2) 1/4,0,z (2 <sub>z</sub>   1/2,0,1/2)	(3) 2 0,y,0 (2 <sub>y</sub>   0,0,0)	(4) 2 x,1/4,1/4 (2 <sub>x</sub>   0,1/2,1/2)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) 3 <sup>+</sup> $\bar{x}$ ,x+1/2, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   0,1/2,1/2)	(7) 3 <sup>+</sup> x+1/2, $\bar{x}$ -1/2, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,0,1/2)	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x (3 <sub>xyz</sub> <sup>-1</sup>   0,0,0)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub>   0,0,0)	(11) 3 <sup>-</sup> $\bar{x}$ +1/2, $\bar{x}$ +1/2, x (3 <sub>xyz</sub>   0,1/2,1/2)	(12) 3 <sup>-</sup> (1/3,-1/3,1/3) x-1/6, x+1/3, $\bar{x}$ (3 <sub>xyz</sub>   1/2,0,1/2)
(13) 2 (1/2,1/2,0) x,x+1/4,3/8 (2 <sub>xy</sub>   1/4,3/4,3/4)	(14) 2 x, $\bar{x}$ +3/4,1/8 (2 <sub>xy</sub>   3/4,3/4,1/4)	(15) 4 <sup>-</sup> (0,0,3/4) 1/2,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   3/4,1/4,3/4)	(16) 4 <sup>+</sup> (0,0,1/4) 0,1/4,z (4 <sub>z</sub>   1/4,1/4,1/4)
(17) 4 <sup>-</sup> (1/4,0,0) x,3/4,0 (4 <sub>x</sub> <sup>-1</sup>   1/4,3/4,3/4)	(18) 2 (0,1/4,1/4) 1/8,y,y (2 <sub>yz</sub>   1/4,1/4,1/4)	(19) 2 (0,1/4,-1/4) 3/8,y+1/2, $\bar{y}$ (2 <sub>yz</sub>   3/4,3/4,1/4)	(20) 4 <sup>+</sup> (3/4,0,0) x,-1/4,1/2 (4 <sub>x</sub>   3/4,1/4,3/4)
(21) 4 <sup>+</sup> (0,3/4,0) 1/2,y,1/4 (4 <sub>y</sub>   1/4,3/4,3/4)	(22) 2 (3/4,0,3/4) x,1/8,x (2 <sub>xz</sub>   3/4,1/4,3/4)	(23) 4 <sup>-</sup> (0,1/4,0) 0,y,1/4 (4 <sub>y</sub> <sup>-1</sup>   1/4,1/4,1/4)	(24) 2 (1/4,0,-1/4) $\bar{x}$ +1/2,3/8,x (2 <sub>xz</sub>   3/4,3/4,1/4)
(25) $\bar{1}$ 3/8,3/8,1/8 ( $\bar{1}$   3/4,3/4,1/4)	(26) d (3/4,1/4,0) x,y,3/8 (m <sub>z</sub>   3/4,1/4,3/4)	(27) d (1/4,0,1/4) x,1/8,z (m <sub>y</sub>   1/4,1/4,1/4)	(28) d (0,3/4,3/4) 1/8,y,z (m <sub>x</sub>   1/4,3/4,3/4)
(29) $\bar{3}^+$ x+1/2,x,x; 5/8,1/8,1/8 ( $\bar{3}_{xyz}$   3/4,3/4,1/4)	(30) $\bar{3}^+$ $\bar{x}$ -3/2,x+1, $\bar{x}$ ; -5/8,1/8,7/8 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/4,3/4,3/4)	(31) $\bar{3}^+$ x+1/2, $\bar{x}$ +1, $\bar{x}$ ; 5/8,7/8,-1/8 ( $\bar{3}_{xyz}$ <sup>-1</sup>   3/4,1/4,3/4)	(32) $\bar{3}^+$ $\bar{x}$ +1/2, $\bar{x}$ ,x; 3/8,-1/8,1/8 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/4,1/4,1/4)
(33) $\bar{3}^-$ x,x+1/2,x; 1/8,5/8,1/8 ( $\bar{3}_{xyz}$ <sup>-1</sup>   3/4,3/4,1/4)	(34) $\bar{3}^-$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ; 1/8,-1/8,3/8 ( $\bar{3}_{xyz}$   1/4,1/4,1/4)	(35) $\bar{3}^-$ $\bar{x}$ -1/2, $\bar{x}$ +1, x; -5/8,7/8,1/8 ( $\bar{3}_{xyz}$   1/4,3/4,3/4)	(36) $\bar{3}^-$ $\bar{x}$ +1, x, $\bar{x}$ ; 7/8,1/8,-1/8 ( $\bar{3}_{xyz}$   3/4,1/4,3/4)
(37) g (-1/4,1/4,1/2) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   0,1/2,1/2)	(38) g (1/2,1/2,0) x,x,z (m <sub>xy</sub>   1/2,1/2,0)	(39) $\bar{4}^-$ 1/4,1/4,z; 1/4,1/4,1/4 ( $\bar{4}_z$ <sup>-1</sup>   1/2,0,1/2)	(40) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}_z$   0,0,0)
(41) $\bar{4}^-$ x,0,1/2; 0,0,1/2 ( $\bar{4}_x$ <sup>-1</sup>   0,1/2,1/2)	(42) m x,y, $\bar{y}$ (m <sub>yz</sub>   0,0,0)	(43) g (1/2,1/4,1/4) x,y+1/4,y (m <sub>yz</sub>   1/2,1/2,0)	(44) $\bar{4}^+$ x,1/4,1/4; 1/4,1/4,1/4 ( $\bar{4}_x$   1/2,0,1/2)
(45) $\bar{4}^+$ -1/4,y,1/4; -1/4,1/4,1/4 ( $\bar{4}_y$   0,1/2,1/2)	(46) m $\bar{x}$ +1/2,y,x (m <sub>xz</sub>   1/2,0,1/2)	(47) $\bar{4}^-$ 0,y,0; 0,0,0 ( $\bar{4}_y$ <sup>-1</sup>   0,0,0)	(48) g (1/4,1/2,1/4) x+1/4,y,x (m <sub>xz</sub>   1/2,1/2,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

192	i	1	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +					
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}$ , $\bar{y}$ +1/2,z+1/2	[ $\bar{u}$ , $\bar{v}$ ,w]	(3)	$\bar{x}$ +1/2,y+1/2, $\bar{z}$	[ $\bar{u}$ ,v, $\bar{w}$ ]	(4)	x+1/2, $\bar{y}$ , $\bar{z}$ +1/2	[u, $\bar{v}$ , $\bar{w}$ ]
(5)	z,x,y	[w,u,v]	(6)	z+1/2, $\bar{x}$ , $\bar{y}$ +1/2	[w, $\bar{u}$ , $\bar{v}$ ]	(7)	$\bar{z}$ , $\bar{x}$ +1/2,y+1/2	[ $\bar{w}$ ,u,v]	(8)	$\bar{z}$ +1/2,x+1/2, $\bar{y}$	[ $\bar{w}$ ,u, $\bar{v}$ ]



- (9)  $y, z, x [v, w, u]$  (10)  $\bar{y}+1/2, z+1/2, \bar{x} [\bar{v}, w, \bar{u}]$  (11)  $y+1/2, \bar{z}, \bar{x}+1/2 [v, \bar{w}, \bar{u}]$  (12)  $\bar{y}, \bar{z}+1/2, x+1/2 [\bar{v}, \bar{w}, u]$   
 (13)  $y+3/4, x+1/4, \bar{z}+3/4 [v, u, \bar{w}]$  (14)  $\bar{y}+1/4, \bar{x}+1/4, \bar{z}+1/4 [\bar{v}, \bar{u}, \bar{w}]$  (15)  $y+1/4, \bar{x}+3/4, z+3/4 [v, \bar{u}, w]$  (16)  $\bar{y}+3/4, x+3/4, z+1/4 [\bar{v}, u, w]$   
 (17)  $x+3/4, z+1/4, \bar{y}+3/4 [u, w, \bar{v}]$  (18)  $\bar{x}+3/4, z+3/4, y+1/4 [\bar{u}, w, v]$  (19)  $\bar{x}+1/4, \bar{z}+1/4, \bar{y}+1/4 [\bar{u}, \bar{w}, \bar{v}]$  (20)  $x+1/4, \bar{z}+3/4, y+3/4 [u, \bar{w}, v]$   
 (21)  $z+3/4, y+1/4, \bar{x}+3/4 [w, v, \bar{u}]$  (22)  $z+1/4, \bar{y}+3/4, x+3/4 [w, \bar{v}, u]$  (23)  $\bar{z}+3/4, y+3/4, x+1/4 [\bar{w}, v, u]$  (24)  $\bar{z}+1/4, \bar{y}+1/4, \bar{x}+1/4 [\bar{w}, \bar{v}, \bar{u}]$   
 (25)  $\bar{x}+1/4, \bar{y}+1/4, \bar{z}+1/4 [u, v, w]$  (26)  $x+1/4, y+3/4, \bar{z}+3/4 [\bar{u}, \bar{v}, w]$  (27)  $x+3/4, \bar{y}+3/4, z+1/4 [\bar{u}, v, \bar{w}]$  (28)  $\bar{x}+3/4, y+1/4, z+3/4 [u, \bar{v}, \bar{w}]$   
 (29)  $\bar{z}+1/4, \bar{x}+1/4, \bar{y}+1/4 [w, u, v]$  (30)  $\bar{z}+3/4, x+1/4, y+3/4 [w, \bar{u}, \bar{v}]$  (31)  $z+1/4, x+3/4, \bar{y}+3/4 [\bar{w}, \bar{u}, v]$  (32)  $z+3/4, \bar{x}+3/4, y+1/4 [\bar{w}, u, \bar{v}]$   
 (33)  $\bar{y}+1/4, \bar{z}+1/4, \bar{x}+1/4 [v, w, u]$  (34)  $y+3/4, \bar{z}+3/4, x+1/4 [\bar{v}, w, \bar{u}]$  (35)  $\bar{y}+3/4, z+1/4, x+3/4 [v, \bar{w}, \bar{u}]$  (36)  $y+1/4, z+3/4, \bar{x}+3/4 [\bar{v}, \bar{w}, u]$   
 (37)  $\bar{y}+1/2, \bar{x}, z+1/2 [v, u, \bar{w}]$  (38)  $y, x, z [\bar{v}, \bar{u}, \bar{w}]$  (39)  $\bar{y}, x+1/2, \bar{z}+1/2 [v, \bar{u}, w]$  (40)  $y+1/2, \bar{x}+1/2, \bar{z} [\bar{v}, u, w]$   
 (41)  $\bar{x}+1/2, \bar{z}, y+1/2 [u, w, \bar{v}]$  (42)  $x+1/2, \bar{z}+1/2, \bar{y} [\bar{u}, w, v]$  (43)  $x, z, y [\bar{u}, \bar{w}, \bar{v}]$  (44)  $\bar{x}, z+1/2, \bar{y}+1/2 [u, \bar{w}, v]$   
 (45)  $\bar{z}+1/2, \bar{y}, x+1/2 [w, v, \bar{u}]$  (46)  $\bar{z}, y+1/2, \bar{x}+1/2 [w, \bar{v}, u]$  (47)  $z+1/2, \bar{y}+1/2, \bar{x} [\bar{w}, v, u]$  (48)  $z, y, x [\bar{w}, \bar{v}, \bar{u}]$

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- $1/8, y, \bar{y}+1/4 [0, \bar{v}, v]$   $7/8, \bar{y}+1/2, \bar{y}+3/4 [0, v, v]$   $3/8, y+1/2, y+3/4 [0, \bar{v}, \bar{v}]$   $5/8, \bar{y}, y+1/4 [0, v, \bar{v}]$   
 $\bar{y}+1/4, 1/8, y [v, 0, \bar{v}]$   $\bar{y}+3/4, 7/8, \bar{y}+1/2 [v, 0, v]$   $y+3/4, 3/8, y+1/2 [\bar{v}, 0, \bar{v}]$   $y+1/4, 5/8, \bar{y} [\bar{v}, 0, v]$   
 $y, \bar{y}+1/4, 1/8 [\bar{v}, v, 0]$   $\bar{y}+1/2, \bar{y}+3/4, 7/8 [v, v, 0]$   $y+1/2, y+3/4, 3/8 [\bar{v}, \bar{v}, 0]$   $\bar{y}, y+1/4, 5/8 [v, \bar{v}, 0]$   
 $1/8, \bar{y}+1/4, y [0, \bar{v}, v]$   $3/8, y+3/4, y+1/2 [0, v, v]$   $7/8, \bar{y}+3/4, \bar{y}+1/2 [0, \bar{v}, \bar{v}]$   $5/8, y+1/4, \bar{y} [0, v, \bar{v}]$   
 $y, 1/8, \bar{y}+1/4 [v, 0, \bar{v}]$   $y+1/2, 3/8, y+3/4 [v, 0, v]$   $\bar{y}+1/2, 7/8, \bar{y}+3/4 [\bar{v}, 0, \bar{v}]$   $\bar{y}, 5/8, y+1/4 [\bar{v}, 0, v]$   
 $\bar{y}+1/4, y, 1/8 [\bar{v}, v, 0]$   $y+3/4, y+1/2, 3/8 [v, v, 0]$   $\bar{y}+3/4, \bar{y}+1/2, 7/8 [\bar{v}, \bar{v}, 0]$   $y+1/4, \bar{y}, 5/8 [v, \bar{v}, 0]$

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- $x, x, z [u, \bar{u}, 0]$   $\bar{x}, \bar{x}+1/2, z+1/2 [\bar{u}, u, 0]$   $\bar{x}+1/2, x+1/2, \bar{z} [\bar{u}, \bar{u}, 0]$   $x+1/2, \bar{x}, \bar{z}+1/2 [u, u, 0]$   
 $z, x, x [0, u, \bar{u}]$   $z+1/2, \bar{x}, \bar{x}+1/2 [0, \bar{u}, u]$   $\bar{z}, \bar{x}+1/2, x+1/2 [0, \bar{u}, \bar{u}]$   $\bar{z}+1/2, x+1/2, \bar{x} [0, u, u]$   
 $x, z, x [\bar{u}, 0, u]$   $\bar{x}+1/2, z+1/2, \bar{x} [u, 0, \bar{u}]$   $x+1/2, \bar{z}, \bar{x}+1/2 [\bar{u}, 0, \bar{u}]$   $\bar{x}, \bar{z}+1/2, x+1/2 [u, 0, u]$   
 $x+3/4, x+1/4, \bar{z}+3/4 [\bar{u}, u, 0]$   $\bar{x}+1/4, \bar{x}+1/4, \bar{z}+1/4 [u, \bar{u}, 0]$   $x+1/4, \bar{x}+3/4, z+3/4 [\bar{u}, \bar{u}, 0]$   $\bar{x}+3/4, x+3/4, z+1/4 [u, u, 0]$   
 $x+3/4, z+1/4, \bar{x}+3/4 [u, 0, u]$   $\bar{x}+3/4, z+3/4, x+1/4 [\bar{u}, 0, \bar{u}]$   $\bar{x}+1/4, \bar{z}+1/4, \bar{x}+1/4 [\bar{u}, 0, u]$   $x+1/4, \bar{z}+3/4, x+3/4 [u, 0, \bar{u}]$   
 $z+3/4, x+1/4, \bar{x}+3/4 [0, \bar{u}, \bar{u}]$   $z+1/4, \bar{x}+3/4, x+3/4 [0, u, u]$   $\bar{z}+3/4, x+3/4, x+1/4 [0, \bar{u}, u]$   $\bar{z}+1/4, \bar{x}+1/4, \bar{x}+1/4 [0, u, \bar{u}]$

- 48 f 2mm  $x, 0, 0 [0, 0, 0]$   $\bar{x}, 1/2, 1/2 [0, 0, 0]$   $0, x, 0 [0, 0, 0]$   $1/2, \bar{x}, 1/2 [0, 0, 0]$   
 $0, 0, x [0, 0, 0]$   $1/2, 1/2, \bar{x} [0, 0, 0]$   $3/4, x+1/4, 3/4 [0, 0, 0]$   $1/4, \bar{x}+1/4, 1/4 [0, 0, 0]$   
 $x+3/4, 1/4, 3/4 [0, 0, 0]$   $\bar{x}+3/4, 3/4, 1/4 [0, 0, 0]$   $3/4, 1/4, \bar{x}+3/4 [0, 0, 0]$   $1/4, 3/4, x+3/4 [0, 0, 0]$

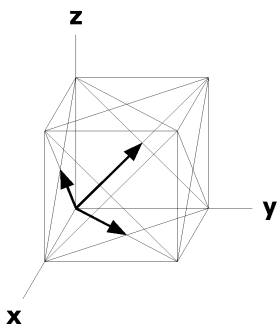
32	e	.3m	$x, x, x [0, 0, 0]$		$\bar{x}, \bar{x}+1/2, x+1/2 [0, 0, 0]$	
			$\bar{x}+1/2, x+1/2, \bar{x} [0, 0, 0]$		$x+1/2, \bar{x}, \bar{x}+1/2 [0, 0, 0]$	
			$x+3/4, x+1/4, \bar{x}+3/4 [0, 0, 0]$		$\bar{x}+1/4, \bar{x}+1/4, \bar{x}+1/4 [0, 0, 0]$	
			$x+1/4, \bar{x}+3/4, x+3/4 [0, 0, 0]$		$\bar{x}+3/4, x+3/4, x+1/4 [0, 0, 0]$	
16	d	$\bar{3}m$	$5/8, 5/8, 5/8 [0, 0, 0]$	$3/8, 7/8, 1/8 [0, 0, 0]$	$7/8, 1/8, 3/8 [0, 0, 0]$	$1/8, 3/8, 7/8 [0, 0, 0]$
16	c	$\bar{3}m$	$1/8, 1/8, 1/8 [0, 0, 0]$	$7/8, 3/8, 5/8 [0, 0, 0]$	$3/8, 5/8, 7/8 [0, 0, 0]$	$5/8, 7/8, 3/8 [0, 0, 0]$
8	b	$\bar{4}3m$	$1/2, 1/2, 1/2 [0, 0, 0]$		$1/4, 3/4, 1/4 [0, 0, 0]$	
8	a	$\bar{4}3m$	$0, 0, 0 [0, 0, 0]$		$3/4, 1/4, 3/4 [0, 0, 0]$	

### Symmetry of Special Projections

Along  $[0, 0, 1]$   $p_6 \cdot 4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/4$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/4$   
 Origin at  $1/4, 0, z$

Along  $[1, 1, 1]$   $p6'mm'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at  $x, x, x$

Along  $[1, 1, 0]$   $c2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at  $x, x, 1/8$



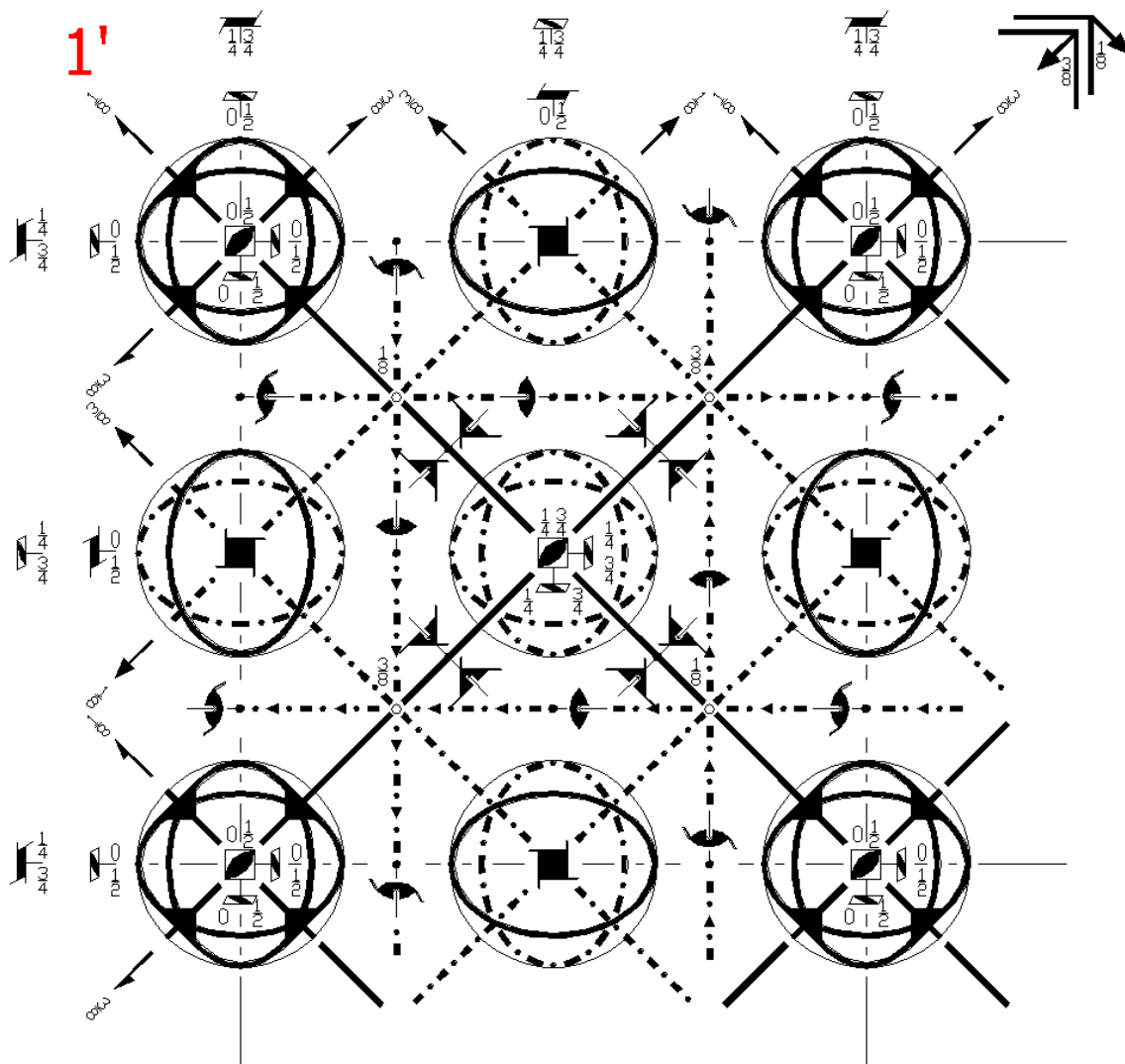
Fd $\bar{3}m1'$

227.2.1629

m $\bar{3}m1'$

F $4_1/d\bar{3}2/m1'$

Cubic



Origin at  $\bar{4}3m1'$ , at  $-1/8, -1/8, -1/8$  from center ( $\bar{3}m1'$ )

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/8$ ;  $-1/8 \leq z \leq 1/8$ ;  $y \leq \min(1/2-x, x)$ ;  $-y \leq z \leq y$

Vertices  $0,0,0$   $1/2,0,0$   $3/8,1/8,1/8$   $1/8,1/8,1/8$   $3/8,1/8,-1/8$   $1/8,1/8,-1/8$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |  |  |   |
|---|--|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)   | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)   | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>  1/2,0,1/2)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> (1/3,-1/3,1/3)<br>x+1/6,x+1/6,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) | (7) 3 <sup>+</sup> (-1/3,1/3,1/3)<br>x+1/3,x-1/6,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2) | (8) 3 <sup>+</sup> (1/3,1/3,-1/3)<br>x+1/6,x+1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x,x̄+1/2,x̄<br>(3 <sub>xyz</sub>  1/2,1/2,0)                                   | (11) 3 <sup>-</sup> x̄+1/2,x̄,x<br>(3 <sub>xyz</sub>  1/2,0,1/2)                                   | (12) 3 <sup>-</sup> x̄-1/2,x+1/2,x̄<br>(3 <sub>xyz</sub>  0,1/2,1/2)                              |

- (13)  $2 (1/2, 1/2, 0) \ x, x-1/4, 3/8$   
 $(2_{xy} | 3/4, 1/4, 3/4)$
- (14)  $2 \ x, \bar{x}+1/4, 1/8$   
 $(2_{xy} | 1/4, 1/4, 1/4)$
- (15)  $4^- (0, 0, 3/4) \ 1/2, 1/4, z$   
 $(4_z^{-1} | 1/4, 3/4, 3/4)$
- (16)  $4^+ (0, 0, 1/4) \ 0, 3/4, z$   
 $(4_z | 3/4, 3/4, 1/4)$
- (17)  $4^- (3/4, 0, 0) \ x, 1/2, 1/4$   
 $(4_x^{-1} | 3/4, 1/4, 3/4)$
- (18)  $2 (0, 1/2, 1/2) \ 3/8, y+1/4, y$   
 $(2_{yz} | 3/4, 3/4, 1/4)$
- (19)  $2 \ 1/8, y+1/4, \bar{y}$   
 $(2_{yz} | 1/4, 1/4, 1/4)$
- (20)  $4^+ (1/4, 0, 0) \ x, 0, 3/4$   
 $(4_x | 1/4, 3/4, 3/4)$
- (21)  $4^+ (0, 1/4, 0) \ 3/4, y, 0$   
 $(4_y | 3/4, 1/4, 3/4)$
- (22)  $2 (1/2, 0, 1/2) \ x-1/4, 3/8, x$   
 $(2_{xz} | 1/4, 3/4, 3/4)$
- (23)  $4^- (0, 3/4, 0) \ 1/4, y, 1/2$   
 $(4_y^{-1} | 3/4, 3/4, 1/4)$
- (24)  $2 \ \bar{x}+1/4, 1/8, x$   
 $(2_{xz} | 1/4, 1/4, 1/4)$
- (25)  $\bar{1} \ 1/8, 1/8, 1/8$   
 $(\bar{1} | 1/4, 1/4, 1/4)$
- (26)  $d (1/4, 3/4, 0) \ x, y, 3/8$   
 $(m_z | 1/4, 3/4, 3/4)$
- (27)  $d (3/4, 0, 1/4) \ x, 3/8, z$   
 $(m_y | 3/4, 3/4, 1/4)$
- (28)  $d (0, 1/4, 3/4) \ 3/8, y, z$   
 $(m_x | 3/4, 1/4, 3/4)$
- (29)  $\bar{3}^+ \ x, x, x;$   
 $1/8, 1/8, 1/8$   
 $(\bar{3}_{xyz} | 1/4, 1/4, 1/4)$
- (30)  $\bar{3}^+ \ \bar{x}-1, x+1, \bar{x};$   
 $-1/8, 1/8, 7/8$   
 $(\bar{3}_{xyz}^{-1} | 3/4, 1/4, 3/4)$
- (31)  $\bar{3}^+ \ x, \bar{x}+1, \bar{x};$   
 $1/8, 7/8, -1/8$   
 $(\bar{3}_{xyz}^{-1} | 1/4, 3/4, 3/4)$
- (32)  $\bar{3}^+ \ \bar{x}+1, \bar{x}, x;$   
 $7/8, -1/8, 1/8$   
 $(\bar{3}_{xyz}^{-1} | 3/4, 3/4, 1/4)$
- (33)  $\bar{3}^- \ x, x, x;$   
 $1/8, 1/8, 1/8$   
 $(\bar{3}_{xyz}^{-1} | 1/4, 1/4, 1/4)$
- (34)  $\bar{3}^- \ x+3/2, \bar{x}-1, \bar{x};$   
 $5/8, -1/8, 7/8$   
 $(\bar{3}_{xyz} | 3/4, 3/4, 1/4)$
- (35)  $\bar{3}^- \ \bar{x}+1/2, \bar{x}+3/2, x;$   
 $-1/8, 7/8, 5/8$   
 $(\bar{3}_{xyz} | 3/4, 1/4, 3/4)$
- (36)  $\bar{3}^- \ \bar{x}+1, x+1/2, \bar{x};$   
 $7/8, 5/8, -1/8$   
 $(\bar{3}_{xyz} | 1/4, 3/4, 3/4)$
- (37)  $g (1/4, -1/4, 1/2) \ x+1/4, \bar{x}, z$   
 $(m_{xy} | 1/2, 0, 1/2)$
- (38)  $m \ x, x, z$   
 $(m_{xy} | 0, 0, 0)$
- (39)  $\bar{4}^- \ -1/4, 1/4, z; \ -1/4, 1/4, 1/4$   
 $(\bar{4}_z^{-1} | 0, 1/2, 1/2)$
- (40)  $\bar{4}^+ \ 1/2, 0, z; \ 1/2, 0, 0$   
 $(\bar{4}_z | 1/2, 1/2, 0)$
- (41)  $\bar{4}^- \ x, -1/4, 1/4; \ 1/4, -1/4, 1/4$   
 $(\bar{4}_x^{-1} | 1/2, 0, 1/2)$
- (42)  $g (1/2, 1/4, -1/4) \ x, y+1/4, \bar{y}$   
 $(m_{yz} | 1/2, 1/2, 0)$
- (43)  $m \ x, y, y$   
 $(m_{yz} | 0, 0, 0)$
- (44)  $\bar{4}^+ \ x, 1/2, 0; \ 0, 1/2, 0$   
 $(\bar{4}_x | 0, 1/2, 1/2)$
- (45)  $\bar{4}^+ \ 0, y, 1/2; \ 0, 0, 1/2$   
 $(\bar{4}_y | 1/2, 0, 1/2)$
- (46)  $g (-1/4, 1/2, 1/4) \ \bar{x}+1/4, y, x$   
 $(m_{xz} | 0, 1/2, 1/2)$
- (47)  $\bar{4}^- \ 1/4, y, -1/4; \ 1/4, 1/4, -1/4$   
 $(\bar{4}_y^{-1} | 1/2, 1/2, 0)$
- (48)  $m \ x, y, x$   
 $(m_{xz} | 0, 0, 0)$

For (0, 1/2, 1/2) + set

- (1)  $t (0, 1/2, 1/2)$   
 $(1 | 0, 1/2, 1/2)$
- (2)  $2 \ 0, 0, z$   
 $(2_z | 0, 0, 0)$
- (3)  $2 \ 1/4, y, 1/4$   
 $(2_y | 1/2, 0, 1/2)$
- (4)  $2 (1/2, 0, 0) \ x, 1/4, 0$   
 $(2_x | 1/2, 1/2, 0)$
- (5)  $3^+ (1/3, 1/3, 1/3)$   
 $x-1/3, x-1/6, x$   
 $(3_{xyz} | 0, 1/2, 1/2)$
- (6)  $3^+ \ \bar{x}+1/2, x, \bar{x}$   
 $(3_{xyz}^{-1} | 1/2, 1/2, 0)$
- (7)  $3^+ \ x, \bar{x}, \bar{x}$   
 $(3_{xyz}^{-1} | 0, 0, 0)$
- (8)  $3^+ \ \bar{x}+1/2, \bar{x}+1/2, x$   
 $(3_{xyz}^{-1} | 1/2, 0, 1/2)$
- (9)  $3^- (1/3, 1/3, 1/3)$   
 $x-1/6, x+1/6, x$   
 $(3_{xyz}^{-1} | 0, 1/2, 1/2)$
- (10)  $3^- \ x+1/2, \bar{x}, \bar{x}$   
 $(3_{xyz} | 1/2, 0, 1/2)$
- (11)  $3^- (1/3, 1/3, -1/3)$   
 $x+1/3, x+1/6, x$   
 $(3_{xyz} | 1/2, 1/2, 0)$
- (12)  $3^- \ \bar{x}, x, \bar{x}$   
 $(3_{xyz} | 0, 0, 0)$
- (13)  $2 (3/4, 3/4, 0) \ x, x, 1/8$   
 $(2_{xy} | 3/4, 3/4, 1/4)$
- (14)  $2 (-1/4, 1/4, 0) \ x, \bar{x}+1/2, 3/8$   
 $(2_{xy} | 1/4, 3/4, 3/4)$
- (15)  $4^- (0, 0, 1/4) \ 1/4, 0, z$   
 $(4_z^{-1} | 1/4, 1/4, 1/4)$
- (16)  $4^+ (0, 0, 3/4) \ 1/4, 1/2, z$   
 $(4_z | 3/4, 1/4, 3/4)$
- (17)  $4^- (3/4, 0, 0) \ x, 1/2, -1/4$   
 $(4_x^{-1} | 3/4, 3/4, 1/4)$
- (18)  $2 (0, 1/2, 1/2) \ 3/8, y-1/4, y$   
 $(2_{yz} | 3/4, 1/4, 3/4)$
- (19)  $2 \ 1/8, y+3/4, \bar{y}$   
 $(2_{yz} | 1/4, 3/4, 3/4)$
- (20)  $4^+ (1/4, 0, 0) \ x, 0, 1/4$   
 $(4_x | 1/4, 1/4, 1/4)$
- (21)  $4^+ (0, 3/4, 0) \ 1/2, y, -1/4$   
 $(4_y | 3/4, 3/4, 1/4)$
- (22)  $2 (1/4, 0, 1/4) \ x, 1/8, x$   
 $(2_{xz} | 1/4, 1/4, 1/4)$
- (23)  $4^- (0, 1/4, 0) \ 0, y, 3/4$   
 $(4_y^{-1} | 3/4, 1/4, 3/4)$
- (24)  $2 (-1/4, 0, 1/4) \ \bar{x}+1/2, 3/8, x$   
 $(2_{xz} | 1/4, 3/4, 3/4)$
- (25)  $\bar{1} \ 1/8, 3/8, 3/8$   
 $(\bar{1} | 1/4, 3/4, 3/4)$
- (26)  $d (1/4, 1/4, 0) \ x, y, 1/8$   
 $(m_z | 1/4, 1/4, 1/4)$
- (27)  $d (3/4, 0, 3/4) \ x, 1/8, z$   
 $(m_y | 3/4, 1/4, 3/4)$
- (28)  $d (0, 3/4, 1/4) \ 3/8, y, z$   
 $(m_x | 3/4, 3/4, 1/4)$
- (29)  $\bar{3}^+ \ x, x+1/2, x;$   
 $1/8, 5/8, 1/8$   
 $(\bar{3}_{xyz} | 1/4, 3/4, 3/4)$
- (30)  $\bar{3}^+ \ \bar{x}-1, x+3/2, \bar{x};$   
 $-1/8, 5/8, 7/8$   
 $(\bar{3}_{xyz}^{-1} | 3/4, 3/4, 1/4)$
- (31)  $\bar{3}^+ \ x, \bar{x}+1/2, \bar{x};$   
 $1/8, 3/8, -1/8$   
 $(\bar{3}_{xyz}^{-1} | 1/4, 1/4, 1/4)$
- (32)  $\bar{3}^+ \ \bar{x}+1, \bar{x}-1/2, x;$   
 $7/8, -5/8, 1/8$   
 $(\bar{3}_{xyz}^{-1} | 3/4, 1/4, 3/4)$

- (33)  $\bar{3}^-$   $x-1/2, x-1/2, x;$   
 $1/8, 1/8, 5/8$   
 $(\bar{3}_{xyz}^{-1} | 1/4, 3/4, 3/4)$
- (34)  $\bar{3}^-$   $x+1, \bar{x}-3/2, \bar{x};$   
 $1/8, -5/8, 7/8$   
 $(\bar{3}_{\bar{xyz}} | 3/4, 1/4, 3/4)$
- (35)  $\bar{3}^-$   $\bar{x}, \bar{x}+1, x;$   
 $-1/8, 7/8, 1/8$   
 $(\bar{3}_{\bar{xyz}} | 3/4, 3/4, 1/4)$
- (36)  $\bar{3}^-$   $\bar{x}+1/2, x, \bar{x};$   
 $3/8, 1/8, -1/8$   
 $(\bar{3}_{\bar{xyz}} | 1/4, 1/4, 1/4)$
- (37)  $m$   $x+1/2, \bar{x}, z$   
 $(m_{xy} | 1/2, 1/2, 0)$
- (38)  $g$   $(1/4, 1/4, 1/2)$   $x-1/4, x, z$   
 $(m_{\bar{xy}} | 0, 1/2, 1/2)$
- (39)  $\bar{4}^-$   $0, 0, z; 0, 0, 0$   
 $(\bar{4}_z^{-1} | 0, 0, 0)$
- (40)  $\bar{4}^+$   $1/4, -1/4, z; 1/4, -1/4, 1/4$   
 $(\bar{4}_z | 1/2, 0, 1/2)$
- (41)  $\bar{4}^-$   $x, 1/4, 1/4; 1/4, 1/4, 1/4$   
 $(\bar{4}_x^{-1} | 1/2, 1/2, 0)$
- (42)  $g$   $(1/2, -1/4, 1/4)$   $x, y+1/4, \bar{y}$   
 $(m_{yz} | 1/2, 0, 1/2)$
- (43)  $g$   $(0, 1/2, 1/2)$   $x, y, y$   
 $(m_{\bar{yz}} | 0, 1/2, 1/2)$
- (44)  $\bar{4}^+$   $x, 0, 0; 0, 0, 0$   
 $(\bar{4}_x | 0, 0, 0)$
- (45)  $\bar{4}^+$   $1/4, y, 1/4; 1/4, 1/4, 1/4$   
 $(\bar{4}_y | 1/2, 1/2, 0)$
- (46)  $m$   $\bar{x}, y, x$   
 $(m_{xz} | 0, 0, 0)$
- (47)  $\bar{4}^-$   $1/2, y, 0; 1/2, 0, 0$   
 $(\bar{4}_y^{-1} | 1/2, 0, 1/2)$
- (48)  $g$   $(1/4, 1/2, 1/4)$   $x-1/4, y, x$   
 $(m_{\bar{xz}} | 0, 1/2, 1/2)$

For  $(1/2, 0, 1/2)$  + set

- (1)  $t$   $(1/2, 0, 1/2)$   
 $(1 | 1/2, 0, 1/2)$
- (2)  $2$   $1/4, 1/4, z$   
 $(2_z | 1/2, 1/2, 0)$
- (3)  $2$   $(0, 1/2, 0)$   $0, y, 1/4$   
 $(2_y | 0, 1/2, 1/2)$
- (4)  $2$   $x, 0, 0$   
 $(2_x | 0, 0, 0)$
- (5)  $3^+$   $(1/3, 1/3, 1/3)$   
 $x+1/6, x-1/6, x$   
 $(3_{xyz} | 1/2, 0, 1/2)$
- (6)  $3^+$   $\bar{x}, x, \bar{x}$   
 $(3_{\bar{xyz}}^{-1} | 0, 0, 0)$
- (7)  $3^+$   $x+1/2, \bar{x}, \bar{x}$   
 $(3_{\bar{xyz}}^{-1} | 1/2, 1/2, 0)$
- (8)  $3^+$   $\bar{x}, \bar{x}+1/2, x$   
 $(3_{xyz}^{-1} | 0, 1/2, 1/2)$
- (9)  $3^-$   $(1/3, 1/3, 1/3)$   
 $x-1/6, x-1/3, x$   
 $(3_{xyz}^{-1} | 1/2, 0, 1/2)$
- (10)  $3^-$   $(-1/3, 1/3, 1/3)$   
 $x+1/6, \bar{x}+1/6, \bar{x}$   
 $(3_{\bar{xyz}} | 0, 1/2, 1/2)$
- (11)  $3^-$   $\bar{x}, \bar{x}, x$   
 $(3_{\bar{yz}} | 0, 0, 0)$
- (12)  $3^-$   $\bar{x}, x+1/2, \bar{x}$   
 $(3_{\bar{yz}} | 1/2, 1/2, 0)$
- (13)  $2$   $(1/4, 1/4, 0)$   $x, x, 1/8$   
 $(2_{xy} | 1/4, 1/4, 1/4)$
- (14)  $2$   $(1/4, -1/4, 0)$   $x, \bar{x}+1/2, 3/8$   
 $(2_{\bar{xy}} | 3/4, 1/4, 3/4)$
- (15)  $4^-$   $(0, 0, 1/4)$   $3/4, 0, z$   
 $(\bar{4}_z^{-1} | 3/4, 3/4, 1/4)$
- (16)  $4^+$   $(0, 0, 3/4)$   $-1/4, 1/2, z$   
 $(\bar{4}_z | 1/4, 3/4, 3/4)$
- (17)  $4^-$   $(1/4, 0, 0)$   $x, 1/4, 0$   
 $(\bar{4}_x^{-1} | 1/4, 1/4, 1/4)$
- (18)  $2$   $(0, 3/4, 3/4)$   $1/8, y, y$   
 $(2_{yz} | 1/4, 3/4, 3/4)$
- (19)  $2$   $(0, -1/4, 1/4)$   $3/8, y+1/2, \bar{y}$   
 $(2_{\bar{yz}} | 3/4, 1/4, 3/4)$
- (20)  $4^+$   $(3/4, 0, 0)$   $x, 1/4, 1/2$   
 $(\bar{4}_x | 3/4, 3/4, 1/4)$
- (21)  $4^+$   $(0, 1/4, 0)$   $1/4, y, 0$   
 $(\bar{4}_y | 1/4, 1/4, 1/4)$
- (22)  $2$   $(1/2, 0, 1/2)$   $x+1/4, 3/8, x$   
 $(2_{xz} | 3/4, 3/4, 1/4)$
- (23)  $4^-$   $(0, 3/4, 0)$   $-1/4, y, 1/2$   
 $(\bar{4}_y^{-1} | 1/4, 3/4, 3/4)$
- (24)  $2$   $\bar{x}+3/4, 1/8, x$   
 $(2_{\bar{xz}} | 3/4, 1/4, 3/4)$
- (25)  $\bar{1}$   $3/8, 1/8, 3/8$   
 $(\bar{1} | 3/4, 1/4, 3/4)$
- (26)  $d$   $(3/4, 3/4, 0)$   $x, y, 1/8$   
 $(m_z | 3/4, 3/4, 1/4)$
- (27)  $d$   $(1/4, 0, 3/4)$   $x, 3/8, z$   
 $(m_y | 1/4, 3/4, 3/4)$
- (28)  $d$   $(0, 1/4, 1/4)$   $1/8, y, z$   
 $(m_x | 1/4, 1/4, 1/4)$
- (29)  $\bar{3}^+$   $x-1/2, x-1/2, x;$   
 $1/8, 1/8, 5/8$   
 $(\bar{3}_{xyz} | 3/4, 1/4, 3/4)$
- (30)  $\bar{3}^+$   $\bar{x}-1/2, x+1/2, \bar{x};$   
 $-1/8, 1/8, 3/8$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 1/4, 1/4, 1/4)$
- (31)  $\bar{3}^+$   $x-1/2, \bar{x}+3/2, \bar{x};$   
 $1/8, 7/8, -5/8$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 3/4, 3/4, 1/4)$
- (32)  $\bar{3}^+$   $\bar{x}+3/2, \bar{x}+1/2, x;$   
 $7/8, -1/8, 5/8$   
 $(\bar{3}_{xyz}^{-1} | 1/4, 3/4, 3/4)$
- (33)  $\bar{3}^-$   $x+1/2, x, x;$   
 $5/8, 1/8, 1/8$   
 $(\bar{3}_{xyz}^{-1} | 3/4, 1/4, 3/4)$
- (34)  $\bar{3}^-$   $x+1, \bar{x}-1, \bar{x};$   
 $1/8, -1/8, 7/8$   
 $(\bar{3}_{\bar{xyz}} | 1/4, 3/4, 3/4)$
- (35)  $\bar{3}^-$   $\bar{x}, \bar{x}+1/2, x;$   
 $-1/8, 3/8, 1/8$   
 $(\bar{3}_{\bar{yz}} | 1/4, 1/4, 1/4)$
- (36)  $\bar{3}^-$   $\bar{x}+3/2, x-1/2, \bar{x};$   
 $7/8, 1/8, -5/8$   
 $(\bar{3}_{\bar{yz}} | 3/4, 3/4, 1/4)$
- (37)  $m$   $x, \bar{x}, z$   
 $(m_{xy} | 0, 0, 0)$
- (38)  $g$   $(1/4, 1/4, 1/2)$   $x+1/4, x, z$   
 $(m_{\bar{xy}} | 1/2, 0, 1/2)$
- (39)  $\bar{4}^-$   $0, 1/2, z; 0, 1/2, 0$   
 $(\bar{4}_z^{-1} | 1/2, 1/2, 0)$
- (40)  $\bar{4}^+$   $1/4, 1/4, z; 1/4, 1/4, 1/4$   
 $(\bar{4}_z | 0, 1/2, 1/2)$
- (41)  $\bar{4}^-$   $x, 0, 0; 0, 0, 0$   
 $(\bar{4}_x^{-1} | 0, 0, 0)$
- (42)  $m$   $x, y+1/2, \bar{y}$   
 $(m_{yz} | 0, 1/2, 1/2)$
- (43)  $g$   $(1/2, 1/4, 1/4)$   $x, y-1/4, y$   
 $(m_{\bar{yz}} | 1/2, 0, 1/2)$
- (44)  $\bar{4}^+$   $x, 1/4, -1/4; 1/4, 1/4, -1/4$   
 $(\bar{4}_x | 1/2, 1/2, 0)$
- (45)  $\bar{4}^+$   $0, y, 0; 0, 0, 0$   
 $(\bar{4}_y | 0, 0, 0)$
- (46)  $g$   $(1/4, 1/2, -1/4)$   $\bar{x}+1/4, y, x$   
 $(m_{xz} | 1/2, 1/2, 0)$
- (47)  $\bar{4}^-$   $1/4, y, 1/4; 1/4, 1/4, 1/4$   
 $(\bar{4}_y^{-1} | 0, 1/2, 1/2)$
- (48)  $g$   $(1/2, 0, 1/2)$   $x, y, x$   
 $(m_{\bar{xz}} | 1/2, 0, 1/2)$

## For (1/2,1/2,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) $t$ (1/2,1/2,0)<br>(1 1/2,1/2,0)   | (2) $2$ (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) $2$ 0,y,0<br>(2 <sub>y</sub>  0,0,0)  | (4) $2$ x,1/4,1/4<br>(2 <sub>x</sub>  0,1/2,1/2)   |
| (5) $3^+$ (1/3,1/3,1/3)<br>x+1/6,x+1/3,x<br>(3 <sub>xyz</sub>  1/2,1/2,0)                            | (6) $3^+$ $\bar{x}$ ,x+1/2, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)                                       | (7) $3^+$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2)                                   | (8) $3^+$ $\bar{x}$ , $\bar{x}$ ,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)  |
| (9) $3^-$ (1/3,1/3,1/3)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0)              | (10) $3^-$ x, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub>  0,0,0)   | (11) $3^-$ $\bar{x}$ +1/2, $\bar{x}$ +1/2, x<br>(3 <sub>xyz</sub>  0,1/2,1/2)   | (12) $3^-$ (1/3,-1/3,1/3)<br>x-1/6, x+1/3, $\bar{x}$<br>(3 <sub>xyz</sub>  1/2,0,1/2)                                    |
| (13) $2$ (1/2,1/2,0) x,x+1/4,3/8<br>(2 <sub>xy</sub>  1/4,3/4,3/4)                                   | (14) $2$ x, $\bar{x}$ +3/4,1/8<br>(2 <sub>xy</sub>  3/4,3/4,1/4)   | (15) $4^-$ (0,0,3/4) 1/2,-1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  3/4,1/4,3/4)  | (16) $4^+$ (0,0,1/4) 0,1/4,z<br>(4 <sub>z</sub>  1/4,1/4,1/4)  |
| (17) $4^-$ (1/4,0,0) x,3/4,0<br>(4 <sub>x</sub> <sup>-1</sup>  1/4,3/4,3/4)                          | (18) $2$ (0,1/4,1/4) 1/8,y,y<br>(2 <sub>yz</sub>  1/4,1/4,1/4)   | (19) $2$ (0,1/4,-1/4) 3/8,y+1/2, $\bar{y}$<br>(2 <sub>yz</sub>  3/4,3/4,1/4)  | (20) $4^+$ (3/4,0,0) x,-1/4,1/2<br>(4 <sub>x</sub>  3/4,1/4,3/4)   |
| (21) $4^+$ (0,3/4,0) 1/2,y,1/4<br>(4 <sub>y</sub>  1/4,3/4,3/4)                                      | (22) $2$ (3/4,0,3/4) x,1/8,x<br>(2 <sub>xz</sub>  3/4,1/4,3/4)   | (23) $4^-$ (0,1/4,0) 0,y,1/4<br>(4 <sub>y</sub> <sup>-1</sup>  1/4,1/4,1/4)   | (24) $2$ (1/4,0,-1/4) $\bar{x}$ +1/2,3/8,x<br>(2 <sub>xz</sub>  3/4,3/4,1/4)   |
| (25) $\bar{1}$ 3/8,3/8,1/8<br>( $\bar{1}$  3/4,3/4,1/4)  | (26) $d$ (3/4,1/4,0) x,y,3/8<br>(m <sub>z</sub>  3/4,1/4,3/4)  | (27) $d$ (1/4,0,1/4) x,1/8,z<br>(m <sub>y</sub>  1/4,1/4,1/4)   | (28) $d$ (0,3/4,3/4) 1/8,y,z<br>(m <sub>x</sub>  1/4,3/4,3/4)  |
| (29) $\bar{3}^+$ x+1/2,x,x;<br>5/8,1/8,1/8<br>( $\bar{3}$ <sub>xyz</sub>  3/4,3/4,1/4)               | (30) $\bar{3}^+$ $\bar{x}$ -3/2,x+1, $\bar{x}$ ;<br>-5/8,1/8,7/8<br>( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>  1/4,3/4,3/4) | (31) $\bar{3}^+$ x+1/2, $\bar{x}$ +1, $\bar{x}$ ;<br>5/8,7/8,-1/8<br>( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>  3/4,1/4,3/4) | (32) $\bar{3}^+$ $\bar{x}$ +1/2, $\bar{x}$ ,x;<br>3/8,-1/8,1/8<br>( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>  1/4,1/4,1/4) |
| (33) $\bar{3}^-$ x,x+1/2,x;<br>1/8,5/8,1/8<br>( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>  3/4,3/4,1/4) | (34) $\bar{3}^-$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ;<br>1/8,-1/8,3/8<br>( $\bar{3}$ <sub>xyz</sub>  1/4,1/4,1/4)            | (35) $\bar{3}^-$ $\bar{x}$ -1/2, $\bar{x}$ +1, x;<br>-5/8,7/8,1/8<br>( $\bar{3}$ <sub>xyz</sub>  1/4,3/4,3/4)               | (36) $\bar{3}^-$ $\bar{x}$ +1, x, $\bar{x}$ ;<br>7/8,1/8,-1/8<br>( $\bar{3}$ <sub>xyz</sub>  3/4,1/4,3/4)                |
| (37) $g$ (-1/4,1/4,1/2) x+1/4, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,1/2,1/2)                          | (38) $g$ (1/2,1/2,0) x,x,z<br>(m <sub>xy</sub>  1/2,1/2,0)   | (39) $\bar{4}^-$ 1/4,1/4,z; 1/4,1/4,1/4<br>( $\bar{4}$ <sub>z</sub> <sup>-1</sup>  1/2,0,1/2)                               | (40) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub>  0,0,0)  |
| (41) $\bar{4}^-$ x,0,1/2; 0,0,1/2<br>( $\bar{4}$ <sub>x</sub> <sup>-1</sup>  0,1/2,1/2)              | (42) $m$ x,y, $\bar{y}$<br>(m <sub>yz</sub>  0,0,0)  | (43) $g$ (1/2,1/4,1/4) x,y+1/4,y<br>(m <sub>yz</sub>  1/2,1/2,0)  | (44) $\bar{4}^+$ x,1/4,1/4; 1/4,1/4,1/4<br>( $\bar{4}$ <sub>x</sub>  1/2,0,1/2)  |
| (45) $\bar{4}^+$ -1/4,y,1/4; -1/4,1/4,1/4<br>( $\bar{4}$ <sub>y</sub>  0,1/2,1/2)                    | (46) $m$ $\bar{x}$ +1/2,y,x<br>(m <sub>xz</sub>  1/2,0,1/2)  | (47) $\bar{4}^-$ 0,y,0; 0,0,0<br>( $\bar{4}$ <sub>y</sub> <sup>-1</sup>  0,0,0)   | (48) $g$ (1/4,1/2,1/4) x+1/4,y,x<br>(m <sub>xz</sub>  1/2,1/2,0)   |

## For (0,0,0)' + set

- |  |  |  |   |
|--|--|--|---|
| (1) $1'$<br>(1 0,0,0)'   | (2) $2'$ (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)'   | (3) $2'$ (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)'   | (4) $2'$ (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>  1/2,0,1/2)'                                  |
| (5) $3^+$ ' x,x,x<br>(3 <sub>xyz</sub>  0,0,0)'                      | (6) $3^+$ ' (1/3,-1/3,1/3)<br>x+1/6,x+1/6, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2)' | (7) $3^+$ ' (-1/3,1/3,1/3)<br>x+1/3,x-1/6, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)' | (8) $3^+$ ' (1/3,1/3,-1/3)<br>x+1/6,x+1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0)' |
| (9) $3^-$ ' x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)'        | (10) $3^-$ ' x, $\bar{x}$ +1/2, $\bar{x}$<br>(3 <sub>xyz</sub>  1/2,1/2,0)'                          | (11) $3^-$ ' $\bar{x}$ +1/2, $\bar{x}$ , x<br>(3 <sub>xyz</sub>  1/2,0,1/2)'                         | (12) $3^-$ ' $\bar{x}$ -1/2, x+1/2, $\bar{x}$<br>(3 <sub>xyz</sub>  0,1/2,1/2)'             |
| (13) $2'$ (1/2,1/2,0) x,x-1/4,3/8<br>(2 <sub>xy</sub>  3/4,1/4,3/4)' | (14) $2'$ x, $\bar{x}$ +1/4,1/8<br>(2 <sub>xy</sub>  1/4,1/4,1/4)'                                   | (15) $4^-$ ' (0,0,3/4) 1/2,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/4,3/4,3/4)'                     | (16) $4^+$ ' (0,0,1/4) 0,3/4,z<br>(4 <sub>z</sub>  3/4,3/4,1/4)'                            |

- (17)  $4^- ' (3/4,0,0) \ x, 1/2, 1/4$   
 $(4_x^{-1} | 3/4, 1/4, 3/4)'$
- (18)  $2' (0, 1/2, 1/2) \ 3/8, y+1/4, y$   
 $(2_{yz} | 3/4, 3/4, 1/4)'$
- (19)  $2' \ 1/8, y+1/4, \bar{y}$   
 $(2_{\bar{y}z} | 1/4, 1/4, 1/4)'$
- (20)  $4^+ ' (1/4, 0, 0) \ x, 0, 3/4$   
 $(4_x | 1/4, 3/4, 3/4)'$
- (21)  $4^+ ' (0, 1/4, 0) \ 3/4, y, 0$   
 $(4_y | 3/4, 1/4, 3/4)'$
- (22)  $2' (1/2, 0, 1/2) \ x-1/4, 3/8, x$   
 $(2_{xz} | 1/4, 3/4, 3/4)'$
- (23)  $4^- ' (0, 3/4, 0) \ 1/4, y, 1/2$   
 $(4_y^{-1} | 3/4, 3/4, 1/4)'$
- (24)  $2' \ \bar{x}+1/4, 1/8, x$   
 $(2_{\bar{x}z} | 1/4, 1/4, 1/4)'$
- (25)  $\bar{1} \ 1/8, 1/8, 1/8$   
 $(\bar{1} | 1/4, 1/4, 1/4)'$
- (26)  $d' (1/4, 3/4, 0) \ x, y, 3/8$   
 $(m_z | 1/4, 3/4, 3/4)'$
- (27)  $d' (3/4, 0, 1/4) \ x, 3/8, z$   
 $(m_y | 3/4, 3/4, 1/4)'$
- (28)  $d' (0, 1/4, 3/4) \ 3/8, y, z$   
 $(m_x | 3/4, 1/4, 3/4)'$
- (29)  $\bar{3}^+ ' \ x, x, x;$   
 $1/8, 1/8, 1/8$   
 $(\bar{3}_{xyz} | 1/4, 1/4, 1/4)'$
- (30)  $\bar{3}^+ ' \ \bar{x}-1, x+1, \bar{x};$   
 $-1/8, 1/8, 7/8$   
 $(\bar{3}_{x\bar{y}z}^{-1} | 3/4, 1/4, 3/4)'$
- (31)  $\bar{3}^+ ' \ x, \bar{x}+1, \bar{x};$   
 $1/8, 7/8, -1/8$   
 $(\bar{3}_{\bar{x}yz}^{-1} | 1/4, 3/4, 3/4)'$
- (32)  $\bar{3}^+ ' \ \bar{x}+1, \bar{x}, x;$   
 $7/8, -1/8, 1/8$   
 $(\bar{3}_{xy\bar{z}}^{-1} | 3/4, 3/4, 1/4)'$
- (33)  $\bar{3}^- ' \ x, x, x;$   
 $1/8, 1/8, 1/8$   
 $(\bar{3}_{xyz}^{-1} | 1/4, 1/4, 1/4)'$
- (34)  $\bar{3}^- ' \ x+3/2, \bar{x}-1, \bar{x};$   
 $5/8, -1/8, 7/8$   
 $(\bar{3}_{\bar{x}yz} | 3/4, 3/4, 1/4)'$
- (35)  $\bar{3}^- ' \ \bar{x}+1/2, \bar{x}+3/2, x;$   
 $-1/8, 7/8, 5/8$   
 $(\bar{3}_{xy\bar{z}} | 3/4, 1/4, 3/4)'$
- (36)  $\bar{3}^- ' \ \bar{x}+1, x+1/2, \bar{x};$   
 $7/8, 5/8, -1/8$   
 $(\bar{3}_{x\bar{y}z} | 1/4, 3/4, 3/4)'$
- (37)  $g' (1/4, -1/4, 1/2) \ x+1/4, \bar{x}, z$   
 $(m_{xy} | 1/2, 0, 1/2)'$
- (38)  $m' \ x, x, z$   
 $(m_{xy} | 0, 0, 0)'$
- (39)  $\bar{4}^- ' \ -1/4, 1/4, z; \ -1/4, 1/4, 1/4$   
 $(\bar{4}_z^{-1} | 0, 1/2, 1/2)'$
- (40)  $\bar{4}^+ ' \ 1/2, 0, z; \ 1/2, 0, 0$   
 $(\bar{4}_z | 1/2, 1/2, 0)'$
- (41)  $\bar{4}^- ' \ x, -1/4, 1/4; \ 1/4, -1/4, 1/4$   
 $(\bar{4}_x^{-1} | 1/2, 0, 1/2)'$
- (42)  $g' (1/2, 1/4, -1/4) \ x, y+1/4, \bar{y}$   
 $(m_{yz} | 1/2, 1/2, 0)'$
- (43)  $m' \ x, y, y$   
 $(m_{\bar{y}z} | 0, 0, 0)'$
- (44)  $\bar{4}^+ ' \ x, 1/2, 0; \ 0, 1/2, 0$   
 $(\bar{4}_x | 0, 1/2, 1/2)'$
- (45)  $\bar{4}^+ ' \ 0, y, 1/2; \ 0, 0, 1/2$   
 $(\bar{4}_y | 1/2, 0, 1/2)'$
- (46)  $g' (-1/4, 1/2, 1/4) \ \bar{x}+1/4, y, x$   
 $(m_{xz} | 0, 1/2, 1/2)'$
- (47)  $\bar{4}^- ' \ 1/4, y, -1/4; \ 1/4, 1/4, -1/4$   
 $(\bar{4}_y^{-1} | 1/2, 1/2, 0)'$
- (48)  $m' \ x, y, x$   
 $(m_{\bar{x}z} | 0, 0, 0)'$

For (0, 1/2, 1/2)' + set

- (1)  $t' (0, 1/2, 1/2)$   
 $(1 | 0, 1/2, 1/2)'$
- (2)  $2' \ 0, 0, z$   
 $(2_z | 0, 0, 0)'$
- (3)  $2' \ 1/4, y, 1/4$   
 $(2_y | 1/2, 0, 1/2)'$
- (4)  $2' (1/2, 0, 0) \ x, 1/4, 0$   
 $(2_x | 1/2, 1/2, 0)'$
- (5)  $3^+ ' (1/3, 1/3, 1/3)$   
 $x-1/3, x-1/6, x$   
 $(3_{xyz} | 0, 1/2, 1/2)'$
- (6)  $3^+ ' \ \bar{x}+1/2, x, \bar{x}$   
 $(3_{x\bar{y}z}^{-1} | 1/2, 1/2, 0)'$
- (7)  $3^+ ' \ x, \bar{x}, \bar{x}$   
 $(3_{\bar{x}yz}^{-1} | 0, 0, 0)'$
- (8)  $3^+ ' \ \bar{x}+1/2, \bar{x}+1/2, x$   
 $(3_{xy\bar{z}}^{-1} | 1/2, 0, 1/2)'$
- (9)  $3^- ' (1/3, 1/3, 1/3)$   
 $x-1/6, x+1/6, x$   
 $(3_{xyz}^{-1} | 0, 1/2, 1/2)'$
- (10)  $3^- ' \ x+1/2, \bar{x}, \bar{x}$   
 $(3_{\bar{x}yz} | 1/2, 0, 1/2)'$
- (11)  $3^- ' (1/3, 1/3, -1/3)$   
 $\bar{x}+1/3, \bar{x}+1/6, x$   
 $(3_{xy\bar{z}} | 1/2, 1/2, 0)'$
- (12)  $3^- ' \ \bar{x}, x, \bar{x}$   
 $(3_{x\bar{y}z} | 0, 0, 0)'$
- (13)  $2' (3/4, 3/4, 0) \ x, x, 1/8$   
 $(2_{xy} | 3/4, 3/4, 1/4)'$
- (14)  $2' (-1/4, 1/4, 0) \ x, \bar{x}+1/2, 3/8$   
 $(2_{\bar{y}z} | 1/4, 3/4, 3/4)'$
- (15)  $4^- ' (0, 0, 1/4) \ 1/4, 0, z$   
 $(4_z^{-1} | 1/4, 1/4, 1/4)'$
- (16)  $4^+ ' (0, 0, 3/4) \ 1/4, 1/2, z$   
 $(4_z | 3/4, 1/4, 3/4)'$
- (17)  $4^- ' (3/4, 0, 0) \ x, 1/2, -1/4$   
 $(4_x^{-1} | 3/4, 3/4, 1/4)'$
- (18)  $2' (0, 1/2, 1/2) \ 3/8, y-1/4, y$   
 $(2_{yz} | 3/4, 1/4, 3/4)'$
- (19)  $2' \ 1/8, y+3/4, \bar{y}$   
 $(2_{\bar{y}z} | 1/4, 3/4, 3/4)'$
- (20)  $4^+ ' (1/4, 0, 0) \ x, 0, 1/4$   
 $(4_x | 1/4, 1/4, 1/4)'$
- (21)  $4^+ ' (0, 3/4, 0) \ 1/2, y, -1/4$   
 $(4_y | 3/4, 3/4, 1/4)'$
- (22)  $2' (1/4, 0, 1/4) \ x, 1/8, x$   
 $(2_{xz} | 1/4, 1/4, 1/4)'$
- (23)  $4^- ' (0, 1/4, 0) \ 0, y, 3/4$   
 $(4_y^{-1} | 3/4, 1/4, 3/4)'$
- (24)  $2' (-1/4, 0, 1/4) \ \bar{x}+1/2, 3/8, x$   
 $(2_{\bar{x}z} | 1/4, 3/4, 3/4)'$
- (25)  $\bar{1} \ 1/8, 3/8, 3/8$   
 $(\bar{1} | 1/4, 3/4, 3/4)'$
- (26)  $d' (1/4, 1/4, 0) \ x, y, 1/8$   
 $(m_z | 1/4, 1/4, 1/4)'$
- (27)  $d' (3/4, 0, 3/4) \ x, 1/8, z$   
 $(m_y | 3/4, 1/4, 3/4)'$
- (28)  $d' (0, 3/4, 1/4) \ 3/8, y, z$   
 $(m_x | 3/4, 3/4, 1/4)'$
- (29)  $\bar{3}^+ ' \ x, x+1/2, x;$   
 $1/8, 5/8, 1/8$   
 $(\bar{3}_{xyz} | 1/4, 3/4, 3/4)'$
- (30)  $\bar{3}^+ ' \ \bar{x}-1, x+3/2, \bar{x};$   
 $-1/8, 5/8, 7/8$   
 $(\bar{3}_{x\bar{y}z}^{-1} | 3/4, 3/4, 1/4)'$
- (31)  $\bar{3}^+ ' \ x, \bar{x}+1/2, \bar{x};$   
 $1/8, 3/8, -1/8$   
 $(\bar{3}_{\bar{x}yz}^{-1} | 1/4, 1/4, 1/4)'$
- (32)  $\bar{3}^+ ' \ \bar{x}+1, \bar{x}-1/2, x;$   
 $7/8, -5/8, 1/8$   
 $(\bar{3}_{xy\bar{z}}^{-1} | 3/4, 1/4, 3/4)'$
- (33)  $\bar{3}^- ' \ x-1/2, x-1/2, x;$   
 $1/8, 1/8, 5/8$   
 $(\bar{3}_{xyz}^{-1} | 1/4, 3/4, 3/4)'$
- (34)  $\bar{3}^- ' \ x+1, \bar{x}-3/2, \bar{x};$   
 $1/8, -5/8, 7/8$   
 $(\bar{3}_{\bar{x}yz} | 3/4, 1/4, 3/4)'$
- (35)  $\bar{3}^- ' \ \bar{x}, \bar{x}+1, x;$   
 $-1/8, 7/8, 1/8$   
 $(\bar{3}_{xy\bar{z}} | 3/4, 3/4, 1/4)'$
- (36)  $\bar{3}^- ' \ \bar{x}+1/2, x, \bar{x};$   
 $3/8, 1/8, -1/8$   
 $(\bar{3}_{x\bar{y}z} | 1/4, 1/4, 1/4)'$

- (37)  $m' \ x+1/2, \bar{x}, z$   
( $m_{xy} | 1/2, 1/2, 0$ )'
- (38)  $g' \ (1/4, 1/4, 1/2) \ x-1/4, x, z$   
( $m_{\bar{xy}} | 0, 1/2, 1/2$ )'
- (39)  $\bar{4}^- \ ' \ 0, 0, z; 0, 0, 0$   
( $\bar{4}_z^{-1} | 0, 0, 0$ )'
- (40)  $\bar{4}^+ \ ' \ 1/4, -1/4, z; 1/4, -1/4, 1/4$   
( $\bar{4}_z | 1/2, 0, 1/2$ )'
- (41)  $\bar{4}^- \ ' \ x, 1/4, 1/4; 1/4, 1/4, 1/4$   
( $\bar{4}_x^{-1} | 1/2, 1/2, 0$ )'
- (42)  $g' \ (1/2, -1/4, 1/4) \ x, y+1/4, \bar{y}$   
( $m_{yz} | 1/2, 0, 1/2$ )'
- (43)  $g' \ (0, 1/2, 1/2) \ x, y, y$   
( $m_{\bar{yz}} | 0, 1/2, 1/2$ )'
- (44)  $\bar{4}^+ \ ' \ x, 0, 0; 0, 0, 0$   
( $\bar{4}_x | 0, 0, 0$ )'
- (45)  $\bar{4}^+ \ ' \ 1/4, y, 1/4; 1/4, 1/4, 1/4$   
( $\bar{4}_y | 1/2, 1/2, 0$ )'
- (46)  $m' \ \bar{x}, y, x$   
( $m_{xz} | 0, 0, 0$ )'
- (47)  $\bar{4}^- \ ' \ 1/2, y, 0; 1/2, 0, 0$   
( $\bar{4}_y^{-1} | 1/2, 0, 1/2$ )'
- (48)  $g' \ (1/4, 1/2, 1/4) \ x-1/4, y, x$   
( $m_{\bar{xz}} | 0, 1/2, 1/2$ )'

For (1/2, 0, 1/2)' + set

- (1)  $t' \ (1/2, 0, 1/2)$   
( $1 | 1/2, 0, 1/2$ )'
- (2)  $2' \ 1/4, 1/4, z$   
( $2_z | 1/2, 1/2, 0$ )'
- (3)  $2' \ (0, 1/2, 0) \ 0, y, 1/4$   
( $2_y | 0, 1/2, 1/2$ )'
- (4)  $2' \ x, 0, 0$   
( $2_x | 0, 0, 0$ )'
- (5)  $3^+ \ ' \ (1/3, 1/3, 1/3)$   
 $x+1/6, x-1/6, x$   
( $3_{xyz} | 1/2, 0, 1/2$ )'
- (6)  $3^+ \ ' \ \bar{x}, x, \bar{x}$   
( $3_{\bar{yz}}^{-1} | 0, 0, 0$ )'
- (7)  $3^+ \ ' \ x+1/2, \bar{x}, \bar{x}$   
( $3_{\bar{yz}}^{-1} | 1/2, 1/2, 0$ )'
- (8)  $3^+ \ ' \ \bar{x}, \bar{x}+1/2, x$   
( $3_{\bar{yz}}^{-1} | 0, 1/2, 1/2$ )'
- (9)  $3^- \ ' \ (1/3, 1/3, 1/3)$   
 $x-1/6, x-1/3, x$   
( $3_{xyz}^{-1} | 1/2, 0, 1/2$ )'
- (10)  $3^- \ ' \ (-1/3, 1/3, 1/3)$   
 $x+1/6, \bar{x}+1/6, \bar{x}$   
( $3_{\bar{yz}} | 0, 1/2, 1/2$ )'
- (11)  $3^- \ ' \ \bar{x}, \bar{x}, x$   
( $3_{\bar{yz}} | 0, 0, 0$ )'
- (12)  $3^- \ ' \ \bar{x}, x+1/2, \bar{x}$   
( $3_{\bar{yz}} | 1/2, 1/2, 0$ )'
- (13)  $2' \ (1/4, 1/4, 0) \ x, x, 1/8$   
( $2_{xy} | 1/4, 1/4, 1/4$ )'
- (14)  $2' \ (1/4, -1/4, 0) \ x, \bar{x}+1/2, 3/8$   
( $2_{\bar{xy}} | 3/4, 1/4, 3/4$ )'
- (15)  $4^- \ ' \ (0, 0, 1/4) \ 3/4, 0, z$   
( $4_z^{-1} | 3/4, 3/4, 1/4$ )'
- (16)  $4^+ \ ' \ (0, 0, 3/4) \ -1/4, 1/2, z$   
( $4_z | 1/4, 3/4, 3/4$ )'
- (17)  $4^- \ ' \ (1/4, 0, 0) \ x, 1/4, 0$   
( $4_x^{-1} | 1/4, 1/4, 1/4$ )'
- (18)  $2' \ (0, 3/4, 3/4) \ 1/8, y, y$   
( $2_{yz} | 1/4, 3/4, 3/4$ )'
- (19)  $2' \ (0, -1/4, 1/4) \ 3/8, y+1/2, \bar{y}$   
( $2_{\bar{yz}} | 3/4, 1/4, 3/4$ )'
- (20)  $4^+ \ ' \ (3/4, 0, 0) \ x, 1/4, 1/2$   
( $4_x | 3/4, 3/4, 1/4$ )'
- (21)  $4^+ \ ' \ (0, 1/4, 0) \ 1/4, y, 0$   
( $4_y | 1/4, 1/4, 1/4$ )'
- (22)  $2' \ (1/2, 0, 1/2) \ x+1/4, 3/8, x$   
( $2_{xz} | 3/4, 3/4, 1/4$ )'
- (23)  $4^- \ ' \ (0, 3/4, 0) \ -1/4, y, 1/2$   
( $4_y^{-1} | 1/4, 3/4, 3/4$ )'
- (24)  $2' \ \bar{x}+3/4, 1/8, x$   
( $2_{\bar{xz}} | 3/4, 1/4, 3/4$ )'
- (25)  $\bar{1} \ ' \ 3/8, 1/8, 3/8$   
( $\bar{1} | 3/4, 1/4, 3/4$ )'
- (26)  $d' \ (3/4, 3/4, 0) \ x, y, 1/8$   
( $m_z | 3/4, 3/4, 1/4$ )'
- (27)  $d' \ (1/4, 0, 3/4) \ x, 3/8, z$   
( $m_y | 1/4, 3/4, 3/4$ )'
- (28)  $d' \ (0, 1/4, 1/4) \ 1/8, y, z$   
( $m_x | 1/4, 1/4, 1/4$ )'
- (29)  $\bar{3}^+ \ ' \ x-1/2, x-1/2, x;$   
 $1/8, 1/8, 5/8$   
( $\bar{3}_{xyz} | 3/4, 1/4, 3/4$ )'
- (30)  $\bar{3}^+ \ ' \ \bar{x}-1/2, x+1/2, \bar{x};$   
 $-1/8, 1/8, 3/8$   
( $\bar{3}_{\bar{yz}}^{-1} | 1/4, 1/4, 1/4$ )'
- (31)  $\bar{3}^+ \ ' \ x-1/2, \bar{x}+3/2, \bar{x};$   
 $1/8, 7/8, -5/8$   
( $\bar{3}_{\bar{yz}}^{-1} | 3/4, 3/4, 1/4$ )'
- (32)  $\bar{3}^+ \ ' \ \bar{x}+3/2, \bar{x}+1/2, x;$   
 $7/8, -1/8, 5/8$   
( $\bar{3}_{\bar{yz}}^{-1} | 1/4, 3/4, 3/4$ )'
- (33)  $\bar{3}^- \ ' \ x+1/2, x, x;$   
 $5/8, 1/8, 1/8$   
( $\bar{3}_{xyz}^{-1} | 3/4, 1/4, 3/4$ )'
- (34)  $\bar{3}^- \ ' \ x+1, \bar{x}-1, \bar{x};$   
 $1/8, -1/8, 7/8$   
( $\bar{3}_{\bar{yz}} | 1/4, 3/4, 3/4$ )'
- (35)  $\bar{3}^- \ ' \ \bar{x}, \bar{x}+1/2, x;$   
 $-1/8, 3/8, 1/8$   
( $\bar{3}_{\bar{yz}} | 1/4, 1/4, 1/4$ )'
- (36)  $\bar{3}^- \ ' \ \bar{x}+3/2, x-1/2, \bar{x};$   
 $7/8, 1/8, -5/8$   
( $\bar{3}_{\bar{yz}} | 3/4, 3/4, 1/4$ )'
- (37)  $m' \ x, \bar{x}, z$   
( $m_{xy} | 0, 0, 0$ )'
- (38)  $g' \ (1/4, 1/4, 1/2) \ x+1/4, x, z$   
( $m_{\bar{xy}} | 1/2, 0, 1/2$ )'
- (39)  $\bar{4}^- \ ' \ 0, 1/2, z; 0, 1/2, 0$   
( $\bar{4}_z^{-1} | 1/2, 1/2, 0$ )'
- (40)  $\bar{4}^+ \ ' \ 1/4, 1/4, z; 1/4, 1/4, 1/4$   
( $\bar{4}_z | 0, 1/2, 1/2$ )'
- (41)  $\bar{4}^- \ ' \ x, 0, 0; 0, 0, 0$   
( $\bar{4}_x^{-1} | 0, 0, 0$ )'
- (42)  $m' \ x, y+1/2, \bar{y}$   
( $m_{yz} | 0, 1/2, 1/2$ )'
- (43)  $g' \ (1/2, 1/4, 1/4) \ x, y-1/4, y$   
( $m_{\bar{yz}} | 1/2, 0, 1/2$ )'
- (44)  $\bar{4}^+ \ ' \ x, 1/4, -1/4; 1/4, 1/4, -1/4$   
( $\bar{4}_x | 1/2, 1/2, 0$ )'
- (45)  $\bar{4}^+ \ ' \ 0, y, 0; 0, 0, 0$   
( $\bar{4}_y | 0, 0, 0$ )'
- (46)  $g' \ (1/4, 1/2, -1/4) \ \bar{x}+1/4, y, x$   
( $m_{xz} | 1/2, 1/2, 0$ )'
- (47)  $\bar{4}^- \ ' \ 1/4, y, 1/4; 1/4, 1/4, 1/4$   
( $\bar{4}_y^{-1} | 0, 1/2, 1/2$ )'
- (48)  $g' \ (1/2, 0, 1/2) \ x, y, x$   
( $m_{\bar{xz}} | 1/2, 0, 1/2$ )'

For (1/2, 1/2, 0)' + set

- (1)  $t' \ (1/2, 1/2, 0)$   
( $1 | 1/2, 1/2, 0$ )'
- (2)  $2' \ (0, 0, 1/2) \ 1/4, 0, z$   
( $2_z | 1/2, 0, 1/2$ )'
- (3)  $2' \ 0, y, 0$   
( $2_y | 0, 0, 0$ )'
- (4)  $2' \ x, 1/4, 1/4$   
( $2_x | 0, 1/2, 1/2$ )'



(5) $3^+ ' (1/3, 1/3, 1/3)$ $x+1/6, x+1/3, x$ $(3_{xyz}^{-1}   1/2, 1/2, 0)'$	(6) $3^+ ' \bar{x}, x+1/2, \bar{x}$ $(3_{x\bar{y}\bar{z}}^{-1}   0, 1/2, 1/2)'$	(7) $3^+ ' x+1/2, \bar{x}-1/2, \bar{x}$ $(3_{x\bar{y}\bar{z}}^{-1}   1/2, 0, 1/2)'$	(8) $3^+ ' \bar{x}, \bar{x}, x$ $(3_{x\bar{y}\bar{z}}^{-1}   0, 0, 0)'$
(9) $3^- ' (1/3, 1/3, 1/3)$ $x+1/3, x+1/6, x$ $(3_{xyz}^{-1}   1/2, 1/2, 0)'$	(10) $3^- ' x, \bar{x}, \bar{x}$ $(3_{x\bar{y}\bar{z}}   0, 0, 0)'$	(11) $3^- ' \bar{x}+1/2, \bar{x}+1/2, x$ $(3_{x\bar{y}\bar{z}}   0, 1/2, 1/2)'$	(12) $3^- ' (1/3, -1/3, 1/3)$ $x-1/6, x+1/3, \bar{x}$ $(3_{x\bar{y}\bar{z}}   1/2, 0, 1/2)'$
(13) $2' (1/2, 1/2, 0)$ $x, x+1/4, 3/8$ $(2_{xy}   1/4, 3/4, 3/4)'$	(14) $2' x, \bar{x}+3/4, 1/8$ $(2_{xy}   3/4, 3/4, 1/4)'$	(15) $4^- ' (0, 0, 3/4)$ $1/2, -1/4, z$ $(4_z^{-1}   3/4, 1/4, 3/4)'$	(16) $4^+ ' (0, 0, 1/4)$ $0, 1/4, z$ $(4_z   1/4, 1/4, 1/4)'$
(17) $4^- ' (1/4, 0, 0)$ $x, 3/4, 0$ $(4_x^{-1}   1/4, 3/4, 3/4)'$	(18) $2' (0, 1/4, 1/4)$ $1/8, y, y$ $(2_{yz}   1/4, 1/4, 1/4)'$	(19) $2' (0, 1/4, -1/4)$ $3/8, y+1/2, \bar{y}$ $(2_{yz}   3/4, 3/4, 1/4)'$	(20) $4^+ ' (3/4, 0, 0)$ $x, -1/4, 1/2$ $(4_x   3/4, 1/4, 3/4)'$
(21) $4^+ ' (0, 3/4, 0)$ $1/2, y, 1/4$ $(4_y   1/4, 3/4, 3/4)'$	(22) $2' (3/4, 0, 3/4)$ $x, 1/8, x$ $(2_{xz}   3/4, 1/4, 3/4)'$	(23) $4^- ' (0, 1/4, 0)$ $0, y, 1/4$ $(4_y^{-1}   1/4, 1/4, 1/4)'$	(24) $2' (1/4, 0, -1/4)$ $\bar{x}+1/2, 3/8, x$ $(2_{xz}   3/4, 3/4, 1/4)'$
(25) $\bar{1}' 3/8, 3/8, 1/8$ $(\bar{1}   3/4, 3/4, 1/4)'$	(26) $d' (3/4, 1/4, 0)$ $x, y, 3/8$ $(m_z   3/4, 1/4, 3/4)'$	(27) $d' (1/4, 0, 1/4)$ $x, 1/8, z$ $(m_y   1/4, 1/4, 1/4)'$	(28) $d' (0, 3/4, 3/4)$ $1/8, y, z$ $(m_x   1/4, 3/4, 3/4)'$
(29) $\bar{3}^+ ' x+1/2, x, x;$ $5/8, 1/8, 1/8$ $(\bar{3}_{xyz}   3/4, 3/4, 1/4)'$	(30) $\bar{3}^+ ' \bar{x}-3/2, x+1, \bar{x};$ $-5/8, 1/8, 7/8$ $(\bar{3}_{x\bar{y}\bar{z}}^{-1}   1/4, 3/4, 3/4)'$	(31) $\bar{3}^+ ' x+1/2, \bar{x}+1, \bar{x};$ $5/8, 7/8, -1/8$ $(\bar{3}_{x\bar{y}\bar{z}}^{-1}   3/4, 1/4, 3/4)'$	(32) $\bar{3}^+ ' \bar{x}+1/2, \bar{x}, x;$ $3/8, -1/8, 1/8$ $(\bar{3}_{x\bar{y}\bar{z}}^{-1}   1/4, 1/4, 1/4)'$
(33) $\bar{3}^- ' x, x+1/2, x;$ $1/8, 5/8, 1/8$ $(\bar{3}_{xyz}^{-1}   3/4, 3/4, 1/4)'$	(34) $\bar{3}^- ' x+1/2, \bar{x}-1/2, \bar{x};$ $1/8, -1/8, 3/8$ $(\bar{3}_{x\bar{y}\bar{z}}   1/4, 1/4, 1/4)'$	(35) $\bar{3}^- ' \bar{x}-1/2, \bar{x}+1, x;$ $-5/8, 7/8, 1/8$ $(\bar{3}_{x\bar{y}\bar{z}}   1/4, 3/4, 3/4)'$	(36) $\bar{3}^- ' \bar{x}+1, x, \bar{x};$ $7/8, 1/8, -1/8$ $(\bar{3}_{x\bar{y}\bar{z}}   3/4, 1/4, 3/4)'$
(37) $g' (-1/4, 1/4, 1/2)$ $x+1/4, \bar{x}, z$ $(m_{xy}   0, 1/2, 1/2)'$	(38) $g' (1/2, 1/2, 0)$ $x, x, z$ $(m_{xy}   1/2, 1/2, 0)'$	(39) $\bar{4}^- ' 1/4, 1/4, z;$ $1/4, 1/4, 1/4$ $(\bar{4}_z^{-1}   1/2, 0, 1/2)'$	(40) $\bar{4}^+ ' 0, 0, z;$ $0, 0, 0$ $(\bar{4}_z   0, 0, 0)'$
(41) $\bar{4}^- ' x, 0, 1/2;$ $0, 0, 1/2$ $(\bar{4}_x^{-1}   0, 1/2, 1/2)'$	(42) $m' x, y, \bar{y}$ $(m_{yz}   0, 0, 0)'$	(43) $g' (1/2, 1/4, 1/4)$ $x, y+1/4, y$ $(m_{yz}   1/2, 1/2, 0)'$	(44) $\bar{4}^+ ' x, 1/4, 1/4;$ $1/4, 1/4, 1/4$ $(\bar{4}_x   1/2, 0, 1/2)'$
(45) $\bar{4}^+ ' -1/4, y, 1/4;$ $-1/4, 1/4, 1/4$ $(\bar{4}_y   0, 1/2, 1/2)'$	(46) $m' \bar{x}+1/2, y, x$ $(m_{xz}   1/2, 0, 1/2)'$	(47) $\bar{4}^- ' 0, y, 0;$ $0, 0, 0$ $(\bar{4}_y^{-1}   0, 0, 0)'$	(48) $g' (1/4, 1/2, 1/4)$ $x+1/4, y, x$ $(m_{xz}   1/2, 1/2, 0)'$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25); 1'.

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

### Coordinates

(0,0,0) + (0,1/2,1/2,) + (1/2,0,1/2) + (1/2,1/2,0) +  
(0,0,0)' + (0,1/2,1/2,)' + (1/2,0,1/2)' + (1/2,1/2,0)'

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(1) $x, y, z$ [0,0,0]	(2) $\bar{x}, \bar{y}+1/2, z+1/2$ [0,0,0]	(3) $\bar{x}+1/2, y+1/2, \bar{z}$ [0,0,0]	(4) $x+1/2, \bar{y}, \bar{z}+1/2$ [0,0,0]
(5) $z, x, y$ [0,0,0]	(6) $z+1/2, \bar{x}, \bar{y}+1/2$ [0,0,0]	(7) $\bar{z}, \bar{x}+1/2, y+1/2$ [0,0,0]	(8) $\bar{z}+1/2, x+1/2, \bar{y}$ [0,0,0]
(9) $y, z, x$ [0,0,0]	(10) $\bar{y}+1/2, z+1/2, \bar{x}$ [0,0,0]	(11) $y+1/2, \bar{z}, \bar{x}+1/2$ [0,0,0]	(12) $\bar{y}, \bar{z}+1/2, x+1/2$ [0,0,0]
(13) $y+3/4, x+1/4, \bar{z}+3/4$ [0,0,0]	(14) $\bar{y}+1/4, \bar{x}+1/4, \bar{z}+1/4$ [0,0,0]	(15) $y+1/4, \bar{x}+3/4, z+3/4$ [0,0,0]	(16) $\bar{y}+3/4, x+3/4, z+1/4$ [0,0,0]

(17) $x+3/4, z+1/4, \bar{y}+3/4$ [0,0,0]	(18) $\bar{x}+3/4, z+3/4, y+1/4$ [0,0,0]	(19) $\bar{x}+1/4, \bar{z}+1/4, \bar{y}+1/4$ [0,0,0]	(20) $x+1/4, \bar{z}+3/4, y+3/4$ [0,0,0]
(21) $z+3/4, y+1/4, \bar{x}+3/4$ [0,0,0]	(22) $z+1/4, \bar{y}+3/4, x+3/4$ [0,0,0]	(23) $\bar{z}+3/4, y+3/4, x+1/4$ [0,0,0]	(24) $\bar{z}+1/4, \bar{y}+1/4, \bar{x}+1/4$ [0,0,0]
(25) $\bar{x}+1/4, \bar{y}+1/4, \bar{z}+1/4$ [0,0,0]	(26) $x+1/4, y+3/4, \bar{z}+3/4$ [0,0,0]	(27) $x+3/4, \bar{y}+3/4, z+1/4$ [0,0,0]	(28) $\bar{x}+3/4, y+1/4, z+3/4$ [0,0,0]
(29) $\bar{z}+1/4, \bar{x}+1/4, \bar{y}+1/4$ [0,0,0]	(30) $\bar{z}+3/4, x+1/4, y+3/4$ [0,0,0]	(31) $z+1/4, x+3/4, \bar{y}+3/4$ [0,0,0]	(32) $z+3/4, \bar{x}+3/4, y+1/4$ [0,0,0]
(33) $\bar{y}+1/4, \bar{z}+1/4, \bar{x}+1/4$ [0,0,0]	(34) $y+3/4, \bar{z}+3/4, x+1/4$ [0,0,0]	(35) $\bar{y}+3/4, z+1/4, x+3/4$ [0,0,0]	(36) $y+1/4, z+3/4, \bar{x}+3/4$ [0,0,0]
(37) $\bar{y}+1/2, \bar{x}, z+1/2$ [0,0,0]	(38) $y, x, z$ [0,0,0]	(39) $\bar{y}, x+1/2, \bar{z}+1/2$ [0,0,0]	(40) $y+1/2, \bar{x}+1/2, \bar{z}$ [0,0,0]
(41) $\bar{x}+1/2, \bar{z}, y+1/2$ [0,0,0]	(42) $x+1/2, \bar{z}+1/2, \bar{y}$ [0,0,0]	(43) $x, z, y$ [0,0,0]	(44) $\bar{x}, z+1/2, \bar{y}+1/2$ [0,0,0]
(45) $\bar{z}+1/2, \bar{y}, x+1/2$ [0,0,0]	(46) $\bar{z}, y+1/2, \bar{x}+1/2$ [0,0,0]	(47) $z+1/2, \bar{y}+1/2, \bar{x}$ [0,0,0]	(48) $z, y, x$ [0,0,0]

96 h ..21'

$1/8, y, \bar{y}+1/4$ [0,0,0]	$7/8, \bar{y}+1/2, \bar{y}+3/4$ [0,0,0]	$3/8, y+1/2, y+3/4$ [0,0,0]	$5/8, \bar{y}, y+1/4$ [0,0,0]
$\bar{y}+1/4, 1/8, y$ [0,0,0]	$\bar{y}+3/4, 7/8, \bar{y}+1/2$ [0,0,0]	$y+3/4, 3/8, y+1/2$ [0,0,0]	$y+1/4, 5/8, \bar{y}$ [0,0,0]
$y, \bar{y}+1/4, 1/8$ [0,0,0]	$\bar{y}+1/2, \bar{y}+3/4, 7/8$ [0,0,0]	$y+1/2, y+3/4, 3/8$ [0,0,0]	$\bar{y}, y+1/4, 5/8$ [0,0,0]
$1/8, \bar{y}+1/4, y$ [0,0,0]	$3/8, y+3/4, y+1/2$ [0,0,0]	$7/8, \bar{y}+3/4, \bar{y}+1/2$ [0,0,0]	$5/8, y+1/4, \bar{y}$ [0,0,0]
$y, 1/8, \bar{y}+1/4$ [0,0,0]	$y+1/2, 3/8, y+3/4$ [0,0,0]	$\bar{y}+1/2, 7/8, \bar{y}+3/4$ [0,0,0]	$\bar{y}, 5/8, y+1/4$ [0,0,0]
$\bar{y}+1/4, y, 1/8$ [0,0,0]	$y+3/4, y+1/2, 3/8$ [0,0,0]	$\bar{y}+3/4, \bar{y}+1/2, 7/8$ [0,0,0]	$y+1/4, \bar{y}, 5/8$ [0,0,0]

96 g ..m1'

$x, x, z$ [0,0,0]	$\bar{x}, \bar{x}+1/2, z+1/2$ [0,0,0]	$\bar{x}+1/2, x+1/2, \bar{z}$ [0,0,0]	$x+1/2, \bar{x}, \bar{z}+1/2$ [0,0,0]
$z, x, x$ [0,0,0]	$z+1/2, \bar{x}, \bar{x}+1/2$ [0,0,0]	$\bar{z}, \bar{x}+1/2, x+1/2$ [0,0,0]	$\bar{z}+1/2, x+1/2, \bar{x}$ [0,0,0]
$x, z, x$ [0,0,0]	$\bar{x}+1/2, z+1/2, \bar{x}$ [0,0,0]	$x+1/2, \bar{z}, \bar{x}+1/2$ [0,0,0]	$\bar{x}, \bar{z}+1/2, x+1/2$ [0,0,0]
$x+3/4, x+1/4, \bar{z}+3/4$ [0,0,0]	$\bar{x}+1/4, \bar{x}+1/4, \bar{z}+1/4$ [0,0,0]	$x+1/4, \bar{x}+3/4, z+3/4$ [0,0,0]	$\bar{x}+3/4, x+3/4, z+1/4$ [0,0,0]
$x+3/4, z+1/4, \bar{x}+3/4$ [0,0,0]	$\bar{x}+3/4, z+3/4, x+1/4$ [0,0,0]	$\bar{x}+1/4, \bar{z}+1/4, \bar{x}+1/4$ [0,0,0]	$x+1/4, \bar{z}+3/4, x+3/4$ [0,0,0]
$z+3/4, x+1/4, \bar{x}+3/4$ [0,0,0]	$z+1/4, \bar{x}+3/4, x+3/4$ [0,0,0]	$\bar{z}+3/4, x+3/4, x+1/4$ [0,0,0]	$\bar{z}+1/4, \bar{x}+1/4, \bar{x}+1/4$ [0,0,0]

48 f 2.mm1'	$x, 0, 0$ [0,0,0]	$\bar{x}, 1/2, 1/2$ [0,0,0]	$0, x, 0$ [0,0,0]	$1/2, \bar{x}, 1/2$ [0,0,0]
	$0, 0, x$ [0,0,0]	$1/2, 1/2, \bar{x}$ [0,0,0]	$3/4, x+1/4, 3/4$ [0,0,0]	$1/4, \bar{x}+1/4, 1/4$ [0,0,0]
	$x+3/4, 1/4, 3/4$ [0,0,0]	$\bar{x}+3/4, 3/4, 1/4$ [0,0,0]	$3/4, 1/4, \bar{x}+3/4$ [0,0,0]	$1/4, 3/4, x+3/4$ [0,0,0]

32 e .3m1'	$x, x, x$ [0,0,0]	$\bar{x}, \bar{x}+1/2, x+1/2$ [0,0,0]
	$\bar{x}+1/2, x+1/2, \bar{x}$ [0,0,0]	$x+1/2, \bar{x}, \bar{x}+1/2$ [0,0,0]
	$x+3/4, x+1/4, \bar{x}+3/4$ [0,0,0]	$\bar{x}+1/4, \bar{x}+1/4, \bar{x}+1/4$ [0,0,0]
	$x+1/4, \bar{x}+3/4, x+3/4$ [0,0,0]	$\bar{x}+3/4, x+3/4, x+1/4$ [0,0,0]

Continued

227.2.1629

Fd $\bar{3}$ m1'

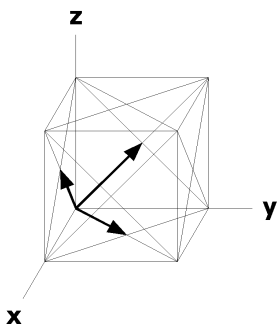
16	d	$\bar{3}m1'$	5/8,5/8,5/8 [0,0,0]	3/8,7/8,1/8 [0,0,0]	7/8,1/8,3/8 [0,0,0]	1/8,3/8,7/8 [0,0,0]
16	c	$\bar{3}m1'$	1/8,1/8,1/8 [0,0,0]	7/8,3/8,5/8 [0,0,0]	3/8,5/8,7/8 [0,0,0]	5/8,7/8,3/8 [0,0,0]
8	b	$\bar{4}3m1'$	1/2,1/2,1/2 [0,0,0]		1/4,3/4,1/4 [0,0,0]	
8	a	$\bar{4}3m1'$	0,0,0 [0,0,0]		3/4,1/4,3/4 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1]  $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/4$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/4$   
 Origin at 0,0,z

Along [1,1,1]  $p6mm1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

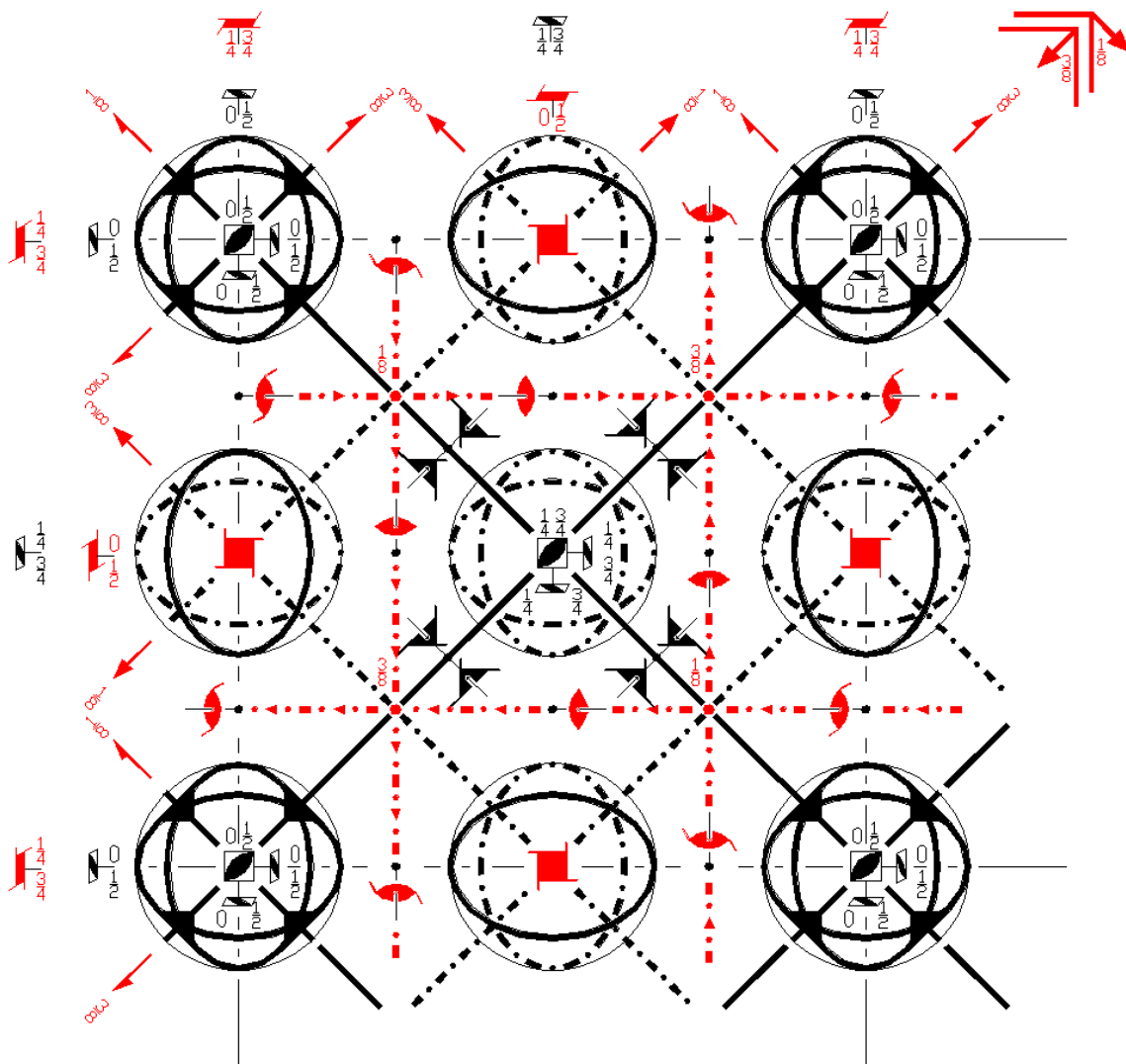
Along [1,1,0]  $c2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x,x,1/8



Fd' $\bar{3}$ 'm  
227.3.1630

m' $\bar{3}$ 'm  
F4<sub>1</sub>'d' $\bar{3}$ '2'/m

Cubic



Origin at  $\bar{4}3m$ , at  $-1/8, -1/8, -1/8$  from center ( $\bar{3}'m$ )

Asymmetric unit  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/8$ ;  $-1/8 \leq z \leq 1/8$ ;  $y \leq \min(1/2-x, x)$ ;  $-y \leq z \leq y$

Vertices  $0,0,0$   $1/2,0,0$   $3/8,1/8,1/8$   $1/8,1/8,1/8$   $3/8,1/8,-1/8$   $1/8,1/8,-1/8$

### Symmetry Operations

For  $(0,0,0)$  + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)   | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)   | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>  1/2,0,1/2)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> (1/3,-1/3,1/3)<br>x+1/6,x+1/6,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) | (7) 3 <sup>+</sup> (-1/3,1/3,1/3)<br>x+1/3,x-1/6,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2) | (8) 3 <sup>+</sup> (1/3,1/3,-1/3)<br>x+1/6,x+1/3,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x,x̄+1/2,x̄<br>(3 <sub>xyz</sub>  1/2,1/2,0)                                   | (11) 3 <sup>-</sup> x̄+1/2,x̄,x<br>(3 <sub>xyz</sub>  1/2,0,1/2)                                   | (12) 3 <sup>-</sup> x̄-1/2,x+1/2,x̄<br>(3 <sub>xyz</sub>  0,1/2,1/2)                               |

- |   |  |  |  |
|---|--|--|--|
| (13) 2' (1/2,1/2,0) x,x-1/4,3/8<br>(2 <sub>xy</sub>  3/4,1/4,3/4)'              | (14) 2' x,x+1/4,1/8<br>(2 <sub>xy</sub>  1/4,1/4,1/4)'                               | (15) 4' (0,0,3/4) 1/2,1/4,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/4,3/4,3/4)'        | (16) 4+ (0,0,1/4) 0,3/4,z<br>(4 <sub>z</sub>  3/4,3/4,1/4)'                        |
| (17) 4' (3/4,0,0) x,1/2,1/4<br>(4 <sub>x</sub> <sup>-1</sup>  3/4,1/4,3/4)'     | (18) 2' (0,1/2,1/2) 3/8,y+1/4,y<br>(2 <sub>yz</sub>  3/4,3/4,1/4)'                   | (19) 2' 1/8,y+1/4,y<br>(2 <sub>yz</sub>  1/4,1/4,1/4)'                             | (20) 4+ (1/4,0,0) x,0,3/4<br>(4 <sub>x</sub>  1/4,3/4,3/4)'                        |
| (21) 4+ (0,1/4,0) 3/4,y,0<br>(4 <sub>y</sub>  3/4,1/4,3/4)'                     | (22) 2' (1/2,0,1/2) x-1/4,3/8,x<br>(2 <sub>xz</sub>  1/4,3/4,3/4)'                   | (23) 4' (0,3/4,0) 1/4,y,1/2<br>(4 <sub>y</sub> <sup>-1</sup>  3/4,3/4,1/4)'        | (24) 2' x+1/4,1/8,x<br>(2 <sub>xz</sub>  1/4,1/4,1/4)'                             |
| (25) 1' 1/8,1/8,1/8<br>(1 1/4,1/4,1/4)'   | (26) d' (1/4,3/4,0) x,y,3/8<br>(m <sub>z</sub>  1/4,3/4,3/4)'                        | (27) d' (3/4,0,1/4) x,3/8,z<br>(m <sub>y</sub>  3/4,3/4,1/4)'                      | (28) d' (0,1/4,3/4) 3/8,y,z<br>(m <sub>x</sub>  3/4,1/4,3/4)'                      |
| (29) 3+ x,x,x;<br>1/8,1/8,1/8<br>(3 <sub>xyz</sub>  1/4,1/4,1/4)'               | (30) 3+ x-1,x+1,x;<br>-1/8,1/8,7/8<br>(3 <sub>xyz</sub> <sup>-1</sup>  3/4,1/4,3/4)' | (31) 3+ x,x+1,x;<br>1/8,7/8,-1/8<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/4,3/4,3/4)' | (32) 3+ x+1,x,x;<br>7/8,-1/8,1/8<br>(3 <sub>xyz</sub> <sup>-1</sup>  3/4,3/4,1/4)' |
| (33) 3- x,x,x;<br>1/8,1/8,1/8<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/4,1/4,1/4)' | (34) 3- x+3/2,x-1,x;<br>5/8,-1/8,7/8<br>(3 <sub>xyz</sub>  3/4,3/4,1/4)'             | (35) 3- x+1/2,x+3/2,x;<br>-1/8,7/8,5/8<br>(3 <sub>xyz</sub>  3/4,1/4,3/4)'         | (36) 3- x+1,x+1/2,x;<br>7/8,5/8,-1/8<br>(3 <sub>xyz</sub>  1/4,3/4,3/4)'           |
| (37) g (1/4,-1/4,1/2) x+1/4,x,z<br>(m <sub>xy</sub>  1/2,0,1/2)                 | (38) m x,x,z<br>(m <sub>xy</sub>  0,0,0)   | (39) 4- -1/4,1/4,z; -1/4,1/4,1/4<br>(4 <sub>z</sub> <sup>-1</sup>  0,1/2,1/2)      | (40) 4+ 1/2,0,z; 1/2,0,0<br>(4 <sub>z</sub>  1/2,1/2,0)                            |
| (41) 4- x,-1/4,1/4; 1/4,-1/4,1/4<br>(4 <sub>x</sub> <sup>-1</sup>  1/2,0,1/2)   | (42) g (1/2,1/4,-1/4) x,y+1/4,y<br>(m <sub>yz</sub>  1/2,1/2,0)                      | (43) m x,y,y<br>(m <sub>yz</sub>  0,0,0)   | (44) 4+ x,1/2,0; 0,1/2,0<br>(4 <sub>x</sub>  0,1/2,1/2)                            |
| (45) 4+ 0,y,1/2; 0,0,1/2<br>(4 <sub>y</sub>  1/2,0,1/2)                         | (46) g (-1/4,1/2,1/4) x+1/4,y,x<br>(m <sub>xz</sub>  0,1/2,1/2)                      | (47) 4- 1/4,y,-1/4; 1/4,1/4,-1/4<br>(4 <sub>y</sub> <sup>-1</sup>  1/2,1/2,0)      | (48) m x,y,x<br>(m <sub>xz</sub>  0,0,0)   |

For (0,1/2,1/2) + set

- |  |  |  |  |
|--|--|--|--|
| (1) t (0,1/2,1/2)<br>(1 0,1/2,1/2)   | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)   | (3) 2 1/4,y,1/4<br>(2 <sub>y</sub>  1/2,0,1/2)                                       | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)                                 |
| (5) 3+ (1/3,1/3,1/3)<br>x-1/3,x-1/6,x<br>(3 <sub>xyz</sub>  0,1/2,1/2)               | (6) 3+ x+1/2,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0)                        | (7) 3+ x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)                              | (8) 3+ x+1/2,x+1/2,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2)                    |
| (9) 3- (1/3,1/3,1/3)<br>x-1/6,x+1/6,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2) | (10) 3- x+1/2,x,x<br>(3 <sub>xyz</sub>  1/2,0,1/2)                                     | (11) 3- (1/3,1/3,-1/3)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub>  1/2,1/2,0)             | (12) 3- x,x,x<br>(3 <sub>xyz</sub>  0,0,0)   |
| (13) 2' (3/4,3/4,0) x,x,1/8<br>(2 <sub>xy</sub>  3/4,3/4,1/4)'                       | (14) 2' (-1/4,1/4,0) x,x+1/2,3/8<br>(2 <sub>xy</sub>  1/4,3/4,3/4)'                    | (15) 4' (0,0,1/4) 1/4,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/4,1/4,1/4)'            | (16) 4+ (0,0,3/4) 1/4,1/2,z<br>(4 <sub>z</sub>  3/4,1/4,3/4)'                          |
| (17) 4' (3/4,0,0) x,1/2,-1/4<br>(4 <sub>x</sub> <sup>-1</sup>  3/4,3/4,1/4)'         | (18) 2' (0,1/2,1/2) 3/8,y-1/4,y<br>(2 <sub>yz</sub>  3/4,1/4,3/4)'                     | (19) 2' 1/8,y+3/4,y<br>(2 <sub>yz</sub>  1/4,3/4,3/4)'                               | (20) 4+ (1/4,0,0) x,0,1/4<br>(4 <sub>x</sub>  1/4,1/4,1/4)'                            |
| (21) 4+ (0,3/4,0) 1/2,y,-1/4<br>(4 <sub>y</sub>  3/4,3/4,1/4)'                       | (22) 2' (1/4,0,1/4) x,1/8,x<br>(2 <sub>xz</sub>  1/4,1/4,1/4)'                         | (23) 4' (0,1/4,0) 0,y,3/4<br>(4 <sub>y</sub> <sup>-1</sup>  3/4,1/4,3/4)'            | (24) 2' (-1/4,0,1/4) x+1/2,3/8,x<br>(2 <sub>xz</sub>  1/4,3/4,3/4)'                    |
| (25) 1' 1/8,3/8,3/8<br>(1 1/4,3/4,3/4)'  | (26) d' (1/4,1/4,0) x,y,1/8<br>(m <sub>z</sub>  1/4,1/4,1/4)'                          | (27) d' (3/4,0,3/4) x,1/8,z<br>(m <sub>y</sub>  3/4,1/4,3/4)'                        | (28) d' (0,3/4,1/4) 3/8,y,z<br>(m <sub>x</sub>  3/4,3/4,1/4)'                          |
| (29) 3+ x,x+1/2,x;<br>1/8,5/8,1/8<br>(3 <sub>xyz</sub>  1/4,3/4,3/4)'                | (30) 3+ x-1,x+3/2,x;<br>-1/8,5/8,7/8<br>(3 <sub>xyz</sub> <sup>-1</sup>  3/4,3/4,1/4)' | (31) 3+ x,x+1/2,x;<br>1/8,3/8,-1/8<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/4,1/4,1/4)' | (32) 3+ x+1,x-1/2,x;<br>7/8,-5/8,1/8<br>(3 <sub>xyz</sub> <sup>-1</sup>  3/4,1/4,3/4)' |

- |   |   |   |   |
|---|---|---|---|
| (33) $\bar{3}^-$ ' x-1/2,x-1/2,x;<br>1/8,1/8,5/8<br>( $\bar{3}_{xyz}^{-1}$  1/4,3/4,3/4)' | (34) $\bar{3}^-$ ' x+1, $\bar{x}$ -3/2, $\bar{x}$ ;<br>1/8,-5/8,7/8<br>( $\bar{3}_{xyz}$  3/4,1/4,3/4)' | (35) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ +1, x;<br>-1/8,7/8,1/8<br>( $\bar{3}_{xyz}$  3/4,3/4,1/4)' | (36) $\bar{3}^-$ ' $\bar{x}$ +1/2, x, $\bar{x}$ ;<br>3/8,1/8,-1/8<br>( $\bar{3}_{xyz}$  1/4,1/4,1/4)' |
| (37) m x+1/2, $\bar{x}$ ,z<br>( $m_{xy}$  1/2,1/2,0)                                      | (38) g (1/4,1/4,1/2) x-1/4,x,z<br>( $m_{xy}$  0,1/2,1/2)  | (39) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1}$  0,0,0)   | (40) $\bar{4}^+$ 1/4,-1/4,z; 1/4,-1/4,1/4<br>( $\bar{4}_z$  1/2,0,1/2)                                |
| (41) $\bar{4}^-$ x,1/4,1/4; 1/4,1/4,1/4<br>( $\bar{4}_x^{-1}$  1/2,1/2,0)                 | (42) g (1/2,-1/4,1/4) x,y+1/4, $\bar{y}$<br>( $m_{yz}$  1/2,0,1/2)                                      | (43) g (0,1/2,1/2) x,y,y<br>( $m_{yz}$  0,1/2,1/2)  | (44) $\bar{4}^+$ x,0,0; 0,0,0<br>( $\bar{4}_x$  0,0,0)  |
| (45) $\bar{4}^+$ 1/4,y,1/4; 1/4,1/4,1/4<br>( $\bar{4}_y$  1/2,1/2,0)                      | (46) m $\bar{x}$ ,y,x<br>( $m_{xz}$  0,0,0)   | (47) $\bar{4}^-$ 1/2,y,0; 1/2,0,0<br>( $\bar{4}_y^{-1}$  1/2,0,1/2)                                 | (48) g (1/4,1/2,1/4) x-1/4,y,x<br>( $m_{xz}$  0,1/2,1/2)  |

For (1/2,0,1/2) + set

- |  |   |  |   |
|--|---|--|---|
| (1) t (1/2,0,1/2)<br>(1 1/2,0,1/2)   | (2) 2 1/4,1/4,z<br>(2 <sub>z</sub>  1/2,1/2,0)  | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> (1/3,1/3,1/3)<br>x+1/6,x-1/6,x<br>(3 <sub>xyz</sub>  1/2,0,1/2)               | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)                         | (7) 3 <sup>+</sup> x+1/2, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0)                 | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ +1/2,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)                |
| (9) 3 <sup>-</sup> (1/3,1/3,1/3)<br>x-1/6,x-1/3,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) | (10) 3 <sup>-</sup> (-1/3,1/3,1/3)<br>x+1/6, $\bar{x}$ +1/6, $\bar{x}$<br>(3 <sub>xyz</sub>  0,1/2,1/2)       | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ , x<br>(3 <sub>xyz</sub>  0,0,0)                                     | (12) 3 <sup>-</sup> $\bar{x}$ , x+1/2, $\bar{x}$<br>(3 <sub>xyz</sub>  1/2,1/2,0)                             |
| (13) 2' (1/4,1/4,0) x,x,1/8<br>(2 <sub>xy</sub>  1/4,1/4,1/4)'                                   | (14) 2' (1/4,-1/4,0) x, $\bar{x}$ +1/2,3/8<br>(2 <sub>xy</sub>  3/4,1/4,3/4)'                                 | (15) 4 <sup>-</sup> ' (0,0,1/4) 3/4,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  3/4,3/4,1/4)'                        | (16) 4 <sup>+</sup> ' (0,0,3/4) -1/4,1/2,z<br>(4 <sub>z</sub>  1/4,3/4,3/4)'                                  |
| (17) 4 <sup>-</sup> ' (1/4,0,0) x,1/4,0<br>(4 <sub>x</sub> <sup>-1</sup>  1/4,1/4,1/4)'          | (18) 2' (0,3/4,3/4) 1/8,y,y<br>(2 <sub>yz</sub>  1/4,3/4,3/4)'  | (19) 2' (0,-1/4,1/4) 3/8,y+1/2, $\bar{y}$<br>(2 <sub>yz</sub>  3/4,1/4,3/4)'                                   | (20) 4 <sup>+</sup> ' (3/4,0,0) x,1/4,1/2<br>(4 <sub>x</sub>  3/4,3/4,1/4)'                                   |
| (21) 4 <sup>+</sup> ' (0,1/4,0) 1/4,y,0<br>(4 <sub>y</sub>  1/4,1/4,1/4)'                        | (22) 2' (1/2,0,1/2) x+1/4,3/8,x<br>(2 <sub>xz</sub>  3/4,3/4,1/4)'  | (23) 4 <sup>-</sup> ' (0,3/4,0) -1/4,y,1/2<br>(4 <sub>y</sub> <sup>-1</sup>  1/4,3/4,3/4)'                     | (24) 2' $\bar{x}$ +3/4,1/8,x<br>(2 <sub>xz</sub>  3/4,1/4,3/4)'   |
| (25) $\bar{1}^-$ 3/8,1/8,3/8<br>( $\bar{1}$  3/4,1/4,3/4)'                                       | (26) d' (3/4,3/4,0) x,y,1/8<br>( $m_z$  3/4,3/4,1/4)'   | (27) d' (1/4,0,3/4) x,3/8,z<br>( $m_y$  1/4,3/4,3/4)'  | (28) d' (0,1/4,1/4) 1/8,y,z<br>( $m_x$  1/4,1/4,1/4)'   |
| (29) $\bar{3}^+$ ' x-1/2,x-1/2,x;<br>1/8,1/8,5/8<br>( $\bar{3}_{xyz}$  3/4,1/4,3/4)'             | (30) $\bar{3}^+$ ' $\bar{x}$ -1/2,x+1/2, $\bar{x}$ ;<br>-1/8,1/8,3/8<br>( $\bar{3}_{xyz}^{-1}$  1/4,1/4,1/4)' | (31) $\bar{3}^+$ ' x-1/2, $\bar{x}$ +3/2, $\bar{x}$ ;<br>1/8,7/8,-5/8<br>( $\bar{3}_{xyz}^{-1}$  3/4,3/4,1/4)' | (32) $\bar{3}^+$ ' $\bar{x}$ +3/2, $\bar{x}$ +1/2,x;<br>7/8,-1/8,5/8<br>( $\bar{3}_{xyz}^{-1}$  1/4,3/4,3/4)' |
| (33) $\bar{3}^-$ ' x+1/2,x,x;<br>5/8,1/8,1/8<br>( $\bar{3}_{xyz}^{-1}$  3/4,1/4,3/4)'            | (34) $\bar{3}^-$ ' x+1, $\bar{x}$ -1, $\bar{x}$ ;<br>1/8,-1/8,7/8<br>( $\bar{3}_{xyz}$  1/4,3/4,3/4)'         | (35) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ +1/2, x;<br>-1/8,3/8,1/8<br>( $\bar{3}_{xyz}$  1/4,1/4,1/4)'          | (36) $\bar{3}^-$ ' $\bar{x}$ +3/2, x-1/2, $\bar{x}$ ;<br>7/8,1/8,-5/8<br>( $\bar{3}_{xyz}$  3/4,3/4,1/4)'     |
| (37) m x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0)   | (38) g (1/4,1/4,1/2) x+1/4,x,z<br>( $m_{xy}$  1/2,0,1/2)  | (39) $\bar{4}^-$ 0,1/2,z; 0,1/2,0<br>( $\bar{4}_z^{-1}$  1/2,1/2,0)  | (40) $\bar{4}^+$ 1/4,1/4,z; 1/4,1/4,1/4<br>( $\bar{4}_z$  0,1/2,1/2)  |
| (41) $\bar{4}^-$ x,0,0; 0,0,0<br>( $\bar{4}_x^{-1}$  0,0,0)                                      | (42) m x,y+1/2, $\bar{y}$<br>( $m_{yz}$  0,1/2,1/2)   | (43) g (1/2,1/4,1/4) x,y-1/4,y<br>( $m_{yz}$  1/2,0,1/2)   | (44) $\bar{4}^+$ x,1/4,-1/4; 1/4,1/4,-1/4<br>( $\bar{4}_x$  1/2,1/2,0)  |
| (45) $\bar{4}^+$ 0,y,0; 0,0,0<br>( $\bar{4}_y$  0,0,0)   | (46) g (1/4,1/2,-1/4) $\bar{x}$ +1/4,y,x<br>( $m_{xz}$  1/2,1/2,0)  | (47) $\bar{4}^-$ 1/4,y,1/4; 1/4,1/4,1/4<br>( $\bar{4}_y^{-1}$  0,1/2,1/2)                                      | (48) g (1/2,0,1/2) x,y,x<br>( $m_{xz}$  1/2,0,1/2)  |

For (1/2,1/2,0) + set

(1) $t$ (1/2,1/2,0) (1   1/2,1/2,0)	(2) $2$ (0,0,1/2) 1/4,0,z (2 <sub>z</sub>   1/2,0,1/2)	(3) $2$ 0,y,0 (2 <sub>y</sub>   0,0,0)	(4) $2$ x,1/4,1/4 (2 <sub>x</sub>   0,1/2,1/2)
(5) $3^+$ (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) $3^+$ $\bar{x}$ ,x+1/2, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   0,1/2,1/2)	(7) $3^+$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,0,1/2)	(8) $3^+$ $\bar{x}$ , $\bar{x}$ ,x (3 <sub>xyz</sub> <sup>-1</sup>   0,0,0)
(9) $3^-$ (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) $3^-$ x, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub>   0,0,0)	(11) $3^-$ $\bar{x}$ +1/2, $\bar{x}$ +1/2, x (3 <sub>xyz</sub>   0,1/2,1/2)	(12) $3^-$ (1/3,-1/3,1/3) x-1/6, x+1/3, $\bar{x}$ (3 <sub>xyz</sub>   1/2,0,1/2)
(13) $2'$ (1/2,1/2,0) x,x+1/4,3/8 (2 <sub>xy</sub>   1/4,3/4,3/4)'	(14) $2'$ x, $\bar{x}$ +3/4,1/8 (2 <sub>xy</sub>   3/4,3/4,1/4)'	(15) $4^-$ (0,0,3/4) 1/2,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   3/4,1/4,3/4)'	(16) $4^+$ (0,0,1/4) 0,1/4,z (4 <sub>z</sub>   1/4,1/4,1/4)'
(17) $4^-$ (1/4,0,0) x,3/4,0 (4 <sub>x</sub> <sup>-1</sup>   1/4,3/4,3/4)'	(18) $2'$ (0,1/4,1/4) 1/8,y,y (2 <sub>yz</sub>   1/4,1/4,1/4)'	(19) $2'$ (0,1/4,-1/4) 3/8,y+1/2, $\bar{y}$ (2 <sub>yz</sub>   3/4,3/4,1/4)'	(20) $4^+$ (3/4,0,0) x,-1/4,1/2 (4 <sub>x</sub>   3/4,1/4,3/4)'
(21) $4^+$ (0,3/4,0) 1/2,y,1/4 (4 <sub>y</sub>   1/4,3/4,3/4)'	(22) $2'$ (3/4,0,3/4) x,1/8,x (2 <sub>xz</sub>   3/4,1/4,3/4)'	(23) $4^-$ (0,1/4,0) 0,y,1/4 (4 <sub>y</sub> <sup>-1</sup>   1/4,1/4,1/4)'	(24) $2'$ (1/4,0,-1/4) $\bar{x}$ +1/2,3/8,x (2 <sub>xz</sub>   3/4,3/4,1/4)'
(25) $\bar{1}$ 3/8,3/8,1/8 ( $\bar{1}$   3/4,3/4,1/4)'	(26) $d'$ (3/4,1/4,0) x,y,3/8 (m <sub>z</sub>   3/4,1/4,3/4)'	(27) $d'$ (1/4,0,1/4) x,1/8,z (m <sub>y</sub>   1/4,1/4,1/4)'	(28) $d'$ (0,3/4,3/4) 1/8,y,z (m <sub>x</sub>   1/4,3/4,3/4)'
(29) $\bar{3}^+$ x+1/2,x,x; 5/8,1/8,1/8 ( $\bar{3}$ <sub>xyz</sub>   3/4,3/4,1/4)'	(30) $\bar{3}^+$ $\bar{x}$ -3/2,x+1, $\bar{x}$ ; -5/8,1/8,7/8 ( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>   1/4,3/4,3/4)'	(31) $\bar{3}^+$ x+1/2, $\bar{x}$ +1, $\bar{x}$ ; 5/8,7/8,-1/8 ( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>   3/4,1/4,3/4)'	(32) $\bar{3}^+$ $\bar{x}$ +1/2, $\bar{x}$ ,x; 3/8,-1/8,1/8 ( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>   1/4,1/4,1/4)'
(33) $\bar{3}^-$ x,x+1/2,x; 1/8,5/8,1/8 ( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>   3/4,3/4,1/4)'	(34) $\bar{3}^-$ x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ; 1/8,-1/8,3/8 ( $\bar{3}$ <sub>xyz</sub>   1/4,1/4,1/4)'	(35) $\bar{3}^-$ $\bar{x}$ -1/2, $\bar{x}$ +1, x; -5/8,7/8,1/8 ( $\bar{3}$ <sub>xyz</sub>   1/4,3/4,3/4)'	(36) $\bar{3}^-$ $\bar{x}$ +1, x, $\bar{x}$ ; 7/8,1/8,-1/8 ( $\bar{3}$ <sub>xyz</sub>   3/4,1/4,3/4)'
(37) $g$ (-1/4,1/4,1/2) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   0,1/2,1/2)	(38) $g$ (1/2,1/2,0) x,x,z (m <sub>xy</sub>   1/2,1/2,0)	(39) $\bar{4}$ 1/4,1/4,z; 1/4,1/4,1/4 ( $\bar{4}$ <sub>z</sub> <sup>-1</sup>   1/2,0,1/2)	(40) $\bar{4}^+$ 0,0,z; 0,0,0 ( $\bar{4}$ <sub>z</sub>   0,0,0)
(41) $\bar{4}$ x,0,1/2; 0,0,1/2 ( $\bar{4}$ <sub>x</sub> <sup>-1</sup>   0,1/2,1/2)	(42) $m$ x,y, $\bar{y}$ (m <sub>yz</sub>   0,0,0)	(43) $g$ (1/2,1/4,1/4) x,y+1/4,y (m <sub>yz</sub>   1/2,1/2,0)	(44) $\bar{4}^+$ x,1/4,1/4; 1/4,1/4,1/4 ( $\bar{4}$ <sub>x</sub>   1/2,0,1/2)
(45) $\bar{4}^+$ -1/4,y,1/4; -1/4,1/4,1/4 ( $\bar{4}$ <sub>y</sub>   0,1/2,1/2)	(46) $m$ $\bar{x}$ +1/2,y,x (m <sub>xz</sub>   1/2,0,1/2)	(47) $\bar{4}$ 0,y,0; 0,0,0 ( $\bar{4}$ <sub>y</sub> <sup>-1</sup>   0,0,0)	(48) $g$ (1/4,1/2,1/4) x+1/4,y,x (m <sub>xz</sub>   1/2,1/2,0)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

192	i	1	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +					
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}$ , $\bar{y}$ +1/2,z+1/2	[ $\bar{u}$ , $\bar{v}$ ,w]	(3)	$\bar{x}$ +1/2,y+1/2, $\bar{z}$	[ $\bar{u}$ ,v, $\bar{w}$ ]	(4)	x+1/2, $\bar{y}$ , $\bar{z}$ +1/2	[u, $\bar{v}$ , $\bar{w}$ ]
(5)	z,x,y	[w,u,v]	(6)	z+1/2, $\bar{x}$ , $\bar{y}$ +1/2	[w, $\bar{u}$ , $\bar{v}$ ]	(7)	$\bar{z}$ , $\bar{x}$ +1/2,y+1/2	[ $\bar{w}$ , $\bar{u}$ ,v]	(8)	$\bar{z}$ +1/2,x+1/2, $\bar{y}$	[ $\bar{w}$ ,u, $\bar{v}$ ]

- (9)  $y, z, x [v, w, u]$  (10)  $\bar{y}+1/2, z+1/2, \bar{x} [\bar{v}, w, \bar{u}]$  (11)  $y+1/2, \bar{z}, \bar{x}+1/2 [v, \bar{w}, \bar{u}]$  (12)  $\bar{y}, \bar{z}+1/2, x+1/2 [\bar{v}, \bar{w}, u]$   
 (13)  $y+3/4, x+1/4, \bar{z}+3/4 [\bar{v}, \bar{u}, w]$  (14)  $\bar{y}+1/4, \bar{x}+1/4, \bar{z}+1/4 [v, u, w]$  (15)  $y+1/4, \bar{x}+3/4, z+3/4 [\bar{v}, u, \bar{w}]$  (16)  $\bar{y}+3/4, x+3/4, z+1/4 [v, \bar{u}, \bar{w}]$   
 (17)  $x+3/4, z+1/4, \bar{y}+3/4 [\bar{u}, \bar{w}, v]$  (18)  $\bar{x}+3/4, z+3/4, y+1/4 [u, \bar{w}, \bar{v}]$  (19)  $\bar{x}+1/4, \bar{z}+1/4, \bar{y}+1/4 [u, w, v]$  (20)  $x+1/4, \bar{z}+3/4, y+3/4 [\bar{u}, w, \bar{v}]$   
 (21)  $z+3/4, y+1/4, \bar{x}+3/4 [\bar{w}, \bar{v}, u]$  (22)  $z+1/4, \bar{y}+3/4, x+3/4 [\bar{w}, v, \bar{u}]$  (23)  $\bar{z}+3/4, y+3/4, x+1/4 [w, \bar{v}, \bar{u}]$  (24)  $\bar{z}+1/4, \bar{y}+1/4, \bar{x}+1/4 [w, v, u]$   
 (25)  $\bar{x}+1/4, \bar{y}+1/4, \bar{z}+1/4 [\bar{u}, \bar{v}, \bar{w}]$  (26)  $x+1/4, y+3/4, \bar{z}+3/4 [u, v, \bar{w}]$  (27)  $x+3/4, \bar{y}+3/4, z+1/4 [u, \bar{v}, w]$  (28)  $\bar{x}+3/4, y+1/4, z+3/4 [\bar{u}, v, w]$   
 (29)  $\bar{z}+1/4, \bar{x}+1/4, \bar{y}+1/4 [\bar{w}, \bar{u}, \bar{v}]$  (30)  $\bar{z}+3/4, x+1/4, y+3/4 [\bar{w}, u, v]$  (31)  $z+1/4, x+3/4, \bar{y}+3/4 [w, u, \bar{v}]$  (32)  $z+3/4, \bar{x}+3/4, y+1/4 [w, \bar{u}, v]$   
 (33)  $\bar{y}+1/4, \bar{z}+1/4, \bar{x}+1/4 [\bar{v}, \bar{w}, \bar{u}]$  (34)  $y+3/4, \bar{z}+3/4, x+1/4 [v, \bar{w}, u]$  (35)  $\bar{y}+3/4, z+1/4, x+3/4 [\bar{v}, w, u]$  (36)  $y+1/4, z+3/4, \bar{x}+3/4 [v, w, \bar{u}]$   
 (37)  $\bar{y}+1/2, \bar{x}, z+1/2 [v, u, \bar{w}]$  (38)  $y, x, z [\bar{v}, \bar{u}, \bar{w}]$  (39)  $\bar{y}, x+1/2, \bar{z}+1/2 [v, \bar{u}, w]$  (40)  $y+1/2, \bar{x}+1/2, \bar{z} [\bar{v}, u, w]$   
 (41)  $\bar{x}+1/2, \bar{z}, y+1/2 [u, w, \bar{v}]$  (42)  $x+1/2, \bar{z}+1/2, \bar{y} [\bar{u}, w, v]$  (43)  $x, z, y [\bar{u}, \bar{w}, \bar{v}]$  (44)  $\bar{x}, z+1/2, \bar{y}+1/2 [u, \bar{w}, v]$   
 (45)  $\bar{z}+1/2, \bar{y}, x+1/2 [w, v, \bar{u}]$  (46)  $\bar{z}, y+1/2, \bar{x}+1/2 [w, \bar{v}, u]$  (47)  $z+1/2, \bar{y}+1/2, \bar{x} [\bar{w}, v, u]$  (48)  $z, y, x [\bar{w}, \bar{v}, \bar{u}]$

96 h ..2'

- $1/8, y, \bar{y}+1/4 [u, v, \bar{v}]$   $7/8, \bar{y}+1/2, \bar{y}+3/4 [\bar{u}, \bar{v}, \bar{v}]$   $3/8, y+1/2, y+3/4 [\bar{u}, v, v]$   $5/8, \bar{y}, y+1/4 [u, \bar{v}, v]$   
 $\bar{y}+1/4, 1/8, y [\bar{v}, u, v]$   $\bar{y}+3/4, 7/8, \bar{y}+1/2 [\bar{v}, \bar{u}, \bar{v}]$   $y+3/4, 3/8, y+1/2 [v, \bar{u}, v]$   $y+1/4, 5/8, \bar{y} [v, u, \bar{v}]$   
 $y, \bar{y}+1/4, 1/8 [v, \bar{v}, u]$   $\bar{y}+1/2, \bar{y}+3/4, 7/8 [\bar{v}, \bar{v}, \bar{u}]$   $y+1/2, y+3/4, 3/8 [v, v, \bar{u}]$   $\bar{y}, y+1/4, 5/8 [\bar{v}, v, u]$   
 $1/8, \bar{y}+1/4, y [\bar{u}, \bar{v}, v]$   $3/8, y+3/4, y+1/2 [u, v, v]$   $7/8, \bar{y}+3/4, \bar{y}+1/2 [u, \bar{v}, \bar{v}]$   $5/8, y+1/4, \bar{y} [\bar{u}, v, \bar{v}]$   
 $y, 1/8, \bar{y}+1/4 [v, \bar{u}, \bar{v}]$   $y+1/2, 3/8, y+3/4 [v, u, v]$   $\bar{y}+1/2, 7/8, \bar{y}+3/4 [\bar{v}, u, \bar{v}]$   $\bar{y}, 5/8, y+1/4 [\bar{v}, \bar{u}, v]$   
 $\bar{y}+1/4, y, 1/8 [\bar{v}, v, \bar{u}]$   $y+3/4, y+1/2, 3/8 [v, v, u]$   $\bar{y}+3/4, \bar{y}+1/2, 7/8 [\bar{v}, \bar{v}, u]$   $y+1/4, \bar{y}, 5/8 [v, \bar{v}, \bar{u}]$

96 g ..m

- $x, x, z [u, \bar{u}, 0]$   $\bar{x}, \bar{x}+1/2, z+1/2 [\bar{u}, u, 0]$   $\bar{x}+1/2, x+1/2, \bar{z} [\bar{u}, \bar{u}, 0]$   $x+1/2, \bar{x}, \bar{z}+1/2 [u, u, 0]$   
 $z, x, x [0, u, \bar{u}]$   $z+1/2, \bar{x}, \bar{x}+1/2 [0, \bar{u}, u]$   $\bar{z}, \bar{x}+1/2, x+1/2 [0, \bar{u}, \bar{u}]$   $\bar{z}+1/2, x+1/2, \bar{x} [0, u, u]$   
 $x, z, x [\bar{u}, 0, u]$   $\bar{x}+1/2, z+1/2, \bar{x} [u, 0, \bar{u}]$   $x+1/2, \bar{z}, \bar{x}+1/2 [\bar{u}, 0, \bar{u}]$   $\bar{x}, \bar{z}+1/2, x+1/2 [u, 0, u]$   
 $x+3/4, x+1/4, \bar{z}+3/4 [u, \bar{u}, 0]$   $\bar{x}+1/4, \bar{x}+1/4, \bar{z}+1/4 [\bar{u}, u, 0]$   $x+1/4, \bar{x}+3/4, z+3/4 [u, u, 0]$   $\bar{x}+3/4, x+3/4, z+1/4 [\bar{u}, \bar{u}, 0]$   
 $x+3/4, z+1/4, \bar{x}+3/4 [\bar{u}, 0, \bar{u}]$   $\bar{x}+3/4, z+3/4, x+1/4 [u, 0, u]$   $\bar{x}+1/4, \bar{z}+1/4, \bar{x}+1/4 [u, 0, \bar{u}]$   $x+1/4, \bar{z}+3/4, x+3/4 [\bar{u}, 0, u]$   
 $z+3/4, x+1/4, \bar{x}+3/4 [0, u, u]$   $z+1/4, \bar{x}+3/4, x+3/4 [0, \bar{u}, \bar{u}]$   $\bar{z}+3/4, x+3/4, x+1/4 [0, u, \bar{u}]$   $\bar{z}+1/4, \bar{x}+1/4, \bar{x}+1/4 [0, \bar{u}, u]$

- 48 f 2mm  $x, 0, 0 [0, 0, 0]$   $\bar{x}, 1/2, 1/2 [0, 0, 0]$   $0, x, 0 [0, 0, 0]$   $1/2, \bar{x}, 1/2 [0, 0, 0]$   
 $0, 0, x [0, 0, 0]$   $1/2, 1/2, \bar{x} [0, 0, 0]$   $3/4, x+1/4, 3/4 [0, 0, 0]$   $1/4, \bar{x}+1/4, 1/4 [0, 0, 0]$   
 $x+3/4, 1/4, 3/4 [0, 0, 0]$   $\bar{x}+3/4, 3/4, 1/4 [0, 0, 0]$   $3/4, 1/4, \bar{x}+3/4 [0, 0, 0]$   $1/4, 3/4, x+3/4 [0, 0, 0]$



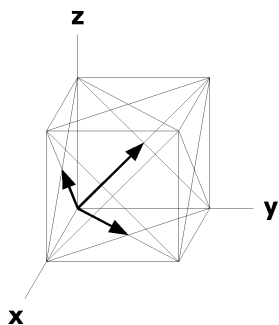
32	e	.3m	x,x,x [0,0,0]		$\bar{x}, \bar{x}+1/2, x+1/2$ [0,0,0]	
			$\bar{x}+1/2, x+1/2, \bar{x}$ [0,0,0]		$x+1/2, \bar{x}, \bar{x}+1/2$ [0,0,0]	
			$x+3/4, x+1/4, \bar{x}+3/4$ [0,0,0]		$\bar{x}+1/4, \bar{x}+1/4, \bar{x}+1/4$ [0,0,0]	
			$x+1/4, \bar{x}+3/4, x+3/4$ [0,0,0]		$\bar{x}+3/4, x+3/4, x+1/4$ [0,0,0]	
16	d	$\bar{3}$ 'm	5/8,5/8,5/8 [0,0,0]	3/8,7/8,1/8 [0,0,0]	7/8,1/8,3/8 [0,0,0]	1/8,3/8,7/8 [0,0,0]
16	c	$\bar{3}$ 'm	1/8,1/8,1/8 [0,0,0]	7/8,3/8,5/8 [0,0,0]	3/8,5/8,7/8 [0,0,0]	5/8,7/8,3/8 [0,0,0]
8	b	$\bar{4}3$ m	1/2,1/2,1/2 [0,0,0]		1/4,3/4,1/4 [0,0,0]	
8	a	$\bar{4}3$ m	0,0,0 [0,0,0]		3/4,1/4,3/4 [0,0,0]	

### Symmetry of Special Projections

Along [0,0,1]  $p_6$ -4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/4$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/4$   
 Origin at 0,0,z

Along [1,1,1]  $p6$ mm  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

Along [1,1,0]  $c2'$ mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at x,x,1/8



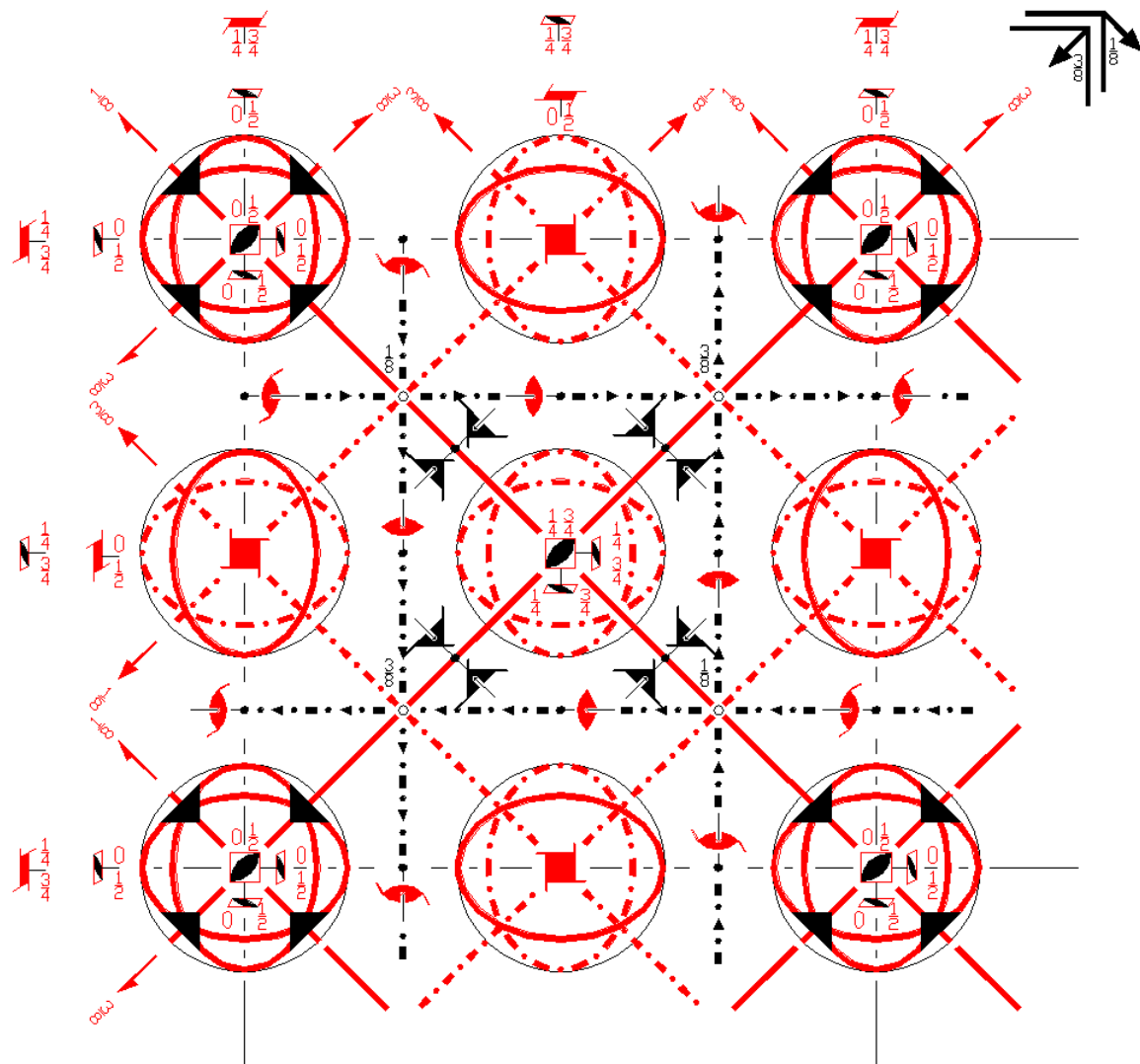
Fd $\bar{3}m'$

227.4.1631

m $\bar{3}m'$

F $4_1'/d\bar{3}2'/m'$

Cubic



Origin at  $\bar{4}'3m'$ , at  $-1/8, -1/8, -1/8$  from center ( $\bar{3}m'$ )

Asymmetric unit  $0 \leq x \leq 1/2; 0 \leq y \leq 1/8; -1/8 \leq z \leq 1/8; y \leq \min(1/2-x, x); -y \leq z \leq y$

Vertices  $0,0,0 \quad 1/2,0,0 \quad 3/8,1/8,1/8 \quad 1/8,1/8,1/8 \quad 3/8,1/8,-1/8 \quad 1/8,1/8,-1/8$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)   | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)   | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>  1/2,0,1/2)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> (1/3,-1/3,1/3)<br>x+1/6,x+1/6,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) | (7) 3 <sup>+</sup> (-1/3,1/3,1/3)<br>x+1/3,x-1/6,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2) | (8) 3 <sup>+</sup> (1/3,1/3,-1/3)<br>x+1/6,x+1/3,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x,x̄+1/2,x̄<br>(3 <sub>xyz</sub>  1/2,1/2,0)                                   | (11) 3 <sup>-</sup> x̄+1/2,x̄,x<br>(3 <sub>xyz</sub>  1/2,0,1/2)                                   | (12) 3 <sup>-</sup> x̄-1/2,x+1/2,x̄<br>(3 <sub>xyz</sub>  0,1/2,1/2)                               |

- (13)  $2'$  (1/2,1/2,0)  $x, x-1/4, 3/8$   
( $2_{xy}$  | 3/4, 1/4, 3/4)'
- (14)  $2'$   $x, \bar{x}+1/4, 1/8$   
( $2_{xy}$  | 1/4, 1/4, 1/4)'
- (15)  $4^-$  (0,0,3/4) 1/2, 1/4, z  
( $4_z^{-1}$  | 1/4, 3/4, 3/4)'
- (16)  $4^+$  (0,0,1/4) 0, 3/4, z  
( $4_z$  | 3/4, 3/4, 1/4)'
- (17)  $4^-$  (3/4,0,0)  $x, 1/2, 1/4$   
( $4_x^{-1}$  | 3/4, 1/4, 3/4)'
- (18)  $2'$  (0,1/2,1/2) 3/8, y+1/4, y  
( $2_{yz}$  | 3/4, 3/4, 1/4)'
- (19)  $2'$  1/8, y+1/4,  $\bar{y}$   
( $2_{yz}$  | 1/4, 1/4, 1/4)'
- (20)  $4^+$  (1/4,0,0)  $x, 0, 3/4$   
( $4_x$  | 1/4, 3/4, 3/4)'
- (21)  $4^+$  (0,1/4,0) 3/4, y, 0  
( $4_y$  | 3/4, 1/4, 3/4)'
- (22)  $2'$  (1/2,0,1/2)  $x-1/4, 3/8, x$   
( $2_{xz}$  | 1/4, 3/4, 3/4)'
- (23)  $4^-$  (0,3/4,0) 1/4, y, 1/2  
( $4_y^{-1}$  | 3/4, 3/4, 1/4)'
- (24)  $2'$   $\bar{x}+1/4, 1/8, x$   
( $2_{xz}$  | 1/4, 1/4, 1/4)'
- (25)  $\bar{1}$  1/8, 1/8, 1/8  
( $\bar{1}$  | 1/4, 1/4, 1/4)
- (26) d (1/4, 3/4, 0)  $x, y, 3/8$   
( $m_z$  | 1/4, 3/4, 3/4)
- (27) d (3/4, 0, 1/4)  $x, 3/8, z$   
( $m_y$  | 3/4, 3/4, 1/4)
- (28) d (0, 1/4, 3/4) 3/8, y, z  
( $m_x$  | 3/4, 1/4, 3/4)
- (29)  $\bar{3}^+$   $x, x, x;$   
1/8, 1/8, 1/8  
( $\bar{3}_{xyz}$  | 1/4, 1/4, 1/4)
- (30)  $\bar{3}^+$   $\bar{x}-1, x+1, \bar{x};$   
-1/8, 1/8, 7/8  
( $\bar{3}_{xyz}^{-1}$  | 3/4, 1/4, 3/4)
- (31)  $\bar{3}^+$   $x, \bar{x}+1, \bar{x};$   
1/8, 7/8, -1/8  
( $\bar{3}_{xyz}^{-1}$  | 1/4, 3/4, 3/4)
- (32)  $\bar{3}^+$   $\bar{x}+1, \bar{x}, x;$   
7/8, -1/8, 1/8  
( $\bar{3}_{xyz}^{-1}$  | 3/4, 3/4, 1/4)
- (33)  $\bar{3}^-$   $x, x, x;$   
1/8, 1/8, 1/8  
( $\bar{3}_{xyz}^{-1}$  | 1/4, 1/4, 1/4)
- (34)  $\bar{3}^-$   $x+3/2, \bar{x}-1, \bar{x};$   
5/8, -1/8, 7/8  
( $\bar{3}_{xyz}$  | 3/4, 3/4, 1/4)
- (35)  $\bar{3}^-$   $\bar{x}+1/2, \bar{x}+3/2, x;$   
-1/8, 7/8, 5/8  
( $\bar{3}_{xyz}$  | 3/4, 1/4, 3/4)
- (36)  $\bar{3}^-$   $\bar{x}+1, x+1/2, \bar{x};$   
7/8, 5/8, -1/8  
( $\bar{3}_{xyz}$  | 1/4, 3/4, 3/4)
- (37)  $g'$  (1/4, -1/4, 1/2)  $x+1/4, \bar{x}, z$   
( $m_{xy}$  | 1/2, 0, 1/2)'
- (38)  $m'$   $x, x, z$   
( $m_{xy}$  | 0, 0, 0)'
- (39)  $\bar{4}^-$  -1/4, 1/4, z; -1/4, 1/4, 1/4  
( $\bar{4}_z^{-1}$  | 0, 1/2, 1/2)'
- (40)  $\bar{4}^+$  1/2, 0, z; 1/2, 0, 0  
( $\bar{4}_z$  | 1/2, 1/2, 0)'
- (41)  $\bar{4}^-$   $x, -1/4, 1/4; 1/4, -1/4, 1/4$   
( $\bar{4}_x^{-1}$  | 1/2, 0, 1/2)'
- (42)  $g'$  (1/2, 1/4, -1/4)  $x, y+1/4, \bar{y}$   
( $m_{yz}$  | 1/2, 1/2, 0)'
- (43)  $m'$   $x, y, y$   
( $m_{yz}$  | 0, 0, 0)'
- (44)  $\bar{4}^+$   $x, 1/2, 0; 0, 1/2, 0$   
( $\bar{4}_x$  | 0, 1/2, 1/2)'
- (45)  $\bar{4}^+$  0, y, 1/2; 0, 0, 1/2  
( $\bar{4}_y$  | 1/2, 0, 1/2)'
- (46)  $g'$  (-1/4, 1/2, 1/4)  $\bar{x}+1/4, y, x$   
( $m_{xz}$  | 0, 1/2, 1/2)'
- (47)  $\bar{4}^-$  1/4, y, -1/4; 1/4, 1/4, -1/4  
( $\bar{4}_y^{-1}$  | 1/2, 1/2, 0)'
- (48)  $m'$   $x, y, x$   
( $m_{xz}$  | 0, 0, 0)'

For (0, 1/2, 1/2) + set

- (1) t (0, 1/2, 1/2)  
( $\bar{1}$  | 0, 1/2, 1/2)
- (2) 2 0, 0, z  
( $2_z$  | 0, 0, 0)
- (3) 2 1/4, y, 1/4  
( $2_y$  | 1/2, 0, 1/2)
- (4) 2 (1/2, 0, 0)  $x, 1/4, 0$   
( $2_x$  | 1/2, 1/2, 0)
- (5)  $3^+$  (1/3, 1/3, 1/3)  
 $x-1/3, x-1/6, x$   
( $3_{xyz}$  | 0, 1/2, 1/2)
- (6)  $3^+$   $\bar{x}+1/2, x, \bar{x}$   
( $3_{xyz}^{-1}$  | 1/2, 1/2, 0)
- (7)  $3^+$   $x, \bar{x}, \bar{x}$   
( $3_{xyz}^{-1}$  | 0, 0, 0)
- (8)  $3^+$   $\bar{x}+1/2, \bar{x}+1/2, x$   
( $3_{xyz}^{-1}$  | 1/2, 0, 1/2)
- (9)  $3^-$  (1/3, 1/3, 1/3)  
 $x-1/6, x+1/6, x$   
( $3_{xyz}^{-1}$  | 0, 1/2, 1/2)
- (10)  $3^-$   $x+1/2, \bar{x}, \bar{x}$   
( $3_{xyz}$  | 1/2, 0, 1/2)
- (11)  $3^-$  (1/3, 1/3, -1/3)  
 $x+1/3, x+1/6, x$   
( $3_{xyz}$  | 1/2, 1/2, 0)
- (12)  $3^-$   $\bar{x}, x, \bar{x}$   
( $3_{xyz}$  | 0, 0, 0)
- (13)  $2'$  (3/4, 3/4, 0)  $x, x, 1/8$   
( $2_{xy}$  | 3/4, 3/4, 1/4)'
- (14)  $2'$  (-1/4, 1/4, 0)  $x, \bar{x}+1/2, 3/8$   
( $2_{xy}$  | 1/4, 3/4, 3/4)'
- (15)  $4^-$  (0,0,1/4) 1/4, 0, z  
( $4_z^{-1}$  | 1/4, 1/4, 1/4)'
- (16)  $4^+$  (0,0,3/4) 1/4, 1/2, z  
( $4_z$  | 3/4, 1/4, 3/4)'
- (17)  $4^-$  (3/4,0,0)  $x, 1/2, -1/4$   
( $4_x^{-1}$  | 3/4, 3/4, 1/4)'
- (18)  $2'$  (0,1/2,1/2) 3/8, y-1/4, y  
( $2_{yz}$  | 3/4, 1/4, 3/4)'
- (19)  $2'$  1/8, y+3/4,  $\bar{y}$   
( $2_{yz}$  | 1/4, 3/4, 3/4)'
- (20)  $4^+$  (1/4,0,0)  $x, 0, 1/4$   
( $4_x$  | 1/4, 1/4, 1/4)'
- (21)  $4^+$  (0,3/4,0) 1/2, y, -1/4  
( $4_y$  | 3/4, 3/4, 1/4)'
- (22)  $2'$  (1/4,0,1/4)  $x, 1/8, x$   
( $2_{xz}$  | 1/4, 1/4, 1/4)'
- (23)  $4^-$  (0,1/4,0) 0, y, 3/4  
( $4_y^{-1}$  | 3/4, 1/4, 3/4)'
- (24)  $2'$  (-1/4,0,1/4)  $\bar{x}+1/2, 3/8, x$   
( $2_{xz}$  | 1/4, 3/4, 3/4)'
- (25)  $\bar{1}$  1/8, 3/8, 3/8  
( $\bar{1}$  | 1/4, 3/4, 3/4)
- (26) d (1/4, 1/4, 0)  $x, y, 1/8$   
( $m_z$  | 1/4, 1/4, 1/4)
- (27) d (3/4, 0, 3/4)  $x, 1/8, z$   
( $m_y$  | 3/4, 1/4, 3/4)
- (28) d (0, 3/4, 1/4) 3/8, y, z  
( $m_x$  | 3/4, 3/4, 1/4)
- (29)  $\bar{3}^+$   $x, x+1/2, x;$   
1/8, 5/8, 1/8  
( $\bar{3}_{xyz}$  | 1/4, 3/4, 3/4)
- (30)  $\bar{3}^+$   $\bar{x}-1, x+3/2, \bar{x};$   
-1/8, 5/8, 7/8  
( $\bar{3}_{xyz}^{-1}$  | 3/4, 3/4, 1/4)
- (31)  $\bar{3}^+$   $x, \bar{x}+1/2, \bar{x};$   
1/8, 3/8, -1/8  
( $\bar{3}_{xyz}^{-1}$  | 1/4, 1/4, 1/4)
- (32)  $\bar{3}^+$   $\bar{x}+1, \bar{x}-1/2, x;$   
7/8, -5/8, 1/8  
( $\bar{3}_{xyz}^{-1}$  | 3/4, 1/4, 3/4)

- (33)  $\bar{3}^-$   $x-1/2, x-1/2, x;$   
 $1/8, 1/8, 5/8$   
 $(\bar{3}_{xyz}^{-1} | 1/4, 3/4, 3/4)$
- (34)  $\bar{3}^-$   $x+1, \bar{x}-3/2, \bar{x};$   
 $1/8, -5/8, 7/8$   
 $(\bar{3}_{\bar{xyz}} | 3/4, 1/4, 3/4)$
- (35)  $\bar{3}^-$   $\bar{x}, \bar{x}+1, x;$   
 $-1/8, 7/8, 1/8$   
 $(\bar{3}_{\bar{xyz}} | 3/4, 3/4, 1/4)$
- (36)  $\bar{3}^-$   $\bar{x}+1/2, x, \bar{x};$   
 $3/8, 1/8, -1/8$   
 $(\bar{3}_{\bar{xyz}} | 1/4, 1/4, 1/4)$
- (37)  $m'$   $x+1/2, \bar{x}, z$   
 $(m_{xy} | 1/2, 1/2, 0)'$
- (38)  $g'$   $(1/4, 1/4, 1/2)$   $x-1/4, x, z$   
 $(m_{\bar{xy}} | 0, 1/2, 1/2)'$
- (39)  $\bar{4}^-$   $0, 0, z; 0, 0, 0$   
 $(\bar{4}_z^{-1} | 0, 0, 0)'$
- (40)  $\bar{4}^+$   $1/4, -1/4, z; 1/4, -1/4, 1/4$   
 $(\bar{4}_z | 1/2, 0, 1/2)'$
- (41)  $\bar{4}^-$   $x, 1/4, 1/4; 1/4, 1/4, 1/4$   
 $(\bar{4}_x^{-1} | 1/2, 1/2, 0)'$
- (42)  $g'$   $(1/2, -1/4, 1/4)$   $x, y+1/4, \bar{y}$   
 $(m_{yz} | 1/2, 0, 1/2)'$
- (43)  $g'$   $(0, 1/2, 1/2)$   $x, y, y$   
 $(m_{\bar{yz}} | 0, 1/2, 1/2)'$
- (44)  $\bar{4}^+$   $x, 0, 0; 0, 0, 0$   
 $(\bar{4}_x | 0, 0, 0)'$
- (45)  $\bar{4}^+$   $1/4, y, 1/4; 1/4, 1/4, 1/4$   
 $(\bar{4}_y | 1/2, 1/2, 0)'$
- (46)  $m'$   $\bar{x}, y, x$   
 $(m_{xz} | 0, 0, 0)'$
- (47)  $\bar{4}^-$   $1/2, y, 0; 1/2, 0, 0$   
 $(\bar{4}_y^{-1} | 1/2, 0, 1/2)'$
- (48)  $g'$   $(1/4, 1/2, 1/4)$   $x-1/4, y, x$   
 $(m_{\bar{xz}} | 0, 1/2, 1/2)'$

For  $(1/2, 0, 1/2) + \text{set}$ 

- (1)  $t$   $(1/2, 0, 1/2)$   
 $(1 | 1/2, 0, 1/2)$
- (2)  $2$   $1/4, 1/4, z$   
 $(2_z | 1/2, 1/2, 0)$
- (3)  $2$   $(0, 1/2, 0)$   $0, y, 1/4$   
 $(2_y | 0, 1/2, 1/2)$
- (4)  $2$   $x, 0, 0$   
 $(2_x | 0, 0, 0)$
- (5)  $3^+$   $(1/3, 1/3, 1/3)$   
 $x+1/6, x-1/6, x$   
 $(3_{xyz} | 1/2, 0, 1/2)$
- (6)  $3^+$   $\bar{x}, x, \bar{x}$   
 $(3_{\bar{xyz}}^{-1} | 0, 0, 0)$
- (7)  $3^+$   $x+1/2, \bar{x}, \bar{x}$   
 $(3_{\bar{xyz}}^{-1} | 1/2, 1/2, 0)$
- (8)  $3^+$   $\bar{x}, \bar{x}+1/2, x$   
 $(3_{xyz}^{-1} | 0, 1/2, 1/2)$
- (9)  $3^-$   $(1/3, 1/3, 1/3)$   
 $x-1/6, x-1/3, x$   
 $(3_{xyz}^{-1} | 1/2, 0, 1/2)$
- (10)  $3^-$   $(-1/3, 1/3, 1/3)$   
 $x+1/6, x+1/6, \bar{x}$   
 $(3_{\bar{xyz}} | 0, 1/2, 1/2)$
- (11)  $3^-$   $\bar{x}, \bar{x}, x$   
 $(3_{\bar{yz}} | 0, 0, 0)$
- (12)  $3^-$   $\bar{x}, x+1/2, \bar{x}$   
 $(3_{\bar{yz}} | 1/2, 1/2, 0)$
- (13)  $2'$   $(1/4, 1/4, 0)$   $x, x, 1/8$   
 $(2_{xy} | 1/4, 1/4, 1/4)'$
- (14)  $2'$   $(1/4, -1/4, 0)$   $x, \bar{x}+1/2, 3/8$   
 $(2_{xy} | 3/4, 1/4, 3/4)'$
- (15)  $4^-$   $(0, 0, 1/4)$   $3/4, 0, z$   
 $(4_z^{-1} | 3/4, 3/4, 1/4)'$
- (16)  $4^+$   $(0, 0, 3/4)$   $-1/4, 1/2, z$   
 $(4_z | 1/4, 3/4, 3/4)'$
- (17)  $4^-$   $(1/4, 0, 0)$   $x, 1/4, 0$   
 $(4_x^{-1} | 1/4, 1/4, 1/4)'$
- (18)  $2'$   $(0, 3/4, 3/4)$   $1/8, y, y$   
 $(2_{yz} | 1/4, 3/4, 3/4)'$
- (19)  $2'$   $(0, -1/4, 1/4)$   $3/8, y+1/2, \bar{y}$   
 $(2_{yz} | 3/4, 1/4, 3/4)'$
- (20)  $4^+$   $(3/4, 0, 0)$   $x, 1/4, 1/2$   
 $(4_x | 3/4, 3/4, 1/4)'$
- (21)  $4^+$   $(0, 1/4, 0)$   $1/4, y, 0$   
 $(4_y | 1/4, 1/4, 1/4)'$
- (22)  $2'$   $(1/2, 0, 1/2)$   $x+1/4, 3/8, x$   
 $(2_{xz} | 3/4, 3/4, 1/4)'$
- (23)  $4^-$   $(0, 3/4, 0)$   $-1/4, y, 1/2$   
 $(4_y^{-1} | 1/4, 3/4, 3/4)'$
- (24)  $2'$   $\bar{x}+3/4, 1/8, x$   
 $(2_{\bar{xz}} | 3/4, 1/4, 3/4)'$
- (25)  $\bar{1}$   $3/8, 1/8, 3/8$   
 $(\bar{1} | 3/4, 1/4, 3/4)$
- (26)  $d$   $(3/4, 3/4, 0)$   $x, y, 1/8$   
 $(m_z | 3/4, 3/4, 1/4)$
- (27)  $d$   $(1/4, 0, 3/4)$   $x, 3/8, z$   
 $(m_y | 1/4, 3/4, 3/4)$
- (28)  $d$   $(0, 1/4, 1/4)$   $1/8, y, z$   
 $(m_x | 1/4, 1/4, 1/4)$
- (29)  $\bar{3}^+$   $x-1/2, x-1/2, x;$   
 $1/8, 1/8, 5/8$   
 $(\bar{3}_{xyz} | 3/4, 1/4, 3/4)$
- (30)  $\bar{3}^+$   $\bar{x}-1/2, x+1/2, \bar{x};$   
 $-1/8, 1/8, 3/8$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 1/4, 1/4, 1/4)$
- (31)  $\bar{3}^+$   $x-1/2, \bar{x}+3/2, \bar{x};$   
 $1/8, 7/8, -5/8$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 3/4, 3/4, 1/4)$
- (32)  $\bar{3}^+$   $\bar{x}+3/2, \bar{x}+1/2, x;$   
 $7/8, -1/8, 5/8$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 1/4, 3/4, 3/4)$
- (33)  $\bar{3}^-$   $x+1/2, x, x;$   
 $5/8, 1/8, 1/8$   
 $(\bar{3}_{xyz}^{-1} | 3/4, 1/4, 3/4)$
- (34)  $\bar{3}^-$   $x+1, \bar{x}-1, \bar{x};$   
 $1/8, -1/8, 7/8$   
 $(\bar{3}_{\bar{xyz}} | 1/4, 3/4, 3/4)$
- (35)  $\bar{3}^-$   $\bar{x}, \bar{x}+1/2, x;$   
 $-1/8, 3/8, 1/8$   
 $(\bar{3}_{\bar{xyz}} | 1/4, 1/4, 1/4)$
- (36)  $\bar{3}^-$   $\bar{x}+3/2, x-1/2, \bar{x};$   
 $7/8, 1/8, -5/8$   
 $(\bar{3}_{\bar{xyz}} | 3/4, 3/4, 1/4)$
- (37)  $m'$   $x, \bar{x}, z$   
 $(m_{xy} | 0, 0, 0)'$
- (38)  $g'$   $(1/4, 1/4, 1/2)$   $x+1/4, x, z$   
 $(m_{\bar{xy}} | 1/2, 0, 1/2)'$
- (39)  $\bar{4}^-$   $0, 1/2, z; 0, 1/2, 0$   
 $(\bar{4}_z^{-1} | 1/2, 1/2, 0)'$
- (40)  $\bar{4}^+$   $1/4, 1/4, z; 1/4, 1/4, 1/4$   
 $(\bar{4}_z | 0, 1/2, 1/2)'$
- (41)  $\bar{4}^-$   $x, 0, 0; 0, 0, 0$   
 $(\bar{4}_x^{-1} | 0, 0, 0)'$
- (42)  $m'$   $x, y+1/2, \bar{y}$   
 $(m_{yz} | 0, 1/2, 1/2)'$
- (43)  $g'$   $(1/2, 1/4, 1/4)$   $x, y-1/4, y$   
 $(m_{\bar{yz}} | 1/2, 0, 1/2)'$
- (44)  $\bar{4}^+$   $x, 1/4, -1/4; 1/4, 1/4, -1/4$   
 $(\bar{4}_x | 1/2, 1/2, 0)'$
- (45)  $\bar{4}^+$   $0, y, 0; 0, 0, 0$   
 $(\bar{4}_y | 0, 0, 0)'$
- (46)  $g'$   $(1/4, 1/2, -1/4)$   $\bar{x}+1/4, y, x$   
 $(m_{xz} | 1/2, 1/2, 0)'$
- (47)  $\bar{4}^-$   $1/4, y, 1/4; 1/4, 1/4, 1/4$   
 $(\bar{4}_y^{-1} | 0, 1/2, 1/2)'$
- (48)  $g'$   $(1/2, 0, 1/2)$   $x, y, x$   
 $(m_{\bar{xz}} | 1/2, 0, 1/2)'$

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (1   1/2,1/2,0)	(2) 2 (0,0,1/2) 1/4,0,z (2 <sub>z</sub>   1/2,0,1/2)	(3) 2 0,y,0 (2 <sub>y</sub>   0,0,0)	(4) 2 x,1/4,1/4 (2 <sub>x</sub>   0,1/2,1/2)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) 3 <sup>+</sup> $\bar{x}$ ,x+1/2, $\bar{x}$ (3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>   0,1/2,1/2)	(7) 3 <sup>+</sup> x+1/2, $\bar{x}$ -1/2, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,0,1/2)	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x (3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>   0,0,0)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$ (3 <sub>x<math>\bar{y}z</math></sub>   0,0,0)	(11) 3 <sup>-</sup> $\bar{x}$ +1/2, $\bar{x}$ +1/2, x (3 <sub>x<math>\bar{y}z</math></sub>   0,1/2,1/2)	(12) 3 <sup>-</sup> (1/3,-1/3,1/3) $\bar{x}$ -1/6, x+1/3, $\bar{x}$ (3 <sub>x<math>\bar{y}z</math></sub>   1/2,0,1/2)
(13) 2' (1/2,1/2,0) x,x+1/4,3/8 (2 <sub>xy</sub>   1/4,3/4,3/4)'	(14) 2' x, $\bar{x}$ +3/4,1/8 (2 <sub>xy</sub>   3/4,3/4,1/4)'	(15) 4 <sup>-</sup> (0,0,3/4) 1/2,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   3/4,1/4,3/4)'	(16) 4 <sup>+</sup> (0,0,1/4) 0,1/4,z (4 <sub>z</sub>   1/4,1/4,1/4)'
(17) 4 <sup>-</sup> (1/4,0,0) x,3/4,0 (4 <sub>x</sub> <sup>-1</sup>   1/4,3/4,3/4)'	(18) 2' (0,1/4,1/4) 1/8,y,y (2 <sub>yz</sub>   1/4,1/4,1/4)'	(19) 2' (0,1/4,-1/4) 3/8,y+1/2, $\bar{y}$ (2 <sub>yz</sub>   3/4,3/4,1/4)'	(20) 4 <sup>+</sup> (3/4,0,0) x,-1/4,1/2 (4 <sub>x</sub>   3/4,1/4,3/4)'
(21) 4 <sup>+</sup> (0,3/4,0) 1/2,y,1/4 (4 <sub>y</sub>   1/4,3/4,3/4)'	(22) 2' (3/4,0,3/4) x,1/8,x (2 <sub>xz</sub>   3/4,1/4,3/4)'	(23) 4 <sup>-</sup> (0,1/4,0) 0,y,1/4 (4 <sub>y</sub> <sup>-1</sup>   1/4,1/4,1/4)'	(24) 2' (1/4,0,-1/4) $\bar{x}$ +1/2,3/8,x (2 <sub>xz</sub>   3/4,3/4,1/4)'
(25) $\bar{1}$ 3/8,3/8,1/8 ( $\bar{1}$   3/4,3/4,1/4)	(26) d (3/4,1/4,0) x,y,3/8 (m <sub>z</sub>   3/4,1/4,3/4)	(27) d (1/4,0,1/4) x,1/8,z (m <sub>y</sub>   1/4,1/4,1/4)	(28) d (0,3/4,3/4) 1/8,y,z (m <sub>x</sub>   1/4,3/4,3/4)
(29) 3 <sup>+</sup> x+1/2,x,x; 5/8,1/8,1/8 (3 <sub>xyz</sub>   3/4,3/4,1/4)	(30) 3 <sup>+</sup> $\bar{x}$ -3/2,x+1, $\bar{x}$ ; -5/8,1/8,7/8 (3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>   1/4,3/4,3/4)	(31) 3 <sup>+</sup> x+1/2, $\bar{x}$ +1, $\bar{x}$ ; 5/8,7/8,-1/8 (3 <sub>xyz</sub> <sup>-1</sup>   3/4,1/4,3/4)	(32) 3 <sup>+</sup> $\bar{x}$ +1/2, $\bar{x}$ ,x; 3/8,-1/8,1/8 (3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>   1/4,1/4,1/4)
(33) 3 <sup>-</sup> x,x+1/2,x; 1/8,5/8,1/8 (3 <sub>xyz</sub> <sup>-1</sup>   3/4,3/4,1/4)	(34) 3 <sup>-</sup> x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ; 1/8,-1/8,3/8 (3 <sub>x<math>\bar{y}z</math></sub>   1/4,1/4,1/4)	(35) 3 <sup>-</sup> $\bar{x}$ -1/2, $\bar{x}$ +1, x; -5/8,7/8,1/8 (3 <sub>x<math>\bar{y}z</math></sub>   1/4,3/4,3/4)	(36) 3 <sup>-</sup> $\bar{x}$ +1, x, $\bar{x}$ ; 7/8,1/8,-1/8 (3 <sub>x<math>\bar{y}z</math></sub>   3/4,1/4,3/4)
(37) g' (-1/4,1/4,1/2) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   0,1/2,1/2)'	(38) g' (1/2,1/2,0) x,x,z (m <sub>xy</sub>   1/2,1/2,0)'	(39) 4 <sup>-</sup> 1/4,1/4,z; 1/4,1/4,1/4 (4 <sub>z</sub> <sup>-1</sup>   1/2,0,1/2)'	(40) 4 <sup>+</sup> 0,0,z; 0,0,0 (4 <sub>z</sub>   0,0,0)'
(41) 4 <sup>-</sup> x,0,1/2; 0,0,1/2 (4 <sub>x</sub> <sup>-1</sup>   0,1/2,1/2)'	(42) m' x,y, $\bar{y}$ (m <sub>yz</sub>   0,0,0)'	(43) g' (1/2,1/4,1/4) x,y+1/4,y (m <sub>yz</sub>   1/2,1/2,0)'	(44) 4 <sup>+</sup> x,1/4,1/4; 1/4,1/4,1/4 (4 <sub>x</sub>   1/2,0,1/2)'
(45) 4 <sup>+</sup> -1/4,y,1/4; -1/4,1/4,1/4 (4 <sub>y</sub>   0,1/2,1/2)'	(46) m' $\bar{x}$ +1/2,y,x (m <sub>xz</sub>   1/2,0,1/2)'	(47) 4 <sup>-</sup> 0,y,0; 0,0,0 (4 <sub>y</sub> <sup>-1</sup>   0,0,0)'	(48) g' (1/4,1/2,1/4) x+1/4,y,x (m <sub>xz</sub>   1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

192	i	1	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +					
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}$ , $\bar{y}$ +1/2,z+1/2	[ $\bar{u}$ , $\bar{v}$ ,w]	(3)	$\bar{x}$ +1/2,y+1/2, $\bar{z}$	[ $\bar{u}$ ,v, $\bar{w}$ ]	(4)	x+1/2, $\bar{y}$ , $\bar{z}$ +1/2	[u, $\bar{v}$ , $\bar{w}$ ]
(5)	z,x,y	[w,u,v]	(6)	z+1/2, $\bar{x}$ , $\bar{y}$ +1/2	[w, $\bar{u}$ , $\bar{v}$ ]	(7)	$\bar{z}$ , $\bar{x}$ +1/2,y+1/2	[ $\bar{w}$ ,u,v]	(8)	$\bar{z}$ +1/2,x+1/2, $\bar{y}$	[ $\bar{w}$ ,u, $\bar{v}$ ]

- (9)  $y, z, x [v, w, u]$  (10)  $\bar{y}+1/2, \bar{z}+1/2, \bar{x} [\bar{v}, \bar{w}, \bar{u}]$  (11)  $y+1/2, \bar{z}, \bar{x}+1/2 [v, \bar{w}, \bar{u}]$  (12)  $\bar{y}, \bar{z}+1/2, x+1/2 [\bar{v}, \bar{w}, u]$   
 (13)  $y+3/4, x+1/4, \bar{z}+3/4 [\bar{v}, \bar{u}, w]$  (14)  $\bar{y}+1/4, \bar{x}+1/4, \bar{z}+1/4 [v, u, w]$  (15)  $y+1/4, \bar{x}+3/4, \bar{z}+3/4 [\bar{v}, \bar{u}, \bar{w}]$  (16)  $\bar{y}+3/4, x+3/4, \bar{z}+1/4 [v, \bar{u}, \bar{w}]$   
 (17)  $x+3/4, \bar{z}+1/4, \bar{y}+3/4 [\bar{u}, \bar{w}, v]$  (18)  $\bar{x}+3/4, \bar{z}+3/4, y+1/4 [u, \bar{w}, \bar{v}]$  (19)  $\bar{x}+1/4, \bar{z}+1/4, \bar{y}+1/4 [u, w, v]$  (20)  $x+1/4, \bar{z}+3/4, y+3/4 [\bar{u}, w, \bar{v}]$   
 (21)  $\bar{z}+3/4, y+1/4, \bar{x}+3/4 [\bar{w}, \bar{v}, u]$  (22)  $\bar{z}+1/4, \bar{y}+3/4, x+3/4 [\bar{w}, v, \bar{u}]$  (23)  $\bar{z}+3/4, y+3/4, x+1/4 [w, \bar{v}, \bar{u}]$  (24)  $\bar{z}+1/4, \bar{y}+1/4, \bar{x}+1/4 [w, v, u]$   
 (25)  $\bar{x}+1/4, \bar{y}+1/4, \bar{z}+1/4 [u, v, w]$  (26)  $x+1/4, y+3/4, \bar{z}+3/4 [\bar{u}, \bar{v}, w]$  (27)  $x+3/4, \bar{y}+3/4, \bar{z}+1/4 [\bar{u}, v, \bar{w}]$  (28)  $\bar{x}+3/4, y+1/4, \bar{z}+3/4 [u, \bar{v}, \bar{w}]$   
 (29)  $\bar{z}+1/4, \bar{x}+1/4, \bar{y}+1/4 [w, u, v]$  (30)  $\bar{z}+3/4, x+1/4, y+3/4 [w, \bar{u}, \bar{v}]$  (31)  $\bar{z}+1/4, x+3/4, \bar{y}+3/4 [\bar{w}, \bar{u}, v]$  (32)  $\bar{z}+3/4, \bar{x}+3/4, y+1/4 [\bar{w}, u, \bar{v}]$   
 (33)  $\bar{y}+1/4, \bar{z}+1/4, \bar{x}+1/4 [v, w, u]$  (34)  $y+3/4, \bar{z}+3/4, x+1/4 [\bar{v}, w, \bar{u}]$  (35)  $\bar{y}+3/4, \bar{z}+1/4, x+3/4 [v, \bar{w}, \bar{u}]$  (36)  $y+1/4, \bar{z}+3/4, \bar{x}+3/4 [\bar{v}, \bar{w}, u]$   
 (37)  $\bar{y}+1/2, \bar{x}, \bar{z}+1/2 [\bar{v}, \bar{u}, w]$  (38)  $y, x, z [v, u, w]$  (39)  $\bar{y}, x+1/2, \bar{z}+1/2 [\bar{v}, u, \bar{w}]$  (40)  $y+1/2, \bar{x}+1/2, \bar{z} [v, \bar{u}, \bar{w}]$   
 (41)  $\bar{x}+1/2, \bar{z}, y+1/2 [\bar{u}, \bar{w}, v]$  (42)  $x+1/2, \bar{z}+1/2, \bar{y} [u, \bar{w}, \bar{v}]$  (43)  $x, z, y [u, w, v]$  (44)  $\bar{x}, \bar{z}+1/2, \bar{y}+1/2 [\bar{u}, w, \bar{v}]$   
 (45)  $\bar{z}+1/2, \bar{y}, x+1/2 [\bar{w}, \bar{v}, u]$  (46)  $\bar{z}, y+1/2, \bar{x}+1/2 [\bar{w}, v, \bar{u}]$  (47)  $\bar{z}+1/2, \bar{y}+1/2, \bar{x} [w, \bar{v}, \bar{u}]$  (48)  $z, y, x [w, v, u]$

96 h ..2'

- $1/8, y, \bar{y}+1/4 [u, v, \bar{v}]$   $7/8, \bar{y}+1/2, \bar{y}+3/4 [\bar{u}, \bar{v}, \bar{v}]$   $3/8, y+1/2, y+3/4 [\bar{u}, v, v]$   $5/8, \bar{y}, y+1/4 [u, \bar{v}, v]$   
 $\bar{y}+1/4, 1/8, y [\bar{v}, u, v]$   $\bar{y}+3/4, 7/8, \bar{y}+1/2 [\bar{v}, \bar{u}, \bar{v}]$   $y+3/4, 3/8, y+1/2 [v, \bar{u}, v]$   $y+1/4, 5/8, \bar{y} [v, u, \bar{v}]$   
 $y, \bar{y}+1/4, 1/8 [v, \bar{v}, u]$   $\bar{y}+1/2, \bar{y}+3/4, 7/8 [\bar{v}, \bar{v}, \bar{u}]$   $y+1/2, y+3/4, 3/8 [v, v, \bar{u}]$   $\bar{y}, y+1/4, 5/8 [\bar{v}, v, u]$   
 $1/8, \bar{y}+1/4, y [u, v, \bar{v}]$   $3/8, y+3/4, y+1/2 [\bar{u}, \bar{v}, \bar{v}]$   $7/8, \bar{y}+3/4, \bar{y}+1/2 [\bar{u}, v, v]$   $5/8, y+1/4, \bar{y} [u, \bar{v}, v]$   
 $y, 1/8, \bar{y}+1/4 [\bar{v}, u, v]$   $y+1/2, 3/8, y+3/4 [\bar{v}, \bar{u}, \bar{v}]$   $\bar{y}+1/2, 7/8, \bar{y}+3/4 [v, \bar{u}, v]$   $\bar{y}, 5/8, y+1/4 [v, u, \bar{v}]$   
 $\bar{y}+1/4, y, 1/8 [v, \bar{v}, u]$   $y+3/4, y+1/2, 3/8 [\bar{v}, \bar{v}, \bar{u}]$   $\bar{y}+3/4, \bar{y}+1/2, 7/8 [v, v, \bar{u}]$   $y+1/4, \bar{y}, 5/8 [\bar{v}, v, u]$

96 g ..m'

- $x, x, z [u, u, w]$   $\bar{x}, \bar{x}+1/2, \bar{z}+1/2 [\bar{u}, \bar{u}, w]$   $\bar{x}+1/2, x+1/2, \bar{z} [\bar{u}, u, \bar{w}]$   $x+1/2, \bar{x}, \bar{z}+1/2 [u, \bar{u}, \bar{w}]$   
 $z, x, x [w, u, u]$   $\bar{z}+1/2, \bar{x}, \bar{x}+1/2 [w, \bar{u}, \bar{u}]$   $\bar{z}, \bar{x}+1/2, x+1/2 [w, \bar{u}, u]$   $\bar{z}+1/2, x+1/2, \bar{x} [w, u, \bar{u}]$   
 $x, z, x [u, w, u]$   $\bar{x}+1/2, \bar{z}+1/2, \bar{x} [\bar{u}, w, \bar{u}]$   $x+1/2, \bar{z}, \bar{x}+1/2 [u, \bar{w}, \bar{u}]$   $\bar{x}, \bar{z}+1/2, x+1/2 [\bar{u}, \bar{w}, u]$   
 $x+3/4, x+1/4, \bar{z}+3/4 [\bar{u}, \bar{u}, w]$   $\bar{x}+1/4, \bar{x}+1/4, \bar{z}+1/4 [u, u, w]$   $x+1/4, \bar{x}+3/4, \bar{z}+3/4 [\bar{u}, u, \bar{w}]$   $\bar{x}+3/4, x+3/4, \bar{z}+1/4 [u, \bar{u}, \bar{w}]$   
 $x+3/4, \bar{z}+1/4, \bar{x}+3/4 [\bar{u}, \bar{w}, u]$   $\bar{x}+3/4, \bar{z}+3/4, x+1/4 [u, \bar{w}, \bar{u}]$   $\bar{x}+1/4, \bar{z}+1/4, \bar{x}+1/4 [u, w, u]$   $x+1/4, \bar{z}+3/4, x+3/4 [\bar{u}, w, \bar{u}]$   
 $\bar{z}+3/4, x+1/4, \bar{x}+3/4 [\bar{w}, \bar{u}, u]$   $\bar{z}+1/4, \bar{x}+3/4, x+3/4 [\bar{w}, u, \bar{u}]$   $\bar{z}+3/4, x+3/4, x+1/4 [w, \bar{u}, \bar{u}]$   $\bar{z}+1/4, \bar{x}+1/4, \bar{x}+1/4 [\bar{w}, u, \bar{u}]$

- 48 f 2.m'm'  $x, 0, 0 [u, 0, 0]$   $\bar{x}, 1/2, 1/2 [\bar{u}, 0, 0]$   $0, x, 0 [0, u, 0]$   $1/2, \bar{x}, 1/2 [0, \bar{u}, 0]$   
 $0, 0, x [0, 0, u]$   $1/2, 1/2, \bar{x} [0, 0, \bar{u}]$   $3/4, x+1/4, 3/4 [0, \bar{u}, 0]$   $1/4, \bar{x}+1/4, 1/4 [0, u, 0]$   
 $x+3/4, 1/4, 3/4 [\bar{u}, 0, 0]$   $\bar{x}+3/4, 3/4, 1/4 [u, 0, 0]$   $3/4, 1/4, \bar{x}+3/4 [0, 0, u]$   $1/4, 3/4, x+3/4 [0, 0, \bar{u}]$

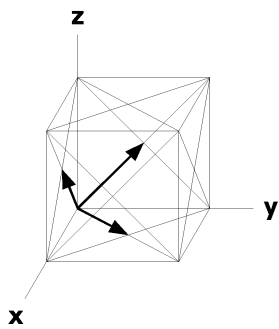
32	e	.3m'	x,x,x [u,u,u]		$\bar{x}, \bar{x}+1/2, x+1/2$ [ $\bar{u}, \bar{u}, u$ ]	
			$\bar{x}+1/2, x+1/2, \bar{x}$ [ $\bar{u}, u, \bar{u}$ ]		$x+1/2, \bar{x}, \bar{x}+1/2$ [u, $\bar{u}, \bar{u}$ ]	
			$x+3/4, x+1/4, \bar{x}+3/4$ [ $\bar{u}, \bar{u}, u$ ]		$\bar{x}+1/4, \bar{x}+1/4, \bar{x}+1/4$ [u, u, u]	
			$x+1/4, \bar{x}+3/4, x+3/4$ [ $\bar{u}, u, \bar{u}$ ]		$\bar{x}+3/4, x+3/4, x+1/4$ [u, $\bar{u}, \bar{u}$ ]	
16	d	$\bar{3}m'$	5/8, 5/8, 5/8 [u, u, u]	3/8, 7/8, 1/8 [ $\bar{u}, \bar{u}, u$ ]	7/8, 1/8, 3/8 [ $\bar{u}, u, \bar{u}$ ]	1/8, 3/8, 7/8 [u, $\bar{u}, \bar{u}$ ]
16	c	$\bar{3}m'$	1/8, 1/8, 1/8 [u, u, u]	7/8, 3/8, 5/8 [ $\bar{u}, \bar{u}, u$ ]	3/8, 5/8, 7/8 [ $\bar{u}, u, \bar{u}$ ]	5/8, 7/8, 3/8 [u, $\bar{u}, \bar{u}$ ]
8	b	$\bar{4}'3m'$	1/2, 1/2, 1/2 [0, 0, 0]		1/4, 3/4, 1/4 [0, 0, 0]	
8	a	$\bar{4}'3m'$	0, 0, 0 [0, 0, 0]		3/4, 1/4, 3/4 [0, 0, 0]	

### Symmetry of Special Projections

Along [0, 0, 1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/4$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/4$   
 Origin at 0, 0, z

Along [1, 1, 1] p6'mm'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x, x, x

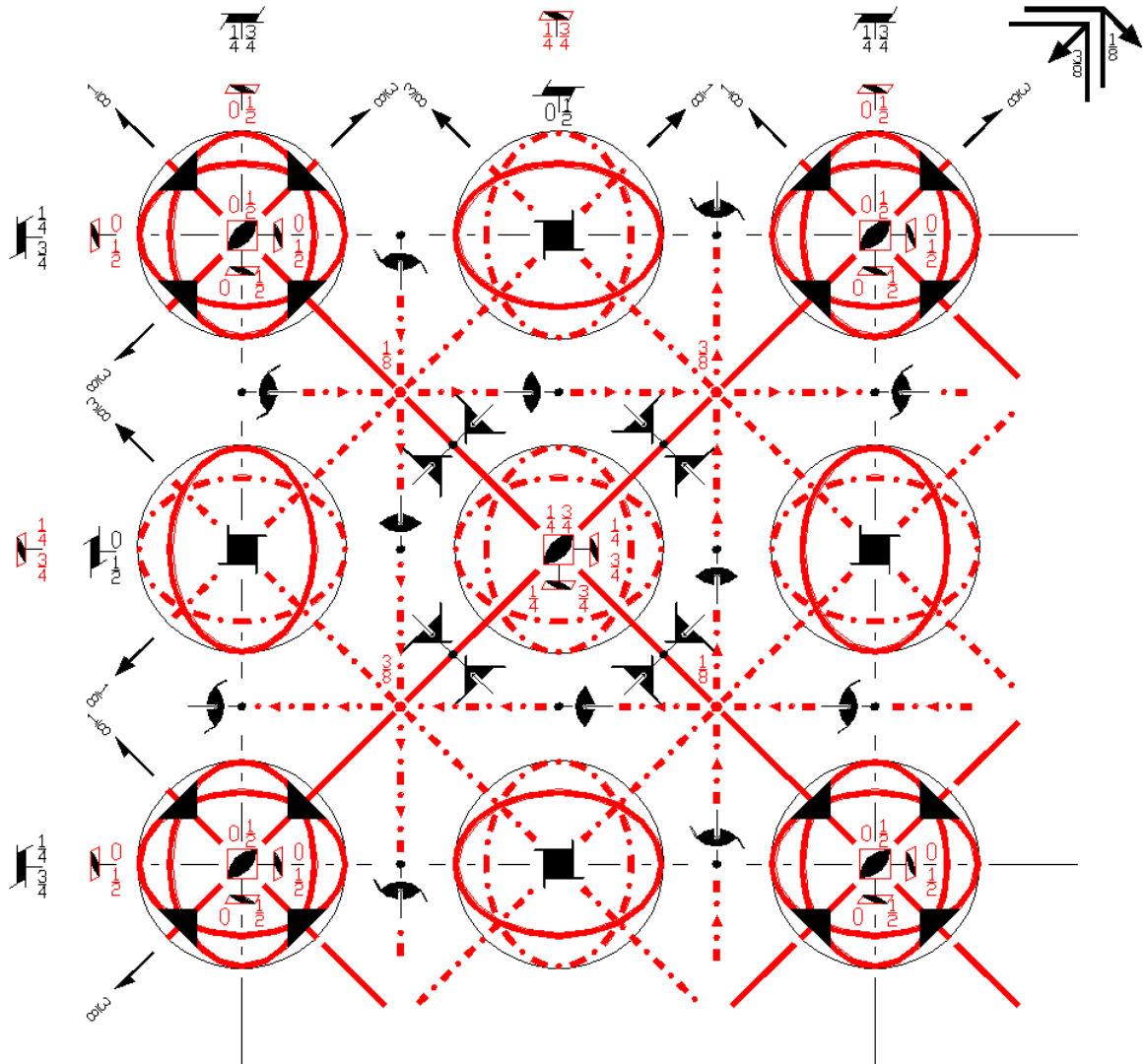
Along [1, 1, 0] c2'mm'  
 $\mathbf{a}^* = \mathbf{c}$   $\mathbf{b}^* = -(-\mathbf{a} + \mathbf{b})/2$   
 Origin at x, x, 1/8



Fd' $\bar{3}$ 'm'  
227.5.1632

m' $\bar{3}$ 'm'  
F4<sub>1</sub>/d' $\bar{3}$ '2/m'

Cubic



**Origin** at  $\bar{4}$ '3m', at  $-1/8, -1/8, -1/8$  from center ( $\bar{3}$ 'm')

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/8$ ;  $-1/8 \leq z \leq 1/8$ ;  $y \leq \min(1/2-x, x)$ ;  $-y \leq z \leq y$

**Vertices** 0,0,0    1/2,0,0    3/8,1/8,1/8    1/8,1/8,1/8    3/8,1/8,-1/8    1/8,1/8,-1/8

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |  |
|---|--|--|--|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,1/2)   | (3) 2 (0,1/2,0) 1/4,y,0<br>(2 <sub>y</sub>  1/2,1/2,0)   | (4) 2 (1/2,0,0) x,0,1/4<br>(2 <sub>x</sub>  1/2,0,1/2)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> (1/3,-1/3,1/3)<br>x+1/6,x+1/6,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2) | (7) 3 <sup>+</sup> (-1/3,1/3,1/3)<br>x+1/3,x-1/6,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2) | (8) 3 <sup>+</sup> (1/3,1/3,-1/3)<br>x+1/6,x+1/3,x̄<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> x,x̄+1/2,x̄<br>(3 <sub>xyz</sub>  1/2,1/2,0)                                   | (11) 3 <sup>-</sup> x̄+1/2,x̄,x<br>(3 <sub>xyz</sub>  1/2,0,1/2)                                   | (12) 3 <sup>-</sup> x̄-1/2,x+1/2,x̄<br>(3 <sub>xyz</sub>  0,1/2,1/2)                               |



- (13)  $2 (1/2, 1/2, 0) \ x, x-1/4, 3/8$   
 $(2_{xy} | 3/4, 1/4, 3/4)$
- (14)  $2 \ x, \bar{x}+1/4, 1/8$   
 $(2_{xy} | 1/4, 1/4, 1/4)$
- (15)  $4^- (0, 0, 3/4) \ 1/2, 1/4, z$   
 $(4_z^{-1} | 1/4, 3/4, 3/4)$
- (16)  $4^+ (0, 0, 1/4) \ 0, 3/4, z$   
 $(4_z | 3/4, 3/4, 1/4)$
- (17)  $4^- (3/4, 0, 0) \ x, 1/2, 1/4$   
 $(4_x^{-1} | 3/4, 1/4, 3/4)$
- (18)  $2 (0, 1/2, 1/2) \ 3/8, y+1/4, y$   
 $(2_{yz} | 3/4, 3/4, 1/4)$
- (19)  $2 \ 1/8, y+1/4, \bar{y}$   
 $(2_{yz} | 1/4, 1/4, 1/4)$
- (20)  $4^+ (1/4, 0, 0) \ x, 0, 3/4$   
 $(4_x | 1/4, 3/4, 3/4)$
- (21)  $4^+ (0, 1/4, 0) \ 3/4, y, 0$   
 $(4_y | 3/4, 1/4, 3/4)$
- (22)  $2 (1/2, 0, 1/2) \ x-1/4, 3/8, x$   
 $(2_{xz} | 1/4, 3/4, 3/4)$
- (23)  $4^- (0, 3/4, 0) \ 1/4, y, 1/2$   
 $(4_y^{-1} | 3/4, 3/4, 1/4)$
- (24)  $2 \ \bar{x}+1/4, 1/8, x$   
 $(2_{xz} | 1/4, 1/4, 1/4)$
- (25)  $\bar{1} \ 1/8, 1/8, 1/8$   
 $(\bar{1} | 1/4, 1/4, 1/4)'$
- (26)  $d' (1/4, 3/4, 0) \ x, y, 3/8$   
 $(m_z | 1/4, 3/4, 3/4)'$
- (27)  $d' (3/4, 0, 1/4) \ x, 3/8, z$   
 $(m_y | 3/4, 3/4, 1/4)'$
- (28)  $d' (0, 1/4, 3/4) \ 3/8, y, z$   
 $(m_x | 3/4, 1/4, 3/4)'$
- (29)  $\bar{3}^+ \ x, x, x;$   
 $1/8, 1/8, 1/8$   
 $(\bar{3}_{xyz} | 1/4, 1/4, 1/4)'$
- (30)  $\bar{3}^+ \ \bar{x}-1, x+1, \bar{x};$   
 $-1/8, 1/8, 7/8$   
 $(\bar{3}_{xyz}^{-1} | 3/4, 1/4, 3/4)'$
- (31)  $\bar{3}^+ \ x, \bar{x}+1, \bar{x};$   
 $1/8, 7/8, -1/8$   
 $(\bar{3}_{xyz}^{-1} | 1/4, 3/4, 3/4)'$
- (32)  $\bar{3}^+ \ \bar{x}+1, \bar{x}, x;$   
 $7/8, -1/8, 1/8$   
 $(\bar{3}_{xyz}^{-1} | 3/4, 3/4, 1/4)'$
- (33)  $\bar{3}^- \ x, x, x;$   
 $1/8, 1/8, 1/8$   
 $(\bar{3}_{xyz}^{-1} | 1/4, 1/4, 1/4)'$
- (34)  $\bar{3}^- \ x+3/2, \bar{x}-1, \bar{x};$   
 $5/8, -1/8, 7/8$   
 $(\bar{3}_{xyz} | 3/4, 3/4, 1/4)'$
- (35)  $\bar{3}^- \ \bar{x}+1/2, \bar{x}+3/2, x;$   
 $-1/8, 7/8, 5/8$   
 $(\bar{3}_{xyz} | 3/4, 1/4, 3/4)'$
- (36)  $\bar{3}^- \ \bar{x}+1, x+1/2, \bar{x};$   
 $7/8, 5/8, -1/8$   
 $(\bar{3}_{xyz} | 1/4, 3/4, 3/4)'$
- (37)  $g' (1/4, -1/4, 1/2) \ x+1/4, \bar{x}, z$   
 $(m_{xy} | 1/2, 0, 1/2)'$
- (38)  $m' \ x, x, z$   
 $(m_{xy} | 0, 0, 0)'$
- (39)  $\bar{4}^- \ -1/4, 1/4, z; \ -1/4, 1/4, 1/4$   
 $(\bar{4}_z^{-1} | 0, 1/2, 1/2)'$
- (40)  $\bar{4}^+ \ 1/2, 0, z; \ 1/2, 0, 0$   
 $(\bar{4}_z | 1/2, 1/2, 0)'$
- (41)  $\bar{4}^- \ x, -1/4, 1/4; \ 1/4, -1/4, 1/4$   
 $(\bar{4}_x^{-1} | 1/2, 0, 1/2)'$
- (42)  $g' (1/2, 1/4, -1/4) \ x, y+1/4, \bar{y}$   
 $(m_{yz} | 1/2, 1/2, 0)'$
- (43)  $m' \ x, y, y$   
 $(m_{yz} | 0, 0, 0)'$
- (44)  $\bar{4}^+ \ x, 1/2, 0; \ 0, 1/2, 0$   
 $(\bar{4}_x | 0, 1/2, 1/2)'$
- (45)  $\bar{4}^+ \ 0, y, 1/2; \ 0, 0, 1/2$   
 $(\bar{4}_y | 1/2, 0, 1/2)'$
- (46)  $g' (-1/4, 1/2, 1/4) \ \bar{x}+1/4, y, x$   
 $(m_{xz} | 0, 1/2, 1/2)'$
- (47)  $\bar{4}^- \ 1/4, y, -1/4; \ 1/4, 1/4, -1/4$   
 $(\bar{4}_y^{-1} | 1/2, 1/2, 0)'$
- (48)  $m' \ x, y, x$   
 $(m_{xz} | 0, 0, 0)'$

For (0, 1/2, 1/2) + set

- (1)  $t (0, 1/2, 1/2)$   
 $(1 | 0, 1/2, 1/2)$
- (2)  $2 \ 0, 0, z$   
 $(2_z | 0, 0, 0)$
- (3)  $2 \ 1/4, y, 1/4$   
 $(2_y | 1/2, 0, 1/2)$
- (4)  $2 (1/2, 0, 0) \ x, 1/4, 0$   
 $(2_x | 1/2, 1/2, 0)$
- (5)  $3^+ (1/3, 1/3, 1/3)$   
 $x-1/3, x-1/6, x$   
 $(3_{xyz} | 0, 1/2, 1/2)$
- (6)  $3^+ \ \bar{x}+1/2, x, \bar{x}$   
 $(3_{xyz}^{-1} | 1/2, 1/2, 0)$
- (7)  $3^+ \ x, \bar{x}, \bar{x}$   
 $(3_{xyz}^{-1} | 0, 0, 0)$
- (8)  $3^+ \ \bar{x}+1/2, \bar{x}+1/2, x$   
 $(3_{xyz}^{-1} | 1/2, 0, 1/2)$
- (9)  $3^- (1/3, 1/3, 1/3)$   
 $x-1/6, x+1/6, x$   
 $(3_{xyz}^{-1} | 0, 1/2, 1/2)$
- (10)  $3^- \ x+1/2, \bar{x}, \bar{x}$   
 $(3_{xyz} | 1/2, 0, 1/2)$
- (11)  $3^- (1/3, 1/3, -1/3)$   
 $x+1/3, x+1/6, x$   
 $(3_{xyz} | 1/2, 1/2, 0)$
- (12)  $3^- \ \bar{x}, x, \bar{x}$   
 $(3_{xyz} | 0, 0, 0)$
- (13)  $2 (3/4, 3/4, 0) \ x, x, 1/8$   
 $(2_{xy} | 3/4, 3/4, 1/4)$
- (14)  $2 (-1/4, 1/4, 0) \ x, \bar{x}+1/2, 3/8$   
 $(2_{xy} | 1/4, 3/4, 3/4)$
- (15)  $4^- (0, 0, 1/4) \ 1/4, 0, z$   
 $(4_z^{-1} | 1/4, 1/4, 1/4)$
- (16)  $4^+ (0, 0, 3/4) \ 1/4, 1/2, z$   
 $(4_z | 3/4, 1/4, 3/4)$
- (17)  $4^- (3/4, 0, 0) \ x, 1/2, -1/4$   
 $(4_x^{-1} | 3/4, 3/4, 1/4)$
- (18)  $2 (0, 1/2, 1/2) \ 3/8, y-1/4, y$   
 $(2_{yz} | 3/4, 1/4, 3/4)$
- (19)  $2 \ 1/8, y+3/4, \bar{y}$   
 $(2_{yz} | 1/4, 3/4, 3/4)$
- (20)  $4^+ (1/4, 0, 0) \ x, 0, 1/4$   
 $(4_x | 1/4, 1/4, 1/4)$
- (21)  $4^+ (0, 3/4, 0) \ 1/2, y, -1/4$   
 $(4_y | 3/4, 3/4, 1/4)$
- (22)  $2 (1/4, 0, 1/4) \ x, 1/8, x$   
 $(2_{xz} | 1/4, 1/4, 1/4)$
- (23)  $4^- (0, 1/4, 0) \ 0, y, 3/4$   
 $(4_y^{-1} | 3/4, 1/4, 3/4)$
- (24)  $2 (-1/4, 0, 1/4) \ \bar{x}+1/2, 3/8, x$   
 $(2_{xz} | 1/4, 3/4, 3/4)$
- (25)  $\bar{1} \ 1/8, 3/8, 3/8$   
 $(\bar{1} | 1/4, 3/4, 3/4)'$
- (26)  $d' (1/4, 1/4, 0) \ x, y, 1/8$   
 $(m_z | 1/4, 1/4, 1/4)'$
- (27)  $d' (3/4, 0, 3/4) \ x, 1/8, z$   
 $(m_y | 3/4, 1/4, 3/4)'$
- (28)  $d' (0, 3/4, 1/4) \ 3/8, y, z$   
 $(m_x | 3/4, 3/4, 1/4)'$
- (29)  $\bar{3}^+ \ x, x+1/2, x;$   
 $1/8, 5/8, 1/8$   
 $(\bar{3}_{xyz} | 1/4, 3/4, 3/4)'$
- (30)  $\bar{3}^+ \ \bar{x}-1, x+3/2, \bar{x};$   
 $-1/8, 5/8, 7/8$   
 $(\bar{3}_{xyz}^{-1} | 3/4, 3/4, 1/4)'$
- (31)  $\bar{3}^+ \ x, \bar{x}+1/2, \bar{x};$   
 $1/8, 3/8, -1/8$   
 $(\bar{3}_{xyz}^{-1} | 1/4, 1/4, 1/4)'$
- (32)  $\bar{3}^+ \ \bar{x}+1, \bar{x}-1/2, x;$   
 $7/8, -5/8, 1/8$   
 $(\bar{3}_{xyz}^{-1} | 3/4, 1/4, 3/4)'$

- (33)  $\bar{3}^-$  ' x-1/2,x-1/2,x;  
1/8,1/8,5/8  
( $\bar{3}_{xyz}^{-1}$  | 1/4,3/4,3/4)'
- (34)  $\bar{3}^-$  ' x+1, $\bar{x}$ -3/2, $\bar{x}$ ;  
1/8,-5/8,7/8  
( $\bar{3}_{xyz}$  | 3/4,1/4,3/4)'
- (35)  $\bar{3}^-$  '  $\bar{x}$ , $\bar{x}$ +1, x;  
-1/8,7/8,1/8  
( $\bar{3}_{xyz}$  | 3/4,3/4,1/4)'
- (36)  $\bar{3}^-$  '  $\bar{x}$ +1/2, x, $\bar{x}$ ;  
3/8,1/8,-1/8  
( $\bar{3}_{xyz}$  | 1/4,1/4,1/4)'
- (37) m' x+1/2, $\bar{x}$ ,z  
( $m_{xy}$  | 1/2,1/2,0)'
- (38) g' (1/4,1/4,1/2) x-1/4,x,z  
( $m_{xy}$  | 0,1/2,1/2)'
- (39)  $\bar{4}^-$  ' 0,0,z; 0,0,0  
( $\bar{4}_z^{-1}$  | 0,0,0)'
- (40)  $\bar{4}^+$  ' 1/4,-1/4,z; 1/4,-1/4,1/4  
( $\bar{4}_z$  | 1/2,0,1/2)'
- (41)  $\bar{4}^-$  ' x,1/4,1/4; 1/4,1/4,1/4  
( $\bar{4}_x^{-1}$  | 1/2,1/2,0)'
- (42) g' (1/2,-1/4,1/4) x,y+1/4, $\bar{y}$   
( $m_{yz}$  | 1/2,0,1/2)'
- (43) g' (0,1/2,1/2) x,y,y  
( $m_{yz}$  | 0,1/2,1/2)'
- (44)  $\bar{4}^+$  ' x,0,0; 0,0,0  
( $\bar{4}_x$  | 0,0,0)'
- (45)  $\bar{4}^+$  ' 1/4,y,1/4; 1/4,1/4,1/4  
( $\bar{4}_y$  | 1/2,1/2,0)'
- (46) m'  $\bar{x}$ ,y,x  
( $m_{xz}$  | 0,0,0)'
- (47)  $\bar{4}^-$  ' 1/2,y,0; 1/2,0,0  
( $\bar{4}_y^{-1}$  | 1/2,0,1/2)'
- (48) g' (1/4,1/2,1/4) x-1/4,y,x  
( $m_{xz}$  | 0,1/2,1/2)'

For (1/2,0,1/2) + set

- (1) t (1/2,0,1/2)  
(1 | 1/2,0,1/2)
- (2) 2 1/4,1/4,z  
(2<sub>z</sub> | 1/2,1/2,0)
- (3) 2 (0,1/2,0) 0,y,1/4  
(2<sub>y</sub> | 0,1/2,1/2)
- (4) 2 x,0,0  
(2<sub>x</sub> | 0,0,0)
- (5) 3<sup>+</sup> (1/3,1/3,1/3)  
x+1/6,x-1/6,x  
(3<sub>xyz</sub> | 1/2,0,1/2)
- (6) 3<sup>+</sup>  $\bar{x}$ ,x, $\bar{x}$   
(3<sub>xyz</sub><sup>-1</sup> | 0,0,0)
- (7) 3<sup>+</sup> x+1/2, $\bar{x}$ , $\bar{x}$   
(3<sub>xyz</sub><sup>-1</sup> | 1/2,1/2,0)
- (8) 3<sup>+</sup>  $\bar{x}$ , $\bar{x}$ +1/2,x  
(3<sub>xyz</sub><sup>-1</sup> | 0,1/2,1/2)
- (9) 3<sup>-</sup> (1/3,1/3,1/3)  
x-1/6,x-1/3,x  
(3<sub>xyz</sub><sup>-1</sup> | 1/2,0,1/2)
- (10) 3<sup>-</sup> (-1/3,1/3,1/3)  
x+1/6, $\bar{x}$ +1/6, $\bar{x}$   
(3<sub>xyz</sub> | 0,1/2,1/2)
- (11) 3<sup>-</sup>  $\bar{x}$ , $\bar{x}$ , x  
(3<sub>xyz</sub> | 0,0,0)
- (12) 3<sup>-</sup>  $\bar{x}$ , x+1/2, $\bar{x}$   
(3<sub>xyz</sub> | 1/2,1/2,0)
- (13) 2 (1/4,1/4,0) x,x,1/8  
(2<sub>xy</sub> | 1/4,1/4,1/4)
- (14) 2 (1/4,-1/4,0) x, $\bar{x}$ +1/2,3/8  
(2<sub>xy</sub> | 3/4,1/4,3/4)
- (15) 4<sup>-</sup> (0,0,1/4) 3/4,0,z  
(4<sub>z</sub><sup>-1</sup> | 3/4,3/4,1/4)
- (16) 4<sup>+</sup> (0,0,3/4) -1/4,1/2,z  
(4<sub>z</sub> | 1/4,3/4,3/4)
- (17) 4<sup>-</sup> (1/4,0,0) x,1/4,0  
(4<sub>x</sub><sup>-1</sup> | 1/4,1/4,1/4)
- (18) 2 (0,3/4,3/4) 1/8,y,y  
(2<sub>yz</sub> | 1/4,3/4,3/4)
- (19) 2 (0,-1/4,1/4) 3/8,y+1/2, $\bar{y}$   
(2<sub>yz</sub> | 3/4,1/4,3/4)
- (20) 4<sup>+</sup> (3/4,0,0) x,1/4,1/2  
(4<sub>x</sub> | 3/4,3/4,1/4)
- (21) 4<sup>+</sup> (0,1/4,0) 1/4,y,0  
(4<sub>y</sub> | 1/4,1/4,1/4)
- (22) 2 (1/2,0,1/2) x+1/4,3/8,x  
(2<sub>xz</sub> | 3/4,3/4,1/4)
- (23) 4<sup>-</sup> (0,3/4,0) -1/4,y,1/2  
(4<sub>y</sub><sup>-1</sup> | 1/4,3/4,3/4)
- (24) 2  $\bar{x}$ +3/4,1/8,x  
(2<sub>xz</sub> | 3/4,1/4,3/4)
- (25)  $\bar{1}$  3/8,1/8,3/8  
( $\bar{1}$  | 3/4,1/4,3/4)'
- (26) d' (3/4,3/4,0) x,y,1/8  
( $m_z$  | 3/4,3/4,1/4)'
- (27) d' (1/4,0,3/4) x,3/8,z  
( $m_y$  | 1/4,3/4,3/4)'
- (28) d' (0,1/4,1/4) 1/8,y,z  
( $m_x$  | 1/4,1/4,1/4)'
- (29)  $\bar{3}^+$  ' x-1/2,x-1/2,x;  
1/8,1/8,5/8  
( $\bar{3}_{xyz}$  | 3/4,1/4,3/4)'
- (30)  $\bar{3}^+$  '  $\bar{x}$ -1/2,x+1/2, $\bar{x}$ ;  
-1/8,1/8,3/8  
( $\bar{3}_{xyz}^{-1}$  | 1/4,1/4,1/4)'
- (31)  $\bar{3}^+$  ' x-1/2, $\bar{x}$ +3/2, $\bar{x}$ ;  
1/8,7/8,-5/8  
( $\bar{3}_{xyz}^{-1}$  | 3/4,3/4,1/4)'
- (32)  $\bar{3}^+$  '  $\bar{x}$ +3/2, $\bar{x}$ +1/2,x;  
7/8,-1/8,5/8  
( $\bar{3}_{xyz}^{-1}$  | 1/4,3/4,3/4)'
- (33)  $\bar{3}^-$  ' x+1/2,x,x;  
5/8,1/8,1/8  
( $\bar{3}_{xyz}^{-1}$  | 3/4,1/4,3/4)'
- (34)  $\bar{3}^-$  ' x+1, $\bar{x}$ -1, $\bar{x}$ ;  
1/8,-1/8,7/8  
( $\bar{3}_{xyz}$  | 1/4,3/4,3/4)'
- (35)  $\bar{3}^-$  '  $\bar{x}$ , $\bar{x}$ +1/2, x;  
-1/8,3/8,1/8  
( $\bar{3}_{xyz}$  | 1/4,1/4,1/4)'
- (36)  $\bar{3}^-$  '  $\bar{x}$ +3/2, x-1/2, $\bar{x}$ ;  
7/8,1/8,-5/8  
( $\bar{3}_{xyz}$  | 3/4,3/4,1/4)'
- (37) m' x, $\bar{x}$ ,z  
( $m_{xy}$  | 0,0,0)'
- (38) g' (1/4,1/4,1/2) x+1/4,x,z  
( $m_{xy}$  | 1/2,0,1/2)'
- (39)  $\bar{4}^-$  ' 0,1/2,z; 0,1/2,0  
( $\bar{4}_z^{-1}$  | 1/2,1/2,0)'
- (40)  $\bar{4}^+$  ' 1/4,1/4,z; 1/4,1/4,1/4  
( $\bar{4}_z$  | 0,1/2,1/2)'
- (41)  $\bar{4}^-$  ' x,0,0; 0,0,0  
( $\bar{4}_x^{-1}$  | 0,0,0)'
- (42) m' x,y+1/2, $\bar{y}$   
( $m_{yz}$  | 0,1/2,1/2)'
- (43) g' (1/2,1/4,1/4) x,y-1/4,y  
( $m_{yz}$  | 1/2,0,1/2)'
- (44)  $\bar{4}^+$  ' x,1/4,-1/4; 1/4,1/4,-1/4  
( $\bar{4}_x$  | 1/2,1/2,0)'
- (45)  $\bar{4}^+$  ' 0,y,0; 0,0,0  
( $\bar{4}_y$  | 0,0,0)'
- (46) g' (1/4,1/2,-1/4)  $\bar{x}$ +1/4,y,x  
( $m_{xz}$  | 1/2,1/2,0)'
- (47)  $\bar{4}^-$  ' 1/4,y,1/4; 1/4,1/4,1/4  
( $\bar{4}_y^{-1}$  | 0,1/2,1/2)'
- (48) g' (1/2,0,1/2) x,y,x  
( $m_{xz}$  | 1/2,0,1/2)'

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (1   1/2,1/2,0)	(2) 2 (0,0,1/2) 1/4,0,z (2 <sub>z</sub>   1/2,0,1/2)	(3) 2 0,y,0 (2 <sub>y</sub>   0,0,0)	(4) 2 x,1/4,1/4 (2 <sub>x</sub>   0,1/2,1/2)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) 3 <sup>+</sup> $\bar{x}$ ,x+1/2, $\bar{x}$ (3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>   0,1/2,1/2)	(7) 3 <sup>+</sup> x+1/2, $\bar{x}$ -1/2, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   1/2,0,1/2)	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x (3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>   0,0,0)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$ (3 <sub>x<math>\bar{y}z</math></sub>   0,0,0)	(11) 3 <sup>-</sup> $\bar{x}$ +1/2, $\bar{x}$ +1/2, x (3 <sub>x<math>\bar{y}z</math></sub>   0,1/2,1/2)	(12) 3 <sup>-</sup> (1/3,-1/3,1/3) $\bar{x}$ -1/6, x+1/3, $\bar{x}$ (3 <sub>x<math>\bar{y}z</math></sub>   1/2,0,1/2)
(13) 2 (1/2,1/2,0) x,x+1/4,3/8 (2 <sub>xy</sub>   1/4,3/4,3/4)	(14) 2 x, $\bar{x}$ +3/4,1/8 (2 <sub>x<math>\bar{y}</math></sub>   3/4,3/4,1/4)	(15) 4 <sup>-</sup> (0,0,3/4) 1/2,-1/4,z (4 <sub>z</sub> <sup>-1</sup>   3/4,1/4,3/4)	(16) 4 <sup>+</sup> (0,0,1/4) 0,1/4,z (4 <sub>z</sub>   1/4,1/4,1/4)
(17) 4 <sup>-</sup> (1/4,0,0) x,3/4,0 (4 <sub>x</sub> <sup>-1</sup>   1/4,3/4,3/4)	(18) 2 (0,1/4,1/4) 1/8,y,y (2 <sub>yz</sub>   1/4,1/4,1/4)	(19) 2 (0,1/4,-1/4) 3/8,y+1/2, $\bar{y}$ (2 <sub>yz</sub>   3/4,3/4,1/4)	(20) 4 <sup>+</sup> (3/4,0,0) x,-1/4,1/2 (4 <sub>x</sub>   3/4,1/4,3/4)
(21) 4 <sup>+</sup> (0,3/4,0) 1/2,y,1/4 (4 <sub>y</sub>   1/4,3/4,3/4)	(22) 2 (3/4,0,3/4) x,1/8,x (2 <sub>xz</sub>   3/4,1/4,3/4)	(23) 4 <sup>-</sup> (0,1/4,0) 0,y,1/4 (4 <sub>y</sub> <sup>-1</sup>   1/4,1/4,1/4)	(24) 2 (1/4,0,-1/4) $\bar{x}$ +1/2,3/8,x (2 <sub>xz</sub>   3/4,3/4,1/4)
(25) $\bar{1}$ ' 3/8,3/8,1/8 ( $\bar{1}$   3/4,3/4,1/4)'	(26) d' (3/4,1/4,0) x,y,3/8 (m <sub>z</sub>   3/4,1/4,3/4)'	(27) d' (1/4,0,1/4) x,1/8,z (m <sub>y</sub>   1/4,1/4,1/4)'	(28) d' (0,3/4,3/4) 1/8,y,z (m <sub>x</sub>   1/4,3/4,3/4)'
(29) $\bar{3}^+$ ' x+1/2,x,x; 5/8,1/8,1/8 ( $\bar{3}$ <sub>xyz</sub>   3/4,3/4,1/4)'	(30) $\bar{3}^+$ ' $\bar{x}$ -3/2,x+1, $\bar{x}$ ; -5/8,1/8,7/8 ( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>   1/4,3/4,3/4)'	(31) $\bar{3}^+$ ' x+1/2, $\bar{x}$ +1, $\bar{x}$ ; 5/8,7/8,-1/8 ( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>   3/4,1/4,3/4)'	(32) $\bar{3}^+$ ' $\bar{x}$ +1/2, $\bar{x}$ ,x; 3/8,-1/8,1/8 ( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>   1/4,1/4,1/4)'
(33) $\bar{3}^-$ ' x,x+1/2,x; 1/8,5/8,1/8 ( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>   3/4,3/4,1/4)'	(34) $\bar{3}^-$ ' x+1/2, $\bar{x}$ -1/2, $\bar{x}$ ; 1/8,-1/8,3/8 ( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub>   1/4,1/4,1/4)'	(35) $\bar{3}^-$ ' $\bar{x}$ -1/2, $\bar{x}$ +1, x; -5/8,7/8,1/8 ( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub>   1/4,3/4,3/4)'	(36) $\bar{3}^-$ ' $\bar{x}$ +1, x, $\bar{x}$ ; 7/8,1/8,-1/8 ( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub>   3/4,1/4,3/4)'
(37) g' (-1/4,1/4,1/2) x+1/4, $\bar{x}$ ,z (m <sub>xy</sub>   0,1/2,1/2)'	(38) g' (1/2,1/2,0) x,x,z (m <sub>x<math>\bar{y}</math></sub>   1/2,1/2,0)'	(39) $\bar{4}^-$ ' 1/4,1/4,z; 1/4,1/4,1/4 ( $\bar{4}$ <sub>z</sub> <sup>-1</sup>   1/2,0,1/2)'	(40) $\bar{4}^+$ ' 0,0,z; 0,0,0 ( $\bar{4}$ <sub>z</sub>   0,0,0)'
(41) $\bar{4}^-$ ' x,0,1/2; 0,0,1/2 ( $\bar{4}$ <sub>x</sub> <sup>-1</sup>   0,1/2,1/2)'	(42) m' x,y, $\bar{y}$ (m <sub>yz</sub>   0,0,0)'	(43) g' (1/2,1/4,1/4) x,y+1/4,y (m <sub>yz</sub>   1/2,1/2,0)'	(44) $\bar{4}^+$ ' x,1/4,1/4; 1/4,1/4,1/4 ( $\bar{4}$ <sub>x</sub>   1/2,0,1/2)'
(45) $\bar{4}^+$ ' -1/4,y,1/4; -1/4,1/4,1/4 ( $\bar{4}$ <sub>y</sub>   0,1/2,1/2)'	(46) m' $\bar{x}$ +1/2,y,x (m <sub>xz</sub>   1/2,0,1/2)'	(47) $\bar{4}^-$ ' 0,y,0; 0,0,0 ( $\bar{4}$ <sub>y</sub> <sup>-1</sup>   0,0,0)'	(48) g' (1/4,1/2,1/4) x+1/4,y,x (m <sub>xz</sub>   1/2,1/2,0)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

192	i	1	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +					
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}$ , $\bar{y}$ +1/2,z+1/2	[ $\bar{u}$ , $\bar{v}$ ,w]	(3)	$\bar{x}$ +1/2,y+1/2, $\bar{z}$	[ $\bar{u}$ ,v, $\bar{w}$ ]	(4)	x+1/2, $\bar{y}$ , $\bar{z}$ +1/2	[u, $\bar{v}$ , $\bar{w}$ ]
(5)	z,x,y	[w,u,v]	(6)	z+1/2, $\bar{x}$ , $\bar{y}$ +1/2	[w, $\bar{u}$ , $\bar{v}$ ]	(7)	$\bar{z}$ , $\bar{x}$ +1/2,y+1/2	[ $\bar{w}$ ,u,v]	(8)	$\bar{z}$ +1/2,x+1/2, $\bar{y}$	[ $\bar{w}$ ,u, $\bar{v}$ ]

- (9)  $y, z, x [v, w, u]$  (10)  $\bar{y}+1/2, z+1/2, \bar{x} [\bar{v}, w, \bar{u}]$  (11)  $y+1/2, \bar{z}, \bar{x}+1/2 [v, \bar{w}, \bar{u}]$  (12)  $\bar{y}, \bar{z}+1/2, x+1/2 [\bar{v}, \bar{w}, u]$   
 (13)  $y+3/4, x+1/4, \bar{z}+3/4 [v, u, \bar{w}]$  (14)  $\bar{y}+1/4, \bar{x}+1/4, \bar{z}+1/4 [\bar{v}, \bar{u}, \bar{w}]$  (15)  $y+1/4, \bar{x}+3/4, z+3/4 [v, \bar{u}, w]$  (16)  $\bar{y}+3/4, x+3/4, z+1/4 [\bar{v}, u, w]$   
 (17)  $x+3/4, z+1/4, \bar{y}+3/4 [u, w, \bar{v}]$  (18)  $\bar{x}+3/4, z+3/4, y+1/4 [\bar{u}, w, v]$  (19)  $\bar{x}+1/4, \bar{z}+1/4, \bar{y}+1/4 [\bar{u}, \bar{w}, \bar{v}]$  (20)  $x+1/4, \bar{z}+3/4, y+3/4 [u, \bar{w}, v]$   
 (21)  $z+3/4, y+1/4, \bar{x}+3/4 [w, v, \bar{u}]$  (22)  $z+1/4, \bar{y}+3/4, x+3/4 [w, \bar{v}, u]$  (23)  $\bar{z}+3/4, y+3/4, x+1/4 [\bar{w}, v, u]$  (24)  $\bar{z}+1/4, \bar{y}+1/4, \bar{x}+1/4 [\bar{w}, \bar{v}, \bar{u}]$   
 (25)  $\bar{x}+1/4, \bar{y}+1/4, \bar{z}+1/4 [\bar{u}, \bar{v}, \bar{w}]$  (26)  $x+1/4, y+3/4, \bar{z}+3/4 [u, v, \bar{w}]$  (27)  $x+3/4, \bar{y}+3/4, z+1/4 [u, \bar{v}, w]$  (28)  $\bar{x}+3/4, y+1/4, z+3/4 [\bar{u}, v, w]$   
 (29)  $\bar{z}+1/4, \bar{x}+1/4, \bar{y}+1/4 [\bar{w}, \bar{u}, \bar{v}]$  (30)  $\bar{z}+3/4, x+1/4, y+3/4 [\bar{w}, u, v]$  (31)  $z+1/4, x+3/4, \bar{y}+3/4 [w, u, \bar{v}]$  (32)  $z+3/4, \bar{x}+3/4, y+1/4 [w, \bar{u}, v]$   
 (33)  $\bar{y}+1/4, \bar{z}+1/4, \bar{x}+1/4 [\bar{v}, \bar{w}, \bar{u}]$  (34)  $y+3/4, \bar{z}+3/4, x+1/4 [v, \bar{w}, u]$  (35)  $\bar{y}+3/4, z+1/4, x+3/4 [\bar{v}, w, u]$  (36)  $y+1/4, z+3/4, \bar{x}+3/4 [v, w, \bar{u}]$   
 (37)  $\bar{y}+1/2, \bar{x}, z+1/2 [\bar{v}, \bar{u}, w]$  (38)  $y, x, z [v, u, w]$  (39)  $\bar{y}, x+1/2, \bar{z}+1/2 [\bar{v}, u, \bar{w}]$  (40)  $y+1/2, \bar{x}+1/2, \bar{z} [v, \bar{u}, \bar{w}]$   
 (41)  $\bar{x}+1/2, \bar{z}, y+1/2 [\bar{u}, \bar{w}, v]$  (42)  $x+1/2, \bar{z}+1/2, \bar{y} [u, \bar{w}, \bar{v}]$  (43)  $x, z, y [u, w, v]$  (44)  $\bar{x}, z+1/2, \bar{y}+1/2 [\bar{u}, w, \bar{v}]$   
 (45)  $\bar{z}+1/2, \bar{y}, x+1/2 [\bar{w}, \bar{v}, u]$  (46)  $\bar{z}, y+1/2, \bar{x}+1/2 [\bar{w}, v, \bar{u}]$  (47)  $z+1/2, \bar{y}+1/2, \bar{x} [w, \bar{v}, \bar{u}]$  (48)  $z, y, x [w, v, u]$

96 h ..2

- $1/8, y, \bar{y}+1/4 [0, \bar{v}, v]$   $7/8, \bar{y}+1/2, \bar{y}+3/4 [0, v, v]$   $3/8, y+1/2, y+3/4 [0, \bar{v}, \bar{v}]$   $5/8, \bar{y}, y+1/4 [0, v, \bar{v}]$   
 $\bar{y}+1/4, 1/8, y [v, 0, \bar{v}]$   $\bar{y}+3/4, 7/8, \bar{y}+1/2 [v, 0, v]$   $y+3/4, 3/8, y+1/2 [\bar{v}, 0, \bar{v}]$   $y+1/4, 5/8, \bar{y} [\bar{v}, 0, v]$   
 $y, \bar{y}+1/4, 1/8 [\bar{v}, v, 0]$   $\bar{y}+1/2, \bar{y}+3/4, 7/8 [v, v, 0]$   $y+1/2, y+3/4, 3/8 [\bar{v}, \bar{v}, 0]$   $\bar{y}, y+1/4, 5/8 [v, \bar{v}, 0]$   
 $1/8, \bar{y}+1/4, y [0, v, \bar{v}]$   $3/8, y+3/4, y+1/2 [0, \bar{v}, \bar{v}]$   $7/8, \bar{y}+3/4, \bar{y}+1/2 [0, v, v]$   $5/8, y+1/4, \bar{y} [0, \bar{v}, v]$   
 $y, 1/8, \bar{y}+1/4 [\bar{v}, 0, v]$   $y+1/2, 3/8, y+3/4 [\bar{v}, 0, \bar{v}]$   $\bar{y}+1/2, 7/8, \bar{y}+3/4 [v, 0, v]$   $\bar{y}, 5/8, y+1/4 [v, 0, \bar{v}]$   
 $\bar{y}+1/4, y, 1/8 [v, \bar{v}, 0]$   $y+3/4, y+1/2, 3/8 [\bar{v}, \bar{v}, 0]$   $\bar{y}+3/4, \bar{y}+1/2, 7/8 [v, v, 0]$   $y+1/4, \bar{y}, 5/8 [\bar{v}, v, 0]$

96 g ..m'

- $x, x, z [u, u, w]$   $\bar{x}, \bar{x}+1/2, z+1/2 [\bar{u}, \bar{u}, w]$   $\bar{x}+1/2, x+1/2, \bar{z} [\bar{u}, u, \bar{w}]$   $x+1/2, \bar{x}, \bar{z}+1/2 [u, \bar{u}, \bar{w}]$   
 $z, x, x [w, u, u]$   $z+1/2, \bar{x}, \bar{x}+1/2 [w, \bar{u}, \bar{u}]$   $\bar{z}, \bar{x}+1/2, x+1/2 [\bar{w}, \bar{u}, u]$   $\bar{z}+1/2, x+1/2, \bar{x} [\bar{w}, u, \bar{u}]$   
 $x, z, x [u, w, u]$   $\bar{x}+1/2, z+1/2, \bar{x} [\bar{u}, w, \bar{u}]$   $x+1/2, \bar{z}, \bar{x}+1/2 [u, \bar{w}, \bar{u}]$   $\bar{x}, \bar{z}+1/2, x+1/2 [\bar{u}, \bar{w}, u]$   
 $x+3/4, x+1/4, \bar{z}+3/4 [u, u, \bar{w}]$   $\bar{x}+1/4, \bar{x}+1/4, \bar{z}+1/4 [\bar{u}, \bar{u}, \bar{w}]$   $x+1/4, \bar{x}+3/4, z+3/4 [u, \bar{u}, w]$   $\bar{x}+3/4, x+3/4, z+1/4 [\bar{u}, u, w]$   
 $x+3/4, z+1/4, \bar{x}+3/4 [u, w, \bar{u}]$   $\bar{x}+3/4, z+3/4, x+1/4 [\bar{u}, w, u]$   $\bar{x}+1/4, \bar{z}+1/4, \bar{x}+1/4 [\bar{u}, \bar{w}, \bar{u}]$   $x+1/4, \bar{z}+3/4, x+3/4 [u, \bar{w}, u]$   
 $z+3/4, x+1/4, \bar{x}+3/4 [w, u, \bar{u}]$   $z+1/4, \bar{x}+3/4, x+3/4 [w, \bar{u}, u]$   $\bar{z}+3/4, x+3/4, x+1/4 [\bar{w}, u, u]$   $\bar{z}+1/4, \bar{x}+1/4, \bar{x}+1/4 [\bar{w}, \bar{u}, \bar{u}]$

- 48 f 2.m'm'  $x, 0, 0 [u, 0, 0]$   $\bar{x}, 1/2, 1/2 [\bar{u}, 0, 0]$   $0, x, 0 [0, u, 0]$   $1/2, \bar{x}, 1/2 [0, \bar{u}, 0]$   
 $0, 0, x [0, 0, u]$   $1/2, 1/2, \bar{x} [0, 0, \bar{u}]$   $3/4, x+1/4, 3/4 [0, u, 0]$   $1/4, \bar{x}+1/4, 1/4 [0, \bar{u}, 0]$   
 $x+3/4, 1/4, 3/4 [u, 0, 0]$   $\bar{x}+3/4, 3/4, 1/4 [0, \bar{u}, 0]$   $3/4, 1/4, \bar{x}+3/4 [0, 0, \bar{u}]$   $1/4, 3/4, x+3/4 [0, 0, u]$

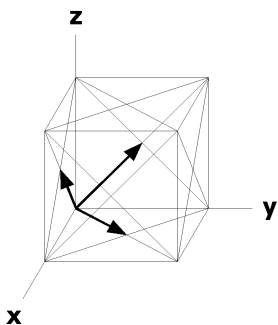
32	e	.3m'	x,x,x [u,u,u]	$\bar{x}, \bar{x}+1/2, x+1/2$ [ $\bar{u}, \bar{u}, u$ ]		
			$\bar{x}+1/2, x+1/2, \bar{x}$ [ $\bar{u}, u, \bar{u}$ ]	$x+1/2, \bar{x}, \bar{x}+1/2$ [u, $\bar{u}, \bar{u}$ ]		
			$x+3/4, x+1/4, \bar{x}+3/4$ [u, u, $\bar{u}$ ]	$\bar{x}+1/4, \bar{x}+1/4, \bar{x}+1/4$ [ $\bar{u}, \bar{u}, \bar{u}$ ]		
			$x+1/4, \bar{x}+3/4, x+3/4$ [u, $\bar{u}, u$ ]	$\bar{x}+3/4, x+3/4, x+1/4$ [ $\bar{u}, u, u$ ]		
16	d	$\bar{3}$ m'	5/8, 5/8, 5/8 [u, u, u]	3/8, 7/8, 1/8 [ $\bar{u}, \bar{u}, u$ ]	7/8, 1/8, 3/8 [ $\bar{u}, u, \bar{u}$ ]	1/8, 3/8, 7/8 [u, $\bar{u}, \bar{u}$ ]
16	c	$\bar{3}$ m'	1/8, 1/8, 1/8 [u, u, u]	7/8, 3/8, 5/8 [ $\bar{u}, \bar{u}, u$ ]	3/8, 5/8, 7/8 [ $\bar{u}, u, \bar{u}$ ]	5/8, 7/8, 3/8 [u, $\bar{u}, \bar{u}$ ]
8	b	$\bar{4}$ '3m'	1/2, 1/2, 1/2 [0, 0, 0]	1/4, 3/4, 1/4 [0, 0, 0]		
8	a	$\bar{4}$ '3m'	0, 0, 0 [0, 0, 0]	3/4, 1/4, 3/4 [0, 0, 0]		

### Symmetry of Special Projections

Along [0, 0, 1] p4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/4$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/4$   
 Origin at 0, 0, z

Along [1, 1, 1] p6m'm'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x, x, x

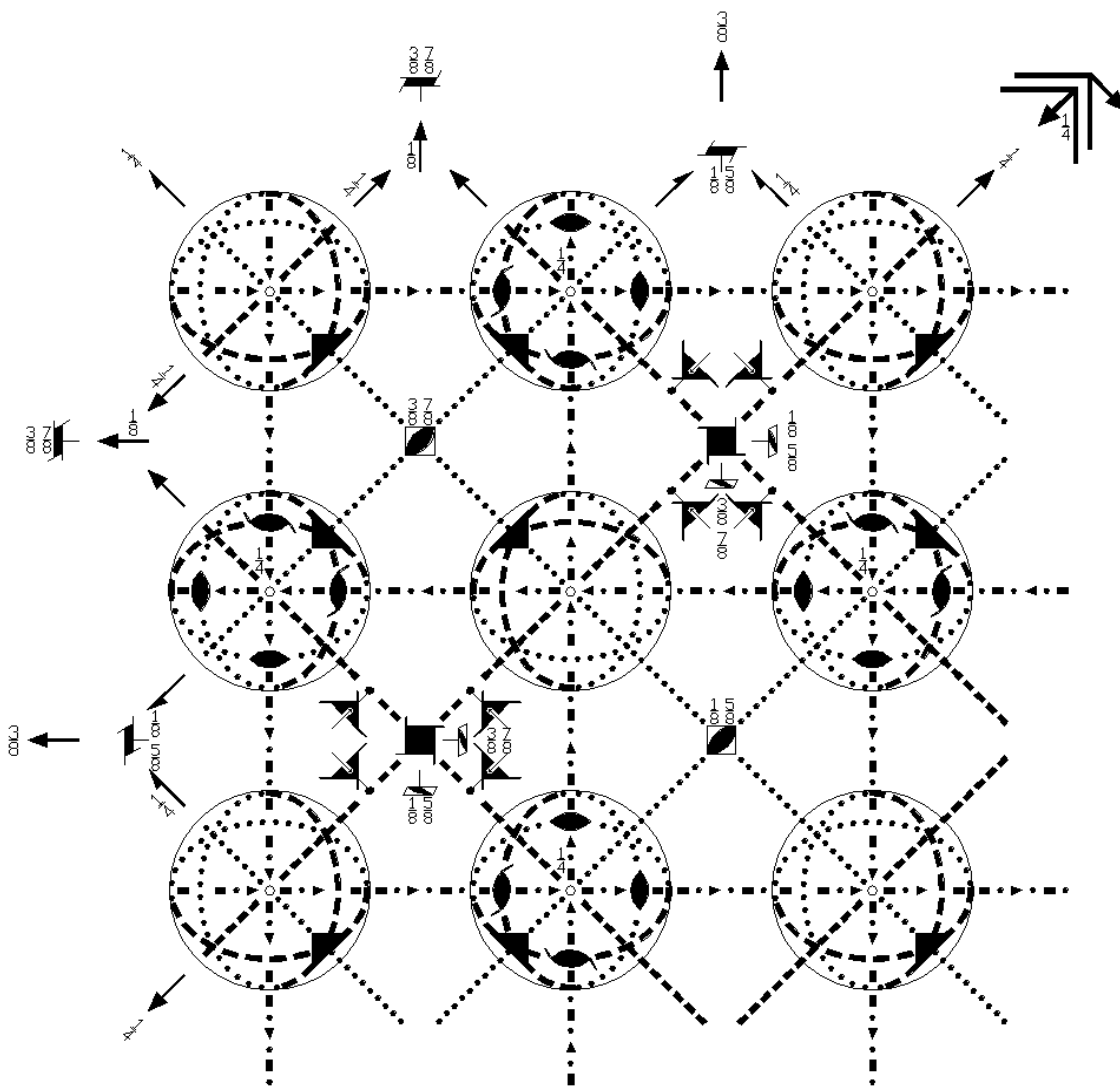
Along [1, 1, 0] c2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}$   
 Origin at x, x, 1/8



$Fd\bar{3}c$   
228.1.1633

$m\bar{3}m$   
 $F4_1/d\bar{3}2/c$

Cubic



**Origin** at center ( $\bar{3}$ ), at  $3/8, 3/8, 3/8$  from 23

**Asymmetric unit**  $-1/8 \leq x \leq 3/8$ ;  $-1/8 \leq y \leq 0$ ;  $-1/4 \leq z \leq 0$ ;  $y \leq \min(1/4-x, x)$ ;  $-y-1/4 \leq z \leq y$

**Vertices**  $-1/8, -1/8, -1/8$   $3/8, -1/8, -1/8$   $1/4, 0, 0$   $0, 0, 0$   $1/4, 0, -1/4$   $0, 0, -1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |  |  |   |
|---|--|--|---|
| (1) 1<br>(1 0,0,0)                              | (2) 2 $(0,0,1/2)$ $1/8, 3/8, z$<br>( $2_z$   $1/4, 3/4, 1/2$ )                                   | (3) 2 $(0,1/2,0)$ $3/8, y, 1/8$<br>( $2_y$   $3/4, 1/2, 1/4$ )                                   | (4) 2 $(1/2,0,0)$ $x, 1/8, 3/8$<br>( $2_x$   $1/2, 1/4, 3/4$ )  |
| (5) $3^+$ $x, x, x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $(1/3, -1/3, 1/3)$<br>$x+1/6, x+5/12, \bar{x}$<br>( $3_{xyz}^{-1}$   $1/2, 1/4, 3/4$ ) | (7) $3^+$ $(-1/3, 1/3, 1/3)$<br>$x+7/12, x-1/6, \bar{x}$<br>( $3_{xyz}^{-1}$   $1/4, 3/4, 1/2$ ) | (8) $3^+$ $(1/3, 1/3, -1/3)$<br>$\bar{x}+5/12, \bar{x}+7/12, x$<br>( $3_{xyz}^{-1}$   $3/4, 1/2, 1/4$ ) |
| (9) $3^-$ $x, x, x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x+1/4, \bar{x}+1/2, \bar{x}$<br>( $3_{xyz}$   $3/4, 1/2, 1/4$ )                      | (11) $3^-$ $\bar{x}+3/4, \bar{x}+1/4, x$<br>( $3_{xy\bar{z}}$   $1/2, 1/4, 3/4$ )                | (12) $3^-$ $\bar{x}-1/2, x+3/4, \bar{x}$<br>( $3_{xy\bar{z}}$   $1/4, 3/4, 1/2$ )                       |

- (13)  $2 (1/2, 1/2, 0) \ x, x-1/4, 0$   
 $(2_{xy} | 3/4, 1/4, 0)$
- (14)  $2 \ x, \bar{x}+1/2, 1/4$   
 $(2_{\bar{xy}} | 1/2, 1/2, 1/2)$
- (15)  $4^- (0, 0, 3/4) \ 1/8, -1/8, z$   
 $(4_z^{-1} | 1/4, 0, 3/4)$
- (16)  $4^+ (0, 0, 1/4) \ -3/8, 3/8, z$   
 $(4_z | 0, 3/4, 1/4)$
- (17)  $4^- (3/4, 0, 0) \ x, 1/8, -1/8$   
 $(4_x^{-1} | 3/4, 1/4, 0)$
- (18)  $2 (0, 1/2, 1/2) \ 0, y+1/4, y$   
 $(2_{yz} | 0, 3/4, 1/4)$
- (19)  $2 \ 1/4, y+1/2, \bar{y}$   
 $(2_{\bar{yz}} | 1/2, 1/2, 1/2)$
- (20)  $4^+ (1/4, 0, 0) \ x, -3/8, 3/8$   
 $(4_x | 1/4, 0, 3/4)$
- (21)  $4^+ (0, 1/4, 0) \ 3/8, y, -3/8$   
 $(4_y | 3/4, 1/4, 0)$
- (22)  $2 (1/2, 0, 1/2) \ x-1/4, 0, x$   
 $(2_{xz} | 1/4, 0, 3/4)$
- (23)  $4^- (0, 3/4, 0) \ -1/8, y, 1/8$   
 $(4_y^{-1} | 0, 3/4, 1/4)$
- (24)  $2 \ \bar{x}+1/2, 1/4, x$   
 $(2_{\bar{xz}} | 1/2, 1/2, 1/2)$
- (25)  $\bar{1} \ 0, 0, 0$   
 $(\bar{1} | 0, 0, 0)$
- (26)  $d (3/4, 1/4, 0) \ x, y, 1/4$   
 $(m_z | 3/4, 1/4, 1/2)$
- (27)  $d (1/4, 0, 3/4) \ x, 1/4, z$   
 $(m_y | 1/4, 1/2, 3/4)$
- (28)  $d (0, 3/4, 1/4) \ 1/4, y, z$   
 $(m_x | 1/2, 3/4, 1/4)$
- (29)  $\bar{3}^+ \ x, x, x;$   
 $0, 0, 0$   
 $(\bar{3}_{xyz} | 0, 0, 0)$
- (30)  $\bar{3}^+ \ \bar{x}-1, x+5/4, \bar{x};$   
 $-1/4, 1/2, 3/4$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 1/2, 3/4, 1/4)$
- (31)  $\bar{3}^+ \ x+1/4, \bar{x}+1, \bar{x};$   
 $1/2, 3/4, -1/4$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 3/4, 1/4, 1/2)$
- (32)  $\bar{3}^+ \ \bar{x}+5/4, \bar{x}+1/4, x;$   
 $3/4, -1/4, 1/2$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 1/4, 1/2, 3/4)$
- (33)  $\bar{3}^- \ x, x, x;$   
 $0, 0, 0$   
 $(\bar{3}_{xyz}^{-1} | 0, 0, 0)$
- (34)  $\bar{3}^- \ x+3/4, \bar{x}-1, \bar{x};$   
 $0, -1/4, 3/4$   
 $(\bar{3}_{\bar{xyz}} | 1/4, 1/2, 3/4)$
- (35)  $\bar{3}^- \ \bar{x}-1/4, \bar{x}+3/4, x;$   
 $-1/4, 3/4, 0$   
 $(\bar{3}_{\bar{xyz}} | 1/2, 3/4, 1/4)$
- (36)  $\bar{3}^- \ \bar{x}+1, x-1/4, \bar{x};$   
 $3/4, 0, -1/4$   
 $(\bar{3}_{\bar{xyz}} | 3/4, 1/4, 1/2)$
- (37)  $g (-1/4, 1/4, 1/2) \ x+1/2, \bar{x}, z$   
 $(m_{xy} | 1/4, 3/4, 0)$
- (38)  $n (1/2, 1/2, 1/2) \ x, x, z$   
 $(m_{\bar{xy}} | 1/2, 1/2, 1/2)$
- (39)  $\bar{4}^- \ 3/8, 3/8, z; \ 3/8, 3/8, 1/8$   
 $(\bar{4}_z^{-1} | 3/4, 0, 1/4)$
- (40)  $\bar{4}^+ \ 1/8, 1/8, z; \ 1/8, 1/8, 3/8$   
 $(\bar{4}_z | 0, 1/4, 3/4)$
- (41)  $\bar{4}^- \ x, 3/8, 3/8; \ 1/8, 3/8, 3/8$   
 $(\bar{4}_x^{-1} | 1/4, 3/4, 0)$
- (42)  $g (0, -1/4, 1/4) \ x, y+1/2, \bar{y}$   
 $(m_{yz} | 0, 1/4, 3/4)$
- (43)  $n (1/2, 1/2, 1/2) \ x, y, y$   
 $(m_{\bar{yz}} | 1/2, 1/2, 1/2)$
- (44)  $\bar{4}^+ \ x, 1/8, 1/8; \ 3/8, 1/8, 1/8$   
 $(\bar{4}_x | 3/4, 0, 1/4)$
- (45)  $\bar{4}^+ \ 1/8, y, 1/8; \ 1/8, 3/8, 1/8$   
 $(\bar{4}_y | 1/4, 3/4, 0)$
- (46)  $g (1/4, 0, -1/4) \ \bar{x}+1/2, y, x$   
 $(m_{xz} | 3/4, 0, 1/4)$
- (47)  $\bar{4}^- \ 3/8, y, 3/8; \ 3/8, 1/8, 3/8$   
 $(\bar{4}_y^{-1} | 0, 1/4, 3/4)$
- (48)  $n (1/2, 1/2, 1/2) \ x, y, x$   
 $(m_{\bar{xz}} | 1/2, 1/2, 1/2)$

For (0, 1/2, 1/2) + set

- (1)  $t (0, 1/2, 1/2)$   
 $(1 | 0, 1/2, 1/2)$
- (2)  $2 \ 1/8, 1/8, z$   
 $(2_z | 1/4, 1/4, 0)$
- (3)  $2 \ 3/8, y, 3/8$   
 $(2_y | 3/4, 0, 3/4)$
- (4)  $2 (1/2, 0, 0) \ x, 3/8, 1/8$   
 $(2_x | 1/2, 3/4, 1/4)$
- (5)  $3^+ (1/3, 1/3, 1/3)$   
 $x-1/3, x-1/6, x$   
 $(3_{xyz} | 0, 1/2, 1/2)$
- (6)  $3^+ \ \bar{x}+1/2, x+1/4, \bar{x}$   
 $(3_{\bar{xyz}}^{-1} | 1/2, 3/4, 1/4)$
- (7)  $3^+ \ x+1/4, \bar{x}, \bar{x}$   
 $(3_{\bar{xyz}}^{-1} | 1/4, 1/4, 0)$
- (8)  $3^+ \ \bar{x}+3/4, \bar{x}+3/4, x$   
 $(3_{\bar{xyz}}^{-1} | 3/4, 0, 3/4)$
- (9)  $3^- (1/3, 1/3, 1/3)$   
 $x-1/6, x+1/6, x$   
 $(3_{xyz}^{-1} | 0, 1/2, 1/2)$
- (10)  $3^- \ x+3/4, \bar{x}, \bar{x}$   
 $(3_{\bar{xyz}} | 3/4, 0, 3/4)$
- (11)  $3^- (1/3, 1/3, -1/3)$   
 $x+7/12, \bar{x}+5/12, x$   
 $(3_{\bar{xyz}} | 1/2, 3/4, 1/4)$
- (12)  $3^- \ \bar{x}, x+1/4, \bar{x}$   
 $(3_{\bar{xyz}} | 1/4, 1/4, 0)$
- (13)  $2 (3/4, 3/4, 0) \ x, x, 1/4$   
 $(2_{xy} | 3/4, 3/4, 1/2)$
- (14)  $2 (1/4, -1/4, 0) \ x, \bar{x}+1/4, 0$   
 $(2_{\bar{xy}} | 1/2, 0, 0)$
- (15)  $4^- (0, 0, 1/4) \ 3/8, 1/8, z$   
 $(4_z^{-1} | 1/4, 1/2, 1/4)$
- (16)  $4^+ (0, 0, 3/4) \ -1/8, 1/8, z$   
 $(4_z | 0, 1/4, 3/4)$
- (17)  $4^- (3/4, 0, 0) \ 5/8, -1/8$   
 $(4_x^{-1} | 3/4, 3/4, 1/2)$
- (18)  $2 (0, 1/2, 1/2) \ 0, y-1/4, y$   
 $(2_{yz} | 0, 1/4, 3/4)$
- (19)  $2 \ 1/4, y, \bar{y}$   
 $(2_{\bar{yz}} | 1/2, 0, 0)$
- (20)  $4^+ (1/4, 0, 0) \ x, 1/8, 3/8$   
 $(4_x | 1/4, 1/2, 1/4)$
- (21)  $4^+ (0, 3/4, 0) \ 5/8, y, -1/8$   
 $(4_y | 3/4, 3/4, 1/2)$
- (22)  $2 (1/4, 0, 1/4) \ x, 1/4, x$   
 $(2_{xz} | 1/4, 1/2, 1/4)$
- (23)  $4^- (0, 1/4, 0) \ -3/8, y, 3/8$   
 $(4_y^{-1} | 0, 1/4, 3/4)$
- (24)  $2 (1/4, 0, -1/4) \ \bar{x}+1/4, 0, x$   
 $(2_{\bar{xz}} | 1/2, 0, 0)$
- (25)  $\bar{1} \ 0, 1/4, 1/4$   
 $(\bar{1} | 0, 1/2, 1/2)$
- (26)  $d (3/4, 3/4, 0) \ x, y, 0$   
 $(m_z | 3/4, 3/4, 0)$
- (27)  $d (1/4, 0, 1/4) \ x, 0, z$   
 $(m_y | 1/4, 0, 1/4)$
- (28)  $d (0, 1/4, 3/4) \ 1/4, y, z$   
 $(m_x | 1/2, 1/4, 3/4)$
- (29)  $\bar{3}^+ \ x, x+1/2, x;$   
 $0, 1/2, 0$   
 $(\bar{3}_{xyz} | 0, 1/2, 1/2)$
- (30)  $\bar{3}^+ \ \bar{x}-1, x+3/4, \bar{x};$   
 $-1/4, 0, 3/4$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 1/2, 1/4, 3/4)$
- (31)  $\bar{3}^+ \ x-3/4, \bar{x}+3/2, \bar{x};$   
 $0, 3/4, -3/4$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 3/4, 3/4, 0)$
- (32)  $\bar{3}^+ \ \bar{x}+1/4, \bar{x}-1/4, x;$   
 $1/4, -1/4, 0$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 1/4, 0, 1/4)$

- |   |   |  |  |
|---|---|--|--|
| (33) $\bar{3}^-$ $x-1/2, x-1/2, x;$<br>0,0,1/2<br>( $\bar{3}_{xyz}^{-1}$   0,1/2,1/2) | (34) $\bar{3}^-$ $x+1/4, \bar{x}-1/2, \bar{x};$<br>0,-1/4,1/4<br>( $\bar{3}_{\bar{xyz}}$   1/4,0,1/4) | (35) $\bar{3}^-$ $\bar{x}+1/4, \bar{x}+5/4, x;$<br>-1/4,3/4,1/2<br>( $\bar{3}_{\bar{yz}}$   1/2,1/4,3/4) | (36) $\bar{3}^-$ $\bar{x}+3/2, x-3/4, \bar{x};$<br>3/4,0,-3/4<br>( $\bar{3}_{\bar{yz}}$   3/4,3/4,0) |
| (37) c (0,0,1/2) $x+1/4, \bar{x}, z$<br>( $m_{xy}$   1/4,1/4,1/2)                     | (38) g (1/4,1/4,0) $x+1/4, x, z$<br>( $m_{\bar{xy}}$   1/2,0,0)                                       | (39) $\bar{4}^-$ 1/8,5/8,z; 1/8,5/8,3/8<br>( $\bar{4}_z^{-1}$   3/4,1/2,3/4)                             | (40) $\bar{4}^+$ 3/8,3/8,z; 3/8,3/8,1/8<br>( $\bar{4}_z$   0,3/4,1/4)                                |
| (41) $\bar{4}^-$ $x,-1/8,3/8; 1/8,-1/8,3/8$<br>( $\bar{4}_x^{-1}$   1/4,1/4,1/2)      | (42) g (0,1/4,-1/4) $x,y+1/2, \bar{y}$<br>( $m_{yz}$   0,3/4,1/4)                                     | (43) a (1/2,0,0) $x,y,y$<br>( $m_{\bar{yz}}$   1/2,0,0)  | (44) $\bar{4}^+$ $x,5/8,1/8; 3/8,5/8,1/8$<br>( $\bar{4}_x$   3/4,0,3/4)                              |
| (45) $\bar{4}^+$ -1/8,y,3/8; -1/8,1/8,3/8<br>( $\bar{4}_y$   1/4,1/4,1/2)             | (46) b (0,1/2,0) $\bar{x}+3/4,y,x$<br>( $m_{xz}$   3/4,1/2,3/4)                                       | (47) $\bar{4}^-$ 1/8,y,1/8; 1/8,3/8,1/8<br>( $\bar{4}_y^{-1}$   0,3/4,1/4)                               | (48) g (1/4,0,1/4) $x+1/4,y,x$<br>( $m_{\bar{xz}}$   1/2,0,0)  |

For (1/2,0,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,0,1/2)<br>(1   1/2,0,1/2)  | (2) 2 3/8,3/8,z<br>(2 $_z$   3/4,3/4,0)   | (3) 2 (0,1/2,0) 1/8,y,3/8<br>(2 $_y$   1/4,1/2,3/4)   | (4) 2 $x,1/8,1/8$<br>(2 $_x$   0,1/4,1/4)   |
| (5) $3^+$ (1/3,1/3,1/3)<br>$x+1/6, x-1/6, x$<br>( $3_{xyz}$   1/2,0,1/2)          | (6) $3^+$ $\bar{x}, x+1/4, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}$   0,1/4,1/4)                                | (7) $3^+$ $x+3/4, \bar{x}, \bar{x}$<br>( $3_{\bar{yz}}^{-1}$   3/4,3/4,0)                                 | (8) $3^+$ $\bar{x}+1/4, \bar{x}+3/4, x$<br>( $3_{\bar{yz}}^{-1}$   1/4,1/2,3/4)                             |
| (9) $3^-$ (1/3,1/3,1/3)<br>$x-1/6, x-1/3, x$<br>( $3_{xyz}^{-1}$   1/2,0,1/2)     | (10) $3^-$ (-1/3,1/3,1/3)<br>$x+5/12, \bar{x}+1/6, \bar{x}$<br>( $3_{\bar{yz}}$   1/4,1/2,3/4)            | (11) $3^-$ $\bar{x}+1/4, \bar{x}+1/4, x$<br>( $3_{\bar{yz}}$   0,1/4,1/4)                                 | (12) $3^-$ $\bar{x}, x+3/4, \bar{x}$<br>( $3_{\bar{yz}}$   3/4,3/4,0)                                       |
| (13) 2 (1/4,1/4,0) $x,x,1/4$<br>(2 $_{xy}$   1/4,1/4,1/2)                         | (14) 2 (-1/4,1/4,0) $x, \bar{x}+1/4, 0$<br>(2 $_{\bar{xy}}$   0,1/2,0)                                    | (15) $4^-$ (0,0,1/4) 3/8,-3/8,z<br>( $4_z^{-1}$   3/4,0,1/4)  | (16) $4^+$ (0,0,3/4) -1/8,5/8,z<br>( $4_z$   1/2,3/4,3/4)   |
| (17) $4^-$ (1/4,0,0) $x,3/8,1/8$<br>( $4_x^{-1}$   1/4,1/4,1/2)                   | (18) 2 (0,3/4,3/4) 1/4,y,y<br>(2 $_{yz}$   1/2,3/4,3/4)   | (19) 2 (0,1/4,-1/4) 0,y+1/4, $\bar{y}$<br>(2 $_{\bar{yz}}$   0,1/2,0)                                     | (20) $4^+$ (3/4,0,0) $x,-1/8,1/8$<br>( $4_x$   3/4,0,1/4)   |
| (21) $4^+$ (0,1/4,0) 3/8,y,1/8<br>( $4_y$   1/4,1/4,1/2)                          | (22) 2 (1/2,0,1/2) $x+1/4,0,x$<br>(2 $_{xz}$   3/4,0,1/4)   | (23) $4^-$ (0,3/4,0) -1/8,y,5/8<br>( $4_y^{-1}$   1/2,3/4,3/4)  | (24) 2 $\bar{x},1/4,x$<br>(2 $_{\bar{xz}}$   0,1/2,0)   |
| (25) $\bar{1}$ 1/4,0,1/4<br>( $\bar{1}$   1/2,0,1/2)                              | (26) d (1/4,1/4,0) $x,y,0$<br>( $m_z$   1/4,1/4,0)  | (27) d (3/4,0,1/4) $x,1/4,z$<br>( $m_y$   3/4,1/2,1/4)  | (28) d (0,3/4,3/4) 0,y,z<br>( $m_x$   0,3/4,3/4)  |
| (29) $\bar{3}^+$ $x-1/2, x-1/2, x;$<br>0,0,1/2<br>( $\bar{3}_{xyz}$   1/2,0,1/2)  | (30) $\bar{3}^+$ $\bar{x}-3/2, x+3/4, \bar{x};$<br>-3/4,0,3/4<br>( $\bar{3}_{\bar{yz}}^{-1}$   0,3/4,3/4) | (31) $\bar{3}^+$ $x-1/4, \bar{x}+1/2, \bar{x};$<br>0,1/4,-1/4<br>( $\bar{3}_{\bar{yz}}^{-1}$   1/4,1/4,0) | (32) $\bar{3}^+$ $\bar{x}+3/4, \bar{x}-1/4, x;$<br>3/4,-1/4,0<br>( $\bar{3}_{\bar{yz}}^{-1}$   3/4,1/2,1/4) |
| (33) $\bar{3}^-$ $x+1/2, x, x;$<br>1/2,0,0<br>( $\bar{3}_{xyz}^{-1}$   1/2,0,1/2) | (34) $\bar{3}^-$ $x+5/4, \bar{x}-1, \bar{x};$<br>1/2,-1/4,3/4<br>( $\bar{3}_{\bar{yz}}$   3/4,1/2,1/4)    | (35) $\bar{3}^-$ $\bar{x}-3/4, \bar{x}+3/4, x;$<br>-3/4,3/4,0<br>( $\bar{3}_{\bar{yz}}$   0,3/4,3/4)      | (36) $\bar{3}^-$ $\bar{x}+1/2, x-1/4, \bar{x};$<br>1/4,0,-1/4<br>( $\bar{3}_{\bar{yz}}$   1/4,1/4,0)        |
| (37) c (0,0,1/2) $x+3/4, \bar{x}, z$<br>( $m_{xy}$   3/4,3/4,1/2)                 | (38) g (1/4,1/4,0) $x-1/4, x, z$<br>( $m_{\bar{xy}}$   0,1/2,0)   | (39) $\bar{4}^-$ 1/8,1/8,z; 1/8,1/8,3/8<br>( $\bar{4}_z^{-1}$   1/4,0,3/4)                                | (40) $\bar{4}^+$ 3/8,-1/8,z; 3/8,-1/8,1/8<br>( $\bar{4}_z$   1/2,1/4,1/4)                                   |
| (41) $\bar{4}^-$ $x,1/8,5/8; 3/8,1/8,5/8$<br>( $\bar{4}_x^{-1}$   3/4,3/4,1/2)    | (42) a (1/2,0,0) $x,y+1/4, \bar{y}$<br>( $m_{yz}$   1/2,1/4,1/4)  | (43) g (0,1/4,1/4) $x,y+1/4,y$<br>( $m_{\bar{yz}}$   0,1/2,0)   | (44) $\bar{4}^+$ $x,3/8,3/8; 1/8,3/8,3/8$<br>( $\bar{4}_x$   1/4,0,3/4)                                     |
| (45) $\bar{4}^+$ 1/8,y,5/8; 1/8,3/8,5/8<br>( $\bar{4}_y$   3/4,3/4,1/2)           | (46) g (-1/4,0,1/4) $\bar{x}+1/2,y,x$<br>( $m_{xz}$   1/4,0,3/4)  | (47) $\bar{4}^-$ 3/8,y,-1/8; 3/8,1/8,-1/8<br>( $\bar{4}_y^{-1}$   1/2,1/4,1/4)                            | (48) b (0,1/2,0) $x,y,x$<br>( $m_{\bar{xz}}$   0,1/2,0)   |



For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (1   1/2,1/2,0)	(2) 2 (0,0,1/2) 3/8,1/8,z (2 <sub>z</sub>   3/4,1/4,1/2)	(3) 2 1/8,y,1/8 (2 <sub>y</sub>   1/4,0,1/4)	(4) 2 x,3/8,3/8 (2 <sub>x</sub>   0,3/4,3/4)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) 3 <sup>+</sup> $\bar{x}$ ,x+3/4, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   0,3/4,3/4)	(7) 3 <sup>+</sup> x+3/4, $\bar{x}$ -1/2, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   3/4,1/4,1/2)	(8) 3 <sup>+</sup> $\bar{x}$ +1/4, $\bar{x}$ +1/4,x (3 <sub>xyz</sub> <sup>-1</sup>   1/4,0,1/4)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) 3 <sup>-</sup> x+1/4, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub>   1/4,0,1/4)	(11) 3 <sup>-</sup> $\bar{x}$ +3/4, $\bar{x}$ +3/4, x (3 <sub>xyz</sub>   0,3/4,3/4)	(12) 3 <sup>-</sup> (1/3,-1/3,1/3) $\bar{x}$ -1/6, x+7/12, $\bar{x}$ (3 <sub>xyz</sub>   3/4,1/4,1/2)
(13) 2 (1/2,1/2,0) x,x+1/4,0 (2 <sub>xy</sub>   1/4,3/4,0)	(14) 2 x, $\bar{x}$ ,1/4 (2 <sub>xy</sub>   0,0,1/2)	(15) 4 <sup>-</sup> (0,0,3/4) 5/8,-1/8,z (4 <sub>z</sub> <sup>-1</sup>   3/4,1/2,3/4)	(16) 4 <sup>+</sup> (0,0,1/4) 1/8,3/8,z (4 <sub>z</sub>   1/2,1/4,1/4)
(17) 4 <sup>-</sup> (1/4,0,0) x,3/8,-3/8 (4 <sub>x</sub> <sup>-1</sup>   1/4,3/4,0)	(18) 2 (0,1/4,1/4) 1/4,y,y (2 <sub>yz</sub>   1/2,1/4,1/4)	(19) 2 (0,-1/4,1/4) 0,y+1/4, $\bar{y}$ (2 <sub>yz</sub>   0,0,1/2)	(20) 4 <sup>+</sup> (3/4,0,0) x,-1/8,5/8 (4 <sub>x</sub>   3/4,1/2,3/4)
(21) 4 <sup>+</sup> (0,3/4,0) 1/8,y,-1/8 (4 <sub>y</sub>   1/4,3/4,0)	(22) 2 (3/4,0,3/4) x,1/4,x (2 <sub>xz</sub>   3/4,1/2,3/4)	(23) 4 <sup>-</sup> (0,1/4,0) 1/8,y,3/8 (4 <sub>y</sub> <sup>-1</sup>   1/2,1/4,1/4)	(24) 2 (-1/4,0,1/4) $\bar{x}$ +1/4,0,x (2 <sub>xz</sub>   0,0,1/2)
(25) $\bar{1}$ 1/4,1/4,0 ( $\bar{1}$   1/2,1/2,0)	(26) d (1/4,3/4,0) x,y,1/4 (m <sub>z</sub>   1/4,3/4,1/2)	(27) d (3/4,0,3/4) x,0,z (m <sub>y</sub>   3/4,0,3/4)	(28) d (0,1/4,1/4) 0,y,z (m <sub>x</sub>   0,1/4,1/4)
(29) $\bar{3}^+$ x+1/2,x,x; 1/2,0,0 ( $\bar{3}_{xyz}$   1/2,1/2,0)	(30) $\bar{3}^+$ $\bar{x}$ -1/2,x+1/4, $\bar{x}$ ; -1/4,0,1/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>   0,1/4,1/4)	(31) $\bar{3}^+$ x-1/4, $\bar{x}$ +1, $\bar{x}$ ; 0,3/4,-1/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/4,3/4,1/2)	(32) $\bar{3}^+$ $\bar{x}$ +3/4, $\bar{x}$ -3/4,x; 3/4,-3/4,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>   3/4,0,3/4)
(33) $\bar{3}^-$ x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)	(34) $\bar{3}^-$ x+3/4, $\bar{x}$ -3/2, $\bar{x}$ ; 0,-3/4,3/4 ( $\bar{3}_{xyz}$   3/4,0,3/4)	(35) $\bar{3}^-$ $\bar{x}$ -1/4, $\bar{x}$ +1/4, x; -1/4,1/4,0 ( $\bar{3}_{xyz}$   0,1/4,1/4)	(36) $\bar{3}^-$ $\bar{x}$ +1, x+1/4, $\bar{x}$ ; 3/4,1/2,-1/4 ( $\bar{3}_{xyz}$   1/4,3/4,1/2)
(37) g (1/4,-1/4,0) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   3/4,1/4,0)	(38) c (0,0,1/2) x,x,z (m <sub>xy</sub>   0,0,1/2)	(39) $\bar{4}^-$ -1/8,3/8,z; -1/8,3/8,1/8 ( $\bar{4}_z$ <sup>-1</sup>   1/4,1/2,1/4)	(40) $\bar{4}^+$ 5/8,1/8,z; 5/8,1/8,3/8 ( $\bar{4}_z$   1/2,3/4,3/4)
(41) $\bar{4}^-$ x,1/8,1/8; 3/8,1/8,1/8 ( $\bar{4}_x$ <sup>-1</sup>   3/4,1/4,0)	(42) a (1/2,0,0) x,y+3/4, $\bar{y}$ (m <sub>yz</sub>   1/2,3/4,3/4)	(43) g (0,1/4,1/4) x,y-1/4,y (m <sub>yz</sub>   0,0,1/2)	(44) $\bar{4}^+$ x,3/8,-1/8; 1/8,3/8,-1/8 ( $\bar{4}_x$   1/4,1/2,1/4)
(45) $\bar{4}^+$ 3/8,y,3/8; 3/8,1/8,3/8 ( $\bar{4}_y$   3/4,1/4,0)	(46) b (0,1/2,0) $\bar{x}$ +1/4,y,x (m <sub>xz</sub>   1/4,1/2,1/4)	(47) $\bar{4}^-$ 5/8,y,1/8; 5/8,3/8,1/8 ( $\bar{4}_y$ <sup>-1</sup>   1/2,3/4,3/4)	(48) g (1/4,0,1/4) x-1/4,y,x (m <sub>xz</sub>   0,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

192	h	1	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +		
(1)	x,y,z	[u,v,w]	(2) $\bar{x}$ +1/4, $\bar{y}$ +3/4,z+1/2	[ $\bar{u}$ , $\bar{v}$ ,w]	(3) $\bar{x}$ +3/4,y+1/2, $\bar{z}$ +1/4	[ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x+1/2, $\bar{y}$ +1/4, $\bar{z}$ +3/4	[u, $\bar{v}$ , $\bar{w}$ ]
(5)	z,x,y	[w,u,v]	(6) z+1/2, $\bar{x}$ +1/4, $\bar{y}$ +3/4	[w, $\bar{u}$ , $\bar{v}$ ]	(7) $\bar{z}$ +1/4, $\bar{x}$ +3/4,y+1/2	[ $\bar{w}$ , $\bar{u}$ ,v]	(8) $\bar{z}$ +3/4,x+1/2, $\bar{y}$ +1/4	[ $\bar{w}$ ,u, $\bar{v}$ ]

- (9)  $y, z, x [v, w, u]$  (10)  $\bar{y}+3/4, z+1/2, \bar{x}+1/4 [\bar{v}, w, \bar{u}]$  (11)  $y+1/2, \bar{z}+1/4, \bar{x}+3/4 [v, \bar{w}, \bar{u}]$  (12)  $\bar{y}+1/4, \bar{z}+3/4, x+1/2 [\bar{v}, \bar{w}, u]$   
 (13)  $y+3/4, x+1/4, \bar{z} [v, u, \bar{w}]$  (14)  $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2 [\bar{v}, \bar{u}, \bar{w}]$  (15)  $y+1/4, \bar{x}, z+3/4 [v, \bar{u}, w]$  (16)  $\bar{y}, x+3/4, z+1/4 [\bar{v}, u, w]$   
 (17)  $x+3/4, z+1/4, \bar{y} [u, w, \bar{v}]$  (18)  $\bar{x}, z+3/4, y+1/4 [\bar{u}, w, v]$  (19)  $\bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2 [\bar{u}, \bar{w}, \bar{v}]$  (20)  $x+1/4, \bar{z}, y+3/4 [u, \bar{w}, v]$   
 (21)  $z+3/4, y+1/4, \bar{x} [w, v, \bar{u}]$  (22)  $z+1/4, \bar{y}, x+3/4 [w, \bar{v}, u]$  (23)  $\bar{z}, y+3/4, x+1/4 [\bar{w}, v, u]$  (24)  $\bar{z}+1/2, \bar{y}+1/2, \bar{x}+1/2 [\bar{w}, \bar{v}, \bar{u}]$   
 (25)  $\bar{x}, \bar{y}, \bar{z} [u, v, w]$  (26)  $x+3/4, y+1/4, \bar{z}+1/2 [\bar{u}, \bar{v}, w]$  (27)  $x+1/4, \bar{y}+1/2, z+3/4 [\bar{u}, v, \bar{w}]$  (28)  $\bar{x}+1/2, y+3/4, z+1/4 [u, \bar{v}, \bar{w}]$   
 (29)  $\bar{z}, \bar{x}, \bar{y} [w, u, v]$  (30)  $\bar{z}+1/2, x+3/4, y+1/4 [w, \bar{u}, \bar{v}]$  (31)  $z+3/4, x+1/4, \bar{y}+1/2 [\bar{w}, \bar{u}, v]$  (32)  $z+1/4, \bar{x}+1/2, y+3/4 [\bar{w}, u, \bar{v}]$   
 (33)  $\bar{y}, \bar{z}, \bar{x} [v, w, u]$  (34)  $y+1/4, \bar{z}+1/2, x+3/4 [\bar{v}, w, \bar{u}]$  (35)  $\bar{y}+1/2, z+3/4, x+1/4 [v, \bar{w}, \bar{u}]$  (36)  $y+3/4, z+1/4, \bar{x}+1/2 [\bar{v}, \bar{w}, u]$   
 (37)  $\bar{y}+1/4, \bar{x}+3/4, z [v, u, \bar{w}]$  (38)  $y+1/2, x+1/2, z+1/2 [\bar{v}, \bar{u}, \bar{w}]$  (39)  $\bar{y}+3/4, x, \bar{z}+1/4 [v, \bar{u}, w]$  (40)  $y, \bar{x}+1/4, \bar{z}+3/4 [\bar{v}, u, w]$   
 (41)  $\bar{x}+1/4, \bar{z}+3/4, y [u, w, \bar{v}]$  (42)  $x, \bar{z}+1/4, \bar{y}+3/4 [\bar{u}, w, v]$  (43)  $x+1/2, z+1/2, y+1/2 [\bar{u}, \bar{w}, \bar{v}]$  (44)  $\bar{x}+3/4, z, \bar{y}+1/4 [u, \bar{w}, v]$   
 (45)  $\bar{z}+1/4, \bar{y}+3/4, x [w, v, \bar{u}]$  (46)  $\bar{z}+3/4, y, \bar{x}+1/4 [w, \bar{v}, u]$  (47)  $z, \bar{y}+1/4, \bar{x}+3/4 [\bar{w}, v, u]$  (48)  $z+1/2, y+1/2, x+1/2 [\bar{w}, \bar{v}, \bar{u}]$

96 g ..2

- $1/4, y, \bar{y} [0, \bar{v}, v]$   $0, \bar{y}+3/4, \bar{y}+1/2 [0, v, v]$   $1/2, y+1/2, y+1/4 [0, \bar{v}, \bar{v}]$   $3/4, \bar{y}+1/4, y+3/4 [0, v, \bar{v}]$   
 $\bar{y}, 1/4, y [v, 0, \bar{v}]$   $\bar{y}+1/2, 0, \bar{y}+3/4 [v, 0, v]$   $y+1/4, 1/2, y+1/2 [\bar{v}, 0, \bar{v}]$   $y+3/4, 3/4, \bar{y}+1/4 [\bar{v}, 0, v]$   
 $y, \bar{y}, 1/4 [\bar{v}, v, 0]$   $\bar{y}+3/4, \bar{y}+1/2, 0 [v, v, 0]$   $y+1/2, y+1/4, 1/2 [\bar{v}, \bar{v}, 0]$   $\bar{y}+1/4, y+3/4, 3/4 [v, \bar{v}, 0]$   
 $3/4, \bar{y}, y [0, \bar{v}, v]$   $0, y+1/4, y+1/2 [0, v, v]$   $1/2, \bar{y}+1/2, \bar{y}+3/4 [0, \bar{v}, \bar{v}]$   $1/4, y+3/4, \bar{y}+1/4 [0, v, \bar{v}]$   
 $y, 3/4, \bar{y} [v, 0, \bar{v}]$   $y+1/2, 0, y+1/4 [v, 0, v]$   $\bar{y}+3/4, 1/2, \bar{y}+1/2 [\bar{v}, 0, \bar{v}]$   $\bar{y}+1/4, 1/4, y+3/4 [\bar{v}, 0, v]$   
 $\bar{y}, y, 3/4 [\bar{v}, v, 0]$   $y+1/4, y+1/2, 0 [v, v, 0]$   $\bar{y}+1/2, \bar{y}+3/4, 1/2 [\bar{v}, \bar{v}, 0]$   $y+3/4, \bar{y}+1/4, 1/4 [v, \bar{v}, 0]$

- 96 f 2..  $x, 1/8, 1/8 [u, 0, 0]$   $\bar{x}+1/4, 5/8, 5/8 [\bar{u}, 0, 0]$   $1/8, x, 1/8 [0, u, 0]$   $5/8, \bar{x}+1/4, 5/8 [0, \bar{u}, 0]$   
 $1/8, 1/8, x [0, 0, u]$   $5/8, 5/8, \bar{x}+1/4 [0, 0, \bar{u}]$   $7/8, x+1/4, 7/8 [0, u, 0]$   $3/8, \bar{x}+1/2, 3/8 [0, \bar{u}, 0]$   
 $x+3/4, 3/8, 7/8 [u, 0, 0]$   $\bar{x}, 7/8, 3/8 [\bar{u}, 0, 0]$   $7/8, 3/8, \bar{x} [0, 0, \bar{u}]$   $3/8, 7/8, x+3/4 [0, 0, u]$   
 $\bar{x}, 7/8, 7/8 [u, 0, 0]$   $x+3/4, 3/8, 3/8 [\bar{u}, 0, 0]$   $7/8, \bar{x}, 7/8 [0, u, 0]$   $3/8, x+3/4, 3/8 [0, \bar{u}, 0]$   
 $7/8, 7/8, \bar{x} [0, 0, u]$   $3/8, 3/8, x+3/4 [0, 0, \bar{u}]$   $1/8, \bar{x}+3/4, 1/8 [0, u, 0]$   $5/8, x+1/2, 5/8 [0, \bar{u}, 0]$   
 $\bar{x}+1/4, 5/8, 1/8 [u, 0, 0]$   $x, 1/8, 5/8 [\bar{u}, 0, 0]$   $1/8, 5/8, x [0, 0, \bar{u}]$   $5/8, 1/8, \bar{x}+1/4 [0, 0, u]$

- 64 e .3.  $x, x, x [u, u, u]$   $\bar{x}+1/4, \bar{x}+3/4, x+1/2 [\bar{u}, \bar{u}, u]$   
 $\bar{x}+3/4, x+1/2, \bar{x}+1/4 [\bar{u}, u, \bar{u}]$   $x+1/2, \bar{x}+1/4, \bar{x}+3/4 [u, \bar{u}, \bar{u}]$   
 $x+3/4, x+1/4, \bar{x} [u, u, \bar{u}]$   $\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, \bar{u}]$   
 $x+1/4, \bar{x}, x+3/4 [u, \bar{u}, u]$   $\bar{x}, x+3/4, x+1/4 [\bar{u}, u, u]$   
 $\bar{x}, \bar{x}, \bar{x} [u, u, u]$   $x+3/4, x+1/4, \bar{x}+1/2 [\bar{u}, \bar{u}, u]$   
 $x+1/4, \bar{x}+1/2, x+3/4 [\bar{u}, u, \bar{u}]$   $\bar{x}+1/2, x+3/4, x+1/4 [u, \bar{u}, \bar{u}]$

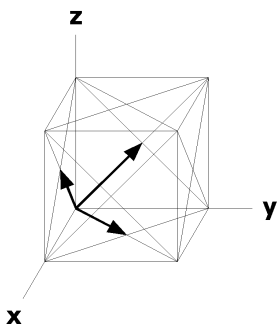
			$\bar{x}+1/4, \bar{x}+3/4, x$ [u, u, $\bar{u}$ ]	$x+1/2, x+1/2, x+1/2$ [ $\bar{u}, \bar{u}, \bar{u}$ ]		
			$\bar{x}+3/4, x, \bar{x}+1/4$ [u, $\bar{u}, u$ ]	$x, \bar{x}+1/4, \bar{x}+3/4$ [ $\bar{u}, u, u$ ]		
48	d	$\bar{4}..$	7/8, 1/8, 1/8 [u, 0, 0]	3/8, 5/8, 5/8 [ $\bar{u}, 0, 0$ ]	1/8, 7/8, 1/8 [0, u, 0]	5/8, 3/8, 5/8 [0, $\bar{u}, 0$ ]
			1/8, 1/8, 7/8 [0, 0, u]	5/8, 5/8, 3/8 [0, 0, $\bar{u}$ ]	7/8, 1/8, 7/8 [0, u, 0]	3/8, 5/8, 3/8 [0, $\bar{u}, 0$ ]
			5/8, 3/8, 7/8 [u, 0, 0]	1/8, 7/8, 3/8 [ $\bar{u}, 0, 0$ ]	7/8, 3/8, 1/8 [0, 0, $\bar{u}$ ]	3/8, 7/8, 5/8 [0, 0, u]
32	c	$\bar{3}.$	0, 0, 0 [u, u, u]	1/4, 3/4, 1/2 [ $\bar{u}, \bar{u}, u$ ]	3/4, 1/2, 1/4 [ $\bar{u}, u, \bar{u}$ ]	1/2, 1/4, 3/4 [u, $\bar{u}, \bar{u}$ ]
			3/4, 1/4, 0 [u, u, $\bar{u}$ ]	1/2, 1/2, 1/2 [ $\bar{u}, \bar{u}, \bar{u}$ ]	1/4, 0, 3/4 [u, $\bar{u}, u$ ]	0, 3/4, 1/4 [ $\bar{u}, u, u$ ]
32	b	.32	1/4, 1/4, 1/4 [0, 0, 0]	0, 1/2, 3/4 [0, 0, 0]	1/2, 3/4, 0 [0, 0, 0]	3/4, 0, 1/2 [0, 0, 0]
			3/4, 3/4, 3/4 [0, 0, 0]	0, 1/2, 1/4 [0, 0, 0]	1/2, 1/4, 0 [0, 0, 0]	1/4, 0, 1/2 [0, 0, 0]
16	a	23.	1/8, 1/8, 1/8 [0, 0, 0]	7/8, 3/8, 7/8 [0, 0, 0]	7/8, 7/8, 7/8 [0, 0, 0]	1/8, 5/8, 1/8 [0, 0, 0]

### Symmetry of Special Projections

Along [0, 0, 1]  $p_6 \cdot 4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/4$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/4$   
 Origin at 1/8, 3/8, z

Along [1, 1, 1]  $p_6'm'm$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x, x, x

Along [1, 1, 0]  $p_6 \cdot 2mm$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/4$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x-1/4, x+1/4, 0$



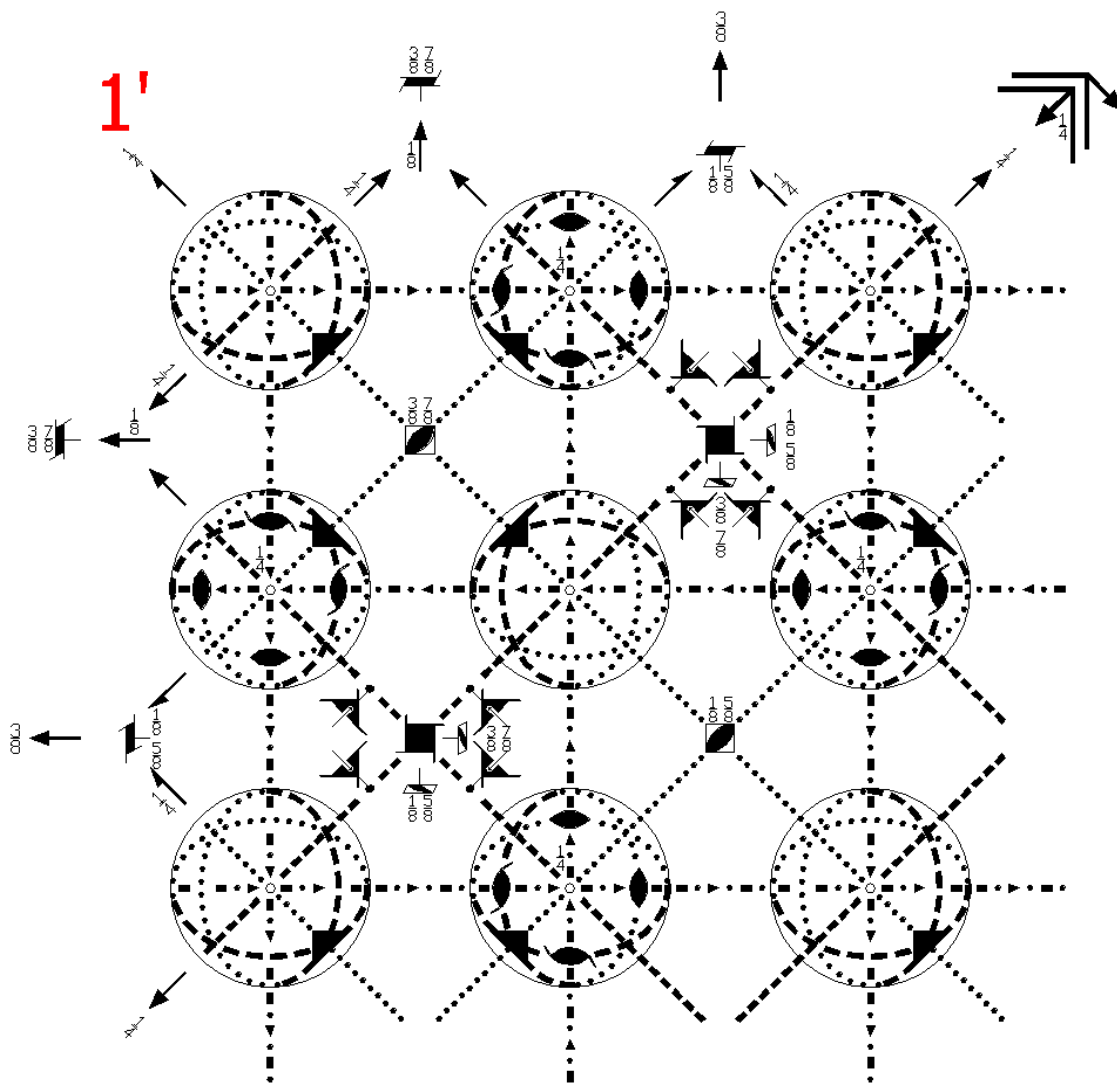
Fd $\bar{3}c1'$

228.2.1634

m $\bar{3}m1'$

F $4_1/d\bar{3}2/c1'$

Cubic



**Origin** at center ( $\bar{3}1'$ ), at  $3/8, 3/8, 3/8$  from  $231'$

**Asymmetric unit**  $-1/8 \leq x \leq 3/8$ ;  $-1/8 \leq y \leq 0$ ;  $-1/4 \leq z \leq 0$ ;  $y \leq \min(1/4-x, x)$ ;  $-y-1/4 \leq z \leq y$

**Vertices**  $-1/8, -1/8, -1/8$   $3/8, -1/8, -1/8$   $1/4, 0, 0$   $0, 0, 0$   $1/4, 0, -1/4$   $0, 0, -1/4$

**Symmetry Operations**

For (0,0,0) + set

- |  |   |   |  |
|--|---|---|--|
| (1) 1<br>(1 0,0,0)                                   | (2) 2 (0,0,1/2) $1/8, 3/8, z$<br>( $2_z$   $1/4, 3/4, 1/2$ )  | (3) 2 (0,1/2,0) $3/8, y, 1/8$<br>( $2_y$   $3/4, 1/2, 1/4$ )  | (4) 2 (1/2,0,0) $x, 1/8, 3/8$<br>( $2_x$   $1/2, 1/4, 3/4$ )   |
| (5) 3 <sup>+</sup> x,x,x<br>( $3_{xyz}$  0,0,0)      | (6) 3 <sup>+</sup> (1/3,-1/3,1/3)<br>$x+1/6, x+5/12, \bar{x}$<br>( $3_{xyz}^{-1}$   $1/2, 1/4, 3/4$ ) | (7) 3 <sup>+</sup> (-1/3,1/3,1/3)<br>$x+7/12, x-1/6, \bar{x}$<br>( $3_{xyz}^{-1}$   $1/4, 3/4, 1/2$ ) | (8) 3 <sup>+</sup> (1/3,1/3,-1/3)<br>$\bar{x}+5/12, \bar{x}+7/12, x$<br>( $3_{xyz}^{-1}$   $3/4, 1/2, 1/4$ ) |
| (9) 3 <sup>-</sup> x,x,x<br>( $3_{xyz}^{-1}$  0,0,0) | (10) 3 <sup>-</sup> $x+1/4, \bar{x}+1/2, \bar{x}$<br>( $3_{\bar{y}\bar{z}}$   $3/4, 1/2, 1/4$ )       | (11) 3 <sup>-</sup> $\bar{x}+3/4, \bar{x}+1/4, x$<br>( $3_{\bar{y}\bar{z}}$   $1/2, 1/4, 3/4$ )       | (12) 3 <sup>-</sup> $\bar{x}-1/2, x+3/4, \bar{x}$<br>( $3_{\bar{y}\bar{z}}$   $1/4, 3/4, 1/2$ )              |

(13) 2 (1/2,1/2,0) x,x-1/4,0 (2 <sub>xy</sub>  3/4,1/4,0)	(14) 2 x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)	(15) 4 <sup>-</sup> (0,0,3/4) 1/8,-1/8,z (4 <sub>z</sub> <sup>-1</sup>  1/4,0,3/4)	(16) 4 <sup>+</sup> (0,0,1/4) -3/8,3/8,z (4 <sub>z</sub>  0,3/4,1/4)
(17) 4 <sup>-</sup> (3/4,0,0) x,1/8,-1/8 (4 <sub>x</sub> <sup>-1</sup>  3/4,1/4,0)	(18) 2 (0,1/2,1/2) 0,y+1/4,y (2 <sub>yz</sub>  0,3/4,1/4)	(19) 2 1/4,y+1/2, $\bar{y}$ (2 <sub>yz</sub>  1/2,1/2,1/2)	(20) 4 <sup>+</sup> (1/4,0,0) x,-3/8,3/8 (4 <sub>x</sub>  1/4,0,3/4)
(21) 4 <sup>+</sup> (0,1/4,0) 3/8,y,-3/8 (4 <sub>y</sub>  3/4,1/4,0)	(22) 2 (1/2,0,1/2) x-1/4,0,x (2 <sub>xz</sub>  1/4,0,3/4)	(23) 4 <sup>-</sup> (0,3/4,0) -1/8,y,1/8 (4 <sub>y</sub> <sup>-1</sup>  0,3/4,1/4)	(24) 2 $\bar{x}$ +1/2,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)
(25) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(26) d (3/4,1/4,0) x,y,1/4 (m <sub>z</sub>  3/4,1/4,1/2)	(27) d (1/4,0,3/4) x,1/4,z (m <sub>y</sub>  1/4,1/2,3/4)	(28) d (0,3/4,1/4) 1/4,y,z (m <sub>x</sub>  1/2,3/4,1/4)
(29) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)	(30) $\bar{3}^+$ $\bar{x}$ -1,x+5/4, $\bar{x}$ ; -1/4,1/2,3/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,3/4,1/4)	(31) $\bar{3}^+$ x+1/4, $\bar{x}$ +1, $\bar{x}$ ; 1/2,3/4,-1/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  3/4,1/4,1/2)	(32) $\bar{3}^+$ $\bar{x}$ +5/4, $\bar{x}$ +1/4,x; 3/4,-1/4,1/2 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/4,1/2,3/4)
(33) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)	(34) $\bar{3}^-$ x+3/4, $\bar{x}$ -1, $\bar{x}$ ; 0,-1/4,3/4 ( $\bar{3}_{xyz}$  1/4,1/2,3/4)	(35) $\bar{3}^-$ $\bar{x}$ -1/4, $\bar{x}$ +3/4,x; -1/4,3/4,0 ( $\bar{3}_{xyz}$  1/2,3/4,1/4)	(36) $\bar{3}^-$ $\bar{x}$ +1,x-1/4, $\bar{x}$ ; 3/4,0,-1/4 ( $\bar{3}_{xyz}$  3/4,1/4,1/2)
(37) g (-1/4,1/4,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/4,3/4,0)	(38) n (1/2,1/2,1/2) x,x,z (m <sub>xy</sub>  1/2,1/2,1/2)	(39) $\bar{4}^-$ 3/8,3/8,z; 3/8,3/8,1/8 (4 <sub>z</sub> <sup>-1</sup>  3/4,0,1/4)	(40) $\bar{4}^+$ 1/8,1/8,z; 1/8,1/8,3/8 (4 <sub>z</sub>  0,1/4,3/4)
(41) $\bar{4}^-$ x,3/8,3/8; 1/8,3/8,3/8 (4 <sub>x</sub> <sup>-1</sup>  1/4,3/4,0)	(42) g (0,-1/4,1/4) x,y+1/2, $\bar{y}$ (m <sub>yz</sub>  0,1/4,3/4)	(43) n (1/2,1/2,1/2) x,y,y (m <sub>yz</sub>  1/2,1/2,1/2)	(44) $\bar{4}^+$ x,1/8,1/8; 3/8,1/8,1/8 (4 <sub>x</sub>  3/4,0,1/4)
(45) $\bar{4}^+$ 1/8,y,1/8; 1/8,3/8,1/8 (4 <sub>y</sub>  1/4,3/4,0)	(46) g (1/4,0,-1/4) $\bar{x}$ +1/2,y,x (m <sub>xz</sub>  3/4,0,1/4)	(47) $\bar{4}^-$ 3/8,y,3/8; 3/8,1/8,3/8 (4 <sub>y</sub> <sup>-1</sup>  0,1/4,3/4)	(48) n (1/2,1/2,1/2) x,y,x (m <sub>xz</sub>  1/2,1/2,1/2)

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2) (1 0,1/2,1/2)	(2) 2 1/8,1/8,z (2 <sub>z</sub>  1/4,1/4,0)	(3) 2 3/8,y,3/8 (2 <sub>y</sub>  3/4,0,3/4)	(4) 2 (1/2,0,0) x,3/8,1/8 (2 <sub>x</sub>  1/2,3/4,1/4)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x-1/3,x-1/6,x (3 <sub>xyz</sub>  0,1/2,1/2)	(6) 3 <sup>+</sup> $\bar{x}$ +1/2,x+1/4, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  1/2,3/4,1/4)	(7) 3 <sup>+</sup> x+1/4, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  1/4,1/4,0)	(8) 3 <sup>+</sup> $\bar{x}$ +3/4, $\bar{x}$ +3/4,x (3 <sub>xyz</sub> <sup>-1</sup>  3/4,0,3/4)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x-1/6,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(10) 3 <sup>-</sup> x+3/4, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub>  3/4,0,3/4)	(11) 3 <sup>-</sup> (1/3,1/3,-1/3) x+7/12, $\bar{x}$ +5/12,x (3 <sub>xyz</sub>  1/2,3/4,1/4)	(12) 3 <sup>-</sup> $\bar{x}$ ,x+1/4, $\bar{x}$ (3 <sub>xyz</sub>  1/4,1/4,0)
(13) 2 (3/4,3/4,0) x,x,1/4 (2 <sub>xy</sub>  3/4,3/4,1/2)	(14) 2 (1/4,-1/4,0) x, $\bar{x}$ +1/4,0 (2 <sub>xy</sub>  1/2,0,0)	(15) 4 <sup>-</sup> (0,0,1/4) 3/8,1/8,z (4 <sub>z</sub> <sup>-1</sup>  1/4,1/2,1/4)	(16) 4 <sup>+</sup> (0,0,3/4) -1/8,1/8,z (4 <sub>z</sub>  0,1/4,3/4)
(17) 4 <sup>-</sup> (3/4,0,0) 5/8,-1/8 (4 <sub>x</sub> <sup>-1</sup>  3/4,3/4,1/2)	(18) 2 (0,1/2,1/2) 0,y-1/4,y (2 <sub>yz</sub>  0,1/4,3/4)	(19) 2 1/4,y, $\bar{y}$ (2 <sub>yz</sub>  1/2,0,0)	(20) 4 <sup>+</sup> (1/4,0,0) x,1/8,3/8 (4 <sub>x</sub>  1/4,1/2,1/4)
(21) 4 <sup>+</sup> (0,3/4,0) 5/8,y,-1/8 (4 <sub>y</sub>  3/4,3/4,1/2)	(22) 2 (1/4,0,1/4) x,1/4,x (2 <sub>xz</sub>  1/4,1/2,1/4)	(23) 4 <sup>-</sup> (0,1/4,0) -3/8,y,3/8 (4 <sub>y</sub> <sup>-1</sup>  0,1/4,3/4)	(24) 2 (1/4,0,-1/4) $\bar{x}$ +1/4,0,x (2 <sub>xz</sub>  1/2,0,0)
(25) $\bar{1}$ 0,1/4,1/4 ( $\bar{1}$  0,1/2,1/2)	(26) d (3/4,3/4,0) x,y,0 (m <sub>z</sub>  3/4,3/4,0)	(27) d (1/4,0,1/4) x,0,z (m <sub>y</sub>  1/4,0,1/4)	(28) d (0,1/4,3/4) 1/4,y,z (m <sub>x</sub>  1/2,1/4,3/4)
(29) $\bar{3}^+$ x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$  0,1/2,1/2)	(30) $\bar{3}^+$ $\bar{x}$ -1,x+3/4, $\bar{x}$ ; -1/4,0,3/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,1/4,3/4)	(31) $\bar{3}^+$ x-3/4, $\bar{x}$ +3/2, $\bar{x}$ ; 0,3/4,-3/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  3/4,3/4,0)	(32) $\bar{3}^+$ $\bar{x}$ +1/4, $\bar{x}$ -1/4,x; 1/4,-1/4,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/4,0,1/4)

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| (33) $\bar{3}^-$ $x-1/2, x-1/2, x;$<br>0,0,1/2<br>( $\bar{3}_{xyz}^{-1}   0, 1/2, 1/2$ ) | (34) $\bar{3}^-$ $x+1/4, \bar{x}-1/2, \bar{x};$<br>0, -1/4, 1/4<br>( $\bar{3}_{\bar{xyz}}   1/4, 0, 1/4$ ) | (35) $\bar{3}^-$ $\bar{x}+1/4, \bar{x}+5/4, x;$<br>-1/4, 3/4, 1/2<br>( $\bar{3}_{\bar{xyz}}   1/2, 1/4, 3/4$ ) | (36) $\bar{3}^-$ $\bar{x}+3/2, x-3/4, \bar{x};$<br>3/4, 0, -3/4<br>( $\bar{3}_{\bar{xyz}}   3/4, 3/4, 0$ ) |
| (37) c (0,0,1/2) $x+1/4, \bar{x}, z$<br>( $m_{xy}   1/4, 1/4, 1/2$ )                     | (38) g (1/4, 1/4, 0) $x+1/4, x, z$<br>( $m_{\bar{xy}}   1/2, 0, 0$ )                                       | (39) $\bar{4}^-$ 1/8, 5/8, z; 1/8, 5/8, 3/8<br>( $\bar{4}_z^{-1}   3/4, 1/2, 3/4$ )                            | (40) $\bar{4}^+$ 3/8, 3/8, z; 3/8, 3/8, 1/8<br>( $\bar{4}_z   0, 3/4, 1/4$ )                               |
| (41) $\bar{4}^-$ $x, -1/8, 3/8; 1/8, -1/8, 3/8$<br>( $\bar{4}_x^{-1}   1/4, 1/4, 1/2$ )  | (42) g (0, 1/4, -1/4) $x, y+1/2, \bar{y}$<br>( $m_{yz}   0, 3/4, 1/4$ )                                    | (43) a (1/2, 0, 0) $x, y, y$<br>( $m_{\bar{yz}}   1/2, 0, 0$ )   | (44) $\bar{4}^+$ $x, 5/8, 1/8; 3/8, 5/8, 1/8$<br>( $\bar{4}_x   3/4, 0, 3/4$ )                             |
| (45) $\bar{4}^+$ -1/8, y, 3/8; -1/8, 1/8, 3/8<br>( $\bar{4}_y   1/4, 1/4, 1/2$ )         | (46) b (0, 1/2, 0) $\bar{x}+3/4, y, x$<br>( $m_{xz}   3/4, 1/2, 3/4$ )                                     | (47) $\bar{4}^-$ 1/8, y, 1/8; 1/8, 3/8, 1/8<br>( $\bar{4}_y^{-1}   0, 3/4, 1/4$ )                              | (48) g (1/4, 0, 1/4) $x+1/4, y, x$<br>( $m_{\bar{xz}}   1/2, 0, 0$ )                                       |

For (1/2, 0, 1/2) + set

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| (1) t (1/2, 0, 1/2)<br>(1   1/2, 0, 1/2)   | (2) 2 3/8, 3/8, z<br>(2 <sub>z</sub>   3/4, 3/4, 0)   | (3) 2 (0, 1/2, 0) 1/8, y, 3/8<br>(2 <sub>y</sub>   1/4, 1/2, 3/4)  | (4) 2 $x, 1/8, 1/8$<br>(2 <sub>x</sub>   0, 1/4, 1/4)   |
| (5) $3^+$ (1/3, 1/3, 1/3)<br>$x+1/6, x-1/6, x$<br>( $3_{xyz}   1/2, 0, 1/2$ )          | (6) $3^+$ $\bar{x}, x+1/4, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   0, 1/4, 1/4$ )                                   | (7) $3^+$ $x+3/4, \bar{x}, \bar{x}$<br>( $3_{\bar{xyz}}^{-1}   3/4, 3/4, 0$ )                                  | (8) $3^+$ $\bar{x}+1/4, \bar{x}+3/4, x$<br>( $3_{\bar{xyz}}^{-1}   1/4, 1/2, 3/4$ )                               |
| (9) $3^-$ (1/3, 1/3, 1/3)<br>$x-1/6, x-1/3, x$<br>( $3_{xyz}^{-1}   1/2, 0, 1/2$ )     | (10) $3^-$ (-1/3, 1/3, 1/3)<br>$x+5/12, \bar{x}+1/6, \bar{x}$<br>( $3_{\bar{xyz}}   1/4, 1/2, 3/4$ )            | (11) $3^-$ $\bar{x}+1/4, \bar{x}+1/4, x$<br>( $3_{\bar{yz}}   0, 1/4, 1/4$ )                                   | (12) $3^-$ $\bar{x}, x+3/4, \bar{x}$<br>( $3_{\bar{yz}}   3/4, 3/4, 0$ )  |
| (13) 2 (1/4, 1/4, 0) $x, x, 1/4$<br>(2 <sub>xy</sub>   1/4, 1/4, 1/2)                  | (14) 2 (-1/4, 1/4, 0) $x, \bar{x}+1/4, 0$<br>(2 <sub>xy</sub>   0, 1/2, 0)                                      | (15) $4^-$ (0, 0, 1/4) 3/8, -3/8, z<br>( $4_z^{-1}   3/4, 0, 1/4$ )  | (16) $4^+$ (0, 0, 3/4) -1/8, 5/8, z<br>( $4_z   1/2, 3/4, 3/4$ )  |
| (17) $4^-$ (1/4, 0, 0) $x, 3/8, 1/8$<br>( $4_x^{-1}   1/4, 1/4, 1/2$ )                 | (18) 2 (0, 3/4, 3/4) 1/4, y, y<br>(2 <sub>yz</sub>   1/2, 3/4, 3/4)   | (19) 2 (0, 1/4, -1/4) 0, y+1/4, $\bar{y}$<br>(2 <sub>yz</sub>   0, 1/2, 0)                                     | (20) $4^+$ (3/4, 0, 0) $x, -1/8, 1/8$<br>( $4_x   3/4, 0, 1/4$ )  |
| (21) $4^+$ (0, 1/4, 0) 3/8, y, 1/8<br>( $4_y   1/4, 1/4, 1/2$ )                        | (22) 2 (1/2, 0, 1/2) $x+1/4, 0, x$<br>(2 <sub>xz</sub>   3/4, 0, 1/4)   | (23) $4^-$ (0, 3/4, 0) -1/8, y, 5/8<br>( $4_y^{-1}   1/2, 3/4, 3/4$ )  | (24) 2 $\bar{x}, 1/4, x$<br>(2 <sub>z</sub>   0, 1/2, 0)  |
| (25) $\bar{1}$ 1/4, 0, 1/4<br>( $\bar{1}   1/2, 0, 1/2$ )                              | (26) d (1/4, 1/4, 0) $x, y, 0$<br>( $m_z   1/4, 1/4, 0$ )   | (27) d (3/4, 0, 1/4) $x, 1/4, z$<br>( $m_y   3/4, 1/2, 1/4$ )  | (28) d (0, 3/4, 3/4) 0, y, z<br>( $m_x   0, 3/4, 3/4$ )   |
| (29) $\bar{3}^+$ $x-1/2, x-1/2, x;$<br>0,0,1/2<br>( $\bar{3}_{xyz}   1/2, 0, 1/2$ )    | (30) $\bar{3}^+$ $\bar{x}-3/2, x+3/4, \bar{x};$<br>-3/4, 0, 3/4<br>( $\bar{3}_{\bar{xyz}}^{-1}   0, 3/4, 3/4$ ) | (31) $\bar{3}^+$ $x-1/4, \bar{x}+1/2, \bar{x};$<br>0, 1/4, -1/4<br>( $\bar{3}_{\bar{yz}}^{-1}   1/4, 1/4, 0$ ) | (32) $\bar{3}^+$ $\bar{x}+3/4, \bar{x}-1/4, x;$<br>3/4, -1/4, 0<br>( $\bar{3}_{\bar{xyz}}^{-1}   3/4, 1/2, 1/4$ ) |
| (33) $\bar{3}^-$ $x+1/2, x, x;$<br>1/2, 0, 0<br>( $\bar{3}_{xyz}^{-1}   1/2, 0, 1/2$ ) | (34) $\bar{3}^-$ $x+5/4, \bar{x}-1, \bar{x};$<br>1/2, -1/4, 3/4<br>( $\bar{3}_{\bar{yz}}   3/4, 1/2, 1/4$ )     | (35) $\bar{3}^-$ $\bar{x}-3/4, \bar{x}+3/4, x;$<br>-3/4, 3/4, 0<br>( $\bar{3}_{\bar{yz}}   0, 3/4, 3/4$ )      | (36) $\bar{3}^-$ $\bar{x}+1/2, x-1/4, \bar{x};$<br>1/4, 0, -1/4<br>( $\bar{3}_{\bar{yz}}   1/4, 1/4, 0$ )         |
| (37) c (0, 0, 1/2) $x+3/4, \bar{x}, z$<br>( $m_{xy}   3/4, 3/4, 1/2$ )                 | (38) g (1/4, 1/4, 0) $x-1/4, x, z$<br>( $m_{\bar{xy}}   0, 1/2, 0$ )  | (39) $\bar{4}^-$ 1/8, 1/8, z; 1/8, 1/8, 3/8<br>( $\bar{4}_z^{-1}   1/4, 0, 3/4$ )                              | (40) $\bar{4}^+$ 3/8, -1/8, z; 3/8, -1/8, 1/8<br>( $\bar{4}_z   1/2, 1/4, 1/4$ )                                  |
| (41) $\bar{4}^-$ $x, 1/8, 5/8; 3/8, 1/8, 5/8$<br>( $\bar{4}_x^{-1}   3/4, 3/4, 1/2$ )  | (42) a (1/2, 0, 0) $x, y+1/4, \bar{y}$<br>( $m_{yz}   1/2, 1/4, 1/4$ )  | (43) g (0, 1/4, 1/4) $x, y+1/4, y$<br>( $m_{\bar{yz}}   0, 1/2, 0$ )   | (44) $\bar{4}^+$ $x, 3/8, 3/8; 1/8, 3/8, 3/8$<br>( $\bar{4}_x   1/4, 0, 3/4$ )                                    |
| (45) $\bar{4}^+$ 1/8, y, 5/8; 1/8, 3/8, 5/8<br>( $\bar{4}_y   3/4, 3/4, 1/2$ )         | (46) g (-1/4, 0, 1/4) $\bar{x}+1/2, y, x$<br>( $m_{xz}   1/4, 0, 3/4$ )   | (47) $\bar{4}^-$ 3/8, y, -1/8; 3/8, 1/8, -1/8<br>( $\bar{4}_y^{-1}   1/2, 1/4, 1/4$ )                          | (48) b (0, 1/2, 0) $x, y, x$<br>( $m_{\bar{xz}}   0, 1/2, 0$ )  |

## For (1/2,1/2,0) + set

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|--|---|--|---|
| (1) t (1/2,1/2,0)<br>(1 1/2,1/2,0)   | (2) 2 (0,0,1/2) 3/8,1/8,z<br>(2 <sub>z</sub>  3/4,1/4,1/2)  | (3) 2 1/8,y,1/8<br>(2 <sub>y</sub>  1/4,0,1/4)   | (4) 2 x,3/8,3/8<br>(2 <sub>x</sub>  0,3/4,3/4)  |
| (5) 3 <sup>+</sup> (1/3,1/3,1/3)<br>x+1/6,x+1/3,x<br>(3 <sub>xyz</sub>  1/2,1/2,0)               | (6) 3 <sup>+</sup> $\bar{x}$ ,x+3/4, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,3/4,3/4)                   | (7) 3 <sup>+</sup> x+3/4, $\bar{x}$ -1/2, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  3/4,1/4,1/2)             | (8) 3 <sup>+</sup> $\bar{x}$ +1/4, $\bar{x}$ +1/4,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/4,0,1/4)              |
| (9) 3 <sup>-</sup> (1/3,1/3,1/3)<br>x+1/3,x+1/6,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/2,0) | (10) 3 <sup>-</sup> x+1/4, $\bar{x}$ , $\bar{x}$<br>(3 <sub>xyz</sub>  1/4,0,1/4)                               | (11) 3 <sup>-</sup> $\bar{x}$ +3/4, $\bar{x}$ +3/4, x<br>(3 <sub>xyz</sub>  0,3/4,3/4)                           | (12) 3 <sup>-</sup> (1/3,-1/3,1/3)<br>$\bar{x}$ -1/6, x+7/12, $\bar{x}$<br>(3 <sub>xyz</sub>  3/4,1/4,1/2)      |
| (13) 2 (1/2,1/2,0) x,x+1/4,0<br>(2 <sub>xy</sub>  1/4,3/4,0)                                     | (14) 2 x, $\bar{x}$ ,1/4<br>(2 <sub>xy</sub>  0,0,1/2)  | (15) 4 <sup>-</sup> (0,0,3/4) 5/8,-1/8,z<br>(4 <sub>z</sub> <sup>-1</sup>  3/4,1/2,3/4)                          | (16) 4 <sup>+</sup> (0,0,1/4) 1/8,3/8,z<br>(4 <sub>z</sub>  1/2,1/4,1/4)  |
| (17) 4 <sup>-</sup> (1/4,0,0) x,3/8,-3/8<br>(4 <sub>x</sub> <sup>-1</sup>  1/4,3/4,0)            | (18) 2 (0,1/4,1/4) 1/4,y,y<br>(2 <sub>yz</sub>  1/2,1/4,1/4)  | (19) 2 (0,-1/4,1/4) 0,y+1/4, $\bar{y}$<br>(2 <sub>yz</sub>  0,0,1/2)   | (20) 4 <sup>+</sup> (3/4,0,0) x,-1/8,5/8<br>(4 <sub>x</sub>  3/4,1/2,3/4)                                       |
| (21) 4 <sup>+</sup> (0,3/4,0) 1/8,y,-1/8<br>(4 <sub>y</sub>  1/4,3/4,0)                          | (22) 2 (3/4,0,3/4) x,1/4,x<br>(2 <sub>xz</sub>  3/4,1/2,3/4)  | (23) 4 <sup>-</sup> (0,1/4,0) 1/8,y,3/8<br>(4 <sub>y</sub> <sup>-1</sup>  1/2,1/4,1/4)                           | (24) 2 (-1/4,0,1/4) $\bar{x}$ +1/4,0,x<br>(2 <sub>xz</sub>  0,0,1/2)  |
| (25) $\bar{1}$ 1/4,1/4,0<br>( $\bar{1}$  1/2,1/2,0)  | (26) d (1/4,3/4,0) x,y,1/4<br>(m <sub>z</sub>  1/4,3/4,1/2)   | (27) d (3/4,0,3/4) x,0,z<br>(m <sub>y</sub>  3/4,0,3/4)  | (28) d (0,1/4,1/4) 0,y,z<br>(m <sub>x</sub>  0,1/4,1/4)   |
| (29) $\bar{3}^+$ x+1/2,x,x;<br>1/2,0,0<br>( $\bar{3}_{xyz}$  1/2,1/2,0)                          | (30) $\bar{3}^+$ $\bar{x}$ -1/2,x+1/4, $\bar{x}$ ;<br>-1/4,0,1/4<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  0,1/4,1/4) | (31) $\bar{3}^+$ x-1/4, $\bar{x}$ +1, $\bar{x}$ ;<br>0,3/4,-1/4<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  1/4,3/4,1/2) | (32) $\bar{3}^+$ $\bar{x}$ +3/4, $\bar{x}$ -3/4,x;<br>3/4,-3/4,0<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  3/4,0,3/4) |
| (33) $\bar{3}^-$ x,x+1/2,x;<br>0,1/2,0<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,1/2,0)            | (34) $\bar{3}^-$ x+3/4, $\bar{x}$ -3/2, $\bar{x}$ ;<br>0,-3/4,3/4<br>( $\bar{3}_{xyz}$  3/4,0,3/4)              | (35) $\bar{3}^-$ $\bar{x}$ -1/4, $\bar{x}$ +1/4, x;<br>-1/4,1/4,0<br>( $\bar{3}_{xyz}$  0,1/4,1/4)               | (36) $\bar{3}^-$ $\bar{x}$ +1, x+1/4, $\bar{x}$ ;<br>3/4,1/2,-1/4<br>( $\bar{3}_{xyz}$  1/4,3/4,1/2)            |
| (37) g (1/4,-1/4,0) x+1/2, $\bar{x}$ ,z<br>(m <sub>xy</sub>  3/4,1/4,0)                          | (38) c (0,0,1/2) x,x,z<br>(m <sub>xy</sub>  0,0,1/2)  | (39) $\bar{4}^-$ -1/8,3/8,z; -1/8,3/8,1/8<br>( $\bar{4}_z$ <sup>-1</sup>  1/4,1/2,1/4)                           | (40) $\bar{4}^+$ 5/8,1/8,z; 5/8,1/8,3/8<br>( $\bar{4}_z$  1/2,3/4,3/4)  |
| (41) $\bar{4}^-$ x,1/8,1/8; 3/8,1/8,1/8<br>( $\bar{4}_x$ <sup>-1</sup>  3/4,1/4,0)               | (42) a (1/2,0,0) x,y+3/4, $\bar{y}$<br>(m <sub>yz</sub>  1/2,3/4,3/4)   | (43) g (0,1/4,1/4) x,y-1/4,y<br>(m <sub>yz</sub>  0,0,1/2)   | (44) $\bar{4}^+$ x,3/8,-1/8; 1/8,3/8,-1/8<br>( $\bar{4}_x$  1/4,1/2,1/4)  |
| (45) $\bar{4}^+$ 3/8,y,3/8; 3/8,1/8,3/8<br>( $\bar{4}_y$  3/4,1/4,0)                             | (46) b (0,1/2,0) $\bar{x}$ +1/4,y,x<br>(m <sub>xz</sub>  1/4,1/2,1/4)   | (47) $\bar{4}^-$ 5/8,y,1/8; 5/8,3/8,1/8<br>( $\bar{4}_y$ <sup>-1</sup>  1/2,3/4,3/4)                             | (48) g (1/4,0,1/4) x-1/4,y,x<br>(m <sub>xz</sub>  0,0,1/2)  |

## For (0,0,0)' + set

- |  |  |   |   |
|--|--|---|---|
| (1) 1'<br>(1 0,0,0)'   | (2) 2' (0,0,1/2) 1/8,3/8,z<br>(2 <sub>z</sub>  1/4,3/4,1/2)'   | (3) 2' (0,1/2,0) 3/8,y,1/8<br>(2 <sub>y</sub>  3/4,1/2,1/4)'  | (4) 2' (1/2,0,0) x,1/8,3/8<br>(2 <sub>x</sub>  1/2,1/4,3/4)'  |
| (5) 3 <sup>+</sup> ' x,x,x<br>(3 <sub>xyz</sub>  0,0,0)'               | (6) 3 <sup>+</sup> ' (1/3,-1/3,1/3)<br>x+1/6,x+5/12, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,1/4,3/4)' | (7) 3 <sup>+</sup> ' (-1/3,1/3,1/3)<br>x+7/12, x-1/6, $\bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/4,3/4,1/2)' | (8) 3 <sup>+</sup> ' (1/3,1/3,-1/3)<br>x+5/12, x+7/12,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  3/4,1/2,1/4)' |
| (9) 3 <sup>-</sup> ' x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)' | (10) 3 <sup>-</sup> ' x+1/4, $\bar{x}$ +1/2, $\bar{x}$<br>(3 <sub>xyz</sub>  3/4,1/2,1/4)'                       | (11) 3 <sup>-</sup> ' $\bar{x}$ +3/4, $\bar{x}$ +1/4, x<br>(3 <sub>xyz</sub>  1/2,1/4,3/4)'                       | (12) 3 <sup>-</sup> ' $\bar{x}$ -1/2, x+3/4, $\bar{x}$<br>(3 <sub>xyz</sub>  1/4,3/4,1/2)'                |
| (13) 2' (1/2,1/2,0) x,x-1/4,0<br>(2 <sub>xy</sub>  3/4,1/4,0)'         | (14) 2' x, $\bar{x}$ +1/2,1/4<br>(2 <sub>xy</sub>  1/2,1/2,1/2)'   | (15) 4 <sup>-</sup> ' (0,0,3/4) 1/8,-1/8,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/4,0,3/4)'                          | (16) 4 <sup>+</sup> ' (0,0,1/4) -3/8,3/8,z<br>(4 <sub>z</sub>  0,3/4,1/4)'                                |

- |  |  |  |  |
|--|--|--|--|
| (17) $4^- ' (3/4,0,0) \ x, 1/8, -1/8$<br>$(4_x^{-1}   3/4, 1/4, 0)'$                   | (18) $2' (0, 1/2, 1/2) \ 0, y+1/4, y$<br>$(2_{yz}   0, 3/4, 1/4)'$   | (19) $2' \ 1/4, y+1/2, \bar{y}$<br>$(2_{\bar{y}z}   1/2, 1/2, 1/2)'$   | (20) $4^+ ' (1/4, 0, 0) \ x, -3/8, 3/8$<br>$(4_x   1/4, 0, 3/4)'$  |
| (21) $4^+ ' (0, 1/4, 0) \ 3/8, y, -3/8$<br>$(4_y   3/4, 1/4, 0)'$                      | (22) $2' (1/2, 0, 1/2) \ x-1/4, 0, x$<br>$(2_{xz}   1/4, 0, 3/4)'$   | (23) $4^- ' (0, 3/4, 0) \ -1/8, y, 1/8$<br>$(4_y^{-1}   0, 3/4, 1/4)'$   | (24) $2' \ \bar{x}+1/2, 1/4, x$<br>$(2_{\bar{x}z}   1/2, 1/2, 1/2)'$   |
| (25) $\bar{1} \ 0, 0, 0$<br>$(\bar{1}   0, 0, 0)'$                                     | (26) $d' (3/4, 1/4, 0) \ x, y, 1/4$<br>$(m_z   3/4, 1/4, 1/2)'$  | (27) $d' (1/4, 0, 3/4) \ x, 1/4, z$<br>$(m_y   1/4, 1/2, 3/4)'$  | (28) $d' (0, 3/4, 1/4) \ 1/4, y, z$<br>$(m_x   1/2, 3/4, 1/4)'$  |
| (29) $\bar{3}^+ ' \ x, x, x;$<br>$0, 0, 0$<br>$(\bar{3}_{xyz}   0, 0, 0)'$             | (30) $\bar{3}^+ ' \ \bar{x}-1, x+5/4, \bar{x};$<br>$-1/4, 1/2, 3/4$<br>$(\bar{3}_{x\bar{y}z}^{-1}   1/2, 3/4, 1/4)'$ | (31) $\bar{3}^+ ' \ x+1/4, \bar{x}+1, \bar{x};$<br>$1/2, 3/4, -1/4$<br>$(\bar{3}_{\bar{x}yz}^{-1}   3/4, 1/4, 1/2)'$ | (32) $\bar{3}^+ ' \ \bar{x}+5/4, \bar{x}+1/4, x;$<br>$3/4, -1/4, 1/2$<br>$(\bar{3}_{x\bar{y}z}^{-1}   1/4, 1/2, 3/4)'$ |
| (33) $\bar{3}^- ' \ x, x, x;$<br>$0, 0, 0$<br>$(\bar{3}_{xyz}^{-1}   0, 0, 0)'$        | (34) $\bar{3}^- ' \ x+3/4, \bar{x}-1, \bar{x};$<br>$0, -1/4, 3/4$<br>$(\bar{3}_{x\bar{y}z}   1/4, 1/2, 3/4)'$        | (35) $\bar{3}^- ' \ \bar{x}-1/4, \bar{x}+3/4, x;$<br>$-1/4, 3/4, 0$<br>$(\bar{3}_{\bar{x}yz}   1/2, 3/4, 1/4)'$      | (36) $\bar{3}^- ' \ \bar{x}+1, x-1/4, \bar{x};$<br>$3/4, 0, -1/4$<br>$(\bar{3}_{x\bar{y}z}   3/4, 1/4, 1/2)'$          |
| (37) $g' (-1/4, 1/4, 1/2) \ x+1/2, \bar{x}, z$<br>$(m_{xy}   1/4, 3/4, 0)'$            | (38) $n' (1/2, 1/2, 1/2) \ x, x, z$<br>$(m_{\bar{xy}}   1/2, 1/2, 1/2)'$   | (39) $\bar{4}^- ' \ 3/8, 3/8, z; \ 3/8, 3/8, 1/8$<br>$(\bar{4}_z^{-1}   3/4, 0, 1/4)'$                               | (40) $\bar{4}^+ ' \ 1/8, 1/8, z; \ 1/8, 1/8, 3/8$<br>$(\bar{4}_z   1/2, 1/2, 0)'$                                      |
| (41) $\bar{4}^- ' \ x, 3/8, 3/8; \ 1/8, 3/8, 3/8$<br>$(\bar{4}_x^{-1}   1/4, 3/4, 0)'$ | (42) $g' (0, -1/4, 1/4) \ x, y+1/2, \bar{y}$<br>$(m_{yz}   0, 1/4, 3/4)'$  | (43) $n' (1/2, 1/2, 1/2) \ x, y, y$<br>$(m_{\bar{y}z}   1/2, 1/2, 1/2)'$   | (44) $\bar{4}^+ ' \ x, 1/8, 1/8; \ 3/8, 1/8, 1/8$<br>$(\bar{4}_x   0, 1/4, 3/4)'$                                      |
| (45) $\bar{4}^+ ' \ 1/8, y, 1/8; \ 1/8, 3/8, 1/8$<br>$(\bar{4}_y   1/4, 3/4, 0)'$      | (46) $g' (1/4, 0, -1/4) \ \bar{x}+1/2, y, x$<br>$(m_{xz}   3/4, 0, 1/4)'$  | (47) $\bar{4}^- ' \ 3/8, y, 3/8; \ 3/8, 1/8, 3/8$<br>$(\bar{4}_y^{-1}   0, 1/4, 3/4)'$                               | (48) $n' (1/2, 1/2, 1/2) \ x, y, x$<br>$(m_{\bar{x}z}   1/2, 1/2, 1/2)'$   |

For (0, 1/2, 1/2)' + set

- |   |  |  |  |
|---|--|--|--|
| (1) $t' (0, 1/2, 1/2)$<br>$(1   0, 1/2, 1/2)'$  | (2) $2' \ 1/8, 1/8, z$<br>$(2_z   1/4, 1/4, 0)'$   | (3) $2' \ 3/8, y, 3/8$<br>$(2_y   3/4, 0, 3/4)'$   | (4) $2' (1/2, 0, 0) \ x, 3/8, 1/8$<br>$(2_x   1/2, 3/4, 1/4)'$   |
| (5) $3^+ ' (1/3, 1/3, 1/3)$<br>$x-1/3, x-1/6, x$<br>$(3_{xyz}   0, 1/2, 1/2)'$                | (6) $3^+ ' \ \bar{x}+1/2, x+1/4, \bar{x}$<br>$(3_{x\bar{y}z}^{-1}   1/2, 3/4, 1/4)'$                               | (7) $3^+ ' \ x+1/4, \bar{x}, \bar{x}$<br>$(3_{\bar{x}yz}^{-1}   1/4, 1/4, 0)'$                                     | (8) $3^+ ' \ \bar{x}+3/4, \bar{x}+3/4, x$<br>$(3_{x\bar{y}z}^{-1}   3/4, 0, 3/4)'$                                 |
| (9) $3^- ' (1/3, 1/3, 1/3)$<br>$x-1/6, x+1/6, x$<br>$(3_{xyz}^{-1}   0, 1/2, 1/2)'$           | (10) $3^- ' \ x+3/4, \bar{x}, \bar{x}$<br>$(3_{x\bar{y}z}   3/4, 0, 3/4)'$   | (11) $3^- ' (1/3, 1/3, -1/3)$<br>$\bar{x}+7/12, \bar{x}+5/12, x$<br>$(3_{x\bar{y}z}   1/2, 3/4, 1/4)'$             | (12) $3^- ' \ \bar{x}, x+1/4, \bar{x}$<br>$(3_{x\bar{y}z}   1/4, 1/4, 0)'$   |
| (13) $2' (3/4, 3/4, 0) \ x, x, 1/4$<br>$(2_{xy}   3/4, 3/4, 1/2)'$                            | (14) $2' (1/4, -1/4, 0) \ x, \bar{x}+1/4, 0$<br>$(2_{\bar{xy}}   1/2, 0, 0)'$                                      | (15) $4^- ' (0, 0, 1/4) \ 3/8, 1/8, z$<br>$(4_z^{-1}   1/4, 1/2, 1/4)'$  | (16) $4^+ ' (0, 0, 3/4) \ -1/8, 1/8, z$<br>$(4_z   0, 1/4, 3/4)'$  |
| (17) $4^- ' (3/4, 0, 0) \ 5/8, -1/8$<br>$(4_x^{-1}   3/4, 3/4, 1/2)'$                         | (18) $2' (0, 1/2, 1/2) \ 0, y-1/4, y$<br>$(2_{yz}   0, 1/4, 3/4)'$   | (19) $2' \ 1/4, y, \bar{y}$<br>$(2_{\bar{y}z}   1/2, 0, 0)'$   | (20) $4^+ ' (1/4, 0, 0) \ x, 1/8, 3/8$<br>$(4_x   1/4, 1/2, 1/4)'$   |
| (21) $4^+ ' (0, 3/4, 0) \ 5/8, y, -1/8$<br>$(4_y   3/4, 3/4, 1/2)'$                           | (22) $2' (1/4, 0, 1/4) \ x, 1/4, x$<br>$(2_{xz}   1/4, 1/2, 1/4)'$   | (23) $4^- ' (0, 1/4, 0) \ -3/8, y, 3/8$<br>$(4_y^{-1}   0, 1/4, 3/4)'$   | (24) $2' (1/4, 0, -1/4) \ \bar{x}+1/4, 0, x$<br>$(2_{\bar{x}z}   1/2, 0, 0)'$                                      |
| (25) $\bar{1} \ 0, 1/4, 1/4$<br>$(\bar{1}   0, 1/2, 1/2)'$                                    | (26) $d' (3/4, 3/4, 0) \ x, y, 0$<br>$(m_z   3/4, 3/4, 0)'$  | (27) $d' (1/4, 0, 1/4) \ x, 0, z$<br>$(m_y   1/4, 0, 1/4)'$  | (28) $d' (0, 1/4, 3/4) \ 1/4, y, z$<br>$(m_x   1/2, 1/4, 3/4)'$  |
| (29) $\bar{3}^+ ' \ x, x+1/2, x;$<br>$0, 1/2, 0$<br>$(\bar{3}_{xyz}   0, 1/2, 1/2)'$          | (30) $\bar{3}^+ ' \ \bar{x}-1, x+3/4, \bar{x};$<br>$-1/4, 0, 3/4$<br>$(\bar{3}_{x\bar{y}z}^{-1}   1/2, 1/4, 3/4)'$ | (31) $\bar{3}^+ ' \ x-3/4, \bar{x}+3/2, \bar{x};$<br>$0, 3/4, -3/4$<br>$(\bar{3}_{\bar{x}yz}^{-1}   3/4, 3/4, 0)'$ | (32) $\bar{3}^+ ' \ \bar{x}+1/4, \bar{x}-1/4, x;$<br>$1/4, -1/4, 0$<br>$(\bar{3}_{x\bar{y}z}^{-1}   1/4, 0, 1/4)'$ |
| (33) $\bar{3}^- ' \ x-1/2, x-1/2, x;$<br>$0, 0, 1/2$<br>$(\bar{3}_{xyz}^{-1}   0, 1/2, 1/2)'$ | (34) $\bar{3}^- ' \ x+1/4, \bar{x}-1/2, \bar{x};$<br>$0, -1/4, 1/4$<br>$(\bar{3}_{x\bar{y}z}   1/4, 0, 1/4)'$      | (35) $\bar{3}^- ' \ \bar{x}+1/4, \bar{x}+5/4, x;$<br>$-1/4, 3/4, 1/2$<br>$(\bar{3}_{\bar{x}yz}   1/2, 1/4, 3/4)'$  | (36) $\bar{3}^- ' \ \bar{x}+3/2, x-3/4, \bar{x};$<br>$3/4, 0, -3/4$<br>$(\bar{3}_{x\bar{y}z}   3/4, 3/4, 0)'$      |



- (37)  $c'$  (0,0,1/2)  $x+1/4,\bar{x},z$  (38)  $g'$  (1/4,1/4,0)  $x+1/4,x,z$  (39)  $\bar{4}^-$  ' 1/8,5/8,z; 1/8,5/8,3/8 (40)  $\bar{4}^+$  ' 3/8,3/8,z; 3/8,3/8,1/8  
 $(m_{xy}|1/4,1/4,1/2)'$   $(m_{\bar{xy}}|1/2,0,0)'$   $(\bar{4}_z^{-1}|3/4,1/2,3/4)'$   $(\bar{4}_z|0,3/4,1/4)'$
- (41)  $\bar{4}^-$  '  $x,-1/8,3/8; 1/8,-1/8,3/8$  (42)  $g'$  (0,1/4,-1/4)  $x,y+1/2,\bar{y}$  (43)  $a'$  (1/2,0,0)  $x,y,y$  (44)  $\bar{4}^+$  '  $x,5/8,1/8; 3/8,5/8,1/8$   
 $(\bar{4}_x^{-1}|1/4,1/4,1/2)'$   $(m_{yz}|0,3/4,1/4)'$   $(m_{\bar{yz}}|1/2,0,0)'$   $(\bar{4}_x|3/4,0,3/4)'$
- (45)  $\bar{4}^+$  '  $-1/8,y,3/8; -1/8,1/8,3/8$  (46)  $b'$  (0,1/2,0)  $\bar{x}+3/4,y,x$  (47)  $\bar{4}^-$  ' 1/8,y,1/8; 1/8,3/8,1/8 (48)  $g'$  (1/4,0,1/4)  $x+1/4,y,x$   
 $(\bar{4}_y|1/4,1/4,1/2)'$   $(m_{xz}|3/4,1/2,3/4)'$   $(\bar{4}_y^{-1}|0,3/4,1/4)'$   $(m_{\bar{xz}}|1/2,0,0)'$

For (1/2,0,1/2)' + set

- (1)  $t'$  (1/2,0,1/2) (2)  $2'$  3/8,3/8,z (3)  $2'$  (0,1/2,0) 1/8,y,3/8 (4)  $2'$   $x,1/8,1/8$   
 $(1|1/2,0,1/2)'$   $(2_z|3/4,3/4,0)'$   $(2_y|1/4,1/2,3/4)'$   $(2_x|0,1/4,1/4)'$
- (5)  $3^+$  ' (1/3,1/3,1/3) (6)  $3^+$  '  $\bar{x},x+1/4,\bar{x}$  (7)  $3^+$  '  $x+3/4,\bar{x},\bar{x}$  (8)  $3^+$  '  $\bar{x}+1/4,\bar{x}+3/4,x$   
 $x+1/6,x-1/6,x$   $(3_{xyz}|1/2,0,1/2)'$   $(3_{\bar{xyz}}^{-1}|0,1/4,1/4)'$   $(3_{\bar{xyz}}^{-1}|3/4,3/4,0)'$   $(3_{xyz}^{-1}|1/4,1/2,3/4)'$
- (9)  $3^-$  ' (1/3,1/3,1/3) (10)  $3^-$  ' (-1/3,1/3,1/3) (11)  $3^-$  '  $\bar{x}+1/4,\bar{x}+1/4,x$  (12)  $3^-$  '  $\bar{x},x+3/4,\bar{x}$   
 $x-1/6,x-1/3,x$   $(3_{xyz}^{-1}|1/2,0,1/2)'$   $x+5/12,\bar{x}+1/6,\bar{x}$   $(3_{xyz}|1/4,1/2,3/4)'$   $(3_{\bar{xyz}}|0,1/4,1/4)'$   $(3_{\bar{xyz}}|3/4,3/4,0)'$
- (13)  $2'$  (1/4,1/4,0)  $x,x,1/4$  (14)  $2'$  (-1/4,1/4,0)  $x,\bar{x}+1/4,0$  (15)  $4^-$  ' (0,0,1/4) 3/8,-3/8,z (16)  $4^+$  ' (0,0,3/4) -1/8,5/8,z  
 $(2_{xy}|1/4,1/4,1/2)'$   $(2_{\bar{xy}}|0,1/2,0)'$   $(4_z^{-1}|3/4,0,1/4)'$   $(4_z|1/2,3/4,3/4)'$
- (17)  $4^-$  ' (1/4,0,0)  $x,3/8,1/8$  (18)  $2'$  (0,3/4,3/4) 1/4,y,y (19)  $2'$  (0,1/4,-1/4) 0,y+1/4, $\bar{y}$  (20)  $4^+$  ' (3/4,0,0)  $x,-1/8,1/8$   
 $(4_x^{-1}|1/4,1/4,1/2)'$   $(2_{yz}|1/2,3/4,3/4)'$   $(2_{\bar{yz}}|0,1/2,0)'$   $(4_x|3/4,0,1/4)'$
- (21)  $4^+$  ' (0,1/4,0) 3/8,y,1/8 (22)  $2'$  (1/2,0,1/2)  $x+1/4,0,x$  (23)  $4^-$  ' (0,3/4,0) -1/8,y,5/8 (24)  $2'$   $\bar{x},1/4,x$   
 $(4_y|1/4,1/4,1/2)'$   $(2_{xz}|3/4,0,1/4)'$   $(4_y^{-1}|1/2,3/4,3/4)'$   $(2_{\bar{xz}}|0,1/2,0)'$
- (25)  $\bar{1}$  ' 1/4,0,1/4 (26)  $d'$  (1/4,1/4,0)  $x,y,0$  (27)  $d'$  (3/4,0,1/4)  $x,1/4,z$  (28)  $d'$  (0,3/4,3/4) 0,y,z  
 $(\bar{1}|1/2,0,1/2)'$   $(m_z|1/4,1/4,0)'$   $(m_y|3/4,1/2,1/4)'$   $(m_x|0,3/4,3/4)'$
- (29)  $\bar{3}^+$  '  $x-1/2,x-1/2,x;$  (30)  $\bar{3}^+$  '  $\bar{x}-3/2,x+3/4,\bar{x};$  (31)  $\bar{3}^+$  '  $x-1/4,\bar{x}+1/2,\bar{x};$  (32)  $\bar{3}^+$  '  $\bar{x}+3/4,\bar{x}-1/4,x;$   
 $0,0,1/2$   $-3/4,0,3/4$   $0,1/4,-1/4$   $3/4,-1/4,0$   
 $(\bar{3}_{xyz}|1/2,0,1/2)'$   $(\bar{3}_{\bar{xyz}}^{-1}|0,3/4,3/4)'$   $(\bar{3}_{\bar{xyz}}^{-1}|1/4,1/4,0)'$   $(\bar{3}_{xyz}^{-1}|3/4,1/2,1/4)'$
- (33)  $\bar{3}^-$  '  $x+1/2,x,x;$  (34)  $\bar{3}^-$  '  $x+5/4,\bar{x}-1,\bar{x};$  (35)  $\bar{3}^-$  '  $\bar{x}-3/4,\bar{x}+3/4,x;$  (36)  $\bar{3}^-$  '  $\bar{x}+1/2,x-1/4,\bar{x};$   
 $1/2,0,0$   $1/2,-1/4,3/4$   $-3/4,3/4,0$   $1/4,0,-1/4$   
 $(\bar{3}_{xyz}^{-1}|1/2,0,1/2)'$   $(\bar{3}_{\bar{xyz}}|3/4,1/2,1/4)'$   $(\bar{3}_{\bar{xyz}}|0,3/4,3/4)'$   $(\bar{3}_{xyz}|1/4,1/4,0)'$
- (37)  $c'$  (0,0,1/2)  $x+3/4,\bar{x},z$  (38)  $g'$  (1/4,1/4,0)  $x-1/4,x,z$  (39)  $\bar{4}^-$  ' 1/8,1/8,z; 1/8,1/8,3/8 (40)  $\bar{4}^+$  ' 3/8,-1/8,z; 3/8,-1/8,1/8  
 $(m_{xy}|3/4,3/4,1/2)'$   $(m_{\bar{xy}}|0,1/2,0)'$   $(\bar{4}_z^{-1}|1/4,0,3/4)'$   $(\bar{4}_z|1/2,1/4,1/4)'$
- (41)  $\bar{4}^-$  '  $x,1/8,5/8; 3/8,1/8,5/8$  (42)  $a'$  (1/2,0,0)  $x,y+1/4,\bar{y}$  (43)  $g'$  (0,1/4,1/4)  $x,y+1/4,y$  (44)  $\bar{4}^+$  '  $x,3/8,3/8; 1/8,3/8,3/8$   
 $(\bar{4}_x^{-1}|3/4,3/4,1/2)'$   $(m_{yz}|1/2,1/4,1/4)'$   $(m_{\bar{yz}}|0,1/2,0)'$   $(\bar{4}_x|1/4,0,3/4)'$
- (45)  $\bar{4}^+$  ' 1/8,y,5/8; 1/8,3/8,5/8 (46)  $g'$  (-1/4,0,1/4)  $\bar{x}+1/2,y,x$  (47)  $\bar{4}^-$  ' 3/8,y,-1/8; 3/8,1/8,-1/8 (48)  $b'$  (0,1/2,0)  $x,y,x$   
 $(\bar{4}_y|3/4,3/4,1/2)'$   $(m_{xz}|1/4,0,3/4)'$   $(\bar{4}_y^{-1}|1/2,1/4,1/4)'$   $(m_{\bar{xz}}|0,1/2,0)'$

For (1/2,1/2,0)' + set

- (1)  $t'$  (1/2,1/2,0) (2)  $2'$  (0,0,1/2) 3/8,1/8,z (3)  $2'$  1/8,y,1/8 (4)  $2'$   $x,3/8,3/8$   
 $(1|1/2,1/2,0)'$   $(2_z|3/4,1/4,1/2)'$   $(2_y|1/4,0,1/4)'$   $(2_x|0,3/4,3/4)'$

(5) $3^+ ' (1/3, 1/3, 1/3)$ $x+1/6, x+1/3, x$ $(3_{xyz}^{-1}   1/2, 1/2, 0)'$	(6) $3^+ ' \bar{x}, x+3/4, \bar{x}$ $(3_{xyz}^{-1}   0, 3/4, 3/4)'$	(7) $3^+ ' x+3/4, \bar{x}-1/2, \bar{x}$ $(3_{xyz}^{-1}   3/4, 1/4, 1/2)'$	(8) $3^+ ' \bar{x}+1/4, \bar{x}+1/4, x$ $(3_{xyz}^{-1}   1/4, 0, 1/4)'$
(9) $3^- ' (1/3, 1/3, 1/3)$ $x+1/3, x+1/6, x$ $(3_{xyz}^{-1}   1/2, 1/2, 0)'$	(10) $3^- ' x+1/4, \bar{x}, \bar{x}$ $(3_{xyz}   1/4, 0, 1/4)'$	(11) $3^- ' \bar{x}+3/4, \bar{x}+3/4, x$ $(3_{xyz}   0, 3/4, 3/4)'$	(12) $3^- ' (1/3, -1/3, 1/3)$ $\bar{x}-1/6, x+7/12, \bar{x}$ $(3_{xyz}   3/4, 1/4, 1/2)'$
(13) $2' (1/2, 1/2, 0)$ $x, x+1/4, 0$ $(2_{xy}   1/4, 3/4, 0)'$	(14) $2' x, \bar{x}, 1/4$ $(2_{xy}   0, 0, 1/2)'$	(15) $4^- ' (0, 0, 3/4)$ $5/8, -1/8, z$ $(4_z^{-1}   3/4, 1/2, 3/4)'$	(16) $4^+ ' (0, 0, 1/4)$ $1/8, 3/8, z$ $(4_z   1/2, 1/4, 1/4)'$
(17) $4^- ' (1/4, 0, 0)$ $x, 3/8, -3/8$ $(4_x^{-1}   1/4, 3/4, 0)'$	(18) $2' (0, 1/4, 1/4)$ $1/4, y, y$ $(2_{yz}   1/2, 1/4, 1/4)'$	(19) $2' (0, -1/4, 1/4)$ $0, y+1/4, \bar{y}$ $(2_{yz}   0, 0, 1/2)'$	(20) $4^+ ' (3/4, 0, 0)$ $x, -1/8, 5/8$ $(4_x   3/4, 1/2, 3/4)'$
(21) $4^+ ' (0, 3/4, 0)$ $1/8, y, -1/8$ $(4_y   1/4, 3/4, 0)'$	(22) $2' (3/4, 0, 3/4)$ $x, 1/4, x$ $(2_{xz}   3/4, 1/2, 3/4)'$	(23) $4^- ' (0, 1/4, 0)$ $1/8, y, 3/8$ $(4_y^{-1}   1/2, 1/4, 1/4)'$	(24) $2' (-1/4, 0, 1/4)$ $\bar{x}+1/4, 0, x$ $(2_{xz}   0, 0, 1/2)'$
(25) $\bar{1} 1/4, 1/4, 0$ $(\bar{1}   1/2, 1/2, 0)'$	(26) $d' (1/4, 3/4, 0)$ $x, y, 1/4$ $(m_z   1/4, 3/4, 1/2)'$	(27) $d' (3/4, 0, 3/4)$ $x, 0, z$ $(m_y   3/4, 0, 3/4)'$	(28) $d' (0, 1/4, 1/4)$ $0, y, z$ $(m_x   0, 1/4, 1/4)'$
(29) $\bar{3}^+ ' x+1/2, x, x;$ $1/2, 0, 0$ $(\bar{3}_{xyz}   1/2, 1/2, 0)'$	(30) $\bar{3}^+ ' \bar{x}-1/2, x+1/4, \bar{x};$ $-1/4, 0, 1/4$ $(\bar{3}_{xyz}^{-1}   0, 1/4, 1/4)'$	(31) $\bar{3}^+ ' x-1/4, \bar{x}+1, \bar{x};$ $0, 3/4, -1/4$ $(\bar{3}_{xyz}^{-1}   1/4, 3/4, 1/2)'$	(32) $\bar{3}^+ ' \bar{x}+3/4, \bar{x}-3/4, x;$ $3/4, -3/4, 0$ $(\bar{3}_{xyz}^{-1}   3/4, 0, 3/4)'$
(33) $\bar{3}^- ' x, x+1/2, x;$ $0, 1/2, 0$ $(\bar{3}_{xyz}^{-1}   1/2, 1/2, 0)'$	(34) $\bar{3}^- ' x+3/4, \bar{x}-3/2, \bar{x};$ $0, -3/4, 3/4$ $(\bar{3}_{xyz}   3/4, 0, 3/4)'$	(35) $\bar{3}^- ' \bar{x}-1/4, \bar{x}+1/4, x;$ $-1/4, 1/4, 0$ $(\bar{3}_{xyz}   0, 1/4, 1/4)'$	(36) $\bar{3}^- ' \bar{x}+1, x+1/4, \bar{x};$ $3/4, 1/2, -1/4$ $(\bar{3}_{xyz}   1/4, 3/4, 1/2)'$
(37) $g' (1/4, -1/4, 0)$ $x+1/2, \bar{x}, z$ $(m_{xy}   3/4, 1/4, 0)'$	(38) $c' (0, 0, 1/2)$ $x, x, z$ $(m_{xy}   0, 0, 1/2)'$	(39) $\bar{4}^- ' -1/8, 3/8, z;$ $-1/8, 3/8, 1/8$ $(\bar{4}_z^{-1}   1/4, 1/2, 1/4)'$	(40) $\bar{4}^+ ' 5/8, 1/8, z;$ $5/8, 1/8, 3/8$ $(\bar{4}_z   1/2, 3/4, 3/4)'$
(41) $\bar{4}^- ' x, 1/8, 1/8;$ $3/8, 1/8, 1/8$ $(\bar{4}_x^{-1}   3/4, 1/4, 0)'$	(42) $a' (1/2, 0, 0)$ $x, y+3/4, \bar{y}$ $(m_{yz}   1/2, 3/4, 3/4)'$	(43) $g' (0, 1/4, 1/4)$ $x, y-1/4, y$ $(m_{yz}   0, 0, 1/2)'$	(44) $\bar{4}^+ ' x, 3/8, -1/8;$ $1/8, 3/8, -1/8$ $(\bar{4}_x   1/4, 1/2, 1/4)'$
(45) $\bar{4}^+ ' 3/8, y, 3/8;$ $3/8, 1/8, 3/8$ $(\bar{4}_y   3/4, 1/4, 0)'$	(46) $b' (0, 1/2, 0)$ $\bar{x}+1/4, y, x$ $(m_{xz}   1/4, 1/2, 1/4)'$	(47) $\bar{4}^- ' 5/8, y, 1/8;$ $5/8, 3/8, 1/8$ $(\bar{4}_y^{-1}   1/2, 3/4, 3/4)'$	(48) $g' (1/4, 0, 1/4)$ $x-1/4, y, x$ $(m_{xz}   0, 0, 1/2)'$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25); 1'.

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

### Coordinates

192	h	11'	(0,0,0) + (0,0,0)'	(0,1/2,1/2.) + (0,1/2,1/2.)'	(1/2,0,1/2) + (1/2,0,1/2)'	(1/2,1/2,0) + (1/2,1/2,0)'					
(1)	x,y,z	[0,0,0]	(2)	$\bar{x}+1/4, \bar{y}+3/4, z+1/2$	[0,0,0]	(3)	$\bar{x}+3/4, y+1/2, \bar{z}+1/4$	[0,0,0]	(4)	$x+1/2, \bar{y}+1/4, \bar{z}+3/4$	[0,0,0]
(5)	z,x,y	[0,0,0]	(6)	$z+1/2, \bar{x}+1/4, \bar{y}+3/4$	[0,0,0]	(7)	$\bar{z}+1/4, \bar{x}+3/4, y+1/2$	[0,0,0]	(8)	$\bar{z}+3/4, x+1/2, \bar{y}+1/4$	[0,0,0]
(9)	y,z,x	[0,0,0]	(10)	$\bar{y}+3/4, z+1/2, \bar{x}+1/4$	[0,0,0]	(11)	$y+1/2, \bar{z}+1/4, \bar{x}+3/4$	[0,0,0]	(12)	$\bar{y}+1/4, \bar{z}+3/4, x+1/2$	[0,0,0]
(13)	$y+3/4, x+1/4, \bar{z}$	[0,0,0]	(14)	$\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2$	[0,0,0]	(15)	$y+1/4, \bar{x}, z+3/4$	[0,0,0]	(16)	$\bar{y}, x+3/4, z+1/4$	[0,0,0]
(17)	$x+3/4, z+1/4, \bar{y}$	[0,0,0]	(18)	$\bar{x}, z+3/4, y+1/4$	[0,0,0]	(19)	$\bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2$	[0,0,0]	(20)	$x+1/4, \bar{z}, y+3/4$	[0,0,0]

(21) $z+3/4, y+1/4, \bar{x}$ [0,0,0]	(22) $z+1/4, \bar{y}, x+3/4$ [0,0,0]	(23) $\bar{z}, y+3/4, x+1/4$ [0,0,0]	(24) $\bar{z}+1/2, \bar{y}+1/2, \bar{x}+1/2$ [0,0,0]
(25) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]	(26) $x+3/4, y+1/4, \bar{z}+1/2$ [0,0,0]	(27) $x+1/4, \bar{y}+1/2, z+3/4$ [0,0,0]	(28) $\bar{x}+1/2, y+3/4, z+1/4$ [0,0,0]
(29) $\bar{z}, \bar{x}, \bar{y}$ [0,0,0]	(30) $\bar{z}+1/2, x+3/4, y+1/4$ [0,0,0]	(31) $z+3/4, x+1/4, \bar{y}+1/2$ [0,0,0]	(32) $z+1/4, \bar{x}+1/2, y+3/4$ [0,0,0]
(33) $\bar{y}, \bar{z}, \bar{x}$ [0,0,0]	(34) $y+1/4, \bar{z}+1/2, x+3/4$ [0,0,0]	(35) $\bar{y}+1/2, z+3/4, x+1/4$ [0,0,0]	(36) $y+3/4, z+1/4, \bar{x}+1/2$ [0,0,0]
(37) $\bar{y}+1/4, \bar{x}+3/4, z$ [0,0,0]	(38) $y+1/2, x+1/2, z+1/2$ [0,0,0]	(39) $\bar{y}+3/4, x, \bar{z}+1/4$ [0,0,0]	(40) $y, \bar{x}+1/4, \bar{z}+3/4$ [0,0,0]
(41) $\bar{x}+1/4, \bar{z}+3/4, y$ [0,0,0]	(42) $x, \bar{z}+1/4, \bar{y}+3/4$ [0,0,0]	(43) $x+1/2, z+1/2, y+1/2$ [0,0,0]	(44) $\bar{x}+3/4, z, \bar{y}+1/4$ [0,0,0]
(45) $\bar{z}+1/4, \bar{y}+3/4, x$ [0,0,0]	(46) $\bar{z}+3/4, y, \bar{x}+1/4$ [0,0,0]	(47) $z, \bar{y}+1/4, \bar{x}+3/4$ [0,0,0]	(48) $z+1/2, y+1/2, x+1/2$ [0,0,0]

96 g ..21'

$1/4, y, \bar{y}$ [0,0,0]	$0, \bar{y}+3/4, \bar{y}+1/2$ [0,0,0]	$1/2, y+1/2, y+1/4$ [0,0,0]	$3/4, \bar{y}+1/4, y+3/4$ [0,0,0]
$\bar{y}, 1/4, y$ [0,0,0]	$\bar{y}+1/2, 0, \bar{y}+3/4$ [0,0,0]	$y+1/4, 1/2, y+1/2$ [0,0,0]	$y+3/4, 3/4, \bar{y}+1/4$ [0,0,0]
$y, \bar{y}, 1/4$ [0,0,0]	$\bar{y}+3/4, \bar{y}+1/2, 0$ [0,0,0]	$y+1/2, y+1/4, 1/2$ [0,0,0]	$\bar{y}+1/4, y+3/4, 3/4$ [0,0,0]
$3/4, \bar{y}, y$ [0,0,0]	$0, y+1/4, y+1/2$ [0,0,0]	$1/2, \bar{y}+1/2, \bar{y}+3/4$ [0,0,0]	$1/4, y+3/4, \bar{y}+1/4$ [0,0,0]
$y, 3/4, \bar{y}$ [0,0,0]	$y+1/2, 0, y+1/4$ [0,0,0]	$\bar{y}+3/4, 1/2, \bar{y}+1/2$ [0,0,0]	$\bar{y}+1/4, 1/4, y+3/4$ [0,0,0]
$\bar{y}, y, 3/4$ [0,0,0]	$y+1/4, y+1/2, 0$ [0,0,0]	$\bar{y}+1/2, \bar{y}+3/4, 1/2$ [0,0,0]	$y+3/4, \bar{y}+1/4, 1/4$ [0,0,0]

96 f 2..1'	$x, 1/8, 1/8$ [0,0,0]	$\bar{x}+1/4, 5/8, 5/8$ [0,0,0]	$1/8, x, 1/8$ [0,0,0]	$5/8, \bar{x}+1/4, 5/8$ [0,0,0]
	$1/8, 1/8, x$ [0,0,0]	$5/8, 5/8, \bar{x}+1/4$ [0,0,0]	$7/8, x+1/4, 7/8$ [0,0,0]	$3/8, \bar{x}+1/2, 3/8$ [0,0,0]
	$x+3/4, 3/8, 7/8$ [0,0,0]	$\bar{x}, 7/8, 3/8$ [0,0,0]	$7/8, 3/8, \bar{x}$ [0,0,0]	$3/8, 7/8, x+3/4$ [0,0,0]
	$\bar{x}, 7/8, 7/8$ [0,0,0]	$x+3/4, 3/8, 3/8$ [0,0,0]	$7/8, \bar{x}, 7/8$ [0,0,0]	$3/8, x+3/4, 3/8$ [0,0,0]
	$7/8, 7/8, \bar{x}$ [0,0,0]	$3/8, 3/8, x+3/4$ [0,0,0]	$1/8, \bar{x}+3/4, 1/8$ [0,0,0]	$5/8, x+1/2, 5/8$ [0,0,0]
	$\bar{x}+1/4, 5/8, 1/8$ [0,0,0]	$x, 1/8, 5/8$ [0,0,0]	$1/8, 5/8, x$ [0,0,0]	$5/8, 1/8, \bar{x}+1/4$ [0,0,0]

64 e .3.1'	$x, x, x$ [0,0,0]	$\bar{x}+1/4, \bar{x}+3/4, x+1/2$ [0,0,0]
	$\bar{x}+3/4, x+1/2, \bar{x}+1/4$ [0,0,0]	$x+1/2, \bar{x}+1/4, \bar{x}+3/4$ [0,0,0]
	$x+3/4, x+1/4, \bar{x}$ [0,0,0]	$\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2$ [0,0,0]
	$x+1/4, \bar{x}, x+3/4$ [0,0,0]	$\bar{x}, x+3/4, x+1/4$ [0,0,0]
	$\bar{x}, \bar{x}, \bar{x}$ [0,0,0]	$x+3/4, x+1/4, \bar{x}+1/2$ [0,0,0]
	$x+1/4, \bar{x}+1/2, x+3/4$ [0,0,0]	$\bar{x}+1/2, x+3/4, x+1/4$ [0,0,0]
	$\bar{x}+1/4, \bar{x}+3/4, x$ [0,0,0]	$x+1/2, x+1/2, x+1/2$ [0,0,0]
	$\bar{x}+3/4, x, \bar{x}+1/4$ [0,0,0]	$x, \bar{x}+1/4, \bar{x}+3/4$ [0,0,0]

Continued

228.2.1634

Fd $\bar{3}c1'$ 

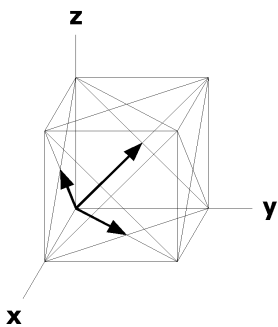
48	d	$\bar{4}..1'$	7/8,1/8,1/8 [0,0,0]	3/8,5/8,5/8 [0,0,0]	1/8,7/8,1/8 [0,0,0]	5/8,3/8,5/8 [0,0,0]
			1/8,1/8,7/8 [0,0,0]	5/8,5/8,3/8 [0,0,0]	7/8,1/8,7/8 [0,0,0]	3/8,5/8,3/8 [0,0,0]
			5/8,3/8,7/8 [0,0,0]	1/8,7/8,3/8 [0,0,0]	7/8,3/8,1/8 [0,0,0]	3/8,7/8,5/8 [0,0,0]
32	c	$\bar{3}.1'$	0,0,0 [0,0,0]	1/4,3/4,1/2 [0,0,0]	3/4,1/2,1/4 [0,0,0]	1/2,1/4,3/4 [0,0,0]
			3/4,1/4,0 [0,0,0]	1/2,1/2,1/2 [0,0,0]	1/4,0,3/4 [0,0,0]	0,3/4,1/4 [0,0,0]
32	b	.321'	1/4,1/4,1/4 [0,0,0]	0,1/2,3/4 [0,0,0]	1/2,3/4,0 [0,0,0]	3/4,0,1/2 [0,0,0]
			3/4,3/4,3/4 [0,0,0]	0,1/2,1/4 [0,0,0]	1/2,1/4,0 [0,0,0]	1/4,0,1/2 [0,0,0]
16	a	23.1'	1/8,1/8,1/8 [0,0,0]	7/8,3/8,7/8 [0,0,0]	7/8,7/8,7/8 [0,0,0]	1/8,5/8,1/8 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/4$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/4$   
 Origin at 1/8,3/8,z

Along [1,1,1] p6mm1'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

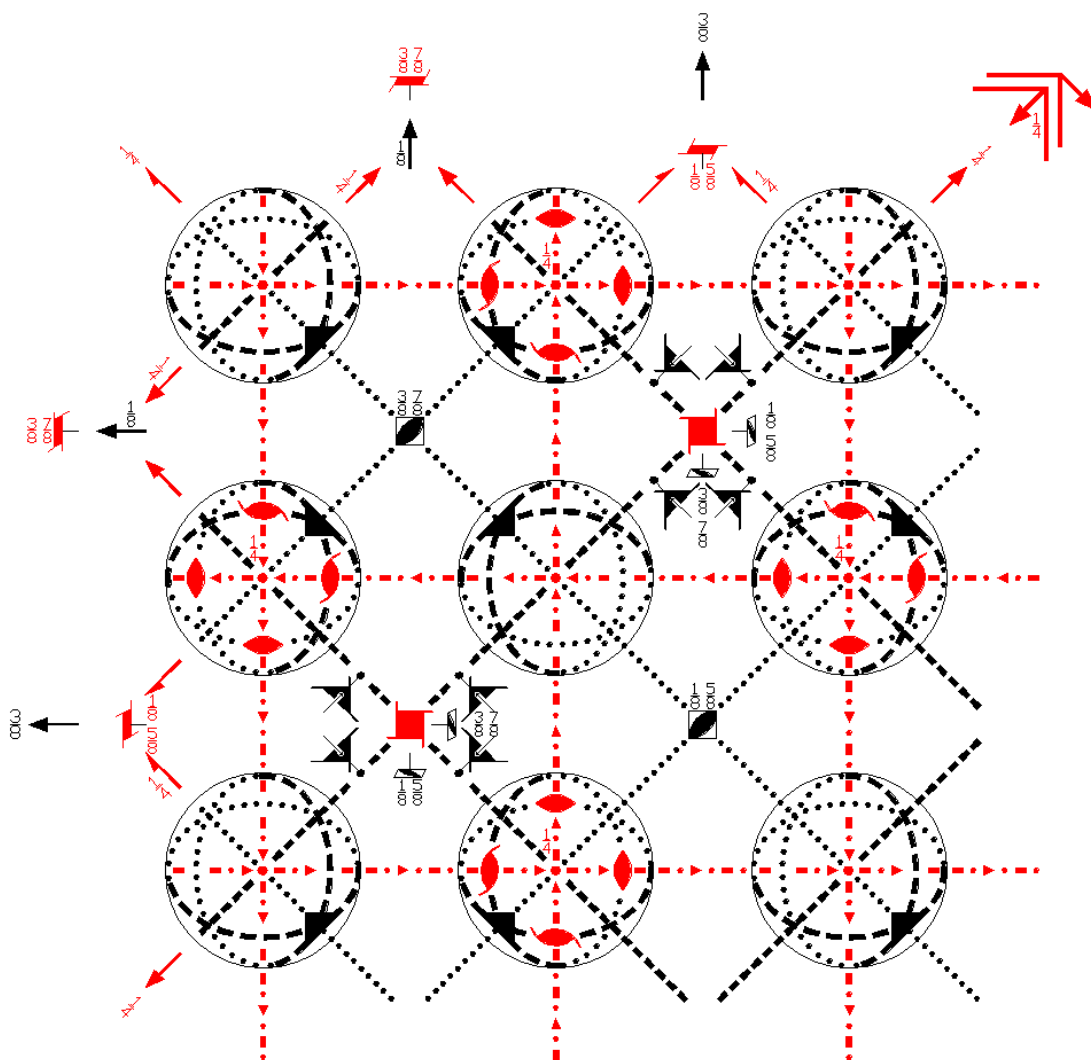
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/4$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



Fd'3'c  
228.3.1635

m'3'm  
F4<sub>1</sub>'d'3'2'/c

Cubic



**Origin** at center ( $\bar{3}'$ ), at  $3/8, 3/8, 3/8$  from 23

**Asymmetric unit**  $-1/8 \leq x \leq 3/8$ ;  $-1/8 \leq y \leq 0$ ;  $-1/4 \leq z \leq 0$ ;  $y \leq \min(1/4-x, x)$ ;  $-y-1/4 \leq z \leq y$

**Vertices**  $-1/8, -1/8, -1/8$   $3/8, -1/8, -1/8$   $1/4, 0, 0$   $0, 0, 0$   $1/4, 0, -1/4$   $0, 0, -1/4$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |   |
|---|--|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) $1/8, 3/8, z$<br>(2 <sub>z</sub>  1/4, 3/4, 1/2)   | (3) 2 (0,1/2,0) $3/8, y, 1/8$<br>(2 <sub>y</sub>  3/4, 1/2, 1/4)   | (4) 2 (1/2,0,0) $x, 1/8, 3/8$<br>(2 <sub>x</sub>  1/2, 1/4, 3/4)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)               | (6) 3 <sup>+</sup> (1/3,-1/3,1/3)<br>$x+1/6, x+5/12, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2, 1/4, 3/4) | (7) 3 <sup>+</sup> (-1/3,1/3,1/3)<br>$x+7/12, x-1/6, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/4, 3/4, 1/2) | (8) 3 <sup>+</sup> (1/3,1/3,-1/3)<br>$x+5/12, x+7/12, x$<br>(3 <sub>xyz</sub> <sup>-1</sup>  3/4, 1/2, 1/4) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0) | (10) 3 <sup>-</sup> $x+1/4, \bar{x}+1/2, \bar{x}$<br>(3 <sub>xyz</sub>  3/4, 1/2, 1/4)                           | (11) 3 <sup>-</sup> $\bar{x}+3/4, \bar{x}+1/4, x$<br>(3 <sub>xy</sub>  1/2, 1/4, 3/4)                            | (12) 3 <sup>-</sup> $\bar{x}-1/2, x+3/4, \bar{x}$<br>(3 <sub>xy</sub>  1/4, 3/4, 1/2)                       |

(13) 2' (1/2,1/2,0) x,x-1/4,0 (2 <sub>xy</sub>  3/4,1/4,0)'	(14) 2' x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(15) 4' (0,0,3/4) 1/8,-1/8,z (4 <sub>z</sub> <sup>-1</sup>  1/4,0,3/4)'	(16) 4 <sup>+</sup> (0,0,1/4) -3/8,3/8,z (4 <sub>z</sub>  0,3/4,1/4)'
(17) 4' (3/4,0,0) x,1/8,-1/8 (4 <sub>x</sub> <sup>-1</sup>  3/4,1/4,0)'	(18) 2' (0,1/2,1/2) 0,y+1/4,y (2 <sub>yz</sub>  0,3/4,1/4)'	(19) 2' 1/4,y+1/2, $\bar{y}$ (2 <sub>yz</sub>  1/2,1/2,1/2)'	(20) 4 <sup>+</sup> (1/4,0,0) x,-3/8,3/8 (4 <sub>x</sub>  1/4,0,3/4)'
(21) 4 <sup>+</sup> (0,1/4,0) 3/8,y,-3/8 (4 <sub>y</sub>  3/4,1/4,0)'	(22) 2' (1/2,0,1/2) x-1/4,0,x (2 <sub>xz</sub>  1/4,0,3/4)'	(23) 4' (0,3/4,0) -1/8,y,1/8 (4 <sub>y</sub> <sup>-1</sup>  0,3/4,1/4)'	(24) 2' $\bar{x}$ +1/2,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)'
(25) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)'	(26) d' (3/4,1/4,0) x,y,1/4 (m <sub>z</sub>  3/4,1/4,1/2)'	(27) d' (1/4,0,3/4) x,1/4,z (m <sub>y</sub>  1/4,1/2,3/4)'	(28) d' (0,3/4,1/4) 1/4,y,z (m <sub>x</sub>  1/2,3/4,1/4)'
(29) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)'	(30) $\bar{3}^+$ $\bar{x}$ -1,x+5/4, $\bar{x}$ ; -1/4,1/2,3/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,3/4,1/4)'	(31) $\bar{3}^+$ x+1/4, $\bar{x}$ +1, $\bar{x}$ ; 1/2,3/4,-1/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  3/4,1/4,1/2)'	(32) $\bar{3}^+$ $\bar{x}$ +5/4, $\bar{x}$ +1/4,x; 3/4,-1/4,1/2 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/4,1/2,3/4)'
(33) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'	(34) $\bar{3}^-$ x+3/4, $\bar{x}$ -1, $\bar{x}$ ; 0,-1/4,3/4 ( $\bar{3}_{xyz}$  1/4,1/2,3/4)'	(35) $\bar{3}^-$ $\bar{x}$ -1/4, $\bar{x}$ +3/4,x; -14,3/4,0 ( $\bar{3}_{xyz}$  1/2,3/4,1/4)'	(36) $\bar{3}^-$ $\bar{x}$ +1,x-1/4, $\bar{x}$ ; 3/4,0,-1/4 ( $\bar{3}_{xyz}$  3/4,1/4,1/2)'
(37) g (-1/4,1/4,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/4,3/4,0)	(38) n (1/2,1/2,1/2) x,x,z (m <sub>xy</sub>  1/2,1/2,1/2)	(39) $\bar{4}^-$ 3/8,3/8,z; 3/8,3/8,1/8 (4 <sub>z</sub> <sup>-1</sup>  3/4,0,1/4)	(40) $\bar{4}^+$ 1/8,1/8,z; 1/8,1/8,3/8 (4 <sub>z</sub>  0,1/4,3/4)
(41) $\bar{4}^-$ x,3/8,3/8; 1/8,3/8,3/8 (4 <sub>x</sub> <sup>-1</sup>  1/4,3/4,0)	(42) g (0,-1/4,1/4) x,y+1/2, $\bar{y}$ (m <sub>yz</sub>  0,1/4,3/4)	(43) n (1/2,1/2,1/2) x,y,y (m <sub>yz</sub>  1/2,1/2,1/2)	(44) $\bar{4}^+$ x,1/8,1/8; 3/8,1/8,1/8 (4 <sub>x</sub>  3/4,0,1/4)
(45) $\bar{4}^+$ 1/8,y,1/8; 1/8,3/8,1/8 (4 <sub>y</sub>  1/4,3/4,0)	(46) g (1/4,0,-1/4) $\bar{x}$ +1/2,y,x (m <sub>xz</sub>  3/4,0,1/4)	(47) $\bar{4}^-$ 3/8,y,3/8; 3/8,1/8,3/8 (4 <sub>y</sub> <sup>-1</sup>  0,1/4,3/4)	(48) n (1/2,1/2,1/2) x,y,x (m <sub>xz</sub>  1/2,1/2,1/2)

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2) (1 0,1/2,1/2)	(2) 2 1/8,1/8,z (2 <sub>z</sub>  1/4,1/4,0)	(3) 2 3/8,y,3/8 (2 <sub>y</sub>  3/4,0,3/4)	(4) 2 (1/2,0,0) x,3/8,1/8 (2 <sub>x</sub>  1/2,3/4,1/4)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x-1/3,x-1/6,x (3 <sub>xyz</sub>  0,1/2,1/2)	(6) 3 <sup>+</sup> $\bar{x}$ +1/2,x+1/4, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  1/2,3/4,1/4)	(7) 3 <sup>+</sup> x+1/4, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  1/4,1/4,0)	(8) 3 <sup>+</sup> $\bar{x}$ +3/4, $\bar{x}$ +3/4,x (3 <sub>xyz</sub> <sup>-1</sup>  3/4,0,3/4)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x-1/6,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(10) 3 <sup>-</sup> x+3/4, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub>  3/4,0,3/4)	(11) 3 <sup>-</sup> (1/3,1/3,-1/3) x+7/12, $\bar{x}$ +5/12,x (3 <sub>xyz</sub>  1/2,3/4,1/4)	(12) 3 <sup>-</sup> $\bar{x}$ ,x+1/4, $\bar{x}$ (3 <sub>xyz</sub>  1/4,1/4,0)
(13) 2' (3/4,3/4,0) x,x,1/4 (2 <sub>xy</sub>  3/4,3/4,1/2)'	(14) 2' (1/4,-1/4,0) x, $\bar{x}$ +1/4,0 (2 <sub>xy</sub>  1/2,0,0)'	(15) 4' (0,0,1/4) 3/8,1/8,z (4 <sub>z</sub> <sup>-1</sup>  1/4,1/2,1/4)'	(16) 4 <sup>+</sup> (0,0,3/4) -1/8,1/8,z (4 <sub>z</sub>  0,1/4,3/4)'
(17) 4' (3/4,0,0) 5/8,-1/8 (4 <sub>x</sub> <sup>-1</sup>  3/4,3/4,1/2)'	(18) 2' (0,1/2,1/2) 0,y-1/4,y (2 <sub>yz</sub>  0,1/4,3/4)'	(19) 2' 1/4,y, $\bar{y}$ (2 <sub>yz</sub> <sup>-1</sup>  1/2,0,0)'	(20) 4 <sup>+</sup> (1/4,0,0) x,1/8,3/8 (4 <sub>x</sub>  1/4,1/2,1/4)'
(21) 4 <sup>+</sup> (0,3/4,0) 5/8,y,-1/8 (4 <sub>y</sub>  3/4,3/4,1/2)'	(22) 2' (1/4,0,1/4) x,1/4,x (2 <sub>xz</sub>  1/4,1/2,1/4)'	(23) 4' (0,1/4,0) -3/8,y,3/8 (4 <sub>y</sub> <sup>-1</sup>  0,1/4,3/4)'	(24) 2' (1/4,0,-1/4) $\bar{x}$ +1/4,0,x (2 <sub>xz</sub>  1/2,0,0)'
(25) $\bar{1}$ 0,1/4,1/4 ( $\bar{1}$  0,1/2,1/2)'	(26) d' (3/4,3/4,0) x,y,0 (m <sub>z</sub>  3/4,3/4,0)'	(27) d' (1/4,0,1/4) x,0,z (m <sub>y</sub>  1/4,0,1/4)'	(28) d' (0,1/4,3/4) 1/4,y,z (m <sub>x</sub>  1/2,1/4,3/4)'
(29) $\bar{3}^+$ x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$  0,1/2,1/2)'	(30) $\bar{3}^+$ $\bar{x}$ -1,x+3/4, $\bar{x}$ ; -1/4,0,3/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,1/4,3/4)'	(31) $\bar{3}^+$ x-3/4, $\bar{x}$ +3/2, $\bar{x}$ ; 0,3/4,-3/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  3/4,3/4,0)'	(32) $\bar{3}^+$ $\bar{x}$ +1/4, $\bar{x}$ -1/4,x; 1/4,-1/4,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/4,0,1/4)'

(33) $\bar{3}^-$ ' x-1/2,x-1/2,x; 0,0,1/2 ( $\bar{3}_{xyz}^{-1}$   0,1/2,1/2)'	(34) $\bar{3}^-$ ' x+1/4, $\bar{x}$ -1/2, $\bar{x}$ ; 0,-1/4,1/4 ( $\bar{3}_{\bar{xyz}}$   1/4,0,1/4)'	(35) $\bar{3}^-$ ' $\bar{x}$ +1/4, $\bar{x}$ +5/4,x; -1/4,3/4,1/2 ( $\bar{3}_{\bar{yz}}$   1/2,1/4,3/4)'	(36) $\bar{3}^-$ ' $\bar{x}$ +3/2,x-3/4, $\bar{x}$ ; 3/4,0,-3/4 ( $\bar{3}_{\bar{yz}}$   3/4,3/4,0)'
(37) c (0,0,1/2) x+1/4, $\bar{x}$ ,z ( $m_{xy}$   1/4,1/4,1/2)	(38) g (1/4,1/4,0) x+1/4,x,z ( $m_{\bar{xy}}$   1/2,0,0)	(39) $\bar{4}^-$ 1/8,5/8,z; 1/8,5/8,3/8 ( $\bar{4}_z^{-1}$   3/4,1/2,3/4)	(40) $\bar{4}^+$ 3/8,3/8,z; 3/8,3/8,1/8 ( $\bar{4}_z$   0,3/4,1/4)
(41) $\bar{4}^-$ x,-1/8,3/8; 1/8,-1/8,3/8 ( $\bar{4}_x^{-1}$   1/4,1/4,1/2)	(42) g (0,1/4,-1/4) x,y+1/2, $\bar{y}$ ( $m_{yz}$   0,3/4,1/4)	(43) a (1/2,0,0) x,y,y ( $m_{\bar{yz}}$   1/2,0,0)	(44) $\bar{4}^+$ x,5/8,1/8; 3/8,5/8,1/8 ( $\bar{4}_x$   3/4,0,3/4)
(45) $\bar{4}^+$ -1/8,y,3/8; -1/8,1/8,3/8 ( $\bar{4}_y$   1/4,1/4,1/2)	(46) b (0,1/2,0) $\bar{x}$ +3/4,y,x ( $m_{xz}$   3/4,1/2,3/4)	(47) $\bar{4}^-$ 1/8,y,1/8; 1/8,3/8,1/8 ( $\bar{4}_y^{-1}$   0,3/4,1/4)	(48) g (1/4,0,1/4) x+1/4,y,x ( $m_{\bar{xz}}$   1/2,0,0)

For (1/2,0,1/2) + set

(1) t (1/2,0,1/2) (1   1/2,0,1/2)	(2) 2 3/8,3/8,z (2 <sub>z</sub>   3/4,3/4,0)	(3) 2 (0,1/2,0) 1/8,y,3/8 (2 <sub>y</sub>   1/4,1/2,3/4)	(4) 2 x,1/8,1/8 (2 <sub>x</sub>   0,1/4,1/4)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x+1/6,x-1/6,x (3 <sub>xyz</sub>   1/2,0,1/2)	(6) 3 <sup>+</sup> $\bar{x}$ ,x+1/4, $\bar{x}$ (3 <sub>x<math>\bar{yz}</math></sub> <sup>-1</sup>   0,1/4,1/4)	(7) 3 <sup>+</sup> x+3/4, $\bar{x}$ , $\bar{x}$ (3 <sub>x<math>\bar{yz}</math></sub> <sup>-1</sup>   3/4,3/4,0)	(8) 3 <sup>+</sup> $\bar{x}$ +1/4, $\bar{x}$ +3/4,x (3 <sub>x<math>\bar{yz}</math></sub> <sup>-1</sup>   1/4,1/2,3/4)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x-1/6,x-1/3,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,0,1/2)	(10) 3 <sup>-</sup> (-1/3,1/3,1/3) x+5/12, $\bar{x}$ +1/6, $\bar{x}$ (3 <sub>x<math>\bar{yz}</math></sub>   1/4,1/2,3/4)	(11) 3 <sup>-</sup> $\bar{x}$ +1/4, $\bar{x}$ +1/4,x (3 <sub>x<math>\bar{yz}</math></sub>   0,1/4,1/4)	(12) 3 <sup>-</sup> $\bar{x}$ ,x+3/4, $\bar{x}$ (3 <sub>x<math>\bar{yz}</math></sub>   3/4,3/4,0)
(13) 2' (1/4,1/4,0) x,x,1/4 (2 <sub>xy</sub>   1/4,1/4,1/2)'	(14) 2' (-1/4,1/4,0) x, $\bar{x}$ +1/4,0 (2 <sub>xy</sub>   0,1/2,0)'	(15) 4 <sup>-</sup> ' (0,0,1/4) 3/8,-3/8,z (4 <sub>z</sub> <sup>-1</sup>   3/4,0,1/4)'	(16) 4 <sup>+</sup> ' (0,0,3/4) -1/8,5/8,z (4 <sub>z</sub>   1/2,3/4,3/4)'
(17) 4 <sup>-</sup> ' (1/4,0,0) x,3/8,1/8 (4 <sub>x</sub> <sup>-1</sup>   1/4,1/4,1/2)'	(18) 2' (0,3/4,3/4) 1/4,y,y (2 <sub>yz</sub>   1/2,3/4,3/4)'	(19) 2' (0,1/4,-1/4) 0,y+1/4, $\bar{y}$ (2 <sub>yz</sub>   0,1/2,0)'	(20) 4 <sup>+</sup> ' (3/4,0,0) x,-1/8,1/8 (4 <sub>x</sub>   3/4,0,1/4)'
(21) 4 <sup>+</sup> ' (0,1/4,0) 3/8,y,1/8 (4 <sub>y</sub>   1/4,1/4,1/2)'	(22) 2' (1/2,0,1/2) x+1/4,0,x (2 <sub>xz</sub>   3/4,0,1/4)'	(23) 4 <sup>-</sup> ' (0,3/4,0) -1/8,y,5/8 (4 <sub>y</sub> <sup>-1</sup>   1/2,3/4,3/4)'	(24) 2' $\bar{x}$ ,1/4,x (2 <sub>xz</sub>   0,1/2,0)'
(25) $\bar{1}^-$ 1/4,0,1/4 ( $\bar{1}$   1/2,0,1/2)'	(26) d' (1/4,1/4,0) x,y,0 ( $m_z$   1/4,1/4,0)'	(27) d' (3/4,0,1/4) x,1/4,z ( $m_y$   3/4,1/2,1/4)'	(28) d' (0,3/4,3/4) 0,y,z ( $m_x$   0,3/4,3/4)'
(29) $\bar{3}^+$ ' x-1/2,x-1/2,x; 0,0,1/2 ( $\bar{3}_{xyz}$   1/2,0,1/2)'	(30) $\bar{3}^+$ ' $\bar{x}$ -3/2,x+3/4, $\bar{x}$ ; -3/4,0,3/4 ( $\bar{3}_{x\bar{yz}}$   0,3/4,3/4)'	(31) $\bar{3}^+$ ' x-1/4, $\bar{x}$ +1/2, $\bar{x}$ ; 0,1/4,-1/4 ( $\bar{3}_{x\bar{yz}}$   1/4,1/4,0)'	(32) $\bar{3}^+$ ' $\bar{x}$ +3/4, $\bar{x}$ -1/4,x; 3/4,-1/4,0 ( $\bar{3}_{x\bar{yz}}$   3/4,1/2,1/4)'
(33) $\bar{3}^-$ ' x+1/2,x,x; 1/2,0,0 ( $\bar{3}_{xyz}$   1/2,0,1/2)'	(34) $\bar{3}^-$ ' x+5/4, $\bar{x}$ -1, $\bar{x}$ ; 1/2,-1/4,3/4 ( $\bar{3}_{x\bar{yz}}$   3/4,1/2,1/4)'	(35) $\bar{3}^-$ ' $\bar{x}$ -3/4, $\bar{x}$ +3/4,x; -3/4,3/4,0 ( $\bar{3}_{x\bar{yz}}$   0,3/4,3/4)'	(36) $\bar{3}^-$ ' $\bar{x}$ +1/2,x-1/4, $\bar{x}$ ; 1/4,0,-1/4 ( $\bar{3}_{x\bar{yz}}$   1/4,1/4,0)'
(37) c (0,0,1/2) x+3/4, $\bar{x}$ ,z ( $m_{xy}$   3/4,3/4,1/2)	(38) g (1/4,1/4,0) x-1/4,x,z ( $m_{\bar{xy}}$   0,1/2,0)	(39) $\bar{4}^-$ 1/8,1/8,z; 1/8,1/8,3/8 ( $\bar{4}_z^{-1}$   1/4,0,3/4)	(40) $\bar{4}^+$ 3/8,-1/8,z; 3/8,-1/8,1/8 ( $\bar{4}_z$   1/2,1/4,1/4)
(41) $\bar{4}^-$ x,1/8,5/8; 3/8,1/8,5/8 ( $\bar{4}_x^{-1}$   3/4,3/4,1/2)	(42) a (1/2,0,0) x,y+1/4, $\bar{y}$ ( $m_{yz}$   1/2,1/4,1/4)	(43) g (0,1/4,1/4) x,y+1/4,y ( $m_{\bar{yz}}$   0,1/2,0)	(44) $\bar{4}^+$ x,3/8,3/8; 1/8,3/8,3/8 ( $\bar{4}_x$   1/4,0,3/4)
(45) $\bar{4}^+$ 1/8,y,5/8; 1/8,3/8,5/8 ( $\bar{4}_y$   3/4,3/4,1/2)	(46) g (-1/4,0,1/4) $\bar{x}$ +1/2,y,x ( $m_{xz}$   1/4,0,3/4)	(47) $\bar{4}^-$ 3/8,y,-1/8; 3/8,1/8,-1/8 ( $\bar{4}_y^{-1}$   1/2,1/4,1/4)	(48) b (0,1/2,0) x,y,x ( $m_{\bar{xz}}$   0,1/2,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (1   1/2,1/2,0)	(2) 2 (0,0,1/2) 3/8,1/8,z (2 <sub>z</sub>   3/4,1/4,1/2)	(3) 2 1/8,y,1/8 (2 <sub>y</sub>   1/4,0,1/4)	(4) 2 x,3/8,3/8 (2 <sub>x</sub>   0,3/4,3/4)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) 3 <sup>+</sup> $\bar{x}$ ,x+3/4, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   0,3/4,3/4)	(7) 3 <sup>+</sup> x+3/4, $\bar{x}$ -1/2, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   3/4,1/4,1/2)	(8) 3 <sup>+</sup> $\bar{x}$ +1/4, $\bar{x}$ +1/4,x (3 <sub>xyz</sub> <sup>-1</sup>   1/4,0,1/4)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) 3 <sup>-</sup> x+1/4, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub>   1/4,0,1/4)	(11) 3 <sup>-</sup> $\bar{x}$ +3/4, $\bar{x}$ +3/4, x (3 <sub>xyz</sub>   0,3/4,3/4)	(12) 3 <sup>-</sup> (1/3,-1/3,1/3) $\bar{x}$ -1/6, x+7/12, $\bar{x}$ (3 <sub>xyz</sub>   3/4,1/4,1/2)
(13) 2' (1/2,1/2,0) x,x+1/4,0 (2 <sub>xy</sub>   1/4,3/4,0)'	(14) 2' x, $\bar{x}$ ,1/4 (2 <sub>xy</sub>   0,0,1/2)'	(15) 4' (0,0,3/4) 5/8,-1/8,z (4 <sub>z</sub> <sup>-1</sup>   3/4,1/2,3/4)'	(16) 4' (0,0,1/4) 1/8,3/8,z (4 <sub>z</sub>   1/2,1/4,1/4)'
(17) 4' (1/4,0,0) x,3/8,-3/8 (4 <sub>x</sub> <sup>-1</sup>   1/4,3/4,0)'	(18) 2' (0,1/4,1/4) 1/4,y,y (2 <sub>yz</sub>   1/2,1/4,1/4)'	(19) 2' (0,-1/4,1/4) 0,y+1/4, $\bar{y}$ (2 <sub>yz</sub>   0,0,1/2)'	(20) 4' (3/4,0,0) x,-1/8,5/8 (4 <sub>x</sub>   3/4,1/2,3/4)'
(21) 4' (0,3/4,0) 1/8,y,-1/8 (4 <sub>y</sub>   1/4,3/4,0)'	(22) 2' (3/4,0,3/4) x,1/4,x (2 <sub>xz</sub>   3/4,1/2,3/4)'	(23) 4' (0,1/4,0) 1/8,y,3/8 (4 <sub>y</sub> <sup>-1</sup>   1/2,1/4,1/4)'	(24) 2' (-1/4,0,1/4) $\bar{x}$ +1/4,0,x (2 <sub>xz</sub>   0,0,1/2)'
(25) 1' 1/4,1/4,0 (1   1/2,1/2,0)'	(26) d' (1/4,3/4,0) x,y,1/4 (m <sub>z</sub>   1/4,3/4,1/2)'	(27) d' (3/4,0,3/4) x,0,z (m <sub>y</sub>   3/4,0,3/4)'	(28) d' (0,1/4,1/4) 0,y,z (m <sub>x</sub>   0,1/4,1/4)'
(29) 3 <sup>+</sup> x+1/2,x,x; 1/2,0,0 (3 <sub>xyz</sub>   1/2,1/2,0)'	(30) 3 <sup>+</sup> $\bar{x}$ -1/2,x+1/4, $\bar{x}$ ; -1/4,0,1/4 (3 <sub>xyz</sub> <sup>-1</sup>   0,1/4,1/4)'	(31) 3 <sup>+</sup> x-1/4, $\bar{x}$ +1, $\bar{x}$ ; 0,3/4,-1/4 (3 <sub>xyz</sub> <sup>-1</sup>   1/4,3/4,1/2)'	(32) 3 <sup>+</sup> $\bar{x}$ +3/4, $\bar{x}$ -3/4,x; 3/4,-3/4,0 (3 <sub>xyz</sub> <sup>-1</sup>   3/4,0,3/4)'
(33) 3 <sup>-</sup> x,x+1/2,x; 0,1/2,0 (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)'	(34) 3 <sup>-</sup> x+3/4, $\bar{x}$ -3/2, $\bar{x}$ ; 0,-3/4,3/4 (3 <sub>xyz</sub>   3/4,0,3/4)'	(35) 3 <sup>-</sup> $\bar{x}$ -1/4, $\bar{x}$ +1/4, x; -1/4,1/4,0 (3 <sub>xyz</sub>   0,1/4,1/4)'	(36) 3 <sup>-</sup> $\bar{x}$ +1, x+1/4, $\bar{x}$ ; 3/4,1/2,-1/4 (3 <sub>xyz</sub> <sup>-1</sup>   1/4,3/4,1/2)'
(37) g (1/4,-1/4,0) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   3/4,1/4,0)	(38) c (0,0,1/2) x,x,z (m <sub>xy</sub>   0,0,1/2)	(39) 4 <sup>-</sup> -1/8,3/8,z; -1/8,3/8,1/8 (4 <sub>z</sub> <sup>-1</sup>   1/4,1/2,1/4)	(40) 4 <sup>+</sup> 5/8,1/8,z; 5/8,1/8,3/8 (4 <sub>z</sub>   1/2,3/4,3/4)
(41) 4 <sup>-</sup> x,1/8,1/8; 3/8,1/8,1/8 (4 <sub>x</sub> <sup>-1</sup>   3/4,1/4,0)	(42) a (1/2,0,0) x,y+3/4, $\bar{y}$ (m <sub>yz</sub>   1/2,3/4,3/4)	(43) g (0,1/4,1/4) x,y-1/4,y (m <sub>yz</sub>   0,0,1/2)	(44) 4 <sup>+</sup> x,3/8,-1/8; 1/8,3/8,-1/8 (4 <sub>x</sub>   1/4,1/2,1/4)
(45) 4 <sup>+</sup> 3/8,y,3/8; 3/8,1/8,3/8 (4 <sub>y</sub>   3/4,1/4,0)	(46) b (0,1/2,0) $\bar{x}$ +1/4,y,x (m <sub>xz</sub>   1/4,1/2,1/4)	(47) 4 <sup>-</sup> 5/8,y,1/8; 5/8,3/8,1/8 (4 <sub>y</sub> <sup>-1</sup>   1/2,3/4,3/4)	(48) g (1/4,0,1/4) x-1/4,y,x (m <sub>xz</sub>   0,0,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

192	h	1	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +		
(1)	x,y,z	[u,v,w]	(2) $\bar{x}$ +1/4, $\bar{y}$ +3/4,z+1/2	[ $\bar{u}$ , $\bar{v}$ ,w]	(3) $\bar{x}$ +3/4,y+1/2, $\bar{z}$ +1/4	[ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x+1/2, $\bar{y}$ +1/4, $\bar{z}$ +3/4	[u, $\bar{v}$ , $\bar{w}$ ]
(5)	z,x,y	[w,u,v]	(6) z+1/2, $\bar{x}$ +1/4, $\bar{y}$ +3/4	[w, $\bar{u}$ , $\bar{v}$ ]	(7) $\bar{z}$ +1/4, $\bar{x}$ +3/4,y+1/2	[ $\bar{w}$ , $\bar{u}$ ,v]	(8) $\bar{z}$ +3/4,x+1/2, $\bar{y}$ +1/4	[ $\bar{w}$ ,u,v]



- (9)  $y, z, x [v, w, u]$  (10)  $\bar{y}+3/4, z+1/2, \bar{x}+1/4 [\bar{v}, w, \bar{u}]$  (11)  $y+1/2, \bar{z}+1/4, \bar{x}+3/4 [v, \bar{w}, \bar{u}]$  (12)  $\bar{y}+1/4, \bar{z}+3/4, x+1/2 [\bar{v}, \bar{w}, u]$   
 (13)  $y+3/4, x+1/4, \bar{z} [\bar{v}, \bar{u}, w]$  (14)  $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2 [v, u, w]$  (15)  $y+1/4, \bar{x}, z+3/4 [v, u, \bar{w}]$  (16)  $\bar{y}, x+3/4, z+1/4 [v, \bar{u}, \bar{w}]$   
 (17)  $x+3/4, z+1/4, \bar{y} [\bar{u}, \bar{w}, v]$  (18)  $\bar{x}, z+3/4, y+1/4 [u, \bar{w}, \bar{v}]$  (19)  $\bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2 [u, w, v]$  (20)  $x+1/4, \bar{z}, y+3/4 [\bar{u}, w, \bar{v}]$   
 (21)  $z+3/4, y+1/4, \bar{x} [\bar{w}, \bar{v}, u]$  (22)  $z+1/4, \bar{y}, x+3/4 [\bar{w}, v, \bar{u}]$  (23)  $\bar{z}, y+3/4, x+1/4 [w, \bar{v}, \bar{u}]$  (24)  $\bar{z}+1/2, \bar{y}+1/2, \bar{x}+1/2 [w, v, u]$   
 (25)  $\bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$  (26)  $x+3/4, y+1/4, \bar{z}+1/2 [u, v, \bar{w}]$  (27)  $x+1/4, \bar{y}+1/2, z+3/4 [u, \bar{v}, w]$  (28)  $\bar{x}+1/2, y+3/4, z+1/4 [\bar{u}, v, w]$   
 (29)  $\bar{z}, \bar{x}, \bar{y} [\bar{w}, \bar{u}, \bar{v}]$  (30)  $\bar{z}+1/2, x+3/4, y+1/4 [\bar{w}, u, v]$  (31)  $z+3/4, x+1/4, \bar{y}+1/2 [w, u, \bar{v}]$  (32)  $z+1/4, \bar{x}+1/2, y+3/4 [w, \bar{u}, v]$   
 (33)  $\bar{y}, \bar{z}, \bar{x} [\bar{v}, \bar{w}, \bar{u}]$  (34)  $y+1/4, \bar{z}+1/2, x+3/4 [v, \bar{w}, u]$  (35)  $\bar{y}+1/2, z+3/4, x+1/4 [\bar{v}, w, u]$  (36)  $y+3/4, z+1/4, \bar{x}+1/2 [v, w, \bar{u}]$   
 (37)  $\bar{y}+1/4, \bar{x}+3/4, z [v, u, \bar{w}]$  (38)  $y+1/2, x+1/2, z+1/2 [\bar{v}, \bar{u}, \bar{w}]$  (39)  $\bar{y}+3/4, x, \bar{z}+1/4 [v, \bar{u}, w]$  (40)  $y, \bar{x}+1/4, \bar{z}+3/4 [\bar{v}, u, w]$   
 (41)  $\bar{x}+1/4, \bar{z}+3/4, y [u, w, \bar{v}]$  (42)  $x, \bar{z}+1/4, \bar{y}+3/4 [\bar{u}, w, v]$  (43)  $x+1/2, z+1/2, y+1/2 [\bar{u}, \bar{w}, \bar{v}]$  (44)  $\bar{x}+3/4, z, \bar{y}+1/4 [u, \bar{w}, v]$   
 (45)  $\bar{z}+1/4, \bar{y}+3/4, x [w, v, \bar{u}]$  (46)  $\bar{z}+3/4, y, \bar{x}+1/4 [w, \bar{v}, u]$  (47)  $z, \bar{y}+1/4, \bar{x}+3/4 [\bar{w}, v, u]$  (48)  $z+1/2, y+1/2, x+1/2 [\bar{w}, \bar{v}, \bar{u}]$

96 g ..2'

- $1/4, y, \bar{y} [u, v, v]$   $0, \bar{y}+3/4, \bar{y}+1/2 [\bar{u}, \bar{v}, v]$   $1/2, y+1/2, y+1/4 [\bar{u}, v, \bar{v}]$   $3/4, \bar{y}+1/4, y+3/4 [u, \bar{v}, \bar{v}]$   
 $\bar{y}, 1/4, y [v, u, v]$   $\bar{y}+1/2, 0, \bar{y}+3/4 [v, \bar{u}, \bar{v}]$   $y+1/4, 1/2, y+1/2 [\bar{v}, \bar{u}, v]$   $y+3/4, 3/4, \bar{y}+1/4 [\bar{v}, u, \bar{v}]$   
 $y, \bar{y}, 1/4 [v, v, u]$   $\bar{y}+3/4, \bar{y}+1/2, 0 [\bar{v}, v, \bar{u}]$   $y+1/2, y+1/4, 1/2 [v, \bar{v}, \bar{u}]$   $\bar{y}+1/4, y+3/4, 3/4 [\bar{v}, \bar{v}, u]$   
 $3/4, \bar{y}, y [\bar{u}, \bar{v}, \bar{v}]$   $0, y+1/4, y+1/2 [u, v, \bar{v}]$   $1/2, \bar{y}+1/2, \bar{y}+3/4 [u, \bar{v}, v]$   $1/4, y+3/4, \bar{y}+1/4 [\bar{u}, v, v]$   
 $y, 3/4, \bar{y} [\bar{v}, \bar{u}, \bar{v}]$   $y+1/2, 0, y+1/4 [\bar{v}, u, v]$   $\bar{y}+3/4, 1/2, \bar{y}+1/2 [v, u, \bar{v}]$   $\bar{y}+1/4, 1/4, y+3/4 [v, \bar{u}, v]$   
 $\bar{y}, y, 3/4 [\bar{v}, \bar{v}, \bar{u}]$   $y+1/4, y+1/2, 0 [v, \bar{v}, u]$   $\bar{y}+1/2, \bar{y}+3/4, 1/2 [\bar{v}, v, u]$   $y+3/4, \bar{y}+1/4, 1/4 [v, v, \bar{u}]$

- 96 f 2..  $x, 1/8, 1/8 [u, 0, 0]$   $\bar{x}+1/4, 5/8, 5/8 [\bar{u}, 0, 0]$   $1/8, x, 1/8 [0, u, 0]$   $5/8, \bar{x}+1/4, 5/8 [0, \bar{u}, 0]$   
 $1/8, 1/8, x [0, 0, u]$   $5/8, 5/8, \bar{x}+1/4 [0, 0, \bar{u}]$   $7/8, x+1/4, 7/8 [0, \bar{u}, 0]$   $3/8, \bar{x}+1/2, 3/8 [0, u, 0]$   
 $x+3/4, 3/8, 7/8 [\bar{u}, 0, 0]$   $\bar{x}, 7/8, 3/8 [u, 0, 0]$   $7/8, 3/8, \bar{x} [0, 0, u]$   $3/8, 7/8, x+3/4 [0, 0, \bar{u}]$   
 $\bar{x}, 7/8, 7/8 [\bar{u}, 0, 0]$   $x+3/4, 3/8, 3/8 [u, 0, 0]$   $7/8, \bar{x}, 7/8 [0, \bar{u}, 0]$   $3/8, x+3/4, 3/8 [0, u, 0]$   
 $7/8, 7/8, \bar{x} [0, 0, \bar{u}]$   $3/8, 3/8, x+3/4 [0, 0, u]$   $1/8, \bar{x}+3/4, 1/8 [0, u, 0]$   $5/8, x+1/2, 5/8 [0, \bar{u}, 0]$   
 $\bar{x}+1/4, 5/8, 1/8 [u, 0, 0]$   $x, 1/8, 5/8 [\bar{u}, 0, 0]$   $1/8, 5/8, x [0, 0, \bar{u}]$   $5/8, 1/8, \bar{x}+1/4 [0, 0, u]$

- 64 e .3.  $x, x, x [u, u, u]$   $\bar{x}+1/4, \bar{x}+3/4, x+1/2 [\bar{u}, \bar{u}, u]$   
 $\bar{x}+3/4, x+1/2, \bar{x}+1/4 [\bar{u}, u, \bar{u}]$   $x+1/2, \bar{x}+1/4, \bar{x}+3/4 [u, \bar{u}, \bar{u}]$   
 $x+3/4, x+1/4, \bar{x} [\bar{u}, \bar{u}, u]$   $\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [u, u, u]$   
 $x+1/4, \bar{x}, x+3/4 [\bar{u}, u, \bar{u}]$   $\bar{x}, x+3/4, x+1/4 [u, \bar{u}, \bar{u}]$   
 $\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$   $x+3/4, x+1/4, \bar{x}+1/2 [u, u, \bar{u}]$   
 $x+1/4, \bar{x}+1/2, x+3/4 [u, \bar{u}, u]$   $\bar{x}+1/2, x+3/4, x+1/4 [\bar{u}, u, u]$

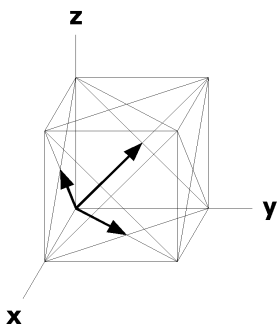
			$\bar{x}+1/4, \bar{x}+3/4, x$ [u,u, $\bar{u}$ ]		$x+1/2, x+1/2, x+1/2$ [ $\bar{u}, \bar{u}, \bar{u}$ ]	
			$\bar{x}+3/4, x, \bar{x}+1/4$ [u, $\bar{u}, u$ ]		$x, \bar{x}+1/4, \bar{x}+3/4$ [ $\bar{u}, u, u$ ]	
48	d	$\bar{4}..$	7/8, 1/8, 1/8 [u,0,0]	3/8, 5/8, 5/8 [ $\bar{u}, 0, 0$ ]	1/8, 7/8, 1/8 [0,u,0]	5/8, 3/8, 5/8 [0, $\bar{u}, 0$ ]
			1/8, 1/8, 7/8 [0,0,u]	5/8, 5/8, 3/8 [0,0, $\bar{u}$ ]	7/8, 1/8, 7/8 [0, $\bar{u}, 0$ ]	3/8, 5/8, 3/8 [0,u,0]
			5/8, 3/8, 7/8 [ $\bar{u}, 0, 0$ ]	1/8, 7/8, 3/8 [u,0,0]	7/8, 3/8, 1/8 [0,0,u]	3/8, 7/8, 5/8 [0,0, $\bar{u}$ ]
32	c	$\bar{3}'$	0,0,0 [0,0,0]	1/4, 3/4, 1/2 [0,0,0]	3/4, 1/2, 1/4 [0,0,0]	1/2, 1/4, 3/4 [0,0,0]
			3/4, 1/4, 0 [0,0,0]	1/2, 1/2, 1/2 [0,0,0]	1/4, 0, 3/4 [0,0,0]	0, 3/4, 1/4 [0,0,0]
32	b	.32'	1/4, 1/4, 1/4 [u,u,u]	0, 1/2, 3/4 [ $\bar{u}, \bar{u}, u$ ]	1/2, 3/4, 0 [ $\bar{u}, u, \bar{u}$ ]	3/4, 0, 1/2 [u, $\bar{u}, \bar{u}$ ]
			3/4, 3/4, 3/4 [ $\bar{u}, \bar{u}, \bar{u}$ ]	0, 1/2, 1/4 [u,u, $\bar{u}$ ]	1/2, 1/4, 0 [u, $\bar{u}, u$ ]	1/4, 0, 1/2 [ $\bar{u}, u, u$ ]
16	a	23.	1/8, 1/8, 1/8 [0,0,0]	7/8, 3/8, 7/8 [0,0,0]	7/8, 7/8, 7/8 [0,0,0]	1/8, 5/8, 1/8 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4'mm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/4$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/4$   
 Origin at 1/8, 3/8, z

Along [1,1,1] p6mm  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

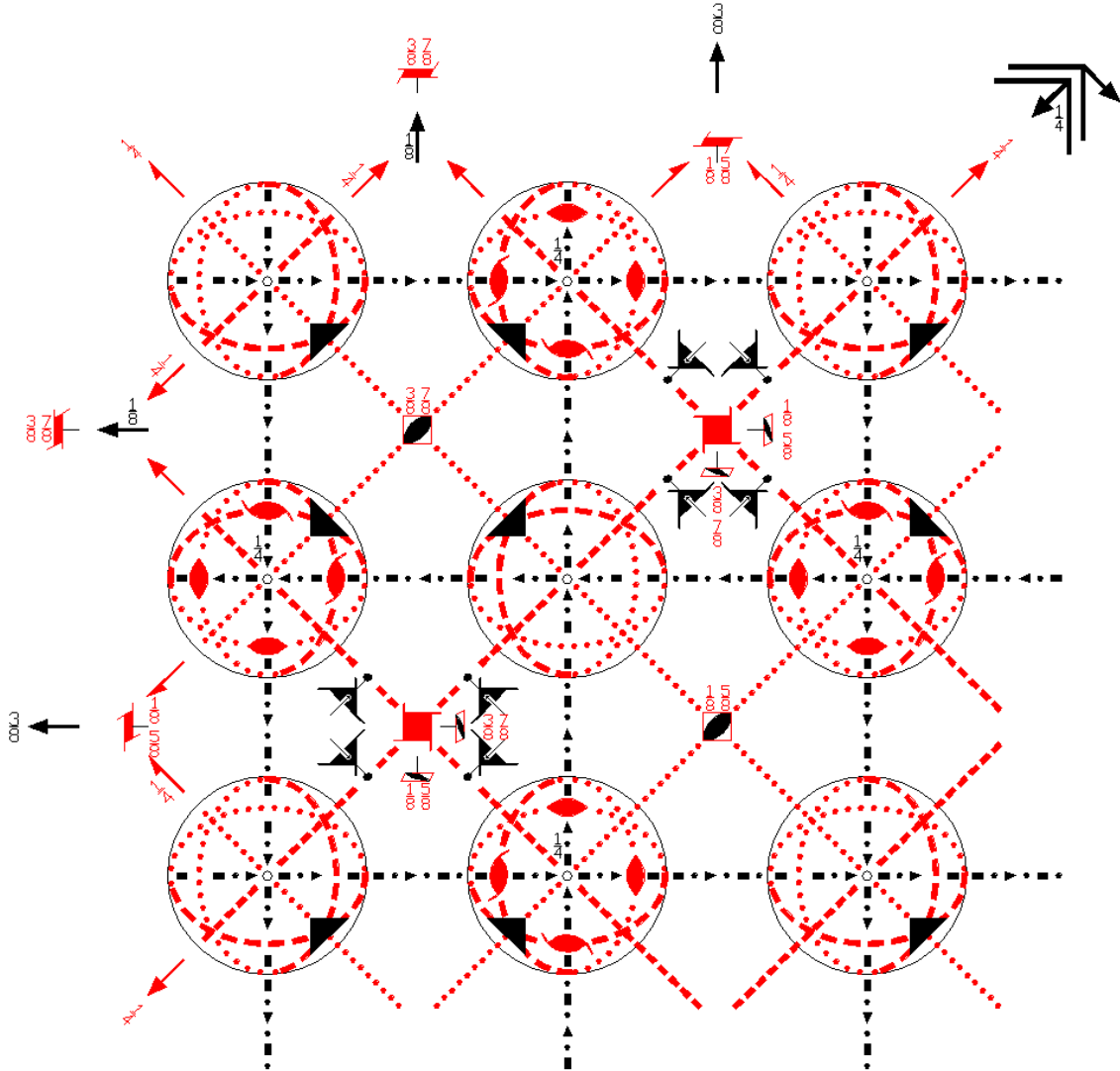
Along [1,1,0] p2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/4$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$Fd\bar{3}c'$   
228.4.1636

$m\bar{3}m'$   
 $F4_1'/d\bar{3}2'/c'$

Cubic



**Origin** at center ( $\bar{3}$ ), at  $3/8, 3/8, 3/8$  from 23

**Asymmetric unit**  $-1/8 \leq x \leq 3/8$ ;  $-1/8 \leq y \leq 0$ ;  $-1/4 \leq z \leq 0$ ;  $y \leq \min(1/4-x, x)$ ;  $-y-1/4 \leq z \leq y$

**Vertices**  $-1/8, -1/8, -1/8$   $3/8, -1/8, -1/8$   $1/4, 0, 0$   $0, 0, 0$   $1/4, 0, -1/4$   $0, 0, -1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |  |  |   |
|---|--|--|---|
| (1) 1<br>(1 0,0,0)                              | (2) 2 (0,0,1/2) $1/8, 3/8, z$<br>( $2_z$   $1/4, 3/4, 1/2$ )                                   | (3) 2 (0,1/2,0) $3/8, y, 1/8$<br>( $2_y$   $3/4, 1/2, 1/4$ )                                   | (4) 2 (1/2,0,0) $x, 1/8, 3/8$<br>( $2_x$   $1/2, 1/4, 3/4$ )  |
| (5) $3^+$ $x, x, x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ (1/3, -1/3, 1/3)<br>$x+1/6, x+5/12, \bar{x}$<br>( $3_{xyz}^{-1}$   $1/2, 1/4, 3/4$ ) | (7) $3^+$ (-1/3, 1/3, 1/3)<br>$x+7/12, x-1/6, \bar{x}$<br>( $3_{xyz}^{-1}$   $1/4, 3/4, 1/2$ ) | (8) $3^+$ (1/3, 1/3, -1/3)<br>$\bar{x}+5/12, \bar{x}+7/12, x$<br>( $3_{xyz}^{-1}$   $3/4, 1/2, 1/4$ ) |
| (9) $3^-$ $x, x, x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x+1/4, \bar{x}+1/2, \bar{x}$<br>( $3_{xyz}$   $3/4, 1/2, 1/4$ )                    | (11) $3^-$ $\bar{x}+3/4, \bar{x}+1/4, x$<br>( $3_{xy\bar{z}}$   $1/2, 1/4, 3/4$ )              | (12) $3^-$ $\bar{x}-1/2, x+3/4, \bar{x}$<br>( $3_{xy\bar{z}}$   $1/4, 3/4, 1/2$ )                     |

(13) 2' (1/2,1/2,0) x,x-1/4,0 (2 <sub>xy</sub>  3/4,1/4,0)'	(14) 2' x, $\bar{x}$ +1/2,1/4 (2 <sub>xy</sub>  1/2,1/2,1/2)'	(15) 4' (0,0,3/4) 1/8,-1/8,z (4 <sub>z</sub> <sup>-1</sup>  1/4,0,3/4)'	(16) 4 <sup>+</sup> (0,0,1/4) -3/8,3/8,z (4 <sub>z</sub>  0,3/4,1/4)'
(17) 4' (3/4,0,0) x,1/8,-1/8 (4 <sub>x</sub> <sup>-1</sup>  3/4,1/4,0)'	(18) 2' (0,1/2,1/2) 0,y+1/4,y (2 <sub>yz</sub>  0,3/4,1/4)'	(19) 2' 1/4,y+1/2, $\bar{y}$ (2 <sub>yz</sub>  1/2,1/2,1/2)'	(20) 4 <sup>+</sup> (1/4,0,0) x,-3/8,3/8 (4 <sub>x</sub>  1/4,0,3/4)'
(21) 4 <sup>+</sup> (0,1/4,0) 3/8,y,-3/8 (4 <sub>y</sub>  3/4,1/4,0)'	(22) 2' (1/2,0,1/2) x-1/4,0,x (2 <sub>xz</sub>  1/4,0,3/4)'	(23) 4' (0,3/4,0) -1/8,y,1/8 (4 <sub>y</sub> <sup>-1</sup>  0,3/4,1/4)'	(24) 2' $\bar{x}$ +1/2,1/4,x (2 <sub>xz</sub>  1/2,1/2,1/2)'
(25) $\bar{1}$ 0,0,0 ( $\bar{1}$  0,0,0)	(26) d (3/4,1/4,0) x,y,1/4 (m <sub>z</sub>  3/4,1/4,1/2)	(27) d (1/4,0,3/4) x,1/4,z (m <sub>y</sub>  1/4,1/2,3/4)	(28) d (0,3/4,1/4) 1/4,y,z (m <sub>x</sub>  1/2,3/4,1/4)
(29) $\bar{3}^+$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$  0,0,0)	(30) $\bar{3}^+$ $\bar{x}$ -1,x+5/4, $\bar{x}$ ; -1/4,1/2,3/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,3/4,1/4)	(31) $\bar{3}^+$ x+1/4, $\bar{x}$ +1, $\bar{x}$ ; 1/2,3/4,-1/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  3/4,1/4,1/2)	(32) $\bar{3}^+$ $\bar{x}$ +5/4, $\bar{x}$ +1/4,x; 3/4,-1/4,1/2 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/4,1/2,3/4)
(33) $\bar{3}^-$ x,x,x; 0,0,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)	(34) $\bar{3}^-$ x+3/4, $\bar{x}$ -1, $\bar{x}$ ; 0,-1/4,3/4 ( $\bar{3}_{xyz}$  1/4,1/2,3/4)	(35) $\bar{3}^-$ $\bar{x}$ -1/4, $\bar{x}$ +3/4,x; -14,3/4,0 ( $\bar{3}_{xyz}$  1/2,3/4,1/4)	(36) $\bar{3}^-$ $\bar{x}$ +1,x-1/4, $\bar{x}$ ; 3/4,0,-1/4 ( $\bar{3}_{xyz}$  3/4,1/4,1/2)
(37) g' (-1/4,1/4,1/2) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>  1/4,3/4,0)'	(38) n' (1/2,1/2,1/2) x,x,z (m <sub>xy</sub>  1/2,1/2,1/2)'	(39) $\bar{4}^-$ (3/8,3/8,z; 3/8,3/8,1/8) (4 <sub>z</sub> <sup>-1</sup>  3/4,0,1/4)'	(40) $\bar{4}^+$ (1/8,1/8,z; 1/8,1/8,3/8) (4 <sub>z</sub>  0,1/4,3/4)'
(41) $\bar{4}^-$ (x,3/8,3/8; 1/8,3/8,3/8) (4 <sub>x</sub> <sup>-1</sup>  1/4,3/4,0)'	(42) g' (0,-1/4,1/4) x,y+1/2, $\bar{y}$ (m <sub>yz</sub>  0,1/4,3/4)'	(43) n' (1/2,1/2,1/2) x,y,y (m <sub>yz</sub>  1/2,1/2,1/2)'	(44) $\bar{4}^+$ (x,1/8,1/8; 3/8,1/8,1/8) (4 <sub>x</sub>  3/4,0,1/4)'
(45) $\bar{4}^+$ (1/8,y,1/8; 1/8,3/8,1/8) (4 <sub>y</sub>  1/4,3/4,0)'	(46) g' (1/4,0,-1/4) $\bar{x}$ +1/2,y,x (m <sub>xz</sub>  3/4,0,1/4)'	(47) $\bar{4}^-$ (3/8,y,3/8; 3/8,1/8,3/8) (4 <sub>y</sub> <sup>-1</sup>  0,1/4,3/4)'	(48) n' (1/2,1/2,1/2) x,y,x (m <sub>xz</sub>  1/2,1/2,1/2)'

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2) (1 0,1/2,1/2)	(2) 2 (1/8,1/8,z) (2 <sub>z</sub>  1/4,1/4,0)	(3) 2 (3/8,y,3/8) (2 <sub>y</sub>  3/4,0,3/4)	(4) 2 (1/2,0,0) x,3/8,1/8 (2 <sub>x</sub>  1/2,3/4,1/4)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x-1/3,x-1/6,x (3 <sub>xyz</sub>  0,1/2,1/2)	(6) 3 <sup>+</sup> $\bar{x}$ +1/2,x+1/4, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  1/2,3/4,1/4)	(7) 3 <sup>+</sup> x+1/4, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>  1/4,1/4,0)	(8) 3 <sup>+</sup> $\bar{x}$ +3/4, $\bar{x}$ +3/4,x (3 <sub>xyz</sub> <sup>-1</sup>  3/4,0,3/4)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x-1/6,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,1/2)	(10) 3 <sup>-</sup> x+3/4, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub>  3/4,0,3/4)	(11) 3 <sup>-</sup> (1/3,1/3,-1/3) x+7/12, $\bar{x}$ +5/12,x (3 <sub>xyz</sub>  1/2,3/4,1/4)	(12) 3 <sup>-</sup> $\bar{x}$ ,x+1/4, $\bar{x}$ (3 <sub>xyz</sub>  1/4,1/4,0)
(13) 2' (3/4,3/4,0) x,x,1/4 (2 <sub>xy</sub>  3/4,3/4,1/2)'	(14) 2' (1/4,-1/4,0) x, $\bar{x}$ +1/4,0 (2 <sub>xy</sub>  1/2,0,0)'	(15) 4' (0,0,1/4) 3/8,1/8,z (4 <sub>z</sub> <sup>-1</sup>  1/4,1/2,1/4)'	(16) 4 <sup>+</sup> (0,0,3/4) -1/8,1/8,z (4 <sub>z</sub>  0,1/4,3/4)'
(17) 4' (3/4,0,0) 5/8,-1/8 (4 <sub>x</sub> <sup>-1</sup>  3/4,3/4,1/2)'	(18) 2' (0,1/2,1/2) 0,y-1/4,y (2 <sub>yz</sub>  0,1/4,3/4)'	(19) 2' 1/4,y, $\bar{y}$ (2 <sub>yz</sub> <sup>-1</sup>  1/2,0,0)'	(20) 4 <sup>+</sup> (1/4,0,0) x,1/8,3/8 (4 <sub>x</sub>  1/4,1/2,1/4)'
(21) 4 <sup>+</sup> (0,3/4,0) 5/8,y,-1/8 (4 <sub>y</sub>  3/4,3/4,1/2)'	(22) 2' (1/4,0,1/4) x,1/4,x (2 <sub>xz</sub>  1/4,1/2,1/4)'	(23) 4' (0,1/4,0) -3/8,y,3/8 (4 <sub>y</sub> <sup>-1</sup>  0,1/4,3/4)'	(24) 2' (1/4,0,-1/4) $\bar{x}$ +1/4,0,x (2 <sub>xz</sub>  1/2,0,0)'
(25) $\bar{1}$ 0,1/4,1/4 ( $\bar{1}$  0,1/2,1/2)	(26) d (3/4,3/4,0) x,y,0 (m <sub>z</sub>  3/4,3/4,0)	(27) d (1/4,0,1/4) x,0,z (m <sub>y</sub>  1/4,0,1/4)	(28) d (0,1/4,3/4) 1/4,y,z (m <sub>x</sub>  1/2,1/4,3/4)
(29) $\bar{3}^+$ x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$  0,1/2,1/2)	(30) $\bar{3}^+$ $\bar{x}$ -1,x+3/4, $\bar{x}$ ; -1/4,0,3/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,1/4,3/4)	(31) $\bar{3}^+$ x-3/4, $\bar{x}$ +3/2, $\bar{x}$ ; 0,3/4,-3/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>  3/4,3/4,0)	(32) $\bar{3}^+$ $\bar{x}$ +1/4, $\bar{x}$ -1/4,x; 1/4,-1/4,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>  1/4,0,1/4)

- (33)  $\bar{3}^-$   $x-1/2, x-1/2, x;$   
 $0, 0, 1/2$   
 $(\bar{3}_{xyz}^{-1} | 0, 1/2, 1/2)$
- (34)  $\bar{3}^-$   $x+1/4, \bar{x}-1/2, \bar{x};$   
 $0, -1/4, 1/4$   
 $(\bar{3}_{\bar{xyz}} | 1/4, 0, 1/4)$
- (35)  $\bar{3}^-$   $\bar{x}+1/4, \bar{x}+5/4, x;$   
 $-1/4, 3/4, 1/2$   
 $(\bar{3}_{\bar{xyz}} | 1/2, 1/4, 3/4)$
- (36)  $\bar{3}^-$   $\bar{x}+3/2, x-3/4, \bar{x};$   
 $3/4, 0, -3/4$   
 $(\bar{3}_{\bar{xyz}} | 3/4, 3/4, 0)$
- (37)  $c'$   $(0, 0, 1/2)$   $x+1/4, \bar{x}, z$   
 $(m_{xy} | 1/4, 1/4, 1/2)'$
- (38)  $g'$   $(1/4, 1/4, 0)$   $x+1/4, x, z$   
 $(m_{\bar{xy}} | 1/2, 0, 0)'$
- (39)  $\bar{4}^-$   $1/8, 5/8, z;$   $1/8, 5/8, 3/8$   
 $(\bar{4}_z^{-1} | 3/4, 1/2, 3/4)'$
- (40)  $\bar{4}^+$   $3/8, 3/8, z;$   $3/8, 3/8, 1/8$   
 $(\bar{4}_z | 0, 3/4, 1/4)'$
- (41)  $\bar{4}^-$   $x, -1/8, 3/8;$   $1/8, -1/8, 3/8$   
 $(\bar{4}_x^{-1} | 1/4, 1/4, 1/2)'$
- (42)  $g'$   $(0, 1/4, -1/4)$   $x, y+1/2, \bar{y}$   
 $(m_{yz} | 0, 3/4, 1/4)'$
- (43)  $a'$   $(1/2, 0, 0)$   $x, y, y$   
 $(m_{\bar{yz}} | 1/2, 0, 0)'$
- (44)  $\bar{4}^+$   $x, 5/8, 1/8;$   $3/8, 5/8, 1/8$   
 $(\bar{4}_x | 3/4, 0, 3/4)'$
- (45)  $\bar{4}^+$   $-1/8, y, 3/8;$   $-1/8, 1/8, 3/8$   
 $(\bar{4}_y | 1/4, 1/4, 1/2)'$
- (46)  $b'$   $(0, 1/2, 0)$   $\bar{x}+3/4, y, x$   
 $(m_{xz} | 3/4, 1/2, 3/4)'$
- (47)  $\bar{4}^-$   $1/8, y, 1/8;$   $1/8, 3/8, 1/8$   
 $(\bar{4}_y^{-1} | 0, 3/4, 1/4)'$
- (48)  $g'$   $(1/4, 0, 1/4)$   $x+1/4, y, x$   
 $(m_{\bar{xz}} | 1/2, 0, 0)'$

For  $(1/2, 0, 1/2)$  + set

- (1)  $t$   $(1/2, 0, 1/2)$   
 $(1 | 1/2, 0, 1/2)$
- (2)  $2$   $3/8, 3/8, z$   
 $(2_z | 3/4, 3/4, 0)$
- (3)  $2$   $(0, 1/2, 0)$   $1/8, y, 3/8$   
 $(2_y | 1/4, 1/2, 3/4)$
- (4)  $2$   $x, 1/8, 1/8$   
 $(2_x | 0, 1/4, 1/4)$
- (5)  $3^+$   $(1/3, 1/3, 1/3)$   
 $x+1/6, x-1/6, x$   
 $(3_{xyz} | 1/2, 0, 1/2)$
- (6)  $3^+$   $\bar{x}, x+1/4, \bar{x}$   
 $(3_{\bar{xyz}}^{-1} | 0, 1/4, 1/4)$
- (7)  $3^+$   $x+3/4, \bar{x}, \bar{x}$   
 $(3_{\bar{xyz}}^{-1} | 3/4, 3/4, 0)$
- (8)  $3^+$   $\bar{x}+1/4, \bar{x}+3/4, x$   
 $(3_{\bar{xyz}}^{-1} | 1/4, 1/2, 3/4)$
- (9)  $3^-$   $(1/3, 1/3, 1/3)$   
 $x-1/6, x-1/3, x$   
 $(3_{xyz}^{-1} | 1/2, 0, 1/2)$
- (10)  $3^-$   $(-1/3, 1/3, 1/3)$   
 $x+5/12, \bar{x}+1/6, \bar{x}$   
 $(3_{\bar{xyz}} | 1/4, 1/2, 3/4)$
- (11)  $3^-$   $\bar{x}+1/4, \bar{x}+1/4, x$   
 $(3_{\bar{yz}} | 0, 1/4, 1/4)$
- (12)  $3^-$   $\bar{x}, x+3/4, \bar{x}$   
 $(3_{\bar{yz}} | 3/4, 3/4, 0)$
- (13)  $2'$   $(1/4, 1/4, 0)$   $x, x, 1/4$   
 $(2_{xy} | 1/4, 1/4, 1/2)'$
- (14)  $2'$   $(-1/4, 1/4, 0)$   $x, \bar{x}+1/4, 0$   
 $(2_{\bar{xy}} | 0, 1/2, 0)'$
- (15)  $4^-$   $(0, 0, 1/4)$   $3/8, -3/8, z$   
 $(4_z^{-1} | 3/4, 0, 1/4)'$
- (16)  $4^+$   $(0, 0, 3/4)$   $-1/8, 5/8, z$   
 $(4_z | 1/2, 3/4, 3/4)'$
- (17)  $4^-$   $(1/4, 0, 0)$   $x, 3/8, 1/8$   
 $(4_x^{-1} | 1/4, 1/4, 1/2)'$
- (18)  $2'$   $(0, 3/4, 3/4)$   $1/4, y, y$   
 $(2_{yz} | 1/2, 3/4, 3/4)'$
- (19)  $2'$   $(0, 1/4, -1/4)$   $0, y+1/4, \bar{y}$   
 $(2_{\bar{yz}} | 0, 1/2, 0)'$
- (20)  $4^+$   $(3/4, 0, 0)$   $x, -1/8, 1/8$   
 $(4_x | 3/4, 0, 1/4)'$
- (21)  $4^+$   $(0, 1/4, 0)$   $3/8, y, 1/8$   
 $(4_y | 1/4, 1/4, 1/2)'$
- (22)  $2'$   $(1/2, 0, 1/2)$   $x+1/4, 0, x$   
 $(2_{xz} | 3/4, 0, 1/4)'$
- (23)  $4^-$   $(0, 3/4, 0)$   $-1/8, y, 5/8$   
 $(4_y^{-1} | 1/2, 3/4, 3/4)'$
- (24)  $2'$   $\bar{x}, 1/4, x$   
 $(2_{\bar{xz}} | 0, 1/2, 0)'$
- (25)  $\bar{1}$   $1/4, 0, 1/4$   
 $(\bar{1} | 1/2, 0, 1/2)$
- (26)  $d$   $(1/4, 1/4, 0)$   $x, y, 0$   
 $(m_z | 1/4, 1/4, 0)$
- (27)  $d$   $(3/4, 0, 1/4)$   $x, 1/4, z$   
 $(m_y | 3/4, 1/2, 1/4)$
- (28)  $d$   $(0, 3/4, 3/4)$   $0, y, z$   
 $(m_x | 0, 3/4, 3/4)$
- (29)  $\bar{3}^+$   $x-1/2, x-1/2, x;$   
 $0, 0, 1/2$   
 $(\bar{3}_{xyz} | 1/2, 0, 1/2)$
- (30)  $\bar{3}^+$   $\bar{x}-3/2, x+3/4, \bar{x};$   
 $-3/4, 0, 3/4$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 0, 3/4, 3/4)$
- (31)  $\bar{3}^+$   $x-1/4, \bar{x}+1/2, \bar{x};$   
 $0, 1/4, -1/4$   
 $(\bar{3}_{\bar{yz}}^{-1} | 1/4, 1/4, 0)$
- (32)  $\bar{3}^+$   $\bar{x}+3/4, \bar{x}-1/4, x;$   
 $3/4, -1/4, 0$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 3/4, 1/2, 1/4)$
- (33)  $\bar{3}^-$   $x+1/2, x, x;$   
 $1/2, 0, 0$   
 $(\bar{3}_{xyz}^{-1} | 1/2, 0, 1/2)$
- (34)  $\bar{3}^-$   $x+5/4, \bar{x}-1, \bar{x};$   
 $1/2, -1/4, 3/4$   
 $(\bar{3}_{\bar{yz}} | 3/4, 1/2, 1/4)$
- (35)  $\bar{3}^-$   $\bar{x}-3/4, \bar{x}+3/4, x;$   
 $-3/4, 3/4, 0$   
 $(\bar{3}_{\bar{yz}} | 0, 3/4, 3/4)$
- (36)  $\bar{3}^-$   $\bar{x}+1/2, x-1/4, \bar{x};$   
 $1/4, 0, -1/4$   
 $(\bar{3}_{\bar{yz}} | 1/4, 1/4, 0)$
- (37)  $c'$   $(0, 0, 1/2)$   $x+3/4, \bar{x}, z$   
 $(m_{xy} | 3/4, 3/4, 1/2)'$
- (38)  $g'$   $(1/4, 1/4, 0)$   $x-1/4, x, z$   
 $(m_{\bar{xy}} | 0, 1/2, 0)'$
- (39)  $\bar{4}^-$   $1/8, 1/8, z;$   $1/8, 1/8, 3/8$   
 $(\bar{4}_z^{-1} | 1/4, 0, 3/4)'$
- (40)  $\bar{4}^+$   $3/8, -1/8, z;$   $3/8, -1/8, 1/8$   
 $(\bar{4}_z | 1/2, 1/4, 1/4)'$
- (41)  $\bar{4}^-$   $x, 1/8, 5/8;$   $3/8, 1/8, 5/8$   
 $(\bar{4}_x^{-1} | 3/4, 3/4, 1/2)'$
- (42)  $a'$   $(1/2, 0, 0)$   $x, y+1/4, \bar{y}$   
 $(m_{yz} | 1/2, 1/4, 1/4)'$
- (43)  $g'$   $(0, 1/4, 1/4)$   $x, y+1/4, y$   
 $(m_{\bar{yz}} | 0, 1/2, 0)'$
- (44)  $\bar{4}^+$   $x, 3/8, 3/8;$   $1/8, 3/8, 3/8$   
 $(\bar{4}_x | 1/4, 0, 3/4)'$
- (45)  $\bar{4}^+$   $1/8, y, 5/8;$   $1/8, 3/8, 5/8$   
 $(\bar{4}_y | 3/4, 3/4, 1/2)'$
- (46)  $g'$   $(-1/4, 0, 1/4)$   $\bar{x}+1/2, y, x$   
 $(m_{xz} | 1/4, 0, 3/4)'$
- (47)  $\bar{4}^-$   $3/8, y, -1/8;$   $3/8, 1/8, -1/8$   
 $(\bar{4}_y^{-1} | 1/2, 1/4, 1/4)'$
- (48)  $b'$   $(0, 1/2, 0)$   $x, y, x$   
 $(m_{\bar{xz}} | 0, 1/2, 0)'$

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (1   1/2,1/2,0)	(2) 2 (0,0,1/2) 3/8,1/8,z (2 <sub>z</sub>   3/4,1/4,1/2)	(3) 2 1/8,y,1/8 (2 <sub>y</sub>   1/4,0,1/4)	(4) 2 x,3/8,3/8 (2 <sub>x</sub>   0,3/4,3/4)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) 3 <sup>+</sup> $\bar{x}$ ,x+3/4, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   0,3/4,3/4)	(7) 3 <sup>+</sup> x+3/4, $\bar{x}$ -1/2, $\bar{x}$ (3 <sub>xyz</sub> <sup>-1</sup>   3/4,1/4,1/2)	(8) 3 <sup>+</sup> $\bar{x}$ +1/4, $\bar{x}$ +1/4,x (3 <sub>xyz</sub> <sup>-1</sup>   1/4,0,1/4)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) 3 <sup>-</sup> x+1/4, $\bar{x}$ , $\bar{x}$ (3 <sub>xyz</sub>   1/4,0,1/4)	(11) 3 <sup>-</sup> $\bar{x}$ +3/4, $\bar{x}$ +3/4, x (3 <sub>xyz</sub>   0,3/4,3/4)	(12) 3 <sup>-</sup> (1/3,-1/3,1/3) $\bar{x}$ -1/6, x+7/12, $\bar{x}$ (3 <sub>xyz</sub>   3/4,1/4,1/2)
(13) 2' (1/2,1/2,0) x,x+1/4,0 (2 <sub>xy</sub>   1/4,3/4,0)'	(14) 2' x, $\bar{x}$ ,1/4 (2 <sub>xy</sub>   0,0,1/2)'	(15) 4' (0,0,3/4) 5/8,-1/8,z (4 <sub>z</sub> <sup>-1</sup>   3/4,1/2,3/4)'	(16) 4' (0,0,1/4) 1/8,3/8,z (4 <sub>z</sub>   1/2,1/4,1/4)'
(17) 4' (1/4,0,0) x,3/8,-3/8 (4 <sub>x</sub> <sup>-1</sup>   1/4,3/4,0)'	(18) 2' (0,1/4,1/4) 1/4,y,y (2 <sub>yz</sub>   1/2,1/4,1/4)'	(19) 2' (0,-1/4,1/4) 0,y+1/4, $\bar{y}$ (2 <sub>yz</sub>   0,0,1/2)'	(20) 4' (3/4,0,0) x,-1/8,5/8 (4 <sub>x</sub>   3/4,1/2,3/4)'
(21) 4' (0,3/4,0) 1/8,y,-1/8 (4 <sub>y</sub>   1/4,3/4,0)'	(22) 2' (3/4,0,3/4) x,1/4,x (2 <sub>xz</sub>   3/4,1/2,3/4)'	(23) 4' (0,1/4,0) 1/8,y,3/8 (4 <sub>y</sub> <sup>-1</sup>   1/2,1/4,1/4)'	(24) 2' (-1/4,0,1/4) $\bar{x}$ +1/4,0,x (2 <sub>xz</sub>   0,0,1/2)'
(25) $\bar{1}$ 1/4,1/4,0 ( $\bar{1}$   1/2,1/2,0)	(26) d (1/4,3/4,0) x,y,1/4 (m <sub>z</sub>   1/4,3/4,1/2)	(27) d (3/4,0,3/4) x,0,z (m <sub>y</sub>   3/4,0,3/4)	(28) d (0,1/4,1/4) 0,y,z (m <sub>x</sub>   0,1/4,1/4)
(29) $\bar{3}^+$ x+1/2,x,x; 1/2,0,0 ( $\bar{3}_{xyz}$   1/2,1/2,0)	(30) $\bar{3}^+$ $\bar{x}$ -1/2,x+1/4, $\bar{x}$ ; -1/4,0,1/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>   0,1/4,1/4)	(31) $\bar{3}^+$ x-1/4, $\bar{x}$ +1, $\bar{x}$ ; 0,3/4,-1/4 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/4,3/4,1/2)	(32) $\bar{3}^+$ $\bar{x}$ +3/4, $\bar{x}$ -3/4,x; 3/4,-3/4,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>   3/4,0,3/4)
(33) $\bar{3}^-$ x,x+1/2,x; 0,1/2,0 ( $\bar{3}_{xyz}$ <sup>-1</sup>   1/2,1/2,0)	(34) $\bar{3}^-$ x+3/4, $\bar{x}$ -3/2, $\bar{x}$ ; 0,-3/4,3/4 ( $\bar{3}_{xyz}$   3/4,0,3/4)	(35) $\bar{3}^-$ $\bar{x}$ -1/4, $\bar{x}$ +1/4, x; -1/4,1/4,0 ( $\bar{3}_{xyz}$   0,1/4,1/4)	(36) $\bar{3}^-$ $\bar{x}$ +1, x+1/4, $\bar{x}$ ; 3/4,1/2,-1/4 ( $\bar{3}_{xyz}$   1/4,3/4,1/2)
(37) g' (1/4,-1/4,0) x+1/2, $\bar{x}$ ,z (m <sub>xy</sub>   3/4,1/4,0)'	(38) c' (0,0,1/2) x,x,z (m <sub>xy</sub>   0,0,1/2)'	(39) $\bar{4}^-$ -1/8,3/8,z; -1/8,3/8,1/8 ( $\bar{4}_z$ <sup>-1</sup>   1/4,1/2,1/4)'	(40) $\bar{4}^+$ 5/8,1/8,z; 5/8,1/8,3/8 ( $\bar{4}_z$   1/2,3/4,3/4)'
(41) $\bar{4}^-$ x,1/8,1/8; 3/8,1/8,1/8 ( $\bar{4}_x$ <sup>-1</sup>   3/4,1/4,0)'	(42) a' (1/2,0,0) x,y+3/4, $\bar{y}$ (m <sub>yz</sub>   1/2,3/4,3/4)'	(43) g' (0,1/4,1/4) x,y-1/4,y (m <sub>yz</sub>   0,0,1/2)'	(44) $\bar{4}^+$ x,3/8,-1/8; 1/8,3/8,-1/8 ( $\bar{4}_x$   1/4,1/2,1/4)'
(45) $\bar{4}^+$ 3/8,y,3/8; 3/8,1/8,3/8 ( $\bar{4}_y$   3/4,1/4,0)'	(46) b' (0,1/2,0) $\bar{x}$ +1/4,y,x (m <sub>xz</sub>   1/4,1/2,1/4)'	(47) $\bar{4}^-$ 5/8,y,1/8; 5/8,3/8,1/8 ( $\bar{4}_y$ <sup>-1</sup>   1/2,3/4,3/4)'	(48) g' (1/4,0,1/4) x-1/4,y,x (m <sub>xz</sub>   0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

192	h	1	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +		
(1)	x,y,z	[u,v,w]	(2) $\bar{x}$ +1/4, $\bar{y}$ +3/4,z+1/2	[ $\bar{u}$ , $\bar{v}$ ,w]	(3) $\bar{x}$ +3/4,y+1/2, $\bar{z}$ +1/4	[ $\bar{u}$ ,v, $\bar{w}$ ]	(4) x+1/2, $\bar{y}$ +1/4, $\bar{z}$ +3/4	[u, $\bar{v}$ , $\bar{w}$ ]
(5)	z,x,y	[w,u,v]	(6) z+1/2, $\bar{x}$ +1/4, $\bar{y}$ +3/4	[w, $\bar{u}$ , $\bar{v}$ ]	(7) $\bar{z}$ +1/4, $\bar{x}$ +3/4,y+1/2	[ $\bar{w}$ , $\bar{u}$ ,v]	(8) $\bar{z}$ +3/4,x+1/2, $\bar{y}$ +1/4	[ $\bar{w}$ ,u, $\bar{v}$ ]

- (9)  $y, z, x$  [ $v, w, u$ ] (10)  $\bar{y}+3/4, z+1/2, \bar{x}+1/4$  [ $\bar{v}, w, \bar{u}$ ] (11)  $y+1/2, \bar{z}+1/4, \bar{x}+3/4$  [ $v, \bar{w}, \bar{u}$ ] (12)  $\bar{y}+1/4, \bar{z}+3/4, x+1/2$  [ $\bar{v}, \bar{w}, u$ ]  
 (13)  $y+3/4, x+1/4, \bar{z}$  [ $\bar{v}, \bar{u}, w$ ] (14)  $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2$  [ $v, u, w$ ] (15)  $y+1/4, \bar{x}, z+3/4$  [ $\bar{v}, u, \bar{w}$ ] (16)  $\bar{y}, x+3/4, z+1/4$  [ $v, \bar{u}, \bar{w}$ ]  
 (17)  $x+3/4, z+1/4, \bar{y}$  [ $\bar{u}, \bar{w}, v$ ] (18)  $\bar{x}, z+3/4, y+1/4$  [ $u, \bar{w}, \bar{v}$ ] (19)  $\bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2$  [ $u, w, v$ ] (20)  $x+1/4, \bar{z}, y+3/4$  [ $\bar{u}, w, \bar{v}$ ]  
 (21)  $z+3/4, y+1/4, \bar{x}$  [ $\bar{w}, \bar{v}, u$ ] (22)  $z+1/4, \bar{y}, x+3/4$  [ $\bar{w}, v, \bar{u}$ ] (23)  $\bar{z}, y+3/4, x+1/4$  [ $w, \bar{v}, \bar{u}$ ] (24)  $\bar{z}+1/2, \bar{y}+1/2, \bar{x}+1/2$  [ $w, v, u$ ]  
 (25)  $\bar{x}, \bar{y}, \bar{z}$  [ $u, v, w$ ] (26)  $x+3/4, y+1/4, \bar{z}+1/2$  [ $\bar{u}, \bar{v}, w$ ] (27)  $x+1/4, \bar{y}+1/2, z+3/4$  [ $\bar{u}, v, \bar{w}$ ] (28)  $\bar{x}+1/2, y+3/4, z+1/4$  [ $u, \bar{v}, \bar{w}$ ]  
 (29)  $\bar{z}, \bar{x}, \bar{y}$  [ $w, u, v$ ] (30)  $\bar{z}+1/2, x+3/4, y+1/4$  [ $w, \bar{u}, \bar{v}$ ] (31)  $z+3/4, x+1/4, \bar{y}+1/2$  [ $\bar{w}, \bar{u}, v$ ] (32)  $z+1/4, \bar{x}+1/2, y+3/4$  [ $\bar{w}, u, \bar{v}$ ]  
 (33)  $\bar{y}, \bar{z}, \bar{x}$  [ $v, w, u$ ] (34)  $y+1/4, \bar{z}+1/2, x+3/4$  [ $\bar{v}, w, \bar{u}$ ] (35)  $\bar{y}+1/2, z+3/4, x+1/4$  [ $v, \bar{w}, \bar{u}$ ] (36)  $y+3/4, z+1/4, \bar{x}+1/2$  [ $\bar{v}, \bar{w}, u$ ]  
 (37)  $\bar{y}+1/4, \bar{x}+3/4, z$  [ $\bar{v}, \bar{u}, w$ ] (38)  $y+1/2, x+1/2, z+1/2$  [ $v, u, w$ ] (39)  $\bar{y}+3/4, x, \bar{z}+1/4$  [ $\bar{v}, u, \bar{w}$ ] (40)  $y, \bar{x}+1/4, \bar{z}+3/4$  [ $v, \bar{u}, \bar{w}$ ]  
 (41)  $\bar{x}+1/4, \bar{z}+3/4, y$  [ $\bar{u}, \bar{w}, v$ ] (42)  $x, \bar{z}+1/4, \bar{y}+3/4$  [ $u, \bar{w}, \bar{v}$ ] (43)  $x+1/2, z+1/2, y+1/2$  [ $u, w, v$ ] (44)  $\bar{x}+3/4, z, \bar{y}+1/4$  [ $\bar{u}, w, \bar{v}$ ]  
 (45)  $\bar{z}+1/4, \bar{y}+3/4, x$  [ $\bar{w}, \bar{v}, u$ ] (46)  $\bar{z}+3/4, y, \bar{x}+1/4$  [ $\bar{w}, v, \bar{u}$ ] (47)  $z, \bar{y}+1/4, \bar{x}+3/4$  [ $w, \bar{v}, \bar{u}$ ] (48)  $z+1/2, y+1/2, x+1/2$  [ $w, v, u$ ]

96 g ..2'

- $1/4, y, \bar{y}$  [ $u, v, v$ ]  $0, \bar{y}+3/4, \bar{y}+1/2$  [ $\bar{u}, \bar{v}, v$ ]  $1/2, y+1/2, y+1/4$  [ $\bar{u}, v, \bar{v}$ ]  $3/4, \bar{y}+1/4, y+3/4$  [ $u, \bar{v}, \bar{v}$ ]  
 $\bar{y}, 1/4, y$  [ $v, u, v$ ]  $\bar{y}+1/2, 0, \bar{y}+3/4$  [ $v, \bar{u}, \bar{v}$ ]  $y+1/4, 1/2, y+1/2$  [ $\bar{v}, \bar{u}, v$ ]  $y+3/4, 3/4, \bar{y}+1/4$  [ $\bar{v}, u, \bar{v}$ ]  
 $y, \bar{y}, 1/4$  [ $v, v, u$ ]  $\bar{y}+3/4, \bar{y}+1/2, 0$  [ $\bar{v}, v, \bar{u}$ ]  $y+1/2, y+1/4, 1/2$  [ $v, \bar{v}, \bar{u}$ ]  $\bar{y}+1/4, y+3/4, 3/4$  [ $\bar{v}, \bar{v}, u$ ]  
 $3/4, \bar{y}, y$  [ $u, v, v$ ]  $0, y+1/4, y+1/2$  [ $\bar{u}, \bar{v}, v$ ]  $1/2, \bar{y}+1/2, \bar{y}+3/4$  [ $\bar{u}, v, \bar{v}$ ]  $1/4, y+3/4, \bar{y}+1/4$  [ $u, \bar{v}, \bar{v}$ ]  
 $y, 3/4, \bar{y}$  [ $v, u, v$ ]  $y+1/2, 0, y+1/4$  [ $v, \bar{u}, \bar{v}$ ]  $\bar{y}+3/4, 1/2, \bar{y}+1/2$  [ $\bar{v}, \bar{u}, v$ ]  $\bar{y}+1/4, 1/4, y+3/4$  [ $\bar{v}, u, \bar{v}$ ]  
 $\bar{y}, y, 3/4$  [ $v, v, u$ ]  $y+1/4, y+1/2, 0$  [ $\bar{v}, v, \bar{u}$ ]  $\bar{y}+1/2, \bar{y}+3/4, 1/2$  [ $v, \bar{v}, \bar{u}$ ]  $y+3/4, \bar{y}+1/4, 1/4$  [ $\bar{v}, \bar{v}, u$ ]

- 96 f 2..  $x, 1/8, 1/8$  [ $u, 0, 0$ ]  $\bar{x}+1/4, 5/8, 5/8$  [ $\bar{u}, 0, 0$ ]  $1/8, x, 1/8$  [ $0, u, 0$ ]  $5/8, \bar{x}+1/4, 5/8$  [ $0, \bar{u}, 0$ ]  
 $1/8, 1/8, x$  [ $0, 0, u$ ]  $5/8, 5/8, \bar{x}+1/4$  [ $0, 0, \bar{u}$ ]  $7/8, x+1/4, 7/8$  [ $0, \bar{u}, 0$ ]  $3/8, \bar{x}+1/2, 3/8$  [ $0, u, 0$ ]  
 $x+3/4, 3/8, 7/8$  [ $\bar{u}, 0, 0$ ]  $\bar{x}, 7/8, 3/8$  [ $u, 0, 0$ ]  $7/8, 3/8, \bar{x}$  [ $0, 0, u$ ]  $3/8, 7/8, x+3/4$  [ $0, 0, \bar{u}$ ]  
 $\bar{x}, 7/8, 7/8$  [ $u, 0, 0$ ]  $x+3/4, 3/8, 3/8$  [ $\bar{u}, 0, 0$ ]  $7/8, \bar{x}, 7/8$  [ $0, u, 0$ ]  $3/8, x+3/4, 3/8$  [ $0, \bar{u}, 0$ ]  
 $7/8, 7/8, \bar{x}$  [ $0, 0, u$ ]  $3/8, 3/8, x+3/4$  [ $0, 0, \bar{u}$ ]  $1/8, \bar{x}+3/4, 1/8$  [ $0, \bar{u}, 0$ ]  $5/8, x+1/2, 5/8$  [ $0, u, 0$ ]  
 $\bar{x}+1/4, 5/8, 1/8$  [ $\bar{u}, 0, 0$ ]  $x, 1/8, 5/8$  [ $u, 0, 0$ ]  $1/8, 5/8, x$  [ $0, 0, u$ ]  $5/8, 1/8, \bar{x}+1/4$  [ $0, 0, \bar{u}$ ]

- 64 e .3.  $x, x, x$  [ $u, u, u$ ]  $\bar{x}+1/4, \bar{x}+3/4, x+1/2$  [ $\bar{u}, \bar{u}, u$ ]  
 $\bar{x}+3/4, x+1/2, \bar{x}+1/4$  [ $\bar{u}, u, \bar{u}$ ]  $x+1/2, \bar{x}+1/4, \bar{x}+3/4$  [ $u, \bar{u}, \bar{u}$ ]  
 $x+3/4, x+1/4, \bar{x}$  [ $\bar{u}, \bar{u}, u$ ]  $\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2$  [ $u, u, u$ ]  
 $x+1/4, \bar{x}, x+3/4$  [ $\bar{u}, u, \bar{u}$ ]  $\bar{x}, x+3/4, x+1/4$  [ $\bar{u}, u, \bar{u}$ ]  
 $\bar{x}, \bar{x}, \bar{x}$  [ $u, u, u$ ]  $x+3/4, x+1/4, \bar{x}+1/2$  [ $\bar{u}, \bar{u}, u$ ]  
 $x+1/4, \bar{x}+1/2, x+3/4$  [ $\bar{u}, u, \bar{u}$ ]  $\bar{x}+1/2, x+3/4, x+1/4$  [ $u, \bar{u}, \bar{u}$ ]

			$\bar{x}+1/4, \bar{x}+3/4, x [\bar{u}, \bar{u}, u]$	$x+1/2, x+1/2, x+1/2 [u, u, u]$		
			$\bar{x}+3/4, x, \bar{x}+1/4 [\bar{u}, u, \bar{u}]$	$x, \bar{x}+1/4, \bar{x}+3/4 [\bar{u}, u, \bar{u}]$		
48	d	$\bar{4}'$	7/8, 1/8, 1/8 [0,0,0]	3/8, 5/8, 5/8 [0,0,0]	1/8, 7/8, 1/8 [0,0,0]	5/8, 3/8, 5/8 [0,0,0]
			1/8, 1/8, 7/8 [0,0,0]	5/8, 5/8, 3/8 [0,0,0]	7/8, 1/8, 7/8 [0,0,0]	3/8, 5/8, 3/8 [0,0,0]
			5/8, 3/8, 7/8 [0,0,0]	1/8, 7/8, 3/8 [0,0,0]	7/8, 3/8, 1/8 [0,0,0]	3/8, 7/8, 5/8 [0,0,0]
32	c	$\bar{3}$	0,0,0 [u,u,u]	1/4, 3/4, 1/2 [ $\bar{u}, \bar{u}, u$ ]	3/4, 1/2, 1/4 [ $\bar{u}, u, \bar{u}$ ]	1/2, 1/4, 3/4 [u, $\bar{u}, \bar{u}$ ]
			3/4, 1/4, 0 [ $\bar{u}, \bar{u}, u$ ]	1/2, 1/2, 1/2 [u,u,u]	1/4, 0, 3/4 [ $\bar{u}, u, \bar{u}$ ]	0, 3/4, 1/4 [u, $\bar{u}, \bar{u}$ ]
32	b	.32'	1/4, 1/4, 1/4 [u,u,u]	0, 1/2, 3/4 [ $\bar{u}, \bar{u}, u$ ]	1/2, 3/4, 0 [ $\bar{u}, u, \bar{u}$ ]	3/4, 0, 1/2 [u, $\bar{u}, \bar{u}$ ]
			3/4, 3/4, 3/4 [u,u,u]	0, 1/2, 1/4 [ $\bar{u}, \bar{u}, u$ ]	1/2, 1/4, 0 [ $\bar{u}, u, \bar{u}$ ]	1/4, 0, 1/2 [u, $\bar{u}, \bar{u}$ ]
16	a	23.	1/8, 1/8, 1/8 [0,0,0]	7/8, 3/8, 7/8 [0,0,0]	7/8, 7/8, 7/8 [0,0,0]	1/8, 5/8, 1/8 [0,0,0]

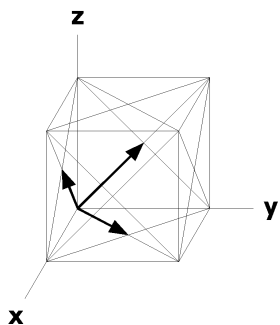
### Symmetry of Special Projections

Along [0,0,1]  $p_6, 4m'm'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/4$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/4$   
 Origin at 1/8, 5/8, z

Along [1,1,1]  $p6'mm'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

Along [1,1,0]  $p2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/4$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0





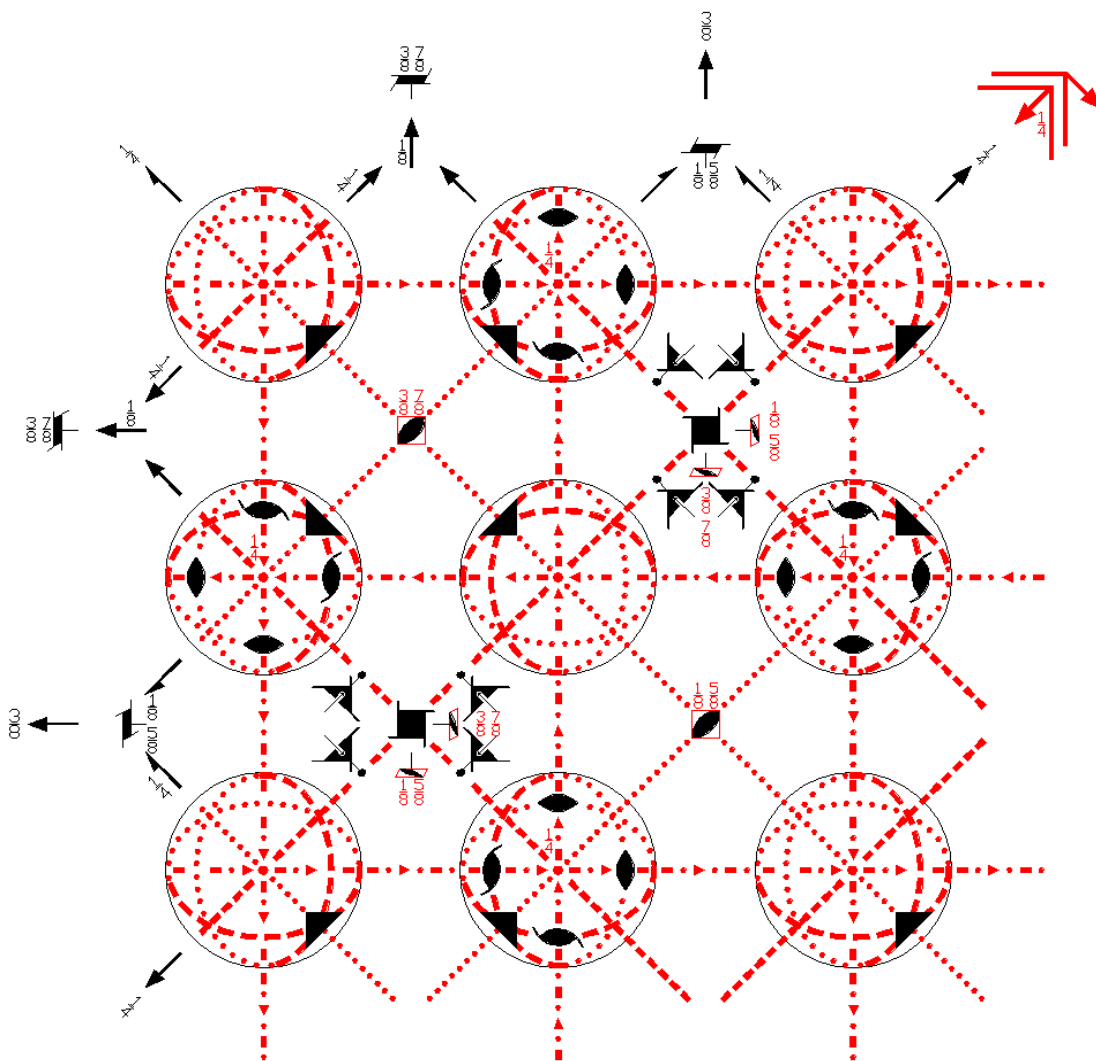
$Fd\bar{3}'c'$

228.5.1637

$m'\bar{3}'m'$

$F4_1/d'\bar{3}'2'/c'$

Cubic



**Origin** at center ( $\bar{3}'$ ), at  $3/8, 3/8, 3/8$  from 23

**Asymmetric unit**  $-1/8 \leq x \leq 3/8$ ;  $-1/8 \leq y \leq 0$ ;  $-1/4 \leq z \leq 0$ ;  $y \leq \min(1/4-x, x)$ ;  $-y-1/4 \leq z \leq y$

**Vertices**  $-1/8, -1/8, -1/8$   $3/8, -1/8, -1/8$   $1/4, 0, 0$   $0, 0, 0$   $1/4, 0, -1/4$   $0, 0, -1/4$

**Symmetry Operations**

For (0,0,0) + set

- |   |  |  |   |
|---|--|--|---|
| (1) 1<br>(1 0,0,0)                              | (2) 2 (0,0,1/2) $1/8, 3/8, z$<br>( $2_z$   $1/4, 3/4, 1/2$ )                                   | (3) 2 (0,1/2,0) $3/8, y, 1/8$<br>( $2_y$   $3/4, 1/2, 1/4$ )                                   | (4) 2 (1/2,0,0) $x, 1/8, 3/8$<br>( $2_x$   $1/2, 1/4, 3/4$ )                              |
| (5) $3^+$ $x, x, x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ (1/3, -1/3, 1/3)<br>$x+1/6, x+5/12, \bar{x}$<br>( $3_{xyz}^{-1}$   $1/2, 1/4, 3/4$ ) | (7) $3^+$ (-1/3, 1/3, 1/3)<br>$x+7/12, x-1/6, \bar{x}$<br>( $3_{xyz}^{-1}$   $1/4, 3/4, 1/2$ ) | (8) $3^+$ (1/3, 1/3, -1/3)<br>$x+5/12, x+7/12, x$<br>( $3_{xyz}^{-1}$   $3/4, 1/2, 1/4$ ) |
| (9) $3^-$ $x, x, x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x+1/4, \bar{x}+1/2, \bar{x}$<br>( $3_{xyz}$   $3/4, 1/2, 1/4$ )                    | (11) $3^-$ $\bar{x}+3/4, \bar{x}+1/4, x$<br>( $3_{xy\bar{z}}$   $1/2, 1/4, 3/4$ )              | (12) $3^-$ $\bar{x}-1/2, x+3/4, \bar{x}$<br>( $3_{xy\bar{z}}$   $1/4, 3/4, 1/2$ )         |

(13) $2 (1/2, 1/2, 0) \ x, x-1/4, 0$ ( $2_{xy}   3/4, 1/4, 0$ )	(14) $2 \ x, \bar{x}+1/2, 1/4$ ( $2_{\bar{xy}}   1/2, 1/2, 1/2$ )	(15) $4^- (0, 0, 3/4) \ 1/8, -1/8, z$ ( $4_z^{-1}   1/4, 0, 3/4$ )	(16) $4^+ (0, 0, 1/4) \ -3/8, 3/8, z$ ( $4_z   0, 3/4, 1/4$ )
(17) $4^- (3/4, 0, 0) \ x, 1/8, -1/8$ ( $4_x^{-1}   3/4, 1/4, 0$ )	(18) $2 (0, 1/2, 1/2) \ 0, y+1/4, y$ ( $2_{yz}   0, 3/4, 1/4$ )	(19) $2 \ 1/4, y+1/2, \bar{y}$ ( $2_{\bar{yz}}   1/2, 1/2, 1/2$ )	(20) $4^+ (1/4, 0, 0) \ x, -3/8, 3/8$ ( $4_x   1/4, 0, 3/4$ )
(21) $4^+ (0, 1/4, 0) \ 3/8, y, -3/8$ ( $4_y   3/4, 1/4, 0$ )	(22) $2 (1/2, 0, 1/2) \ x-1/4, 0, x$ ( $2_{xz}   1/4, 0, 3/4$ )	(23) $4^- (0, 3/4, 0) \ -1/8, y, 1/8$ ( $4_y^{-1}   0, 3/4, 1/4$ )	(24) $2 \ \bar{x}+1/2, 1/4, x$ ( $2_{\bar{xz}}   1/2, 1/2, 1/2$ )
(25) $\bar{1}^- \ 0, 0, 0$ ( $\bar{1}   0, 0, 0$ )'	(26) $d' (3/4, 1/4, 0) \ x, y, 1/4$ ( $m_z   3/4, 1/4, 1/2$ )'	(27) $d' (1/4, 0, 3/4) \ x, 1/4, z$ ( $m_y   1/4, 1/2, 3/4$ )'	(28) $d' (0, 3/4, 1/4) \ 1/4, y, z$ ( $m_x   1/2, 3/4, 1/4$ )'
(29) $\bar{3}^+ \ x, x, x;$ $0, 0, 0$ ( $\bar{3}_{xyz}   0, 0, 0$ )'	(30) $\bar{3}^+ \ \bar{x}-1, x+5/4, \bar{x};$ $-1/4, 1/2, 3/4$ ( $\bar{3}_{\bar{xyz}}^{-1}   1/2, 3/4, 1/4$ )'	(31) $\bar{3}^+ \ x+1/4, \bar{x}+1, \bar{x};$ $1/2, 3/4, -1/4$ ( $\bar{3}_{\bar{xyz}}^{-1}   3/4, 1/4, 1/2$ )'	(32) $\bar{3}^+ \ \bar{x}+5/4, \bar{x}+1/4, x;$ $3/4, -1/4, 1/2$ ( $\bar{3}_{\bar{xyz}}^{-1}   1/4, 1/2, 3/4$ )'
(33) $\bar{3}^- \ x, x, x;$ $0, 0, 0$ ( $\bar{3}_{xyz}^{-1}   0, 0, 0$ )'	(34) $\bar{3}^- \ x+3/4, \bar{x}-1, \bar{x};$ $0, -1/4, 3/4$ ( $\bar{3}_{\bar{xyz}}   1/4, 1/2, 3/4$ )'	(35) $\bar{3}^- \ \bar{x}-1/4, \bar{x}+3/4, x;$ $-14, 3/4, 0$ ( $\bar{3}_{\bar{xyz}}   1/2, 3/4, 1/4$ )'	(36) $\bar{3}^- \ \bar{x}+1, x-1/4, \bar{x};$ $3/4, 0, -1/4$ ( $\bar{3}_{\bar{xyz}}   3/4, 1/4, 1/2$ )'
(37) $g' (-1/4, 1/4, 1/2) \ x+1/2, \bar{x}, z$ ( $m_{xy}   1/4, 3/4, 0$ )'	(38) $n' (1/2, 1/2, 1/2) \ x, x, z$ ( $m_{\bar{xy}}   1/2, 1/2, 1/2$ )'	(39) $\bar{4}^- \ 3/8, 3/8, z; \ 3/8, 3/8, 1/8$ ( $\bar{4}_z^{-1}   3/4, 0, 1/4$ )'	(40) $\bar{4}^+ \ 1/8, 1/8, z; \ 1/8, 1/8, 3/8$ ( $\bar{4}_z   0, 1/4, 3/4$ )'
(41) $\bar{4}^- \ x, 3/8, 3/8; \ 1/8, 3/8, 3/8$ ( $\bar{4}_x^{-1}   1/4, 3/4, 0$ )'	(42) $g' (0, -1/4, 1/4) \ x, y+1/2, \bar{y}$ ( $m_{yz}   0, 1/4, 3/4$ )'	(43) $n' (1/2, 1/2, 1/2) \ x, y, y$ ( $m_{\bar{yz}}   1/2, 1/2, 1/2$ )'	(44) $\bar{4}^+ \ x, 1/8, 1/8; \ 3/8, 1/8, 1/8$ ( $\bar{4}_x   3/4, 0, 1/4$ )'
(45) $\bar{4}^+ \ 1/8, y, 1/8; \ 1/8, 3/8, 1/8$ ( $\bar{4}_y   1/4, 3/4, 0$ )'	(46) $g' (1/4, 0, -1/4) \ \bar{x}+1/2, y, x$ ( $m_{xz}   3/4, 0, 1/4$ )'	(47) $\bar{4}^- \ 3/8, y, 3/8; \ 3/8, 1/8, 3/8$ ( $\bar{4}_y^{-1}   0, 1/4, 3/4$ )'	(48) $n' (1/2, 1/2, 1/2) \ x, y, x$ ( $m_{\bar{xz}}   1/2, 1/2, 1/2$ )'

For (0, 1/2, 1/2) + set

(1) $t (0, 1/2, 1/2)$ ( $1   0, 1/2, 1/2$ )	(2) $2 \ 1/8, 1/8, z$ ( $2_z   1/4, 1/4, 0$ )	(3) $2 \ 3/8, y, 3/8$ ( $2_y   3/4, 0, 3/4$ )	(4) $2 (1/2, 0, 0) \ x, 3/8, 1/8$ ( $2_x   1/2, 3/4, 1/4$ )
(5) $3^+ (1/3, 1/3, 1/3)$ $x-1/3, x-1/6, x$ ( $3_{xyz}   0, 1/2, 1/2$ )	(6) $3^+ \ \bar{x}+1/2, x+1/4, \bar{x}$ ( $3_{\bar{xyz}}^{-1}   1/2, 3/4, 1/4$ )	(7) $3^+ \ x+1/4, \bar{x}, \bar{x}$ ( $3_{\bar{xyz}}^{-1}   1/4, 1/4, 0$ )	(8) $3^+ \ \bar{x}+3/4, \bar{x}+3/4, x$ ( $3_{\bar{xyz}}^{-1}   3/4, 0, 3/4$ )
(9) $3^- (1/3, 1/3, 1/3)$ $x-1/6, x+1/6, x$ ( $3_{xyz}^{-1}   0, 1/2, 1/2$ )	(10) $3^- \ x+3/4, \bar{x}, \bar{x}$ ( $3_{\bar{xyz}}   3/4, 0, 3/4$ )	(11) $3^- (1/3, 1/3, -1/3)$ $x+7/12, \bar{x}+5/12, x$ ( $3_{\bar{xyz}}   1/2, 3/4, 1/4$ )	(12) $3^- \ \bar{x}, x+1/4, \bar{x}$ ( $3_{\bar{xyz}}   1/4, 1/4, 0$ )
(13) $2 (3/4, 3/4, 0) \ x, x, 1/4$ ( $2_{xy}   3/4, 3/4, 1/2$ )	(14) $2 (1/4, -1/4, 0) \ x, \bar{x}+1/4, 0$ ( $2_{\bar{xy}}   1/2, 0, 0$ )	(15) $4^- (0, 0, 1/4) \ 3/8, 1/8, z$ ( $4_z^{-1}   1/4, 1/2, 1/4$ )	(16) $4^+ (0, 0, 3/4) \ -1/8, 1/8, z$ ( $4_z   0, 1/4, 3/4$ )
(17) $4^- (3/4, 0, 0) \ 5/8, -1/8$ ( $4_x^{-1}   3/4, 3/4, 1/2$ )	(18) $2 (0, 1/2, 1/2) \ 0, y-1/4, y$ ( $2_{yz}   0, 1/4, 3/4$ )	(19) $2 \ 1/4, y, \bar{y}$ ( $2_{\bar{yz}}   1/2, 0, 0$ )	(20) $4^+ (1/4, 0, 0) \ x, 1/8, 3/8$ ( $4_x   1/4, 1/2, 1/4$ )
(21) $4^+ (0, 3/4, 0) \ 5/8, y, -1/8$ ( $4_y   3/4, 3/4, 1/2$ )	(22) $2 (1/4, 0, 1/4) \ x, 1/4, x$ ( $2_{xz}   1/4, 1/2, 1/4$ )	(23) $4^- (0, 1/4, 0) \ -3/8, y, 3/8$ ( $4_y^{-1}   0, 1/4, 3/4$ )	(24) $2 (1/4, 0, -1/4) \ \bar{x}+1/4, 0, x$ ( $2_{\bar{xz}}   1/2, 0, 0$ )
(25) $\bar{1}^- \ 0, 1/4, 1/4$ ( $\bar{1}   0, 1/2, 1/2$ )'	(26) $d' (3/4, 3/4, 0) \ x, y, 0$ ( $m_z   3/4, 3/4, 0$ )'	(27) $d' (1/4, 0, 1/4) \ x, 0, z$ ( $m_y   1/4, 0, 1/4$ )'	(28) $d' (0, 1/4, 3/4) \ 1/4, y, z$ ( $m_x   1/2, 1/4, 3/4$ )'
(29) $\bar{3}^+ \ x, x+1/2, x;$ $0, 1/2, 0$ ( $\bar{3}_{xyz}   0, 1/2, 1/2$ )'	(30) $\bar{3}^+ \ \bar{x}-1, x+3/4, \bar{x};$ $-1/4, 0, 3/4$ ( $\bar{3}_{\bar{xyz}}^{-1}   1/2, 1/4, 3/4$ )'	(31) $\bar{3}^+ \ x-3/4, \bar{x}+3/2, \bar{x};$ $0, 3/4, -3/4$ ( $\bar{3}_{\bar{xyz}}^{-1}   3/4, 3/4, 0$ )'	(32) $\bar{3}^+ \ \bar{x}+1/4, \bar{x}-1/4, x;$ $1/4, -1/4, 0$ ( $\bar{3}_{\bar{xyz}}^{-1}   1/4, 0, 1/4$ )'

- |  |  |  |  |
|--|--|--|--|
| (33) $\bar{3}^- \mid x-1/2, x-1/2, x; 0, 0, 1/2$<br>( $\bar{3}_{xyz}^{-1} \mid 0, 1/2, 1/2$ )' | (34) $\bar{3}^- \mid x+1/4, \bar{x}-1/2, \bar{x}; 0, -1/4, 1/4$<br>( $\bar{3}_{xyz} \mid 1/4, 0, 1/4$ )' | (35) $\bar{3}^- \mid \bar{x}+1/4, \bar{x}+5/4, x; -1/4, 3/4, 1/2$<br>( $\bar{3}_{xyz} \mid 1/2, 1/4, 3/4$ )' | (36) $\bar{3}^- \mid \bar{x}+3/2, x-3/4, \bar{x}; 3/4, 0, -3/4$<br>( $\bar{3}_{xyz} \mid 3/4, 3/4, 0$ )' |
| (37) $c' (0, 0, 1/2) \mid x+1/4, \bar{x}, z$<br>( $m_{xy} \mid 1/4, 1/4, 1/2$ )'               | (38) $g' (1/4, 1/4, 0) \mid x+1/4, x, z$<br>( $m_{xy} \mid 1/2, 0, 0$ )'                                 | (39) $\bar{4}^- \mid 1/8, 5/8, z; 1/8, 5/8, 3/8$<br>( $\bar{4}_z^{-1} \mid 3/4, 1/2, 3/4$ )'                 | (40) $\bar{4}^+ \mid 3/8, 3/8, z; 3/8, 3/8, 1/8$<br>( $\bar{4}_z \mid 0, 3/4, 1/4$ )'                    |
| (41) $\bar{4}^- \mid x, -1/8, 3/8; 1/8, -1/8, 3/8$<br>( $\bar{4}_x^{-1} \mid 1/4, 1/4, 1/2$ )' | (42) $g' (0, 1/4, -1/4) \mid x, y+1/2, \bar{y}$<br>( $m_{yz} \mid 0, 3/4, 1/4$ )'                        | (43) $a' (1/2, 0, 0) \mid x, y, y$<br>( $m_{yz} \mid 1/2, 0, 0$ )'   | (44) $\bar{4}^+ \mid x, 5/8, 1/8; 3/8, 5/8, 1/8$<br>( $\bar{4}_x \mid 3/4, 0, 3/4$ )'                    |
| (45) $\bar{4}^+ \mid -1/8, y, 3/8; -1/8, 1/8, 3/8$<br>( $\bar{4}_y \mid 1/4, 1/4, 1/2$ )'      | (46) $b' (0, 1/2, 0) \mid \bar{x}+3/4, y, x$<br>( $m_{xz} \mid 3/4, 1/2, 3/4$ )'                         | (47) $\bar{4}^- \mid 1/8, y, 1/8; 1/8, 3/8, 1/8$<br>( $\bar{4}_y^{-1} \mid 0, 3/4, 1/4$ )'                   | (48) $g' (1/4, 0, 1/4) \mid x+1/4, y, x$<br>( $m_{xz} \mid 1/2, 0, 0$ )'                                 |

For (1/2, 0, 1/2) + set

- |  |   |   |   |
|--|---|---|---|
| (1) $t (1/2, 0, 1/2)$<br>( $1 \mid 1/2, 0, 1/2$ )  | (2) $2 \mid 3/8, 3/8, z$<br>( $2_z \mid 3/4, 3/4, 0$ )  | (3) $2 (0, 1/2, 0) \mid 1/8, y, 3/8$<br>( $2_y \mid 1/4, 1/2, 3/4$ )  | (4) $2 \mid x, 1/8, 1/8$<br>( $2_x \mid 0, 1/4, 1/4$ )  |
| (5) $3^+ (1/3, 1/3, 1/3)$<br>$x+1/6, x-1/6, x$<br>( $3_{xyz} \mid 1/2, 0, 1/2$ )             | (6) $3^+ \mid \bar{x}, x+1/4, \bar{x}$<br>( $3_{xyz}^{-1} \mid 0, 1/4, 1/4$ )                                 | (7) $3^+ \mid x+3/4, \bar{x}, \bar{x}$<br>( $3_{xyz}^{-1} \mid 3/4, 3/4, 0$ )                                 | (8) $3^+ \mid \bar{x}+1/4, \bar{x}+3/4, x$<br>( $3_{xyz}^{-1} \mid 1/4, 1/2, 3/4$ )                             |
| (9) $3^- (1/3, 1/3, 1/3)$<br>$x-1/6, x-1/3, x$<br>( $3_{xyz}^{-1} \mid 1/2, 0, 1/2$ )        | (10) $3^- (-1/3, 1/3, 1/3)$<br>$x+5/12, \bar{x}+1/6, \bar{x}$<br>( $3_{xyz} \mid 1/4, 1/2, 3/4$ )             | (11) $3^- \mid \bar{x}+1/4, \bar{x}+1/4, x$<br>( $3_{xyz} \mid 0, 1/4, 1/4$ )                                 | (12) $3^- \mid \bar{x}, x+3/4, \bar{x}$<br>( $3_{xyz} \mid 3/4, 3/4, 0$ )                                       |
| (13) $2 (1/4, 1/4, 0) \mid x, x, 1/4$<br>( $2_{xy} \mid 1/4, 1/4, 1/2$ )                     | (14) $2 (-1/4, 1/4, 0) \mid x, \bar{x}+1/4, 0$<br>( $2_{xy} \mid 0, 1/2, 0$ )                                 | (15) $4^- (0, 0, 1/4) \mid 3/8, -3/8, z$<br>( $4_z^{-1} \mid 3/4, 0, 1/4$ )                                   | (16) $4^+ (0, 0, 3/4) \mid -1/8, 5/8, z$<br>( $4_z \mid 1/2, 3/4, 3/4$ )  |
| (17) $4^- (1/4, 0, 0) \mid x, 3/8, 1/8$<br>( $4_x^{-1} \mid 1/4, 1/4, 1/2$ )                 | (18) $2 (0, 3/4, 3/4) \mid 1/4, y, y$<br>( $2_{yz} \mid 1/2, 3/4, 3/4$ )                                      | (19) $2 (0, 1/4, -1/4) \mid 0, y+1/4, \bar{y}$<br>( $2_{yz} \mid 0, 1/2, 0$ )                                 | (20) $4^+ (3/4, 0, 0) \mid x, -1/8, 1/8$<br>( $4_x \mid 3/4, 0, 1/4$ )  |
| (21) $4^+ (0, 1/4, 0) \mid 3/8, y, 1/8$<br>( $4_y \mid 1/4, 1/4, 1/2$ )                      | (22) $2 (1/2, 0, 1/2) \mid x+1/4, 0, x$<br>( $2_{xz} \mid 3/4, 0, 1/4$ )                                      | (23) $4^- (0, 3/4, 0) \mid -1/8, y, 5/8$<br>( $4_y^{-1} \mid 1/2, 3/4, 3/4$ )                                 | (24) $2 \mid \bar{x}, 1/4, x$<br>( $2_{xz} \mid 0, 1/2, 0$ )  |
| (25) $\bar{1} \mid 1/4, 0, 1/4$<br>( $\bar{1} \mid 1/2, 0, 1/2$ )'                           | (26) $d' (1/4, 1/4, 0) \mid x, y, 0$<br>( $m_z \mid 1/4, 1/4, 0$ )'   | (27) $d' (3/4, 0, 1/4) \mid x, 1/4, z$<br>( $m_y \mid 3/4, 1/2, 1/4$ )'                                       | (28) $d' (0, 3/4, 3/4) \mid 0, y, z$<br>( $m_x \mid 0, 3/4, 3/4$ )'   |
| (29) $\bar{3}^+ \mid x-1/2, x-1/2, x; 0, 0, 1/2$<br>( $\bar{3}_{xyz} \mid 1/2, 0, 1/2$ )'    | (30) $\bar{3}^+ \mid \bar{x}-3/2, x+3/4, \bar{x}; -3/4, 0, 3/4$<br>( $\bar{3}_{xyz}^{-1} \mid 0, 3/4, 3/4$ )' | (31) $\bar{3}^+ \mid x-1/4, \bar{x}+1/2, \bar{x}; 0, 1/4, -1/4$<br>( $\bar{3}_{xyz}^{-1} \mid 1/4, 1/4, 0$ )' | (32) $\bar{3}^+ \mid \bar{x}+3/4, \bar{x}-1/4, x; 3/4, -1/4, 0$<br>( $\bar{3}_{xyz}^{-1} \mid 3/4, 1/2, 1/4$ )' |
| (33) $\bar{3}^- \mid x+1/2, x, x; 1/2, 0, 0$<br>( $\bar{3}_{xyz}^{-1} \mid 1/2, 0, 1/2$ )'   | (34) $\bar{3}^- \mid x+5/4, \bar{x}-1, \bar{x}; 1/2, -1/4, 3/4$<br>( $\bar{3}_{xyz} \mid 3/4, 1/2, 1/4$ )'    | (35) $\bar{3}^- \mid \bar{x}-3/4, \bar{x}+3/4, x; -3/4, 3/4, 0$<br>( $\bar{3}_{xyz} \mid 0, 3/4, 3/4$ )'      | (36) $\bar{3}^- \mid \bar{x}+1/2, x-1/4, \bar{x}; 1/4, 0, -1/4$<br>( $\bar{3}_{xyz} \mid 1/4, 1/4, 0$ )'        |
| (37) $c' (0, 0, 1/2) \mid x+3/4, \bar{x}, z$<br>( $m_{xy} \mid 3/4, 3/4, 1/2$ )'             | (38) $g' (1/4, 1/4, 0) \mid x-1/4, x, z$<br>( $m_{xy} \mid 0, 1/2, 0$ )'                                      | (39) $\bar{4}^- \mid 1/8, 1/8, z; 1/8, 1/8, 3/8$<br>( $\bar{4}_z^{-1} \mid 1/4, 0, 3/4$ )'                    | (40) $\bar{4}^+ \mid 3/8, -1/8, z; 3/8, -1/8, 1/8$<br>( $\bar{4}_z \mid 1/2, 1/4, 1/4$ )'                       |
| (41) $\bar{4}^- \mid x, 1/8, 5/8; 3/8, 1/8, 5/8$<br>( $\bar{4}_x^{-1} \mid 3/4, 3/4, 1/2$ )' | (42) $a' (1/2, 0, 0) \mid x, y+1/4, \bar{y}$<br>( $m_{yz} \mid 1/2, 1/4, 1/4$ )'                              | (43) $g' (0, 1/4, 1/4) \mid x, y+1/4, y$<br>( $m_{yz} \mid 0, 1/2, 0$ )'                                      | (44) $\bar{4}^+ \mid x, 3/8, 3/8; 1/8, 3/8, 3/8$<br>( $\bar{4}_x \mid 1/4, 0, 3/4$ )'                           |
| (45) $\bar{4}^+ \mid 1/8, y, 5/8; 1/8, 3/8, 5/8$<br>( $\bar{4}_y \mid 3/4, 3/4, 1/2$ )'      | (46) $g' (-1/4, 0, 1/4) \mid \bar{x}+1/2, y, x$<br>( $m_{xz} \mid 1/4, 0, 3/4$ )'                             | (47) $\bar{4}^- \mid 3/8, y, -1/8; 3/8, 1/8, -1/8$<br>( $\bar{4}_y^{-1} \mid 1/2, 1/4, 1/4$ )'                | (48) $b' (0, 1/2, 0) \mid x, y, x$<br>( $m_{xz} \mid 0, 1/2, 0$ )'  |

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (1   1/2,1/2,0)	(2) 2 (0,0,1/2) 3/8,1/8,z (2 <sub>z</sub>   3/4,1/4,1/2)	(3) 2 1/8,y,1/8 (2 <sub>y</sub>   1/4,0,1/4)	(4) 2 x,3/8,3/8 (2 <sub>x</sub>   0,3/4,3/4)
(5) 3 <sup>+</sup> (1/3,1/3,1/3) x+1/6,x+1/3,x (3 <sub>xyz</sub>   1/2,1/2,0)	(6) 3 <sup>+</sup> x̄,x+3/4,x̄ (3 <sub>xyz</sub> <sup>-1</sup>   0,3/4,3/4)	(7) 3 <sup>+</sup> x+3/4,x̄-1/2,x̄ (3 <sub>xyz</sub> <sup>-1</sup>   3/4,1/4,1/2)	(8) 3 <sup>+</sup> x̄+1/4,x̄+1/4,x (3 <sub>xyz</sub> <sup>-1</sup>   1/4,0,1/4)
(9) 3 <sup>-</sup> (1/3,1/3,1/3) x+1/3,x+1/6,x (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)	(10) 3 <sup>-</sup> x+1/4,x̄,x̄ (3 <sub>xyz</sub>   1/4,0,1/4)	(11) 3 <sup>-</sup> x̄+3/4,x̄+3/4,x (3 <sub>xyz</sub>   0,3/4,3/4)	(12) 3 <sup>-</sup> (1/3,-1/3,1/3) x̄-1/6,x+7/12,x̄ (3 <sub>xyz</sub>   3/4,1/4,1/2)
(13) 2 (1/2,1/2,0) x,x+1/4,0 (2 <sub>xy</sub>   1/4,3/4,0)	(14) 2 x,x̄,1/4 (2 <sub>xy</sub>   0,0,1/2)	(15) 4 <sup>-</sup> (0,0,3/4) 5/8,-1/8,z (4 <sub>z</sub> <sup>-1</sup>   3/4,1/2,3/4)	(16) 4 <sup>+</sup> (0,0,1/4) 1/8,3/8,z (4 <sub>z</sub>   1/2,1/4,1/4)
(17) 4 <sup>-</sup> (1/4,0,0) x,3/8,-3/8 (4 <sub>x</sub> <sup>-1</sup>   1/4,3/4,0)	(18) 2 (0,1/4,1/4) 1/4,y,y (2 <sub>yz</sub>   1/2,1/4,1/4)	(19) 2 (0,-1/4,1/4) 0,y+1/4,ȳ (2 <sub>yz</sub>   0,0,1/2)	(20) 4 <sup>+</sup> (3/4,0,0) x,-1/8,5/8 (4 <sub>x</sub>   3/4,1/2,3/4)
(21) 4 <sup>+</sup> (0,3/4,0) 1/8,y,-1/8 (4 <sub>y</sub>   1/4,3/4,0)	(22) 2 (3/4,0,3/4) x,1/4,x (2 <sub>xz</sub>   3/4,1/2,3/4)	(23) 4 <sup>-</sup> (0,1/4,0) 1/8,y,3/8 (4 <sub>y</sub> <sup>-1</sup>   1/2,1/4,1/4)	(24) 2 (-1/4,0,1/4) x̄+1/4,0,x (2 <sub>xz</sub>   0,0,1/2)
(25) 1 <sup>-</sup> 1/4,1/4,0 (1   1/2,1/2,0)'	(26) d' (1/4,3/4,0) x,y,1/4 (m <sub>z</sub>   1/4,3/4,1/2)'	(27) d' (3/4,0,3/4) x,0,z (m <sub>y</sub>   3/4,0,3/4)'	(28) d' (0,1/4,1/4) 0,y,z (m <sub>x</sub>   0,1/4,1/4)'
(29) 3 <sup>+</sup> x+1/2,x,x; 1/2,0,0 (3 <sub>xyz</sub>   1/2,1/2,0)'	(30) 3 <sup>+</sup> x̄-1/2,x+1/4,x̄; -1/4,0,1/4 (3 <sub>xyz</sub> <sup>-1</sup>   0,1/4,1/4)'	(31) 3 <sup>+</sup> x-1/4,x̄+1,x̄; 0,3/4,-1/4 (3 <sub>xyz</sub> <sup>-1</sup>   1/4,3/4,1/2)'	(32) 3 <sup>+</sup> x̄+3/4,x̄-3/4,x; 3/4,-3/4,0 (3 <sub>xyz</sub> <sup>-1</sup>   3/4,0,3/4)'
(33) 3 <sup>-</sup> x,x+1/2,x; 0,1/2,0 (3 <sub>xyz</sub> <sup>-1</sup>   1/2,1/2,0)'	(34) 3 <sup>-</sup> x+3/4,x̄-3/2,x̄; 0,-3/4,3/4 (3 <sub>xyz</sub>   3/4,0,3/4)'	(35) 3 <sup>-</sup> x̄-1/4,x̄+1/4,x; -1/4,1/4,0 (3 <sub>xyz</sub>   0,1/4,1/4)'	(36) 3 <sup>-</sup> x̄+1,x+1/4,x̄; 3/4,1/2,-1/4 (3 <sub>xyz</sub>   1/4,3/4,1/2)'
(37) g' (1/4,-1/4,0) x+1/2,x̄,z (m <sub>xy</sub>   3/4,1/4,0)'	(38) c' (0,0,1/2) x,x,z (m <sub>xy</sub>   0,0,1/2)'	(39) 4 <sup>-</sup> -1/8,3/8,z; -1/8,3/8,1/8 (4 <sub>z</sub> <sup>-1</sup>   1/4,1/2,1/4)'	(40) 4 <sup>+</sup> 5/8,1/8,z; 5/8,1/8,3/8 (4 <sub>z</sub>   1/2,3/4,3/4)'
(41) 4 <sup>-</sup> x,1/8,1/8; 3/8,1/8,1/8 (4 <sub>x</sub> <sup>-1</sup>   3/4,1/4,0)'	(42) a' (1/2,0,0) x,y+3/4,ȳ (m <sub>yz</sub>   1/2,3/4,3/4)'	(43) g' (0,1/4,1/4) x,y-1/4,y (m <sub>yz</sub>   0,0,1/2)'	(44) 4 <sup>+</sup> x,3/8,-1/8; 1/8,3/8,-1/8 (4 <sub>x</sub>   1/4,1/2,1/4)'
(45) 4 <sup>+</sup> 3/8,y,3/8; 3/8,1/8,3/8 (4 <sub>y</sub>   3/4,1/4,0)'	(46) b' (0,1/2,0) x̄+1/4,y,x (m <sub>xz</sub>   1/4,1/2,1/4)'	(47) 4 <sup>-</sup> 5/8,y,1/8; 5/8,3/8,1/8 (4 <sub>y</sub> <sup>-1</sup>   1/2,3/4,3/4)'	(48) g' (1/4,0,1/4) x-1/4,y,x (m <sub>xz</sub>   0,0,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

**Positions**

## Coordinates

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

192	h	1	(0,0,0) +	(0,1/2,1/2) +	(1/2,0,1/2) +	(1/2,1/2,0) +		
(1)	x,y,z	[u,v,w]	(2) x̄+1/4,ȳ+3/4,z+1/2	[ū,v̄,w]	(3) x̄+3/4,y+1/2,z̄+1/4	[ū,v̄,w̄]	(4) x+1/2,ȳ+1/4,z̄+3/4	[u,v̄,w̄]
(5)	z,x,y	[w,u,v]	(6) z+1/2,x̄+1/4,ȳ+3/4	[w̄,ū,v̄]	(7) z̄+1/4,x̄+3/4,y+1/2	[w̄,ū,v]	(8) z̄+3/4,x+1/2,ȳ+1/4	[w̄,u,v̄]

- (9)  $y, z, x [v, w, u]$  (10)  $\bar{y}+3/4, z+1/2, \bar{x}+1/4 [\bar{v}, w, \bar{u}]$  (11)  $y+1/2, \bar{z}+1/4, \bar{x}+3/4 [v, \bar{w}, \bar{u}]$  (12)  $\bar{y}+1/4, \bar{z}+3/4, x+1/2 [\bar{v}, \bar{w}, u]$   
 (13)  $y+3/4, x+1/4, \bar{z} [v, u, \bar{w}]$  (14)  $\bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2 [\bar{v}, \bar{u}, \bar{w}]$  (15)  $y+1/4, \bar{x}, z+3/4 [v, \bar{u}, w]$  (16)  $\bar{y}, x+3/4, z+1/4 [\bar{v}, u, w]$   
 (17)  $x+3/4, z+1/4, \bar{y} [u, w, \bar{v}]$  (18)  $\bar{x}, z+3/4, y+1/4 [\bar{u}, w, v]$  (19)  $\bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2 [\bar{u}, \bar{w}, \bar{v}]$  (20)  $x+1/4, \bar{z}, y+3/4 [u, \bar{w}, v]$   
 (21)  $z+3/4, y+1/4, \bar{x} [w, v, \bar{u}]$  (22)  $z+1/4, \bar{y}, x+3/4 [w, \bar{v}, u]$  (23)  $\bar{z}, y+3/4, x+1/4 [\bar{w}, v, u]$  (24)  $\bar{z}+1/2, \bar{y}+1/2, \bar{x}+1/2 [\bar{w}, \bar{v}, \bar{u}]$   
 (25)  $\bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}]$  (26)  $x+3/4, y+1/4, \bar{z}+1/2 [u, v, \bar{w}]$  (27)  $x+1/4, \bar{y}+1/2, z+3/4 [u, \bar{v}, w]$  (28)  $\bar{x}+1/2, y+3/4, z+1/4 [\bar{u}, v, w]$   
 (29)  $\bar{z}, \bar{x}, \bar{y} [\bar{w}, \bar{u}, \bar{v}]$  (30)  $\bar{z}+1/2, x+3/4, y+1/4 [\bar{w}, u, v]$  (31)  $z+3/4, x+1/4, \bar{y}+1/2 [w, u, \bar{v}]$  (32)  $z+1/4, \bar{x}+1/2, y+3/4 [w, \bar{u}, v]$   
 (33)  $\bar{y}, \bar{z}, \bar{x} [\bar{v}, \bar{w}, \bar{u}]$  (34)  $y+1/4, \bar{z}+1/2, x+3/4 [v, \bar{w}, u]$  (35)  $\bar{y}+1/2, z+3/4, x+1/4 [\bar{v}, w, u]$  (36)  $y+3/4, z+1/4, \bar{x}+1/2 [v, w, \bar{u}]$   
 (37)  $\bar{y}+1/4, \bar{x}+3/4, z [\bar{v}, \bar{u}, w]$  (38)  $y+1/2, x+1/2, z+1/2 [v, u, w]$  (39)  $\bar{y}+3/4, x, \bar{z}+1/4 [\bar{v}, u, \bar{w}]$  (40)  $y, \bar{x}+1/4, \bar{z}+3/4 [v, \bar{u}, \bar{w}]$   
 (41)  $\bar{x}+1/4, \bar{z}+3/4, y [\bar{u}, \bar{w}, v]$  (42)  $x, \bar{z}+1/4, \bar{y}+3/4 [u, \bar{w}, \bar{v}]$  (43)  $x+1/2, z+1/2, y+1/2 [u, w, v]$  (44)  $\bar{x}+3/4, z, \bar{y}+1/4 [\bar{u}, w, \bar{v}]$   
 (45)  $\bar{z}+1/4, \bar{y}+3/4, x [\bar{w}, \bar{v}, u]$  (46)  $\bar{z}+3/4, y, \bar{x}+1/4 [\bar{w}, v, \bar{u}]$  (47)  $z, \bar{y}+1/4, \bar{x}+3/4 [w, \bar{v}, \bar{u}]$  (48)  $z+1/2, y+1/2, x+1/2 [w, v, u]$

96 g ..2

- $1/4, y, \bar{y} [0, \bar{v}, v]$   $0, \bar{y}+3/4, \bar{y}+1/2 [0, v, v]$   $1/2, y+1/2, y+1/4 [0, \bar{v}, \bar{v}]$   $3/4, \bar{y}+1/4, y+3/4 [0, v, \bar{v}]$   
 $\bar{y}, 1/4, y [v, 0, \bar{v}]$   $\bar{y}+1/2, 0, \bar{y}+3/4 [v, 0, v]$   $y+1/4, 1/2, y+1/2 [\bar{v}, 0, \bar{v}]$   $y+3/4, 3/4, \bar{y}+1/4 [\bar{v}, 0, v]$   
 $y, \bar{y}, 1/4 [\bar{v}, v, 0]$   $\bar{y}+3/4, \bar{y}+1/2, 0 [v, v, 0]$   $y+1/2, y+1/4, 1/2 [\bar{v}, \bar{v}, 0]$   $\bar{y}+1/4, y+3/4, 3/4 [v, \bar{v}, 0]$   
 $3/4, \bar{y}, y [0, v, \bar{v}]$   $0, y+1/4, y+1/2 [0, \bar{v}, \bar{v}]$   $1/2, \bar{y}+1/2, \bar{y}+3/4 [0, v, v]$   $1/4, y+3/4, \bar{y}+1/4 [0, \bar{v}, v]$   
 $y, 3/4, \bar{y} [\bar{v}, 0, v]$   $y+1/2, 0, y+1/4 [\bar{v}, 0, \bar{v}]$   $\bar{y}+3/4, 1/2, \bar{y}+1/2 [v, 0, v]$   $\bar{y}+1/4, 1/4, y+3/4 [v, 0, \bar{v}]$   
 $\bar{y}, y, 3/4 [v, \bar{v}, 0]$   $y+1/4, y+1/2, 0 [\bar{v}, \bar{v}, 0]$   $\bar{y}+1/2, \bar{y}+3/4, 1/2 [v, v, 0]$   $y+3/4, \bar{y}+1/4, 1/4 [\bar{v}, v, 0]$

- 96 f 2..  $x, 1/8, 1/8 [u, 0, 0]$   $\bar{x}+1/4, 5/8, 5/8 [\bar{u}, 0, 0]$   $1/8, x, 1/8 [0, u, 0]$   $5/8, \bar{x}+1/4, 5/8 [0, \bar{u}, 0]$   
 $1/8, 1/8, x [0, 0, u]$   $5/8, 5/8, \bar{x}+1/4 [0, 0, \bar{u}]$   $7/8, x+1/4, 7/8 [0, u, 0]$   $3/8, \bar{x}+1/2, 3/8 [0, \bar{u}, 0]$   
 $x+3/4, 3/8, 7/8 [u, 0, 0]$   $\bar{x}, 7/8, 3/8 [\bar{u}, 0, 0]$   $7/8, 3/8, \bar{x} [0, 0, \bar{u}]$   $3/8, 7/8, x+3/4 [0, 0, u]$   
 $\bar{x}, 7/8, 7/8 [\bar{u}, 0, 0]$   $x+3/4, 3/8, 3/8 [u, 0, 0]$   $7/8, \bar{x}, 7/8 [0, \bar{u}, 0]$   $3/8, x+3/4, 3/8 [0, u, 0]$   
 $7/8, 7/8, \bar{x} [0, 0, \bar{u}]$   $3/8, 3/8, x+3/4 [0, 0, u]$   $1/8, \bar{x}+3/4, 1/8 [0, \bar{u}, 0]$   $5/8, x+1/2, 5/8 [0, u, 0]$   
 $\bar{x}+1/4, 5/8, 1/8 [\bar{u}, 0, 0]$   $x, 1/8, 5/8 [u, 0, 0]$   $1/8, 5/8, x [0, 0, u]$   $5/8, 1/8, \bar{x}+1/4 [0, 0, \bar{u}]$

- 64 e .3.  $x, x, x [u, u, u]$   $\bar{x}+1/4, \bar{x}+3/4, x+1/2 [\bar{u}, \bar{u}, u]$   
 $\bar{x}+3/4, x+1/2, \bar{x}+1/4 [\bar{u}, u, \bar{u}]$   $x+1/2, \bar{x}+1/4, \bar{x}+3/4 [\bar{u}, u, \bar{u}]$   
 $x+3/4, x+1/4, \bar{x} [u, u, \bar{u}]$   $\bar{x}+1/2, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, \bar{u}]$   
 $x+1/4, \bar{x}, x+3/4 [u, \bar{u}, u]$   $\bar{x}, x+3/4, x+1/4 [\bar{u}, u, u]$   
 $\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$   $x+3/4, x+1/4, \bar{x}+1/2 [u, u, \bar{u}]$   
 $x+1/4, \bar{x}+1/2, x+3/4 [u, \bar{u}, u]$   $\bar{x}+1/2, x+3/4, x+1/4 [\bar{u}, u, u]$

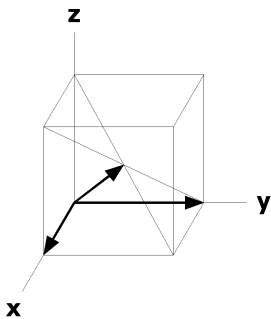
			$\bar{x}+1/4, \bar{x}+3/4, x$ [ $\bar{u}, \bar{u}, u$ ]	$x+1/2, x+1/2, x+1/2$ [ $u, u, u$ ]		
			$\bar{x}+3/4, x, \bar{x}+1/4$ [ $\bar{u}, u, \bar{u}$ ]	$x, \bar{x}+1/4, \bar{x}+3/4$ [ $\bar{u}, u, \bar{u}$ ]		
48	d	$\bar{4}'..$	7/8, 1/8, 1/8 [0,0,0]	3/8, 5/8, 5/8 [0,0,0]	1/8, 7/8, 1/8 [0,0,0]	5/8, 3/8, 5/8 [0,0,0]
			1/8, 1/8, 7/8 [0,0,0]	5/8, 5/8, 3/8 [0,0,0]	7/8, 1/8, 7/8 [0,0,0]	3/8, 5/8, 3/8 [0,0,0]
			5/8, 3/8, 7/8 [0,0,0]	1/8, 7/8, 3/8 [0,0,0]	7/8, 3/8, 1/8 [0,0,0]	3/8, 7/8, 5/8 [0,0,0]
32	c	$\bar{3}'.$	0,0,0 [0,0,0]	1/4, 3/4, 1/2 [0,0,0]	3/4, 1/2, 1/4 [0,0,0]	1/2, 1/4, 3/4 [0,0,0]
			3/4, 1/4, 0 [0,0,0]	1/2, 1/2, 1/2 [0,0,0]	1/4, 0, 3/4 [0,0,0]	0, 3/4, 1/4 [0,0,0]
32	b	.32	1/4, 1/4, 1/4 [0,0,0]	0, 1/2, 3/4 [0,0,0]	1/2, 3/4, 0 [0,0,0]	3/4, 0, 1/2 [0,0,0]
			3/4, 3/4, 3/4 [0,0,0]	0, 1/2, 1/4 [0,0,0]	1/2, 1/4, 0 [0,0,0]	1/4, 0, 1/2 [0,0,0]
16	a	23.	1/8, 1/8, 1/8 [0,0,0]	7/8, 3/8, 7/8 [0,0,0]	7/8, 7/8, 7/8 [0,0,0]	1/8, 5/8, 1/8 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/4$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/4$   
 Origin at 1/8, 3/8, z

Along [1,1,1] p6m'm'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6$   
 Origin at x,x,x

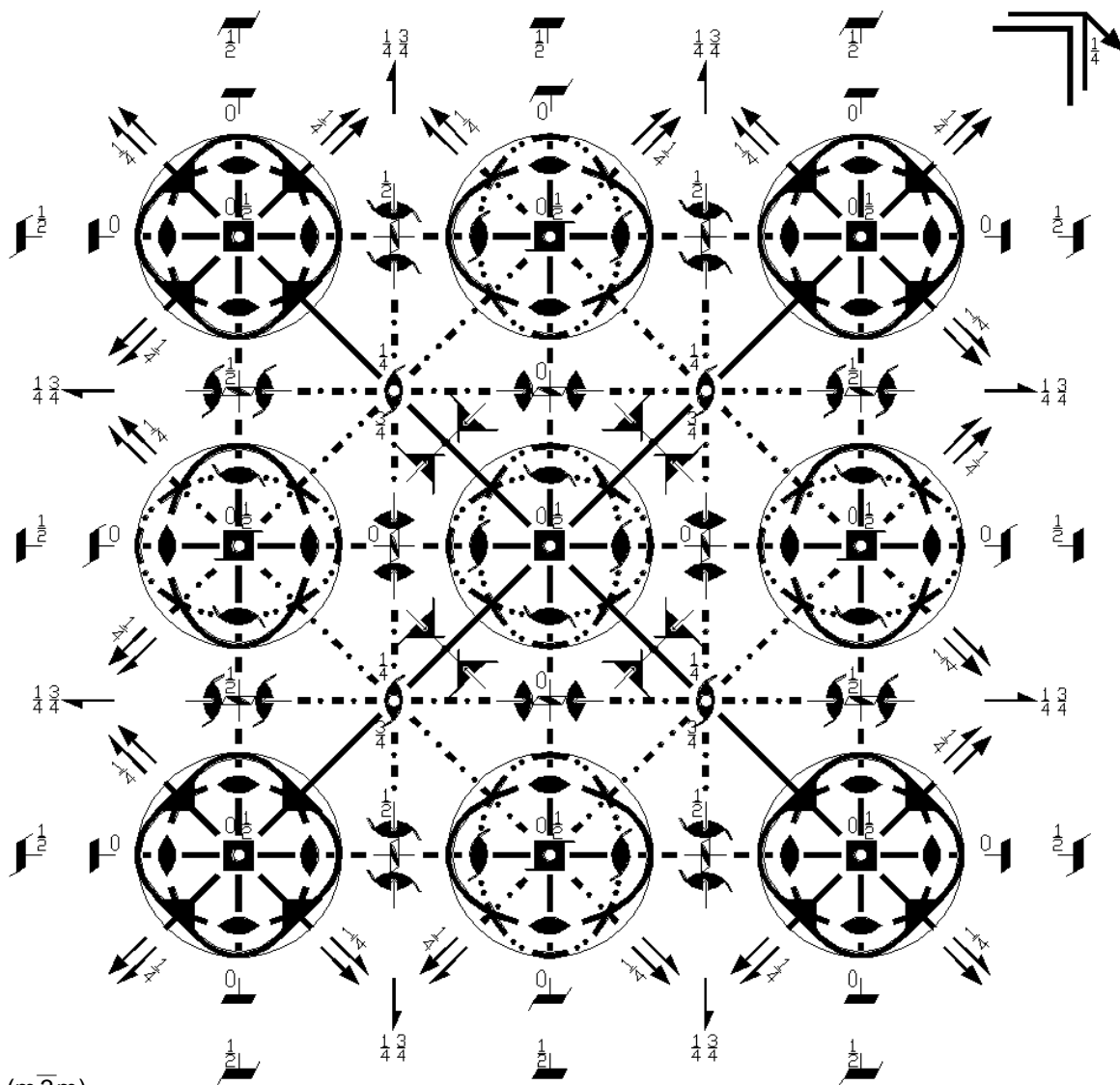
Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/4$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0



$Im\bar{3}m$   
229.1.1638

$m\bar{3}m$   
 $I4/m\bar{3}2/m$

Cubic



Origin at center ( $m\bar{3}m$ )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/4;$   $y \leq x;$   $z \leq \min(1/2-x,y)$   
**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/4,1/4,1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                         | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)    | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)      | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)     |

(13) $2 \ x,x,0$ ( $2_{xy} 0,0,0$ )	(14) $2 \ x,\bar{x},0$ ( $2_{\bar{xy}} 0,0,0$ )	(15) $4^- \ 0,0,z$ ( $4_z^{-1} 0,0,0$ )	(16) $4^+ \ 0,0,z$ ( $4_z 0,0,0$ )
(17) $4^- \ x,0,0$ ( $4_x^{-1} 0,0,0$ )	(18) $2 \ 0,y,y$ ( $2_{yz} 0,0,0$ )	(19) $2 \ 0,y,\bar{y}$ ( $2_{\bar{yz}} 0,0,0$ )	(20) $4^+ \ x,0,0$ ( $4_x 0,0,0$ )
(21) $4^+ \ 0,y,0$ ( $4_y 0,0,0$ )	(22) $2 \ x,0,x$ ( $2_{xz} 0,0,0$ )	(23) $4^- \ 0,y,0$ ( $4_y^{-1} 0,0,0$ )	(24) $2 \ \bar{x},0,x$ ( $2_{\bar{xz}} 0,0,0$ )
(25) $\bar{1} \ 0,0,0$ ( $\bar{1} 0,0,0$ )	(26) $m \ x,y,0$ ( $m_z 0,0,0$ )	(27) $m \ x,0,z$ ( $m_y 0,0,0$ )	(28) $m \ 0,y,z$ ( $m_x 0,0,0$ )
(29) $\bar{3}^+ \ x,x,x; 0,0,0$ ( $\bar{3}_{xyz} 0,0,0$ )	(30) $\bar{3}^+ \ \bar{x},x,\bar{x}; 0,0,0$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1} 0,0,0$ )	(31) $\bar{3}^+ \ x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{x}yz}^{-1} 0,0,0$ )	(32) $\bar{3}^+ \ \bar{x},\bar{x},x; 0,0,0$ ( $\bar{3}_{\bar{x}y\bar{z}}^{-1} 0,0,0$ )
(33) $\bar{3}^- \ x,x,x; 0,0,0$ ( $\bar{3}_{xyz}^{-1} 0,0,0$ )	(34) $\bar{3}^- \ x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{x\bar{y}\bar{z}} 0,0,0$ )	(35) $\bar{3}^- \ \bar{x},x,\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{x}yz} 0,0,0$ )	(36) $\bar{3}^- \ \bar{x},x,x; 0,0,0$ ( $\bar{3}_{x\bar{y}\bar{z}} 0,0,0$ )
(37) $m \ x,\bar{x},z$ ( $m_{xy} 0,0,0$ )	(38) $m \ x,x,z$ ( $m_{\bar{xy}} 0,0,0$ )	(39) $\bar{4}^- \ 0,0,z; 0,0,0$ ( $\bar{4}_z^{-1} 0,0,0$ )	(40) $\bar{4}^+ \ 0,0,z; 0,0,0$ ( $\bar{4}_z 0,0,0$ )
(41) $\bar{4}^- \ x,0,0; 0,0,0$ ( $\bar{4}_x^{-1} 0,0,0$ )	(42) $m \ x,y,\bar{y}$ ( $m_{yz} 0,0,0$ )	(43) $m \ x,y,y$ ( $m_{\bar{yz}} 0,0,0$ )	(44) $\bar{4}^+ \ x,0,0; 0,0,0$ ( $\bar{4}_x 0,0,0$ )
(45) $\bar{4}^+ \ 0,y,0; 0,0,0$ ( $\bar{4}_y 0,0,0$ )	(46) $m \ \bar{x},y,x$ ( $m_{xz} 0,0,0$ )	(47) $\bar{4}^- \ 0,y,0; 0,0,0$ ( $\bar{4}_y^{-1} 0,0,0$ )	(48) $m \ x,y,x$ ( $m_{\bar{xz}} 0,0,0$ )

## For (1/2,1/2,1/2) + set

(1) $t \ (1/2,1/2,1/2)$ ( $\bar{1} 1/2,1/2,1/2$ )	(2) $2 \ (0,0,1/2) \ 1/4,1/4,z$ ( $2_z 1/2,1/2,1/2$ )	(3) $2 \ (0,1/2,0) \ 1/4,y,1/4$ ( $2_y 1/2,1/2,1/2$ )	(4) $2 \ (1/2,0,0) \ x,1/4,1/4$ ( $2_x 1/2,1/2,1/2$ )
(5) $3^+ \ (1/2,1/2,1/2) \ x,x,x$ ( $3_{xyz} 1/2,1/2,1/2$ )	(6) $3^+ \ (1/6,-1/6,1/6)$ $x+1/3, x+1/3, \bar{x}$ ( $3_{x\bar{y}\bar{z}}^{-1} 1/2,1/2,1/2$ )	(7) $3^+ \ (-1/6,1/6,1/6)$ $x+2/3, \bar{x}-1/3, \bar{x}$ ( $3_{\bar{x}yz}^{-1} 1/2,1/2,1/2$ )	(8) $3^+ \ (1/6,1/6,-1/6)$ $\bar{x}+1/3, \bar{x}+2/3, x$ ( $3_{x\bar{y}\bar{z}}^{-1} 1/2,1/2,1/2$ )
(9) $3^- \ (1/2,1/2,1/2) \ x,x,x$ ( $3_{xyz}^{-1} 1/2,1/2,1/2$ )	(10) $3^- \ (-1/6,1/6,1/6)$ $x+1/3, \bar{x}+1/3, \bar{x}$ ( $3_{x\bar{y}\bar{z}} 1/2,1/2,1/2$ )	(11) $3^- \ (1/6,1/6,-1/6)$ $\bar{x}+2/3, \bar{x}+1/3, x$ ( $3_{\bar{x}yz} 1/2,1/2,1/2$ )	(12) $3^- \ (1/6,-1/6,1/6)$ $\bar{x}-1/3, x+2/3, \bar{x}$ ( $3_{x\bar{y}\bar{z}} 1/2,1/2,1/2$ )
(13) $2 \ (1/2,1/2,0) \ x,x,1/4$ ( $2_{xy} 1/2,1/2,1/2$ )	(14) $2 \ x,\bar{x}+1/2,1/4$ ( $2_{\bar{xy}} 1/2,1/2,1/2$ )	(15) $4^- \ (0,0,1/2) \ 1/2,0,z$ ( $4_z^{-1} 1/2,1/2,1/2$ )	(16) $4^+ \ (0,0,1/2) \ 0,1/2,z$ ( $4_z 1/2,1/2,1/2$ )
(17) $4^- \ (1/2,0,0) \ x,1/2,0$ ( $4_x^{-1} 1/2,1/2,1/2$ )	(18) $2 \ (0,1/2,1/2) \ 1/4,y,y$ ( $2_{yz} 1/2,1/2,1/2$ )	(19) $2 \ 1/4,y+1/2,\bar{y}$ ( $2_{\bar{yz}} 1/2,1/2,1/2$ )	(20) $4^+ \ (1/2,0,0) \ x,0,1/2$ ( $4_x 1/2,1/2,1/2$ )
(21) $4^+ \ (0,1/2,0) \ 1/2,y,0$ ( $4_y 1/2,1/2,1/2$ )	(22) $2 \ (1/2,0,1/2) \ x,1/4,x$ ( $2_{xz} 1/2,1/2,1/2$ )	(23) $4^- \ (0,1/2,0) \ 0,y,1/2$ ( $4_y^{-1} 1/2,1/2,1/2$ )	(24) $2 \ \bar{x}+1/2,1/4,x$ ( $2_{\bar{xz}} 1/2,1/2,1/2$ )
(25) $\bar{1} \ 1/4,1/4,1/4$ ( $\bar{1} 1/2,1/2,1/2$ )	(26) $n \ (1/2,1/2,0) \ x,y,1/4$ ( $m_z 1/2,1/2,1/2$ )	(27) $n \ (1/2,0,1/2) \ x,1/4,z$ ( $m_y 1/2,1/2,1/2$ )	(28) $n \ (0,1/2,1/2) \ 1/4,y,z$ ( $m_x 1/2,1/2,1/2$ )
(29) $\bar{3}^+ \ x,x,x;$ $1/4,1/4,1/4$ ( $\bar{3}_{xyz} 1/2,1/2,1/2$ )	(30) $\bar{3}^+ \ \bar{x}-1,x+1,\bar{x};$ $-1/4,1/4,3/4$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1} 1/2,1/2,1/2$ )	(31) $\bar{3}^+ \ x,\bar{x}+1,\bar{x};$ $1/4,3/4,-1/4$ ( $\bar{3}_{\bar{x}yz}^{-1} 1/2,1/2,1/2$ )	(32) $\bar{3}^+ \ \bar{x}+1,\bar{x},x;$ $3/4,-1/4,1/4$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1} 1/2,1/2,1/2$ )



(33) $\bar{3}^-$ $x,x,x;$ 1/4,1/4,1/4 ( $\bar{3}_{xyz}^{-1} 1/2,1/2,1/2$ )	(34) $\bar{3}^-$ $x+1,\bar{x}-1,\bar{x};$ 1/4,-1/4,3/4 ( $\bar{3}_{xyz}^{-1} 1/2,1/2,1/2$ )	(35) $\bar{3}^-$ $\bar{x},\bar{x}+1,x;$ -1/4,3/4,1/4 ( $\bar{3}_{xyz}^{-1} 1/2,1/2,1/2$ )	(36) $\bar{3}^-$ $\bar{x}+1,x,\bar{x};$ 3/4,1/4,-1/4 ( $\bar{3}_{xyz}^{-1} 1/2,1/2,1/2$ )
(37) $c$ (0,0,1/2) $x+1/2,\bar{x},z$ ( $m_{xy} 1/2,1/2,1/2$ )	(38) $n$ (1/2,1/2,1/2) $x,x,z$ ( $m_{xy} 1/2,1/2,1/2$ )	(39) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1} 1/2,1/2,1/2$ )	(40) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z 1/2,1/2,1/2$ )
(41) $\bar{4}^-$ $x,0,1/2; 1/4,0,1/2$ ( $\bar{4}_x^{-1} 1/2,1/2,1/2$ )	(42) $a$ (1/2,0,0) $x,y+1/2,\bar{y}$ ( $m_{yz} 1/2,1/2,1/2$ )	(43) $n$ (1/2,1/2,1/2) $x,y,y$ ( $m_{yz} 1/2,1/2,1/2$ )	(44) $\bar{4}^+$ $x,1/2,0; 1/4,1/2,0$ ( $\bar{4}_x 1/2,1/2,1/2$ )
(45) $\bar{4}^+$ 0,y,1/2; 0,1/4,1/2 ( $\bar{4}_y 1/2,1/2,1/2$ )	(46) $b$ (0,1/2,0) $\bar{x}+1/2,y,x$ ( $m_{xz} 1/2,1/2,1/2$ )	(47) $\bar{4}^-$ 1/2,y,0; 1/2,1/4,0 ( $\bar{4}_y^{-1} 1/2,1/2,1/2$ )	(48) $n$ (1/2,1/2,1/2) $x,y,x$ ( $m_{xz} 1/2,1/2,1/2$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

		(0,0,0) +	(1/2,1/2,1/2) +			
96	l	1				
(1)	$x,y,z$	[u,v,w]	(2)	$\bar{x},\bar{y},z$	[ $\bar{u},\bar{v},w$ ]	
(5)	$z,x,y$	[w,u,v]	(6)	$z,\bar{x},\bar{y}$	[w, $\bar{u},\bar{v}$ ]	
(9)	$y,z,x$	[v,w,u]	(10)	$\bar{y},z,\bar{x}$	[ $\bar{v},w,\bar{u}$ ]	
(13)	$y,x,\bar{z}$	[v,u, $\bar{w}$ ]	(14)	$\bar{y},\bar{x},\bar{z}$	[ $\bar{v},\bar{u},\bar{w}$ ]	
(17)	$x,z,\bar{y}$	[u,w, $\bar{v}$ ]	(18)	$\bar{x},z,y$	[ $\bar{u},w,v$ ]	
(21)	$z,y,\bar{x}$	[w,v, $\bar{u}$ ]	(22)	$z,\bar{y},x$	[w, $\bar{v},u$ ]	
(25)	$\bar{x},\bar{y},\bar{z}$	[ $\bar{u},\bar{v},\bar{w}$ ]	(26)	$x,y,\bar{z}$	[ $\bar{u},\bar{v},w$ ]	
(29)	$\bar{z},\bar{x},\bar{y}$	[w,u,v]	(30)	$\bar{z},x,y$	[w, $\bar{u},\bar{v}$ ]	
(33)	$\bar{y},\bar{z},\bar{x}$	[v,w,u]	(34)	$y,\bar{z},x$	[ $\bar{v},w,\bar{u}$ ]	
(37)	$\bar{y},\bar{x},z$	[v,u, $\bar{w}$ ]	(38)	$y,x,z$	[ $\bar{v},\bar{u},\bar{w}$ ]	
(41)	$\bar{x},\bar{z},y$	[u,w, $\bar{v}$ ]	(42)	$x,\bar{z},y$	[ $\bar{u},w,\bar{v}$ ]	
(45)	$\bar{z},\bar{y},x$	[w,v, $\bar{u}$ ]	(46)	$\bar{z},y,\bar{x}$	[w, $\bar{v},u$ ]	
48	k	..m	$x,x,z$	[u, $\bar{u},0$ ]	$\bar{x},\bar{x},z$	[ $\bar{u},\bar{u},0$ ]
			$z,x,x$	[0, $\bar{u},\bar{u}$ ]	$\bar{z},\bar{x},x$	[0, $\bar{u},\bar{u}$ ]
			$x,z,x$	[ $\bar{u},0,u$ ]	$\bar{x},z,\bar{x}$	[ $\bar{u},0,\bar{u}$ ]
			$x,x,\bar{z}$	[ $\bar{u},u,0$ ]	$\bar{x},\bar{x},\bar{z}$	[ $\bar{u},\bar{u},0$ ]
			$x,z,\bar{x}$	[u,0,u]	$\bar{x},z,\bar{x}$	[ $\bar{u},0,\bar{u}$ ]

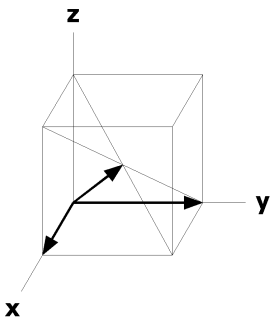
			$z, x, \bar{x} [0, \bar{u}, \bar{u}]$	$z, \bar{x}, x [0, u, u]$	$\bar{z}, x, x [0, \bar{u}, u]$	$\bar{z}, \bar{x}, \bar{x} [0, u, \bar{u}]$
48	j	m..	$0, y, z [u, 0, 0]$	$0, \bar{y}, z [\bar{u}, 0, 0]$	$0, y, \bar{z} [\bar{u}, 0, 0]$	$0, \bar{y}, \bar{z} [u, 0, 0]$
			$z, 0, y [0, u, 0]$	$z, 0, \bar{y} [0, \bar{u}, 0]$	$\bar{z}, 0, y [0, \bar{u}, 0]$	$\bar{z}, 0, \bar{y} [0, u, 0]$
			$y, z, 0 [0, 0, u]$	$\bar{y}, z, 0 [0, 0, \bar{u}]$	$y, \bar{z}, 0 [0, 0, \bar{u}]$	$\bar{y}, \bar{z}, 0 [0, 0, u]$
			$y, 0, \bar{z} [0, u, 0]$	$\bar{y}, 0, \bar{z} [0, \bar{u}, 0]$	$y, 0, z [0, \bar{u}, 0]$	$\bar{y}, 0, z [0, u, 0]$
			$0, z, \bar{y} [u, 0, 0]$	$0, z, y [\bar{u}, 0, 0]$	$0, \bar{z}, \bar{y} [\bar{u}, 0, 0]$	$0, \bar{z}, y [u, 0, 0]$
			$z, y, 0 [0, 0, \bar{u}]$	$z, \bar{y}, 0 [0, 0, u]$	$\bar{z}, y, 0 [0, 0, u]$	$\bar{z}, \bar{y}, 0 [0, 0, \bar{u}]$
48	i	..2				
			$1/4, y, \bar{y} + 1/2 [0, \bar{v}, v]$	$3/4, \bar{y}, \bar{y} + 1/2 [0, v, v]$	$3/4, y, y + 1/2 [0, \bar{v}, \bar{v}]$	$1/4, \bar{y}, y + 1/2 [0, v, \bar{v}]$
			$\bar{y} + 1/2, 1/4, y [v, 0, \bar{v}]$	$\bar{y} + 1/2, 3/4, \bar{y} [v, 0, v]$	$y + 1/2, 3/4, y [\bar{v}, 0, \bar{v}]$	$y + 1/2, 1/4, \bar{y} [\bar{v}, 0, v]$
			$y, \bar{y} + 1/2, 1/4 [\bar{v}, v, 0]$	$\bar{y}, \bar{y} + 1/2, 3/4 [v, v, 0]$	$y, y + 1/2, 3/4 [\bar{v}, \bar{v}, 0]$	$\bar{y}, y + 1/2, 1/4 [v, \bar{v}, 0]$
			$3/4, \bar{y}, y + 1/2 [0, \bar{v}, v]$	$1/4, y, y + 1/2 [0, v, v]$	$1/4, \bar{y}, \bar{y} + 1/2 [0, \bar{v}, \bar{v}]$	$3/4, y, \bar{y} + 1/2 [0, v, \bar{v}]$
			$y + 1/2, 3/4, \bar{y} [v, 0, \bar{v}]$	$y + 1/2, 1/4, y [v, 0, v]$	$\bar{y} + 1/2, 1/4, \bar{y} [\bar{v}, 0, \bar{v}]$	$\bar{y} + 1/2, 3/4, y [\bar{v}, 0, v]$
			$\bar{y}, y + 1/2, 3/4 [\bar{v}, v, 0]$	$y, y + 1/2, 1/4 [v, v, 0]$	$\bar{y}, \bar{y} + 1/2, 1/4 [\bar{v}, \bar{v}, 0]$	$y, \bar{y} + 1/2, 3/4 [v, \bar{v}, 0]$
24	h	m.m2	$0, y, y [0, 0, 0]$	$0, \bar{y}, y [0, 0, 0]$	$0, y, \bar{y} [0, 0, 0]$	$0, \bar{y}, \bar{y} [0, 0, 0]$
			$y, 0, y [0, 0, 0]$	$y, 0, \bar{y} [0, 0, 0]$	$\bar{y}, 0, y [0, 0, 0]$	$\bar{y}, 0, \bar{y} [0, 0, 0]$
			$y, y, 0 [0, 0, 0]$	$\bar{y}, y, 0 [0, 0, 0]$	$y, \bar{y}, 0 [0, 0, 0]$	$\bar{y}, \bar{y}, 0 [0, 0, 0]$
24	g	mm2..	$x, 0, 1/2 [0, 0, 0]$	$\bar{x}, 0, 1/2 [0, 0, 0]$	$1/2, x, 0 [0, 0, 0]$	$1/2, \bar{x}, 0 [0, 0, 0]$
			$0, 1/2, x [0, 0, 0]$	$0, 1/2, \bar{x} [0, 0, 0]$	$0, x, 1/2 [0, 0, 0]$	$0, \bar{x}, 1/2 [0, 0, 0]$
			$x, 1/2, 0 [0, 0, 0]$	$\bar{x}, 1/2, 0 [0, 0, 0]$	$1/2, 0, \bar{x} [0, 0, 0]$	$1/2, 0, x [0, 0, 0]$
16	f	.3m	$x, x, x [0, 0, 0]$	$\bar{x}, \bar{x}, x [0, 0, 0]$	$\bar{x}, x, \bar{x} [0, 0, 0]$	$x, \bar{x}, \bar{x} [0, 0, 0]$
			$x, x, \bar{x} [0, 0, 0]$	$\bar{x}, \bar{x}, \bar{x} [0, 0, 0]$	$x, \bar{x}, x [0, 0, 0]$	$\bar{x}, x, x [0, 0, 0]$
12	e	4m.m	$x, 0, 0 [0, 0, 0]$	$\bar{x}, 0, 0 [0, 0, 0]$		$0, x, 0 [0, 0, 0]$
			$0, \bar{x}, 0 [0, 0, 0]$	$0, 0, x [0, 0, 0]$		$0, 0, \bar{x} [0, 0, 0]$
12	d	$\bar{4}m.2$	$1/4, 0, 1/2 [0, 0, 0]$	$3/4, 0, 1/2 [0, 0, 0]$		$1/2, 1/4, 0 [0, 0, 0]$
			$1/2, 3/4, 0 [0, 0, 0]$	$0, 1/2, 1/4 [0, 0, 0]$		$0, 1/2, 3/4 [0, 0, 0]$
8	c	$\bar{3}m$	$1/4, 1/4, 1/4 [0, 0, 0]$	$3/4, 3/4, 1/4 [0, 0, 0]$	$3/4, 1/4, 3/4 [0, 0, 0]$	$1/4, 3/4, 3/4 [0, 0, 0]$
6	b	4/mm.m	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$		$1/2, 1/2, 0 [0, 0, 0]$
2	a	m $\bar{3}m$	$0, 0, 0 [0, 0, 0]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $0,0,z$

Along  $[1,1,1]$   $p6'm'm$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
Origin at  $x,x,x$

Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at  $x,x,0$



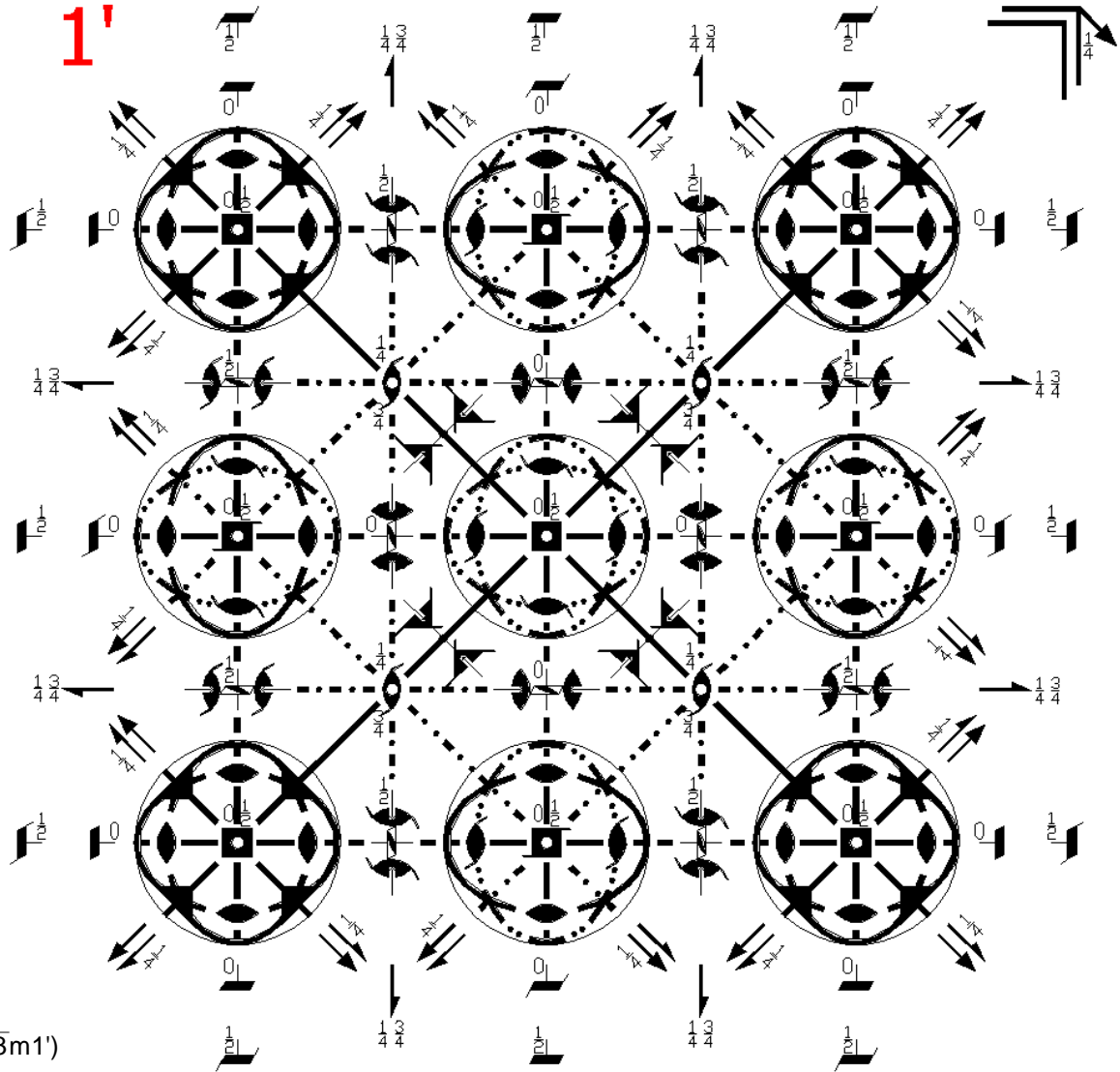
$Im\bar{3}m1'$

229.2.1639

$m\bar{3}m1'$

$I4/m\bar{3}2/m1'$

Cubic



**Origin** at center ( $m\bar{3}m1'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/4;$   $y \leq x;$   $z \leq \min(1/2-x,y)$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/4,1/4,1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |   |   |   |
|--|---|---|---|
| (1) 1<br>(1 0,0,0)                                   | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                  | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                                  | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                  |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)             | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0)  |
| (9) $3^-$ $x,x,x$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) |

(13) $2 \ x,x,0$ ( $2_{xy} 0,0,0$ )	(14) $2 \ x,\bar{x},0$ ( $2_{\bar{xy}} 0,0,0$ )	(15) $4^- \ 0,0,z$ ( $4_z^{-1} 0,0,0$ )	(16) $4^+ \ 0,0,z$ ( $4_z 0,0,0$ )
(17) $4^- \ x,0,0$ ( $4_x^{-1} 0,0,0$ )	(18) $2 \ 0,y,y$ ( $2_{yz} 0,0,0$ )	(19) $2 \ 0,y,\bar{y}$ ( $2_{\bar{yz}} 0,0,0$ )	(20) $4^+ \ x,0,0$ ( $4_x 0,0,0$ )
(21) $4^+ \ 0,y,0$ ( $4_y 0,0,0$ )	(22) $2 \ x,0,x$ ( $2_{xz} 0,0,0$ )	(23) $4^- \ 0,y,0$ ( $4_y^{-1} 0,0,0$ )	(24) $2 \ \bar{x},0,x$ ( $2_{\bar{xz}} 0,0,0$ )
(25) $\bar{1} \ 0,0,0$ ( $\bar{1} 0,0,0$ )	(26) $m \ x,y,0$ ( $m_z 0,0,0$ )	(27) $m \ x,0,z$ ( $m_y 0,0,0$ )	(28) $m \ 0,y,z$ ( $m_x 0,0,0$ )
(29) $\bar{3}^+ \ x,x,x; 0,0,0$ ( $\bar{3}_{xyz} 0,0,0$ )	(30) $\bar{3}^+ \ \bar{x},x,\bar{x}; 0,0,0$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1} 0,0,0$ )	(31) $\bar{3}^+ \ x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{x}yz}^{-1} 0,0,0$ )	(32) $\bar{3}^+ \ \bar{x},\bar{x},x; 0,0,0$ ( $\bar{3}_{\bar{x}y\bar{z}}^{-1} 0,0,0$ )
(33) $\bar{3}^- \ x,x,x; 0,0,0$ ( $\bar{3}_{xyz}^{-1} 0,0,0$ )	(34) $\bar{3}^- \ x,\bar{x},\bar{x}; 0,0,0$ ( $\bar{3}_{x\bar{y}\bar{z}} 0,0,0$ )	(35) $\bar{3}^- \ \bar{x},x,\bar{x}; 0,0,0$ ( $\bar{3}_{\bar{x}yz} 0,0,0$ )	(36) $\bar{3}^- \ \bar{x},x,x; 0,0,0$ ( $\bar{3}_{x\bar{y}\bar{z}} 0,0,0$ )
(37) $m \ x,\bar{x},z$ ( $m_{xy} 0,0,0$ )	(38) $m \ x,x,z$ ( $m_{\bar{xy}} 0,0,0$ )	(39) $\bar{4}^- \ 0,0,z; 0,0,0$ ( $\bar{4}_z^{-1} 0,0,0$ )	(40) $\bar{4}^+ \ 0,0,z; 0,0,0$ ( $\bar{4}_z 0,0,0$ )
(41) $\bar{4}^- \ x,0,0; 0,0,0$ ( $\bar{4}_x^{-1} 0,0,0$ )	(42) $m \ x,y,\bar{y}$ ( $m_{yz} 0,0,0$ )	(43) $m \ x,y,y$ ( $m_{\bar{yz}} 0,0,0$ )	(44) $\bar{4}^+ \ x,0,0; 0,0,0$ ( $\bar{4}_x 0,0,0$ )
(45) $\bar{4}^+ \ 0,y,0; 0,0,0$ ( $\bar{4}_y 0,0,0$ )	(46) $m \ \bar{x},y,x$ ( $m_{xz} 0,0,0$ )	(47) $\bar{4}^- \ 0,y,0; 0,0,0$ ( $\bar{4}_y^{-1} 0,0,0$ )	(48) $m \ x,y,x$ ( $m_{\bar{xz}} 0,0,0$ )

For  $(1/2,1/2,1/2) + \text{set}$ 

(1) $t \ (1/2,1/2,1/2)$ ( $1 1/2,1/2,1/2$ )	(2) $2 \ (0,0,1/2) \ 1/4,1/4,z$ ( $2_z 1/2,1/2,1/2$ )	(3) $2 \ (0,1/2,0) \ 1/4,y,1/4$ ( $2_y 1/2,1/2,1/2$ )	(4) $2 \ (1/2,0,0) \ x,1/4,1/4$ ( $2_x 1/2,1/2,1/2$ )
(5) $3^+ \ (1/2,1/2,1/2) \ x,x,x$ ( $3_{xyz} 1/2,1/2,1/2$ )	(6) $3^+ \ (1/6,-1/6,1/6)$ $x+1/3, x+1/3, \bar{x}$ ( $3_{x\bar{y}\bar{z}}^{-1} 1/2,1/2,1/2$ )	(7) $3^+ \ (-1/6,1/6,1/6)$ $x+2/3, \bar{x}-1/3, \bar{x}$ ( $3_{\bar{x}yz}^{-1} 1/2,1/2,1/2$ )	(8) $3^+ \ (1/6,1/6,-1/6)$ $\bar{x}+1/3, \bar{x}+2/3, x$ ( $3_{x\bar{y}\bar{z}}^{-1} 1/2,1/2,1/2$ )
(9) $3^- \ (1/2,1/2,1/2) \ x,x,x$ ( $3_{xyz}^{-1} 1/2,1/2,1/2$ )	(10) $3^- \ (-1/6,1/6,1/6)$ $x+1/3, \bar{x}+1/3, \bar{x}$ ( $3_{x\bar{y}\bar{z}} 1/2,1/2,1/2$ )	(11) $3^- \ (1/6,1/6,-1/6)$ $\bar{x}+2/3, \bar{x}+1/3, x$ ( $3_{\bar{x}yz} 1/2,1/2,1/2$ )	(12) $3^- \ (1/6,-1/6,1/6)$ $\bar{x}-1/3, x+2/3, \bar{x}$ ( $3_{x\bar{y}\bar{z}} 1/2,1/2,1/2$ )
(13) $2 \ (1/2,1/2,0) \ x,x,1/4$ ( $2_{xy} 1/2,1/2,1/2$ )	(14) $2 \ x,\bar{x}+1/2,1/4$ ( $2_{\bar{xy}} 1/2,1/2,1/2$ )	(15) $4^- \ (0,0,1/2) \ 1/2,0,z$ ( $4_z^{-1} 1/2,1/2,1/2$ )	(16) $4^+ \ (0,0,1/2) \ 0,1/2,z$ ( $4_z 1/2,1/2,1/2$ )
(17) $4^- \ (1/2,0,0) \ x,1/2,0$ ( $4_x^{-1} 1/2,1/2,1/2$ )	(18) $2 \ (0,1/2,1/2) \ 1/4,y,y$ ( $2_{yz} 1/2,1/2,1/2$ )	(19) $2 \ 1/4,y+1/2,\bar{y}$ ( $2_{\bar{yz}} 1/2,1/2,1/2$ )	(20) $4^+ \ (1/2,0,0) \ x,0,1/2$ ( $4_x 1/2,1/2,1/2$ )
(21) $4^+ \ (0,1/2,0) \ 1/2,y,0$ ( $4_y 1/2,1/2,1/2$ )	(22) $2 \ (1/2,0,1/2) \ x,1/4,x$ ( $2_{xz} 1/2,1/2,1/2$ )	(23) $4^- \ (0,1/2,0) \ 0,y,1/2$ ( $4_y^{-1} 1/2,1/2,1/2$ )	(24) $2 \ \bar{x}+1/2,1/4,x$ ( $2_{\bar{xz}} 1/2,1/2,1/2$ )
(25) $\bar{1} \ 1/4,1/4,1/4$ ( $\bar{1} 1/2,1/2,1/2$ )	(26) $n \ (1/2,1/2,0) \ x,y,1/4$ ( $m_z 1/2,1/2,1/2$ )	(27) $n \ (1/2,0,1/2) \ x,1/4,z$ ( $m_y 1/2,1/2,1/2$ )	(28) $n \ (0,1/2,1/2) \ 1/4,y,z$ ( $m_x 1/2,1/2,1/2$ )
(29) $\bar{3}^+ \ x,x,x;$ $1/4,1/4,1/4$ ( $\bar{3}_{xyz} 1/2,1/2,1/2$ )	(30) $\bar{3}^+ \ \bar{x}-1,x+1,\bar{x};$ $-1/4,1/4,3/4$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1} 1/2,1/2,1/2$ )	(31) $\bar{3}^+ \ x,\bar{x}+1,\bar{x};$ $1/4,3/4,-1/4$ ( $\bar{3}_{\bar{x}yz}^{-1} 1/2,1/2,1/2$ )	(32) $\bar{3}^+ \ \bar{x}+1,\bar{x},x;$ $3/4,-1/4,1/4$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1} 1/2,1/2,1/2$ )

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| (33) $\bar{3}^-$ $x,x,x;$<br>1/4,1/4,1/4<br>( $\bar{3}_{xyz}^{-1} 1/2,1/2,1/2$ ) | (34) $\bar{3}^-$ $x+1,\bar{x}-1,\bar{x};$<br>1/4,-1/4,3/4<br>( $\bar{3}_{\bar{xyz}} 1/2,1/2,1/2$ ) | (35) $\bar{3}^-$ $\bar{x},\bar{x}+1,x;$<br>-1/4,3/4,1/4<br>( $\bar{3}_{\bar{yz}} 1/2,1/2,1/2$ ) | (36) $\bar{3}^-$ $\bar{x}+1,x,\bar{x};$<br>3/4,1/4,-1/4<br>( $\bar{3}_{\bar{yz}} 1/2,1/2,1/2$ ) |
| (37) $c$ (0,0,1/2) $x+1/2,\bar{x},z$<br>( $m_{xy} 1/2,1/2,1/2$ )                 | (38) $n$ (1/2,1/2,1/2) $x,x,z$<br>( $m_{\bar{xy}} 1/2,1/2,1/2$ )                                   | (39) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4<br>( $\bar{4}_z^{-1} 1/2,1/2,1/2$ )                         | (40) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4<br>( $\bar{4}_z 1/2,1/2,1/2$ )                              |
| (41) $\bar{4}^-$ $x,0,1/2; 1/4,0,1/2$<br>( $\bar{4}_x^{-1} 1/2,1/2,1/2$ )        | (42) $a$ (1/2,0,0) $x,y+1/2,\bar{y}$<br>( $m_{yz} 1/2,1/2,1/2$ )                                   | (43) $n$ (1/2,1/2,1/2) $x,y,y$<br>( $m_{\bar{yz}} 1/2,1/2,1/2$ )                                | (44) $\bar{4}^+$ $x,1/2,0; 1/4,1/2,0$<br>( $\bar{4}_x 1/2,1/2,1/2$ )                            |
| (45) $\bar{4}^+$ 0,y,1/2; 0,1/4,1/2<br>( $\bar{4}_y 1/2,1/2,1/2$ )               | (46) $b$ (0,1/2,0) $\bar{x}+1/2,y,x$<br>( $m_{xz} 1/2,1/2,1/2$ )                                   | (47) $\bar{4}^-$ 1/2,y,0; 1/2,1/4,0<br>( $\bar{4}_y^{-1} 1/2,1/2,1/2$ )                         | (48) $n$ (1/2,1/2,1/2) $x,y,x$<br>( $m_{\bar{xz}} 1/2,1/2,1/2$ )                                |

For (0,0,0)' + set

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| (1) $1'$<br>( $1 0,0,0$ )'   | (2) $2'$ 0,0,z<br>( $2_z 0,0,0$ )'   | (3) $2'$ 0,y,0<br>( $2_y 0,0,0$ )'  | (4) $2'$ x,0,0<br>( $2_x 0,0,0$ )'  |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz} 0,0,0$ )'                                | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{\bar{xyz}}^{-1} 0,0,0$ )'                     | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{\bar{xyz}}^{-1} 0,0,0$ )'                    | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{\bar{yz}}^{-1} 0,0,0$ )'                     |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1} 0,0,0$ )'                           | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{\bar{xyz}} 0,0,0$ )'                         | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{\bar{yz}} 0,0,0$ )'                         | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{\bar{yz}} 0,0,0$ )'                         |
| (13) $2'$ x,x,0<br>( $2_{xy} 0,0,0$ )'                                   | (14) $2'$ x, $\bar{x}$ ,0<br>( $2_{\bar{xy}} 0,0,0$ )'                               | (15) $4^-$ 0,0,z<br>( $4_z^{-1} 0,0,0$ )'   | (16) $4^+$ 0,0,z<br>( $4_z 0,0,0$ )'  |
| (17) $4^-$ x,0,0<br>( $4_x^{-1} 0,0,0$ )'                                | (18) $2'$ 0,y,y<br>( $2_{yz} 0,0,0$ )'   | (19) $2'$ 0,y, $\bar{y}$<br>( $2_{\bar{yz}} 0,0,0$ )'                               | (20) $4^+$ x,0,0<br>( $4_x 0,0,0$ )'  |
| (21) $4^+$ 0,y,0<br>( $4_y 0,0,0$ )'                                     | (22) $2'$ x,0,x<br>( $2_{xz} 0,0,0$ )'   | (23) $4^-$ 0,y,0<br>( $4_y^{-1} 0,0,0$ )'   | (24) $2'$ $\bar{x}$ ,0,x<br>( $2_{\bar{xz}} 0,0,0$ )'                               |
| (25) $\bar{1}'$ 0,0,0<br>( $\bar{1} 0,0,0$ )'                            | (26) $m'$ x,y,0<br>( $m_z 0,0,0$ )'  | (27) $m'$ x,0,z<br>( $m_y 0,0,0$ )'   | (28) $m'$ 0,y,z<br>( $m_x 0,0,0$ )'   |
| (29) $\bar{3}^+$ $x,x,x; 0,0,0$<br>( $\bar{3}_{xyz} 0,0,0$ )'            | (30) $\bar{3}^+$ $\bar{x},x,\bar{x}; 0,0,0$<br>( $\bar{3}_{\bar{xyz}}^{-1} 0,0,0$ )' | (31) $\bar{3}^+$ $x,\bar{x},\bar{x}; 0,0,0$<br>( $\bar{3}_{\bar{yz}}^{-1} 0,0,0$ )' | (32) $\bar{3}^+$ $\bar{x},\bar{x},x; 0,0,0$<br>( $\bar{3}_{\bar{yz}}^{-1} 0,0,0$ )' |
| (33) $\bar{3}^-$ $x,x,x; 0,0,0$<br>( $\bar{3}_{\bar{xyz}}^{-1} 0,0,0$ )' | (34) $\bar{3}^-$ $x,\bar{x},\bar{x}; 0,0,0$<br>( $\bar{3}_{\bar{xyz}} 0,0,0$ )'      | (35) $\bar{3}^-$ $\bar{x},\bar{x},x; 0,0,0$<br>( $\bar{3}_{\bar{yz}} 0,0,0$ )'      | (36) $\bar{3}^-$ $\bar{x},x,\bar{x}; 0,0,0$<br>( $\bar{3}_{\bar{yz}} 0,0,0$ )'      |
| (37) $m'$ x, $\bar{x}$ ,z<br>( $m_{xy} 0,0,0$ )'                         | (38) $m'$ x,x,z<br>( $m_{\bar{xy}} 0,0,0$ )'   | (39) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^{-1} 0,0,0$ )'                        | (40) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z 0,0,0$ )'                             |
| (41) $\bar{4}^-$ x,0,0; 0,0,0<br>( $\bar{4}_x^{-1} 0,0,0$ )'             | (42) $m'$ x,y, $\bar{y}$<br>( $m_{yz} 0,0,0$ )'                                      | (43) $m'$ x,y,y<br>( $m_{\bar{yz}} 0,0,0$ )'  | (44) $\bar{4}^+$ x,0,0; 0,0,0<br>( $\bar{4}_x 0,0,0$ )'                             |
| (45) $\bar{4}^+$ 0,y,0; 0,0,0<br>( $\bar{4}_y 0,0,0$ )'                  | (46) $m'$ $\bar{x}$ ,y,x<br>( $m_{xz} 0,0,0$ )'                                      | (47) $\bar{4}^-$ 0,y,0; 0,0,0<br>( $\bar{4}_y^{-1} 0,0,0$ )'                        | (48) $m'$ x,y,x<br>( $m_{\bar{xz}} 0,0,0$ )'  |

For (1/2,1/2,1/2)' + set

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| (1) $t'$ (1/2,1/2,1/2)<br>( $1 1/2,1/2,1/2$ )' | (2) $2'$ (0,0,1/2) 1/4,1/4,z<br>( $2_z 1/2,1/2,1/2$ )' | (3) $2'$ (0,1/2,0) 1/4,y,1/4<br>( $2_y 1/2,1/2,1/2$ )' | (4) $2'$ (1/2,0,0) x,1/4,1/4<br>( $2_x 1/2,1/2,1/2$ )' |
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(5) $3^+ ' (1/2, 1/2, 1/2) \ x, x, x$ $(3_{xyz}   1/2, 1/2, 1/2)'$	(6) $3^+ ' (1/6, -1/6, 1/6) \frac{\bar{x}}{x+1/3, x+1/3, \bar{x}}$ $(3_{xyz}^{-1}   1/2, 1/2, 1/2)'$	(7) $3^+ ' (-1/6, 1/6, 1/6) \frac{\bar{x}}{x+2/3, \bar{x}-1/3, \bar{x}}$ $(3_{xyz}^{-1}   1/2, 1/2, 1/2)'$	(8) $3^+ ' (1/6, 1/6, -1/6) \frac{\bar{x}}{x+1/3, x+2/3, \bar{x}}$ $(3_{xyz}^{-1}   1/2, 1/2, 1/2)'$
(9) $3^- ' (1/2, 1/2, 1/2) \ x, x, x$ $(3_{xyz}^{-1}   1/2, 1/2, 1/2)'$	(10) $3^- ' (-1/6, 1/6, 1/6) \frac{\bar{x}}{x+1/3, \bar{x}+1/3, \bar{x}}$ $(3_{xyz}   1/2, 1/2, 1/2)'$	(11) $3^- ' (1/6, 1/6, -1/6) \frac{\bar{x}}{x+2/3, \bar{x}+1/3, \bar{x}}$ $(3_{xyz}   1/2, 1/2, 1/2)'$	(12) $3^- ' (1/6, -1/6, 1/6) \frac{\bar{x}}{x-1/3, x+2/3, \bar{x}}$ $(3_{xyz}   1/2, 1/2, 1/2)'$
(13) $2' (1/2, 1/2, 0) \ x, x, 1/4$ $(2_{xy}   1/2, 1/2, 1/2)'$	(14) $2' \ x, \bar{x}+1/2, 1/4$ $(2_{xy}   1/2, 1/2, 1/2)'$	(15) $4^- ' (0, 0, 1/2) \ 1/2, 0, z$ $(4_z^{-1}   1/2, 1/2, 1/2)'$	(16) $4^+ ' (0, 0, 1/2) \ 0, 1/2, z$ $(4_z   1/2, 1/2, 1/2)'$
(17) $4^- ' (1/2, 0, 0) \ x, 1/2, 0$ $(4_x^{-1}   1/2, 1/2, 1/2)'$	(18) $2' (0, 1/2, 1/2) \ 1/4, y, y$ $(2_{yz}   1/2, 1/2, 1/2)'$	(19) $2' \ 1/4, y+1/2, \bar{y}$ $(2_{yz}   1/2, 1/2, 1/2)'$	(20) $4^+ ' (1/2, 0, 0) \ x, 0, 1/2$ $(4_x   1/2, 1/2, 1/2)'$
(21) $4^+ ' (0, 1/2, 0) \ 1/2, y, 0$ $(4_y   1/2, 1/2, 1/2)'$	(22) $2' (1/2, 0, 1/2) \ x, 1/4, x$ $(2_{xz}   1/2, 1/2, 1/2)'$	(23) $4^- ' (0, 1/2, 0) \ 0, y, 1/2$ $(4_y^{-1}   1/2, 1/2, 1/2)'$	(24) $2' \ \bar{x}+1/2, 1/4, x$ $(2_{xz}   1/2, 1/2, 1/2)'$
(25) $\bar{1}' \ 1/4, 1/4, 1/4$ $(\bar{1}   1/2, 1/2, 1/2)'$	(26) $n' (1/2, 1/2, 0) \ x, y, 1/4$ $(m_z   1/2, 1/2, 1/2)'$	(27) $n' (1/2, 0, 1/2) \ x, 1/4, z$ $(m_y   1/2, 1/2, 1/2)'$	(28) $n' (0, 1/2, 1/2) \ 1/4, y, z$ $(m_x   1/2, 1/2, 1/2)'$
(29) $\bar{3}^+ ' \ x, x, x;$ $1/4, 1/4, 1/4$ $(\bar{3}_{xyz}   1/2, 1/2, 1/2)'$	(30) $\bar{3}^+ ' \ \bar{x}-1, x+1, \bar{x};$ $-1/4, 1/4, 3/4$ $(\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2)'$	(31) $\bar{3}^+ ' \ x, \bar{x}+1, \bar{x};$ $1/4, 3/4, -1/4$ $(\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2)'$	(32) $\bar{3}^+ ' \ \bar{x}+1, \bar{x}, x;$ $3/4, -1/4, 1/4$ $(\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2)'$
(33) $\bar{3}^- ' \ x, x, x;$ $1/4, 1/4, 1/4$ $(\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2)'$	(34) $\bar{3}^- ' \ x+1, \bar{x}-1, \bar{x};$ $1/4, -1/4, 3/4$ $(\bar{3}_{xyz}   1/2, 1/2, 1/2)'$	(35) $\bar{3}^- ' \ \bar{x}, \bar{x}+1, x;$ $-1/4, 3/4, 1/4$ $(\bar{3}_{xyz}   1/2, 1/2, 1/2)'$	(36) $\bar{3}^- ' \ \bar{x}+1, x, \bar{x};$ $3/4, 1/4, -1/4$ $(\bar{3}_{xyz}   1/2, 1/2, 1/2)'$
(37) $c' (0, 0, 1/2) \ x+1/2, \bar{x}, z$ $(m_{xy}   1/2, 1/2, 1/2)'$	(38) $n' (1/2, 1/2, 1/2) \ x, x, z$ $(m_{xy}   1/2, 1/2, 1/2)'$	(39) $\bar{4}^- ' \ 0, 1/2, z; \ 0, 1/2, 1/4$ $(\bar{4}_z^{-1}   1/2, 1/2, 1/2)'$	(40) $\bar{4}^+ ' \ 1/2, 0, z; \ 1/2, 0, 1/4$ $(\bar{4}_z   1/2, 1/2, 1/2)'$
(41) $\bar{4}^- ' \ x, 0, 1/2; \ 1/4, 0, 1/2$ $(\bar{4}_x^{-1}   1/2, 1/2, 1/2)'$	(42) $a' (1/2, 0, 0) \ x, y+1/2, \bar{y}$ $(m_{yz}   1/2, 1/2, 1/2)'$	(43) $n' (1/2, 1/2, 1/2) \ x, y, y$ $(m_{yz}   1/2, 1/2, 1/2)'$	(44) $\bar{4}^+ ' \ x, 1/2, 0; \ 1/4, 1/2, 0$ $(\bar{4}_x   1/2, 1/2, 1/2)'$
(45) $\bar{4}^+ ' \ 0, y, 1/2; \ 0, 1/4, 1/2$ $(\bar{4}_y   1/2, 1/2, 1/2)'$	(46) $b' (0, 1/2, 0) \ \bar{x}+1/2, y, x$ $(m_{xz}   1/2, 1/2, 1/2)'$	(47) $\bar{4}^- ' \ 1/2, y, 0; \ 1/2, 1/4, 0$ $(\bar{4}_y^{-1}   1/2, 1/2, 1/2)'$	(48) $n' (1/2, 1/2, 1/2) \ x, y, x$ $(m_{xz}   1/2, 1/2, 1/2)'$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25); 1'.

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

### Coordinates

(0,0,0) + (1/2,1/2,1/2) +  
(0,0,0)' + (1/2,1/2,1/2)'

96 | 11'

(1) $x, y, z [0, 0, 0]$	(2) $\bar{x}, \bar{y}, z [0, 0, 0]$	(3) $\bar{x}, y, \bar{z} [0, 0, 0]$	(4) $x, \bar{y}, \bar{z} [0, 0, 0]$
(5) $z, x, y [0, 0, 0]$	(6) $z, \bar{x}, \bar{y} [0, 0, 0]$	(7) $\bar{z}, \bar{x}, y [0, 0, 0]$	(8) $\bar{z}, x, \bar{y} [0, 0, 0]$
(9) $y, z, x [0, 0, 0]$	(10) $\bar{y}, z, \bar{x} [0, 0, 0]$	(11) $y, \bar{z}, \bar{x} [0, 0, 0]$	(12) $\bar{y}, \bar{z}, x [0, 0, 0]$
(13) $y, x, \bar{z} [0, 0, 0]$	(14) $\bar{y}, \bar{x}, \bar{z} [0, 0, 0]$	(15) $y, \bar{x}, z [0, 0, 0]$	(16) $\bar{y}, x, z [0, 0, 0]$

(17) $x,z,\bar{y}$ [0,0,0]	(18) $\bar{x},z,y$ [0,0,0]	(19) $\bar{x},\bar{z},\bar{y}$ [0,0,0]	(20) $x,\bar{z},y$ [0,0,0]
(21) $z,y,\bar{x}$ [0,0,0]	(22) $z,\bar{y},x$ [0,0,0]	(23) $\bar{z},y,x$ [0,0,0]	(24) $\bar{z},\bar{y},\bar{x}$ [0,0,0]
(25) $\bar{x},\bar{y},\bar{z}$ [0,0,0]	(26) $x,y,\bar{z}$ [0,0,0]	(27) $x,\bar{y},z$ [0,0,0]	(28) $\bar{x},y,z$ [0,0,0]
(29) $\bar{z},\bar{x},\bar{y}$ [0,0,0]	(30) $\bar{z},x,y$ [0,0,0]	(31) $z,x,\bar{y}$ [0,0,0]	(32) $z,\bar{x},y$ [0,0,0]
(33) $\bar{y},\bar{z},\bar{x}$ [0,0,0]	(34) $y,\bar{z},x$ [0,0,0]	(35) $\bar{y},z,x$ [0,0,0]	(36) $y,z,\bar{x}$ [0,0,0]
(37) $\bar{y},\bar{x},z$ [0,0,0]	(38) $y,x,z$ [0,0,0]	(39) $\bar{y},x,\bar{z}$ [0,0,0]	(40) $y,\bar{x},\bar{z}$ [0,0,0]
(41) $\bar{x},\bar{z},y$ [0,0,0]	(42) $x,\bar{z},\bar{y}$ [0,0,0]	(43) $x,z,y$ [0,0,0]	(44) $\bar{x},z,\bar{y}$ [0,0,0]
(45) $\bar{z},\bar{y},x$ [0,0,0]	(46) $\bar{z},y,\bar{x}$ [0,0,0]	(47) $z,\bar{y},\bar{x}$ [0,0,0]	(48) $z,y,x$ [0,0,0]
48    k    ..m1'	$x,x,z$ [0,0,0]	$\bar{x},\bar{x},z$ [0,0,0]	$\bar{x},x,\bar{z}$ [0,0,0]
	$z,x,x$ [0,0,0]	$z,\bar{x},\bar{x}$ [0,0,0]	$\bar{z},x,\bar{x}$ [0,0,0]
	$x,z,x$ [0,0,0]	$\bar{x},z,\bar{x}$ [0,0,0]	$x,\bar{z},\bar{x}$ [0,0,0]
	$x,x,\bar{z}$ [0,0,0]	$\bar{x},\bar{x},\bar{z}$ [0,0,0]	$x,\bar{x},z$ [0,0,0]
	$x,z,\bar{x}$ [0,0,0]	$\bar{x},z,x$ [0,0,0]	$\bar{x},\bar{z},\bar{x}$ [0,0,0]
	$z,x,\bar{x}$ [0,0,0]	$z,\bar{x},x$ [0,0,0]	$\bar{z},x,x$ [0,0,0]
48    j    m..1'	$0,y,z$ [0,0,0]	$0,\bar{y},z$ [0,0,0]	$0,y,\bar{z}$ [0,0,0]
	$z,0,y$ [0,0,0]	$z,0,\bar{y}$ [0,0,0]	$\bar{z},0,y$ [0,0,0]
	$y,z,0$ [0,0,0]	$\bar{y},z,0$ [0,0,0]	$y,\bar{z},0$ [0,0,0]
	$y,0,\bar{z}$ [0,0,0]	$\bar{y},0,\bar{z}$ [0,0,0]	$\bar{y},0,z$ [0,0,0]
	$0,z,\bar{y}$ [0,0,0]	$0,z,y$ [0,0,0]	$0,\bar{z},\bar{y}$ [0,0,0]
	$z,y,0$ [0,0,0]	$z,\bar{y},0$ [0,0,0]	$\bar{z},\bar{y},0$ [0,0,0]
48    i    ..21'			
$1/4,y,\bar{y}+1/2$ [0,0,0]	$3/4,\bar{y},\bar{y}+1/2$ [0,0,0]	$3/4,y,y+1/2$ [0,0,0]	$1/4,\bar{y},y+1/2$ [0,0,0]
$\bar{y}+1/2,1/4,y$ [0,0,0]	$\bar{y}+1/2,3/4,\bar{y}$ [0,0,0]	$y+1/2,3/4,y$ [0,0,0]	$y+1/2,1/4,\bar{y}$ [0,0,0]
$y,\bar{y}+1/2,1/4$ [0,0,0]	$\bar{y},\bar{y}+1/2,3/4$ [0,0,0]	$y,y+1/2,3/4$ [0,0,0]	$\bar{y},y+1/2,1/4$ [0,0,0]
$3/4,\bar{y},y+1/2$ [0,0,0]	$1/4,y,y+1/2$ [0,0,0]	$1/4,\bar{y},\bar{y}+1/2$ [0,0,0]	$3/4,y,\bar{y}+1/2$ [0,0,0]
$y+1/2,3/4,\bar{y}$ [0,0,0]	$y+1/2,1/4,y$ [0,0,0]	$\bar{y}+1/2,1/4,\bar{y}$ [0,0,0]	$\bar{y}+1/2,3/4,y$ [0,0,0]
$\bar{y},y+1/2,3/4$ [0,0,0]	$y,y+1/2,1/4$ [0,0,0]	$\bar{y},\bar{y}+1/2,1/4$ [0,0,0]	$y,\bar{y}+1/2,3/4$ [0,0,0]



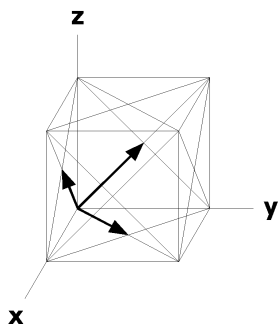
24	h	$m.m21'$	$0,y,y [0,0,0]$	$0,\bar{y},y [0,0,0]$	$0,y,\bar{y} [0,0,0]$	$0,\bar{y},\bar{y} [0,0,0]$
			$y,0,y [0,0,0]$	$y,0,\bar{y} [0,0,0]$	$\bar{y},0,y [0,0,0]$	$\bar{y},0,\bar{y} [0,0,0]$
			$y,y,0 [0,0,0]$	$\bar{y},y,0 [0,0,0]$	$y,\bar{y},0 [0,0,0]$	$\bar{y},\bar{y},0 [0,0,0]$
24	g	$mm2..1'$	$x,0,1/2 [0,0,0]$	$\bar{x},0,1/2 [0,0,0]$	$1/2,x,0 [0,0,0]$	$1/2,\bar{x},0 [0,0,0]$
			$0,1/2,x [0,0,0]$	$0,1/2,\bar{x} [0,0,0]$	$0,x,1/2 [0,0,0]$	$0,\bar{x},1/2 [0,0,0]$
			$x,1/2,0 [0,0,0]$	$\bar{x},1/2,0 [0,0,0]$	$1/2,0,\bar{x} [0,0,0]$	$1/2,0,x [0,0,0]$
16	f	$.3m1'$	$x,x,x [0,0,0]$	$\bar{x},\bar{x},x [0,0,0]$	$\bar{x},x,\bar{x} [0,0,0]$	$x,\bar{x},\bar{x} [0,0,0]$
			$x,x,\bar{x} [0,0,0]$	$\bar{x},\bar{x},\bar{x} [0,0,0]$	$x,\bar{x},x [0,0,0]$	$\bar{x},x,x [0,0,0]$
12	e	$4m.m1'$	$x,0,0 [0,0,0]$	$\bar{x},0,0 [0,0,0]$	$0,x,0 [0,0,0]$	$0,x,0 [0,0,0]$
			$0,\bar{x},0 [0,0,0]$	$0,0,x [0,0,0]$	$0,0,\bar{x} [0,0,0]$	$0,0,\bar{x} [0,0,0]$
12	d	$\bar{4}m.21'$	$1/4,0,1/2 [0,0,0]$	$3/4,0,1/2 [0,0,0]$	$1/2,1/4,0 [0,0,0]$	$1/2,1/4,0 [0,0,0]$
			$1/2,3/4,0 [0,0,0]$	$0,1/2,1/4 [0,0,0]$	$0,1/2,3/4 [0,0,0]$	$0,1/2,3/4 [0,0,0]$
8	c	$\bar{3}m1'$	$1/4,1/4,1/4 [0,0,0]$	$3/4,3/4,1/4 [0,0,0]$	$3/4,1/4,3/4 [0,0,0]$	$1/4,3/4,3/4 [0,0,0]$
6	b	$4/mm.m1'$	$0,1/2,1/2 [0,0,0]$	$1/2,0,1/2 [0,0,0]$	$1/2,1/2,0 [0,0,0]$	$1/2,1/2,0 [0,0,0]$
2	a	$m\bar{3}m1'$	$0,0,0 [0,0,0]$			

### Symmetry of Special Projections

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p6mm1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x,x,x$

Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x,x,0$



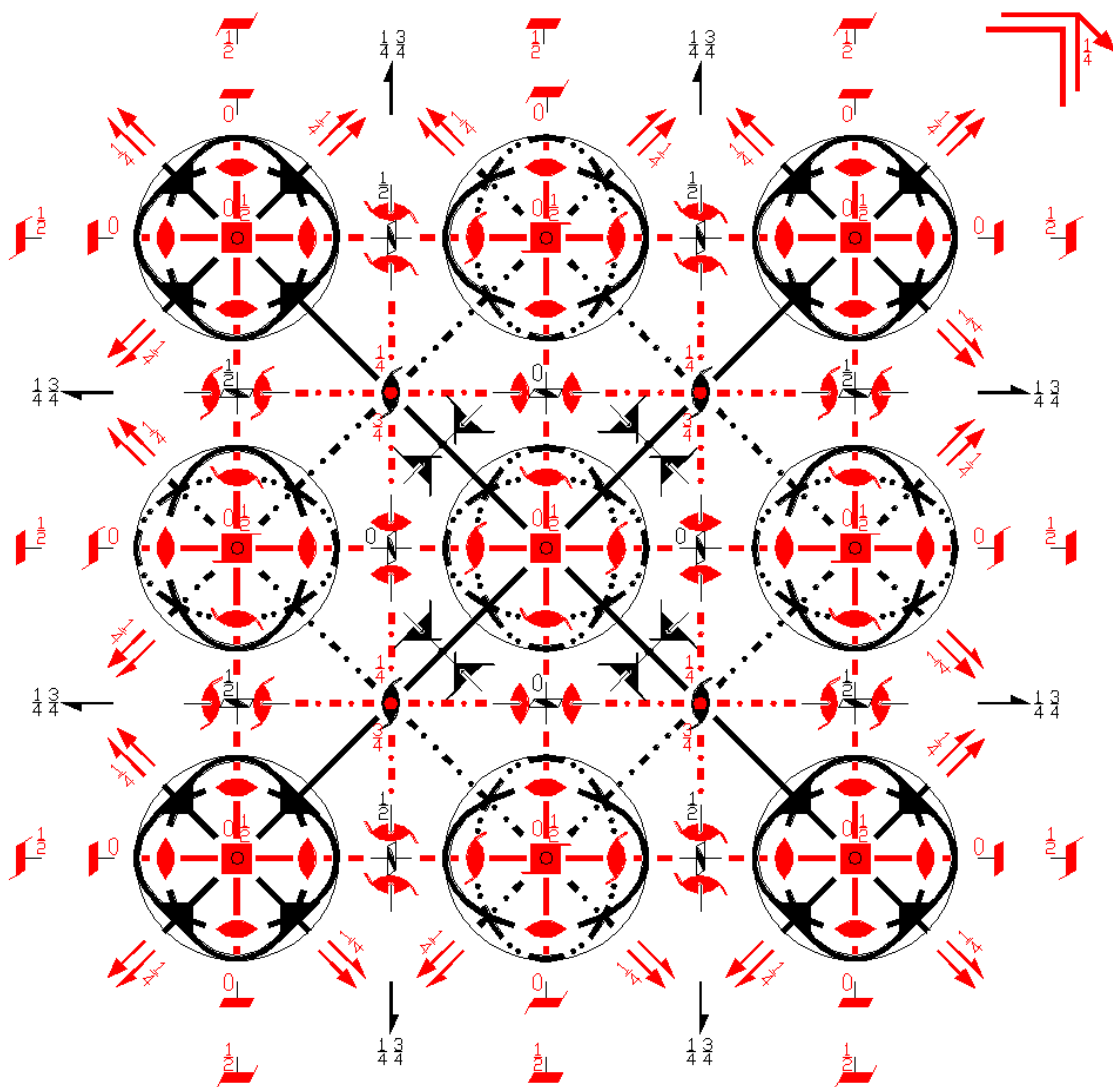
$Im\bar{3}'m$

229.3.1640

$m\bar{3}'m$

$I4'/m\bar{3}'2'/m$

Cubic



**Origin** at center ( $m\bar{3}'m$ )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/4;$   $y \leq x;$   $z \leq \min(1/2-x,y)$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/4,1/4,1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |   |   |  |
|---|---|---|--|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                            | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                 |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  0,0,0) | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)  | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}z}^{-1}$  0,0,0)  |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)     | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}z}$  0,0,0) | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}z}^{-1}$  0,0,0) |

(13) $2' \ x, x, 0$ ( $2_{xy}   0, 0, 0$ )'	(14) $2' \ x, \bar{x}, 0$ ( $2_{\bar{xy}}   0, 0, 0$ )'	(15) $4' \ 0, 0, z$ ( $4_z^{-1}   0, 0, 0$ )'	(16) $4^+ \ 0, 0, z$ ( $4_z   0, 0, 0$ )'
(17) $4' \ x, 0, 0$ ( $4_x^{-1}   0, 0, 0$ )'	(18) $2' \ 0, y, y$ ( $2_{yz}   0, 0, 0$ )'	(19) $2' \ 0, y, \bar{y}$ ( $2_{\bar{yz}}   0, 0, 0$ )'	(20) $4^+ \ x, 0, 0$ ( $4_x   0, 0, 0$ )'
(21) $4^+ \ 0, y, 0$ ( $4_y   0, 0, 0$ )'	(22) $2' \ x, 0, x$ ( $2_{xz}   0, 0, 0$ )'	(23) $4' \ 0, y, 0$ ( $4_y^{-1}   0, 0, 0$ )'	(24) $2' \ \bar{x}, 0, x$ ( $2_{\bar{xz}}   0, 0, 0$ )'
(25) $\bar{1}' \ 0, 0, 0$ ( $\bar{1}   0, 0, 0$ )'	(26) $m' \ x, y, 0$ ( $m_z   0, 0, 0$ )'	(27) $m' \ x, 0, z$ ( $m_y   0, 0, 0$ )'	(28) $m' \ 0, y, z$ ( $m_x   0, 0, 0$ )'
(29) $\bar{3}^+ \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}   0, 0, 0$ )'	(30) $\bar{3}^+ \ \bar{x}, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}^{-1}   0, 0, 0$ )'	(31) $\bar{3}^+ \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}^{-1}   0, 0, 0$ )'	(32) $\bar{3}^+ \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{xyz}^{-1}   0, 0, 0$ )'
(33) $\bar{3}^- \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}^{-1}   0, 0, 0$ )'	(34) $\bar{3}^- \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}   0, 0, 0$ )'	(35) $\bar{3}^- \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{xyz}   0, 0, 0$ )'	(36) $\bar{3}^- \ \bar{x}, x, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}   0, 0, 0$ )'
(37) $m \ x, \bar{x}, z$ ( $m_{xy}   0, 0, 0$ )	(38) $m \ x, x, z$ ( $m_{\bar{xy}}   0, 0, 0$ )	(39) $\bar{4}' \ 0, 0, z; 0, 0, 0$ ( $\bar{4}_z^{-1}   0, 0, 0$ )	(40) $\bar{4}^+ \ 0, 0, z; 0, 0, 0$ ( $\bar{4}_z   0, 0, 0$ )
(41) $\bar{4}' \ x, 0, 0; 0, 0, 0$ ( $\bar{4}_x^{-1}   0, 0, 0$ )	(42) $m \ x, y, \bar{y}$ ( $m_{yz}   0, 0, 0$ )	(43) $m \ x, y, y$ ( $m_{\bar{yz}}   0, 0, 0$ )	(44) $\bar{4}^+ \ x, 0, 0; 0, 0, 0$ ( $\bar{4}_x   0, 0, 0$ )
(45) $\bar{4}^+ \ 0, y, 0; 0, 0, 0$ ( $\bar{4}_y   0, 0, 0$ )	(46) $m \ \bar{x}, y, x$ ( $m_{xz}   0, 0, 0$ )	(47) $\bar{4}' \ 0, y, 0; 0, 0, 0$ ( $\bar{4}_y^{-1}   0, 0, 0$ )	(48) $m \ x, y, x$ ( $m_{\bar{xz}}   0, 0, 0$ )

## For (1/2, 1/2, 1/2) + set

(1) $t \ (1/2, 1/2, 1/2)$ ( $1   1/2, 1/2, 1/2$ )	(2) $2 \ (0, 0, 1/2) \ 1/4, 1/4, z$ ( $2_z   1/2, 1/2, 1/2$ )	(3) $2 \ (0, 1/2, 0) \ 1/4, y, 1/4$ ( $2_y   1/2, 1/2, 1/2$ )	(4) $2 \ (1/2, 0, 0) \ x, 1/4, 1/4$ ( $2_x   1/2, 1/2, 1/2$ )
(5) $3^+ \ (1/2, 1/2, 1/2) \ x, x, x$ ( $3_{xyz}   1/2, 1/2, 1/2$ )	(6) $3^+ \ (1/6, -1/6, 1/6)$ $x+1/3, x+1/3, \bar{x}$ ( $3_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2$ )	(7) $3^+ \ (-1/6, 1/6, 1/6)$ $x+2/3, \bar{x}-1/3, \bar{x}$ ( $3_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(8) $3^+ \ (1/6, 1/6, -1/6)$ $\bar{x}+1/3, \bar{x}+2/3, x$ ( $3_{\bar{yz}}^{-1}   1/2, 1/2, 1/2$ )
(9) $3^- \ (1/2, 1/2, 1/2) \ x, x, x$ ( $3_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(10) $3^- \ (-1/6, 1/6, 1/6)$ $x+1/3, \bar{x}+1/3, \bar{x}$ ( $3_{\bar{xyz}}   1/2, 1/2, 1/2$ )	(11) $3^- \ (1/6, 1/6, -1/6)$ $\bar{x}+2/3, \bar{x}+1/3, x$ ( $3_{xyz}   1/2, 1/2, 1/2$ )	(12) $3^- \ (1/6, -1/6, 1/6)$ $\bar{x}-1/3, x+2/3, \bar{x}$ ( $3_{\bar{yz}}   1/2, 1/2, 1/2$ )
(13) $2' \ (1/2, 1/2, 0) \ x, x, 1/4$ ( $2_{xy}   1/2, 1/2, 1/2$ )'	(14) $2' \ x, \bar{x}+1/2, 1/4$ ( $2_{\bar{xy}}   1/2, 1/2, 1/2$ )'	(15) $4' \ (0, 0, 1/2) \ 1/2, 0, z$ ( $4_z^{-1}   1/2, 1/2, 1/2$ )'	(16) $4^+ \ (0, 0, 1/2) \ 0, 1/2, z$ ( $4_z   1/2, 1/2, 1/2$ )'
(17) $4' \ (1/2, 0, 0) \ x, 1/2, 0$ ( $4_x^{-1}   1/2, 1/2, 1/2$ )'	(18) $2' \ (0, 1/2, 1/2) \ 1/4, y, y$ ( $2_{yz}   1/2, 1/2, 1/2$ )'	(19) $2' \ 1/4, y+1/2, \bar{y}$ ( $2_{\bar{yz}}   1/2, 1/2, 1/2$ )'	(20) $4^+ \ (1/2, 0, 0) \ x, 0, 1/2$ ( $4_x   1/2, 1/2, 1/2$ )'
(21) $4^+ \ (0, 1/2, 0) \ 1/2, y, 0$ ( $4_y   1/2, 1/2, 1/2$ )'	(22) $2' \ (1/2, 0, 1/2) \ x, 1/4, x$ ( $2_{xz}   1/2, 1/2, 1/2$ )'	(23) $4' \ (0, 1/2, 0) \ 0, y, 1/2$ ( $4_y^{-1}   1/2, 1/2, 1/2$ )'	(24) $2' \ \bar{x}+1/2, 1/4, x$ ( $2_{\bar{xz}}   1/2, 1/2, 1/2$ )'
(25) $\bar{1}' \ 1/4, 1/4, 1/4$ ( $\bar{1}   1/2, 1/2, 1/2$ )'	(26) $n' \ (1/2, 1/2, 0) \ x, y, 1/4$ ( $m_z   1/2, 1/2, 1/2$ )'	(27) $n' \ (1/2, 0, 1/2) \ x, 1/4, z$ ( $m_y   1/2, 1/2, 1/2$ )'	(28) $n' \ (0, 1/2, 1/2) \ 1/4, y, z$ ( $m_x   1/2, 1/2, 1/2$ )'
(29) $\bar{3}^+ \ x, x, x;$ $1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 1/2, 1/2$ )'	(30) $\bar{3}^+ \ \bar{x}-1, x+1, \bar{x};$ $-1/4, 1/4, 3/4$ ( $\bar{3}_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2$ )'	(31) $\bar{3}^+ \ x, \bar{x}+1, \bar{x};$ $1/4, 3/4, -1/4$ ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2$ )'	(32) $\bar{3}^+ \ \bar{x}+1, \bar{x}, x;$ $3/4, -1/4, 1/4$ ( $\bar{3}_{\bar{yz}}^{-1}   1/2, 1/2, 1/2$ )'

(33) $\bar{3}^-$ ' x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2)'	(34) $\bar{3}^-$ ' x+1, $\bar{x}$ -1, $\bar{x}$ ; 1/4,-1/4,3/4 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2)'	(35) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ +1, x; -1/4,3/4,1/4 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2)'	(36) $\bar{3}^-$ ' $\bar{x}$ +1, x, $\bar{x}$ ; 3/4,1/4,-1/4 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2)'
(37) c (0,0,1/2) x+1/2, $\bar{x}$ ,z ( $m_{xy}$   1/2,1/2,1/2)	(38) n (1/2,1/2,1/2) x,x,z ( $m_{xy}$   1/2,1/2,1/2)	(39) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$   1/2,1/2,1/2)	(40) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)
(41) $\bar{4}^-$ x,0,1/2; 1/4,0,1/2 ( $\bar{4}_x^{-1}$   1/2,1/2,1/2)	(42) a (1/2,0,0) x,y+1/2, $\bar{y}$ ( $m_{yz}$   1/2,1/2,1/2)	(43) n (1/2,1/2,1/2) x,y,y ( $m_{yz}$   1/2,1/2,1/2)	(44) $\bar{4}^+$ x,1/2,0; 1/4,1/2,0 ( $\bar{4}_x$   1/2,1/2,1/2)
(45) $\bar{4}^+$ 0,y,1/2; 0,1/4,1/2 ( $\bar{4}_y$   1/2,1/2,1/2)	(46) b (0,1/2,0) $\bar{x}$ +1/2,y,x ( $m_{xz}$   1/2,1/2,1/2)	(47) $\bar{4}^-$ 1/2,y,0; 1/2,1/4,0 ( $\bar{4}_y^{-1}$   1/2,1/2,1/2)	(48) n (1/2,1/2,1/2) x,y,x ( $m_{xz}$   1/2,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

### Coordinates

			(0,0,0) +	(1/2,1/2,1/2) +						
96	l	1								
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}$ , $\bar{y}$ ,z	[ $\bar{u}$ , $\bar{v}$ ,w]	(3)	$\bar{x}$ ,y,z	[ $\bar{u}$ ,v, $\bar{w}$ ]		
(5)	z,x,y	[w,u,v]	(6)	z, $\bar{x}$ , $\bar{y}$	[w, $\bar{u}$ , $\bar{v}$ ]	(7)	$\bar{z}$ , $\bar{x}$ ,y	[ $\bar{w}$ , $\bar{u}$ ,v]		
(9)	y,z,x	[v,w,u]	(10)	$\bar{y}$ ,z, $\bar{x}$	[ $\bar{v}$ ,w, $\bar{u}$ ]	(11)	y, $\bar{z}$ , $\bar{x}$	[v, $\bar{w}$ , $\bar{u}$ ]		
(13)	y,x, $\bar{z}$	[ $\bar{v}$ , $\bar{u}$ ,w]	(14)	$\bar{y}$ , $\bar{x}$ , $\bar{z}$	[v,u,w]	(15)	y, $\bar{x}$ ,z	[ $\bar{v}$ ,u, $\bar{w}$ ]		
(17)	x,z, $\bar{y}$	[ $\bar{u}$ , $\bar{w}$ ,v]	(18)	$\bar{x}$ ,z,y	[u, $\bar{w}$ , $\bar{v}$ ]	(19)	$\bar{x}$ , $\bar{z}$ , $\bar{y}$	[u,w,v]		
(21)	z,y, $\bar{x}$	[ $\bar{w}$ , $\bar{v}$ ,u]	(22)	z, $\bar{y}$ ,x	[ $\bar{w}$ ,v, $\bar{u}$ ]	(23)	$\bar{z}$ ,y,x	[w, $\bar{v}$ , $\bar{u}$ ]		
(25)	$\bar{x}$ , $\bar{y}$ , $\bar{z}$	[ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]	(26)	x,y, $\bar{z}$	[u,v, $\bar{w}$ ]	(27)	x, $\bar{y}$ ,z	[u, $\bar{v}$ ,w]		
(29)	$\bar{z}$ , $\bar{x}$ , $\bar{y}$	[ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ]	(30)	$\bar{z}$ ,x,y	[ $\bar{w}$ ,u,v]	(31)	z,x, $\bar{y}$	[w,u, $\bar{v}$ ]		
(33)	$\bar{y}$ , $\bar{z}$ , $\bar{x}$	[ $\bar{v}$ , $\bar{w}$ , $\bar{u}$ ]	(34)	y, $\bar{z}$ ,x	[v, $\bar{w}$ ,u]	(35)	$\bar{y}$ ,z,x	[ $\bar{v}$ ,w,u]		
(37)	$\bar{y}$ , $\bar{x}$ ,z	[v,u, $\bar{w}$ ]	(38)	y,x,z	[ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(39)	$\bar{y}$ ,x, $\bar{z}$	[v, $\bar{u}$ ,w]		
(41)	$\bar{x}$ , $\bar{z}$ ,y	[u,w, $\bar{v}$ ]	(42)	x, $\bar{z}$ , $\bar{y}$	[u,w, $\bar{v}$ ]	(43)	x,z,y	[ $\bar{u}$ , $\bar{w}$ , $\bar{v}$ ]		
(45)	$\bar{z}$ , $\bar{y}$ ,x	[w,v, $\bar{u}$ ]	(46)	$\bar{z}$ ,y, $\bar{x}$	[w, $\bar{v}$ ,u]	(47)	z, $\bar{y}$ , $\bar{x}$	[ $\bar{w}$ ,v,u]		
48	k	..m	x,x,z	[u, $\bar{u}$ ,0]	$\bar{x}$ , $\bar{x}$ ,z	[ $\bar{u}$ ,u,0]	$\bar{x}$ ,x, $\bar{z}$	[ $\bar{u}$ , $\bar{u}$ ,0]	x, $\bar{x}$ , $\bar{z}$	[u,u,0]
			z,x,x	[0,u, $\bar{u}$ ]	z, $\bar{x}$ , $\bar{x}$	[0, $\bar{u}$ ,u]	$\bar{z}$ , $\bar{x}$ ,x	[0, $\bar{u}$ , $\bar{u}$ ]	$\bar{z}$ ,x, $\bar{x}$	[0,u,u]
			x,z,x	[ $\bar{u}$ ,0,u]	$\bar{x}$ ,z, $\bar{x}$	[u,0, $\bar{u}$ ]	x, $\bar{z}$ , $\bar{x}$	[ $\bar{u}$ ,0, $\bar{u}$ ]	$\bar{x}$ , $\bar{z}$ ,x	[u,0,u]
			x,x, $\bar{z}$	[u, $\bar{u}$ ,0]	$\bar{x}$ , $\bar{x}$ , $\bar{z}$	[ $\bar{u}$ ,u,0]	x, $\bar{x}$ ,z	[u,u,0]	$\bar{x}$ ,x,z	[ $\bar{u}$ , $\bar{u}$ ,0]
			x,z, $\bar{x}$	[ $\bar{u}$ ,0, $\bar{u}$ ]	$\bar{x}$ ,z,x	[u,0,u]	$\bar{x}$ , $\bar{z}$ , $\bar{x}$	[u,0, $\bar{u}$ ]	x, $\bar{z}$ ,x	[ $\bar{u}$ ,0,u]

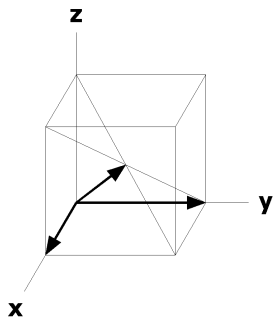
			$z, x, \bar{x} [0, u, u]$	$z, \bar{x}, x [0, \bar{u}, \bar{u}]$	$\bar{z}, x, x [0, u, \bar{u}]$	$\bar{z}, \bar{x}, \bar{x} [0, \bar{u}, u]$
48	j	m'..	$0, y, z [0, v, w]$	$0, \bar{y}, z [0, \bar{v}, w]$	$0, y, \bar{z} [0, v, \bar{w}]$	$0, \bar{y}, \bar{z} [0, \bar{v}, \bar{w}]$
			$z, 0, y [w, 0, v]$	$z, 0, \bar{y} [w, 0, \bar{v}]$	$\bar{z}, 0, y [\bar{w}, 0, v]$	$\bar{z}, 0, \bar{y} [\bar{w}, 0, \bar{v}]$
			$y, z, 0 [v, w, 0]$	$\bar{y}, z, 0 [\bar{v}, w, 0]$	$y, \bar{z}, 0 [v, \bar{w}, 0]$	$\bar{y}, \bar{z}, 0 [\bar{v}, \bar{w}, 0]$
			$y, 0, \bar{z} [\bar{v}, 0, w]$	$\bar{y}, 0, \bar{z} [v, 0, w]$	$y, 0, z [\bar{v}, 0, \bar{w}]$	$\bar{y}, 0, z [v, 0, \bar{w}]$
			$0, z, \bar{y} [0, \bar{w}, v]$	$0, z, y [0, \bar{w}, \bar{v}]$	$0, \bar{z}, \bar{y} [0, w, v]$	$0, \bar{z}, y [0, w, \bar{v}]$
			$z, y, 0 [\bar{w}, \bar{v}, 0]$	$z, \bar{y}, 0 [\bar{w}, v, 0]$	$\bar{z}, y, 0 [w, \bar{v}, 0]$	$\bar{z}, \bar{y}, 0 [w, v, 0]$
48	i	..2'				
			$1/4, y, \bar{y} + 1/2 [u, v, v]$	$3/4, \bar{y}, \bar{y} + 1/2 [\bar{u}, \bar{v}, v]$	$3/4, y, y + 1/2 [\bar{u}, v, \bar{v}]$	$1/4, \bar{y}, y + 1/2 [u, \bar{v}, \bar{v}]$
			$\bar{y} + 1/2, 1/4, y [v, u, v]$	$\bar{y} + 1/2, 3/4, \bar{y} [v, \bar{u}, \bar{v}]$	$y + 1/2, 3/4, y [v, \bar{u}, v]$	$y + 1/2, 1/4, \bar{y} [v, u, \bar{v}]$
			$y, \bar{y} + 1/2, 1/4 [v, v, u]$	$\bar{y}, \bar{y} + 1/2, 3/4 [v, v, \bar{u}]$	$y, y + 1/2, 3/4 [v, \bar{v}, \bar{u}]$	$\bar{y}, y + 1/2, 1/4 [v, \bar{v}, u]$
			$3/4, \bar{y}, y + 1/2 [\bar{u}, \bar{v}, \bar{v}]$	$1/4, y, y + 1/2 [u, v, \bar{v}]$	$1/4, \bar{y}, \bar{y} + 1/2 [u, \bar{v}, v]$	$3/4, y, \bar{y} + 1/2 [\bar{u}, v, v]$
			$y + 1/2, 3/4, \bar{y} [\bar{v}, \bar{u}, \bar{v}]$	$y + 1/2, 1/4, y [v, u, v]$	$\bar{y} + 1/2, 1/4, \bar{y} [v, u, \bar{v}]$	$\bar{y} + 1/2, 3/4, y [v, \bar{u}, v]$
			$\bar{y}, y + 1/2, 3/4 [\bar{v}, \bar{v}, \bar{u}]$	$y, y + 1/2, 1/4 [v, \bar{v}, u]$	$\bar{y}, \bar{y} + 1/2, 1/4 [v, v, u]$	$y, \bar{y} + 1/2, 3/4 [v, v, \bar{u}]$
24	h	m'.m2'	$0, y, y [0, \bar{v}, v]$	$0, \bar{y}, y [0, v, v]$	$0, y, \bar{y} [0, \bar{v}, \bar{v}]$	$0, \bar{y}, \bar{y} [0, v, \bar{v}]$
			$y, 0, y [v, 0, \bar{v}]$	$y, 0, \bar{y} [v, 0, v]$	$\bar{y}, 0, y [\bar{v}, 0, \bar{v}]$	$\bar{y}, 0, \bar{y} [\bar{v}, 0, v]$
			$y, y, 0 [\bar{v}, v, 0]$	$\bar{y}, y, 0 [v, v, 0]$	$y, \bar{y}, 0 [\bar{v}, \bar{v}, 0]$	$\bar{y}, \bar{y}, 0 [v, \bar{v}, 0]$
24	g	m'm'2..	$x, 0, 1/2 [u, 0, 0]$	$\bar{x}, 0, 1/2 [\bar{u}, 0, 0]$	$1/2, x, 0 [0, u, 0]$	$1/2, \bar{x}, 0 [0, \bar{u}, 0]$
			$0, 1/2, x [0, 0, u]$	$0, 1/2, \bar{x} [0, 0, \bar{u}]$	$0, x, 1/2 [0, \bar{u}, 0]$	$0, \bar{x}, 1/2 [0, u, 0]$
			$x, 1/2, 0 [\bar{u}, 0, 0]$	$\bar{x}, 1/2, 0 [u, 0, 0]$	$1/2, 0, \bar{x} [0, 0, u]$	$1/2, 0, x [0, 0, \bar{u}]$
16	f	.3m'	$x, x, x [u, u, u]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$	$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
			$x, x, \bar{x} [\bar{u}, \bar{u}, u]$	$\bar{x}, \bar{x}, \bar{x} [u, u, u]$	$x, \bar{x}, x [\bar{u}, u, \bar{u}]$	$\bar{x}, x, x [u, \bar{u}, \bar{u}]$
12	e	4'm'.m	$x, 0, 0 [0, 0, 0]$	$\bar{x}, 0, 0 [0, 0, 0]$	$0, x, 0 [0, 0, 0]$	$0, x, 0 [0, 0, 0]$
			$0, \bar{x}, 0 [0, 0, 0]$	$0, 0, x [0, 0, 0]$	$0, 0, \bar{x} [0, 0, 0]$	$0, 0, \bar{x} [0, 0, 0]$
12	d	4m'.2'	$1/4, 0, 1/2 [u, 0, 0]$	$3/4, 0, 1/2 [\bar{u}, 0, 0]$	$1/2, 1/4, 0 [0, u, 0]$	$1/2, 1/4, 0 [0, u, 0]$
			$1/2, 3/4, 0 [0, \bar{u}, 0]$	$0, 1/2, 1/4 [0, 0, u]$	$0, 1/2, 3/4 [0, 0, \bar{u}]$	$0, 1/2, 3/4 [0, 0, \bar{u}]$
8	c	.3'm	$1/4, 1/4, 1/4 [0, 0, 0]$	$3/4, 3/4, 1/4 [0, 0, 0]$	$3/4, 1/4, 3/4 [0, 0, 0]$	$1/4, 3/4, 3/4 [0, 0, 0]$
6	b	4'/m'm'.m	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$	$1/2, 1/2, 0 [0, 0, 0]$
2	a	m'3'm	$0, 0, 0 [0, 0, 0]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4'm'm$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $0,0,z$

Along  $[1,1,1]$   $p6mm$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
Origin at  $x,x,x$

Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at  $x,x,0$



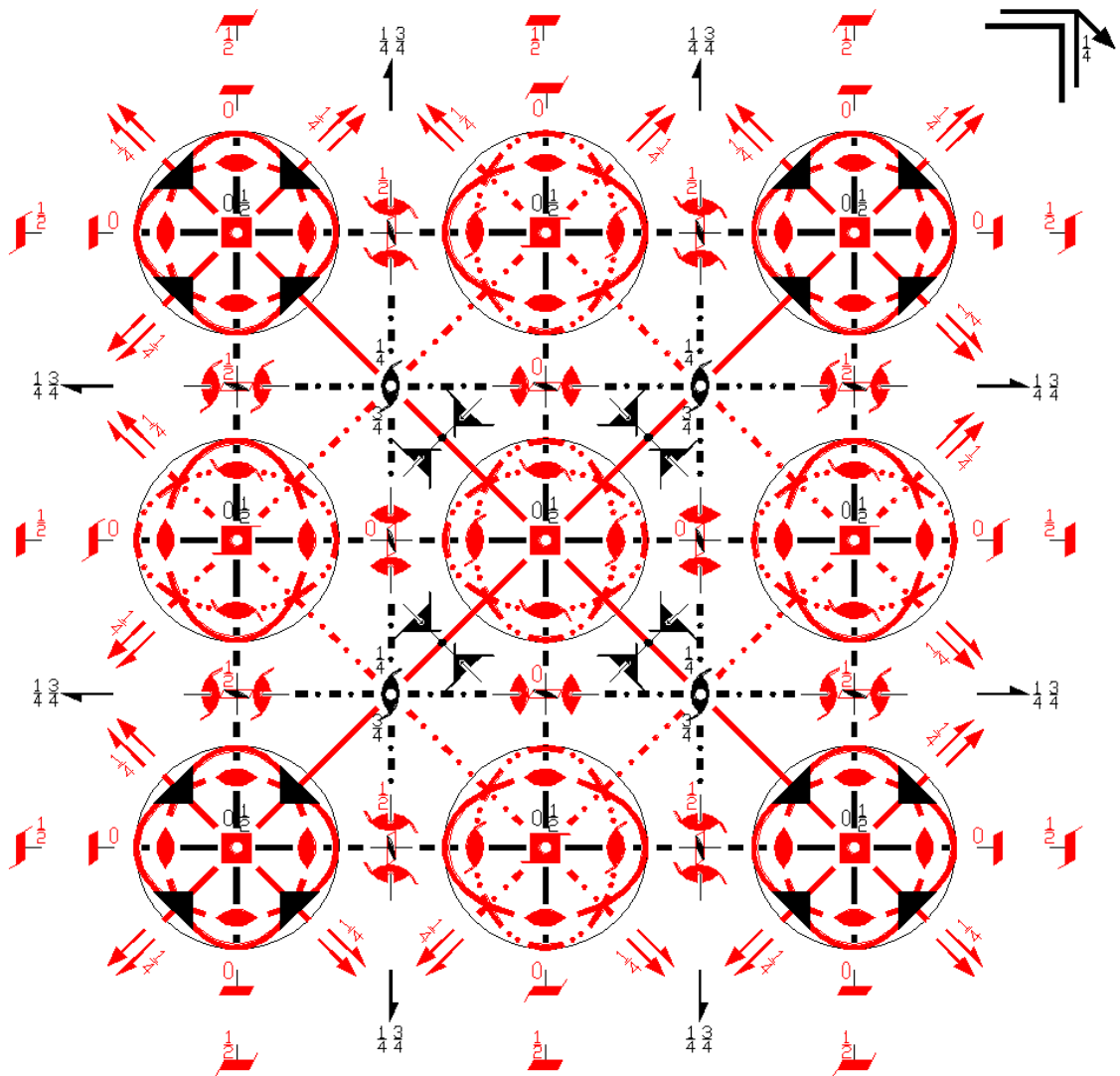
$Im\bar{3}m'$

229.4.1641

$m\bar{3}m'$

$I4'/m\bar{3}2'/m'$

Cubic



**Origin** at center ( $m\bar{3}m'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/4;$   $y \leq x;$   $z \leq \min(1/2-x,y)$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/4,1/4,1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |  |   |   |
|---|--|---|---|
| (1) 1<br>(1 0,0,0)                            | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                                 | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)                            | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)                                  |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)      | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}\bar{z}}$  0,0,0) | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)  | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}yz}$  0,0,0)        |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}^{-1}$  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)      | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{\bar{x}yz}$  0,0,0) | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{\bar{x}y\bar{z}}$  0,0,0) |

(13) $2' x, x, 0$ ( $2_{xy}   0, 0, 0$ )'	(14) $2' x, \bar{x}, 0$ ( $2_{\bar{xy}}   0, 0, 0$ )'	(15) $4' 0, 0, z$ ( $4_z^{-1}   0, 0, 0$ )'	(16) $4^+ 0, 0, z$ ( $4_z   0, 0, 0$ )'
(17) $4' x, 0, 0$ ( $4_x^{-1}   0, 0, 0$ )'	(18) $2' 0, y, y$ ( $2_{yz}   0, 0, 0$ )'	(19) $2' 0, y, \bar{y}$ ( $2_{\bar{yz}}   0, 0, 0$ )'	(20) $4^+ x, 0, 0$ ( $4_x   0, 0, 0$ )'
(21) $4^+ 0, y, 0$ ( $4_y   0, 0, 0$ )'	(22) $2' x, 0, x$ ( $2_{xz}   0, 0, 0$ )'	(23) $4' 0, y, 0$ ( $4_y^{-1}   0, 0, 0$ )'	(24) $2' \bar{x}, 0, x$ ( $2_{\bar{xz}}   0, 0, 0$ )'
(25) $\bar{1} 0, 0, 0$ ( $\bar{1}   0, 0, 0$ )	(26) $m x, y, 0$ ( $m_z   0, 0, 0$ )	(27) $m x, 0, z$ ( $m_y   0, 0, 0$ )	(28) $m 0, y, z$ ( $m_x   0, 0, 0$ )
(29) $\bar{3}^+ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}   0, 0, 0$ )	(30) $\bar{3}^+ \bar{x}, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}^{-1}   0, 0, 0$ )	(31) $\bar{3}^+ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}^{-1}   0, 0, 0$ )	(32) $\bar{3}^+ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{xyz}^{-1}   0, 0, 0$ )
(33) $\bar{3}^- x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}^{-1}   0, 0, 0$ )	(34) $\bar{3}^- \bar{x}, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}   0, 0, 0$ )	(35) $\bar{3}^- \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{xyz}   0, 0, 0$ )	(36) $\bar{3}^- \bar{x}, x, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}   0, 0, 0$ )
(37) $m' x, \bar{x}, z$ ( $m_{xy}   0, 0, 0$ )'	(38) $m' x, x, z$ ( $m_{\bar{xy}}   0, 0, 0$ )'	(39) $\bar{4}' 0, 0, z; 0, 0, 0$ ( $\bar{4}_z^{-1}   0, 0, 0$ )'	(40) $\bar{4}^+ 0, 0, z; 0, 0, 0$ ( $\bar{4}_z   0, 0, 0$ )'
(41) $\bar{4}' x, 0, 0; 0, 0, 0$ ( $\bar{4}_x^{-1}   0, 0, 0$ )'	(42) $m' x, y, \bar{y}$ ( $m_{yz}   0, 0, 0$ )'	(43) $m' x, y, y$ ( $m_{\bar{yz}}   0, 0, 0$ )'	(44) $\bar{4}^+ x, 0, 0; 0, 0, 0$ ( $\bar{4}_x   0, 0, 0$ )'
(45) $\bar{4}^+ 0, y, 0; 0, 0, 0$ ( $\bar{4}_y   0, 0, 0$ )'	(46) $m' \bar{x}, y, x$ ( $m_{xz}   0, 0, 0$ )'	(47) $\bar{4}' 0, y, 0; 0, 0, 0$ ( $\bar{4}_y^{-1}   0, 0, 0$ )'	(48) $m' x, y, x$ ( $m_{\bar{xz}}   0, 0, 0$ )'

For (1/2, 1/2, 1/2) + set

(1) $t (1/2, 1/2, 1/2)$ ( $1   1/2, 1/2, 1/2$ )	(2) $2 (0, 0, 1/2) 1/4, 1/4, z$ ( $2_z   1/2, 1/2, 1/2$ )	(3) $2 (0, 1/2, 0) 1/4, y, 1/4$ ( $2_y   1/2, 1/2, 1/2$ )	(4) $2 (1/2, 0, 0) x, 1/4, 1/4$ ( $2_x   1/2, 1/2, 1/2$ )
(5) $3^+ (1/2, 1/2, 1/2) x, x, x$ ( $3_{xyz}   1/2, 1/2, 1/2$ )	(6) $3^+ (1/6, -1/6, 1/6)$ $x+1/3, x+1/3, \bar{x}$ ( $3_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2$ )	(7) $3^+ (-1/6, 1/6, 1/6)$ $x+2/3, \bar{x}-1/3, \bar{x}$ ( $3_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(8) $3^+ (1/6, 1/6, -1/6)$ $\bar{x}+1/3, \bar{x}+2/3, x$ ( $3_{\bar{yz}}^{-1}   1/2, 1/2, 1/2$ )
(9) $3^- (1/2, 1/2, 1/2) x, x, x$ ( $3_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(10) $3^- (-1/6, 1/6, 1/6)$ $x+1/3, \bar{x}+1/3, \bar{x}$ ( $3_{xyz}   1/2, 1/2, 1/2$ )	(11) $3^- (1/6, 1/6, -1/6)$ $\bar{x}+2/3, \bar{x}+1/3, x$ ( $3_{\bar{yz}}   1/2, 1/2, 1/2$ )	(12) $3^- (1/6, -1/6, 1/6)$ $\bar{x}-1/3, x+2/3, \bar{x}$ ( $3_{xyz}   1/2, 1/2, 1/2$ )
(13) $2' (1/2, 1/2, 0) x, x, 1/4$ ( $2_{xy}   1/2, 1/2, 1/2$ )'	(14) $2' x, \bar{x}+1/2, 1/4$ ( $2_{\bar{xy}}   1/2, 1/2, 1/2$ )'	(15) $4' (0, 0, 1/2) 1/2, 0, z$ ( $4_z^{-1}   1/2, 1/2, 1/2$ )'	(16) $4^+ (0, 0, 1/2) 0, 1/2, z$ ( $4_z   1/2, 1/2, 1/2$ )'
(17) $4' (1/2, 0, 0) x, 1/2, 0$ ( $4_x^{-1}   1/2, 1/2, 1/2$ )'	(18) $2' (0, 1/2, 1/2) 1/4, y, y$ ( $2_{yz}   1/2, 1/2, 1/2$ )'	(19) $2' 1/4, y+1/2, \bar{y}$ ( $2_{\bar{yz}}   1/2, 1/2, 1/2$ )'	(20) $4^+ (1/2, 0, 0) x, 0, 1/2$ ( $4_x   1/2, 1/2, 1/2$ )'
(21) $4^+ (0, 1/2, 0) 1/2, y, 0$ ( $4_y   1/2, 1/2, 1/2$ )'	(22) $2' (1/2, 0, 1/2) x, 1/4, x$ ( $2_{xz}   1/2, 1/2, 1/2$ )'	(23) $4' (0, 1/2, 0) 0, y, 1/2$ ( $4_y^{-1}   1/2, 1/2, 1/2$ )'	(24) $2' \bar{x}+1/2, 1/4, x$ ( $2_{\bar{xz}}   1/2, 1/2, 1/2$ )'
(25) $\bar{1} 1/4, 1/4, 1/4$ ( $\bar{1}   1/2, 1/2, 1/2$ )	(26) $n (1/2, 1/2, 0) x, y, 1/4$ ( $m_z   1/2, 1/2, 1/2$ )	(27) $n (1/2, 0, 1/2) x, 1/4, z$ ( $m_y   1/2, 1/2, 1/2$ )	(28) $n (0, 1/2, 1/2) 1/4, y, z$ ( $m_x   1/2, 1/2, 1/2$ )
(29) $\bar{3}^+ x, x, x;$ $1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 1/2, 1/2$ )	(30) $\bar{3}^+ \bar{x}-1, x+1, \bar{x};$ $-1/4, 1/4, 3/4$ ( $\bar{3}_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2$ )	(31) $\bar{3}^+ x, \bar{x}+1, \bar{x};$ $1/4, 3/4, -1/4$ ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(32) $\bar{3}^+ \bar{x}+1, \bar{x}, x;$ $3/4, -1/4, 1/4$ ( $\bar{3}_{\bar{yz}}^{-1}   1/2, 1/2, 1/2$ )



(33) $\bar{3}^-$ $x,x,x;$ $1/4,1/4,1/4$ $(\bar{3}_{xyz}^{-1} 1/2,1/2,1/2)$	(34) $\bar{3}^-$ $x+1,\bar{x}-1,\bar{x};$ $1/4,-1/4,3/4$ $(\bar{3}_{xyz}^{-1} 1/2,1/2,1/2)$	(35) $\bar{3}^-$ $\bar{x},\bar{x}+1,x;$ $-1/4,3/4,1/4$ $(\bar{3}_{xyz}^{-1} 1/2,1/2,1/2)$	(36) $\bar{3}^-$ $\bar{x}+1,x,\bar{x};$ $3/4,1/4,-1/4$ $(\bar{3}_{xyz}^{-1} 1/2,1/2,1/2)$
(37) $c'$ $(0,0,1/2)$ $x+1/2,\bar{x},z$ $(m_{xy} 1/2,1/2,1/2)'$	(38) $n'$ $(1/2,1/2,1/2)$ $x,x,z$ $(m_{xy} 1/2,1/2,1/2)'$	(39) $\bar{4}^-$ $0,1/2,z; 0,1/2,1/4$ $(\bar{4}_z^{-1} 1/2,1/2,1/2)'$	(40) $\bar{4}^+$ $1/2,0,z; 1/2,0,1/4$ $(\bar{4}_z 1/2,1/2,1/2)'$
(41) $\bar{4}^-$ $x,0,1/2; 1/4,0,1/2$ $(\bar{4}_x^{-1} 1/2,1/2,1/2)'$	(42) $a'$ $(1/2,0,0)$ $x,y+1/2,\bar{y}$ $(m_{yz} 1/2,1/2,1/2)'$	(43) $n'$ $(1/2,1/2,1/2)$ $x,y,y$ $(m_{yz} 1/2,1/2,1/2)'$	(44) $\bar{4}^+$ $x,1/2,0; 1/4,1/2,0$ $(\bar{4}_x 1/2,1/2,1/2)'$
(45) $\bar{4}^+$ $0,y,1/2; 0,1/4,1/2$ $(\bar{4}_y 1/2,1/2,1/2)'$	(46) $b'$ $(0,1/2,0)$ $\bar{x}+1/2,y,x$ $(m_{xz} 1/2,1/2,1/2)'$	(47) $\bar{4}^-$ $1/2,y,0; 1/2,1/4,0$ $(\bar{4}_y^{-1} 1/2,1/2,1/2)'$	(48) $n'$ $(1/2,1/2,1/2)$ $x,y,x$ $(m_{xz} 1/2,1/2,1/2)'$

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(1/2,1/2,1/2)$ ; (2); (3); (5); (13); (25).

**Positions**

			Coordinates						
Multiplicity, Wyckoff letter, Site Symmetry.									
			(0,0,0) +	(1/2,1/2,1/2) +					
96	l	1							
(1)	$x,y,z$	$[u,v,w]$	(2)	$\bar{x},\bar{y},z$	$[\bar{u},\bar{v},w]$	(3)	$\bar{x},y,z$	$[\bar{u},v,\bar{w}]$	
(5)	$z,x,y$	$[w,u,v]$	(6)	$z,\bar{x},\bar{y}$	$[w,\bar{u},\bar{v}]$	(7)	$\bar{z},\bar{x},y$	$[\bar{w},\bar{u},v]$	
(9)	$y,z,x$	$[v,w,u]$	(10)	$\bar{y},z,\bar{x}$	$[\bar{v},w,\bar{u}]$	(11)	$y,\bar{z},\bar{x}$	$[v,\bar{w},\bar{u}]$	
(13)	$y,x,\bar{z}$	$[\bar{v},\bar{u},w]$	(14)	$\bar{y},\bar{x},\bar{z}$	$[v,u,w]$	(15)	$y,\bar{x},z$	$[\bar{v},u,\bar{w}]$	
(17)	$x,z,\bar{y}$	$[\bar{u},\bar{w},v]$	(18)	$\bar{x},z,y$	$[u,\bar{w},\bar{v}]$	(19)	$\bar{x},\bar{z},\bar{y}$	$[u,w,v]$	
(21)	$z,y,\bar{x}$	$[\bar{w},\bar{v},u]$	(22)	$z,\bar{y},x$	$[\bar{w},v,\bar{u}]$	(23)	$\bar{z},y,x$	$[w,\bar{v},\bar{u}]$	
(25)	$\bar{x},\bar{y},\bar{z}$	$[u,v,w]$	(26)	$x,y,\bar{z}$	$[\bar{u},\bar{v},w]$	(27)	$x,\bar{y},z$	$[\bar{u},v,\bar{w}]$	
(29)	$\bar{z},\bar{x},\bar{y}$	$[w,u,v]$	(30)	$\bar{z},x,y$	$[w,\bar{u},\bar{v}]$	(31)	$z,x,\bar{y}$	$[\bar{w},\bar{u},v]$	
(33)	$\bar{y},\bar{z},\bar{x}$	$[v,w,u]$	(34)	$y,\bar{z},x$	$[\bar{v},w,\bar{u}]$	(35)	$\bar{y},z,x$	$[v,\bar{w},\bar{u}]$	
(37)	$\bar{y},\bar{x},z$	$[\bar{v},\bar{u},w]$	(38)	$y,x,z$	$[v,u,w]$	(39)	$\bar{y},x,\bar{z}$	$[v,\bar{u},\bar{w}]$	
(41)	$\bar{x},\bar{z},y$	$[\bar{u},\bar{w},v]$	(42)	$x,\bar{z},\bar{y}$	$[u,\bar{w},\bar{v}]$	(43)	$x,z,y$	$[u,w,v]$	
(45)	$\bar{z},\bar{y},x$	$[\bar{w},\bar{v},u]$	(46)	$\bar{z},y,\bar{x}$	$[\bar{w},v,\bar{u}]$	(47)	$z,\bar{y},\bar{x}$	$[w,\bar{v},\bar{u}]$	
48	k	..m'	$x,x,z$	$[\bar{x},\bar{x},z]$	$[\bar{u},\bar{u},w]$	$\bar{x},x,\bar{z}$	$[\bar{u},u,\bar{w}]$	$x,\bar{x},\bar{z}$	$[u,\bar{u},\bar{w}]$
			$z,x,x$	$[z,\bar{x},\bar{x}]$	$[w,\bar{u},\bar{u}]$	$\bar{z},\bar{x},x$	$[\bar{w},\bar{u},u]$	$\bar{z},x,\bar{x}$	$[\bar{w},u,\bar{u}]$
			$x,z,x$	$[x,\bar{z},\bar{x}]$	$[\bar{u},w,\bar{u}]$	$x,\bar{z},\bar{x}$	$[u,\bar{w},\bar{u}]$	$\bar{x},\bar{z},x$	$[\bar{u},\bar{w},u]$
			$x,x,\bar{z}$	$[\bar{x},\bar{x},\bar{z}]$	$[u,u,w]$	$x,\bar{x},z$	$[\bar{u},u,\bar{w}]$	$\bar{x},x,z$	$[u,\bar{u},\bar{w}]$
			$x,z,\bar{x}$	$[x,\bar{z},\bar{x}]$	$[u,\bar{w},\bar{u}]$	$\bar{x},\bar{z},x$	$[u,w,u]$	$x,\bar{z},x$	$[\bar{u},w,\bar{u}]$

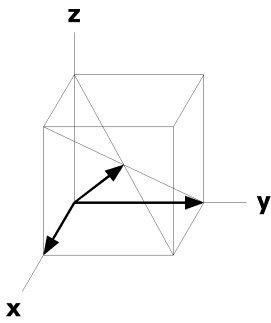
			$z, x, \bar{x} [\bar{w}, \bar{u}, \bar{u}]$	$z, \bar{x}, x [\bar{w}, \bar{u}, \bar{u}]$	$\bar{z}, x, x [w, \bar{u}, \bar{u}]$	$\bar{z}, \bar{x}, \bar{x} [w, u, u]$
48	j	m..	$0, y, z [u, 0, 0]$	$0, \bar{y}, z [\bar{u}, 0, 0]$	$0, y, \bar{z} [\bar{u}, 0, 0]$	$0, \bar{y}, \bar{z} [u, 0, 0]$
			$z, 0, y [0, u, 0]$	$z, 0, \bar{y} [0, \bar{u}, 0]$	$\bar{z}, 0, y [0, \bar{u}, 0]$	$\bar{z}, 0, \bar{y} [0, u, 0]$
			$y, z, 0 [0, 0, u]$	$\bar{y}, z, 0 [0, 0, \bar{u}]$	$y, \bar{z}, 0 [0, 0, \bar{u}]$	$\bar{y}, \bar{z}, 0 [0, 0, u]$
			$y, 0, \bar{z} [0, \bar{u}, 0]$	$\bar{y}, 0, \bar{z} [0, u, 0]$	$y, 0, z [0, u, 0]$	$\bar{y}, 0, z [0, \bar{u}, 0]$
			$0, z, \bar{y} [\bar{u}, 0, 0]$	$0, z, y [u, 0, 0]$	$0, \bar{z}, \bar{y} [u, 0, 0]$	$0, \bar{z}, y [\bar{u}, 0, 0]$
			$z, y, 0 [0, 0, u]$	$z, \bar{y}, 0 [0, 0, \bar{u}]$	$\bar{z}, y, 0 [0, 0, \bar{u}]$	$\bar{z}, \bar{y}, 0 [0, 0, u]$
48	i	..2				
			$1/4, y, \bar{y} + 1/2 [0, \bar{v}, v]$	$3/4, \bar{y}, \bar{y} + 1/2 [0, v, v]$	$3/4, y, y + 1/2 [0, \bar{v}, \bar{v}]$	$1/4, \bar{y}, y + 1/2 [0, v, \bar{v}]$
			$\bar{y} + 1/2, 1/4, y [v, 0, \bar{v}]$	$\bar{y} + 1/2, 3/4, \bar{y} [v, 0, v]$	$y + 1/2, 3/4, y [\bar{v}, 0, \bar{v}]$	$y + 1/2, 1/4, \bar{y} [\bar{v}, 0, v]$
			$y, \bar{y} + 1/2, 1/4 [\bar{v}, v, 0]$	$\bar{y}, \bar{y} + 1/2, 3/4 [v, v, 0]$	$y, y + 1/2, 3/4 [\bar{v}, \bar{v}, 0]$	$\bar{y}, y + 1/2, 1/4 [v, \bar{v}, 0]$
			$3/4, \bar{y}, y + 1/2 [0, \bar{v}, v]$	$1/4, y, y + 1/2 [0, v, v]$	$1/4, \bar{y}, \bar{y} + 1/2 [0, \bar{v}, \bar{v}]$	$3/4, y, \bar{y} + 1/2 [0, v, \bar{v}]$
			$y + 1/2, 3/4, \bar{y} [v, 0, \bar{v}]$	$y + 1/2, 1/4, y [v, 0, v]$	$\bar{y} + 1/2, 1/4, \bar{y} [\bar{v}, 0, \bar{v}]$	$\bar{y} + 1/2, 3/4, y [\bar{v}, 0, v]$
			$\bar{y}, y + 1/2, 3/4 [\bar{v}, v, 0]$	$y, y + 1/2, 1/4 [v, v, 0]$	$\bar{y}, \bar{y} + 1/2, 1/4 [\bar{v}, \bar{v}, 0]$	$y, \bar{y} + 1/2, 3/4 [v, \bar{v}, 0]$
24	h	m.m'2'	$0, y, y [u, 0, 0]$	$0, \bar{y}, y [\bar{u}, 0, 0]$	$0, y, \bar{y} [\bar{u}, 0, 0]$	$0, \bar{y}, \bar{y} [u, 0, 0]$
			$y, 0, y [0, u, 0]$	$y, 0, \bar{y} [0, \bar{u}, 0]$	$\bar{y}, 0, y [0, \bar{u}, 0]$	$\bar{y}, 0, \bar{y} [0, u, 0]$
			$y, y, 0 [0, 0, u]$	$\bar{y}, y, 0 [0, 0, \bar{u}]$	$y, \bar{y}, 0 [0, 0, \bar{u}]$	$\bar{y}, \bar{y}, 0 [0, 0, u]$
24	g	mm2..	$x, 0, 1/2 [0, 0, 0]$	$\bar{x}, 0, 1/2 [0, 0, 0]$	$1/2, x, 0 [0, 0, 0]$	$1/2, \bar{x}, 0 [0, 0, 0]$
			$0, 1/2, x [0, 0, 0]$	$0, 1/2, \bar{x} [0, 0, 0]$	$0, x, 1/2 [0, 0, 0]$	$0, \bar{x}, 1/2 [0, 0, 0]$
			$x, 1/2, 0 [0, 0, 0]$	$\bar{x}, 1/2, 0 [0, 0, 0]$	$1/2, 0, \bar{x} [0, 0, 0]$	$1/2, 0, x [0, 0, 0]$
16	f	.3m'	$x, x, x [u, u, u]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$	$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
			$x, x, \bar{x} [\bar{u}, \bar{u}, u]$	$\bar{x}, \bar{x}, \bar{x} [u, u, u]$	$x, \bar{x}, x [\bar{u}, u, \bar{u}]$	$\bar{x}, x, x [u, \bar{u}, \bar{u}]$
12	e	4'm.m'	$x, 0, 0 [0, 0, 0]$	$\bar{x}, 0, 0 [0, 0, 0]$		$0, x, 0 [0, 0, 0]$
			$0, \bar{x}, 0 [0, 0, 0]$	$0, 0, x [0, 0, 0]$		$0, 0, \bar{x} [0, 0, 0]$
12	d	$\bar{4}'m.2'$	$1/4, 0, 1/2 [0, 0, 0]$	$3/4, 0, 1/2 [0, 0, 0]$		$1/2, 1/4, 0 [0, 0, 0]$
			$1/2, 3/4, 0 [0, 0, 0]$	$0, 1/2, 1/4 [0, 0, 0]$		$0, 1/2, 3/4 [0, 0, 0]$
8	c	. $\bar{3}m'$	$1/4, 1/4, 1/4 [u, u, u]$	$3/4, 3/4, 1/4 [\bar{u}, \bar{u}, u]$	$3/4, 1/4, 3/4 [\bar{u}, u, \bar{u}]$	$1/4, 3/4, 3/4 [u, \bar{u}, \bar{u}]$
6	b	4'/mm.m'	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$		$1/2, 1/2, 0 [0, 0, 0]$
2	a	$m\bar{3}m'$	$0, 0, 0 [0, 0, 0]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $\text{p}4\text{mm}1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $0,0,z$

Along  $[1,1,1]$   $\text{p}6'\text{mm}'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
Origin at  $x,x,x$

Along  $[1,1,0]$   $\text{p}2'\text{mm}'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
Origin at  $x,x,0$



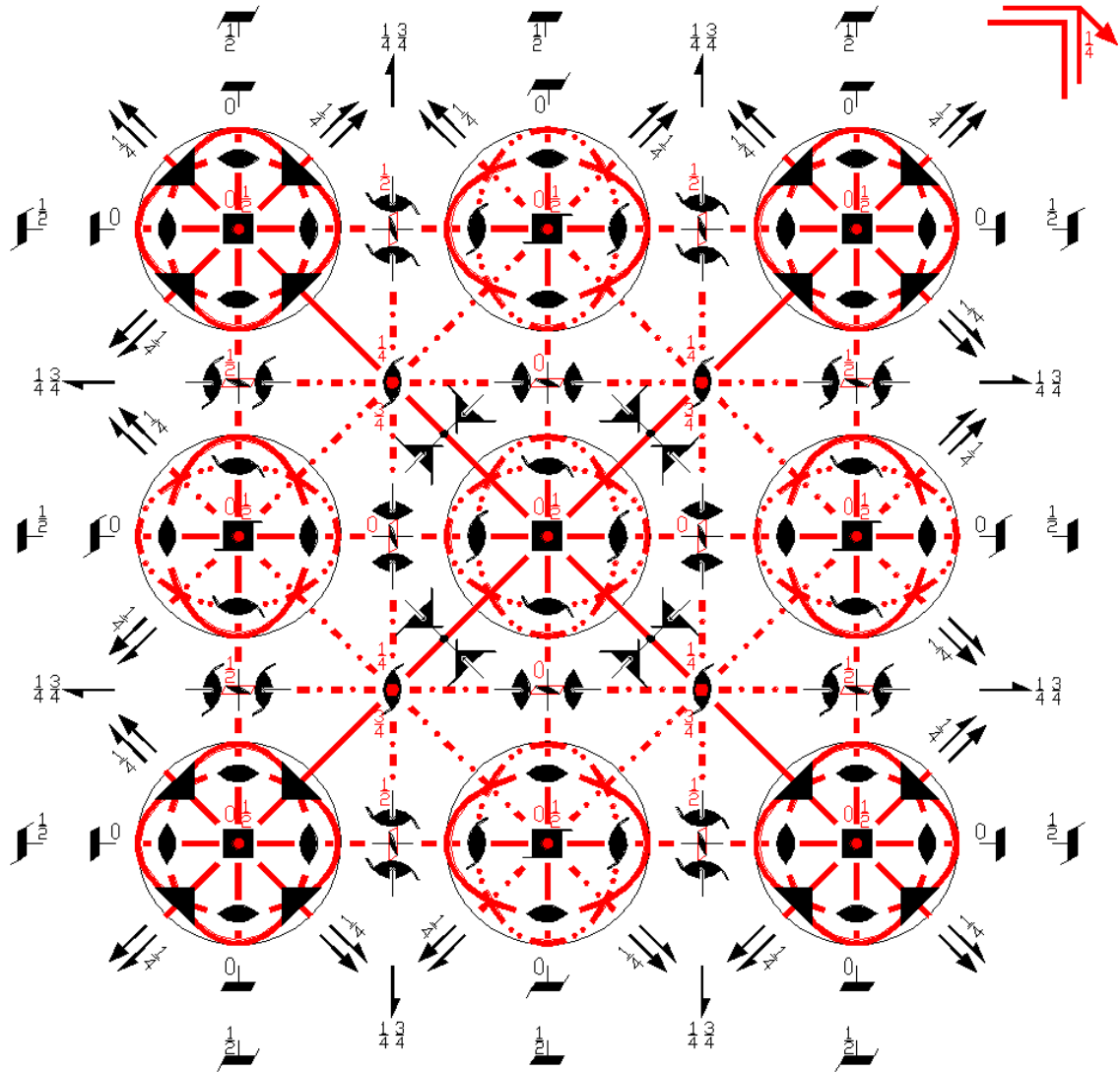
$Im'\bar{3}'m'$

229.5.1642

$m'\bar{3}'m'$

$I4/m'\bar{3}'2/m'$

Cubic



**Origin** at center ( $m'\bar{3}'m'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $y \leq x$ ;  $z \leq \min(1/2-x, y)$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/4,1/4,1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                         | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)    | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)      | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)     |

(13) $2 \ x, x, 0$ ( $2_{xy}   0, 0, 0$ )	(14) $2 \ x, \bar{x}, 0$ ( $2_{\bar{xy}}   0, 0, 0$ )	(15) $4^- \ 0, 0, z$ ( $4_z^{-1}   0, 0, 0$ )	(16) $4^+ \ 0, 0, z$ ( $4_z   0, 0, 0$ )
(17) $4^- \ x, 0, 0$ ( $4_x^{-1}   0, 0, 0$ )	(18) $2 \ 0, y, y$ ( $2_{yz}   0, 0, 0$ )	(19) $2 \ 0, y, \bar{y}$ ( $2_{\bar{yz}}   0, 0, 0$ )	(20) $4^+ \ x, 0, 0$ ( $4_x   0, 0, 0$ )
(21) $4^+ \ 0, y, 0$ ( $4_y   0, 0, 0$ )	(22) $2 \ x, 0, x$ ( $2_{xz}   0, 0, 0$ )	(23) $4^- \ 0, y, 0$ ( $4_y^{-1}   0, 0, 0$ )	(24) $2 \ \bar{x}, 0, x$ ( $2_{\bar{xz}}   0, 0, 0$ )
(25) $\bar{1}' \ 0, 0, 0$ ( $\bar{1}   0, 0, 0$ )'	(26) $m' \ x, y, 0$ ( $m_z   0, 0, 0$ )'	(27) $m' \ x, 0, z$ ( $m_y   0, 0, 0$ )'	(28) $m' \ 0, y, z$ ( $m_x   0, 0, 0$ )'
(29) $\bar{3}^+ \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}   0, 0, 0$ )'	(30) $\bar{3}^+ \ \bar{x}, x, \bar{x}; 0, 0, 0$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1}   0, 0, 0$ )'	(31) $\bar{3}^+ \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xy}\bar{z}}^{-1}   0, 0, 0$ )'	(32) $\bar{3}^+ \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{\bar{xy}\bar{z}}^{-1}   0, 0, 0$ )'
(33) $\bar{3}^- \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}^{-1}   0, 0, 0$ )'	(34) $\bar{3}^- \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{x\bar{y}\bar{z}}   0, 0, 0$ )'	(35) $\bar{3}^- \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{\bar{xy}\bar{z}}   0, 0, 0$ )'	(36) $\bar{3}^- \ \bar{x}, x, \bar{x}; 0, 0, 0$ ( $\bar{3}_{x\bar{y}\bar{z}}   0, 0, 0$ )'
(37) $m' \ x, \bar{x}, z$ ( $m_{xy}   0, 0, 0$ )'	(38) $m' \ x, x, z$ ( $m_{\bar{xy}}   0, 0, 0$ )'	(39) $\bar{4}^- \ 0, 0, z; 0, 0, 0$ ( $\bar{4}_z^{-1}   0, 0, 0$ )'	(40) $\bar{4}^+ \ 0, 0, z; 0, 0, 0$ ( $\bar{4}_z   0, 0, 0$ )'
(41) $\bar{4}^- \ x, 0, 0; 0, 0, 0$ ( $\bar{4}_x^{-1}   0, 0, 0$ )'	(42) $m' \ x, y, \bar{y}$ ( $m_{yz}   0, 0, 0$ )'	(43) $m' \ x, y, y$ ( $m_{\bar{yz}}   0, 0, 0$ )'	(44) $\bar{4}^+ \ x, 0, 0; 0, 0, 0$ ( $\bar{4}_x   0, 0, 0$ )'
(45) $\bar{4}^+ \ 0, y, 0; 0, 0, 0$ ( $\bar{4}_y   0, 0, 0$ )'	(46) $m' \ \bar{x}, y, x$ ( $m_{xz}   0, 0, 0$ )'	(47) $\bar{4}^- \ 0, y, 0; 0, 0, 0$ ( $\bar{4}_y^{-1}   0, 0, 0$ )'	(48) $m' \ x, y, x$ ( $m_{\bar{xz}}   0, 0, 0$ )'

For (1/2, 1/2, 1/2) + set

(1) $t \ (1/2, 1/2, 1/2)$ ( $1   1/2, 1/2, 1/2$ )	(2) $2 \ (0, 0, 1/2) \ 1/4, 1/4, z$ ( $2_z   1/2, 1/2, 1/2$ )	(3) $2 \ (0, 1/2, 0) \ 1/4, y, 1/4$ ( $2_y   1/2, 1/2, 1/2$ )	(4) $2 \ (1/2, 0, 0) \ x, 1/4, 1/4$ ( $2_x   1/2, 1/2, 1/2$ )
(5) $3^+ \ (1/2, 1/2, 1/2) \ x, x, x$ ( $3_{xyz}   1/2, 1/2, 1/2$ )	(6) $3^+ \ (1/6, -1/6, 1/6)$ $x+1/3, x+1/3, \bar{x}$ ( $3_{x\bar{y}\bar{z}}^{-1}   1/2, 1/2, 1/2$ )	(7) $3^+ \ (-1/6, 1/6, 1/6)$ $x+2/3, \bar{x}-1/3, \bar{x}$ ( $3_{\bar{xy}\bar{z}}^{-1}   1/2, 1/2, 1/2$ )	(8) $3^+ \ (1/6, 1/6, -1/6)$ $x+1/3, \bar{x}+2/3, x$ ( $3_{xy\bar{z}}^{-1}   1/2, 1/2, 1/2$ )
(9) $3^- \ (1/2, 1/2, 1/2) \ x, x, x$ ( $3_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(10) $3^- \ (-1/6, 1/6, 1/6)$ $x+1/3, \bar{x}+1/3, \bar{x}$ ( $3_{x\bar{y}\bar{z}}   1/2, 1/2, 1/2$ )	(11) $3^- \ (1/6, 1/6, -1/6)$ $\bar{x}+2/3, \bar{x}+1/3, x$ ( $3_{\bar{xy}\bar{z}}   1/2, 1/2, 1/2$ )	(12) $3^- \ (1/6, -1/6, 1/6)$ $\bar{x}-1/3, x+2/3, \bar{x}$ ( $3_{x\bar{y}\bar{z}}   1/2, 1/2, 1/2$ )
(13) $2 \ (1/2, 1/2, 0) \ x, x, 1/4$ ( $2_{xy}   1/2, 1/2, 1/2$ )	(14) $2 \ x, \bar{x}+1/2, 1/4$ ( $2_{\bar{xy}}   1/2, 1/2, 1/2$ )	(15) $4^- \ (0, 0, 1/2) \ 1/2, 0, z$ ( $4_z^{-1}   1/2, 1/2, 1/2$ )	(16) $4^+ \ (0, 0, 1/2) \ 0, 1/2, z$ ( $4_z   1/2, 1/2, 1/2$ )
(17) $4^- \ (1/2, 0, 0) \ x, 1/2, 0$ ( $4_x^{-1}   1/2, 1/2, 1/2$ )	(18) $2 \ (0, 1/2, 1/2) \ 1/4, y, y$ ( $2_{yz}   1/2, 1/2, 1/2$ )	(19) $2 \ 1/4, y+1/2, \bar{y}$ ( $2_{\bar{yz}}   1/2, 1/2, 1/2$ )	(20) $4^+ \ (1/2, 0, 0) \ x, 0, 1/2$ ( $4_x   1/2, 1/2, 1/2$ )
(21) $4^+ \ (0, 1/2, 0) \ 1/2, y, 0$ ( $4_y   1/2, 1/2, 1/2$ )	(22) $2 \ (1/2, 0, 1/2) \ x, 1/4, x$ ( $2_{xz}   1/2, 1/2, 1/2$ )	(23) $4^- \ (0, 1/2, 0) \ 0, y, 1/2$ ( $4_y^{-1}   1/2, 1/2, 1/2$ )	(24) $2 \ \bar{x}+1/2, 1/4, x$ ( $2_{\bar{xz}}   1/2, 1/2, 1/2$ )
(25) $\bar{1}' \ 1/4, 1/4, 1/4$ ( $\bar{1}   1/2, 1/2, 1/2$ )'	(26) $n' \ (1/2, 1/2, 0) \ x, y, 1/4$ ( $m_z   1/2, 1/2, 1/2$ )'	(27) $n' \ (1/2, 0, 1/2) \ x, 1/4, z$ ( $m_y   1/2, 1/2, 1/2$ )'	(28) $n' \ (0, 1/2, 1/2) \ 1/4, y, z$ ( $m_x   1/2, 1/2, 1/2$ )'
(29) $\bar{3}^+ \ x, x, x;$ $1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 1/2, 1/2$ )'	(30) $\bar{3}^+ \ \bar{x}-1, x+1, \bar{x};$ $-1/4, 1/4, 3/4$ ( $\bar{3}_{x\bar{y}\bar{z}}^{-1}   1/2, 1/2, 1/2$ )'	(31) $\bar{3}^+ \ x, \bar{x}+1, \bar{x};$ $1/4, 3/4, -1/4$ ( $\bar{3}_{\bar{xy}\bar{z}}^{-1}   1/2, 1/2, 1/2$ )'	(32) $\bar{3}^+ \ \bar{x}+1, \bar{x}, x;$ $3/4, -1/4, 1/4$ ( $\bar{3}_{xy\bar{z}}^{-1}   1/2, 1/2, 1/2$ )'

(33) $\bar{3}^-$ ' x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2)'	(34) $\bar{3}^-$ ' x+1, $\bar{x}$ -1, $\bar{x}$ ; 1/4,-1/4,3/4 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2)'	(35) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ +1, x; -1/4,3/4,1/4 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2)'	(36) $\bar{3}^-$ ' $\bar{x}$ +1, x, $\bar{x}$ ; 3/4,1/4,-1/4 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2)'
(37) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z ( $m_{xy}$   1/2,1/2,1/2)'	(38) n' (1/2,1/2,1/2) x,x,z ( $m_{xy}$   1/2,1/2,1/2)'	(39) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$   1/2,1/2,1/2)'	(40) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'
(41) $\bar{4}^-$ ' x,0,1/2; 1/4,0,1/2 ( $\bar{4}_x^{-1}$   1/2,1/2,1/2)'	(42) a' (1/2,0,0) x,y+1/2, $\bar{y}$ ( $m_{yz}$   1/2,1/2,1/2)'	(43) n' (1/2,1/2,1/2) x,y,y ( $m_{yz}$   1/2,1/2,1/2)'	(44) $\bar{4}^+$ ' x,1/2,0; 1/4,1/2,0 ( $\bar{4}_x$   1/2,1/2,1/2)'
(45) $\bar{4}^+$ ' 0,y,1/2; 0,1/4,1/2 ( $\bar{4}_y$   1/2,1/2,1/2)'	(46) b' (0,1/2,0) $\bar{x}$ +1/2,y,x ( $m_{xz}$   1/2,1/2,1/2)'	(47) $\bar{4}^-$ ' 1/2,y,0; 1/2,1/4,0 ( $\bar{4}_y^{-1}$   1/2,1/2,1/2)'	(48) n' (1/2,1/2,1/2) x,y,x ( $m_{xz}$   1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25).

### Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

### Coordinates

		(0,0,0) +	(1/2,1/2,1/2) +				
96	l	1					
(1)	x,y,z [u,v,w]	(2)	$\bar{x}$ , $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w]	(3)	$\bar{x}$ ,y,z [ $\bar{u}$ ,v, $\bar{w}$ ]	(4)	x, $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ , $\bar{w}$ ]
(5)	z,x,y [w,u,v]	(6)	z, $\bar{x}$ , $\bar{y}$ [ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ]	(7)	$\bar{z}$ , $\bar{x}$ ,y [ $\bar{w}$ , $\bar{u}$ ,v]	(8)	$\bar{z}$ ,x,y [ $\bar{w}$ ,u, $\bar{v}$ ]
(9)	y,z,x [v,w,u]	(10)	$\bar{y}$ ,z, $\bar{x}$ [ $\bar{v}$ ,w, $\bar{u}$ ]	(11)	y, $\bar{z}$ , $\bar{x}$ [v, $\bar{w}$ , $\bar{u}$ ]	(12)	$\bar{y}$ , $\bar{z}$ ,x [v, $\bar{w}$ ,u]
(13)	y,x, $\bar{z}$ [v,u, $\bar{w}$ ]	(14)	$\bar{y}$ , $\bar{x}$ ,z [ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]	(15)	y, $\bar{x}$ ,z [v, $\bar{u}$ ,w]	(16)	$\bar{y}$ ,x,z [v, $\bar{u}$ ,w]
(17)	x,z, $\bar{y}$ [u,w, $\bar{v}$ ]	(18)	$\bar{x}$ ,z,y [ $\bar{u}$ ,w,v]	(19)	$\bar{x}$ ,z, $\bar{y}$ [ $\bar{u}$ , $\bar{w}$ , $\bar{v}$ ]	(20)	x, $\bar{z}$ ,y [u, $\bar{w}$ ,v]
(21)	z,y, $\bar{x}$ [w,v, $\bar{u}$ ]	(22)	z, $\bar{y}$ ,x [w, $\bar{v}$ ,u]	(23)	$\bar{z}$ ,y,x [ $\bar{w}$ ,v,u]	(24)	$\bar{z}$ ,y, $\bar{x}$ [ $\bar{w}$ ,v, $\bar{u}$ ]
(25)	$\bar{x}$ , $\bar{y}$ ,z [ $\bar{u}$ , $\bar{v}$ ,w]	(26)	x,y,z [u,v,w]	(27)	x, $\bar{y}$ ,z [u, $\bar{v}$ ,w]	(28)	$\bar{x}$ ,y,z [ $\bar{u}$ ,v,w]
(29)	$\bar{z}$ , $\bar{x}$ , $\bar{y}$ [ $\bar{w}$ , $\bar{u}$ , $\bar{v}$ ]	(30)	$\bar{z}$ ,x,y [ $\bar{w}$ ,u,v]	(31)	z,x,y [w,u,v]	(32)	z, $\bar{x}$ ,y [w, $\bar{u}$ ,v]
(33)	$\bar{y}$ ,z, $\bar{x}$ [v,w,u]	(34)	y,z,x [v,w,u]	(35)	$\bar{y}$ ,z,x [v,w,u]	(36)	y,z, $\bar{x}$ [v,w, $\bar{u}$ ]
(37)	$\bar{y}$ , $\bar{x}$ ,z [v, $\bar{u}$ ,w]	(38)	y,x,z [v,u,w]	(39)	$\bar{y}$ ,x,z [v, $\bar{u}$ ,w]	(40)	y, $\bar{x}$ ,z [v, $\bar{u}$ ,w]
(41)	$\bar{x}$ ,z,y [u,w,v]	(42)	x,z,y [u,w,v]	(43)	x,z,y [u,w,v]	(44)	$\bar{x}$ ,z,y [u,w,v]
(45)	$\bar{z}$ ,y,x [w,v,u]	(46)	$\bar{z}$ ,y,x [w,v,u]	(47)	z,y,x [w,v,u]	(48)	z,y,x [w,v,u]
48	k	..m'	x,x,z [u,u,w]	$\bar{x}$ , $\bar{x}$ ,z [ $\bar{u}$ , $\bar{u}$ ,w]	$\bar{x}$ ,x,z [ $\bar{u}$ ,u, $\bar{w}$ ]	x, $\bar{x}$ ,z [u, $\bar{u}$ , $\bar{w}$ ]	
			z,x,x [w,u,u]	z, $\bar{x}$ , $\bar{x}$ [ $\bar{w}$ , $\bar{u}$ , $\bar{u}$ ]	$\bar{z}$ , $\bar{x}$ ,x [ $\bar{w}$ , $\bar{u}$ ,u]	$\bar{z}$ ,x, $\bar{x}$ [ $\bar{w}$ ,u, $\bar{u}$ ]	
			x,z,x [u,w,u]	$\bar{x}$ ,z, $\bar{x}$ [ $\bar{u}$ ,w, $\bar{u}$ ]	x,z, $\bar{x}$ [u,w, $\bar{u}$ ]	$\bar{x}$ ,z,x [u,w, $\bar{u}$ ]	
			x,x,z [u,u,w]	$\bar{x}$ , $\bar{x}$ ,z [ $\bar{u}$ , $\bar{u}$ ,w]	x, $\bar{x}$ ,z [u, $\bar{u}$ ,w]	$\bar{x}$ ,x,z [u, $\bar{u}$ ,w]	
			x,z, $\bar{x}$ [u,w, $\bar{u}$ ]	$\bar{x}$ ,z,x [u,w, $\bar{u}$ ]	$\bar{x}$ ,z,x [u,w, $\bar{u}$ ]	x,z,x [u,w, $\bar{u}$ ]	

			$z, x, \bar{x} [w, u, \bar{u}]$	$z, \bar{x}, x [w, \bar{u}, u]$	$\bar{z}, x, x [\bar{w}, u, u]$	$\bar{z}, \bar{x}, \bar{x} [\bar{w}, \bar{u}, \bar{u}]$
48	j	m'..	$0, y, z [0, v, w]$	$0, \bar{y}, z [0, \bar{v}, w]$	$0, y, \bar{z} [0, v, \bar{w}]$	$0, \bar{y}, \bar{z} [0, \bar{v}, \bar{w}]$
			$z, 0, y [w, 0, v]$	$z, 0, \bar{y} [w, 0, \bar{v}]$	$\bar{z}, 0, y [\bar{w}, 0, v]$	$\bar{z}, 0, \bar{y} [\bar{w}, 0, \bar{v}]$
			$y, z, 0 [v, w, 0]$	$\bar{y}, z, 0 [\bar{v}, w, 0]$	$y, \bar{z}, 0 [v, \bar{w}, 0]$	$\bar{y}, \bar{z}, 0 [\bar{v}, \bar{w}, 0]$
			$y, 0, \bar{z} [v, 0, \bar{w}]$	$\bar{y}, 0, \bar{z} [\bar{v}, 0, \bar{w}]$	$y, 0, z [v, 0, w]$	$\bar{y}, 0, z [\bar{v}, 0, w]$
			$0, z, \bar{y} [0, w, \bar{v}]$	$0, z, y [0, w, v]$	$0, \bar{z}, \bar{y} [0, \bar{w}, \bar{v}]$	$0, \bar{z}, y [0, \bar{w}, v]$
			$z, y, 0 [w, v, 0]$	$z, \bar{y}, 0 [w, \bar{v}, 0]$	$\bar{z}, y, 0 [\bar{w}, v, 0]$	$\bar{z}, \bar{y}, 0 [\bar{w}, \bar{v}, 0]$
48	i	..2				
			$1/4, y, \bar{y} + 1/2 [0, \bar{v}, v]$	$3/4, \bar{y}, \bar{y} + 1/2 [0, v, v]$	$3/4, y, y + 1/2 [0, \bar{v}, \bar{v}]$	$1/4, \bar{y}, y + 1/2 [0, v, \bar{v}]$
			$\bar{y} + 1/2, 1/4, y [v, 0, \bar{v}]$	$\bar{y} + 1/2, 3/4, \bar{y} [v, 0, v]$	$y + 1/2, 3/4, y [\bar{v}, 0, \bar{v}]$	$y + 1/2, 1/4, \bar{y} [\bar{v}, 0, v]$
			$y, \bar{y} + 1/2, 1/4 [\bar{v}, v, 0]$	$\bar{y}, \bar{y} + 1/2, 3/4 [v, v, 0]$	$y, y + 1/2, 3/4 [\bar{v}, \bar{v}, 0]$	$\bar{y}, y + 1/2, 1/4 [v, \bar{v}, 0]$
			$3/4, \bar{y}, y + 1/2 [0, \bar{v}, v]$	$1/4, y, y + 1/2 [0, v, v]$	$1/4, \bar{y}, \bar{y} + 1/2 [0, \bar{v}, \bar{v}]$	$3/4, y, \bar{y} + 1/2 [0, v, \bar{v}]$
			$y + 1/2, 3/4, \bar{y} [v, 0, \bar{v}]$	$y + 1/2, 1/4, y [v, 0, v]$	$\bar{y} + 1/2, 1/4, \bar{y} [\bar{v}, 0, \bar{v}]$	$\bar{y} + 1/2, 3/4, y [\bar{v}, 0, v]$
			$\bar{y}, y + 1/2, 3/4 [\bar{v}, v, 0]$	$y, y + 1/2, 1/4 [v, v, 0]$	$\bar{y}, \bar{y} + 1/2, 1/4 [\bar{v}, \bar{v}, 0]$	$y, \bar{y} + 1/2, 3/4 [v, \bar{v}, 0]$
24	h	m'.m'2	$0, y, y [0, v, v]$	$0, \bar{y}, y [0, \bar{v}, v]$	$0, y, \bar{y} [0, v, \bar{v}]$	$0, \bar{y}, \bar{y} [0, \bar{v}, \bar{v}]$
			$y, 0, y [v, 0, v]$	$y, 0, \bar{y} [v, 0, \bar{v}]$	$\bar{y}, 0, y [\bar{v}, 0, v]$	$\bar{y}, 0, \bar{y} [\bar{v}, 0, \bar{v}]$
			$y, y, 0 [v, v, 0]$	$\bar{y}, y, 0 [\bar{v}, v, 0]$	$y, \bar{y}, 0 [v, \bar{v}, 0]$	$\bar{y}, \bar{y}, 0 [\bar{v}, \bar{v}, 0]$
24	g	m'm'2..	$x, 0, 1/2 [u, 0, 0]$	$\bar{x}, 0, 1/2 [\bar{u}, 0, 0]$	$1/2, x, 0 [0, u, 0]$	$1/2, \bar{x}, 0 [0, \bar{u}, 0]$
			$0, 1/2, x [0, 0, u]$	$0, 1/2, \bar{x} [0, 0, \bar{u}]$	$0, x, 1/2 [0, u, 0]$	$0, \bar{x}, 1/2 [0, \bar{u}, 0]$
			$x, 1/2, 0 [u, 0, 0]$	$\bar{x}, 1/2, 0 [\bar{u}, 0, 0]$	$1/2, 0, \bar{x} [0, 0, \bar{u}]$	$1/2, 0, x [0, 0, u]$
16	f	.3m'	$x, x, x [u, u, u]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$	$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
			$x, x, \bar{x} [u, u, \bar{u}]$	$\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$	$x, \bar{x}, x [u, \bar{u}, u]$	$\bar{x}, x, x [\bar{u}, u, \bar{u}]$
12	e	4m'.m'	$x, 0, 0 [u, 0, 0]$	$\bar{x}, 0, 0 [\bar{u}, 0, 0]$		$0, x, 0 [0, u, 0]$
			$0, \bar{x}, 0 [0, \bar{u}, 0]$	$0, 0, x [0, 0, u]$		$0, 0, \bar{x} [0, 0, \bar{u}]$
12	d	4m'.2	$1/4, 0, 1/2 [0, 0, 0]$	$3/4, 0, 1/2 [0, 0, 0]$		$1/2, 1/4, 0 [0, 0, 0]$
			$1/2, 3/4, 0 [0, 0, 0]$	$0, 1/2, 1/4 [0, 0, 0]$		$0, 1/2, 3/4 [0, 0, 0]$
8	c	.3m'	$1/4, 1/4, 1/4 [0, 0, 0]$	$3/4, 3/4, 1/4 [0, 0, 0]$	$3/4, 1/4, 3/4 [0, 0, 0]$	$1/4, 3/4, 3/4 [0, 0, 0]$
6	b	4/m'm'.m'	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$		$1/2, 1/2, 0 [0, 0, 0]$
2	a	m'3'm'	$0, 0, 0 [0, 0, 0]$			

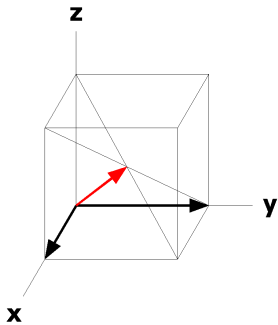
**Symmetry of Special Projections**

Along [0,0,1] p4m'm'  
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at 0,0,z

Along [1,1,1] p6m'm'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

Along [1,1,0] p2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x,0

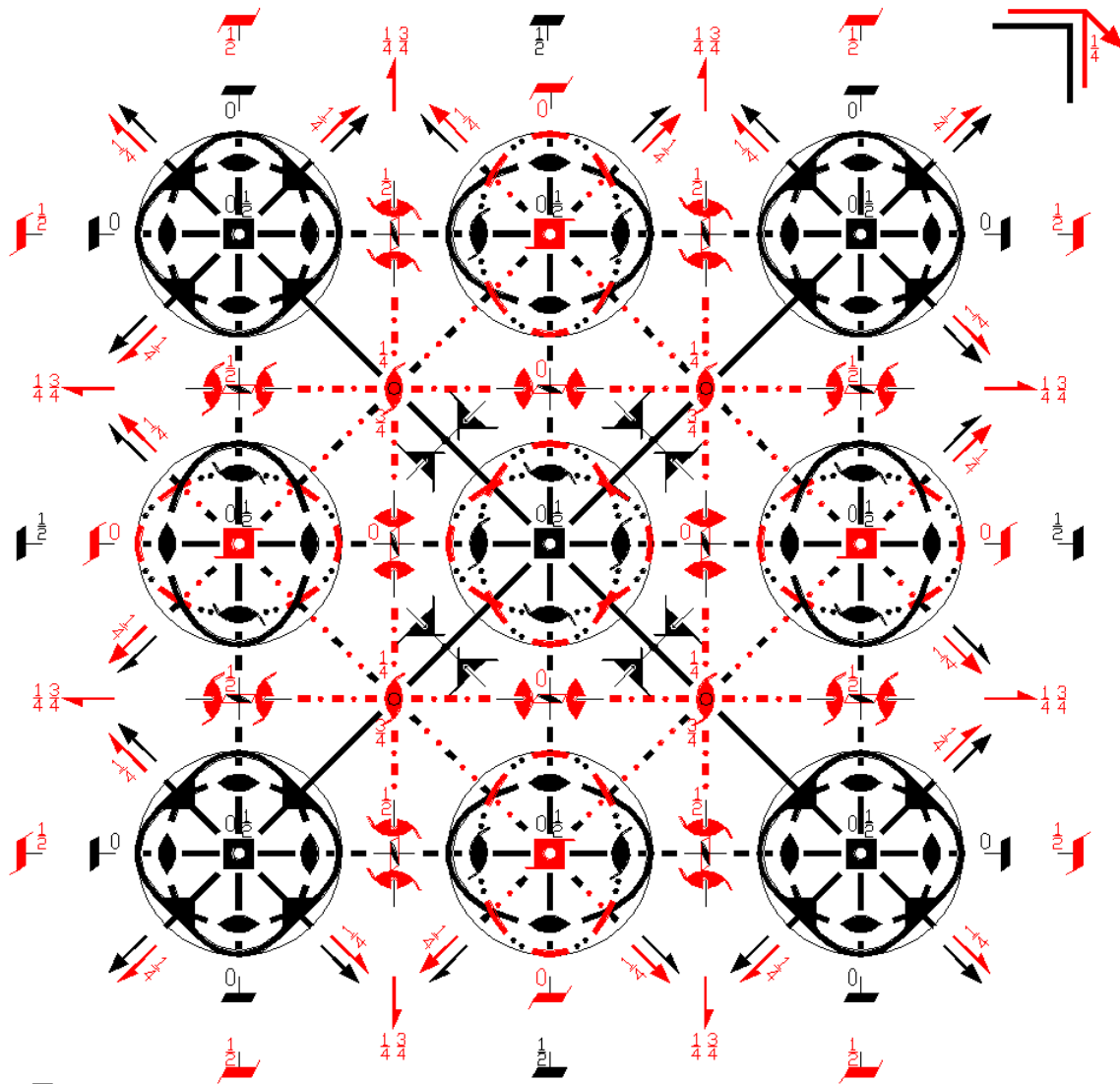




$I_P m\bar{3}m$   
229.6.1643

$m\bar{3}m1'$   
 $I_P 4/m\bar{3}2/m$

Cubic



**Origin** at center ( $m\bar{3}m$ )

**Asymmetric unit**  $0 \leq x \leq 1/2$ ;  $0 \leq y \leq 1/2$ ;  $0 \leq z \leq 1/4$ ;  $y \leq x$ ;  $z \leq \min(1/2-x, y)$

**Vertices** 0,0,0      1/2,0,0      1/2,1/2,0      1/4,1/4,1/4

**Symmetry Operations**

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                         | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)    | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)      | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)     |

(13) $2^- x, x, 0$ ( $2_{xy}^-   0, 0, 0$ )	(14) $2^- x, \bar{x}, 0$ ( $2_{\bar{xy}}^-   0, 0, 0$ )	(15) $4^- 0, 0, z$ ( $4_z^-   0, 0, 0$ )	(16) $4^+ 0, 0, z$ ( $4_z   0, 0, 0$ )
(17) $4^- x, 0, 0$ ( $4_x^-   0, 0, 0$ )	(18) $2^- 0, y, y$ ( $2_{yz}^-   0, 0, 0$ )	(19) $2^- 0, y, \bar{y}$ ( $2_{\bar{yz}}^-   0, 0, 0$ )	(20) $4^+ x, 0, 0$ ( $4_x   0, 0, 0$ )
(21) $4^+ 0, y, 0$ ( $4_y   0, 0, 0$ )	(22) $2^- x, 0, x$ ( $2_{xz}^-   0, 0, 0$ )	(23) $4^- 0, y, 0$ ( $4_y^-   0, 0, 0$ )	(24) $2^- \bar{x}, 0, x$ ( $2_{\bar{xz}}^-   0, 0, 0$ )
(25) $\bar{1}^- 0, 0, 0$ ( $\bar{1}^-   0, 0, 0$ )	(26) $m^- x, y, 0$ ( $m_z^-   0, 0, 0$ )	(27) $m^- x, 0, z$ ( $m_y^-   0, 0, 0$ )	(28) $m^- 0, y, z$ ( $m_x^-   0, 0, 0$ )
(29) $\bar{3}^+ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}^+   0, 0, 0$ )	(30) $\bar{3}^+ \bar{x}, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}^+   0, 0, 0$ )	(31) $\bar{3}^+ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}^+   0, 0, 0$ )	(32) $\bar{3}^+ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{xyz}^+   0, 0, 0$ )
(33) $\bar{3}^- x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}^-   0, 0, 0$ )	(34) $\bar{3}^- \bar{x}, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}^-   0, 0, 0$ )	(35) $\bar{3}^- \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{xy\bar{z}}^-   0, 0, 0$ )	(36) $\bar{3}^- \bar{x}, x, \bar{x}; 0, 0, 0$ ( $\bar{3}_{x\bar{y}\bar{z}}^-   0, 0, 0$ )
(37) $m^- x, \bar{x}, z$ ( $m_{xy}^-   0, 0, 0$ )	(38) $m^- x, x, z$ ( $m_{\bar{xy}}^-   0, 0, 0$ )	(39) $\bar{4}^- 0, 0, z; 0, 0, 0$ ( $\bar{4}_z^-   0, 0, 0$ )	(40) $\bar{4}^+ 0, 0, z; 0, 0, 0$ ( $\bar{4}_z   0, 0, 0$ )
(41) $\bar{4}^- x, 0, 0; 0, 0, 0$ ( $\bar{4}_x^-   0, 0, 0$ )	(42) $m^- x, y, \bar{y}$ ( $m_{yz}^-   0, 0, 0$ )	(43) $m^- x, y, y$ ( $m_{\bar{yz}}^-   0, 0, 0$ )	(44) $\bar{4}^+ x, 0, 0; 0, 0, 0$ ( $\bar{4}_x   0, 0, 0$ )
(45) $\bar{4}^+ 0, y, 0; 0, 0, 0$ ( $\bar{4}_y   0, 0, 0$ )	(46) $m^- \bar{x}, y, x$ ( $m_{xz}^-   0, 0, 0$ )	(47) $\bar{4}^- 0, y, 0; 0, 0, 0$ ( $\bar{4}_y^-   0, 0, 0$ )	(48) $m^- x, y, x$ ( $m_{\bar{xz}}^-   0, 0, 0$ )

For  $(1/2, 1/2, 1/2)'$  + set

(1) $t' (1/2, 1/2, 1/2)$ ( $1   1/2, 1/2, 1/2$ )'	(2) $2' (0, 0, 1/2) \quad 1/4, 1/4, z$ ( $2_z   1/2, 1/2, 1/2$ )'	(3) $2' (0, 1/2, 0) \quad 1/4, y, 1/4$ ( $2_y   1/2, 1/2, 1/2$ )'	(4) $2' (1/2, 0, 0) \quad x, 1/4, 1/4$ ( $2_x   1/2, 1/2, 1/2$ )'
(5) $3^{*'} (1/2, 1/2, 1/2) \quad x, x, x$ ( $3_{xyz}   1/2, 1/2, 1/2$ )'	(6) $3^{*'} (1/6, -1/6, 1/6) \quad \bar{x} + 1/3, x + 1/3, \bar{x}$ ( $3_{\bar{xyz}}   1/2, 1/2, 1/2$ )'	(7) $3^{*'} (-1/6, 1/6, 1/6) \quad \bar{x} + 2/3, x - 1/3, \bar{x}$ ( $3_{\bar{xyz}}   1/2, 1/2, 1/2$ )'	(8) $3^{*'} (1/6, 1/6, -1/6) \quad \bar{x} + 1/3, x + 2/3, \bar{x}$ ( $3_{xy\bar{z}}   1/2, 1/2, 1/2$ )'
(9) $3^{-'} (1/2, 1/2, 1/2) \quad x, x, x$ ( $3_{xyz}^-   1/2, 1/2, 1/2$ )'	(10) $3^{-'} (-1/6, 1/6, 1/6) \quad \bar{x} + 1/3, \bar{x} + 1/3, \bar{x}$ ( $3_{xyz}   1/2, 1/2, 1/2$ )'	(11) $3^{-'} (1/6, 1/6, -1/6) \quad \bar{x} + 2/3, x + 1/3, x$ ( $3_{xy\bar{z}}   1/2, 1/2, 1/2$ )'	(12) $3^{-'} (1/6, -1/6, 1/6) \quad \bar{x} - 1/3, x + 2/3, \bar{x}$ ( $3_{x\bar{y}\bar{z}}   1/2, 1/2, 1/2$ )'
(13) $2' (1/2, 1/2, 0) \quad x, x, 1/4$ ( $2_{xy}   1/2, 1/2, 1/2$ )'	(14) $2' x, \bar{x} + 1/2, 1/4$ ( $2_{\bar{xy}}   1/2, 1/2, 1/2$ )'	(15) $4^{-'} (0, 0, 1/2) \quad 1/2, 0, z$ ( $4_z^-   1/2, 1/2, 1/2$ )'	(16) $4^{*'} (0, 0, 1/2) \quad 0, 1/2, z$ ( $4_z   1/2, 1/2, 1/2$ )'
(17) $4^{-'} (1/2, 0, 0) \quad x, 1/2, 0$ ( $4_x^-   1/2, 1/2, 1/2$ )'	(18) $2' (0, 1/2, 1/2) \quad 1/4, y, y$ ( $2_{yz}   1/2, 1/2, 1/2$ )'	(19) $2' 1/4, y + 1/2, \bar{y}$ ( $2_{\bar{yz}}   1/2, 1/2, 1/2$ )'	(20) $4^{*'} (1/2, 0, 0) \quad x, 0, 1/2$ ( $4_x   1/2, 1/2, 1/2$ )'
(21) $4^{*'} (0, 1/2, 0) \quad 1/2, y, 0$ ( $4_y   1/2, 1/2, 1/2$ )'	(22) $2' (1/2, 0, 1/2) \quad x, 1/4, x$ ( $2_{xz}   1/2, 1/2, 1/2$ )'	(23) $4^{-'} (0, 1/2, 0) \quad 0, y, 1/2$ ( $4_y^-   1/2, 1/2, 1/2$ )'	(24) $2' \bar{x} + 1/2, 1/4, x$ ( $2_{\bar{xz}}   1/2, 1/2, 1/2$ )'
(25) $\bar{1}^- 1/4, 1/4, 1/4$ ( $\bar{1}^-   1/2, 1/2, 1/2$ )'	(26) $n' (1/2, 1/2, 0) \quad x, y, 1/4$ ( $m_z   1/2, 1/2, 1/2$ )'	(27) $n' (1/2, 0, 1/2) \quad x, 1/4, z$ ( $m_y   1/2, 1/2, 1/2$ )'	(28) $n' (0, 1/2, 1/2) \quad 1/4, y, z$ ( $m_x   1/2, 1/2, 1/2$ )'
(29) $\bar{3}^+ x, x, x; \quad 1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 1/2, 1/2$ )'	(30) $\bar{3}^+ \bar{x} - 1, x + 1, \bar{x}; \quad -1/4, 1/4, 3/4$ ( $\bar{3}_{\bar{xyz}}   1/2, 1/2, 1/2$ )'	(31) $\bar{3}^+ x, \bar{x} + 1, \bar{x}; \quad 1/4, 3/4, -1/4$ ( $\bar{3}_{\bar{xyz}}   1/2, 1/2, 1/2$ )'	(32) $\bar{3}^+ \bar{x} + 1, \bar{x}, x; \quad 3/4, -1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 1/2, 1/2$ )'

(33) $\bar{3}^-$ ' x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2)'	(34) $\bar{3}^-$ ' x+1, $\bar{x}$ -1, $\bar{x}$ ; 1/4,-1/4,3/4 ( $\bar{3}_{\bar{xyz}}$   1/2,1/2,1/2)'	(35) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ +1, x; -1/4,3/4,1/4 ( $\bar{3}_{x\bar{z}}$   1/2,1/2,1/2)'	(36) $\bar{3}^-$ ' $\bar{x}$ +1, x, $\bar{x}$ ; 3/4,1/4,-1/4 ( $\bar{3}_{x\bar{yz}}$   1/2,1/2,1/2)'
(37) c' (0,0,1/2) x+1/2, $\bar{x}$ ,z ( $m_{xy}$   1/2,1/2,1/2)'	(38) n' (1/2,1/2,1/2) x,x,z ( $m_{\bar{xy}}$   1/2,1/2,1/2)'	(39) $\bar{4}^-$ ' 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$   1/2,1/2,1/2)'	(40) $\bar{4}^+$ ' 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)'
(41) $\bar{4}^-$ ' x,0,1/2; 1/4,0,1/2 ( $\bar{4}_x^{-1}$   1/2,1/2,1/2)'	(42) a' (1/2,0,0) x,y+1/2, $\bar{y}$ ( $m_{yz}$   1/2,1/2,1/2)'	(43) n' (1/2,1/2,1/2) x,y,y ( $m_{\bar{yz}}$   1/2,1/2,1/2)'	(44) $\bar{4}^+$ ' x,1/2,0; 1/4,1/2,0 ( $\bar{4}_x$   1/2,1/2,1/2)'
(45) $\bar{4}^+$ ' 0,y,1/2; 0,1/4,1/2 ( $\bar{4}_y$   1/2,1/2,1/2)'	(46) b' (0,1/2,0) $\bar{x}$ +1/2,y,x ( $m_{xz}$   1/2,1/2,1/2)'	(47) $\bar{4}^-$ ' 1/2,y,0; 1/2,1/4,0 ( $\bar{4}_y^{-1}$   1/2,1/2,1/2)'	(48) n' (1/2,1/2,1/2) x,y,x ( $m_{\bar{xz}}$   1/2,1/2,1/2)'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13); (25).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

		(0,0,0) +		(1/2,1/2,1/2)' +	
96	l	1			
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}$ , $\bar{y}$ ,z	[ $\bar{u}$ , $\bar{v}$ ,w]
(3)	$\bar{x}$ ,y,z	[ $\bar{u}$ ,v, $\bar{w}$ ]	(4)	x, $\bar{y}$ ,z	[u, $\bar{v}$ , $\bar{w}$ ]
(5)	z,x,y	[w,u,v]	(6)	z, $\bar{x}$ , $\bar{y}$	[w, $\bar{u}$ , $\bar{v}$ ]
(7)	$\bar{z}$ , $\bar{x}$ ,y	[ $\bar{w}$ , $\bar{u}$ ,v]	(8)	$\bar{z}$ ,x, $\bar{y}$	[ $\bar{w}$ ,u, $\bar{v}$ ]
(9)	y,z,x	[v,w,u]	(10)	$\bar{y}$ ,z, $\bar{x}$	[ $\bar{v}$ ,w, $\bar{u}$ ]
(11)	y, $\bar{z}$ , $\bar{x}$	[v, $\bar{w}$ , $\bar{u}$ ]	(12)	$\bar{y}$ ,z,x	[ $\bar{v}$ , $\bar{w}$ ,u]
(13)	y,x, $\bar{z}$	[v,u, $\bar{w}$ ]	(14)	$\bar{y}$ , $\bar{x}$ ,z	[ $\bar{v}$ , $\bar{u}$ , $\bar{w}$ ]
(15)	y, $\bar{x}$ ,z	[v, $\bar{u}$ ,w]	(16)	$\bar{y}$ ,x,z	[ $\bar{v}$ ,u,w]
(17)	x,z, $\bar{y}$	[u,w, $\bar{v}$ ]	(18)	$\bar{x}$ ,z,y	[ $\bar{u}$ ,w,v]
(19)	$\bar{x}$ ,z, $\bar{y}$	[ $\bar{u}$ , $\bar{w}$ , $\bar{v}$ ]	(20)	x, $\bar{z}$ ,y	[u, $\bar{w}$ ,v]
(21)	z,y, $\bar{x}$	[w,v, $\bar{u}$ ]	(22)	z, $\bar{y}$ ,x	[w, $\bar{v}$ ,u]
(23)	$\bar{z}$ ,y,x	[ $\bar{w}$ ,v,u]	(24)	$\bar{z}$ , $\bar{y}$ , $\bar{x}$	[ $\bar{w}$ , $\bar{v}$ , $\bar{u}$ ]
(25)	$\bar{x}$ , $\bar{y}$ ,z	[u,v,w]	(26)	x,y, $\bar{z}$	[u,v, $\bar{w}$ ]
(27)	x, $\bar{y}$ ,z	[u,v, $\bar{w}$ ]	(28)	$\bar{x}$ ,y,z	[u, $\bar{v}$ , $\bar{w}$ ]
(29)	$\bar{z}$ , $\bar{x}$ , $\bar{y}$	[w,u,v]	(30)	$\bar{z}$ ,x,y	[ $\bar{w}$ ,u,v]
(31)	z,x, $\bar{y}$	[w, $\bar{u}$ ,v]	(32)	z, $\bar{x}$ ,y	[ $\bar{w}$ ,u,v]
(33)	$\bar{y}$ ,z, $\bar{x}$	[v,w,u]	(34)	y, $\bar{z}$ ,x	[ $\bar{v}$ ,w,u]
(35)	$\bar{y}$ ,z,x	[v, $\bar{w}$ ,u]	(36)	y,z, $\bar{x}$	[ $\bar{v}$ , $\bar{w}$ ,u]
(37)	$\bar{y}$ , $\bar{x}$ ,z	[v,u, $\bar{w}$ ]	(38)	y,x,z	[ $\bar{v}$ ,u, $\bar{w}$ ]
(39)	$\bar{y}$ ,x,z	[v,u,w]	(40)	y, $\bar{x}$ ,z	[ $\bar{v}$ ,u,w]
(41)	$\bar{x}$ ,z,y	[u,w, $\bar{v}$ ]	(42)	x,z, $\bar{y}$	[u,w,v]
(43)	x,z,y	[u,w, $\bar{v}$ ]	(44)	$\bar{x}$ ,z,y	[u,w,v]
(45)	$\bar{z}$ , $\bar{y}$ ,x	[w,v, $\bar{u}$ ]	(46)	$\bar{z}$ ,y, $\bar{x}$	[w, $\bar{v}$ ,u]
(47)	z, $\bar{y}$ , $\bar{x}$	[ $\bar{w}$ ,v,u]	(48)	z,y,x	[ $\bar{w}$ , $\bar{v}$ , $\bar{u}$ ]
48	k	..m	x,x,z	[u, $\bar{u}$ ,0]	$\bar{x}$ , $\bar{x}$ ,z
			x,x,z	[u,u,0]	$\bar{x}$ ,x,z
			z,x,x	[0,u, $\bar{u}$ ]	$\bar{z}$ , $\bar{x}$ ,x
			z,x,x	[0,u,u]	$\bar{z}$ ,x,x
			x,z,x	[ $\bar{u}$ ,0,u]	$\bar{x}$ ,z,x
			x,z,x	[u,0, $\bar{u}$ ]	$\bar{x}$ ,z,x
			x,x,z	[ $\bar{u}$ ,u,0]	x, $\bar{x}$ ,z
			x,x,z	[u,u,0]	x,x,z
			x,z, $\bar{x}$	[u,0,u]	$\bar{x}$ ,z,x
			x,z,x	[ $\bar{u}$ ,0, $\bar{u}$ ]	$\bar{x}$ ,z,x
			x,z,x	[u,0,u]	$\bar{x}$ ,z,x

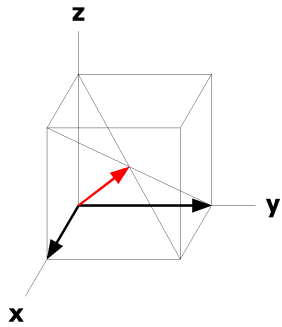
			$z, x, \bar{x} [0, \bar{u}, \bar{u}]$	$z, \bar{x}, x [0, u, u]$	$\bar{z}, x, x [0, \bar{u}, u]$	$\bar{z}, \bar{x}, \bar{x} [0, u, \bar{u}]$
48	j	m..	$0, y, z [u, 0, 0]$	$0, \bar{y}, z [\bar{u}, 0, 0]$	$0, y, \bar{z} [\bar{u}, 0, 0]$	$0, \bar{y}, \bar{z} [u, 0, 0]$
			$z, 0, y [0, u, 0]$	$z, 0, \bar{y} [0, \bar{u}, 0]$	$\bar{z}, 0, y [0, \bar{u}, 0]$	$\bar{z}, 0, \bar{y} [0, u, 0]$
			$y, z, 0 [0, 0, u]$	$\bar{y}, z, 0 [0, 0, \bar{u}]$	$y, \bar{z}, 0 [0, 0, \bar{u}]$	$\bar{y}, \bar{z}, 0 [0, 0, u]$
			$y, 0, \bar{z} [0, u, 0]$	$\bar{y}, 0, \bar{z} [0, \bar{u}, 0]$	$y, 0, z [0, \bar{u}, 0]$	$\bar{y}, 0, z [0, u, 0]$
			$0, z, \bar{y} [u, 0, 0]$	$0, z, y [\bar{u}, 0, 0]$	$0, \bar{z}, \bar{y} [\bar{u}, 0, 0]$	$0, \bar{z}, y [u, 0, 0]$
			$z, y, 0 [0, 0, \bar{u}]$	$z, \bar{y}, 0 [0, 0, u]$	$\bar{z}, y, 0 [0, 0, u]$	$\bar{z}, \bar{y}, 0 [0, 0, \bar{u}]$
48	i	..2'				
			$1/4, y, \bar{y} + 1/2 [u, v, v]$	$3/4, \bar{y}, \bar{y} + 1/2 [\bar{u}, \bar{v}, \bar{v}]$	$3/4, y, y + 1/2 [\bar{u}, v, \bar{v}]$	$1/4, \bar{y}, y + 1/2 [u, \bar{v}, \bar{v}]$
			$\bar{y} + 1/2, 1/4, y [v, u, v]$	$\bar{y} + 1/2, 3/4, \bar{y} [v, \bar{u}, \bar{v}]$	$y + 1/2, 3/4, y [v, \bar{u}, v]$	$y + 1/2, 1/4, \bar{y} [v, u, \bar{v}]$
			$y, \bar{y} + 1/2, 1/4 [v, v, u]$	$\bar{y}, \bar{y} + 1/2, 3/4 [v, \bar{v}, \bar{u}]$	$y, y + 1/2, 3/4 [v, \bar{v}, \bar{u}]$	$\bar{y}, y + 1/2, 1/4 [v, \bar{v}, u]$
			$3/4, \bar{y}, y + 1/2 [u, v, v]$	$1/4, y, y + 1/2 [\bar{u}, \bar{v}, \bar{v}]$	$1/4, \bar{y}, \bar{y} + 1/2 [\bar{u}, v, \bar{v}]$	$3/4, y, \bar{y} + 1/2 [u, \bar{v}, \bar{v}]$
			$y + 1/2, 3/4, \bar{y} [v, u, v]$	$y + 1/2, 1/4, y [v, \bar{u}, \bar{v}]$	$\bar{y} + 1/2, 1/4, \bar{y} [v, \bar{u}, v]$	$\bar{y} + 1/2, 3/4, y [v, u, \bar{v}]$
			$\bar{y}, y + 1/2, 3/4 [v, v, u]$	$y, y + 1/2, 1/4 [v, \bar{v}, \bar{u}]$	$\bar{y}, \bar{y} + 1/2, 1/4 [v, \bar{v}, \bar{u}]$	$y, \bar{y} + 1/2, 3/4 [v, \bar{v}, u]$
24	h	m.m2	$0, y, y [0, 0, 0]$	$0, \bar{y}, y [0, 0, 0]$	$0, y, \bar{y} [0, 0, 0]$	$0, \bar{y}, \bar{y} [0, 0, 0]$
			$y, 0, y [0, 0, 0]$	$y, 0, \bar{y} [0, 0, 0]$	$\bar{y}, 0, y [0, 0, 0]$	$\bar{y}, 0, \bar{y} [0, 0, 0]$
			$y, y, 0 [0, 0, 0]$	$\bar{y}, y, 0 [0, 0, 0]$	$y, \bar{y}, 0 [0, 0, 0]$	$\bar{y}, \bar{y}, 0 [0, 0, 0]$
24	g	mm2..	$x, 0, 1/2 [0, 0, 0]$	$\bar{x}, 0, 1/2 [0, 0, 0]$	$1/2, x, 0 [0, 0, 0]$	$1/2, \bar{x}, 0 [0, 0, 0]$
			$0, 1/2, x [0, 0, 0]$	$0, 1/2, \bar{x} [0, 0, 0]$	$0, x, 1/2 [0, 0, 0]$	$0, \bar{x}, 1/2 [0, 0, 0]$
			$x, 1/2, 0 [0, 0, 0]$	$\bar{x}, 1/2, 0 [0, 0, 0]$	$1/2, 0, \bar{x} [0, 0, 0]$	$1/2, 0, x [0, 0, 0]$
16	f	.3m	$x, x, x [0, 0, 0]$	$\bar{x}, \bar{x}, x [0, 0, 0]$	$\bar{x}, x, \bar{x} [0, 0, 0]$	$x, \bar{x}, \bar{x} [0, 0, 0]$
			$x, x, \bar{x} [0, 0, 0]$	$\bar{x}, \bar{x}, \bar{x} [0, 0, 0]$	$x, \bar{x}, x [0, 0, 0]$	$\bar{x}, x, x [0, 0, 0]$
12	e	4m.m	$x, 0, 0 [0, 0, 0]$	$\bar{x}, 0, 0 [0, 0, 0]$		$0, x, 0 [0, 0, 0]$
			$0, \bar{x}, 0 [0, 0, 0]$	$0, 0, x [0, 0, 0]$		$0, 0, \bar{x} [0, 0, 0]$
12	d	$\bar{4}'m.2'$	$1/4, 0, 1/2 [0, 0, 0]$	$3/4, 0, 1/2 [0, 0, 0]$		$1/2, 1/4, 0 [0, 0, 0]$
			$1/2, 3/4, 0 [0, 0, 0]$	$0, 1/2, 1/4 [0, 0, 0]$		$0, 1/2, 3/4 [0, 0, 0]$
8	c	$\bar{3}'m$	$1/4, 1/4, 1/4 [0, 0, 0]$	$3/4, 3/4, 1/4 [0, 0, 0]$	$3/4, 1/4, 3/4 [0, 0, 0]$	$1/4, 3/4, 3/4 [0, 0, 0]$
6	b	4/mm.m	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$		$1/2, 1/2, 0 [0, 0, 0]$
2	a	$m\bar{3}m$	$0, 0, 0 [0, 0, 0]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $0,0,z$

Along  $[1,1,1]$   $p6mm1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
Origin at  $x,x,x$

Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at  $x,x,0$



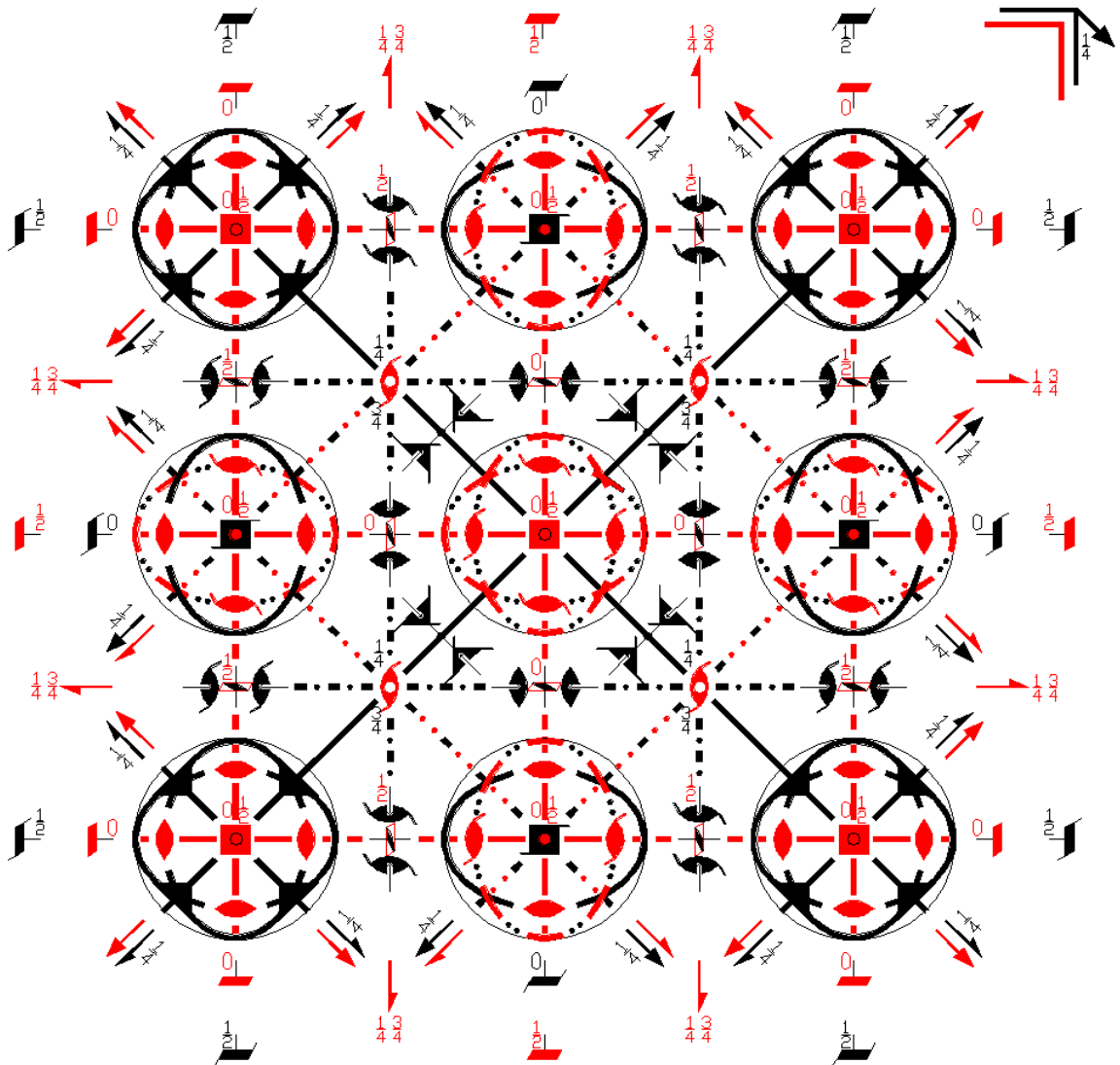
$I_P m\bar{3}m$

229.7.1644

$m\bar{3}m1'$

$I_P 4/m\bar{3}2/m$

Cubic



**Origin** at center ( $m\bar{3}m$ )

**Asymmetric unit**  $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; y \leq x; z \leq \min(1/2-x, y)$

**Vertices**  $0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/4,1/4,1/4$

**Symmetry Operations**

For  $(0,0,0) + \text{set}$

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                         | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)    | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)      | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)     |

(13) $2' x, x, 0$ $(2_{xy}   0, 0, 0)'$	(14) $2' x, \bar{x}, 0$ $(2_{\bar{xy}}   0, 0, 0)'$	(15) $4' 0, 0, z$ $(4_z^{-1}   0, 0, 0)'$	(16) $4^+ 0, 0, z$ $(4_z   0, 0, 0)'$
(17) $4' x, 0, 0$ $(4_x^{-1}   0, 0, 0)'$	(18) $2' 0, y, y$ $(2_{yz}   0, 0, 0)'$	(19) $2' 0, y, \bar{y}$ $(2_{\bar{yz}}   0, 0, 0)'$	(20) $4^+ x, 0, 0$ $(4_x   0, 0, 0)'$
(21) $4^+ 0, y, 0$ $(4_y   0, 0, 0)'$	(22) $2' x, 0, x$ $(2_{xz}   0, 0, 0)'$	(23) $4' 0, y, 0$ $(4_y^{-1}   0, 0, 0)'$	(24) $2' \bar{x}, 0, x$ $(2_{\bar{xz}}   0, 0, 0)'$
(25) $\bar{1}' 0, 0, 0$ $(\bar{1}   0, 0, 0)'$	(26) $m' x, y, 0$ $(m_z   0, 0, 0)'$	(27) $m' x, 0, z$ $(m_y   0, 0, 0)'$	(28) $m' 0, y, z$ $(m_x   0, 0, 0)'$
(29) $\bar{3}^+ x, x, x; 0, 0, 0$ $(\bar{3}_{xyz}   0, 0, 0)'$	(30) $\bar{3}^+ \bar{x}, \bar{x}, \bar{x}; 0, 0, 0$ $(\bar{3}_{\bar{xyz}}^{-1}   0, 0, 0)'$	(31) $\bar{3}^+ x, \bar{x}, \bar{x}; 0, 0, 0$ $(\bar{3}_{\bar{xyz}}^{-1}   0, 0, 0)'$	(32) $\bar{3}^+ \bar{x}, \bar{x}, x; 0, 0, 0$ $(\bar{3}_{\bar{xyz}}^{-1}   0, 0, 0)'$
(33) $\bar{3}^- x, x, x; 0, 0, 0$ $(\bar{3}_{xyz}^{-1}   0, 0, 0)'$	(34) $\bar{3}^- x, \bar{x}, \bar{x}; 0, 0, 0$ $(\bar{3}_{\bar{xyz}}   0, 0, 0)'$	(35) $\bar{3}^- \bar{x}, \bar{x}, x; 0, 0, 0$ $(\bar{3}_{\bar{xyz}}   0, 0, 0)'$	(36) $\bar{3}^- \bar{x}, x, \bar{x}; 0, 0, 0$ $(\bar{3}_{\bar{xyz}}   0, 0, 0)'$
(37) $m x, \bar{x}, z$ $(m_{xy}   0, 0, 0)$	(38) $m x, x, z$ $(m_{\bar{xy}}   0, 0, 0)$	(39) $\bar{4}' 0, 0, z; 0, 0, 0$ $(\bar{4}_z^{-1}   0, 0, 0)$	(40) $\bar{4}^+ 0, 0, z; 0, 0, 0$ $(\bar{4}_z   0, 0, 0)$
(41) $\bar{4}' x, 0, 0; 0, 0, 0$ $(\bar{4}_x^{-1}   0, 0, 0)$	(42) $m x, y, \bar{y}$ $(m_{yz}   0, 0, 0)$	(43) $m x, y, y$ $(m_{\bar{yz}}   0, 0, 0)$	(44) $\bar{4}^+ x, 0, 0; 0, 0, 0$ $(\bar{4}_x   0, 0, 0)$
(45) $\bar{4}^+ 0, y, 0; 0, 0, 0$ $(\bar{4}_y   0, 0, 0)$	(46) $m \bar{x}, y, x$ $(m_{xz}   0, 0, 0)$	(47) $\bar{4}' 0, y, 0; 0, 0, 0$ $(\bar{4}_y^{-1}   0, 0, 0)$	(48) $m x, y, x$ $(m_{\bar{xz}}   0, 0, 0)$

For  $(1/2, 1/2, 1/2)' + \text{set}$ 

(1) $t' (1/2, 1/2, 1/2)$ $(1   1/2, 1/2, 1/2)'$	(2) $2' (0, 0, 1/2) \ 1/4, 1/4, z$ $(2_z   1/2, 1/2, 1/2)'$	(3) $2' (0, 1/2, 0) \ 1/4, y, 1/4$ $(2_y   1/2, 1/2, 1/2)'$	(4) $2' (1/2, 0, 0) \ x, 1/4, 1/4$ $(2_x   1/2, 1/2, 1/2)'$
(5) $3^+ (1/2, 1/2, 1/2) \ x, x, x$ $(3_{xyz}   1/2, 1/2, 1/2)'$	(6) $3^+ (1/6, -1/6, 1/6) \ \bar{x} + 1/3, x + 1/3, \bar{x}$ $(3_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2)'$	(7) $3^+ (-1/6, 1/6, 1/6) \ x + 2/3, \bar{x} - 1/3, x$ $(3_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2)'$	(8) $3^+ (1/6, 1/6, -1/6) \ \bar{x} + 1/3, x + 2/3, \bar{x}$ $(3_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2)'$
(9) $3^- (1/2, 1/2, 1/2) \ x, x, x$ $(3_{xyz}^{-1}   1/2, 1/2, 1/2)'$	(10) $3^- (-1/6, 1/6, 1/6) \ x + 1/3, \bar{x} + 1/3, \bar{x}$ $(3_{xyz}   1/2, 1/2, 1/2)'$	(11) $3^- (1/6, 1/6, -1/6) \ \bar{x} + 2/3, x + 1/3, x$ $(3_{xyz}   1/2, 1/2, 1/2)'$	(12) $3^- (1/6, -1/6, 1/6) \ \bar{x} - 1/3, x + 2/3, \bar{x}$ $(3_{xyz}   1/2, 1/2, 1/2)'$
(13) $2 (1/2, 1/2, 0) \ x, x, 1/4$ $(2_{xy}   1/2, 1/2, 1/2)$	(14) $2 \ x, \bar{x} + 1/2, 1/4$ $(2_{\bar{xy}}   1/2, 1/2, 1/2)$	(15) $4' (0, 0, 1/2) \ 1/2, 0, z$ $(4_z^{-1}   1/2, 1/2, 1/2)$	(16) $4^+ (0, 0, 1/2) \ 0, 1/2, z$ $(4_z   1/2, 1/2, 1/2)$
(17) $4' (1/2, 0, 0) \ x, 1/2, 0$ $(4_x^{-1}   1/2, 1/2, 1/2)$	(18) $2 (0, 1/2, 1/2) \ 1/4, y, y$ $(2_{yz}   1/2, 1/2, 1/2)$	(19) $2 \ 1/4, y + 1/2, \bar{y}$ $(2_{\bar{yz}}   1/2, 1/2, 1/2)$	(20) $4^+ (1/2, 0, 0) \ x, 0, 1/2$ $(4_x   1/2, 1/2, 1/2)$
(21) $4^+ (0, 1/2, 0) \ 1/2, y, 0$ $(4_y   1/2, 1/2, 1/2)$	(22) $2 (1/2, 0, 1/2) \ x, 1/4, x$ $(2_{xz}   1/2, 1/2, 1/2)$	(23) $4' (0, 1/2, 0) \ 0, y, 1/2$ $(4_y^{-1}   1/2, 1/2, 1/2)$	(24) $2 \ \bar{x} + 1/2, 1/4, x$ $(2_{\bar{xz}}   1/2, 1/2, 1/2)$
(25) $\bar{1} \ 1/4, 1/4, 1/4$ $(\bar{1}   1/2, 1/2, 1/2)$	(26) $n (1/2, 1/2, 0) \ x, y, 1/4$ $(m_z   1/2, 1/2, 1/2)$	(27) $n (1/2, 0, 1/2) \ x, 1/4, z$ $(m_y   1/2, 1/2, 1/2)$	(28) $n (0, 1/2, 1/2) \ 1/4, y, z$ $(m_x   1/2, 1/2, 1/2)$
(29) $\bar{3}^+ x, x, x; \ 1/4, 1/4, 1/4$ $(\bar{3}_{xyz}   1/2, 1/2, 1/2)$	(30) $\bar{3}^+ \bar{x} - 1, x + 1, \bar{x}; \ -1/4, 1/4, 3/4$ $(\bar{3}_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2)$	(31) $\bar{3}^+ x, \bar{x} + 1, \bar{x}; \ 1/4, 3/4, -1/4$ $(\bar{3}_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2)$	(32) $\bar{3}^+ \bar{x} + 1, \bar{x}, x; \ 3/4, -1/4, 1/4$ $(\bar{3}_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2)$

(33) $\bar{3}^-$ $x, x, x;$ 1/4, 1/4, 1/4 ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(34) $\bar{3}^-$ $x+1, \bar{x}-1, \bar{x};$ 1/4, -1/4, 3/4 ( $\bar{3}_{\bar{xyz}}   1/2, 1/2, 1/2$ )	(35) $\bar{3}^-$ $\bar{x}, \bar{x}+1, x;$ -1/4, 3/4, 1/4 ( $\bar{3}_{x\bar{z}}   1/2, 1/2, 1/2$ )	(36) $\bar{3}^-$ $\bar{x}+1, x, \bar{x};$ 3/4, 1/4, -1/4 ( $\bar{3}_{x\bar{yz}}   1/2, 1/2, 1/2$ )
(37) $c'$ (0,0,1/2) $x+1/2, \bar{x}, z$ ( $m_{xy}   1/2, 1/2, 1/2$ )'	(38) $n'$ (1/2, 1/2, 1/2) $x, x, z$ ( $m_{\bar{xy}}   1/2, 1/2, 1/2$ )'	(39) $\bar{4}^-$ ' 0, 1/2, z; 0, 1/2, 1/4 ( $\bar{4}_z^{-1}   1/2, 1/2, 1/2$ )'	(40) $\bar{4}^+$ ' 1/2, 0, z; 1/2, 0, 1/4 ( $\bar{4}_z   1/2, 1/2, 1/2$ )'
(41) $\bar{4}^-$ ' $x, 0, 1/2; 1/4, 0, 1/2$ ( $\bar{4}_x^{-1}   1/2, 1/2, 1/2$ )'	(42) $a'$ (1/2, 0, 0) $x, y+1/2, \bar{y}$ ( $m_{yz}   1/2, 1/2, 1/2$ )'	(43) $n'$ (1/2, 1/2, 1/2) $x, y, y$ ( $m_{\bar{yz}}   1/2, 1/2, 1/2$ )'	(44) $\bar{4}^+$ ' $x, 1/2, 0; 1/4, 1/2, 0$ ( $\bar{4}_x   1/2, 1/2, 1/2$ )'
(45) $\bar{4}^+$ ' 0, y, 1/2; 0, 1/4, 1/2 ( $\bar{4}_y   1/2, 1/2, 1/2$ )'	(46) $b'$ (0, 1/2, 0) $\bar{x}+1/2, y, x$ ( $m_{xz}   1/2, 1/2, 1/2$ )'	(47) $\bar{4}^-$ ' 1/2, y, 0; 1/2, 1/4, 0 ( $\bar{4}_y^{-1}   1/2, 1/2, 1/2$ )'	(48) $n'$ (1/2, 1/2, 1/2) $x, y, x$ ( $m_{\bar{xz}}   1/2, 1/2, 1/2$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13); (25).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

		(0,0,0) +		(1/2, 1/2, 1/2)' +	
96	l	1			
(1)	$x, y, z$	[u, v, w]	(2)	$\bar{x}, \bar{y}, z$	[ $\bar{u}, \bar{v}, w$ ]
(5)	$z, x, y$	[w, u, v]	(6)	$z, \bar{x}, \bar{y}$	[w, $\bar{u}, \bar{v}$ ]
(9)	$y, z, x$	[v, w, u]	(10)	$\bar{y}, z, \bar{x}$	[ $\bar{v}, w, \bar{u}$ ]
(13)	$y, x, \bar{z}$	[ $\bar{v}, \bar{u}, w$ ]	(14)	$\bar{y}, \bar{x}, \bar{z}$	[v, u, w]
(17)	$x, z, \bar{y}$	[ $\bar{u}, \bar{w}, v$ ]	(18)	$\bar{x}, z, y$	[u, $\bar{w}, \bar{v}$ ]
(21)	$z, y, \bar{x}$	[ $\bar{w}, \bar{v}, u$ ]	(22)	$z, \bar{y}, x$	[ $\bar{w}, v, \bar{u}$ ]
(25)	$\bar{x}, \bar{y}, \bar{z}$	[ $\bar{u}, \bar{v}, \bar{w}$ ]	(26)	$x, y, \bar{z}$	[u, v, $\bar{w}$ ]
(29)	$\bar{z}, \bar{x}, \bar{y}$	[ $\bar{w}, \bar{u}, \bar{v}$ ]	(30)	$\bar{z}, x, y$	[ $\bar{w}, u, v$ ]
(33)	$\bar{y}, \bar{z}, \bar{x}$	[ $\bar{v}, \bar{w}, \bar{u}$ ]	(34)	$y, \bar{z}, x$	[v, $\bar{w}, u$ ]
(37)	$\bar{y}, \bar{x}, z$	[v, u, $\bar{w}$ ]	(38)	$y, x, z$	[ $\bar{v}, \bar{u}, \bar{w}$ ]
(41)	$\bar{x}, \bar{z}, y$	[u, w, $\bar{v}$ ]	(42)	$x, \bar{z}, y$	[u, w, $\bar{v}$ ]
(45)	$\bar{z}, \bar{y}, x$	[w, v, $\bar{u}$ ]	(46)	$\bar{z}, y, \bar{x}$	[w, $\bar{v}, u$ ]
48	k	..m	$x, x, z$	[u, $\bar{u}, 0$ ]	$\bar{x}, \bar{x}, z$
			$z, x, x$	[0, $\bar{u}, \bar{u}$ ]	$\bar{z}, \bar{x}, \bar{x}$
			$x, z, x$	[ $\bar{u}, 0, u$ ]	$\bar{x}, \bar{z}, \bar{x}$
			$x, x, \bar{z}$	[u, $\bar{u}, 0$ ]	$\bar{x}, \bar{x}, z$
			$x, z, \bar{x}$	[ $\bar{u}, 0, \bar{u}$ ]	$\bar{x}, \bar{z}, \bar{x}$



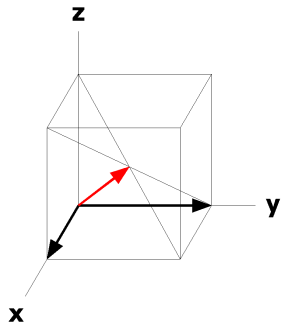
			$z, x, \bar{x} [0, u, u]$	$z, \bar{x}, x [0, \bar{u}, \bar{u}]$	$\bar{z}, x, x [0, u, \bar{u}]$	$\bar{z}, \bar{x}, \bar{x} [0, \bar{u}, u]$
48	j	$m'..$	$0, y, z [0, v, w]$	$0, \bar{y}, z [0, \bar{v}, w]$	$0, y, \bar{z} [0, v, \bar{w}]$	$0, \bar{y}, \bar{z} [0, \bar{v}, \bar{w}]$
			$z, 0, y [w, 0, v]$	$z, 0, \bar{y} [w, 0, \bar{v}]$	$\bar{z}, 0, y [\bar{w}, 0, v]$	$\bar{z}, 0, \bar{y} [\bar{w}, 0, \bar{v}]$
			$y, z, 0 [v, w, 0]$	$\bar{y}, z, 0 [\bar{v}, w, 0]$	$y, \bar{z}, 0 [v, \bar{w}, 0]$	$\bar{y}, \bar{z}, 0 [\bar{v}, \bar{w}, 0]$
			$y, 0, \bar{z} [\bar{v}, 0, w]$	$\bar{y}, 0, \bar{z} [v, 0, w]$	$y, 0, z [\bar{v}, 0, \bar{w}]$	$\bar{y}, 0, z [v, 0, \bar{w}]$
			$0, z, \bar{y} [0, \bar{w}, v]$	$0, z, y [0, \bar{w}, \bar{v}]$	$0, \bar{z}, \bar{y} [0, w, v]$	$0, \bar{z}, y [0, w, \bar{v}]$
			$z, y, 0 [\bar{w}, \bar{v}, 0]$	$z, \bar{y}, 0 [\bar{w}, v, 0]$	$\bar{z}, y, 0 [w, \bar{v}, 0]$	$\bar{z}, \bar{y}, 0 [w, v, 0]$
48	i	$..2$				
			$1/4, y, \bar{y} + 1/2 [0, \bar{v}, v]$	$3/4, \bar{y}, \bar{y} + 1/2 [0, v, v]$	$3/4, y, y + 1/2 [0, \bar{v}, \bar{v}]$	$1/4, \bar{y}, y + 1/2 [0, v, \bar{v}]$
			$\bar{y} + 1/2, 1/4, y [v, 0, \bar{v}]$	$\bar{y} + 1/2, 3/4, \bar{y} [v, 0, v]$	$y + 1/2, 3/4, y [\bar{v}, 0, \bar{v}]$	$y + 1/2, 1/4, \bar{y} [\bar{v}, 0, v]$
			$y, \bar{y} + 1/2, 1/4 [\bar{v}, v, 0]$	$\bar{y}, \bar{y} + 1/2, 3/4 [v, v, 0]$	$y, y + 1/2, 3/4 [\bar{v}, \bar{v}, 0]$	$\bar{y}, y + 1/2, 1/4 [v, \bar{v}, 0]$
			$3/4, \bar{y}, y + 1/2 [0, v, \bar{v}]$	$1/4, y, y + 1/2 [0, \bar{v}, \bar{v}]$	$1/4, \bar{y}, \bar{y} + 1/2 [0, v, v]$	$3/4, y, \bar{y} + 1/2 [0, \bar{v}, v]$
			$y + 1/2, 3/4, \bar{y} [\bar{v}, 0, v]$	$y + 1/2, 1/4, y [\bar{v}, 0, \bar{v}]$	$\bar{y} + 1/2, 1/4, \bar{y} [v, 0, v]$	$\bar{y} + 1/2, 3/4, y [v, 0, \bar{v}]$
			$\bar{y}, y + 1/2, 3/4 [v, \bar{v}, 0]$	$y, y + 1/2, 1/4 [\bar{v}, \bar{v}, 0]$	$\bar{y}, \bar{y} + 1/2, 1/4 [v, v, 0]$	$y, \bar{y} + 1/2, 3/4 [\bar{v}, v, 0]$
24	h	$m'.m2'$	$0, y, y [0, \bar{v}, v]$	$0, \bar{y}, y [0, v, v]$	$0, y, \bar{y} [0, \bar{v}, \bar{v}]$	$0, \bar{y}, \bar{y} [0, v, \bar{v}]$
			$y, 0, y [v, 0, \bar{v}]$	$y, 0, \bar{y} [v, 0, v]$	$\bar{y}, 0, y [\bar{v}, 0, \bar{v}]$	$\bar{y}, 0, \bar{y} [\bar{v}, 0, v]$
			$y, y, 0 [\bar{v}, v, 0]$	$\bar{y}, y, 0 [v, v, 0]$	$y, \bar{y}, 0 [\bar{v}, \bar{v}, 0]$	$\bar{y}, \bar{y}, 0 [v, \bar{v}, 0]$
24	g	$m'm'2..$	$x, 0, 1/2 [u, 0, 0]$	$\bar{x}, 0, 1/2 [\bar{u}, 0, 0]$	$1/2, x, 0 [0, u, 0]$	$1/2, \bar{x}, 0 [0, \bar{u}, 0]$
			$0, 1/2, x [0, 0, u]$	$0, 1/2, \bar{x} [0, 0, \bar{u}]$	$0, x, 1/2 [0, \bar{u}, 0]$	$0, \bar{x}, 1/2 [0, u, 0]$
			$x, 1/2, 0 [\bar{u}, 0, 0]$	$\bar{x}, 1/2, 0 [u, 0, 0]$	$1/2, 0, \bar{x} [0, 0, u]$	$1/2, 0, x [0, 0, \bar{u}]$
16	f	$.3m'$	$x, x, x [u, u, u]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$	$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
			$x, x, \bar{x} [\bar{u}, \bar{u}, u]$	$\bar{x}, \bar{x}, \bar{x} [u, u, u]$	$x, \bar{x}, x [\bar{u}, u, \bar{u}]$	$\bar{x}, x, x [u, \bar{u}, \bar{u}]$
12	e	$4'm'.m$	$x, 0, 0 [0, 0, 0]$	$\bar{x}, 0, 0 [0, 0, 0]$		$0, x, 0 [0, 0, 0]$
			$0, \bar{x}, 0 [0, 0, 0]$	$0, 0, x [0, 0, 0]$		$0, 0, \bar{x} [0, 0, 0]$
12	d	$\bar{4}'m'.2$	$1/4, 0, 1/2 [0, 0, 0]$	$3/4, 0, 1/2 [0, 0, 0]$		$1/2, 1/4, 0 [0, 0, 0]$
			$1/2, 3/4, 0 [0, 0, 0]$	$0, 1/2, 1/4 [0, 0, 0]$		$0, 1/2, 3/4 [0, 0, 0]$
8	c	$.3m'$	$1/4, 1/4, 1/4 [u, u, u]$	$3/4, 3/4, 1/4 [\bar{u}, \bar{u}, u]$	$3/4, 1/4, 3/4 [\bar{u}, u, \bar{u}]$	$1/4, 3/4, 3/4 [u, \bar{u}, \bar{u}]$
6	b	$4'/m'm'.m$	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$		$1/2, 1/2, 0 [0, 0, 0]$
2	a	$m'\bar{3}'m$	$0, 0, 0 [0, 0, 0]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p_4 m' m'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $1/2, 0, z$

Along  $[1,1,1]$   $p6mm1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

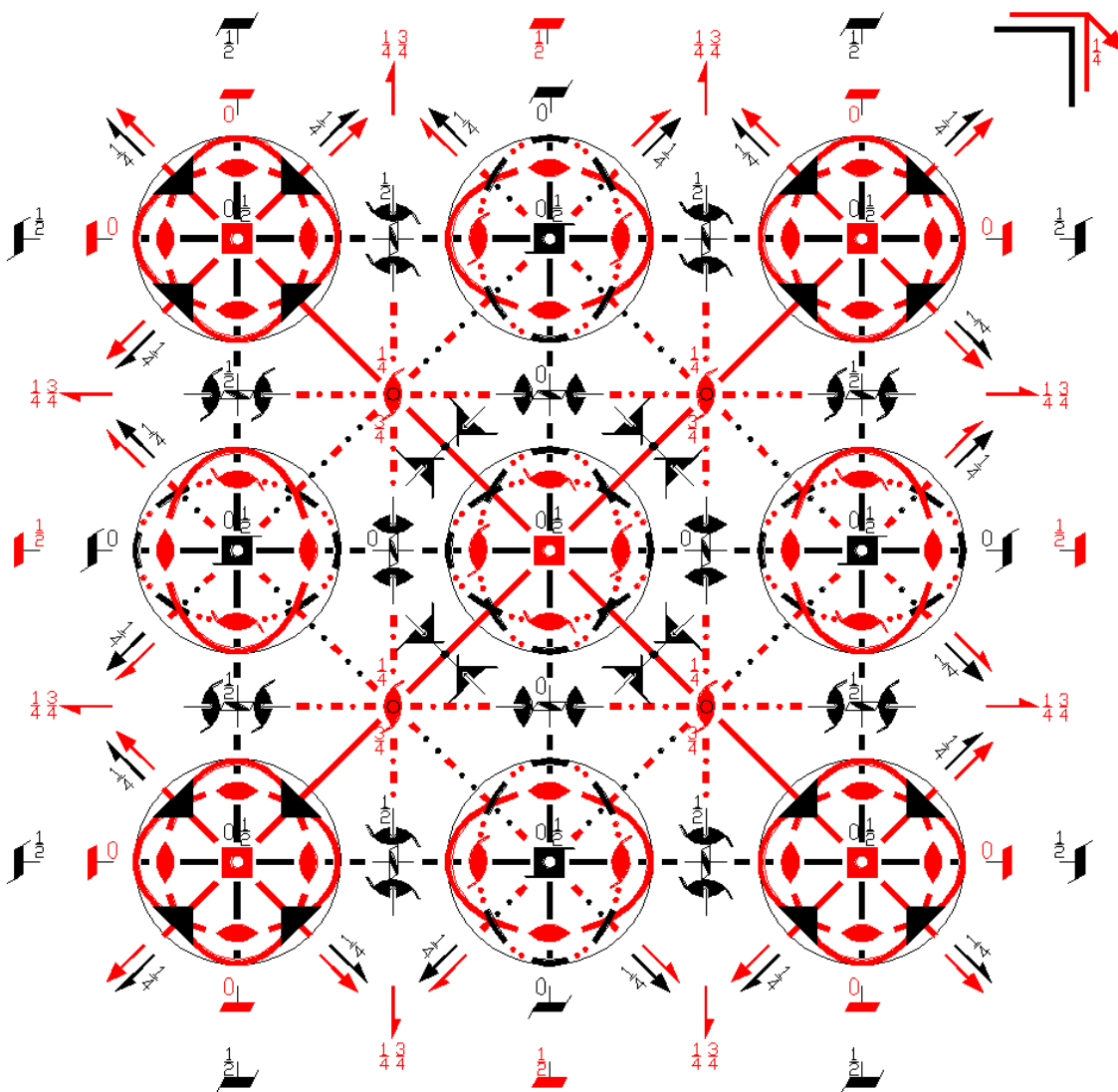
Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, x, 0$



$I_p m\bar{3}m'$   
229.8.1645

$m\bar{3}m1'$   
 $I_p 4'/m\bar{3}2'/m'$

Cubic



**Origin** at center ( $m\bar{3}m'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/4;$   $y \leq x;$   $z \leq \min(1/2-x, y)$

**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/4,1/4,1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)                                     | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)   | (3) 2 $0,y,0$<br>( $2_y$  0,0,0)   | (4) 2 $x,0,0$<br>( $2_x$  0,0,0)   |
| (5) $3^+$ $x,x,x$<br>( $3_{xyz}$  0,0,0)               | (6) $3^+$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}z}$ <sup>-1</sup>  0,0,0) | (7) $3^+$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$ <sup>-1</sup>  0,0,0) | (8) $3^+$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}z}$ <sup>-1</sup>  0,0,0) |
| (9) $3^-$ $x,x,x$<br>( $3_{xyz}$ <sup>-1</sup>  0,0,0) | (10) $3^-$ $x,\bar{x},\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)              | (11) $3^-$ $\bar{x},\bar{x},x$<br>( $3_{x\bar{y}z}$  0,0,0)              | (12) $3^-$ $\bar{x},x,\bar{x}$<br>( $3_{x\bar{y}z}$  0,0,0)              |

- |   |   |   |  |
|---|---|---|--|
| (13) $2' x, x, 0$<br>$(2_{xy}   0, 0, 0)'$                            | (14) $2' x, \bar{x}, 0$<br>$(2_{\bar{xy}}   0, 0, 0)'$  | (15) $4^- ' 0, 0, z$<br>$(4_z^{-1}   0, 0, 0)'$   | (16) $4^+ ' 0, 0, z$<br>$(4_z   0, 0, 0)'$   |
| (17) $4^- ' x, 0, 0$<br>$(4_x^{-1}   0, 0, 0)'$                       | (18) $2' 0, y, y$<br>$(2_{yz}   0, 0, 0)'$  | (19) $2' 0, y, \bar{y}$<br>$(2_{\bar{yz}}   0, 0, 0)'$                                  | (20) $4^+ ' x, 0, 0$<br>$(4_x   0, 0, 0)'$   |
| (21) $4^+ ' 0, y, 0$<br>$(4_y   0, 0, 0)'$                            | (22) $2' x, 0, x$<br>$(2_{xz}   0, 0, 0)'$  | (23) $4^- ' 0, y, 0$<br>$(4_y^{-1}   0, 0, 0)'$   | (24) $2' \bar{x}, 0, x$<br>$(2_{\bar{xz}}   0, 0, 0)'$                                   |
| (25) $\bar{1} 0, 0, 0$<br>$(\bar{1}   0, 0, 0)$                       | (26) $m x, y, 0$<br>$(m_z   0, 0, 0)$   | (27) $m x, 0, z$<br>$(m_y   0, 0, 0)$   | (28) $m 0, y, z$<br>$(m_x   0, 0, 0)$  |
| (29) $\bar{3}^+ x, x, x; 0, 0, 0$<br>$(\bar{3}_{xyz}   0, 0, 0)$      | (30) $\bar{3}^+ \bar{x}, \bar{x}, \bar{x}; 0, 0, 0$<br>$(\bar{3}_{\bar{xyz}}^{-1}   0, 0, 0)$ | (31) $\bar{3}^+ x, \bar{x}, \bar{x}; 0, 0, 0$<br>$(\bar{3}_{\bar{xyz}}^{-1}   0, 0, 0)$ | (32) $\bar{3}^+ \bar{x}, \bar{x}, \bar{x}; 0, 0, 0$<br>$(\bar{3}_{xyz}^{-1}   0, 0, 0)$  |
| (33) $\bar{3}^- x, x, x; 0, 0, 0$<br>$(\bar{3}_{xyz}^{-1}   0, 0, 0)$ | (34) $\bar{3}^- \bar{x}, \bar{x}, \bar{x}; 0, 0, 0$<br>$(\bar{3}_{\bar{xyz}}   0, 0, 0)$      | (35) $\bar{3}^- \bar{x}, \bar{x}, \bar{x}; 0, 0, 0$<br>$(\bar{3}_{xyz}   0, 0, 0)$      | (36) $\bar{3}^- \bar{x}, \bar{x}, \bar{x}; 0, 0, 0$<br>$(\bar{3}_{\bar{xyz}}   0, 0, 0)$ |
| (37) $m' x, \bar{x}, z$<br>$(m_{xy}   0, 0, 0)'$                      | (38) $m' x, x, z$<br>$(m_{\bar{xy}}   0, 0, 0)'$  | (39) $\bar{4}^- ' 0, 0, z; 0, 0, 0$<br>$(\bar{4}_z^{-1}   0, 0, 0)'$                    | (40) $\bar{4}^+ ' 0, 0, z; 0, 0, 0$<br>$(\bar{4}_z   0, 0, 0)'$                          |
| (41) $\bar{4}^- ' x, 0, 0; 0, 0, 0$<br>$(\bar{4}_x^{-1}   0, 0, 0)'$  | (42) $m' x, y, \bar{y}$<br>$(m_{yz}   0, 0, 0)'$  | (43) $m' x, y, y$<br>$(m_{\bar{yz}}   0, 0, 0)'$  | (44) $\bar{4}^+ ' x, 0, 0; 0, 0, 0$<br>$(\bar{4}_x   0, 0, 0)'$                          |
| (45) $\bar{4}^+ ' 0, y, 0; 0, 0, 0$<br>$(\bar{4}_y   0, 0, 0)'$       | (46) $m' \bar{x}, y, x$<br>$(m_{xz}   0, 0, 0)'$  | (47) $\bar{4}^- ' 0, y, 0; 0, 0, 0$<br>$(\bar{4}_y^{-1}   0, 0, 0)'$                    | (48) $m' x, y, x$<br>$(m_{\bar{xz}}   0, 0, 0)'$   |

For  $(1/2, 1/2, 1/2)' + \text{set}$ 

- |   |   |   |  |
|---|---|---|--|
| (1) $t' (1/2, 1/2, 1/2)$<br>$(1   1/2, 1/2, 1/2)'$                                | (2) $2' (0, 0, 1/2) \ 1/4, 1/4, z$<br>$(2_z   1/2, 1/2, 1/2)'$  | (3) $2' (0, 1/2, 0) \ 1/4, y, 1/4$<br>$(2_y   1/2, 1/2, 1/2)'$  | (4) $2' (1/2, 0, 0) \ x, 1/4, 1/4$<br>$(2_x   1/2, 1/2, 1/2)'$   |
| (5) $3^+ ' (1/2, 1/2, 1/2) \ x, x, x$<br>$(3_{xyz}   1/2, 1/2, 1/2)'$             | (6) $3^+ ' (1/6, -1/6, 1/6) \ \bar{x} + 1/3, \bar{x} + 1/3, \bar{x}$<br>$(3_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2)'$         | (7) $3^+ ' (-1/6, 1/6, 1/6) \ \bar{x} + 2/3, \bar{x} - 1/3, \bar{x}$<br>$(3_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2)'$ | (8) $3^+ ' (1/6, 1/6, -1/6) \ \bar{x} + 1/3, \bar{x} + 2/3, \bar{x}$<br>$(3_{\bar{yz}}^{-1}   1/2, 1/2, 1/2)'$ |
| (9) $3^- ' (1/2, 1/2, 1/2) \ x, x, x$<br>$(3_{xyz}^{-1}   1/2, 1/2, 1/2)'$        | (10) $3^- ' (-1/6, 1/6, 1/6) \ \bar{x} + 1/3, \bar{x} + 1/3, \bar{x}$<br>$(3_{xyz}   1/2, 1/2, 1/2)'$                   | (11) $3^- ' (1/6, 1/6, -1/6) \ \bar{x} + 2/3, \bar{x} + 1/3, \bar{x}$<br>$(3_{xyz}   1/2, 1/2, 1/2)'$           | (12) $3^- ' (1/6, -1/6, 1/6) \ \bar{x} - 1/3, \bar{x} + 2/3, \bar{x}$<br>$(3_{\bar{yz}}   1/2, 1/2, 1/2)'$     |
| (13) $2 (1/2, 1/2, 0) \ x, x, 1/4$<br>$(2_{xy}   1/2, 1/2, 1/2)$                  | (14) $2 \ x, \bar{x} + 1/2, 1/4$<br>$(2_{\bar{xy}}   1/2, 1/2, 1/2)$  | (15) $4^- (0, 0, 1/2) \ 1/2, 0, z$<br>$(4_z^{-1}   1/2, 1/2, 1/2)$  | (16) $4^+ (0, 0, 1/2) \ 0, 1/2, z$<br>$(4_z   1/2, 1/2, 1/2)$  |
| (17) $4^- (1/2, 0, 0) \ x, 1/2, 0$<br>$(4_x^{-1}   1/2, 1/2, 1/2)$                | (18) $2 (0, 1/2, 1/2) \ 1/4, y, y$<br>$(2_{yz}   1/2, 1/2, 1/2)$  | (19) $2 \ 1/4, y + 1/2, \bar{y}$<br>$(2_{\bar{yz}}   1/2, 1/2, 1/2)$  | (20) $4^+ (1/2, 0, 0) \ x, 0, 1/2$<br>$(4_x   1/2, 1/2, 1/2)$  |
| (21) $4^+ (0, 1/2, 0) \ 1/2, y, 0$<br>$(4_y   1/2, 1/2, 1/2)$                     | (22) $2 (1/2, 0, 1/2) \ x, 1/4, x$<br>$(2_{xz}   1/2, 1/2, 1/2)$  | (23) $4^- (0, 1/2, 0) \ 0, y, 1/2$<br>$(4_y^{-1}   1/2, 1/2, 1/2)$  | (24) $2 \ \bar{x} + 1/2, 1/4, x$<br>$(2_{\bar{xz}}   1/2, 1/2, 1/2)$   |
| (25) $\bar{1} \ 1/4, 1/4, 1/4$<br>$(\bar{1}   1/2, 1/2, 1/2)'$                    | (26) $n' (1/2, 1/2, 0) \ x, y, 1/4$<br>$(m_z   1/2, 1/2, 1/2)'$   | (27) $n' (1/2, 0, 1/2) \ x, 1/4, z$<br>$(m_y   1/2, 1/2, 1/2)'$   | (28) $n' (0, 1/2, 1/2) \ 1/4, y, z$<br>$(m_x   1/2, 1/2, 1/2)'$  |
| (29) $\bar{3}^+ ' x, x, x; \ 1/4, 1/4, 1/4$<br>$(\bar{3}_{xyz}   1/2, 1/2, 1/2)'$ | (30) $\bar{3}^+ ' \bar{x} - 1, \bar{x} + 1, \bar{x}; \ -1/4, 1/4, 3/4$<br>$(\bar{3}_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2)'$ | (31) $\bar{3}^+ ' x, \bar{x} + 1, \bar{x}; \ 1/4, 3/4, -1/4$<br>$(\bar{3}_{\bar{yz}}^{-1}   1/2, 1/2, 1/2)'$    | (32) $\bar{3}^+ ' \bar{x} + 1, \bar{x}, \bar{x}; \ 3/4, -1/4, 1/4$<br>$(\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2)'$  |

(33) $\bar{3}^-$ ' x,x,x; 1/4,1/4,1/4 ( $\bar{3}_{xyz}^{-1}$   1/2,1/2,1/2)'	(34) $\bar{3}^-$ ' x+1, $\bar{x}$ -1, $\bar{x}$ ; 1/4,-1/4,3/4 ( $\bar{3}_{xyz}$   1/2,1/2,1/2)'	(35) $\bar{3}^-$ ' $\bar{x}$ , $\bar{x}$ +1, x; -1/4,3/4,1/4 ( $\bar{3}_{xy\bar{z}}$   1/2,1/2,1/2)'	(36) $\bar{3}^-$ ' $\bar{x}$ +1, x, $\bar{x}$ ; 3/4,1/4,-1/4 ( $\bar{3}_{x\bar{y}\bar{z}}$   1/2,1/2,1/2)'
(37) c (0,0,1/2) x+1/2, $\bar{x}$ ,z ( $m_{xy}$   1/2,1/2,1/2)	(38) n (1/2,1/2,1/2) x,x,z ( $m_{\bar{xy}}$   1/2,1/2,1/2)	(39) $\bar{4}^-$ 0,1/2,z; 0,1/2,1/4 ( $\bar{4}_z^{-1}$   1/2,1/2,1/2)	(40) $\bar{4}^+$ 1/2,0,z; 1/2,0,1/4 ( $\bar{4}_z$   1/2,1/2,1/2)
(41) $\bar{4}^-$ x,0,1/2; 1/4,0,1/2 ( $\bar{4}_x^{-1}$   1/2,1/2,1/2)	(42) a (1/2,0,0) x,y+1/2, $\bar{y}$ ( $m_{yz}$   1/2,1/2,1/2)	(43) n (1/2,1/2,1/2) x,y,y ( $m_{yz}$   1/2,1/2,1/2)	(44) $\bar{4}^+$ x,1/2,0; 1/4,1/2,0 ( $\bar{4}_x$   1/2,1/2,1/2)
(45) $\bar{4}^+$ 0,y,1/2; 0,1/4,1/2 ( $\bar{4}_y$   1/2,1/2,1/2)	(46) b (0,1/2,0) $\bar{x}$ +1/2,y,x ( $m_{xz}$   1/2,1/2,1/2)	(47) $\bar{4}^-$ 1/2,y,0; 1/2,1/4,0 ( $\bar{4}_y^{-1}$   1/2,1/2,1/2)	(48) n (1/2,1/2,1/2) x,y,x ( $m_{xz}$   1/2,1/2,1/2)

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13); (25).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

		(0,0,0) +	(1/2,1/2,1/2)' +				
96	l	1					
(1)	x,y,z [u,v,w]	(2)	$\bar{x}, \bar{y}, z$ [ $\bar{u}, \bar{v}, w$ ]	(3)	$\bar{x}, y, \bar{z}$ [ $\bar{u}, v, \bar{w}$ ]	(4)	x, $\bar{y}, \bar{z}$ [u, $\bar{v}, \bar{w}$ ]
(5)	z,x,y [w,u,v]	(6)	z, $\bar{x}, \bar{y}$ [ $\bar{w}, \bar{u}, \bar{v}$ ]	(7)	$\bar{z}, \bar{x}, y$ [ $\bar{w}, \bar{u}, v$ ]	(8)	$\bar{z}, x, \bar{y}$ [ $\bar{w}, u, \bar{v}$ ]
(9)	y,z,x [v,w,u]	(10)	$\bar{y}, z, \bar{x}$ [ $\bar{v}, w, \bar{u}$ ]	(11)	y, $\bar{z}, \bar{x}$ [v, $\bar{w}, \bar{u}$ ]	(12)	$\bar{y}, \bar{z}, x$ [ $\bar{v}, \bar{w}, u$ ]
(13)	y,x, $\bar{z}$ [ $\bar{v}, \bar{u}, w$ ]	(14)	$\bar{y}, \bar{x}, \bar{z}$ [ $\bar{v}, u, w$ ]	(15)	y, $\bar{x}, z$ [ $\bar{v}, u, \bar{w}$ ]	(16)	$\bar{y}, x, z$ [ $\bar{v}, u, \bar{w}$ ]
(17)	x,z, $\bar{y}$ [ $\bar{u}, \bar{w}, v$ ]	(18)	$\bar{x}, z, y$ [ $\bar{u}, \bar{w}, \bar{v}$ ]	(19)	$\bar{x}, \bar{z}, \bar{y}$ [ $\bar{u}, w, v$ ]	(20)	x, $\bar{z}, y$ [ $\bar{u}, w, \bar{v}$ ]
(21)	z,y, $\bar{x}$ [ $\bar{w}, \bar{v}, u$ ]	(22)	z, $\bar{y}, x$ [ $\bar{w}, v, \bar{u}$ ]	(23)	$\bar{z}, y, x$ [ $\bar{w}, \bar{v}, \bar{u}$ ]	(24)	$\bar{z}, \bar{y}, \bar{x}$ [ $\bar{w}, v, u$ ]
(25)	$\bar{x}, \bar{y}, \bar{z}$ [u,v,w]	(26)	x,y, $\bar{z}$ [ $\bar{u}, \bar{v}, w$ ]	(27)	x, $\bar{y}, z$ [ $\bar{u}, v, \bar{w}$ ]	(28)	$\bar{x}, y, z$ [u, $\bar{v}, \bar{w}$ ]
(29)	$\bar{z}, \bar{x}, \bar{y}$ [w,u,v]	(30)	$\bar{z}, x, y$ [ $\bar{w}, \bar{u}, \bar{v}$ ]	(31)	z,x, $\bar{y}$ [ $\bar{w}, \bar{u}, v$ ]	(32)	z, $\bar{x}, y$ [ $\bar{w}, u, \bar{v}$ ]
(33)	$\bar{y}, \bar{z}, \bar{x}$ [v,w,u]	(34)	y, $\bar{z}, x$ [ $\bar{v}, w, \bar{u}$ ]	(35)	$\bar{y}, z, x$ [ $\bar{v}, \bar{w}, \bar{u}$ ]	(36)	y, z, $\bar{x}$ [ $\bar{v}, w, u$ ]
(37)	$\bar{y}, \bar{x}, z$ [ $\bar{v}, \bar{u}, w$ ]	(38)	y,x,z [v,u,w]	(39)	$\bar{y}, x, z$ [ $\bar{v}, u, \bar{w}$ ]	(40)	y, $\bar{x}, z$ [ $\bar{v}, u, \bar{w}$ ]
(41)	$\bar{x}, \bar{z}, y$ [ $\bar{u}, \bar{w}, v$ ]	(42)	x, $\bar{z}, \bar{y}$ [ $\bar{u}, \bar{w}, \bar{v}$ ]	(43)	x,z,y [u,w,v]	(44)	$\bar{x}, z, y$ [ $\bar{u}, w, \bar{v}$ ]
(45)	$\bar{z}, \bar{y}, x$ [ $\bar{w}, \bar{v}, u$ ]	(46)	$\bar{z}, y, \bar{x}$ [ $\bar{w}, v, \bar{u}$ ]	(47)	z, $\bar{y}, \bar{x}$ [ $\bar{w}, \bar{v}, \bar{u}$ ]	(48)	z, y, x [w,v,u]
48	k	..m'	x,x,z [u,u,w]	$\bar{x}, \bar{x}, z$ [ $\bar{u}, \bar{u}, w$ ]	$\bar{x}, x, \bar{z}$ [ $\bar{u}, u, \bar{w}$ ]	x, $\bar{x}, \bar{z}$ [u, $\bar{u}, \bar{w}$ ]	
			z,x,x [w,u,u]	z, $\bar{x}, \bar{x}$ [ $\bar{w}, \bar{u}, \bar{u}$ ]	$\bar{z}, \bar{x}, x$ [ $\bar{w}, \bar{u}, u$ ]	$\bar{z}, x, \bar{x}$ [ $\bar{w}, u, \bar{u}$ ]	
			x,z,x [u,w,u]	$\bar{x}, z, \bar{x}$ [ $\bar{u}, w, \bar{u}$ ]	x, $\bar{z}, \bar{x}$ [ $\bar{u}, \bar{w}, \bar{u}$ ]	$\bar{x}, \bar{z}, x$ [ $\bar{u}, w, u$ ]	
			x,x, $\bar{z}$ [ $\bar{u}, \bar{u}, w$ ]	$\bar{x}, \bar{x}, \bar{z}$ [ $\bar{u}, u, w$ ]	x, $\bar{x}, z$ [ $\bar{u}, u, \bar{w}$ ]	$\bar{x}, x, z$ [u, $\bar{u}, \bar{w}$ ]	
			x,z, $\bar{x}$ [ $\bar{u}, \bar{w}, u$ ]	$\bar{x}, z, \bar{x}$ [ $\bar{u}, w, \bar{u}$ ]	$\bar{x}, \bar{z}, \bar{x}$ [ $\bar{u}, w, u$ ]	$\bar{x}, z, x$ [ $\bar{u}, w, \bar{u}$ ]	

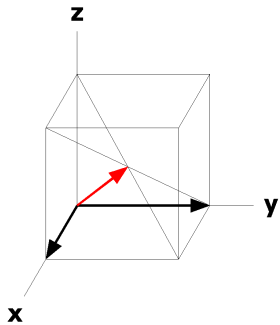
			$z, x, \bar{x} [\bar{w}, \bar{u}, \bar{u}]$	$z, \bar{x}, x [\bar{w}, \bar{u}, \bar{u}]$	$\bar{z}, x, x [w, \bar{u}, \bar{u}]$	$\bar{z}, \bar{x}, \bar{x} [w, u, u]$
48	j	m..	$0, y, z [u, 0, 0]$	$0, \bar{y}, z [\bar{u}, 0, 0]$	$0, y, \bar{z} [\bar{u}, 0, 0]$	$0, \bar{y}, \bar{z} [u, 0, 0]$
			$z, 0, y [0, u, 0]$	$z, 0, \bar{y} [0, \bar{u}, 0]$	$\bar{z}, 0, y [0, \bar{u}, 0]$	$\bar{z}, 0, \bar{y} [0, u, 0]$
			$y, z, 0 [0, 0, u]$	$\bar{y}, z, 0 [0, 0, \bar{u}]$	$y, \bar{z}, 0 [0, 0, \bar{u}]$	$\bar{y}, \bar{z}, 0 [0, 0, u]$
			$y, 0, \bar{z} [0, \bar{u}, 0]$	$\bar{y}, 0, \bar{z} [0, u, 0]$	$y, 0, z [0, u, 0]$	$\bar{y}, 0, z [0, \bar{u}, 0]$
			$0, z, \bar{y} [\bar{u}, 0, 0]$	$0, z, y [u, 0, 0]$	$0, \bar{z}, \bar{y} [u, 0, 0]$	$0, \bar{z}, y [\bar{u}, 0, 0]$
			$z, y, 0 [0, 0, u]$	$z, \bar{y}, 0 [0, 0, \bar{u}]$	$\bar{z}, y, 0 [0, 0, \bar{u}]$	$\bar{z}, \bar{y}, 0 [0, 0, u]$
48	i	..2				
			$1/4, y, \bar{y} + 1/2 [0, \bar{v}, v]$	$3/4, \bar{y}, \bar{y} + 1/2 [0, v, v]$	$3/4, y, y + 1/2 [0, \bar{v}, \bar{v}]$	$1/4, \bar{y}, y + 1/2 [0, v, \bar{v}]$
			$\bar{y} + 1/2, 1/4, y [v, 0, \bar{v}]$	$\bar{y} + 1/2, 3/4, \bar{y} [v, 0, v]$	$y + 1/2, 3/4, y [\bar{v}, 0, \bar{v}]$	$y + 1/2, 1/4, \bar{y} [\bar{v}, 0, v]$
			$y, \bar{y} + 1/2, 1/4 [\bar{v}, v, 0]$	$\bar{y}, \bar{y} + 1/2, 3/4 [v, v, 0]$	$y, y + 1/2, 3/4 [\bar{v}, \bar{v}, 0]$	$\bar{y}, y + 1/2, 1/4 [v, \bar{v}, 0]$
			$3/4, \bar{y}, y + 1/2 [0, \bar{v}, v]$	$1/4, y, y + 1/2 [0, v, v]$	$1/4, \bar{y}, \bar{y} + 1/2 [0, \bar{v}, \bar{v}]$	$3/4, y, \bar{y} + 1/2 [0, v, \bar{v}]$
			$y + 1/2, 3/4, \bar{y} [v, 0, \bar{v}]$	$y + 1/2, 1/4, y [v, 0, v]$	$\bar{y} + 1/2, 1/4, \bar{y} [\bar{v}, 0, \bar{v}]$	$\bar{y} + 1/2, 3/4, y [\bar{v}, 0, v]$
			$\bar{y}, y + 1/2, 3/4 [\bar{v}, v, 0]$	$y, y + 1/2, 1/4 [v, v, 0]$	$\bar{y}, \bar{y} + 1/2, 1/4 [\bar{v}, \bar{v}, 0]$	$y, \bar{y} + 1/2, 3/4 [v, \bar{v}, 0]$
24	h	m.m'2'	$0, y, y [u, 0, 0]$	$0, \bar{y}, y [\bar{u}, 0, 0]$	$0, y, \bar{y} [\bar{u}, 0, 0]$	$0, \bar{y}, \bar{y} [u, 0, 0]$
			$y, 0, y [0, u, 0]$	$y, 0, \bar{y} [0, \bar{u}, 0]$	$\bar{y}, 0, y [0, \bar{u}, 0]$	$\bar{y}, 0, \bar{y} [0, u, 0]$
			$y, y, 0 [0, 0, u]$	$\bar{y}, y, 0 [0, 0, \bar{u}]$	$y, \bar{y}, 0 [0, 0, \bar{u}]$	$\bar{y}, \bar{y}, 0 [0, 0, u]$
24	g	mm2..	$x, 0, 1/2 [0, 0, 0]$	$\bar{x}, 0, 1/2 [0, 0, 0]$	$1/2, x, 0 [0, 0, 0]$	$1/2, \bar{x}, 0 [0, 0, 0]$
			$0, 1/2, x [0, 0, 0]$	$0, 1/2, \bar{x} [0, 0, 0]$	$0, x, 1/2 [0, 0, 0]$	$0, \bar{x}, 1/2 [0, 0, 0]$
			$x, 1/2, 0 [0, 0, 0]$	$\bar{x}, 1/2, 0 [0, 0, 0]$	$1/2, 0, \bar{x} [0, 0, 0]$	$1/2, 0, x [0, 0, 0]$
16	f	.3m'	$x, x, x [u, u, u]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$	$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
			$x, x, \bar{x} [\bar{u}, \bar{u}, u]$	$\bar{x}, \bar{x}, \bar{x} [u, u, u]$	$x, \bar{x}, x [\bar{u}, u, \bar{u}]$	$\bar{x}, x, x [u, \bar{u}, \bar{u}]$
12	e	4'm.m'	$x, 0, 0 [0, 0, 0]$	$\bar{x}, 0, 0 [0, 0, 0]$		$0, x, 0 [0, 0, 0]$
			$0, \bar{x}, 0 [0, 0, 0]$	$0, 0, x [0, 0, 0]$		$0, 0, \bar{x} [0, 0, 0]$
12	d	$\bar{4}m.2$	$1/4, 0, 1/2 [0, 0, 0]$	$3/4, 0, 1/2 [0, 0, 0]$		$1/2, 1/4, 0 [0, 0, 0]$
			$1/2, 3/4, 0 [0, 0, 0]$	$0, 1/2, 1/4 [0, 0, 0]$		$0, 1/2, 3/4 [0, 0, 0]$
8	c	. $\bar{3}$ 'm'	$1/4, 1/4, 1/4 [0, 0, 0]$	$3/4, 3/4, 1/4 [0, 0, 0]$	$3/4, 1/4, 3/4 [0, 0, 0]$	$1/4, 3/4, 3/4 [0, 0, 0]$
6	b	4'/mm.m'	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$		$1/2, 1/2, 0 [0, 0, 0]$
2	a	$m\bar{3}m'$	$0, 0, 0 [0, 0, 0]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
 Origin at  $0,0,z$

Along  $[1,1,1]$   $p6mm1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x,x,x$

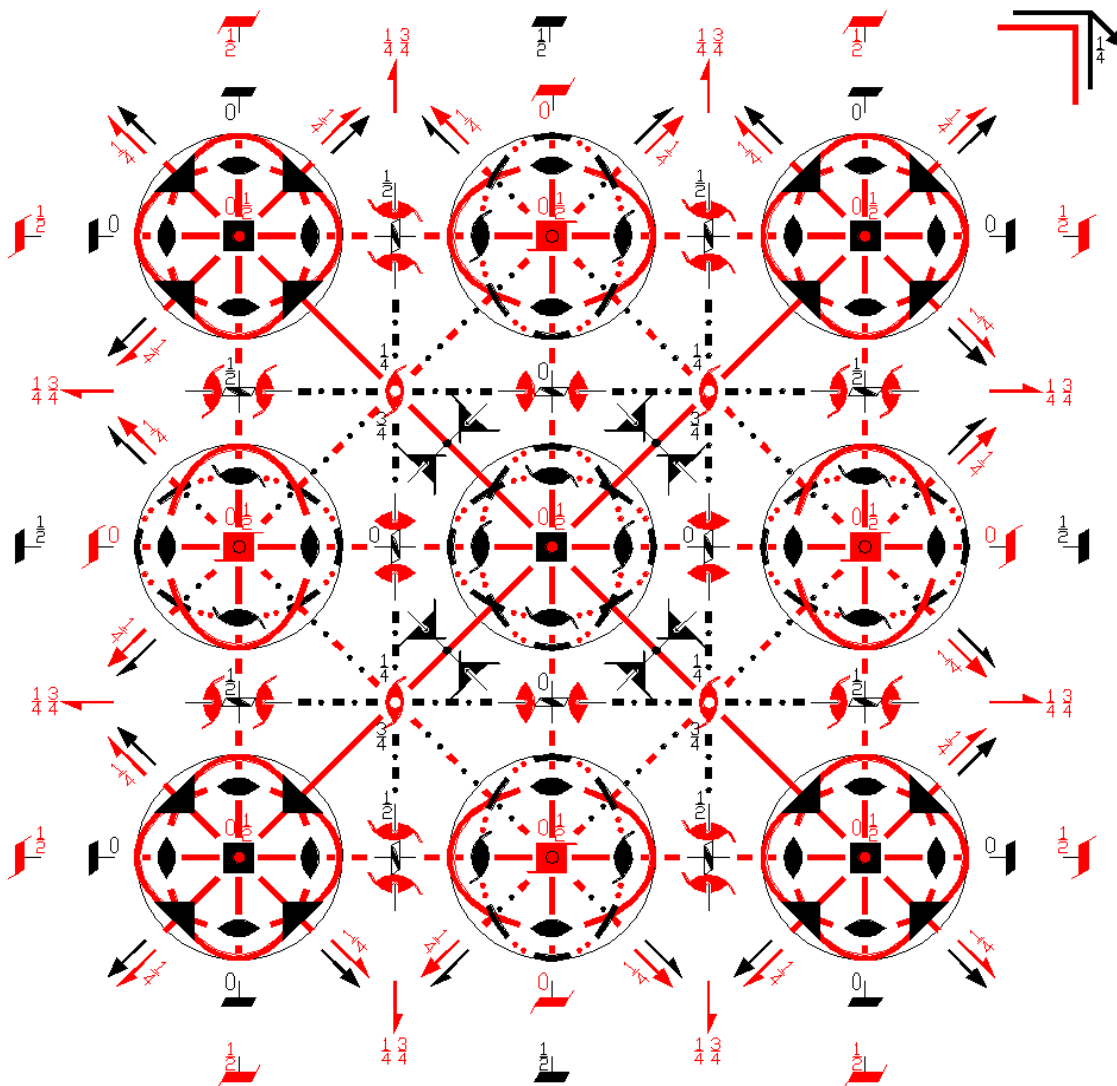
Along  $[1,1,0]$   $p_{2a} 2m'm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x,x,1/4$



$I_p m' \bar{3}' m'$   
229.9.1646

$m \bar{3} m 1'$   
 $I_p 4/m' \bar{3}' 2/m'$

Cubic



**Origin** at center ( $m' \bar{3}' m'$ )

**Asymmetric unit**  $0 \leq x \leq 1/2;$   $0 \leq y \leq 1/2;$   $0 \leq z \leq 1/4;$   $y \leq x;$   $z \leq \min(1/2-x, y)$   
**Vertices**  $0,0,0$   $1/2,0,0$   $1/2,1/2,0$   $1/4,1/4,1/4$

**Symmetry Operations**

For  $(0,0,0)$  + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)   | (4) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                         | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub><math>\bar{x}yz^{-1}</math></sub>  0,0,0) | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)    | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)      | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$<br>(3 <sub><math>\bar{x}yz</math></sub>  0,0,0)     |



(13) $2 \ x, x, 0$ ( $2_{xy}   0, 0, 0$ )	(14) $2 \ x, \bar{x}, 0$ ( $2_{\bar{xy}}   0, 0, 0$ )	(15) $4^- \ 0, 0, z$ ( $4_z^{-1}   0, 0, 0$ )	(16) $4^+ \ 0, 0, z$ ( $4_z   0, 0, 0$ )
(17) $4^- \ x, 0, 0$ ( $4_x^{-1}   0, 0, 0$ )	(18) $2 \ 0, y, y$ ( $2_{yz}   0, 0, 0$ )	(19) $2 \ 0, y, \bar{y}$ ( $2_{\bar{yz}}   0, 0, 0$ )	(20) $4^+ \ x, 0, 0$ ( $4_x   0, 0, 0$ )
(21) $4^+ \ 0, y, 0$ ( $4_y   0, 0, 0$ )	(22) $2 \ x, 0, x$ ( $2_{xz}   0, 0, 0$ )	(23) $4^- \ 0, y, 0$ ( $4_y^{-1}   0, 0, 0$ )	(24) $2 \ \bar{x}, 0, x$ ( $2_{\bar{xz}}   0, 0, 0$ )
(25) $\bar{1} \ 0, 0, 0$ ( $\bar{1}   0, 0, 0$ )'	(26) $m' \ x, y, 0$ ( $m_z   0, 0, 0$ )'	(27) $m' \ x, 0, z$ ( $m_y   0, 0, 0$ )'	(28) $m' \ 0, y, z$ ( $m_x   0, 0, 0$ )'
(29) $\bar{3}^+ \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}   0, 0, 0$ )'	(30) $\bar{3}^+ \ \bar{x}, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}^{-1}   0, 0, 0$ )'	(31) $\bar{3}^+ \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}^{-1}   0, 0, 0$ )'	(32) $\bar{3}^+ \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}^{-1}   0, 0, 0$ )'
(33) $\bar{3}^- \ x, x, x; 0, 0, 0$ ( $\bar{3}_{xyz}^{-1}   0, 0, 0$ )'	(34) $\bar{3}^- \ x, \bar{x}, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}   0, 0, 0$ )'	(35) $\bar{3}^- \ \bar{x}, \bar{x}, x; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}   0, 0, 0$ )'	(36) $\bar{3}^- \ \bar{x}, x, \bar{x}; 0, 0, 0$ ( $\bar{3}_{\bar{xyz}}   0, 0, 0$ )'
(37) $m' \ x, \bar{x}, z$ ( $m_{xy}   0, 0, 0$ )'	(38) $m' \ x, x, z$ ( $m_{\bar{xy}}   0, 0, 0$ )'	(39) $\bar{4}^- \ 0, 0, z; 0, 0, 0$ ( $\bar{4}_z^{-1}   0, 0, 0$ )'	(40) $\bar{4}^+ \ 0, 0, z; 0, 0, 0$ ( $\bar{4}_z   0, 0, 0$ )'
(41) $\bar{4}^- \ x, 0, 0; 0, 0, 0$ ( $\bar{4}_x^{-1}   0, 0, 0$ )'	(42) $m' \ x, y, \bar{y}$ ( $m_{yz}   0, 0, 0$ )'	(43) $m' \ x, y, y$ ( $m_{\bar{yz}}   0, 0, 0$ )'	(44) $\bar{4}^+ \ x, 0, 0; 0, 0, 0$ ( $\bar{4}_x   0, 0, 0$ )'
(45) $\bar{4}^+ \ 0, y, 0; 0, 0, 0$ ( $\bar{4}_y   0, 0, 0$ )'	(46) $m' \ \bar{x}, y, x$ ( $m_{xz}   0, 0, 0$ )'	(47) $\bar{4}^- \ 0, y, 0; 0, 0, 0$ ( $\bar{4}_y^{-1}   0, 0, 0$ )'	(48) $m' \ x, y, x$ ( $m_{\bar{xz}}   0, 0, 0$ )'

For  $(1/2, 1/2, 1/2)'$  + set

(1) $t' \ (1/2, 1/2, 1/2)$ ( $1   1/2, 1/2, 1/2$ )'	(2) $2' \ (0, 0, 1/2) \ 1/4, 1/4, z$ ( $2_z   1/2, 1/2, 1/2$ )'	(3) $2' \ (0, 1/2, 0) \ 1/4, y, 1/4$ ( $2_y   1/2, 1/2, 1/2$ )'	(4) $2' \ (1/2, 0, 0) \ x, 1/4, 1/4$ ( $2_x   1/2, 1/2, 1/2$ )'
(5) $3^+ \ (1/2, 1/2, 1/2) \ x, x, x$ ( $3_{xyz}   1/2, 1/2, 1/2$ )'	(6) $3^+ \ (1/6, -1/6, 1/6) \ \bar{x} + 1/3, \bar{x} + 1/3, \bar{x}$ ( $3_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2$ )'	(7) $3^+ \ (-1/6, 1/6, 1/6) \ x + 2/3, x - 1/3, x$ ( $3_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2$ )'	(8) $3^+ \ (1/6, 1/6, -1/6) \ \bar{x} + 1/3, \bar{x} + 2/3, \bar{x}$ ( $3_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2$ )'
(9) $3^- \ (1/2, 1/2, 1/2) \ x, x, x$ ( $3_{xyz}^{-1}   1/2, 1/2, 1/2$ )'	(10) $3^- \ (-1/6, 1/6, 1/6) \ \bar{x} + 1/3, \bar{x} + 1/3, \bar{x}$ ( $3_{\bar{xyz}}   1/2, 1/2, 1/2$ )'	(11) $3^- \ (1/6, 1/6, -1/6) \ x + 2/3, x + 1/3, x$ ( $3_{\bar{xyz}}   1/2, 1/2, 1/2$ )'	(12) $3^- \ (1/6, -1/6, 1/6) \ \bar{x} - 1/3, \bar{x} + 2/3, \bar{x}$ ( $3_{\bar{xyz}}   1/2, 1/2, 1/2$ )'
(13) $2' \ (1/2, 1/2, 0) \ x, x, 1/4$ ( $2_{xy}   1/2, 1/2, 1/2$ )'	(14) $2' \ x, \bar{x} + 1/2, 1/4$ ( $2_{\bar{xy}}   1/2, 1/2, 1/2$ )'	(15) $4^- \ (0, 0, 1/2) \ 1/2, 0, z$ ( $4_z^{-1}   1/2, 1/2, 1/2$ )'	(16) $4^+ \ (0, 0, 1/2) \ 0, 1/2, z$ ( $4_z   1/2, 1/2, 1/2$ )'
(17) $4^- \ (1/2, 0, 0) \ x, 1/2, 0$ ( $4_x^{-1}   1/2, 1/2, 1/2$ )'	(18) $2' \ (0, 1/2, 1/2) \ 1/4, y, y$ ( $2_{yz}   1/2, 1/2, 1/2$ )'	(19) $2' \ 1/4, y + 1/2, \bar{y}$ ( $2_{\bar{yz}}   1/2, 1/2, 1/2$ )'	(20) $4^+ \ (1/2, 0, 0) \ x, 0, 1/2$ ( $4_x   1/2, 1/2, 1/2$ )'
(21) $4^+ \ (0, 1/2, 0) \ 1/2, y, 0$ ( $4_y   1/2, 1/2, 1/2$ )'	(22) $2' \ (1/2, 0, 1/2) \ x, 1/4, x$ ( $2_{xz}   1/2, 1/2, 1/2$ )'	(23) $4^- \ (0, 1/2, 0) \ 0, y, 1/2$ ( $4_y^{-1}   1/2, 1/2, 1/2$ )'	(24) $2' \ \bar{x} + 1/2, 1/4, x$ ( $2_{\bar{xz}}   1/2, 1/2, 1/2$ )'
(25) $\bar{1} \ 1/4, 1/4, 1/4$ ( $\bar{1}   1/2, 1/2, 1/2$ )	(26) $n \ (1/2, 1/2, 0) \ x, y, 1/4$ ( $m_z   1/2, 1/2, 1/2$ )	(27) $n \ (1/2, 0, 1/2) \ x, 1/4, z$ ( $m_y   1/2, 1/2, 1/2$ )	(28) $n \ (0, 1/2, 1/2) \ 1/4, y, z$ ( $m_x   1/2, 1/2, 1/2$ )
(29) $\bar{3}^+ \ x, x, x; 1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 1/2, 1/2$ )	(30) $\bar{3}^+ \ \bar{x} - 1, \bar{x} + 1, \bar{x}; -1/4, 1/4, 3/4$ ( $\bar{3}_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2$ )	(31) $\bar{3}^+ \ x, \bar{x} + 1, \bar{x}; 1/4, 3/4, -1/4$ ( $\bar{3}_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2$ )	(32) $\bar{3}^+ \ \bar{x} + 1, \bar{x}, x; 3/4, -1/4, 1/4$ ( $\bar{3}_{\bar{xyz}}^{-1}   1/2, 1/2, 1/2$ )

(33) $\bar{3}^-$ $x, x, x;$ 1/4, 1/4, 1/4 ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(34) $\bar{3}^-$ $x+1, \bar{x}-1, \bar{x};$ 1/4, -1/4, 3/4 ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(35) $\bar{3}^-$ $\bar{x}, \bar{x}+1, x;$ -1/4, 3/4, 1/4 ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(36) $\bar{3}^-$ $\bar{x}+1, x, \bar{x};$ 3/4, 1/4, -1/4 ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2$ )
(37) c (0, 0, 1/2) $x+1/2, \bar{x}, z$ ( $m_{xy}   1/2, 1/2, 1/2$ )	(38) n (1/2, 1/2, 1/2) $x, x, z$ ( $m_{xy}   1/2, 1/2, 1/2$ )	(39) $\bar{4}^-$ 0, 1/2, z; 0, 1/2, 1/4 ( $\bar{4}_z^{-1}   1/2, 1/2, 1/2$ )	(40) $\bar{4}^+$ 1/2, 0, z; 1/2, 0, 1/4 ( $\bar{4}_z   1/2, 1/2, 1/2$ )
(41) $\bar{4}^-$ $x, 0, 1/2; 1/4, 0, 1/2$ ( $\bar{4}_x^{-1}   1/2, 1/2, 1/2$ )	(42) a (1/2, 0, 0) $x, y+1/2, \bar{y}$ ( $m_{yz}   1/2, 1/2, 1/2$ )	(43) n (1/2, 1/2, 1/2) $x, y, y$ ( $m_{yz}   1/2, 1/2, 1/2$ )	(44) $\bar{4}^+$ $x, 1/2, 0; 1/4, 1/2, 0$ ( $\bar{4}_x   1/2, 1/2, 1/2$ )
(45) $\bar{4}^+$ 0, y, 1/2; 0, 1/4, 1/2 ( $\bar{4}_y   1/2, 1/2, 1/2$ )	(46) b (0, 1/2, 0) $\bar{x}+1/2, y, x$ ( $m_{xz}   1/2, 1/2, 1/2$ )	(47) $\bar{4}^-$ 1/2, y, 0; 1/2, 1/4, 0 ( $\bar{4}_y^{-1}   1/2, 1/2, 1/2$ )	(48) n (1/2, 1/2, 1/2) $x, y, x$ ( $m_{xz}   1/2, 1/2, 1/2$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13); (25).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

## Coordinates

		(0,0,0) +		(1/2,1/2,1/2)' +	
96	l	1			
(1)	$x, y, z$	[u, v, w]	(2)	$\bar{x}, \bar{y}, z$	[ $\bar{u}, \bar{v}, w$ ]
(5)	$z, x, y$	[w, u, v]	(6)	$z, \bar{x}, \bar{y}$	[w, $\bar{u}, \bar{v}$ ]
(9)	$y, z, x$	[v, w, u]	(10)	$\bar{y}, z, \bar{x}$	[ $\bar{v}, w, \bar{u}$ ]
(13)	$y, x, \bar{z}$	[v, u, $\bar{w}$ ]	(14)	$\bar{y}, \bar{x}, \bar{z}$	[ $\bar{v}, \bar{u}, \bar{w}$ ]
(17)	$x, z, \bar{y}$	[u, w, $\bar{v}$ ]	(18)	$\bar{x}, z, y$	[ $\bar{u}, w, v$ ]
(21)	$z, y, \bar{x}$	[w, v, $\bar{u}$ ]	(22)	$z, \bar{y}, x$	[w, $\bar{v}, u$ ]
(25)	$\bar{x}, \bar{y}, \bar{z}$	[ $\bar{u}, \bar{v}, \bar{w}$ ]	(26)	$x, y, \bar{z}$	[u, v, $\bar{w}$ ]
(29)	$\bar{z}, \bar{x}, \bar{y}$	[ $\bar{w}, \bar{u}, \bar{v}$ ]	(30)	$\bar{z}, x, y$	[ $\bar{w}, u, v$ ]
(33)	$\bar{y}, \bar{z}, \bar{x}$	[ $\bar{v}, \bar{w}, \bar{u}$ ]	(34)	$y, \bar{z}, x$	[v, $\bar{w}, u$ ]
(37)	$\bar{y}, \bar{x}, z$	[ $\bar{v}, \bar{u}, w$ ]	(38)	$y, x, z$	[v, u, w]
(41)	$\bar{x}, \bar{z}, y$	[ $\bar{u}, \bar{w}, v$ ]	(42)	$x, \bar{z}, y$	[u, $\bar{w}, v$ ]
(45)	$\bar{z}, \bar{y}, x$	[ $\bar{w}, \bar{v}, u$ ]	(46)	$\bar{z}, y, \bar{x}$	[ $\bar{w}, v, \bar{u}$ ]
48	k	..m'	$x, x, z$	[u, u, w]	$\bar{x}, \bar{x}, z$
			$z, x, x$	[w, u, u]	$\bar{z}, \bar{x}, x$
			$x, z, x$	[u, w, u]	$\bar{x}, \bar{z}, x$
			$x, x, \bar{z}$	[u, u, $\bar{w}$ ]	$\bar{x}, \bar{x}, z$
			$x, z, \bar{x}$	[u, w, $\bar{u}$ ]	$\bar{x}, \bar{z}, x$

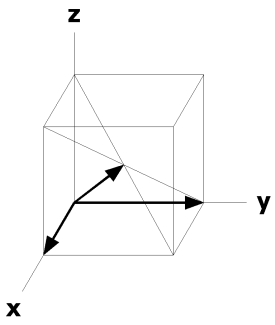
			$z, x, \bar{x} [w, u, \bar{u}]$	$z, \bar{x}, x [w, \bar{u}, u]$	$\bar{z}, x, x [\bar{w}, u, u]$	$\bar{z}, \bar{x}, \bar{x} [\bar{w}, \bar{u}, \bar{u}]$
48	j	$m'..$	$0, y, z [0, v, w]$	$0, \bar{y}, z [0, \bar{v}, w]$	$0, y, \bar{z} [0, v, \bar{w}]$	$0, \bar{y}, \bar{z} [0, \bar{v}, \bar{w}]$
			$z, 0, y [w, 0, v]$	$z, 0, \bar{y} [w, 0, \bar{v}]$	$\bar{z}, 0, y [\bar{w}, 0, v]$	$\bar{z}, 0, \bar{y} [\bar{w}, 0, \bar{v}]$
			$y, z, 0 [v, w, 0]$	$\bar{y}, z, 0 [\bar{v}, w, 0]$	$y, \bar{z}, 0 [v, \bar{w}, 0]$	$\bar{y}, \bar{z}, 0 [\bar{v}, \bar{w}, 0]$
			$y, 0, \bar{z} [v, 0, \bar{w}]$	$\bar{y}, 0, \bar{z} [\bar{v}, 0, \bar{w}]$	$y, 0, z [v, 0, w]$	$\bar{y}, 0, z [\bar{v}, 0, w]$
			$0, z, \bar{y} [0, w, \bar{v}]$	$0, z, y [0, w, v]$	$0, \bar{z}, \bar{y} [0, \bar{w}, \bar{v}]$	$0, \bar{z}, y [0, \bar{w}, v]$
			$z, y, 0 [w, v, 0]$	$z, \bar{y}, 0 [w, \bar{v}, 0]$	$\bar{z}, y, 0 [\bar{w}, v, 0]$	$\bar{z}, \bar{y}, 0 [\bar{w}, \bar{v}, 0]$
48	i	$..2'$				
			$1/4, y, \bar{y} + 1/2 [u, v, v]$	$3/4, \bar{y}, \bar{y} + 1/2 [\bar{u}, \bar{v}, v]$	$3/4, y, y + 1/2 [u, v, \bar{v}]$	$1/4, \bar{y}, y + 1/2 [u, \bar{v}, \bar{v}]$
			$\bar{y} + 1/2, 1/4, y [v, u, v]$	$\bar{y} + 1/2, 3/4, \bar{y} [v, \bar{u}, \bar{v}]$	$y + 1/2, 3/4, y [v, \bar{u}, v]$	$y + 1/2, 1/4, \bar{y} [v, u, \bar{v}]$
			$y, \bar{y} + 1/2, 1/4 [v, v, u]$	$\bar{y}, \bar{y} + 1/2, 3/4 [v, v, \bar{u}]$	$y, y + 1/2, 3/4 [v, \bar{v}, \bar{u}]$	$\bar{y}, y + 1/2, 1/4 [v, \bar{v}, u]$
			$3/4, \bar{y}, y + 1/2 [\bar{u}, \bar{v}, \bar{v}]$	$1/4, y, y + 1/2 [u, v, \bar{v}]$	$1/4, \bar{y}, \bar{y} + 1/2 [u, \bar{v}, v]$	$3/4, y, \bar{y} + 1/2 [\bar{u}, v, v]$
			$y + 1/2, 3/4, \bar{y} [v, \bar{u}, \bar{v}]$	$y + 1/2, 1/4, y [v, u, v]$	$\bar{y} + 1/2, 1/4, \bar{y} [v, u, \bar{v}]$	$\bar{y} + 1/2, 3/4, y [v, \bar{u}, v]$
			$\bar{y}, y + 1/2, 3/4 [v, \bar{v}, \bar{u}]$	$y, y + 1/2, 1/4 [v, \bar{v}, u]$	$\bar{y}, \bar{y} + 1/2, 1/4 [v, v, u]$	$y, \bar{y} + 1/2, 3/4 [v, v, \bar{u}]$
24	h	$m'.m'2$	$0, y, y [0, v, v]$	$0, \bar{y}, y [0, \bar{v}, v]$	$0, y, \bar{y} [0, v, \bar{v}]$	$0, \bar{y}, \bar{y} [0, \bar{v}, \bar{v}]$
			$y, 0, y [v, 0, v]$	$y, 0, \bar{y} [v, 0, \bar{v}]$	$\bar{y}, 0, y [v, 0, v]$	$\bar{y}, 0, \bar{y} [v, 0, \bar{v}]$
			$y, y, 0 [v, v, 0]$	$\bar{y}, y, 0 [v, v, 0]$	$y, \bar{y}, 0 [v, \bar{v}, 0]$	$\bar{y}, \bar{y}, 0 [v, \bar{v}, 0]$
24	g	$m'm'2..$	$x, 0, 1/2 [u, 0, 0]$	$\bar{x}, 0, 1/2 [\bar{u}, 0, 0]$	$1/2, x, 0 [0, u, 0]$	$1/2, \bar{x}, 0 [0, \bar{u}, 0]$
			$0, 1/2, x [0, 0, u]$	$0, 1/2, \bar{x} [0, 0, \bar{u}]$	$0, x, 1/2 [0, u, 0]$	$0, \bar{x}, 1/2 [0, \bar{u}, 0]$
			$x, 1/2, 0 [u, 0, 0]$	$\bar{x}, 1/2, 0 [\bar{u}, 0, 0]$	$1/2, 0, \bar{x} [0, 0, \bar{u}]$	$1/2, 0, x [0, 0, u]$
16	f	$.3m'$	$x, x, x [u, u, u]$	$\bar{x}, \bar{x}, x [\bar{u}, \bar{u}, u]$	$\bar{x}, x, \bar{x} [\bar{u}, u, \bar{u}]$	$x, \bar{x}, \bar{x} [u, \bar{u}, \bar{u}]$
			$x, x, \bar{x} [u, u, \bar{u}]$	$\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$	$x, \bar{x}, x [u, \bar{u}, u]$	$\bar{x}, x, x [\bar{u}, u, \bar{u}]$
12	e	$4m'.m'$	$x, 0, 0 [u, 0, 0]$	$\bar{x}, 0, 0 [\bar{u}, 0, 0]$		$0, x, 0 [0, u, 0]$
			$0, \bar{x}, 0 [0, \bar{u}, 0]$	$0, 0, x [0, 0, u]$		$0, 0, \bar{x} [0, 0, \bar{u}]$
12	d	$\bar{4}m'.2'$	$1/4, 0, 1/2 [u, 0, 0]$	$3/4, 0, 1/2 [\bar{u}, 0, 0]$		$1/2, 1/4, 0 [0, u, 0]$
			$1/2, 3/4, 0 [0, \bar{u}, 0]$	$0, 1/2, 1/4 [0, 0, u]$		$0, 1/2, 3/4 [0, 0, \bar{u}]$
8	c	$.3m'$	$1/4, 1/4, 1/4 [u, u, u]$	$3/4, 3/4, 1/4 [\bar{u}, \bar{u}, u]$	$3/4, 1/4, 3/4 [\bar{u}, u, \bar{u}]$	$1/4, 3/4, 3/4 [u, \bar{u}, \bar{u}]$
6	b	$4/m'm'.m'$	$0, 1/2, 1/2 [0, 0, 0]$	$1/2, 0, 1/2 [0, 0, 0]$		$1/2, 1/2, 0 [0, 0, 0]$
2	a	$m'\bar{3}'m'$	$0, 0, 0 [0, 0, 0]$			

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4mm1'$   
 $\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2$   $\mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$   
Origin at  $0,0,z$

Along  $[1,1,1]$   $p6mm1'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
Origin at  $x,x,x$

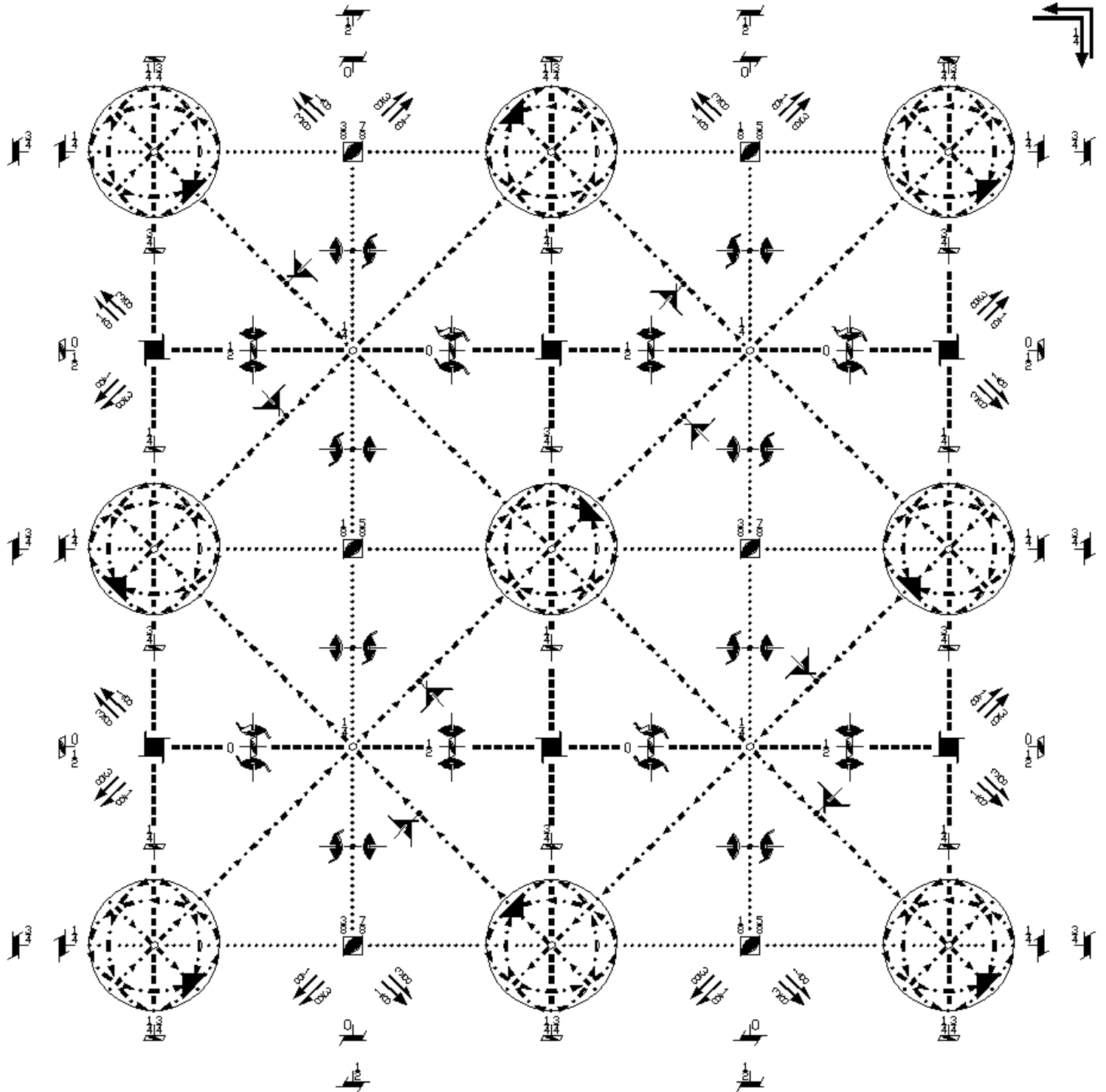
Along  $[1,1,0]$   $p2mm1'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
Origin at  $x,x,0$



$la\bar{3}d$   
230.1.1647

$m\bar{3}m$   
 $I4_1/a\bar{3}2/d$

Cubic



Origin at center ( $\bar{3}$ )

**Asymmetric unit**  $-1/8 \leq x \leq 1/8$ ;  $-1/8 \leq y \leq 1/8$ ;  $0 \leq z \leq 1/4$ ;  $\max(x, -x, y, -y) \leq z$

Vertices  $0,0,0$   $1/8, 1/8, 1/8$   $-1/8, 1/8, 1/8$   $-1/8, -1/8, 1/8$   $1/8, -1/8, 1/8$   
 $1/8, 1/8, 1/4$   $-1/8, 1/8, 1/4$   $-1/8, -1/8, 1/4$   $1/8, -1/8, 1/4$

## Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)                                  | (6) 3 <sup>+</sup> $\bar{x}+1/2, x, \bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,1/2,0)                         | (7) 3 <sup>+</sup> $x+1/2, \bar{x}-1/2, \bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,0,1/2)                       | (8) 3 <sup>+</sup> $\bar{x}, \bar{x}+1/2, x$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,1/2,1/2)                         |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)                                  | (10) 3 <sup>-</sup> (-1/3,1/3,1/3)<br>x+1/6, x+1/6, $\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub>  0,1/2,1/2)                      | (11) 3 <sup>-</sup> (1/3,1/3,-1/3)<br>x+1/3, x+1/6, x<br>(3 <sub>x<math>\bar{y}z</math></sub>  1/2,1/2,0)                                | (12) 3 <sup>-</sup> (1/3,-1/3,1/3)<br>x-1/6, x+1/3, $\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub>  1/2,0,1/2)                      |
| (13) 2 (1/2,1/2,0) x,x-1/4,1/8<br>(2 <sub>xy</sub>  3/4,1/4,1/4)                                     | (14) 2 x, $\bar{x}+3/4, 3/8$<br>(2 <sub>xy</sub>  3/4,3/4,3/4)   | (15) 4 <sup>-</sup> (0,0,3/4) 1/4,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/4,1/4,3/4)   | (16) 4 <sup>+</sup> (0,0,1/4) -1/4,1/2,z<br>(4 <sub>z</sub>  1/4,3/4,1/4)  |
| (17) 4 <sup>-</sup> (3/4,0,0) x,1/4,0<br>(4 <sub>x</sub> <sup>-1</sup>  3/4,1/4,1/4)                 | (18) 2 (0,1/2,1/2) 1/8,y+1/4,y<br>(2 <sub>yz</sub>  1/4,3/4,1/4)   | (19) 2 3/8,y+3/4, $\bar{y}$<br>(2 <sub>yz</sub>  3/4,3/4,3/4)  | (20) 4 <sup>+</sup> (1/4,0,0) x,-1/4,1/2<br>(4 <sub>x</sub>  1/4,1/4,3/4)  |
| (21) 4 <sup>+</sup> (0,1/4,0) 1/2,y,-1/4<br>(4 <sub>y</sub>  3/4,1/4,1/4)                            | (22) 2 (1/2,0,1/2) x-1/4,1/8,x<br>(2 <sub>xz</sub>  1/4,1/4,3/4)   | (23) 4 <sup>-</sup> (0,3/4,0) 0,y,1/4<br>(4 <sub>y</sub> <sup>-1</sup>  1/4,3/4,1/4)   | (24) 2 $\bar{x}+3/4, 3/8, x$<br>(2 <sub>xz</sub>  3/4,3/4,3/4)   |
| (25) $\bar{1}$ 0,0,0<br>(1 0,0,0)  | (26) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)  | (27) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)  | (28) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)  |
| (29) $\bar{3}^+$ x,x,x; 0,0,0<br>( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>  0,0,0)                    | (30) $\bar{3}^+$ $\bar{x}-1/2, x+1, \bar{x}$ ;<br>0,1/2,1/2<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,1/2,0) | (31) $\bar{3}^+$ $x+1/2, \bar{x}+1/2, \bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,0,1/2) | (32) $\bar{3}^+$ $\bar{x}+1, \bar{x}+1/2, x$ ;<br>1/2,0,1/2<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,1/2,1/2) |
| (33) $\bar{3}^-$ x,x,x; 0,0,0<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,0) | (34) $\bar{3}^-$ $x+1/2, \bar{x}-1/2, \bar{x}$ ; 0,0,1/2<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub>  0,1/2,1/2)                  | (35) $\bar{3}^-$ $\bar{x}, \bar{x}+1/2, x$ ; 0,1/2,0<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub>  1/2,1/2,0)                        | (36) $\bar{3}^-$ $\bar{x}+1/2, x, \bar{x}$ ; 1/2,0,0<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub>  1/2,0,1/2)                      |
| (37) d (-1/4,1/4,1/4) x+1/2, $\bar{x}, z$<br>(m <sub>xy</sub>  1/4,3/4,3/4)                          | (38) d (1/4,1/4,1/4) x,x,z<br>(m <sub>xy</sub>  1/4,1/4,1/4)   | (39) $\bar{4}^-$ 0,3/4,z; 0,3/4,1/8<br>( $\bar{4}$ <sub>z</sub> <sup>-1</sup>  3/4,3/4,1/4)  | (40) $\bar{4}^+$ 1/2,-1/4,z; 1/2,-1/4,3/8<br>( $\bar{4}$ <sub>z</sub>  3/4,1/4,3/4)  |
| (41) $\bar{4}^-$ x,0,3/4; 1/8,0,3/4<br>( $\bar{4}$ <sub>x</sub> <sup>-1</sup>  1/4,3/4,3/4)          | (42) d (3/4,-1/4,1/4) x,y+1/2, $\bar{y}$<br>(m <sub>yz</sub>  3/4,1/4,3/4)   | (43) d (1/4,1/4,1/4) x,y,y<br>(m <sub>yz</sub>  1/4,1/4,1/4)   | (44) $\bar{4}^+$ x,1/2,-1/4; 3/8,1/2,-1/4<br>( $\bar{4}$ <sub>x</sub>  3/4,3/4,1/4)  |
| (45) $\bar{4}^+$ -1/4,y,1/2; -1/4,3/8,1/2<br>( $\bar{4}$ <sub>y</sub>  1/4,3/4,3/4)                  | (46) d (1/4,3/4,-1/4) $\bar{x}+1/2, y, x$<br>(m <sub>xz</sub>  3/4,3/4,1/4)  | (47) $\bar{4}^-$ 3/4,y,0; 3/4,1/8,0<br>( $\bar{4}$ <sub>y</sub> <sup>-1</sup>  3/4,1/4,3/4)  | (48) d (1/4,1/4,1/4) x,y,x<br>(m <sub>xz</sub>  1/4,1/4,1/4)   |

For (1/2,1/2,1/2) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                                    | (2) 2 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,0)   | (3) 2 1/4,y,0<br>(2 <sub>y</sub>  1/2,0,0)   | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)   |
| (5) 3 <sup>+</sup> (1/2,1/2,1/2) x,x,x<br>(3 <sub>xyz</sub>  1/2,1/2,1/2) | (6) 3 <sup>+</sup> (1/6,-1/6,1/6)<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,1/2) | (7) 3 <sup>+</sup> (-1/6,1/6,1/6)<br>x+1/6, x+1/6, $\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,1/2,0) | (8) 3 <sup>+</sup> (1/6,1/6,-1/6)<br>$\bar{x}+1/3, \bar{x}+1/6, x$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,0,0) |

(9) $3^- (1/2, 1/2, 1/2) \ x, x, x$ ( $3_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(10) $3^- (1/6, -1/6, -1/6) \ \bar{x}$ $x+1/6, x+1/6, \bar{x}$ ( $3_{xyz}   1/2, 0, 0$ )	(11) $3^- (-1/6, -1/6, 1/6)$ $x+1/3, x+1/6, x$ ( $3_{xyz}   0, 0, 1/2$ )	(12) $3^- (-1/6, 1/6, -1/6) \ \bar{x}$ $x-1/6, x+1/3, \bar{x}$ ( $3_{xyz}   0, 1/2, 0$ )
(13) $2 (1/2, 1/2, 0) \ x, x+1/4, 3/8$ ( $2_{xy}   1/4, 3/4, 3/4$ )	(14) $2 \ x, \bar{x}+1/4, 1/8$ ( $2_{xy}   1/4, 1/4, 1/4$ )	(15) $4^- (0, 0, 1/4) \ 3/4, 0, z$ ( $4_z^{-1}   3/4, 3/4, 1/4$ )	(16) $4^+ (0, 0, 3/4) \ 1/4, 1/2, z$ ( $4_z   3/4, 1/4, 3/4$ )
(17) $4^- (1/4, 0, 0) \ x, 3/4, 0$ ( $4_x^{-1}   1/4, 3/4, 3/4$ )	(18) $2 (0, 1/2, 1/2) \ 3/8, y-1/4, y$ ( $2_{yz}   3/4, 1/4, 3/4$ )	(19) $2 \ 1/8, y+1/4, \bar{y}$ ( $2_{yz}   1/4, 1/4, 1/4$ )	(20) $4^+ (3/4, 0, 0) \ x, 1/4, 1/2$ ( $4_x   3/4, 3/4, 1/4$ )
(21) $4^+ (0, 3/4, 0) \ 1/2, y, 1/4$ ( $4_y   1/4, 3/4, 3/4$ )	(22) $2 (1/2, 0, 1/2) \ x+1/4, 3/8, x$ ( $2_{xz}   3/4, 3/4, 1/4$ )	(23) $4^- (0, 1/2, 0) \ 0, y, 3/4$ ( $4_y^{-1}   3/4, 1/4, 3/4$ )	(24) $2 \ \bar{x}+1/4, 1/8, x$ ( $2_{xz}   1/4, 1/4, 1/4$ )
(25) $\bar{1} \ 1/4, 1/4, 1/4$ ( $\bar{1}   1/2, 1/2, 1/2$ )	(26) $b (0, 1/2, 0) \ x, y, 0$ ( $m_z   0, 1/2, 0$ )	(27) $a (1/2, 0, 0) \ x, 0, z$ ( $m_y   1/2, 0, 0$ )	(28) $c (0, 0, 1/2) \ 0, y, z$ ( $m_x   0, 0, 1/2$ )
(29) $\bar{3}^+ \ x, x, x;$ $1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 1/2, 1/2$ )	(30) $\bar{3}^+ \ \bar{x}-1/2, x, \bar{x};$ $-1/4, -1/4, 1/4$ ( $\bar{3}_{xyz}^{-1}   0, 0, 1/2$ )	(31) $\bar{3}^+ \ x-1/2, \bar{x}+1/2, \bar{x};$ $-1/4, 1/4, -1/4$ ( $\bar{3}_{xyz}^{-1}   0, 1/2, 0$ )	(32) $\bar{3}^+ \ \bar{x}, \bar{x}-1/2, x;$ $1/4, -1/4, -1/4$ ( $\bar{3}_{xyz}^{-1}   1/2, 0, 0$ )
(33) $\bar{3}^- \ x, x, x;$ $1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(34) $\bar{3}^- \ x+1/2, \bar{x}-1/2, \bar{x};$ $1/4, -1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 0, 0$ )	(35) $\bar{3}^- \ \bar{x}, \bar{x}+1/2, x;$ $-1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}   0, 0, 1/2$ )	(36) $\bar{3}^- \ \bar{x}+1/2, x, \bar{x};$ $1/4, 1/4, -1/4$ ( $\bar{3}_{xyz}   0, 1/2, 0$ )
(37) $d (1/4, -1/4, 1/4) \ x+1/2, \bar{x}, z$ ( $m_{xy}   3/4, 1/4, 1/4$ )	(38) $d (3/4, 3/4, 3/4) \ x, x, z$ ( $m_{xy}   3/4, 3/4, 3/4$ )	(39) $\bar{4}^- \ 0, 1/4, z; \ 0, 1/4, 3/8$ ( $\bar{4}_z^{-1}   1/4, 1/4, 3/4$ )	(40) $\bar{4}^+ \ 1/2, 1/4, z; \ 1/2, 1/4, 1/8$ ( $\bar{4}_z   1/4, 3/4, 1/4$ )
(41) $\bar{4}^- \ x, 0, 1/4; \ 3/8, 0, 1/4$ ( $\bar{4}_x^{-1}   3/4, 1/4, 1/4$ )	(42) $d (1/4, 1/4, -1/4) \ x, y+1/2, \bar{y}$ ( $m_{yz}   1/4, 3/4, 1/4$ )	(43) $d (3/4, 3/4, 3/4) \ x, y, y$ ( $m_{yz}   3/4, 3/4, 3/4$ )	(44) $\bar{4}^+ \ x, 1/2, 1/4; \ 1/8, 1/2, 1/4$ ( $\bar{4}_x   1/4, 1/4, 3/4$ )
(45) $\bar{4}^+ \ 1/4, y, 1/2; \ 1/4, 1/8, 1/2$ ( $\bar{4}_y   3/4, 1/4, 1/4$ )	(46) $d (-1/4, 1/4, 1/4) \ \bar{x}+1/2, y, x$ ( $m_{xz}   1/4, 1/4, 3/4$ )	(47) $\bar{4}^- \ 1/4, y, 0; \ 1/4, 3/8, 0$ ( $\bar{4}_y^{-1}   1/4, 3/4, 1/4$ )	(48) $d (3/4, 3/4, 3/4) \ x, y, x$ ( $m_{xz}   3/4, 3/4, 3/4$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates								
96	h	1	(0,0,0) +	(1/2,1/2,1/2) +							
(1)	$x, y, z$	[u,v,w]	(2)	$\bar{x}+1/2, \bar{y}, z+1/2$	[ $\bar{u}, \bar{v}, w$ ]	(3)	$\bar{x}, y+1/2, \bar{z}+1/2$	[ $\bar{u}, v, \bar{w}$ ]	(4)	$x+1/2, \bar{y}+1/2, \bar{z}$	[ $u, \bar{v}, \bar{w}$ ]
(5)	$z, x, y$	[w,u,v]	(6)	$z+1/2, \bar{x}+1/2, \bar{y}$	[ $w, \bar{u}, \bar{v}$ ]	(7)	$\bar{z}+1/2, \bar{x}, y+1/2$	[ $\bar{w}, \bar{u}, v$ ]	(8)	$\bar{z}, x+1/2, \bar{y}+1/2$	[ $\bar{w}, u, \bar{v}$ ]
(9)	$y, z, x$	[v,w,u]	(10)	$\bar{y}, z+1/2, \bar{x}+1/2$	[ $\bar{v}, w, \bar{u}$ ]	(11)	$y+1/2, \bar{z}+1/2, \bar{x}$	[ $v, \bar{w}, \bar{u}$ ]	(12)	$\bar{y}+1/2, \bar{z}, x+1/2$	[ $\bar{v}, \bar{w}, u$ ]
(13)	$y+3/4, x+1/4, \bar{z}+1/4$	[v,u,w]	(14)	$\bar{y}+3/4, \bar{x}+3/4, \bar{z}+3/4$	[ $\bar{v}, \bar{u}, \bar{w}$ ]	(15)	$y+1/4, \bar{x}+1/4, z+3/4$	[v,u,w]	(16)	$\bar{y}+1/4, x+3/4, z+1/4$	[ $\bar{v}, u, w$ ]
(17)	$x+3/4, z+1/4, \bar{y}+1/4$	[u,w,v]	(18)	$\bar{x}+1/4, z+3/4, y+1/4$	[ $\bar{u}, w, v$ ]	(19)	$\bar{x}+3/4, \bar{z}+3/4, \bar{y}+3/4$	[ $\bar{u}, \bar{w}, \bar{v}$ ]	(20)	$x+1/4, \bar{z}+1/4, y+3/4$	[u,w,v]
(21)	$z+3/4, y+1/4, \bar{x}+1/4$	[w,v,u]	(22)	$z+1/4, \bar{y}+1/4, x+3/4$	[w,v,u]	(23)	$\bar{z}+1/4, y+3/4, x+1/4$	[ $\bar{w}, v, u$ ]	(24)	$\bar{z}+3/4, \bar{y}+3/4, \bar{x}+3/4$	[ $\bar{w}, \bar{v}, \bar{u}$ ]
(25)	$\bar{x}, \bar{y}, \bar{z}$	[u,v,w]	(26)	$x+1/2, y, \bar{z}+1/2$	[ $\bar{u}, \bar{v}, w$ ]	(27)	$x, \bar{y}+1/2, z+1/2$	[ $\bar{u}, v, \bar{w}$ ]	(28)	$\bar{x}+1/2, y+1/2, z$	[ $u, \bar{v}, \bar{w}$ ]

- (29)  $\bar{z}, \bar{x}, \bar{y}$  [w,u,v]      (30)  $\bar{z}+1/2, \bar{x}+1/2, \bar{y}$  [w,  $\bar{u}, \bar{v}$ ]      (31)  $z+1/2, x, \bar{y}+1/2$  [ $\bar{w}, \bar{u}, \bar{v}$ ]      (32)  $z, \bar{x}+1/2, \bar{y}+1/2$  [ $\bar{w}, \bar{u}, \bar{v}$ ]  
 (33)  $\bar{y}, \bar{z}, \bar{x}$  [v,w,u]      (34)  $y, \bar{z}+1/2, \bar{x}+1/2$  [ $\bar{v}, \bar{w}, \bar{u}$ ]      (35)  $\bar{y}+1/2, z+1/2, x$  [v,  $\bar{w}, \bar{u}$ ]      (36)  $y+1/2, z, \bar{x}+1/2$  [ $\bar{v}, \bar{w}, \bar{u}$ ]  
 (37)  $\bar{y}+1/4, \bar{x}+3/4, z+3/4$  [v,u, $\bar{w}$ ](38)  $y+1/4, \bar{x}+1/4, z+1/4$  [ $\bar{v}, \bar{u}, \bar{w}$ ](39)  $\bar{y}+3/4, \bar{x}+3/4, \bar{z}+1/4$  [v,  $\bar{u}, \bar{w}$ ](40)  $y+3/4, \bar{x}+1/4, \bar{z}+3/4$  [ $\bar{v}, \bar{u}, \bar{w}$ ]  
 (41)  $\bar{x}+1/4, \bar{z}+3/4, \bar{y}+3/4$  [u,w, $\bar{v}$ ](42)  $x+3/4, \bar{z}+1/4, \bar{y}+3/4$  [ $\bar{u}, \bar{w}, \bar{v}$ ](43)  $x+1/4, z+1/4, \bar{y}+1/4$  [ $\bar{u}, \bar{w}, \bar{v}$ ](44)  $\bar{x}+3/4, z+3/4, \bar{y}+1/4$  [u, $\bar{w}, \bar{v}$ ]  
 (45)  $\bar{z}+1/4, \bar{y}+3/4, \bar{x}+3/4$  [w,v, $\bar{u}$ ](46)  $\bar{z}+3/4, \bar{y}+3/4, \bar{x}+1/4$  [w, $\bar{v}, \bar{u}$ ](47)  $z+3/4, \bar{y}+1/4, \bar{x}+3/4$  [ $\bar{w}, \bar{v}, \bar{u}$ ](48)  $z+1/4, \bar{y}+1/4, \bar{x}+1/4$  [ $\bar{w}, \bar{v}, \bar{u}$ ]

48 g ..2

- $1/8, \bar{y}, \bar{y}+1/4$  [0,  $\bar{v}, \bar{v}$ ]       $3/8, \bar{y}, \bar{y}+3/4$  [0,v,v]       $7/8, \bar{y}+1/2, \bar{y}+1/4$  [0,  $\bar{v}, \bar{v}$ ]       $5/8, \bar{y}+1/2, \bar{y}+3/4$  [0,v, $\bar{v}$ ]  
 $\bar{y}+1/4, 1/8, \bar{y}$  [v,0, $\bar{v}$ ]       $\bar{y}+3/4, 3/8, \bar{y}$  [v,0,v]       $y+1/4, 7/8, \bar{y}+1/2$  [ $\bar{v}, 0, \bar{v}$ ]       $y+3/4, 5/8, \bar{y}+1/2$  [ $\bar{v}, 0, \bar{v}$ ]  
 $y, \bar{y}+1/4, 1/8$  [ $\bar{v}, \bar{v}, 0$ ]       $\bar{y}, \bar{y}+3/4, 3/8$  [v,v,0]       $y+1/2, \bar{y}+1/4, 7/8$  [ $\bar{v}, \bar{v}, 0$ ]       $\bar{y}+1/2, \bar{y}+3/4, 5/8$  [v, $\bar{v}, 0$ ]  
 $7/8, \bar{y}, \bar{y}+3/4$  [0,  $\bar{v}, \bar{v}$ ]       $5/8, \bar{y}, \bar{y}+1/4$  [0,v,v]       $1/8, \bar{y}+1/2, \bar{y}+3/4$  [0,  $\bar{v}, \bar{v}$ ]       $3/8, \bar{y}+1/2, \bar{y}+1/4$  [0,v, $\bar{v}$ ]  
 $y+3/4, 7/8, \bar{y}$  [v,0, $\bar{v}$ ]       $y+1/4, 5/8, \bar{y}$  [v,0,v]       $\bar{y}+3/4, 1/8, \bar{y}+1/2$  [ $\bar{v}, 0, \bar{v}$ ]       $\bar{y}+1/4, 3/8, \bar{y}+1/2$  [ $\bar{v}, 0, \bar{v}$ ]  
 $\bar{y}, \bar{y}+3/4, 7/8$  [ $\bar{v}, \bar{v}, 0$ ]       $y, \bar{y}+1/4, 5/8$  [v,v,0]       $\bar{y}+1/2, \bar{y}+3/4, 1/8$  [ $\bar{v}, \bar{v}, 0$ ]       $y+1/2, \bar{y}+1/4, 3/8$  [v, $\bar{v}, 0$ ]

48 f 2..

- $x, 0, 1/4$  [u,0,0]       $\bar{x}+1/2, 0, 3/4$  [ $\bar{u}, 0, 0$ ]       $1/4, x, 0$  [0,u,0]       $3/4, \bar{x}+1/2, 0$  [0, $\bar{u}, 0$ ]  
 $0, 1/4, x$  [0,0,u]       $0, 3/4, \bar{x}+1/2$  [0,0, $\bar{u}$ ]       $3/4, x+1/4, 0$  [0,u,0]       $3/4, \bar{x}+3/4, 1/2$  [0, $\bar{u}, 0$ ]  
 $x+3/4, 1/2, 1/4$  [u,0,0]       $\bar{x}+1/4, 0, 1/4$  [ $\bar{u}, 0, 0$ ]       $0, 1/4, \bar{x}+1/4$  [0,0, $\bar{u}$ ]       $1/2, 1/4, x+3/4$  [0,0,u]  
 $\bar{x}, 0, 3/4$  [u,0,0]       $x+1/2, 0, 1/4$  [ $\bar{u}, 0, 0$ ]       $3/4, \bar{x}, 0$  [0,u,0]       $1/4, x+1/4, 0$  [0, $\bar{u}, 0$ ]  
 $0, 3/4, \bar{x}$  [0,0,u]       $0, 1/4, x+1/2$  [0,0, $\bar{u}$ ]       $1/4, \bar{x}+3/4, 0$  [0,u,0]       $1/4, x+1/4, 1/2$  [0, $\bar{u}, 0$ ]  
 $\bar{x}+1/4, 1/2, 3/4$  [u,0,0]       $x+3/4, 0, 3/4$  [ $\bar{u}, 0, 0$ ]       $0, 3/4, x+3/4$  [0,0, $\bar{u}$ ]       $1/2, 3/4, \bar{x}+1/4$  [0,0,u]

32 e .3.

- $x, x, x$  [u,u,u]       $\bar{x}+1/2, \bar{x}, \bar{x}+1/2$  [ $\bar{u}, \bar{u}, \bar{u}$ ]       $\bar{x}, \bar{x}+1/2, \bar{x}+1/2$  [ $\bar{u}, \bar{u}, \bar{u}$ ]       $x+1/2, \bar{x}+1/2, \bar{x}$  [u, $\bar{u}, \bar{u}$ ]  
 $x+3/4, \bar{x}+1/4, \bar{x}+1/4$  [u,u, $\bar{u}$ ]       $\bar{x}+3/4, \bar{x}+3/4, \bar{x}+3/4$  [ $\bar{u}, \bar{u}, \bar{u}$ ]       $x+1/4, \bar{x}+1/4, x+3/4$  [u, $\bar{u}, \bar{u}$ ]       $\bar{x}+1/4, x+3/4, \bar{x}+1/4$  [ $\bar{u}, \bar{u}, \bar{u}$ ]  
 $\bar{x}, \bar{x}, \bar{x}$  [u,u,u]       $x+1/2, x, \bar{x}+1/2$  [ $\bar{u}, \bar{u}, \bar{u}$ ]       $x, \bar{x}+1/2, \bar{x}+1/2$  [ $\bar{u}, \bar{u}, \bar{u}$ ]       $\bar{x}+1/2, x+1/2, x$  [u, $\bar{u}, \bar{u}$ ]  
 $\bar{x}+1/4, \bar{x}+3/4, x+3/4$  [u,u, $\bar{u}$ ]       $x+1/4, \bar{x}+1/4, \bar{x}+1/4$  [ $\bar{u}, \bar{u}, \bar{u}$ ]       $\bar{x}+3/4, x+3/4, \bar{x}+1/4$  [u, $\bar{u}, \bar{u}$ ]       $x+3/4, \bar{x}+1/4, \bar{x}+3/4$  [ $\bar{u}, \bar{u}, \bar{u}$ ]

12 d 4..

- $3/8, 0, 1/4$  [u,0,0]       $1/8, 0, 3/4$  [ $\bar{u}, 0, 0$ ]       $1/4, 3/8, 0$  [0,u,0]       $3/4, 1/8, 0$  [0, $\bar{u}, 0$ ]  
 $0, 1/4, 3/8$  [0,0,u]       $0, 3/4, 1/8$  [0,0, $\bar{u}$ ]       $3/4, 5/8, 0$  [0,u,0]       $3/4, 3/8, 1/2$  [0, $\bar{u}, 0$ ]  
 $1/8, 1/2, 1/4$  [u,0,0]       $7/8, 0, 1/4$  [ $\bar{u}, 0, 0$ ]       $0, 1/4, 7/8$  [0,0, $\bar{u}$ ]       $1/2, 1/4, 1/8$  [0,0,u]

24 c 2.22

- $1/8, 0, 1/4$  [0,0,0]       $3/8, 0, 3/4$  [0,0,0]       $1/4, 1/8, 0$  [0,0,0]       $3/4, 3/8, 0$  [0,0,0]  
 $0, 1/4, 1/8$  [0,0,0]       $0, 3/4, 3/8$  [0,0,0]       $7/8, 0, 3/4$  [0,0,0]       $5/8, 0, 1/4$  [0,0,0]  
 $3/4, 7/8, 0$  [0,0,0]       $1/4, 5/8, 0$  [0,0,0]       $0, 3/4, 7/8$  [0,0,0]       $0, 1/4, 5/8$  [0,0,0]



Continued

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Ia $\bar{3}$ d

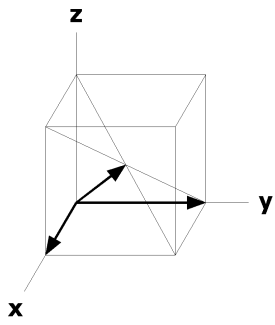
16	b	.32	1/8, 1/8, 1/8 [0,0,0]	3/8, 7/8, 5/8 [0,0,0]	7/8, 5/8, 3/8 [0,0,0]	5/8, 3/8, 7/8 [0,0,0]
			7/8, 7/8, 7/8 [0,0,0]	5/8, 1/8, 3/8 [0,0,0]	1/8, 3/8, 5/8 [0,0,0]	3/8, 5/8, 1/8 [0,0,0]
16	a	$\bar{.3}$ .	0,0,0 [u,u,u]	1/2, 0, 1/2 [ $\bar{u}$ , $\bar{u}$ , u]	0, 1/2, 1/2 [ $\bar{u}$ , u, $\bar{u}$ ]	1/2, 1/2, 0 [u, $\bar{u}$ , $\bar{u}$ ]
			3/4, 1/4, 1/4 [u, u, $\bar{u}$ ]	3/4, 3/4, 3/4 [ $\bar{u}$ , $\bar{u}$ , $\bar{u}$ ]	1/4, 1/4, 3/4 [u, $\bar{u}$ , u]	1/4, 3/4, 1/4 [ $\bar{u}$ , u, u]

### Symmetry of Special Projections

Along [0,0,1]  $p_6$ -4m'm'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,0,z

Along [1,1,1]  $p6$ 'm'm  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

Along [1,1,0]  $c_6$ -2m'm'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x+1/4,1/8



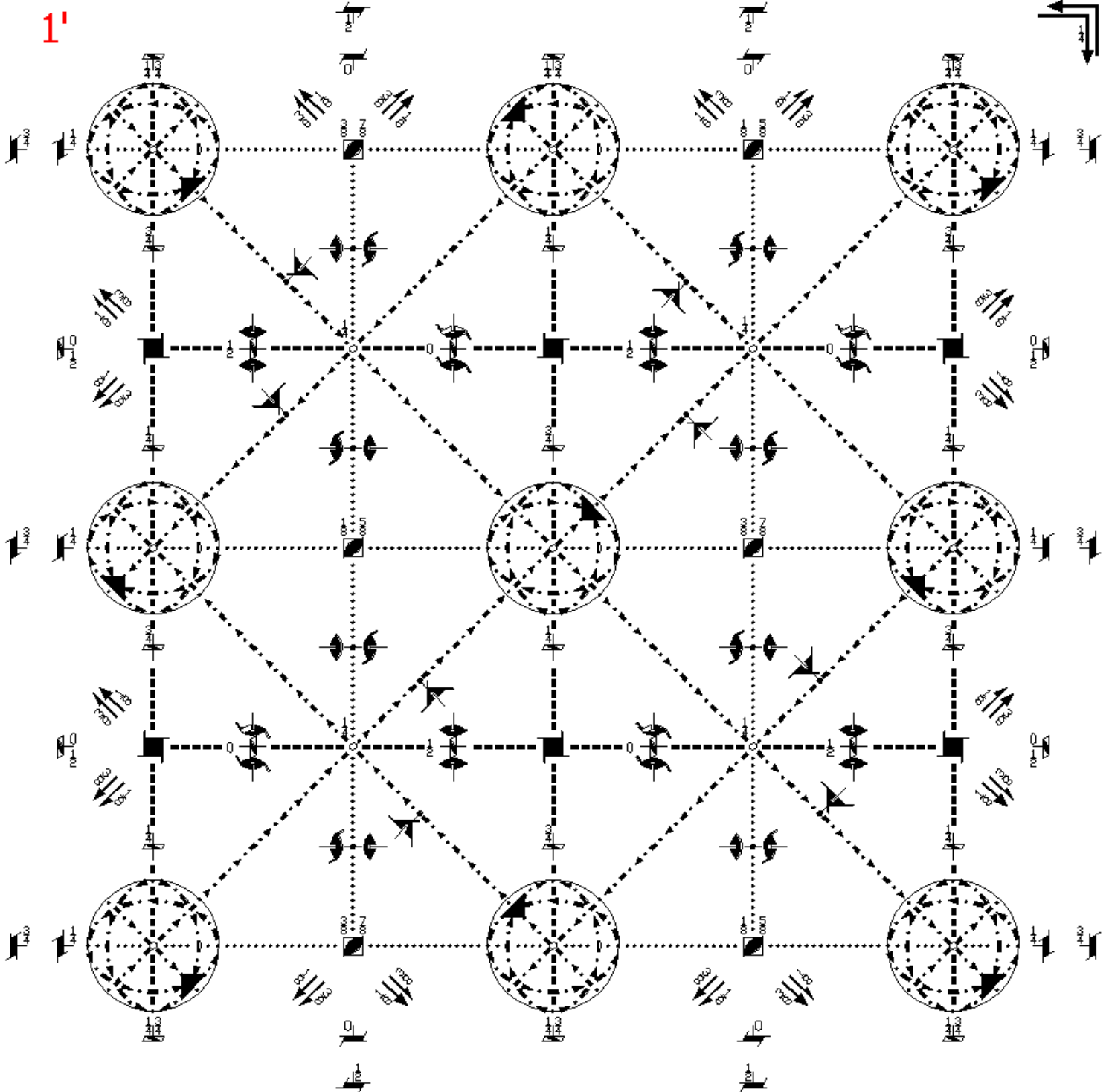
$Ia\bar{3}d1'$

230.2.1648

$m\bar{3}m1'$

$I4_1/a\bar{3}2/d1'$

Cubic



Origin at center ( $\bar{3}1'$ )Asymmetric unit  $-1/8 \leq x \leq 1/8$ ;  $-1/8 \leq y \leq 1/8$ ;  $0 \leq z \leq 1/4$ ;  $\max(x, -x, y, -y) \leq z$ 

Vertices	0,0,0	1/8,1/8,1/8	-1/8,1/8,1/8	-1/8,-1/8,1/8	1/8,-1/8,1/8
	1/8,1/8,1/4	-1/8,1/8,1/4	-1/8,-1/8,1/4	1/8,-1/8,1/4	

## Symmetry Operations

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)  | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub>  0,0,0)                                | (6) 3 <sup>+</sup> $\bar{x}+1/2,x,\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,1/2,0)           | (7) 3 <sup>+</sup> x+1/2, $\bar{x}-1/2,\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,0,1/2) | (8) 3 <sup>+</sup> $\bar{x},\bar{x}+1/2,x$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,1/2,1/2)           |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)                  | (10) 3 <sup>-</sup> (-1/3,1/3,1/3)<br>x+1/6, $\bar{x}+1/6,\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub>  0,1/2,1/2) | (11) 3 <sup>-</sup> (1/3,1/3,-1/3)<br>x+1/3, $\bar{x}+1/6,x$<br>(3 <sub>x<math>\bar{y}z</math></sub>  1/2,1/2,0)  | (12) 3 <sup>-</sup> (1/3,-1/3,1/3)<br>x-1/6, $\bar{x}+1/3,\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub>  1/2,0,1/2) |
| (13) 2 (1/2,1/2,0) x,x-1/4,1/8<br>(2 <sub>xy</sub>  3/4,1/4,1/4)                     | (14) 2 x, $\bar{x}+3/4,3/8$<br>(2 <sub>xy</sub>  3/4,3/4,3/4)  | (15) 4 <sup>-</sup> (0,0,3/4) 1/4,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/4,1/4,3/4)                              | (16) 4 <sup>+</sup> (0,0,1/4) -1/4,1/2,z<br>(4 <sub>z</sub>  1/4,3/4,1/4)  |
| (17) 4 <sup>-</sup> (3/4,0,0) x,1/4,0<br>(4 <sub>x</sub> <sup>-1</sup>  3/4,1/4,1/4) | (18) 2 (0,1/2,1/2) 1/8,y+1/4,y<br>(2 <sub>yz</sub>  1/4,3/4,1/4)   | (19) 2 3/8,y+3/4, $\bar{y}$<br>(2 <sub>yz</sub>  3/4,3/4,3/4)   | (20) 4 <sup>+</sup> (1/4,0,0) x,-1/4,1/2<br>(4 <sub>x</sub>  1/4,1/4,3/4)  |
| (21) 4 <sup>+</sup> (0,1/4,0) 1/2,y,-1/4<br>(4 <sub>y</sub>  3/4,1/4,1/4)            | (22) 2 (1/2,0,1/2) x-1/4,1/8,x<br>(2 <sub>xz</sub>  1/4,1/4,3/4)   | (23) 4 <sup>-</sup> (0,3/4,0) 0,y,1/4<br>(4 <sub>y</sub> <sup>-1</sup>  1/4,3/4,1/4)                              | (24) 2 $\bar{x}+3/4,3/8,x$<br>(2 <sub>xz</sub>  3/4,3/4,3/4)   |
| (25) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)  | (26) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)  | (27) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)   | (28) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)  |
| (29) $\bar{3}^+$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$  0,0,0)                           | (30) $\bar{3}^+$ $\bar{x}-1/2,x+1,\bar{x}$ ;<br>0,1/2,1/2<br>( $\bar{3}_{x\bar{y}z$ <sup>-1</sup>  1/2,1/2,0)          | (31) $\bar{3}^+$ x+1/2, $\bar{x}+1/2,\bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{x\bar{y}z$ <sup>-1</sup>  1/2,0,1/2)  | (32) $\bar{3}^+$ $\bar{x}+1,\bar{x}+1/2,x$ ;<br>1/2,0,1/2<br>( $\bar{3}_{x\bar{y}z$ <sup>-1</sup>  0,1/2,1/2)          |
| (33) $\bar{3}^-$ x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)             | (34) $\bar{3}^-$ x+1/2, $\bar{x}-1/2,\bar{x}$ ; 0,0,1/2<br>( $\bar{3}_{x\bar{y}z$  0,1/2,1/2)                          | (35) $\bar{3}^-$ $\bar{x},\bar{x}+1/2,x$ ; 0,1/2,0<br>( $\bar{3}_{x\bar{y}z$  1/2,1/2,0)                          | (36) $\bar{3}^-$ $\bar{x}+1/2,x,\bar{x}$ ; 1/2,0,0<br>( $\bar{3}_{x\bar{y}z$  1/2,0,1/2)                               |
| (37) d (-1/4,1/4,1/4) x+1/2, $\bar{x},z$<br>(m <sub>xy</sub>  1/4,3/4,3/4)           | (38) d (1/4,1/4,1/4) x,x,z<br>(m <sub>xy</sub>  1/4,1/4,1/4)   | (39) $\bar{4}^-$ 0,3/4,z; 0,3/4,1/8<br>( $\bar{4}_z$ <sup>-1</sup>  3/4,3/4,1/4)                                  | (40) $\bar{4}^+$ 1/2,-1/4,z; 1/2,-1/4,3/8<br>( $\bar{4}_z$  3/4,1/4,3/4)   |
| (41) $\bar{4}^-$ x,0,3/4; 1/8,0,3/4<br>( $\bar{4}_x$ <sup>-1</sup>  1/4,3/4,3/4)     | (42) d (3/4,-1/4,1/4) x,y+1/2, $\bar{y}$<br>(m <sub>yz</sub>  3/4,1/4,3/4)   | (43) d (1/4,1/4,1/4) x,y,y<br>(m <sub>yz</sub>  1/4,1/4,1/4)  | (44) $\bar{4}^+$ x,1/2,-1/4; 3/8,1/2,-1/4<br>( $\bar{4}_x$  3/4,3/4,1/4)   |
| (45) $\bar{4}^+$ -1/4,y,1/2; -1/4,3/8,1/2<br>( $\bar{4}_y$  1/4,3/4,3/4)             | (46) d (1/4,3/4,-1/4) $\bar{x}+1/2,y,x$<br>(m <sub>xz</sub>  3/4,3/4,1/4)  | (47) $\bar{4}^-$ 3/4,y,0; 3/4,1/8,0<br>( $\bar{4}_y$ <sup>-1</sup>  3/4,1/4,3/4)                                  | (48) d (1/4,1/4,1/4) x,y,x<br>(m <sub>xz</sub>  1/4,1/4,1/4)   |

For (1/2,1/2,1/2) + set

- |   |   |   |   |
|---|---|---|---|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                                    | (2) 2 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,0)  | (3) 2 1/4,y,0<br>(2 <sub>y</sub>  1/2,0,0)  | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)  |
| (5) 3 <sup>+</sup> (1/2,1/2,1/2) x,x,x<br>(3 <sub>xyz</sub>  1/2,1/2,1/2) | (6) 3 <sup>+</sup> (1/6,-1/6,1/6)<br>x-1/6,x+1/3, $\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,1/2) | (7) 3 <sup>+</sup> (-1/6,1/6,1/6)<br>x+1/6, $\bar{x}+1/6,\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,1/2,0) | (8) 3 <sup>+</sup> (1/6,1/6,-1/6)<br>x+1/3, $\bar{x}+1/6,x$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,0,0) |

- (9)  $3^- (1/2, 1/2, 1/2) \ x, x, x$   
 $(3_{xyz}^{-1} | 1/2, 1/2, 1/2)$
- (10)  $3^- (1/6, -1/6, -1/6) \ \bar{x} + 1/6, \bar{x} + 1/6, \bar{x}$   
 $(3_{\bar{xyz}} | 1/2, 0, 0)$
- (11)  $3^- (-1/6, -1/6, 1/6) \ \bar{x} + 1/3, \bar{x} + 1/6, \bar{x}$   
 $(3_{\bar{xyz}} | 0, 0, 1/2)$
- (12)  $3^- (-1/6, 1/6, -1/6) \ \bar{x} - 1/6, \bar{x} + 1/3, \bar{x}$   
 $(3_{\bar{xyz}} | 0, 1/2, 0)$
- (13)  $2 (1/2, 1/2, 0) \ x, \bar{x} + 1/4, 3/8$   
 $(2_{xy} | 1/4, 3/4, 3/4)$
- (14)  $2 \ x, \bar{x} + 1/4, 1/8$   
 $(2_{\bar{xy}} | 1/4, 1/4, 1/4)$
- (15)  $4^- (0, 0, 1/4) \ 3/4, 0, z$   
 $(4_z^{-1} | 3/4, 3/4, 1/4)$
- (16)  $4^+ (0, 0, 3/4) \ 1/4, 1/2, z$   
 $(4_z | 3/4, 1/4, 3/4)$
- (17)  $4^- (1/4, 0, 0) \ x, 3/4, 0$   
 $(4_x^{-1} | 1/4, 3/4, 3/4)$
- (18)  $2 (0, 1/2, 1/2) \ 3/8, y - 1/4, y$   
 $(2_{yz} | 3/4, 1/4, 3/4)$
- (19)  $2 \ 1/8, y + 1/4, \bar{y}$   
 $(2_{\bar{yz}} | 1/4, 1/4, 1/4)$
- (20)  $4^+ (3/4, 0, 0) \ x, 1/4, 1/2$   
 $(4_x | 3/4, 3/4, 1/4)$
- (21)  $4^+ (0, 3/4, 0) \ 1/2, y, 1/4$   
 $(4_y | 1/4, 3/4, 3/4)$
- (22)  $2 (1/2, 0, 1/2) \ \bar{x} + 1/4, 3/8, \bar{x}$   
 $(2_{z\bar{x}} | 3/4, 3/4, 1/4)$
- (23)  $4^- (0, 1/2, 0) \ 0, y, 3/4$   
 $(4_y^{-1} | 3/4, 1/4, 3/4)$
- (24)  $2 \ \bar{x} + 1/4, 1/8, \bar{x}$   
 $(2_{z\bar{x}} | 1/4, 1/4, 1/4)$
- (25)  $\bar{1} \ 1/4, 1/4, 1/4$   
 $(\bar{1} | 1/2, 1/2, 1/2)$
- (26)  $b (0, 1/2, 0) \ x, y, 0$   
 $(m_z | 0, 1/2, 0)$
- (27)  $a (1/2, 0, 0) \ x, 0, z$   
 $(m_y | 1/2, 0, 0)$
- (28)  $c (0, 0, 1/2) \ 0, y, z$   
 $(m_x | 0, 0, 1/2)$
- (29)  $\bar{3}^+ \ x, x, x;$   
 $1/4, 1/4, 1/4$   
 $(\bar{3}_{xyz} | 1/2, 1/2, 1/2)$
- (30)  $\bar{3}^+ \ \bar{x} - 1/2, \bar{x}, \bar{x};$   
 $-1/4, -1/4, 1/4$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 0, 0, 1/2)$
- (31)  $\bar{3}^+ \ x - 1/2, \bar{x} + 1/2, \bar{x};$   
 $-1/4, 1/4, -1/4$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 0, 1/2, 0)$
- (32)  $\bar{3}^+ \ \bar{x}, \bar{x} - 1/2, \bar{x};$   
 $1/4, -1/4, -1/4$   
 $(\bar{3}_{\bar{xyz}}^{-1} | 1/2, 0, 0)$
- (33)  $\bar{3}^- \ x, x, x;$   
 $1/4, 1/4, 1/4$   
 $(\bar{3}_{xyz}^{-1} | 1/2, 1/2, 1/2)$
- (34)  $\bar{3}^- \ \bar{x} + 1/2, \bar{x} - 1/2, \bar{x};$   
 $1/4, -1/4, 1/4$   
 $(\bar{3}_{\bar{xyz}} | 1/2, 0, 0)$
- (35)  $\bar{3}^- \ \bar{x}, \bar{x} + 1/2, \bar{x};$   
 $-1/4, 1/4, 1/4$   
 $(\bar{3}_{\bar{xyz}} | 0, 0, 1/2)$
- (36)  $\bar{3}^- \ \bar{x} + 1/2, \bar{x}, \bar{x};$   
 $1/4, 1/4, -1/4$   
 $(\bar{3}_{\bar{xyz}} | 0, 1/2, 0)$
- (37)  $d (1/4, -1/4, 1/4) \ \bar{x} + 1/2, \bar{x}, z$   
 $(m_{xy} | 3/4, 1/4, 1/4)$
- (38)  $d (3/4, 3/4, 3/4) \ x, x, z$   
 $(m_{\bar{xy}} | 3/4, 3/4, 3/4)$
- (39)  $\bar{4}^- \ 0, 1/4, z; \ 0, 1/4, 3/8$   
 $(\bar{4}_z^{-1} | 1/4, 1/4, 3/4)$
- (40)  $\bar{4}^+ \ 1/2, 1/4, z; \ 1/2, 1/4, 1/8$   
 $(\bar{4}_z | 1/4, 3/4, 1/4)$
- (41)  $\bar{4}^- \ x, 0, 1/4; \ 3/8, 0, 1/4$   
 $(\bar{4}_x^{-1} | 3/4, 1/4, 1/4)$
- (42)  $d (1/4, 1/4, -1/4) \ x, y + 1/2, \bar{y}$   
 $(m_{yz} | 1/4, 3/4, 1/4)$
- (43)  $d (3/4, 3/4, 3/4) \ x, y, y$   
 $(m_{\bar{yz}} | 3/4, 3/4, 3/4)$
- (44)  $\bar{4}^+ \ x, 1/2, 1/4; \ 1/8, 1/2, 1/4$   
 $(\bar{4}_x | 1/4, 1/4, 3/4)$
- (45)  $\bar{4}^+ \ 1/4, y, 1/2; \ 1/4, 1/8, 1/2$   
 $(\bar{4}_y | 3/4, 1/4, 1/4)$
- (46)  $d (-1/4, 1/4, 1/4) \ \bar{x} + 1/2, y, x$   
 $(m_{xz} | 1/4, 1/4, 3/4)$
- (47)  $\bar{4}^- \ 1/4, y, 0; \ 1/4, 3/8, 0$   
 $(\bar{4}_y^{-1} | 1/4, 3/4, 1/4)$
- (48)  $d (3/4, 3/4, 3/4) \ x, y, x$   
 $(m_{z\bar{x}} | 3/4, 3/4, 3/4)$

## For (0,0,0)' + set

- (1)  $1'$   
 $(1 | 0, 0, 0)'$
- (2)  $2' (0, 0, 1/2) \ 1/4, 0, z$   
 $(2_z | 1/2, 0, 1/2)'$
- (3)  $2' (0, 1/2, 0) \ 0, y, 1/4$   
 $(2_y | 0, 1/2, 1/2)'$
- (4)  $2' (1/2, 0, 0) \ x, 1/4, 0$   
 $(2_x | 1/2, 1/2, 0)'$
- (5)  $3^+ \ x, x, x$   
 $(3_{xyz} | 0, 0, 0)'$
- (6)  $3^+ \ \bar{x} + 1/2, \bar{x}, \bar{x}$   
 $(3_{\bar{xyz}}^{-1} | 1/2, 1/2, 0)'$
- (7)  $3^+ \ \bar{x} + 1/2, \bar{x} - 1/2, \bar{x}$   
 $(3_{\bar{xyz}}^{-1} | 1/2, 0, 1/2)'$
- (8)  $3^+ \ \bar{x}, \bar{x} + 1/2, \bar{x}$   
 $(3_{\bar{xyz}}^{-1} | 0, 1/2, 1/2)'$
- (9)  $3^- \ x, x, x$   
 $(3_{xyz}^{-1} | 0, 0, 0)'$
- (10)  $3^- \ (-1/3, 1/3, 1/3) \ \bar{x} + 1/6, \bar{x} + 1/6, \bar{x}$   
 $(3_{\bar{xyz}} | 0, 1/2, 1/2)'$
- (11)  $3^- \ (1/3, 1/3, -1/3) \ \bar{x} + 1/3, \bar{x} + 1/6, \bar{x}$   
 $(3_{\bar{xyz}} | 1/2, 1/2, 0)'$
- (12)  $3^- \ (1/3, -1/3, 1/3) \ \bar{x} - 1/6, \bar{x} + 1/3, \bar{x}$   
 $(3_{\bar{xyz}} | 1/2, 0, 1/2)'$
- (13)  $2' (1/2, 1/2, 0) \ x, \bar{x} - 1/4, 1/8$   
 $(2_{xy} | 3/4, 1/4, 1/4)'$
- (14)  $2' \ x, \bar{x} + 3/4, 3/8$   
 $(2_{\bar{xy}} | 3/4, 3/4, 3/4)'$
- (15)  $4^- \ (0, 0, 3/4) \ 1/4, 0, z$   
 $(4_z^{-1} | 1/4, 1/4, 3/4)'$
- (16)  $4^+ \ (0, 0, 1/4) \ -1/4, 1/2, z$   
 $(4_z | 1/4, 3/4, 1/4)'$
- (17)  $4^- \ (3/4, 0, 0) \ x, 1/4, 0$   
 $(4_x^{-1} | 3/4, 1/4, 1/4)'$
- (18)  $2' (0, 1/2, 1/2) \ 1/8, y + 1/4, y$   
 $(2_{yz} | 1/4, 3/4, 1/4)'$
- (19)  $2' \ 3/8, y + 3/4, \bar{y}$   
 $(2_{\bar{yz}} | 3/4, 3/4, 3/4)'$
- (20)  $4^+ \ (1/4, 0, 0) \ x, -1/4, 1/2$   
 $(4_x | 1/4, 1/4, 3/4)'$
- (21)  $4^+ \ (0, 1/4, 0) \ 1/2, y, -1/4$   
 $(4_y | 3/4, 1/4, 1/4)'$
- (22)  $2' (1/2, 0, 1/2) \ \bar{x} - 1/4, 1/8, \bar{x}$   
 $(2_{z\bar{x}} | 1/4, 1/4, 3/4)'$
- (23)  $4^- \ (0, 3/4, 0) \ 0, y, 1/4$   
 $(4_y^{-1} | 1/4, 3/4, 1/4)'$
- (24)  $2' \ \bar{x} + 3/4, 3/8, \bar{x}$   
 $(2_{z\bar{x}} | 3/4, 3/4, 3/4)'$
- (25)  $\bar{1} \ 0, 0, 0$   
 $(\bar{1} | 0, 0, 0)'$
- (26)  $a' (1/2, 0, 0) \ x, y, 1/4$   
 $(m_z | 1/2, 0, 1/2)'$
- (27)  $c' (0, 0, 1/2) \ x, 1/4, z$   
 $(m_y | 0, 1/2, 1/2)'$
- (28)  $b' (0, 1/2, 0) \ 1/4, y, z$   
 $(m_x | 1/2, 1/2, 0)'$

- (29)  $\bar{3}^+ ' x,x,x; 0,0,0$   
 $(\bar{3}_{xyz}|0,0,0)'$
- (30)  $\bar{3}^+ ' \bar{x}-1/2,x+1,\bar{x};$   
 $0,1/2,1/2$   
 $(\bar{3}_{xyz}^{-1}|1/2,1/2,0)'$
- (31)  $\bar{3}^+ ' x+1/2,\bar{x}+1/2,\bar{x};$   
 $1/2,1/2,0$   
 $(\bar{3}_{xyz}^{-1}|1/2,0,1/2)'$
- (32)  $\bar{3}^+ ' \bar{x}+1,\bar{x}+1/2,x;$   
 $1/2,0,1/2$   
 $(\bar{3}_{xyz}^{-1}|0,1/2,1/2)'$
- (33)  $\bar{3}^- ' x,x,x; 0,0,0$   
 $(\bar{3}_{xyz}^{-1}|0,0,0)'$
- (34)  $\bar{3}^- ' x+1/2,\bar{x}-1/2,\bar{x}; 0,0,1/2$   
 $(\bar{3}_{xyz}|0,1/2,1/2)'$
- (35)  $\bar{3}^- ' \bar{x},\bar{x}+1/2,x; 0,1/2,0$   
 $(\bar{3}_{xyz}|1/2,1/2,0)'$
- (36)  $\bar{3}^- ' \bar{x}+1/2,x,\bar{x}; 1/2,0,0$   
 $(\bar{3}_{xyz}|1/2,0,1/2)'$
- (37)  $d' (-1/4,1/4,1/4) x+1/2,\bar{x},z$   
 $(m_{xy}|1/4,3/4,3/4)'$
- (38)  $d' (1/4,1/4,1/4) x,x,z$   
 $(m_{xy}|1/4,1/4,1/4)'$
- (39)  $\bar{4}^- ' 0,3/4,z; 0,3/4,1/8$   
 $(\bar{4}_z^{-1}|3/4,3/4,1/4)'$
- (40)  $\bar{4}^+ ' 1/2,-1/4,z; 1/2,-1/4,3/8$   
 $(\bar{4}_z|3/4,1/4,3/4)'$
- (41)  $\bar{4}^- ' x,0,3/4; 1/8,0,3/4$   
 $(\bar{4}_x^{-1}|1/4,3/4,3/4)'$
- (42)  $d' (3/4,-1/4,1/4) x,y+1/2,\bar{y}$   
 $(m_{yz}|3/4,1/4,3/4)'$
- (43)  $d' (1/4,1/4,1/4) x,y,y$   
 $(m_{yz}|1/4,1/4,1/4)'$
- (44)  $\bar{4}^+ ' x,1/2,-1/4; 3/8,1/2,-1/4$   
 $(\bar{4}_x|3/4,3/4,1/4)'$
- (45)  $\bar{4}^+ ' -1/4,y,1/2; -1/4,3/8,1/2$   
 $(\bar{4}_y|1/4,3/4,3/4)'$
- (46)  $d' (1/4,3/4,-1/4) \bar{x}+1/2,y,x$   
 $(m_{xz}|3/4,3/4,1/4)'$
- (47)  $\bar{4}^- ' 3/4,y,0; 3/4,1/8,0$   
 $(\bar{4}_y^{-1}|3/4,1/4,3/4)'$
- (48)  $d' (1/4,1/4,1/4) x,y,x$   
 $(m_{xz}|1/4,1/4,1/4)'$

For (1/2,1/2,1/2)' + set

- (1)  $t' (1/2,1/2,1/2)$   
 $(1|1/2,1/2,1/2)'$
- (2)  $2' 0,1/4,z$   
 $(2_z|0,1/2,0)'$
- (3)  $2' 1/4,y,0$   
 $(2_y|1/2,0,0)'$
- (4)  $2' x,0,1/4$   
 $(2_x|0,0,1/2)'$
- (5)  $3^+ ' (1/2,1/2,1/2) x,x,x$   
 $(3_{xyz}|1/2,1/2,1/2)'$
- (6)  $3^+ ' (1/6,-1/6,1/6)$   
 $\bar{x}-1/6,x+1/3,\bar{x}$   
 $(3_{xyz}^{-1}|0,0,1/2)'$
- (7)  $3^+ ' (-1/6,1/6,1/6)$   
 $x+1/6,\bar{x}+1/6,\bar{x}$   
 $(3_{xyz}^{-1}|0,1/2,0)'$
- (8)  $3^+ ' (1/6,1/6,-1/6)$   
 $\bar{x}+1/3,\bar{x}+1/6,x$   
 $(3_{xyz}^{-1}|1/2,0,0)'$
- (9)  $3^- ' (1/2,1/2,1/2) x,x,x$   
 $(3_{xyz}^{-1}|1/2,1/2,1/2)'$
- (10)  $3^- ' (1/6,-1/6,-1/6)$   
 $x+1/6,\bar{x}+1/6,\bar{x}$   
 $(3_{xyz}|1/2,0,0)'$
- (11)  $3^- ' (-1/6,-1/6,1/6)$   
 $\bar{x}+1/3,\bar{x}+1/6,x$   
 $(3_{xyz}|0,0,1/2)'$
- (12)  $3^- ' (-1/6,1/6,-1/6)$   
 $\bar{x}-1/6,x+1/3,\bar{x}$   
 $(3_{xyz}|0,1/2,0)'$
- (13)  $2' (1/2,1/2,0) x,x+1/4,3/8$   
 $(2_{xy}|1/4,3/4,3/4)'$
- (14)  $2' x,\bar{x}+1/4,1/8$   
 $(2_{xy}|1/4,1/4,1/4)'$
- (15)  $4^- ' (0,0,1/4) 3/4,0,z$   
 $(\bar{4}_z^{-1}|3/4,3/4,1/4)'$
- (16)  $4^+ ' (0,0,3/4) 1/4,1/2,z$   
 $(\bar{4}_z|3/4,1/4,3/4)'$
- (17)  $4^- ' (1/4,0,0) x,3/4,0$   
 $(\bar{4}_x^{-1}|1/4,3/4,3/4)'$
- (18)  $2' (0,1/2,1/2) 3/8,y-1/4,y$   
 $(2_{yz}|3/4,1/4,3/4)'$
- (19)  $2' 1/8,y+1/4,\bar{y}$   
 $(2_{yz}|1/4,1/4,1/4)'$
- (20)  $4^+ ' (3/4,0,0) x,1/4,1/2$   
 $(\bar{4}_x|3/4,3/4,1/4)'$
- (21)  $4^+ ' (0,3/4,0) 1/2,y,1/4$   
 $(\bar{4}_y|1/4,3/4,3/4)'$
- (22)  $2' (1/2,0,1/2) x+1/4,3/8,x$   
 $(2_{xz}|3/4,3/4,1/4)'$
- (23)  $4^- ' (0,1/2,0) 0,y,3/4$   
 $(\bar{4}_y^{-1}|3/4,1/4,3/4)'$
- (24)  $2' \bar{x}+1/4,1/8,x$   
 $(2_{xz}|1/4,1/4,1/4)'$
- (25)  $\bar{1} ' 1/4,1/4,1/4$   
 $(\bar{1}|1/2,1/2,1/2)'$
- (26)  $b' (0,1/2,0) x,y,0$   
 $(m_z|0,1/2,0)'$
- (27)  $a' (1/2,0,0) x,0,z$   
 $(m_y|1/2,0,0)'$
- (28)  $c' (0,0,1/2) 0,y,z$   
 $(m_x|0,0,1/2)'$
- (29)  $\bar{3}^+ ' x,x,x;$   
 $1/4,1/4,1/4$   
 $(\bar{3}_{xyz}|1/2,1/2,1/2)'$
- (30)  $\bar{3}^+ ' \bar{x}-1/2,x,\bar{x};$   
 $-1/4,-1/4,1/4$   
 $(\bar{3}_{xyz}^{-1}|0,0,1/2)'$
- (31)  $\bar{3}^+ ' x-1/2,\bar{x}+1/2,\bar{x};$   
 $-1/4,1/4,-1/4$   
 $(\bar{3}_{xyz}^{-1}|0,1/2,0)'$
- (32)  $\bar{3}^+ ' \bar{x},\bar{x}-1/2,x;$   
 $1/4,-1/4,-1/4$   
 $(\bar{3}_{xyz}^{-1}|1/2,0,0)'$
- (33)  $\bar{3}^- ' x,x,x;$   
 $1/4,1/4,1/4$   
 $(\bar{3}_{xyz}^{-1}|1/2,1/2,1/2)'$
- (34)  $\bar{3}^- ' x+1/2,\bar{x}-1/2,\bar{x};$   
 $1/4,-1/4,1/4$   
 $(\bar{3}_{xyz}|1/2,0,0)'$
- (35)  $\bar{3}^- ' \bar{x},\bar{x}+1/2,x;$   
 $-1/4,1/4,1/4$   
 $(\bar{3}_{xyz}|0,0,1/2)'$
- (36)  $\bar{3}^- ' \bar{x}+1/2,x,\bar{x};$   
 $1/4,1/4,-1/4$   
 $(\bar{3}_{xyz}|0,1/2,0)'$
- (37)  $d' (1/4,-1/4,1/4) x+1/2,\bar{x},z$   
 $(m_{xy}|3/4,1/4,1/4)'$
- (38)  $d' (3/4,3/4,3/4) x,x,z$   
 $(m_{xy}|3/4,3/4,3/4)'$
- (39)  $\bar{4}^- ' 0,1/4,z; 0,1/4,3/8$   
 $(\bar{4}_z^{-1}|1/4,1/4,3/4)'$
- (40)  $\bar{4}^+ ' 1/2,1/4,z; 1/2,1/4,1/8$   
 $(\bar{4}_z|1/4,3/4,1/4)'$
- (41)  $\bar{4}^- ' x,0,1/4; 3/8,0,1/4$   
 $(\bar{4}_x^{-1}|3/4,1/4,1/4)'$
- (42)  $d' (1/4,1/4,-1/4) x,y+1/2,\bar{y}$   
 $(m_{yz}|1/4,3/4,1/4)'$
- (43)  $d' (3/4,3/4,3/4) x,y,y$   
 $(m_{yz}|3/4,3/4,3/4)'$
- (44)  $\bar{4}^+ ' x,1/2,1/4; 1/8,1/2,1/4$   
 $(\bar{4}_x|1/4,1/4,3/4)'$
- (45)  $\bar{4}^+ ' 1/4,y,1/2; 1/4,1/8,1/2$   
 $(\bar{4}_y|3/4,1/4,1/4)'$
- (46)  $d' (-1/4,1/4,1/4) \bar{x}+1/2,y,x$   
 $(m_{xz}|1/4,1/4,3/4)'$
- (47)  $\bar{4}^- ' 1/4,y,0; 1/4,3/8,0$   
 $(\bar{4}_y^{-1}|1/4,3/4,1/4)'$
- (48)  $d' (3/4,3/4,3/4) x,y,x$   
 $(m_{xz}|3/4,3/4,3/4)'$

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25); 1'.

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.	Coordinates			
	(0,0,0) + (0,0,0)'	(1/2,1/2,1/2) + (1/2,1/2,1/2)'		
96 h 11'				
(1) x,y,z [0,0,0]	(2) $\bar{x}+1/2, \bar{y}, z+1/2$ [0,0,0]	(3) $\bar{x}, y+1/2, \bar{z}+1/2$ [0,0,0]	(4) $x+1/2, \bar{y}+1/2, \bar{z}$ [0,0,0]	
(5) z,x,y [0,0,0]	(6) $z+1/2, \bar{x}+1/2, \bar{y}$ [0,0,0]	(7) $\bar{z}+1/2, \bar{x}, y+1/2$ [0,0,0]	(8) $\bar{z}, x+1/2, \bar{y}+1/2$ [0,0,0]	
(9) y,z,x [0,0,0]	(10) $\bar{y}, z+1/2, \bar{x}+1/2$ [0,0,0]	(11) $y+1/2, \bar{z}+1/2, \bar{x}$ [0,0,0]	(12) $\bar{y}+1/2, \bar{z}, x+1/2$ [0,0,0]	
(13) $y+3/4, x+1/4, \bar{z}+1/4$ [0,0,0]	(14) $\bar{y}+3/4, \bar{x}+3/4, \bar{z}+3/4$ [0,0,0]	(15) $y+1/4, \bar{x}+1/4, z+3/4$ [0,0,0]	(16) $\bar{y}+1/4, x+3/4, z+1/4$ [0,0,0]	
(17) $x+3/4, z+1/4, \bar{y}+1/4$ [0,0,0]	(18) $\bar{x}+1/4, z+3/4, y+1/4$ [0,0,0]	(19) $\bar{x}+3/4, \bar{z}+3/4, \bar{y}+3/4$ [0,0,0]	(20) $x+1/4, \bar{z}+1/4, y+3/4$ [0,0,0]	
(21) $z+3/4, y+1/4, \bar{x}+1/4$ [w,v,u]	(22) $z+1/4, \bar{y}+1/4, x+3/4$ [0,0,0]	(23) $\bar{z}+1/4, y+3/4, x+1/4$ [0,0,0]	(24) $\bar{z}+3/4, \bar{y}+3/4, \bar{x}+3/4$ [0,0,0]	
(25) $\bar{x}, \bar{y}, \bar{z}$ [0,0,0]	(26) $x+1/2, y, \bar{z}+1/2$ [0,0,0]	(27) $x, \bar{y}+1/2, z+1/2$ [0,0,0]	(28) $\bar{x}+1/2, y+1/2, z$ [0,0,0]	
(29) $\bar{z}, \bar{x}, \bar{y}$ [0,0,0]	(30) $\bar{z}+1/2, x+1/2, y$ [0,0,0]	(31) $z+1/2, x, \bar{y}+1/2$ [0,0,0]	(32) $z, \bar{x}+1/2, y+1/2$ [0,0,0]	
(33) $\bar{y}, \bar{z}, \bar{x}$ [0,0,0]	(34) $y, \bar{z}+1/2, x+1/2$ [0,0,0]	(35) $\bar{y}+1/2, z+1/2, x$ [0,0,0]	(36) $y+1/2, z, \bar{x}+1/2$ [0,0,0]	
(37) $\bar{y}+1/4, \bar{x}+3/4, z+3/4$ [0,0,0]	(38) $y+1/4, x+1/4, z+1/4$ [0,0,0]	(39) $\bar{y}+3/4, x+3/4, \bar{z}+1/4$ [0,0,0]	(40) $y+3/4, \bar{x}+1/4, \bar{z}+3/4$ [0,0,0]	
(41) $\bar{x}+1/4, \bar{z}+3/4, y+3/4$ [0,0,0]	(42) $x+3/4, \bar{z}+1/4, \bar{y}+3/4$ [0,0,0]	(43) $x+1/4, z+1/4, y+1/4$ [0,0,0]	(44) $\bar{x}+3/4, z+3/4, \bar{y}+1/4$ [0,0,0]	
(45) $\bar{z}+1/4, \bar{y}+3/4, x+3/4$ [0,0,0]	(46) $\bar{z}+3/4, y+3/4, \bar{x}+1/4$ [0,0,0]	(47) $z+3/4, \bar{y}+1/4, \bar{x}+3/4$ [0,0,0]	(48) $z+1/4, y+1/4, x+1/4$ [0,0,0]	
48 g ..21'				
1/8, y, $\bar{y}+1/4$ [0,0,0]	3/8, $\bar{y}, \bar{y}+3/4$ [0,0,0]	7/8, $y+1/2, y+1/4$ [0,0,0]	5/8, $\bar{y}+1/2, y+3/4$ [0,0,0]	
$\bar{y}+1/4, 1/8, y$ [0,0,0]	$\bar{y}+3/4, 3/8, \bar{y}$ [0,0,0]	$y+1/4, 7/8, y+1/2$ [0,0,0]	$y+3/4, 5/8, \bar{y}+1/2$ [0,0,0]	
$y, \bar{y}+1/4, 1/8$ [0,0,0]	$\bar{y}, \bar{y}+3/4, 3/8$ [0,0,0]	$y+1/2, y+1/4, 7/8$ [0,0,0]	$\bar{y}+1/2, y+3/4, 5/8$ [0,0,0]	
7/8, $\bar{y}, y+3/4$ [0,0,0]	5/8, $y, y+1/4$ [0,0,0]	1/8, $\bar{y}+1/2, \bar{y}+3/4$ [0,0,0]	3/8, $y+1/2, \bar{y}+1/4$ [0,0,0]	
$y+3/4, 7/8, \bar{y}$ [0,0,0]	$y+1/4, 5/8, y$ [0,0,0]	$\bar{y}+3/4, 1/8, \bar{y}+1/2$ [0,0,0]	$\bar{y}+1/4, 3/8, y+1/2$ [0,0,0]	
$\bar{y}, y+3/4, 7/8$ [0,0,0]	$y, y+1/4, 5/8$ [0,0,0]	$\bar{y}+1/2, \bar{y}+3/4, 1/8$ [0,0,0]	$y+1/2, \bar{y}+1/4, 3/8$ [0,0,0]	
48 f 2..1'	$x, 0, 1/4$ [0,0,0]	$\bar{x}+1/2, 0, 3/4$ [0,0,0]	$1/4, x, 0$ [0,0,0]	$3/4, \bar{x}+1/2, 0$ [0,0,0]
	$0, 1/4, x$ [0,0,0]	$0, 3/4, \bar{x}+1/2$ [0,0,0]	$3/4, x+1/4, 0$ [0,0,0]	$3/4, \bar{x}+3/4, 1/2$ [0,0,0]
	$x+3/4, 1/2, 1/4$ [0,0,0]	$\bar{x}+1/4, 0, 1/4$ [0,0,0]	$0, 1/4, \bar{x}+1/4$ [0,0,0]	$1/2, 1/4, x+3/4$ [0,0,0]
	$\bar{x}, 0, 3/4$ [0,0,0]	$x+1/2, 0, 1/4$ [0,0,0]	$3/4, \bar{x}, 0$ [0,0,0]	$1/4, x+1/4, 0$ [0,0,0]

Continued

230.2.1648

Ia $\bar{3}$ d1'

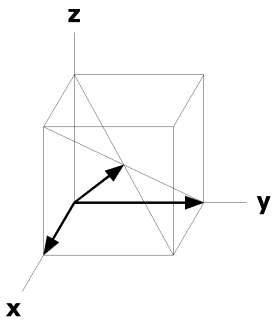
			0,3/4, $\bar{x}$ [0,0,0]	0,1/4,x+1/2 [0,0,0]	1/4, $\bar{x}$ +3/4,0 [0,0,0]	1/4,x+1/4,1/2 [0,0,0]
			$\bar{x}$ +1/4,1/2,3/4 [0,0,0]	x+3/4,0,3/4 [0,0,0]	0,3/4,x+3/4 [0,0,0]	1/2,3/4, $\bar{x}$ +1/4 [0,0,0]
32	e	.3.1'				
			x,x,x [0,0,0]	$\bar{x}$ +1/2, $\bar{x}$ ,x+1/2 [0,0,0]	$\bar{x}$ ,x+1/2, $\bar{x}$ +1/2 [0,0,0]	x+1/2, $\bar{x}$ +1/2, $\bar{x}$ [0,0,0]
			x+3/4,x+1/4, $\bar{x}$ +1/4 [0,0,0]	$\bar{x}$ +3/4, $\bar{x}$ +3/4, $\bar{x}$ +3/4 [0,0,0]	x+1/4, $\bar{x}$ +1/4,x+3/4 [0,0,0]	$\bar{x}$ +1/4,x+3/4,x+1/4 [0,0,0]
			$\bar{x}$ , $\bar{x}$ , $\bar{x}$ [0,0,0]	x+1/2,x, $\bar{x}$ +1/2 [0,0,0]	x, $\bar{x}$ +1/2,x+1/2 [0,0,0]	$\bar{x}$ +1/2,x+1/2,x [0,0,0]
			$\bar{x}$ +1/4, $\bar{x}$ +3/4,x+3/4 [0,0,0]	x+1/4,x+1/4,x+1/4 [0,0,0]	$\bar{x}$ +3/4,x+3/4, $\bar{x}$ +1/4 [0,0,0]	x+3/4, $\bar{x}$ +1/4, $\bar{x}$ +3/4 [0,0,0]
12	d	$\bar{4}$ ..1'	3/8,0,1/4 [0,0,0]	1/8,0,3/4 [0,0,0]	1/4,3/8,0 [0,0,0]	3/4,1/8,0 [0,0,0]
			0,1/4,3/8 [0,0,0]	0,3/4,1/8 [0,0,0]	3/4,5/8,0 [0,0,0]	3/4,3/8,1/2 [0,0,0]
			1/8,1/2,1/4 [0,0,0]	7/8,0,1/4 [0,0,0]	0,1/4,7/8 [0,0,0]	1/2,1/4,1/8 [0,0,0]
24	c	2.221'	1/8,0,1/4 [0,0,0]	3/8,0,3/4 [0,0,0]	1/4,1/8,0 [0,0,0]	3/4,3/8,0 [0,0,0]
			0,1/4,1/8 [0,0,0]	0,3/4,3/8 [0,0,0]	7/8,0,3/4 [0,0,0]	5/8,0,1/4 [0,0,0]
			3/4,7/8,0 [0,0,0]	1/4,5/8,0 [0,0,0]	0,3/4,7/8 [0,0,0]	0,1/4,5/8 [0,0,0]
16	b	.321'	1/8,1/8,1/8 [0,0,0]	3/8,7/8,5/8 [0,0,0]	7/8,5/8,3/8 [0,0,0]	5/8,3/8,7/8 [0,0,0]
			7/8,7/8,7/8 [0,0,0]	5/8,1/8,3/8 [0,0,0]	1/8,3/8,5/8 [0,0,0]	3/8,5/8,1/8 [0,0,0]
16	a	$\bar{3}$ .1'	0,0,0 [0,0,0]	1/2,0,1/2 [0,0,0]	0,1/2,1/2 [0,0,0]	1/2,1/2,0 [0,0,0]
			3/4,1/4,1/4 [0,0,0]	3/4,3/4,3/4 [0,0,0]	1/4,1/4,3/4 [0,0,0]	1/4,3/4,1/4 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4,0,z

Along [1,1,1] p6mm1'  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x,x,x

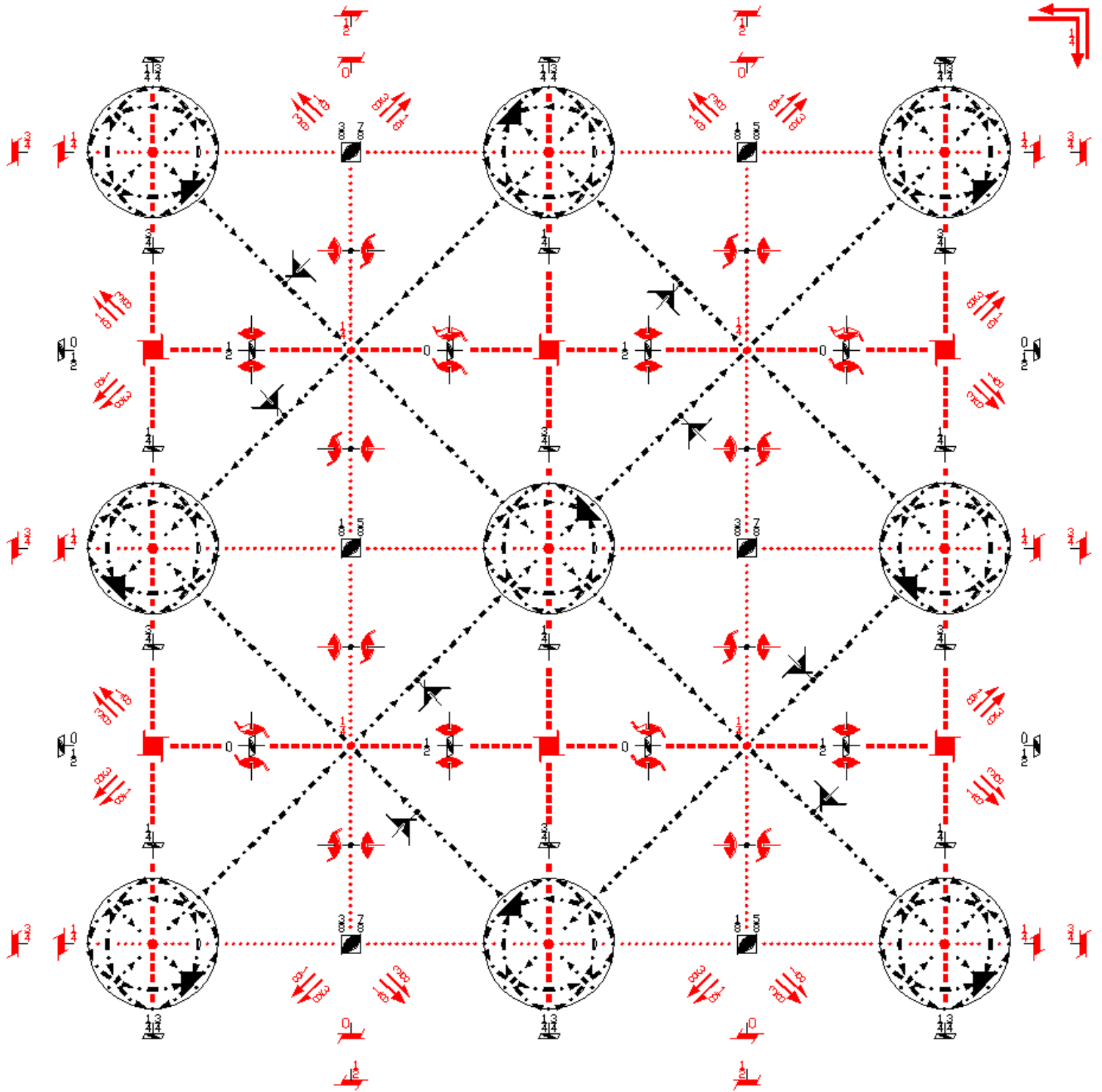
Along [1,1,0] c2mm1'  
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at x,x+1/4,1/8



$1a\bar{3}'d$   
230.3.1649

$m\bar{3}'m$   
 $I4_1'/a\bar{3}'2'/d$

Cubic





Origin at center ( $\bar{3}$ )

**Asymmetric unit**  $-1/8 \leq x \leq 1/8$ ;  $-1/8 \leq y \leq 1/8$ ;  $0 \leq z \leq 1/4$ ;  $\max(x, -x, y, -y) \leq z$

Vertices  $0,0,0$   $1/8, 1/8, 1/8$   $-1/8, 1/8, 1/8$   $-1/8, -1/8, 1/8$   $1/8, -1/8, 1/8$   
 $1/8, 1/8, 1/4$   $-1/8, 1/8, 1/4$   $-1/8, -1/8, 1/4$   $1/8, -1/8, 1/4$

## Symmetry Operations

For (0,0,0) + set

- |   |   |  |   |
|---|---|--|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)  | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)  |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)                         | (6) 3 <sup>+</sup> $\bar{x}+1/2, x, \bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,1/2,0)                          | (7) 3 <sup>+</sup> $x+1/2, \bar{x}-1/2, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2)                        | (8) 3 <sup>+</sup> $\bar{x}, \bar{x}+1/2, x$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,1/2,1/2)                          |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)                         | (10) 3 <sup>-</sup> (-1/3,1/3,1/3)<br>x+1/6, x+1/6, $\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub>  0,1/2,1/2)                       | (11) 3 <sup>-</sup> (1/3,1/3,-1/3)<br>x+1/3, x+1/6, x<br>(3 <sub>x<math>\bar{y}z</math></sub>  1/2,1/2,0)              | (12) 3 <sup>-</sup> (1/3,-1/3,1/3)<br>x-1/6, x+1/3, $\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub>  1/2,0,1/2)                       |
| (13) 2' (1/2,1/2,0) x,x-1/4,1/8<br>(2 <sub>xy</sub>  3/4,1/4,1/4)'                          | (14) 2' x, $\bar{x}+3/4, 3/8$<br>(2 <sub>xy</sub>  3/4,3/4,3/4)'  | (15) 4' (0,0,3/4) 1/4,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/4,1/4,3/4)'  | (16) 4' (0,0,1/4) -1/4,1/2,z<br>(4 <sub>z</sub>  1/4,3/4,1/4)'  |
| (17) 4' (3/4,0,0) x,1/4,0<br>(4 <sub>x</sub> <sup>-1</sup>  3/4,1/4,1/4)'                   | (18) 2' (0,1/2,1/2) 1/8,y+1/4,y<br>(2 <sub>yz</sub>  1/4,3/4,1/4)'  | (19) 2' 3/8,y+3/4, $\bar{y}$<br>(2 <sub>yz</sub>  3/4,3/4,3/4)'  | (20) 4' (1/4,0,0) x,-1/4,1/2<br>(4 <sub>x</sub>  1/4,1/4,3/4)'  |
| (21) 4' (0,1/4,0) 1/2,y,-1/4<br>(4 <sub>y</sub>  3/4,1/4,1/4)'                              | (22) 2' (1/2,0,1/2) x-1/4,1/8,x<br>(2 <sub>xz</sub>  1/4,1/4,3/4)'  | (23) 4' (0,3/4,0) 0,y,1/4<br>(4 <sub>y</sub> <sup>-1</sup>  1/4,3/4,1/4)'  | (24) 2' $\bar{x}+3/4, 3/8, x$<br>(2 <sub>xz</sub>  3/4,3/4,3/4)'  |
| (25) $\bar{1}$ 0,0,0<br>(1 0,0,0)'  | (26) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)'   | (27) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)'  | (28) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)'   |
| (29) $\bar{3}^+$ x,x,x; 0,0,0<br>( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>  0,0,0)'          | (30) $\bar{3}^+$ $\bar{x}-1/2, x+1, \bar{x}$ ;<br>0,1/2,1/2<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,1/2,0)' | (31) $\bar{3}^+$ $x+1/2, \bar{x}+1/2, \bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2)' | (32) $\bar{3}^+$ $\bar{x}+1, \bar{x}+1/2, x$ ;<br>1/2,0,1/2<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,1/2,1/2)' |
| (33) $\bar{3}^-$ x,x,x; 0,0,0<br>( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>  0,0,0)'          | (34) $\bar{3}^-$ $x+1/2, \bar{x}-1/2, \bar{x}$ ; 0,0,1/2<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub>  0,1/2,1/2)'                  | (35) $\bar{3}^-$ $\bar{x}, \bar{x}+1/2, x$ ; 0,1/2,0<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub>  1/2,1/2,0)'     | (36) $\bar{3}^-$ $\bar{x}+1/2, x, \bar{x}$ ; 1/2,0,0<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub>  1/2,0,1/2)'                      |
| (37) d (-1/4,1/4,1/4) x+1/2, $\bar{x}, z$<br>(m <sub>xy</sub>  1/4,3/4,3/4)                 | (38) d (1/4,1/4,1/4) x,x,z<br>(m <sub>xy</sub>  1/4,1/4,1/4)  | (39) $\bar{4}^-$ 0,3/4,z; 0,3/4,1/8<br>( $\bar{4}$ <sub>z</sub> <sup>-1</sup>  3/4,3/4,1/4)                            | (40) $\bar{4}^+$ 1/2,-1/4,z; 1/2,-1/4,3/8<br>( $\bar{4}$ <sub>z</sub>  3/4,1/4,3/4)   |
| (41) $\bar{4}^-$ x,0,3/4; 1/8,0,3/4<br>( $\bar{4}$ <sub>x</sub> <sup>-1</sup>  1/4,3/4,3/4) | (42) d (3/4,-1/4,1/4) x,y+1/2, $\bar{y}$<br>(m <sub>yz</sub>  3/4,1/4,3/4)  | (43) d (1/4,1/4,1/4) x,y,y<br>(m <sub>yz</sub>  1/4,1/4,1/4)   | (44) $\bar{4}^+$ x,1/2,-1/4; 3/8,1/2,-1/4<br>( $\bar{4}$ <sub>x</sub>  3/4,3/4,1/4)   |
| (45) $\bar{4}^+$ -1/4,y,1/2; -1/4,3/8,1/2<br>( $\bar{4}$ <sub>y</sub>  1/4,3/4,3/4)         | (46) d (1/4,3/4,-1/4) $\bar{x}+1/2, y, x$<br>(m <sub>xz</sub>  3/4,3/4,1/4)   | (47) $\bar{4}^-$ 3/4,y,0; 3/4,1/8,0<br>( $\bar{4}$ <sub>y</sub> <sup>-1</sup>  3/4,1/4,3/4)                            | (48) d (1/4,1/4,1/4) x,y,x<br>(m <sub>xz</sub>  1/4,1/4,1/4)  |

For (1/2,1/2,1/2) + set

- |   |  |   |  |
|---|--|---|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                                    | (2) 2 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,0)   | (3) 2 1/4,y,0<br>(2 <sub>y</sub>  1/2,0,0)  | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)   |
| (5) 3 <sup>+</sup> (1/2,1/2,1/2) x,x,x<br>(3 <sub>xyz</sub>  1/2,1/2,1/2) | (6) 3 <sup>+</sup> (1/6,-1/6,1/6)<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,1/2) | (7) 3 <sup>+</sup> (-1/6,1/6,1/6)<br>x+1/6, $\bar{x}+1/6, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,0) | (8) 3 <sup>+</sup> (1/6,1/6,-1/6)<br>$\bar{x}+1/3, \bar{x}+1/6, x$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,0,0) |

(9) $3^- (1/2, 1/2, 1/2) \ x, x, x$ ( $3_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(10) $3^- (1/6, -1/6, -1/6) \ \bar{x}$ $x+1/6, x+1/6, \bar{x}$ ( $3_{xyz}   1/2, 0, 0$ )	(11) $3^- (-1/6, -1/6, 1/6)$ $x+1/3, x+1/6, x$ ( $3_{xyz}   0, 0, 1/2$ )	(12) $3^- (-1/6, 1/6, -1/6) \ \bar{x}$ $x-1/6, x+1/3, \bar{x}$ ( $3_{xyz}   0, 1/2, 0$ )
(13) $2' (1/2, 1/2, 0) \ x, x+1/4, 3/8$ ( $2_{xy}   1/4, 3/4, 3/4$ )	(14) $2' \ x, \bar{x}+1/4, 1/8$ ( $2_{xy}   1/4, 1/4, 1/4$ )	(15) $4^- (0, 0, 1/4) \ 3/4, 0, z$ ( $4_z^{-1}   3/4, 3/4, 1/4$ )	(16) $4^+ (0, 0, 3/4) \ 1/4, 1/2, z$ ( $4_z   3/4, 1/4, 3/4$ )
(17) $4^- (1/4, 0, 0) \ x, 3/4, 0$ ( $4_x^{-1}   1/4, 3/4, 3/4$ )	(18) $2' (0, 1/2, 1/2) \ 3/8, y-1/4, y$ ( $2_{yz}   3/4, 1/4, 3/4$ )	(19) $2' \ 1/8, y+1/4, \bar{y}$ ( $2_{yz}   1/4, 1/4, 1/4$ )	(20) $4^+ (3/4, 0, 0) \ x, 1/4, 1/2$ ( $4_x   3/4, 3/4, 1/4$ )
(21) $4^+ (0, 3/4, 0) \ 1/2, y, 1/4$ ( $4_y   1/4, 3/4, 3/4$ )	(22) $2' (1/2, 0, 1/2) \ x+1/4, 3/8, x$ ( $2_{xz}   3/4, 3/4, 1/4$ )	(23) $4^- (0, 1/2, 0) \ 0, y, 3/4$ ( $4_y^{-1}   3/4, 1/4, 3/4$ )	(24) $2' \ \bar{x}+1/4, 1/8, x$ ( $2_{xz}   1/4, 1/4, 1/4$ )
(25) $\bar{1}^+ \ 1/4, 1/4, 1/4$ ( $\bar{1}   1/2, 1/2, 1/2$ )	(26) $b' (0, 1/2, 0) \ x, y, 0$ ( $m_z   0, 1/2, 0$ )	(27) $a' (1/2, 0, 0) \ x, 0, z$ ( $m_y   1/2, 0, 0$ )	(28) $c' (0, 0, 1/2) \ 0, y, z$ ( $m_x   0, 0, 1/2$ )
(29) $\bar{3}^+ \ x, x, x;$ $1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 1/2, 1/2$ )	(30) $\bar{3}^+ \ \bar{x}-1/2, x, \bar{x};$ $-1/4, -1/4, 1/4$ ( $\bar{3}_{xyz}^{-1}   0, 0, 1/2$ )	(31) $\bar{3}^+ \ x-1/2, \bar{x}+1/2, \bar{x};$ $-1/4, 1/4, -1/4$ ( $\bar{3}_{xyz}^{-1}   0, 1/2, 0$ )	(32) $\bar{3}^+ \ \bar{x}, \bar{x}-1/2, x;$ $1/4, -1/4, -1/4$ ( $\bar{3}_{xyz}^{-1}   1/2, 0, 0$ )
(33) $\bar{3}^- \ x, x, x;$ $1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(34) $\bar{3}^- \ x+1/2, \bar{x}-1/2, \bar{x};$ $1/4, -1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 0, 0$ )	(35) $\bar{3}^- \ \bar{x}, \bar{x}+1/2, x;$ $-1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}   0, 0, 1/2$ )	(36) $\bar{3}^- \ \bar{x}+1/2, x, \bar{x};$ $1/4, 1/4, -1/4$ ( $\bar{3}_{xyz}   0, 1/2, 0$ )
(37) $d (1/4, -1/4, 1/4) \ x+1/2, \bar{x}, z$ ( $m_{xy}   3/4, 1/4, 1/4$ )	(38) $d (3/4, 3/4, 3/4) \ x, x, z$ ( $m_{xy}   3/4, 3/4, 3/4$ )	(39) $\bar{4}^- \ 0, 1/4, z; \ 0, 1/4, 3/8$ ( $\bar{4}_z^{-1}   1/4, 1/4, 3/4$ )	(40) $\bar{4}^+ \ 1/2, 1/4, z; \ 1/2, 1/4, 1/8$ ( $\bar{4}_z   1/4, 3/4, 1/4$ )
(41) $\bar{4}^- \ x, 0, 1/4; \ 3/8, 0, 1/4$ ( $\bar{4}_x^{-1}   3/4, 1/4, 1/4$ )	(42) $d (1/4, 1/4, -1/4) \ x, y+1/2, \bar{y}$ ( $m_{yz}   1/4, 3/4, 1/4$ )	(43) $d (3/4, 3/4, 3/4) \ x, y, y$ ( $m_{yz}   3/4, 3/4, 3/4$ )	(44) $\bar{4}^+ \ x, 1/2, 1/4; \ 1/8, 1/2, 1/4$ ( $\bar{4}_x   1/4, 1/4, 3/4$ )
(45) $\bar{4}^+ \ 1/4, y, 1/2; \ 1/4, 1/8, 1/2$ ( $\bar{4}_y   3/4, 1/4, 1/4$ )	(46) $d (-1/4, 1/4, 1/4) \ \bar{x}+1/2, y, x$ ( $m_{xz}   1/4, 1/4, 3/4$ )	(47) $\bar{4}^- \ 1/4, y, 0; \ 1/4, 3/8, 0$ ( $\bar{4}_y^{-1}   1/4, 3/4, 1/4$ )	(48) $d (3/4, 3/4, 3/4) \ x, y, x$ ( $m_{xz}   3/4, 3/4, 3/4$ )

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates								
96	h	1	(0,0,0) +	(1/2,1/2,1/2) +							
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}+1/2, \bar{y}, z+1/2$	$[\bar{u}, \bar{v}, w]$	(3)	$\bar{x}, y+1/2, \bar{z}+1/2$	$[\bar{u}, v, \bar{w}]$	(4)	$x+1/2, \bar{y}+1/2, \bar{z}$	$[u, \bar{v}, \bar{w}]$
(5)	z,x,y	[w,u,v]	(6)	$z+1/2, \bar{x}+1/2, \bar{y}$	$[w, \bar{u}, \bar{v}]$	(7)	$\bar{z}+1/2, \bar{x}, y+1/2$	$[\bar{w}, \bar{u}, v]$	(8)	$\bar{z}, x+1/2, \bar{y}+1/2$	$[\bar{w}, u, \bar{v}]$
(9)	y,z,x	[v,w,u]	(10)	$\bar{y}, z+1/2, \bar{x}+1/2$	$[\bar{v}, w, \bar{u}]$	(11)	$y+1/2, \bar{z}+1/2, \bar{x}$	$[v, \bar{w}, \bar{u}]$	(12)	$\bar{y}+1/2, \bar{z}, x+1/2$	$[\bar{v}, \bar{w}, u]$
(13)	$y+3/4, x+1/4, \bar{z}+1/4$	$[\bar{v}, \bar{u}, w]$	(14)	$\bar{y}+3/4, \bar{x}+3/4, \bar{z}+3/4$	$[v, u, w]$	(15)	$y+1/4, \bar{x}+1/4, z+3/4$	$[\bar{v}, u, \bar{w}]$	(16)	$\bar{y}+1/4, x+3/4, z+1/4$	$[v, \bar{u}, \bar{w}]$
(17)	$x+3/4, z+1/4, \bar{y}+1/4$	$[\bar{u}, \bar{w}, v]$	(18)	$\bar{x}+1/4, z+3/4, y+1/4$	$[u, \bar{w}, \bar{v}]$	(19)	$\bar{x}+3/4, \bar{z}+3/4, \bar{y}+3/4$	$[u, w, v]$	(20)	$x+1/4, \bar{z}+1/4, y+3/4$	$[\bar{u}, w, \bar{v}]$
(21)	$z+3/4, y+1/4, \bar{x}+1/4$	$[\bar{w}, \bar{v}, u]$	(22)	$z+1/4, \bar{y}+1/4, x+3/4$	$[\bar{w}, v, \bar{u}]$	(23)	$\bar{z}+1/4, y+3/4, x+1/4$	$[w, \bar{v}, \bar{u}]$	(24)	$\bar{z}+3/4, \bar{y}+3/4, \bar{x}+3/4$	$[w, v, u]$
(25)	$\bar{x}, \bar{y}, \bar{z}$	$[\bar{u}, \bar{v}, \bar{w}]$	(26)	$x+1/2, y, \bar{z}+1/2$	$[u, v, \bar{w}]$	(27)	$x, \bar{y}+1/2, z+1/2$	$[u, \bar{v}, w]$	(28)	$\bar{x}+1/2, y+1/2, z$	$[\bar{u}, v, w]$

- (29)  $\bar{z}, \bar{x}, \bar{y} [\bar{w}, \bar{u}, \bar{v}]$  (30)  $\bar{z}+1/2, \bar{x}+1/2, \bar{y} [\bar{w}, \bar{u}, \bar{v}]$  (31)  $z+1/2, x, \bar{y}+1/2 [\bar{w}, \bar{u}, \bar{v}]$  (32)  $z, \bar{x}+1/2, \bar{y}+1/2 [\bar{w}, \bar{u}, \bar{v}]$   
 (33)  $\bar{y}, \bar{z}, \bar{x} [\bar{v}, \bar{w}, \bar{u}]$  (34)  $y, \bar{z}+1/2, \bar{x}+1/2 [\bar{v}, \bar{w}, \bar{u}]$  (35)  $\bar{y}+1/2, z+1/2, x [\bar{v}, \bar{w}, \bar{u}]$  (36)  $y+1/2, z, \bar{x}+1/2 [\bar{v}, \bar{w}, \bar{u}]$   
 (37)  $\bar{y}+1/4, \bar{x}+3/4, z+3/4 [\bar{v}, \bar{u}, \bar{w}]$  (38)  $y+1/4, \bar{x}+1/4, z+1/4 [\bar{v}, \bar{u}, \bar{w}]$  (39)  $\bar{y}+3/4, \bar{x}+3/4, \bar{z}+1/4 [\bar{v}, \bar{u}, \bar{w}]$  (40)  $y+3/4, \bar{x}+1/4, \bar{z}+3/4 [\bar{v}, \bar{u}, \bar{w}]$   
 (41)  $\bar{x}+1/4, \bar{z}+3/4, \bar{y}+3/4 [\bar{u}, \bar{w}, \bar{v}]$  (42)  $x+3/4, \bar{z}+1/4, \bar{y}+3/4 [\bar{u}, \bar{w}, \bar{v}]$  (43)  $x+1/4, z+1/4, \bar{y}+1/4 [\bar{u}, \bar{w}, \bar{v}]$  (44)  $\bar{x}+3/4, \bar{z}+3/4, \bar{y}+1/4 [\bar{u}, \bar{w}, \bar{v}]$   
 (45)  $\bar{z}+1/4, \bar{y}+3/4, \bar{x}+3/4 [\bar{w}, \bar{v}, \bar{u}]$  (46)  $\bar{z}+3/4, \bar{y}+3/4, \bar{x}+1/4 [\bar{w}, \bar{v}, \bar{u}]$  (47)  $z+3/4, \bar{y}+1/4, \bar{x}+3/4 [\bar{w}, \bar{v}, \bar{u}]$  (48)  $z+1/4, \bar{y}+1/4, \bar{x}+1/4 [\bar{w}, \bar{v}, \bar{u}]$

48 g ..2'

- $1/8, \bar{y}, \bar{y}+1/4 [\bar{u}, \bar{v}, \bar{v}]$   $3/8, \bar{y}, \bar{y}+3/4 [\bar{u}, \bar{v}, \bar{v}]$   $7/8, \bar{y}+1/2, \bar{y}+1/4 [\bar{u}, \bar{v}, \bar{v}]$   $5/8, \bar{y}+1/2, \bar{y}+3/4 [\bar{u}, \bar{v}, \bar{v}]$   
 $\bar{y}+1/4, 1/8, \bar{y} [\bar{v}, \bar{u}, \bar{v}]$   $\bar{y}+3/4, 3/8, \bar{y} [\bar{v}, \bar{u}, \bar{v}]$   $\bar{y}+1/4, 7/8, \bar{y}+1/2 [\bar{v}, \bar{u}, \bar{v}]$   $\bar{y}+3/4, 5/8, \bar{y}+1/2 [\bar{v}, \bar{u}, \bar{v}]$   
 $\bar{y}, \bar{y}+1/4, 1/8 [\bar{v}, \bar{v}, \bar{u}]$   $\bar{y}, \bar{y}+3/4, 3/8 [\bar{v}, \bar{v}, \bar{u}]$   $\bar{y}+1/2, \bar{y}+1/4, 7/8 [\bar{v}, \bar{v}, \bar{u}]$   $\bar{y}+1/2, \bar{y}+3/4, 5/8 [\bar{v}, \bar{v}, \bar{u}]$   
 $7/8, \bar{y}, \bar{y}+3/4 [\bar{u}, \bar{v}, \bar{v}]$   $5/8, \bar{y}, \bar{y}+1/4 [\bar{u}, \bar{v}, \bar{v}]$   $1/8, \bar{y}+1/2, \bar{y}+3/4 [\bar{u}, \bar{v}, \bar{v}]$   $3/8, \bar{y}+1/2, \bar{y}+1/4 [\bar{u}, \bar{v}, \bar{v}]$   
 $\bar{y}+3/4, 7/8, \bar{y} [\bar{v}, \bar{u}, \bar{v}]$   $\bar{y}+1/4, 5/8, \bar{y} [\bar{v}, \bar{u}, \bar{v}]$   $\bar{y}+3/4, 1/8, \bar{y}+1/2 [\bar{v}, \bar{u}, \bar{v}]$   $\bar{y}+1/4, 3/8, \bar{y}+1/2 [\bar{v}, \bar{u}, \bar{v}]$   
 $\bar{y}, \bar{y}+3/4, 7/8 [\bar{v}, \bar{v}, \bar{u}]$   $\bar{y}, \bar{y}+1/4, 5/8 [\bar{v}, \bar{v}, \bar{u}]$   $\bar{y}+1/2, \bar{y}+3/4, 1/8 [\bar{v}, \bar{v}, \bar{u}]$   $\bar{y}+1/2, \bar{y}+1/4, 3/8 [\bar{v}, \bar{v}, \bar{u}]$

- 48 f 2..  $x, 0, 1/4 [\bar{u}, 0, 0]$   $\bar{x}+1/2, 0, 3/4 [\bar{u}, 0, 0]$   $1/4, x, 0 [0, \bar{u}, 0]$   $3/4, \bar{x}+1/2, 0 [0, \bar{u}, 0]$   
 $0, 1/4, x [0, 0, \bar{u}]$   $0, 3/4, \bar{x}+1/2 [0, 0, \bar{u}]$   $3/4, x+1/4, 0 [0, \bar{u}, 0]$   $3/4, \bar{x}+3/4, 1/2 [0, \bar{u}, 0]$   
 $x+3/4, 1/2, 1/4 [\bar{u}, 0, 0]$   $\bar{x}+1/4, 0, 1/4 [\bar{u}, 0, 0]$   $0, 1/4, \bar{x}+1/4 [0, 0, \bar{u}]$   $1/2, 1/4, x+3/4 [0, 0, \bar{u}]$   
 $\bar{x}, 0, 3/4 [\bar{u}, 0, 0]$   $x+1/2, 0, 1/4 [\bar{u}, 0, 0]$   $3/4, \bar{x}, 0 [0, \bar{u}, 0]$   $1/4, x+1/4, 0 [0, \bar{u}, 0]$   
 $0, 3/4, \bar{x} [0, 0, \bar{u}]$   $0, 1/4, x+1/2 [0, 0, \bar{u}]$   $1/4, \bar{x}+3/4, 0 [0, \bar{u}, 0]$   $1/4, x+1/4, 1/2 [0, \bar{u}, 0]$   
 $\bar{x}+1/4, 1/2, 3/4 [\bar{u}, 0, 0]$   $x+3/4, 0, 3/4 [\bar{u}, 0, 0]$   $0, 3/4, x+3/4 [0, 0, \bar{u}]$   $1/2, 3/4, \bar{x}+1/4 [0, 0, \bar{u}]$

32 e .3.

- $x, x, x [\bar{u}, \bar{u}, \bar{u}]$   $\bar{x}+1/2, \bar{x}, \bar{x}+1/2 [\bar{u}, \bar{u}, \bar{u}]$   $\bar{x}, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, \bar{u}]$   $x+1/2, \bar{x}+1/2, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$   
 $x+3/4, \bar{x}+1/4, \bar{x}+1/4 [\bar{u}, \bar{u}, \bar{u}]$   $\bar{x}+3/4, \bar{x}+3/4, \bar{x}+3/4 [\bar{u}, \bar{u}, \bar{u}]$   $x+1/4, \bar{x}+1/4, x+3/4 [\bar{u}, \bar{u}, \bar{u}]$   $\bar{x}+1/4, x+3/4, \bar{x}+1/4 [\bar{u}, \bar{u}, \bar{u}]$   
 $\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$   $x+1/2, \bar{x}, \bar{x}+1/2 [\bar{u}, \bar{u}, \bar{u}]$   $x, \bar{x}+1/2, \bar{x}+1/2 [\bar{u}, \bar{u}, \bar{u}]$   $\bar{x}+1/2, \bar{x}+1/2, x [\bar{u}, \bar{u}, \bar{u}]$   
 $\bar{x}+1/4, \bar{x}+3/4, x+3/4 [\bar{u}, \bar{u}, \bar{u}]$   $x+1/4, \bar{x}+1/4, x+1/4 [\bar{u}, \bar{u}, \bar{u}]$   $\bar{x}+3/4, x+3/4, \bar{x}+1/4 [\bar{u}, \bar{u}, \bar{u}]$   $x+3/4, \bar{x}+1/4, \bar{x}+3/4 [\bar{u}, \bar{u}, \bar{u}]$

- 12 d 4..  $3/8, 0, 1/4 [\bar{u}, 0, 0]$   $1/8, 0, 3/4 [\bar{u}, 0, 0]$   $1/4, 3/8, 0 [0, \bar{u}, 0]$   $3/4, 1/8, 0 [0, \bar{u}, 0]$   
 $0, 1/4, 3/8 [0, 0, \bar{u}]$   $0, 3/4, 1/8 [0, 0, \bar{u}]$   $3/4, 5/8, 0 [0, \bar{u}, 0]$   $3/4, 3/8, 1/2 [0, \bar{u}, 0]$   
 $1/8, 1/2, 1/4 [\bar{u}, 0, 0]$   $7/8, 0, 1/4 [\bar{u}, 0, 0]$   $0, 1/4, 7/8 [0, 0, \bar{u}]$   $1/2, 1/4, 1/8 [0, 0, \bar{u}]$

- 24 c 2.2'2'  $1/8, 0, 1/4 [\bar{u}, 0, 0]$   $3/8, 0, 3/4 [\bar{u}, 0, 0]$   $1/4, 1/8, 0 [0, \bar{u}, 0]$   $3/4, 3/8, 0 [0, \bar{u}, 0]$   
 $0, 1/4, 1/8 [0, 0, \bar{u}]$   $0, 3/4, 3/8 [0, 0, \bar{u}]$   $7/8, 0, 3/4 [\bar{u}, 0, 0]$   $5/8, 0, 1/4 [\bar{u}, 0, 0]$   
 $3/4, 7/8, 0 [0, \bar{u}, 0]$   $1/4, 5/8, 0 [0, \bar{u}, 0]$   $0, 3/4, 7/8 [0, 0, \bar{u}]$   $0, 1/4, 5/8 [0, 0, \bar{u}]$

Continued

230.3.1649

Ia $\bar{3}$ 'd

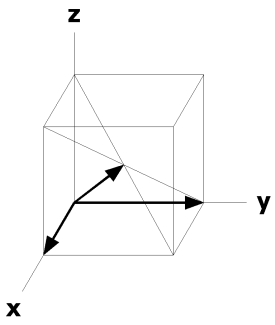
16	b	.32'	1/8, 1/8, 1/8 [u, u, u]	3/8, 7/8, 5/8 [ $\bar{u}$ , $\bar{u}$ , u]	7/8, 5/8, 3/8 [ $\bar{u}$ , u, $\bar{u}$ ]	5/8, 3/8, 7/8 [u, $\bar{u}$ , $\bar{u}$ ]
			7/8, 7/8, 7/8 [ $\bar{u}$ , $\bar{u}$ , $\bar{u}$ ]	5/8, 1/8, 3/8 [u, u, $\bar{u}$ ]	1/8, 3/8, 5/8 [u, $\bar{u}$ , u]	3/8, 5/8, 1/8 [ $\bar{u}$ , u, u]
16	a	$\bar{.3}$ '	0, 0, 0 [0, 0, 0]	1/2, 0, 1/2 [0, 0, 0]	0, 1/2, 1/2 [0, 0, 0]	1/2, 1/2, 0 [0, 0, 0]
			3/4, 1/4, 1/4 [0, 0, 0]	3/4, 3/4, 3/4 [0, 0, 0]	1/4, 1/4, 3/4 [0, 0, 0]	1/4, 3/4, 1/4 [0, 0, 0]

### Symmetry of Special Projections

Along [0, 0, 1] p4'm'm  
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at 1/4, 0, z

Along [1, 1, 1] p6mm  
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at x, x, x

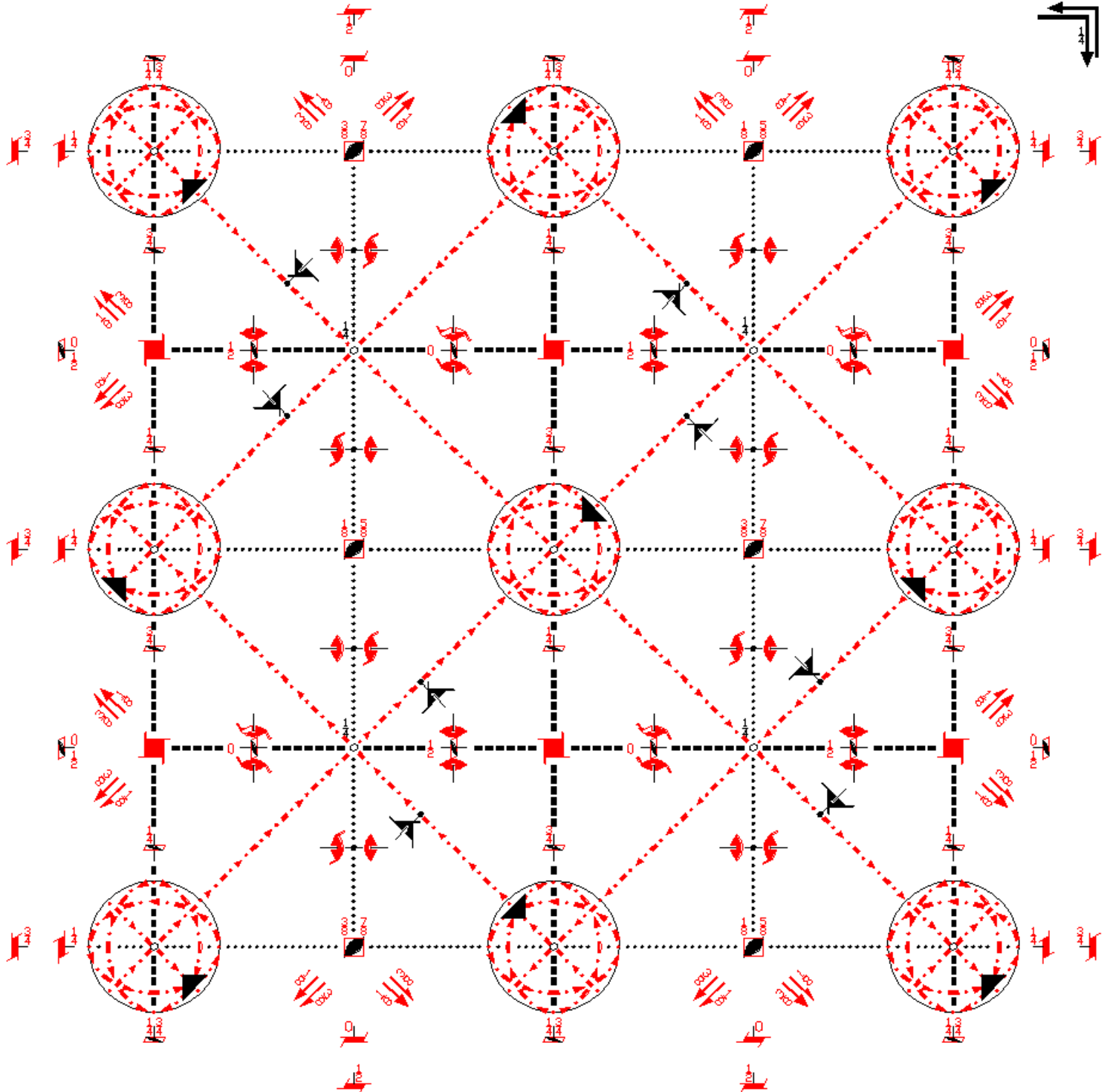
Along [1, 1, 0] c $_p$ -2'mm'  
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at x, x+1/4, 1/8



$1a\bar{3}d'$   
230.4.1650

$m\bar{3}m'$   
 $I4_1'/a\bar{3}2'/d'$

Cubic



Origin at center ( $\bar{3}$ )Asymmetric unit  $-1/8 \leq x \leq 1/8$ ;  $-1/8 \leq y \leq 1/8$ ;  $0 \leq z \leq 1/4$ ;  $\max(x, -x, y, -y) \leq z$ 

Vertices	0,0,0	1/8,1/8,1/8	-1/8,1/8,1/8	-1/8,-1/8,1/8	1/8,-1/8,1/8
	1/8,1/8,1/4	-1/8,1/8,1/4	-1/8,-1/8,1/4	1/8,-1/8,1/4	

## Symmetry Operations

For (0,0,0) + set

- |  |  |  |  |
|--|--|--|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)   | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)                            | (6) 3 <sup>+</sup> $\bar{x}+1/2, x, \bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,1/2,0)                         | (7) 3 <sup>+</sup> $x+1/2, \bar{x}-1/2, \bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,0,1/2)                       | (8) 3 <sup>+</sup> $\bar{x}, \bar{x}+1/2, x$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,1/2,1/2)                         |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)                            | (10) 3 <sup>-</sup> (-1/3,1/3,1/3)<br>x+1/6, x+1/6, $\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub>  0,1/2,1/2)                      | (11) 3 <sup>-</sup> (1/3,1/3,-1/3)<br>x+1/3, x+1/6, x<br>(3 <sub>x<math>\bar{y}z</math></sub>  1/2,1/2,0)                                | (12) 3 <sup>-</sup> (1/3,-1/3,1/3)<br>x-1/6, x+1/3, $\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub>  1/2,0,1/2)                      |
| (13) 2' (1/2,1/2,0) x,x-1/4,1/8<br>(2 <sub>xy</sub>  3/4,1/4,1/4)'                             | (14) 2' x, $\bar{x}+3/4, 3/8$<br>(2 <sub>xy</sub>  3/4,3/4,3/4)'   | (15) 4 <sup>-</sup> (0,0,3/4) 1/4,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/4,1/4,3/4)'  | (16) 4 <sup>+</sup> (0,0,1/4) -1/4,1/2,z<br>(4 <sub>z</sub>  1/4,3/4,1/4)'   |
| (17) 4 <sup>-</sup> (3/4,0,0) x,1/4,0<br>(4 <sub>x</sub> <sup>-1</sup>  3/4,1/4,1/4)'          | (18) 2' (0,1/2,1/2) 1/8,y+1/4,y<br>(2 <sub>yz</sub>  1/4,3/4,1/4)'   | (19) 2' 3/8,y+3/4, $\bar{y}$<br>(2 <sub>yz</sub>  3/4,3/4,3/4)'  | (20) 4 <sup>+</sup> (1/4,0,0) x,-1/4,1/2<br>(4 <sub>x</sub>  1/4,1/4,3/4)'   |
| (21) 4 <sup>+</sup> (0,1/4,0) 1/2,y,-1/4<br>(4 <sub>y</sub>  3/4,1/4,1/4)'                     | (22) 2' (1/2,0,1/2) x-1/4,1/8,x<br>(2 <sub>xz</sub>  1/4,1/4,3/4)'   | (23) 4 <sup>-</sup> (0,3/4,0) 0,y,1/4<br>(4 <sub>y</sub> <sup>-1</sup>  1/4,3/4,1/4)'  | (24) 2' $\bar{x}+3/4, 3/8, x$<br>(2 <sub>xz</sub>  3/4,3/4,3/4)'   |
| (25) $\bar{1}$ 0,0,0<br>(1 0,0,0)  | (26) a (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)  | (27) c (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)  | (28) b (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)  |
| (29) $\bar{3}^+$ x,x,x; 0,0,0<br>( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>  0,0,0)              | (30) $\bar{3}^+$ $\bar{x}-1/2, x+1, \bar{x}$ ;<br>0,1/2,1/2<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,1/2,0) | (31) $\bar{3}^+$ $x+1/2, \bar{x}+1/2, \bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,0,1/2) | (32) $\bar{3}^+$ $\bar{x}+1, \bar{x}+1/2, x$ ;<br>1/2,0,1/2<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,1/2,1/2) |
| (33) $\bar{3}^-$ x,x,x; 0,0,0<br>( $\bar{3}$ <sub>xyz</sub> <sup>-1</sup>  0,0,0)              | (34) $\bar{3}^-$ $x+1/2, \bar{x}-1/2, \bar{x}$ ; 0,0,1/2<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub>  0,1/2,1/2)                  | (35) $\bar{3}^-$ $\bar{x}, \bar{x}+1/2, x$ ; 0,1/2,0<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub>  1/2,1/2,0)                        | (36) $\bar{3}^-$ $\bar{x}+1/2, x, \bar{x}$ ; 1/2,0,0<br>( $\bar{3}$ <sub>x<math>\bar{y}z</math></sub>  1/2,0,1/2)                      |
| (37) d' (-1/4,1/4,1/4) x+1/2, $\bar{x}, z$<br>(m <sub>xy</sub>  1/4,3/4,3/4)'                  | (38) d' (1/4,1/4,1/4) x,x,z<br>(m $\bar{x}y$  1/4,1/4,1/4)'  | (39) $\bar{4}^-$ (0,3/4,z; 0,3/4,1/8)<br>( $\bar{4}$ <sub>z</sub> <sup>-1</sup>  3/4,3/4,1/4)'   | (40) $\bar{4}^+$ (1/2,-1/4,z; 1/2,-1/4,3/8)<br>( $\bar{4}$ <sub>z</sub>  3/4,1/4,3/4)'   |
| (41) $\bar{4}^-$ (x,0,3/4; 1/8,0,3/4)<br>( $\bar{4}$ <sub>x</sub> <sup>-1</sup>  1/4,3/4,3/4)' | (42) d' (3/4,-1/4,1/4) x,y+1/2, $\bar{y}$<br>(m <sub>yz</sub>  3/4,1/4,3/4)'   | (43) d' (1/4,1/4,1/4) x,y,y<br>(m $\bar{y}z$  1/4,1/4,1/4)'  | (44) $\bar{4}^+$ (x,1/2,-1/4; 3/8,1/2,-1/4)<br>( $\bar{4}$ <sub>x</sub>  3/4,3/4,1/4)'   |
| (45) $\bar{4}^+$ (-1/4,y,1/2; -1/4,3/8,1/2)<br>( $\bar{4}$ <sub>y</sub>  1/4,3/4,3/4)'         | (46) d' (1/4,3/4,-1/4) $\bar{x}+1/2, y, x$<br>(m <sub>xz</sub>  3/4,3/4,1/4)'  | (47) $\bar{4}^-$ (3/4,y,0; 3/4,1/8,0)<br>( $\bar{4}$ <sub>y</sub> <sup>-1</sup>  3/4,1/4,3/4)'   | (48) d' (1/4,1/4,1/4) x,y,x<br>(m $\bar{x}z$  1/4,1/4,1/4)'  |

For (1/2,1/2,1/2) + set

- |   |  |  |  |
|---|--|--|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                                    | (2) 2 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,0)   | (3) 2 1/4,y,0<br>(2 <sub>y</sub>  1/2,0,0)   | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)   |
| (5) 3 <sup>+</sup> (1/2,1/2,1/2) x,x,x<br>(3 <sub>xyz</sub>  1/2,1/2,1/2) | (6) 3 <sup>+</sup> (1/6,-1/6,1/6)<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,1/2) | (7) 3 <sup>+</sup> (-1/6,1/6,1/6)<br>x+1/6, $\bar{x}+1/6, \bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,1/2,0) | (8) 3 <sup>+</sup> (1/6,1/6,-1/6)<br>$\bar{x}+1/3, \bar{x}+1/6, x$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,0,0) |

(9) $3^- (1/2, 1/2, 1/2) \ x, x, x$ ( $3_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(10) $3^- (1/6, -1/6, -1/6) \ \bar{x}$ $x+1/6, x+1/6, \bar{x}$ ( $3_{xyz}   1/2, 0, 0$ )	(11) $3^- (-1/6, -1/6, 1/6)$ $x+1/3, x+1/6, x$ ( $3_{xyz}   0, 0, 1/2$ )	(12) $3^- (-1/6, 1/6, -1/6) \ \bar{x}$ $x-1/6, x+1/3, \bar{x}$ ( $3_{xyz}   0, 1/2, 0$ )
(13) $2' (1/2, 1/2, 0) \ x, x+1/4, 3/8$ ( $2_{xy}   1/4, 3/4, 3/4$ )'	(14) $2' \ x, \bar{x}+1/4, 1/8$ ( $2_{xy}   1/4, 1/4, 1/4$ )'	(15) $4^- (0, 0, 1/4) \ 3/4, 0, z$ ( $4_z^{-1}   3/4, 3/4, 1/4$ )'	(16) $4^+ (0, 0, 3/4) \ 1/4, 1/2, z$ ( $4_z   3/4, 1/4, 3/4$ )'
(17) $4^- (1/4, 0, 0) \ x, 3/4, 0$ ( $4_x^{-1}   1/4, 3/4, 3/4$ )'	(18) $2' (0, 1/2, 1/2) \ 3/8, y-1/4, y$ ( $2_{yz}   3/4, 1/4, 3/4$ )'	(19) $2' \ 1/8, y+1/4, \bar{y}$ ( $2_{yz}   1/4, 1/4, 1/4$ )'	(20) $4^+ (3/4, 0, 0) \ x, 1/4, 1/2$ ( $4_x   3/4, 3/4, 1/4$ )'
(21) $4^+ (0, 3/4, 0) \ 1/2, y, 1/4$ ( $4_y   1/4, 3/4, 3/4$ )'	(22) $2' (1/2, 0, 1/2) \ x+1/4, 3/8, x$ ( $2_{xz}   3/4, 3/4, 1/4$ )'	(23) $4^- (0, 1/2, 0) \ 0, y, 3/4$ ( $4_y^{-1}   3/4, 1/4, 3/4$ )'	(24) $2' \ \bar{x}+1/4, 1/8, x$ ( $2_{xz}   1/4, 1/4, 1/4$ )'
(25) $\bar{1} \ 1/4, 1/4, 1/4$ ( $\bar{1}   1/2, 1/2, 1/2$ )	(26) $b (0, 1/2, 0) \ x, y, 0$ ( $m_z   0, 1/2, 0$ )	(27) $a (1/2, 0, 0) \ x, 0, z$ ( $m_y   1/2, 0, 0$ )	(28) $c (0, 0, 1/2) \ 0, y, z$ ( $m_x   0, 0, 1/2$ )
(29) $\bar{3}^+ \ x, x, x;$ $1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 1/2, 1/2$ )	(30) $\bar{3}^+ \ \bar{x}-1/2, x, \bar{x};$ $-1/4, -1/4, 1/4$ ( $\bar{3}_{xyz}^{-1}   0, 0, 1/2$ )	(31) $\bar{3}^+ \ x-1/2, \bar{x}+1/2, \bar{x};$ $-1/4, 1/4, -1/4$ ( $\bar{3}_{xyz}^{-1}   0, 1/2, 0$ )	(32) $\bar{3}^+ \ \bar{x}, \bar{x}-1/2, x;$ $1/4, -1/4, -1/4$ ( $\bar{3}_{xyz}^{-1}   1/2, 0, 0$ )
(33) $\bar{3}^- \ x, x, x;$ $1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(34) $\bar{3}^- \ x+1/2, \bar{x}-1/2, \bar{x};$ $1/4, -1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 0, 0$ )	(35) $\bar{3}^- \ \bar{x}, \bar{x}+1/2, x;$ $-1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}   0, 0, 1/2$ )	(36) $\bar{3}^- \ \bar{x}+1/2, x, \bar{x};$ $1/4, 1/4, -1/4$ ( $\bar{3}_{xyz}   0, 1/2, 0$ )
(37) $d' (1/4, -1/4, 1/4) \ x+1/2, \bar{x}, z$ ( $m_{xy}   3/4, 1/4, 1/4$ )'	(38) $d' (3/4, 3/4, 3/4) \ x, x, z$ ( $m_{xy}   3/4, 3/4, 3/4$ )'	(39) $\bar{4}^- (0, 1/4, z; 0, 1/4, 3/8)$ ( $\bar{4}_z^{-1}   1/4, 1/4, 3/4$ )'	(40) $\bar{4}^+ (1/2, 1/4, z; 1/2, 1/4, 1/8)$ ( $\bar{4}_z   1/4, 3/4, 1/4$ )'
(41) $\bar{4}^- (x, 0, 1/4; 3/8, 0, 1/4)$ ( $\bar{4}_x^{-1}   3/4, 1/4, 1/4$ )'	(42) $d' (1/4, 1/4, -1/4) \ x, y+1/2, \bar{y}$ ( $m_{yz}   1/4, 3/4, 1/4$ )'	(43) $d' (3/4, 3/4, 3/4) \ x, y, y$ ( $m_{yz}   3/4, 3/4, 3/4$ )'	(44) $\bar{4}^+ (x, 1/2, 1/4; 1/8, 1/2, 1/4)$ ( $\bar{4}_x   1/4, 1/4, 3/4$ )'
(45) $\bar{4}^+ (1/4, y, 1/2; 1/4, 1/8, 1/2)$ ( $\bar{4}_y   3/4, 1/4, 1/4$ )'	(46) $d' (-1/4, 1/4, 1/4) \ \bar{x}+1/2, y, x$ ( $m_{xz}   1/4, 1/4, 3/4$ )'	(47) $\bar{4}^- (1/4, y, 0; 1/4, 3/8, 0)$ ( $\bar{4}_y^{-1}   1/4, 3/4, 1/4$ )'	(48) $d' (3/4, 3/4, 3/4) \ x, y, x$ ( $m_{xz}   3/4, 3/4, 3/4$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25).

### Positions

			Coordinates					
Multiplicity, Wyckoff letter, Site Symmetry.								
			(0,0,0) +	(1/2,1/2,1/2) +				
96	h	1						
(1)	$x, y, z$	[u, v, w]	(2)	$\bar{x}+1/2, \bar{y}, z+1/2$	[ $\bar{u}, \bar{v}, w$ ]	(3)	$\bar{x}, y+1/2, \bar{z}+1/2$	[ $\bar{u}, v, \bar{w}$ ]
(5)	$z, x, y$	[w, u, v]	(6)	$z+1/2, \bar{x}+1/2, \bar{y}$	[w, $\bar{u}, \bar{v}$ ]	(7)	$\bar{z}+1/2, \bar{x}, y+1/2$	[ $\bar{w}, \bar{u}, v$ ]
(9)	$y, z, x$	[v, w, u]	(10)	$\bar{y}, z+1/2, \bar{x}+1/2$	[ $\bar{v}, w, \bar{u}$ ]	(11)	$y+1/2, \bar{z}+1/2, \bar{x}$	[v, $\bar{w}, \bar{u}$ ]
(13)	$y+3/4, x+1/4, \bar{z}+1/4$	[ $\bar{v}, \bar{u}, w$ ]	(14)	$\bar{y}+3/4, \bar{x}+3/4, \bar{z}+3/4$	[v, u, w]	(15)	$y+1/4, \bar{x}+1/4, z+3/4$	[ $\bar{v}, \bar{u}, \bar{w}$ ]
(17)	$x+3/4, z+1/4, \bar{y}+1/4$	[ $\bar{u}, \bar{w}, v$ ]	(18)	$\bar{x}+1/4, z+3/4, y+1/4$	[u, $\bar{w}, \bar{v}$ ]	(19)	$\bar{x}+3/4, \bar{z}+3/4, \bar{y}+3/4$	[u, w, v]
(21)	$z+3/4, y+1/4, \bar{x}+1/4$	[ $\bar{w}, \bar{v}, u$ ]	(22)	$z+1/4, \bar{y}+1/4, x+3/4$	[ $\bar{w}, v, \bar{u}$ ]	(23)	$\bar{z}+1/4, y+3/4, x+1/4$	[w, $\bar{v}, \bar{u}$ ]
(25)	$\bar{x}, \bar{y}, \bar{z}$	[u, v, w]	(26)	$x+1/2, y, \bar{z}+1/2$	[ $\bar{u}, \bar{v}, w$ ]	(27)	$x, \bar{y}+1/2, z+1/2$	[ $\bar{u}, v, \bar{w}$ ]
						(28)	$\bar{x}+1/2, y+1/2, z$	[u, $\bar{v}, \bar{w}$ ]

(29) $\bar{z}, \bar{x}, \bar{y}$ [w,u,v]	(30) $\bar{z}+1/2, \bar{x}+1/2, \bar{y}$ [w, $\bar{u}, \bar{v}$ ]	(31) $z+1/2, \bar{x}, \bar{y}+1/2$ [ $\bar{w}, \bar{u}, \bar{v}$ ]	(32) $z, \bar{x}+1/2, \bar{y}+1/2$ [ $\bar{w}, \bar{u}, \bar{v}$ ]
(33) $\bar{y}, \bar{z}, \bar{x}$ [v,w,u]	(34) $y, \bar{z}+1/2, \bar{x}+1/2$ [ $\bar{v}, \bar{w}, \bar{u}$ ]	(35) $\bar{y}+1/2, z+1/2, \bar{x}$ [v, $\bar{w}, \bar{u}$ ]	(36) $y+1/2, z, \bar{x}+1/2$ [ $\bar{v}, \bar{w}, \bar{u}$ ]
(37) $\bar{y}+1/4, \bar{x}+3/4, z+3/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(38) $y+1/4, \bar{x}+1/4, z+1/4$ [v, $\bar{u}, \bar{w}$ ]	(39) $\bar{y}+3/4, \bar{x}+3/4, \bar{z}+1/4$ [ $\bar{v}, \bar{u}, \bar{w}$ ]	(40) $y+3/4, \bar{x}+1/4, \bar{z}+3/4$ [v, $\bar{u}, \bar{w}$ ]
(41) $\bar{x}+1/4, \bar{z}+3/4, \bar{y}+3/4$ [ $\bar{u}, \bar{w}, \bar{v}$ ]	(42) $x+3/4, \bar{z}+1/4, \bar{y}+3/4$ [u, $\bar{w}, \bar{v}$ ]	(43) $x+1/4, z+1/4, \bar{y}+1/4$ [u, $\bar{w}, \bar{v}$ ]	(44) $\bar{x}+3/4, \bar{z}+3/4, \bar{y}+1/4$ [ $\bar{u}, \bar{w}, \bar{v}$ ]
(45) $\bar{z}+1/4, \bar{y}+3/4, \bar{x}+3/4$ [ $\bar{w}, \bar{v}, \bar{u}$ ]	(46) $\bar{z}+3/4, \bar{y}+3/4, \bar{x}+1/4$ [ $\bar{w}, \bar{v}, \bar{u}$ ]	(47) $z+3/4, \bar{y}+1/4, \bar{x}+3/4$ [w, $\bar{v}, \bar{u}$ ]	(48) $z+1/4, \bar{y}+1/4, \bar{x}+1/4$ [w, $\bar{v}, \bar{u}$ ]

48 g ..2'

$1/8, \bar{y}, \bar{y}+1/4$ [u,v,v]	$3/8, \bar{y}, \bar{y}+3/4$ [ $\bar{u}, \bar{v}, \bar{v}$ ]	$7/8, \bar{y}+1/2, \bar{y}+1/4$ [ $\bar{u}, \bar{v}, \bar{v}$ ]	$5/8, \bar{y}+1/2, \bar{y}+3/4$ [ $\bar{u}, \bar{v}, \bar{v}$ ]
$\bar{y}+1/4, 1/8, \bar{y}$ [v,u,v]	$\bar{y}+3/4, 3/8, \bar{y}$ [v, $\bar{u}, \bar{v}$ ]	$y+1/4, 7/8, \bar{y}+1/2$ [ $\bar{v}, \bar{u}, \bar{v}$ ]	$y+3/4, 5/8, \bar{y}+1/2$ [ $\bar{v}, \bar{u}, \bar{v}$ ]
$y, \bar{y}+1/4, 1/8$ [v,v,u]	$\bar{y}, \bar{y}+3/4, 3/8$ [ $\bar{v}, \bar{v}, \bar{u}$ ]	$y+1/2, \bar{y}+1/4, 7/8$ [v, $\bar{v}, \bar{u}$ ]	$\bar{y}+1/2, \bar{y}+3/4, 5/8$ [ $\bar{v}, \bar{v}, \bar{u}$ ]
$7/8, \bar{y}, \bar{y}+3/4$ [u,v,v]	$5/8, \bar{y}, \bar{y}+1/4$ [ $\bar{u}, \bar{v}, \bar{v}$ ]	$1/8, \bar{y}+1/2, \bar{y}+3/4$ [ $\bar{u}, \bar{v}, \bar{v}$ ]	$3/8, \bar{y}+1/2, \bar{y}+1/4$ [ $\bar{u}, \bar{v}, \bar{v}$ ]
$y+3/4, 7/8, \bar{y}$ [v,u,v]	$y+1/4, 5/8, \bar{y}$ [v, $\bar{u}, \bar{v}$ ]	$\bar{y}+3/4, 1/8, \bar{y}+1/2$ [ $\bar{v}, \bar{u}, \bar{v}$ ]	$\bar{y}+1/4, 3/8, \bar{y}+1/2$ [ $\bar{v}, \bar{u}, \bar{v}$ ]
$\bar{y}, \bar{y}+3/4, 7/8$ [v,v,u]	$y, \bar{y}+1/4, 5/8$ [ $\bar{v}, \bar{v}, \bar{u}$ ]	$\bar{y}+1/2, \bar{y}+3/4, 1/8$ [v, $\bar{v}, \bar{u}$ ]	$y+1/2, \bar{y}+1/4, 3/8$ [ $\bar{v}, \bar{v}, \bar{u}$ ]

48 f 2..

$x, 0, 1/4$ [u,0,0]	$\bar{x}+1/2, 0, 3/4$ [ $\bar{u}, 0, 0$ ]	$1/4, x, 0$ [0,u,0]	$3/4, \bar{x}+1/2, 0$ [0, $\bar{u}, 0$ ]
$0, 1/4, x$ [0,0,u]	$0, 3/4, \bar{x}+1/2$ [0,0, $\bar{u}$ ]	$3/4, x+1/4, 0$ [0, $\bar{u}, 0$ ]	$3/4, \bar{x}+3/4, 1/2$ [0,u,0]
$x+3/4, 1/2, 1/4$ [ $\bar{u}, 0, 0$ ]	$\bar{x}+1/4, 0, 1/4$ [u,0,0]	$0, 1/4, \bar{x}+1/4$ [0,0,u]	$1/2, 1/4, x+3/4$ [0,0, $\bar{u}$ ]
$\bar{x}, 0, 3/4$ [u,0,0]	$x+1/2, 0, 1/4$ [ $\bar{u}, 0, 0$ ]	$3/4, \bar{x}, 0$ [0,u,0]	$1/4, x+1/4, 0$ [0, $\bar{u}, 0$ ]
$0, 3/4, \bar{x}$ [0,0,u]	$0, 1/4, x+1/2$ [0,0, $\bar{u}$ ]	$1/4, \bar{x}+3/4, 0$ [0, $\bar{u}, 0$ ]	$1/4, x+1/4, 1/2$ [0,u,0]
$\bar{x}+1/4, 1/2, 3/4$ [ $\bar{u}, 0, 0$ ]	$x+3/4, 0, 3/4$ [u,0,0]	$0, 3/4, x+3/4$ [0,0,u]	$1/2, 3/4, \bar{x}+1/4$ [0,0, $\bar{u}$ ]

32 e .3.

$x, x, x$ [u,u,u]	$\bar{x}+1/2, \bar{x}, \bar{x}+1/2$ [ $\bar{u}, \bar{u}, \bar{u}$ ]	$\bar{x}, \bar{x}+1/2, \bar{x}+1/2$ [ $\bar{u}, \bar{u}, \bar{u}$ ]	$x+1/2, \bar{x}+1/2, \bar{x}$ [u, $\bar{u}, \bar{u}$ ]
$x+3/4, \bar{x}+1/4, \bar{x}+1/4$ [ $\bar{u}, \bar{u}, \bar{u}$ ]	$\bar{x}+3/4, \bar{x}+3/4, \bar{x}+3/4$ [u,u,u]	$x+1/4, \bar{x}+1/4, \bar{x}+3/4$ [ $\bar{u}, \bar{u}, \bar{u}$ ]	$\bar{x}+1/4, \bar{x}+3/4, \bar{x}+1/4$ [u, $\bar{u}, \bar{u}$ ]
$\bar{x}, \bar{x}, \bar{x}$ [u,u,u]	$x+1/2, x, \bar{x}+1/2$ [ $\bar{u}, \bar{u}, \bar{u}$ ]	$x, \bar{x}+1/2, \bar{x}+1/2$ [ $\bar{u}, \bar{u}, \bar{u}$ ]	$\bar{x}+1/2, \bar{x}+1/2, x$ [u, $\bar{u}, \bar{u}$ ]
$\bar{x}+1/4, \bar{x}+3/4, \bar{x}+3/4$ [ $\bar{u}, \bar{u}, \bar{u}$ ]	$x+1/4, \bar{x}+1/4, \bar{x}+1/4$ [u,u,u]	$\bar{x}+3/4, \bar{x}+3/4, \bar{x}+1/4$ [ $\bar{u}, \bar{u}, \bar{u}$ ]	$x+3/4, \bar{x}+1/4, \bar{x}+3/4$ [u, $\bar{u}, \bar{u}$ ]

12 d 4'..

$3/8, 0, 1/4$ [0,0,0]	$1/8, 0, 3/4$ [0,0,0]	$1/4, 3/8, 0$ [0,0,0]	$3/4, 1/8, 0$ [0,0,0]
$0, 1/4, 3/8$ [0,0,0]	$0, 3/4, 1/8$ [0,0,0]	$3/4, 5/8, 0$ [0,0,0]	$3/4, 3/8, 1/2$ [0,0,0]
$1/8, 1/2, 1/4$ [0,0,0]	$7/8, 0, 1/4$ [0,0,0]	$0, 1/4, 7/8$ [0,0,0]	$1/2, 1/4, 1/8$ [0,0,u]

24 c 2.2'2'

$1/8, 0, 1/4$ [u,0,0]	$3/8, 0, 3/4$ [ $\bar{u}, 0, 0$ ]	$1/4, 1/8, 0$ [0,u,0]	$3/4, 3/8, 0$ [0, $\bar{u}, 0$ ]
$0, 1/4, 1/8$ [0,0,u]	$0, 3/4, 3/8$ [0,0, $\bar{u}$ ]	$7/8, 0, 3/4$ [u,0,0]	$5/8, 0, 1/4$ [ $\bar{u}, 0, 0$ ]
$3/4, 7/8, 0$ [0,u,0]	$1/4, 5/8, 0$ [0, $\bar{u}, 0$ ]	$0, 3/4, 7/8$ [0,0,u]	$0, 1/4, 5/8$ [0,0, $\bar{u}$ ]



Continued

230.4.1650

 $1a\bar{3}d'$ 

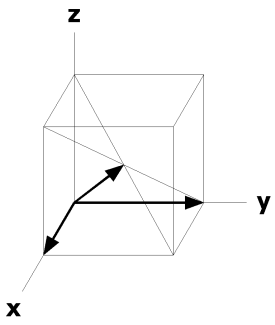
16	b	.32'	$1/8, 1/8, 1/8 [u, u, u]$	$3/8, 7/8, 5/8 [\bar{u}, \bar{u}, u]$	$7/8, 5/8, 3/8 [\bar{u}, u, \bar{u}]$	$5/8, 3/8, 7/8 [u, \bar{u}, \bar{u}]$
			$7/8, 7/8, 7/8 [u, u, u]$	$5/8, 1/8, 3/8 [\bar{u}, \bar{u}, u]$	$1/8, 3/8, 5/8 [\bar{u}, u, \bar{u}]$	$3/8, 5/8, 1/8 [u, \bar{u}, \bar{u}]$
16	a	$\bar{3}$ .	$0, 0, 0 [u, u, u]$	$1/2, 0, 1/2 [\bar{u}, \bar{u}, u]$	$0, 1/2, 1/2 [\bar{u}, u, \bar{u}]$	$1/2, 1/2, 0 [u, \bar{u}, \bar{u}]$
			$3/4, 1/4, 1/4 [\bar{u}, \bar{u}, u]$	$3/4, 3/4, 3/4 [u, u, u]$	$1/4, 1/4, 3/4 [\bar{u}, u, \bar{u}]$	$1/4, 3/4, 1/4 [u, \bar{u}, \bar{u}]$

**Symmetry of Special Projections**

Along  $[0, 0, 1]$   $p_c 4mm$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $1/2, 1/4, z$

Along  $[1, 1, 1]$   $p6'mm'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

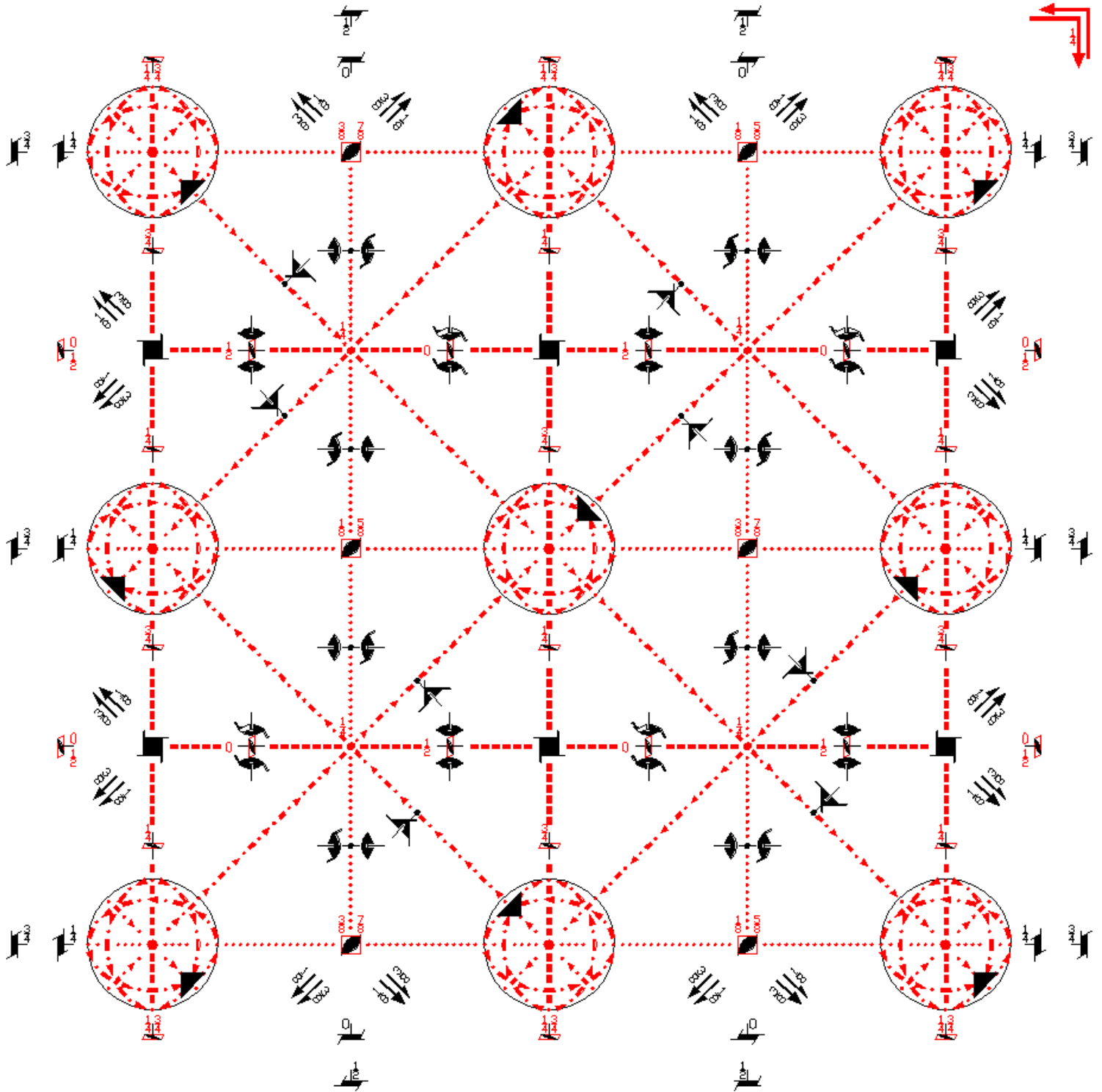
Along  $[1, 1, 0]$   $c2'mm'$   
 $\mathbf{a}^* = \mathbf{c}/2$   $\mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2$   
 Origin at  $x, x+1/4, 1/8$



$la\bar{3}'d'$   
230.5.1651

$m'\bar{3}'m'$   
 $I4_1/a'\bar{3}'2/d'$

Cubic



Origin at center ( $\bar{3}'$ )

**Asymmetric unit**  $-1/8 \leq x \leq 1/8$ ;  $-1/8 \leq y \leq 1/8$ ;  $0 \leq z \leq 1/4$ ;  $\max(x, -x, y, -y) \leq z$

Vertices  $0,0,0$   $1/8, 1/8, 1/8$   $-1/8, 1/8, 1/8$   $-1/8, -1/8, 1/8$   $1/8, -1/8, 1/8$   
 $1/8, 1/8, 1/4$   $-1/8, 1/8, 1/4$   $-1/8, -1/8, 1/4$   $1/8, -1/8, 1/4$

## Symmetry Operations

For (0,0,0) + set

- |  |  |   |  |
|--|--|---|--|
| (1) 1<br>(1 0,0,0)   | (2) 2 (0,0,1/2) 1/4,0,z<br>(2 <sub>z</sub>  1/2,0,1/2)   | (3) 2 (0,1/2,0) 0,y,1/4<br>(2 <sub>y</sub>  0,1/2,1/2)  | (4) 2 (1/2,0,0) x,1/4,0<br>(2 <sub>x</sub>  1/2,1/2,0)   |
| (5) 3 <sup>+</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)                  | (6) 3 <sup>+</sup> $\bar{x}+1/2, x, \bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,1/2,0)     | (7) 3 <sup>+</sup> $x+1/2, \bar{x}-1/2, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  1/2,0,1/2)                 | (8) 3 <sup>+</sup> $\bar{x}, \bar{x}+1/2, x$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,1/2,1/2)     |
| (9) 3 <sup>-</sup> x,x,x<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,0,0)                  | (10) 3 <sup>-</sup> (-1/3,1/3,1/3)<br>x+1/6, x+1/6, $\bar{x}$<br>(3 <sub>xyz</sub>  0,1/2,1/2)                     | (11) 3 <sup>-</sup> (1/3,1/3,-1/3)<br>x+1/3, x+1/6, x<br>(3 <sub>x<math>\bar{y}z</math></sub>  1/2,1/2,0)       | (12) 3 <sup>-</sup> (1/3,-1/3,1/3)<br>x-1/6, x+1/3, $\bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub>  1/2,0,1/2)  |
| (13) 2 (1/2,1/2,0) x,x-1/4,1/8<br>(2 <sub>xy</sub>  3/4,1/4,1/4)                     | (14) 2 x, $\bar{x}+3/4, 3/8$<br>(2 <sub>xy</sub>  3/4,3/4,3/4)   | (15) 4 <sup>-</sup> (0,0,3/4) 1/4,0,z<br>(4 <sub>z</sub> <sup>-1</sup>  1/4,1/4,3/4)                            | (16) 4 <sup>+</sup> (0,0,1/4) -1/4,1/2,z<br>(4 <sub>z</sub>  1/4,3/4,1/4)  |
| (17) 4 <sup>-</sup> (3/4,0,0) x,1/4,0<br>(4 <sub>x</sub> <sup>-1</sup>  3/4,1/4,1/4) | (18) 2 (0,1/2,1/2) 1/8,y+1/4,y<br>(2 <sub>yz</sub>  1/4,3/4,1/4)   | (19) 2 3/8,y+3/4, $\bar{y}$<br>(2 <sub>yz</sub>  3/4,3/4,3/4)   | (20) 4 <sup>+</sup> (1/4,0,0) x,-1/4,1/2<br>(4 <sub>x</sub>  1/4,1/4,3/4)  |
| (21) 4 <sup>+</sup> (0,1/4,0) 1/2,y,-1/4<br>(4 <sub>y</sub>  3/4,1/4,1/4)            | (22) 2 (1/2,0,1/2) x-1/4,1/8,x<br>(2 <sub>xz</sub>  1/4,1/4,3/4)   | (23) 4 <sup>-</sup> (0,3/4,0) 0,y,1/4<br>(4 <sub>y</sub> <sup>-1</sup>  1/4,3/4,1/4)                            | (24) 2 $\bar{x}+3/4, 3/8, x$<br>(2 <sub>xz</sub>  3/4,3/4,3/4)   |
| (25) $\bar{1}'$ 0,0,0<br>(1 0,0,0)'  | (26) a' (1/2,0,0) x,y,1/4<br>(m <sub>z</sub>  1/2,0,1/2)'  | (27) c' (0,0,1/2) x,1/4,z<br>(m <sub>y</sub>  0,1/2,1/2)'   | (28) b' (0,1/2,0) 1/4,y,z<br>(m <sub>x</sub>  1/2,1/2,0)'  |
| (29) $\bar{3}^+$ ' x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'          | (30) $\bar{3}^+$ ' $\bar{x}-1/2, x+1, \bar{x}$ ;<br>0,1/2,1/2<br>( $\bar{3}_{x\bar{y}z$ <sup>-1</sup>  1/2,1/2,0)' | (31) $\bar{3}^+$ ' $x+1/2, \bar{x}+1/2, \bar{x}$ ;<br>1/2,1/2,0<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  1/2,0,1/2)' | (32) $\bar{3}^+$ ' $\bar{x}+1, \bar{x}+1/2, x$ ;<br>1/2,0,1/2<br>( $\bar{3}_{x\bar{y}z$ <sup>-1</sup>  0,1/2,1/2)' |
| (33) $\bar{3}^-$ ' x,x,x; 0,0,0<br>( $\bar{3}_{xyz}$ <sup>-1</sup>  0,0,0)'          | (34) $\bar{3}^-$ ' $x+1/2, \bar{x}-1/2, \bar{x}$ ; 0,0,1/2<br>( $\bar{3}_{xyz}$  0,1/2,1/2)'                       | (35) $\bar{3}^-$ ' $\bar{x}, \bar{x}+1/2, x$ ; 0,1/2,0<br>( $\bar{3}_{x\bar{y}z$  1/2,1/2,0)'                   | (36) $\bar{3}^-$ ' $\bar{x}+1/2, x, \bar{x}$ ; 1/2,0,0<br>( $\bar{3}_{x\bar{y}z$  1/2,0,1/2)'                      |
| (37) d' (-1/4,1/4,1/4) x+1/2, $\bar{x}, z$<br>(m <sub>xy</sub>  1/4,3/4,3/4)'        | (38) d' (1/4,1/4,1/4) x,x,z<br>(m <sub>xy</sub>  1/4,1/4,1/4)'   | (39) $\bar{4}^-$ ' 0,3/4,z; 0,3/4,1/8<br>( $\bar{4}_z$ <sup>-1</sup>  3/4,3/4,1/4)'                             | (40) $\bar{4}^+$ ' 1/2,-1/4,z; 1/2,-1/4,3/8<br>( $\bar{4}_z$  3/4,1/4,3/4)'  |
| (41) $\bar{4}^-$ ' x,0,3/4; 1/8,0,3/4<br>( $\bar{4}_x$ <sup>-1</sup>  1/4,3/4,3/4)'  | (42) d' (3/4,-1/4,1/4) x,y+1/2, $\bar{y}$<br>(m <sub>yz</sub>  3/4,1/4,3/4)'                                       | (43) d' (1/4,1/4,1/4) x,y,y<br>(m <sub>yz</sub>  1/4,1/4,1/4)'  | (44) $\bar{4}^+$ ' x,1/2,-1/4; 3/8,1/2,-1/4<br>( $\bar{4}_x$  3/4,3/4,1/4)'  |
| (45) $\bar{4}^+$ ' -1/4,y,1/2; -1/4,3/8,1/2<br>( $\bar{4}_y$  1/4,3/4,3/4)'          | (46) d' (1/4,3/4,-1/4) $\bar{x}+1/2, y, x$<br>(m <sub>xz</sub>  3/4,3/4,1/4)'                                      | (47) $\bar{4}^-$ ' 3/4,y,0; 3/4,1/8,0<br>( $\bar{4}_y$ <sup>-1</sup>  3/4,1/4,3/4)'                             | (48) d' (1/4,1/4,1/4) x,y,x<br>(m <sub>xz</sub>  1/4,1/4,1/4)'   |

For (1/2,1/2,1/2) + set

- |   |  |   |  |
|---|--|---|--|
| (1) t (1/2,1/2,1/2)<br>(1 1/2,1/2,1/2)                                    | (2) 2 0,1/4,z<br>(2 <sub>z</sub>  0,1/2,0)   | (3) 2 1/4,y,0<br>(2 <sub>y</sub>  1/2,0,0)  | (4) 2 x,0,1/4<br>(2 <sub>x</sub>  0,0,1/2)   |
| (5) 3 <sup>+</sup> (1/2,1/2,1/2) x,x,x<br>(3 <sub>xyz</sub>  1/2,1/2,1/2) | (6) 3 <sup>+</sup> (1/6,-1/6,1/6)<br>$\bar{x}-1/6, x+1/3, \bar{x}$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  0,0,1/2) | (7) 3 <sup>+</sup> (-1/6,1/6,1/6)<br>x+1/6, $\bar{x}+1/6, \bar{x}$<br>(3 <sub>xyz</sub> <sup>-1</sup>  0,1/2,0) | (8) 3 <sup>+</sup> (1/6,1/6,-1/6)<br>$\bar{x}+1/3, \bar{x}+1/6, x$<br>(3 <sub>x<math>\bar{y}z</math></sub> <sup>-1</sup>  1/2,0,0) |

(9) $3^- (1/2, 1/2, 1/2) \ x, x, x$ ( $3_{xyz}^{-1}   1/2, 1/2, 1/2$ )	(10) $3^- (1/6, -1/6, -1/6) \ \bar{x}$ $x+1/6, x+1/6, \bar{x}$ ( $3_{xyz}   1/2, 0, 0$ )	(11) $3^- (-1/6, -1/6, 1/6)$ $x+1/3, x+1/6, x$ ( $3_{xyz}   0, 0, 1/2$ )	(12) $3^- (-1/6, 1/6, -1/6) \ \bar{x}$ $x-1/6, x+1/3, \bar{x}$ ( $3_{xyz}   0, 1/2, 0$ )
(13) $2 (1/2, 1/2, 0) \ x, x+1/4, 3/8$ ( $2_{xy}   1/4, 3/4, 3/4$ )	(14) $2 \ x, \bar{x}+1/4, 1/8$ ( $2_{xy}   1/4, 1/4, 1/4$ )	(15) $4^- (0, 0, 1/4) \ 3/4, 0, z$ ( $4_z^{-1}   3/4, 3/4, 1/4$ )	(16) $4^+ (0, 0, 3/4) \ 1/4, 1/2, z$ ( $4_z   3/4, 1/4, 3/4$ )
(17) $4^- (1/4, 0, 0) \ x, 3/4, 0$ ( $4_x^{-1}   1/4, 3/4, 3/4$ )	(18) $2 (0, 1/2, 1/2) \ 3/8, y-1/4, y$ ( $2_{yz}   3/4, 1/4, 3/4$ )	(19) $2 \ 1/8, y+1/4, \bar{y}$ ( $2_{yz}   1/4, 1/4, 1/4$ )	(20) $4^+ (3/4, 0, 0) \ x, 1/4, 1/2$ ( $4_x   3/4, 3/4, 1/4$ )
(21) $4^+ (0, 3/4, 0) \ 1/2, y, 1/4$ ( $4_y   1/4, 3/4, 3/4$ )	(22) $2 (1/2, 0, 1/2) \ x+1/4, 3/8, x$ ( $2_{xz}   3/4, 3/4, 1/4$ )	(23) $4^- (0, 1/2, 0) \ 0, y, 3/4$ ( $4_y^{-1}   3/4, 1/4, 3/4$ )	(24) $2 \ \bar{x}+1/4, 1/8, x$ ( $2_{xz}   1/4, 1/4, 1/4$ )
(25) $\bar{1}^+ \ 1/4, 1/4, 1/4$ ( $\bar{1}   1/2, 1/2, 1/2$ )'	(26) $b' (0, 1/2, 0) \ x, y, 0$ ( $m_z   0, 1/2, 0$ )'	(27) $a' (1/2, 0, 0) \ x, 0, z$ ( $m_y   1/2, 0, 0$ )'	(28) $c' (0, 0, 1/2) \ 0, y, z$ ( $m_x   0, 0, 1/2$ )'
(29) $\bar{3}^+ \ x, x, x;$ $1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 1/2, 1/2$ )'	(30) $\bar{3}^+ \ \bar{x}-1/2, x, \bar{x};$ $-1/4, -1/4, 1/4$ ( $\bar{3}_{xyz}^{-1}   0, 0, 1/2$ )'	(31) $\bar{3}^+ \ x-1/2, \bar{x}+1/2, \bar{x};$ $-1/4, 1/4, -1/4$ ( $\bar{3}_{xyz}^{-1}   0, 1/2, 0$ )'	(32) $\bar{3}^+ \ \bar{x}, \bar{x}-1/2, x;$ $1/4, -1/4, -1/4$ ( $\bar{3}_{xyz}^{-1}   1/2, 0, 0$ )'
(33) $\bar{3}^- \ x, x, x;$ $1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}^{-1}   1/2, 1/2, 1/2$ )'	(34) $\bar{3}^- \ x+1/2, \bar{x}-1/2, \bar{x};$ $1/4, -1/4, 1/4$ ( $\bar{3}_{xyz}   1/2, 0, 0$ )'	(35) $\bar{3}^- \ \bar{x}, \bar{x}+1/2, x;$ $-1/4, 1/4, 1/4$ ( $\bar{3}_{xyz}   0, 0, 1/2$ )'	(36) $\bar{3}^- \ \bar{x}+1/2, x, \bar{x};$ $1/4, 1/4, -1/4$ ( $\bar{3}_{xyz}   0, 1/2, 0$ )'
(37) $d' (1/4, -1/4, 1/4) \ x+1/2, \bar{x}, z$ ( $m_{xy}   3/4, 1/4, 1/4$ )'	(38) $d' (3/4, 3/4, 3/4) \ x, x, z$ ( $m_{xy}   3/4, 3/4, 3/4$ )'	(39) $\bar{4}^- \ 0, 1/4, z; \ 0, 1/4, 3/8$ ( $\bar{4}_z^{-1}   1/4, 1/4, 3/4$ )'	(40) $\bar{4}^+ \ 1/2, 1/4, z; \ 1/2, 1/4, 1/8$ ( $\bar{4}_z   1/4, 3/4, 1/4$ )'
(41) $\bar{4}^- \ x, 0, 1/4; \ 3/8, 0, 1/4$ ( $\bar{4}_x^{-1}   3/4, 1/4, 1/4$ )'	(42) $d' (1/4, 1/4, -1/4) \ x, y+1/2, \bar{y}$ ( $m_{yz}   1/4, 3/4, 1/4$ )'	(43) $d' (3/4, 3/4, 3/4) \ x, y, y$ ( $m_{yz}   3/4, 3/4, 3/4$ )'	(44) $\bar{4}^+ \ x, 1/2, 1/4; \ 1/8, 1/2, 1/4$ ( $\bar{4}_x   1/4, 1/4, 3/4$ )'
(45) $\bar{4}^+ \ 1/4, y, 1/2; \ 1/4, 1/8, 1/2$ ( $\bar{4}_y   3/4, 1/4, 1/4$ )'	(46) $d' (-1/4, 1/4, 1/4) \ \bar{x}+1/2, y, x$ ( $m_{xz}   1/4, 1/4, 3/4$ )'	(47) $\bar{4}^- \ 1/4, y, 0; \ 1/4, 3/8, 0$ ( $\bar{4}_y^{-1}   1/4, 3/4, 1/4$ )'	(48) $d' (3/4, 3/4, 3/4) \ x, y, x$ ( $m_{xz}   3/4, 3/4, 3/4$ )'

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25).

### Positions

Multiplicity, Wyckoff letter, Site Symmetry.			Coordinates								
96	h	1	(0,0,0) +	(1/2,1/2,1/2) +							
(1)	x,y,z	[u,v,w]	(2)	$\bar{x}+1/2, \bar{y}, z+1/2$	$[\bar{u}, \bar{v}, w]$	(3)	$\bar{x}, y+1/2, \bar{z}+1/2$	$[\bar{u}, v, \bar{w}]$	(4)	$x+1/2, \bar{y}+1/2, \bar{z}$	$[u, \bar{v}, \bar{w}]$
(5)	z,x,y	[w,u,v]	(6)	$z+1/2, \bar{x}+1/2, \bar{y}$	$[w, \bar{u}, \bar{v}]$	(7)	$\bar{z}+1/2, \bar{x}, y+1/2$	$[\bar{w}, \bar{u}, v]$	(8)	$\bar{z}, x+1/2, \bar{y}+1/2$	$[\bar{w}, u, \bar{v}]$
(9)	y,z,x	[v,w,u]	(10)	$\bar{y}, z+1/2, \bar{x}+1/2$	$[\bar{v}, w, \bar{u}]$	(11)	$y+1/2, \bar{z}+1/2, \bar{x}$	$[v, \bar{w}, \bar{u}]$	(12)	$\bar{y}+1/2, \bar{z}, x+1/2$	$[\bar{v}, \bar{w}, u]$
(13)	$y+3/4, x+1/4, \bar{z}+1/4$	$[v, u, \bar{w}]$	(14)	$\bar{y}+3/4, \bar{x}+3/4, \bar{z}+3/4$	$[\bar{v}, \bar{u}, \bar{w}]$	(15)	$y+1/4, \bar{x}+1/4, z+3/4$	$[v, \bar{u}, w]$	(16)	$\bar{y}+1/4, x+3/4, z+1/4$	$[\bar{v}, u, w]$
(17)	$x+3/4, z+1/4, \bar{y}+1/4$	$[u, w, \bar{v}]$	(18)	$\bar{x}+1/4, z+3/4, y+1/4$	$[\bar{u}, w, v]$	(19)	$\bar{x}+3/4, \bar{z}+3/4, \bar{y}+3/4$	$[\bar{u}, \bar{w}, \bar{v}]$	(20)	$x+1/4, \bar{z}+1/4, y+3/4$	$[u, \bar{w}, v]$
(21)	$z+3/4, y+1/4, \bar{x}+1/4$	$[w, v, \bar{u}]$	(22)	$z+1/4, \bar{y}+1/4, x+3/4$	$[w, \bar{v}, u]$	(23)	$\bar{z}+1/4, y+3/4, x+1/4$	$[\bar{w}, v, u]$	(24)	$\bar{z}+3/4, \bar{y}+3/4, \bar{x}+3/4$	$[\bar{w}, \bar{v}, \bar{u}]$
(25)	$\bar{x}, \bar{y}, \bar{z}$	$[\bar{u}, \bar{v}, \bar{w}]$	(26)	$x+1/2, y, \bar{z}+1/2$	$[u, v, \bar{w}]$	(27)	$x, \bar{y}+1/2, z+1/2$	$[u, \bar{v}, w]$	(28)	$\bar{x}+1/2, y+1/2, z$	$[\bar{u}, v, w]$

- (29)  $\bar{z}, \bar{x}, \bar{y} [\bar{w}, \bar{u}, \bar{v}]$  (30)  $\bar{z}+1/2, \bar{x}+1/2, \bar{y} [\bar{w}, \bar{u}, \bar{v}]$  (31)  $z+1/2, x, \bar{y}+1/2 [w, u, \bar{v}]$  (32)  $z, \bar{x}+1/2, \bar{y}+1/2 [w, \bar{u}, \bar{v}]$   
 (33)  $\bar{y}, \bar{z}, \bar{x} [\bar{v}, \bar{w}, \bar{u}]$  (34)  $y, \bar{z}+1/2, \bar{x}+1/2 [v, \bar{w}, \bar{u}]$  (35)  $\bar{y}+1/2, z+1/2, x [\bar{v}, w, \bar{u}]$  (36)  $y+1/2, z, \bar{x}+1/2 [v, w, \bar{u}]$   
 (37)  $\bar{y}+1/4, \bar{x}+3/4, z+3/4 [\bar{v}, \bar{u}, w]$  (38)  $y+1/4, \bar{x}+1/4, z+1/4 [v, u, w]$  (39)  $\bar{y}+3/4, \bar{x}+3/4, \bar{z}+1/4 [\bar{v}, u, \bar{w}]$  (40)  $y+3/4, \bar{x}+1/4, \bar{z}+3/4 [v, \bar{u}, \bar{w}]$   
 (41)  $\bar{x}+1/4, \bar{z}+3/4, y+3/4 [\bar{u}, \bar{w}, \bar{v}]$  (42)  $x+3/4, \bar{z}+1/4, \bar{y}+3/4 [u, \bar{w}, \bar{v}]$  (43)  $x+1/4, z+1/4, y+1/4 [u, w, \bar{v}]$  (44)  $\bar{x}+3/4, z+3/4, \bar{y}+1/4 [\bar{u}, w, \bar{v}]$   
 (45)  $\bar{z}+1/4, \bar{y}+3/4, \bar{x}+3/4 [\bar{w}, \bar{v}, \bar{u}]$  (46)  $\bar{z}+3/4, y+3/4, \bar{x}+1/4 [\bar{w}, v, \bar{u}]$  (47)  $z+3/4, \bar{y}+1/4, \bar{x}+3/4 [w, \bar{v}, \bar{u}]$  (48)  $z+1/4, y+1/4, \bar{x}+1/4 [w, v, \bar{u}]$

48 g ..2

- $1/8, y, \bar{y}+1/4 [0, \bar{v}, v]$   $3/8, \bar{y}, \bar{y}+3/4 [0, v, v]$   $7/8, y+1/2, y+1/4 [0, \bar{v}, \bar{v}]$   $5/8, \bar{y}+1/2, y+3/4 [0, v, \bar{v}]$   
 $\bar{y}+1/4, 1/8, y [v, 0, \bar{v}]$   $\bar{y}+3/4, 3/8, \bar{y} [v, 0, v]$   $y+1/4, 7/8, y+1/2 [\bar{v}, 0, \bar{v}]$   $y+3/4, 5/8, \bar{y}+1/2 [\bar{v}, 0, v]$   
 $y, \bar{y}+1/4, 1/8 [\bar{v}, v, 0]$   $\bar{y}, \bar{y}+3/4, 3/8 [v, v, 0]$   $y+1/2, y+1/4, 7/8 [\bar{v}, \bar{v}, 0]$   $\bar{y}+1/2, y+3/4, 5/8 [v, \bar{v}, 0]$   
 $7/8, \bar{y}, y+3/4 [0, v, \bar{v}]$   $5/8, y, y+1/4 [0, \bar{v}, \bar{v}]$   $1/8, \bar{y}+1/2, \bar{y}+3/4 [0, v, v]$   $3/8, y+1/2, \bar{y}+1/4 [0, \bar{v}, v]$   
 $y+3/4, 7/8, \bar{y} [\bar{v}, 0, v]$   $y+1/4, 5/8, y [\bar{v}, 0, \bar{v}]$   $\bar{y}+3/4, 1/8, \bar{y}+1/2 [v, 0, v]$   $\bar{y}+1/4, 3/8, y+1/2 [v, 0, \bar{v}]$   
 $\bar{y}, y+3/4, 7/8 [v, \bar{v}, 0]$   $y, y+1/4, 5/8 [\bar{v}, \bar{v}, 0]$   $\bar{y}+1/2, \bar{y}+3/4, 1/8 [v, v, 0]$   $y+1/2, \bar{y}+1/4, 3/8 [\bar{v}, v, 0]$

- 48 f 2..  $x, 0, 1/4 [u, 0, 0]$   $\bar{x}+1/2, 0, 3/4 [\bar{u}, 0, 0]$   $1/4, x, 0 [0, u, 0]$   $3/4, \bar{x}+1/2, 0 [0, \bar{u}, 0]$   
 $0, 1/4, x [0, 0, u]$   $0, 3/4, \bar{x}+1/2 [0, 0, \bar{u}]$   $3/4, x+1/4, 0 [0, u, 0]$   $3/4, \bar{x}+3/4, 1/2 [0, \bar{u}, 0]$   
 $x+3/4, 1/2, 1/4 [u, 0, 0]$   $\bar{x}+1/4, 0, 1/4 [\bar{u}, 0, 0]$   $0, 1/4, \bar{x}+1/4 [0, 0, \bar{u}]$   $1/2, 1/4, x+3/4 [0, 0, u]$   
 $\bar{x}, 0, 3/4 [\bar{u}, 0, 0]$   $x+1/2, 0, 1/4 [u, 0, 0]$   $3/4, \bar{x}, 0 [0, \bar{u}, 0]$   $1/4, x+1/4, 0 [0, u, 0]$   
 $0, 3/4, \bar{x} [0, 0, \bar{u}]$   $0, 1/4, x+1/2 [0, 0, u]$   $1/4, \bar{x}+3/4, 0 [0, \bar{u}, 0]$   $1/4, x+1/4, 1/2 [0, u, 0]$   
 $\bar{x}+1/4, 1/2, 3/4 [\bar{u}, 0, 0]$   $x+3/4, 0, 3/4 [u, 0, 0]$   $0, 3/4, x+3/4 [0, 0, u]$   $1/2, 3/4, \bar{x}+1/4 [0, 0, \bar{u}]$

32 e .3.

- $x, x, x [u, u, u]$   $\bar{x}+1/2, \bar{x}, x+1/2 [\bar{u}, \bar{u}, u]$   $\bar{x}, x+1/2, \bar{x}+1/2 [\bar{u}, u, \bar{u}]$   $x+1/2, \bar{x}+1/2, \bar{x} [u, \bar{u}, \bar{u}]$   
 $x+3/4, x+1/4, \bar{x}+1/4 [u, u, \bar{u}]$   $\bar{x}+3/4, \bar{x}+3/4, \bar{x}+3/4 [\bar{u}, \bar{u}, \bar{u}]$   $x+1/4, \bar{x}+1/4, x+3/4 [u, \bar{u}, u]$   $\bar{x}+1/4, x+3/4, x+1/4 [\bar{u}, u, u]$   
 $\bar{x}, \bar{x}, \bar{x} [\bar{u}, \bar{u}, \bar{u}]$   $x+1/2, x, \bar{x}+1/2 [u, u, \bar{u}]$   $x, \bar{x}+1/2, x+1/2 [u, \bar{u}, u]$   $\bar{x}+1/2, x+1/2, x [\bar{u}, u, u]$   
 $\bar{x}+1/4, \bar{x}+3/4, x+3/4 [\bar{u}, \bar{u}, u]$   $x+1/4, x+1/4, x+1/4 [u, u, u]$   $\bar{x}+3/4, x+3/4, \bar{x}+1/4 [\bar{u}, u, \bar{u}]$   $x+3/4, \bar{x}+1/4, \bar{x}+3/4 [u, \bar{u}, \bar{u}]$

- 12 d 4'..  $3/8, 0, 1/4 [0, 0, 0]$   $1/8, 0, 3/4 [0, 0, 0]$   $1/4, 3/8, 0 [0, 0, 0]$   $3/4, 1/8, 0 [0, 0, 0]$   
 $0, 1/4, 3/8 [0, 0, 0]$   $0, 3/4, 1/8 [0, 0, 0]$   $3/4, 5/8, 0 [0, 0, 0]$   $3/4, 3/8, 1/2 [0, 0, 0]$   
 $1/8, 1/2, 1/4 [0, 0, 0]$   $7/8, 0, 1/4 [0, 0, 0]$   $0, 1/4, 7/8 [0, 0, 0]$   $1/2, 1/4, 1/8 [0, 0, 0]$

- 24 c 2.22  $1/8, 0, 1/4 [0, 0, 0]$   $3/8, 0, 3/4 [0, 0, 0]$   $1/4, 1/8, 0 [0, 0, 0]$   $3/4, 3/8, 0 [0, 0, 0]$   
 $0, 1/4, 1/8 [0, 0, 0]$   $0, 3/4, 3/8 [0, 0, 0]$   $7/8, 0, 3/4 [0, 0, 0]$   $5/8, 0, 1/4 [0, 0, 0]$   
 $3/4, 7/8, 0 [0, 0, 0]$   $1/4, 5/8, 0 [0, 0, 0]$   $0, 3/4, 7/8 [0, 0, 0]$   $0, 1/4, 5/8 [0, 0, 0]$

Continued

230.5.1651

 $Ia\bar{3}d'$ 

16	b	.32	$1/8, 1/8, 1/8 [0,0,0]$	$3/8, 7/8, 5/8 [0,0,0]$	$7/8, 5/8, 3/8 [0,0,0]$	$5/8, 3/8, 7/8 [0,0,0]$
			$7/8, 7/8, 7/8 [0,0,0]$	$5/8, 1/8, 3/8 [0,0,0]$	$1/8, 3/8, 5/8 [0,0,0]$	$3/8, 5/8, 1/8 [0,0,0]$
16	a	$\bar{3}$	$0,0,0 [0,0,0]$	$1/2, 0, 1/2 [0,0,0]$	$0, 1/2, 1/2 [0,0,0]$	$1/2, 1/2, 0 [0,0,0]$
			$3/4, 1/4, 1/4 [0,0,0]$	$3/4, 3/4, 3/4 [0,0,0]$	$1/4, 1/4, 3/4 [0,0,0]$	$1/4, 3/4, 1/4 [0,0,0]$

**Symmetry of Special Projections**

Along  $[0,0,1]$   $p4m'm'$   
 $\mathbf{a}^* = \mathbf{a}/2$   $\mathbf{b}^* = \mathbf{b}/2$   
 Origin at  $1/4, 0, z$

Along  $[1,1,1]$   $p6m'm'$   
 $\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3$   $\mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$   
 Origin at  $x, x, x$

Along  $[1,1,0]$   $c2m'm'$   
 $\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2$   $\mathbf{b}^* = \mathbf{c}/2$   
 Origin at  $x, x+1/4, 1/8$